Supporting information for: Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections

Pavlo O. Dral,* Xin Wu, and Walter Thiel*

Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr

E-mail: dral@kofo.mpg.de; thiel@kofo.mpg.de

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1 Parametrization Details

The parametrization program supports the following algorithms:

1. Levenberg–Marquardt method.[S1,S2]

2. Gauss–Newton method with line searches.[S3]

3. Parallel Nelder–Mead simplex method.[S4]

4. Controlled random search method with local mutations.[S5]

5. DIviding RECTangles (DIRECT) method.[S6]

6. Locally-biased DIRECT Method.[S7]

7. Improved stochastic ranking evolution strategy.[S8]

8. PRincipal AXIS (PRAXIS) method.[S9]

9. Modified implementation of the Subplex method.[S10]

We use own implementations of algorithms 1–2, while the code for algorithms 4–9 comes from the NLopt library.[S11] There are two implementations of algorithm 3: our own and one based on NLopt. Algorithm 4 is available in two variants (parallel and serial).

For many parametrization iterations optimizations were performed in parallel with all the above algorithms for the same initial parameter guess. Then we evaluated the most promising parameter sets obtained during optimizations on their own training sets to quickly discard bad parameter sets and to select the best candidate parameter sets. The latter were carefully evaluated manually using our large collection of validation sets (see the main text) and the next parametrization iterations were started with the most promising candidate sets as new initial guess.

We first addressed our objective 1 (see main text) by analyzing how the absolute errors of various properties of small molecules depend on changes in the parameters. We found that adjustments of the orthogonalization correction parameters[S12] can significantly reduce the errors in both ZPVE-exclusive atomization energies at 0 K and heats of formation at 298 K, while affecting other properties much less. Thus, we first optimized only the orthogonalization correction parameters to satisfy objective 1. The resulting parameter sets performed already reasonably well and were of similar accuracy as the OMx-D3T methods. We then proceeded to achieve the other objectives (see main text). In the following we discuss specific details of the ODM2 and ODM3 parametrizations, with focus on the successful steps leading to the final parameters.

In the ODM2 parametrization we first optimized only the orthogonalization correction parameters F_1, F_2, G_1, and G_2 in the following five steps:

Step 1. C and H parameters were optimized for the singlet CH-species of the MGAE109 set (Cartesian gradient norms and ZPVE-exclusive atomization energies at 0 K) and cubane (ZPVE-exclusive atomization energies at 0 K) using the Levenberg–Marquardt method and the OM2-D3T parameters as initial guess. The SSQ value of the relative errors was minimized with OM2-D3T as reference SQC method. The weight of the atomization energy of cubane (w_{si}^{entry}) was increased to 2.

Step 2. O parameters were optimized for the CHO-species of the MGAE109 set (ZPVE-exclusive atomization energies at 0 K) with increased weights for selected molecules ($w_{si}^{\text{entry}} = 5$ for water and ethanol, $w_{si}^{\text{entry}} = 2$ for hydrogen peroxide and oxygen) using the C and H parameters from the first parametrization step. The SSQ value of absolute errors was minimized using the controlled random search method with local mutation.

Step 3. N parameters were optimized for the CHN-species of the MGAE109 and TAE140 sets with increased weights for selected molecules ($w_{si}^{\text{entry}} = 5$ for methylamine, hydrazine, and ammonia in both sets) using the C and H parameters from the first parametrization step. The SSQ value of absolute errors was minimized with the Levenberg–Marquardt method.

Step 4. CHNO parameters obtained in steps 1–3 were re-optimized for the singlet CHNO-species, the HCO radical, and triplet oxygen of the MGAE109 set plus cubane. The SSQ value of the relative errors in Cartesian gradient norms and ZPVE-exclusive atomization energies at 0 K was minimized with OM2-D3T as reference SQC method. The improved stochastic ranking evolution strategy was used.

Step 5. CHNO parameters obtained in step 4 were re-optimized with the same setup as in step 4, using the controlled random search method with local mutation and with increased weights for the atomization energy of cubane ($w_{si}^{\text{entry}} = 3$), acetylene ($w_{si}^{\text{entry}} = 3$), and benzene ($w_{si}^{\text{entry}} = 15$) and for the Cartesian gradient norms of acetylene and benzene ($w_{si}^{\text{entry}} = 15$).

At the next stage we included vertical excitation energies into the training data and optimized all the above ODM2 parameters to minimize the SSQ value of relative errors. This parametrization took another five consecutive steps:

Step 6. Parameters from step 5 were optimized *one by one* for the singlet CHNO-species, the HCO radical, and triplet oxygen of the MGAE109 set (Cartesian gradient norms and ZPVE-exclusive atomization energies at 0 K), the CHNO set (heats of formation at 298 K, bond lengths, angles, dihedral angles, ionization potentials and differences between them, dipole moments, relative energies, barriers, vibrational wavenumbers), the VEE set (vertical excitation energies), and cubane (Cartesian gradient norms and ZPVE-exclusive atomization energies at 0 K). We changed the weights w_{sp}^{prop} of the errors in atomization energies of the MGAE109 set to 3.1324, in bond lengths to 0.47838, and in vertical excitation energies to 10. We also adjusted the weights w_{si}^{entry} for selected errors in atomization energies (acetylene to 3, benzene to 15, water and ammonia to 10), in Cartesian gradient norms (acetylene and benzene to 15), in some barriers and relative energies (to 2), and in the atomization energy of cubane (to 3).

Step 7. Parameters from step 6 were re-optimized one more time using the same setup as in step 6.

Step 8. Parameters from step 7 were re-optimized (with G_2 taken from step 6) using the same setup as in step 7, but with the weights for selected errors set to the following values: w_{sp}^{prop} to 1.48841 for atomization energies of the MGAE109 set and to 10.01827 for vertical excitation energies; w_{si}^{entry} to 5 for the atomization energies and Cartesian gradient norms of acetylene, benzene, C_4H_4O, and C_4H_5N.

Step 9. Parameters from step 8 were re-optimized (with G_2 taken from step 7) using the same setup as in step 8, but *simultaneously* and with the weights w_{sp}^{prop} for selected errors set to the following values: to 1.35838 for bond lengths in the CHNO set, to 2 for other properties in the CHNO set, and to 5 for vertical excitation energies.

Step 10. F parameters were optimized for the CHNOF-species of the MGAE109 and TAE140 sets (ZPVE-exclusive atomization energies at 0 K) and for the FLUOR set (heats of formation at 298 K, bond lengths, angles, dihedral angles, ionization potentials, dipole moments, relative energies, and barriers). The CHNO parameters were taken from step 9 and the initial F parameters from the standard OM2-D3T method.

As reference SQC method we used OM2 for the CHNO and FLUOR sets, and OM2-D3T for the MGAE109 and TAE140 sets and for cubane. To meet objective 4, we scaled the reference SQC (OM2) errors for the VEE set by a factor of 0.6. The Levenberg–Marquardt method was employed for steps 6–9 and the Gauss–Newton method with line searches for step 10.

Finally, we included noncovalent complexes into the training data and re-optimized all the above ODM2 parameters to minimize the SSQ value of the relative errors in two more steps:

Step 11. CHNO parameters from step 9 were re-optimized for the singlet CHNO-species, the HCO radical, and triplet oxygen of the MGAE109 set (Cartesian gradient norms and ZPVE-exclusive atomization energies at 0 K), the CHNO set (heats of formation at 298 K, bond lengths, angles, dihedral angles, ionization potentials and differences between them, dipole moments, relative energies, barriers, vibrational wavenumbers), the VEE set (vertical excitation energies), the S66 set (relative energies, single-point calculations), and cubane (Cartesian gradient norm and ZPVE-exclusive atomization energy at 0 K). The Levenberg–Marquardt method was used. The same weights as in step 9 were adopted and the weight for the relative energies in the S66 set was set to 4.

Step 12. F parameters were optimized for the CHNOF-species of the MGAE109 and TAE140 sets (ZPVE-exclusive atomization energies at 0 K) and for the FLUOR set (heats of formation at 298 K, bond lengths, angles, dihedral angles, ionization potentials, dipole moments, relative energies, and barriers). The CHNO parameters were taken from step 11, initial F parameters were taken from step 10, and the PRAXIS method was used. OM3 served as reference SQC method. The weights (w_{sp}^{prop}) for bond lengths were increased to 5.

The reference SQC method was the same as in steps 6–10 and the OM2-D3 method was used as a reference SQC method for the S66 set. The parameters obtained in steps 11 and 12 are the final ODM2 parameters and their values are given in the main text.

The ODM3 parametrization started with the optimization of the orthogonalization correction parameters F_1 and G_1 to minimize the SSQ value of the absolute errors in ZPVE-exclusive atomization energies at 0 K in four steps:

Step 1. C and H parameters were optimized for the singlet CH-species of the MGAE109 set and cubane.

Step 2. O parameters were optimized for the CHO-species of the MGAE109 set with increased weights for selected molecules ($w_{si}^{\mathrm{entry}} = 5$ for water and ethanol, $w_{si}^{\mathrm{entry}} = 2$ for hydrogen peroxide and oxygen) using the C and H parameters from step 1.

Step 3. N parameters were optimized for the CHN-species of the MGAE109 and TAE140 sets with increased weights for selected molecules ($w_{si}^{\text{entry}} = 5$ for methylamine, hydrazine, and ammonia in both sets) using the C and H parameters from step 1.

Step 4. F parameters were optimized for the CHNOF-species of the MGAE109 and TAE140 sets using the CHNO parameters from steps 1–3.

In all cases, the standard OM3-D3T parameters served as initial guess and a modified implementation of the Subplex method was used. This rather restricted parametrization was sufficient to achieving objectives 1–3 reasonably well.

Next, we minimized the SSQ value of the relative errors in multiple properties by optimizing simultaneously all the above ODM3 parameters in three additional steps:

Step 5. CHNO parameters obtained in steps 1–3 were re-optimized for the singlet CHNO-species, the HCO radical, and triplet oxygen of the MGAE109 set (Cartesian gradient norms and ZPVE-exclusive atomization energies at 0 K, OM3-D3T as reference SQC method), the CHNO set (heats of formation at 298 K, bond lengths, angles, dihedral angles, ionization potentials and differences between them, dipole moments, relative energies, barriers, vibrational wavenumbers, OM3 as reference SQC method), the VEE set (vertical excitation energies, ODM2 as reference SQC method), the S66 set (relative energies, D3-corrected OM3 as reference method, single-point calculations), and cubane (Cartesian gradient norm and ZPVE-exclusive atomization energy at 0 K, OM3-D3T as reference SQC method). The Gauss–Newton method with line searches was used. Increased weights were applied for the atomization energy of cubane ($w_{si}^{\text{entry}} = 2$) and for a few selected barriers and relative energies in the CHNO set ($w_{si}^{\text{entry}} = 2$).

Step 6. CHNO parameters obtained in step 5 were re-optimized using the same setup as in step 5, but with weights (w_{sp}^{prop}) for heats of formation (in the CHNO set) and excited state-energies (in the VEE set) increased to 10.

Step 7. F parameters were optimized for the CHNOF-species of the MGAE109 and TAE140 sets (ZPVE-exclusive atomization energies at 0 K) and for the FLUOR set (heats of formation at 298 K, bond lengths, angles, dihedral angles, ionization potentials, dipole moments, relative energies, and barriers). The CHNO parameters were taken from step 6, the initial F parameters were taken from step 4, and the PRAXIS method was used. OM3 served as the reference SQC method. The weights (w_{sp}^{prop}) for heats of formation and atomization energies were increased to 2.

The parameters obtained in steps 6 and 7 are the final ODM3 parameters and their values are given in the main text.

2 Plots of Resonance Integrals

2.1 ODM2 vs OM2

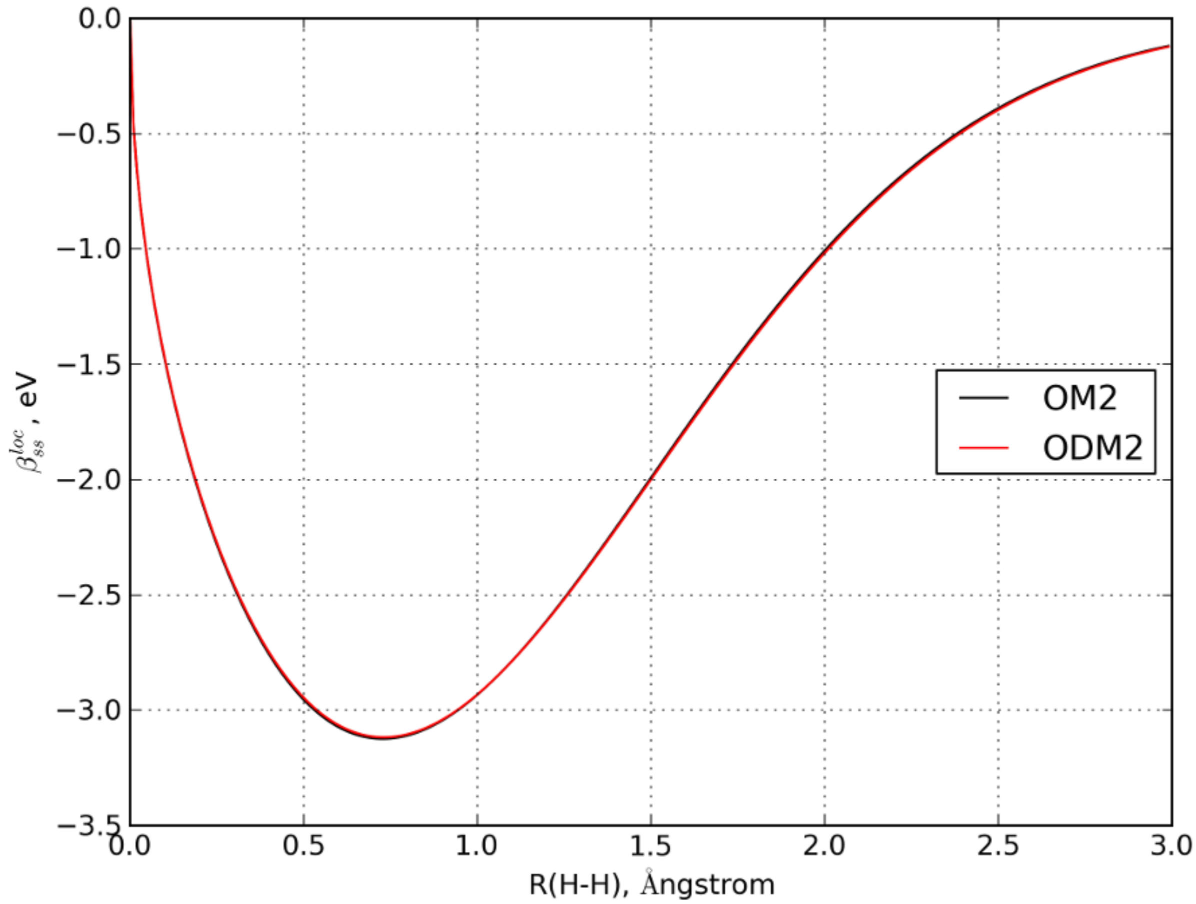

Figure S1: Comparison of *ss* local resonance integrals for the H−H pair calculated using standard OM2 and new ODM2 parameters.

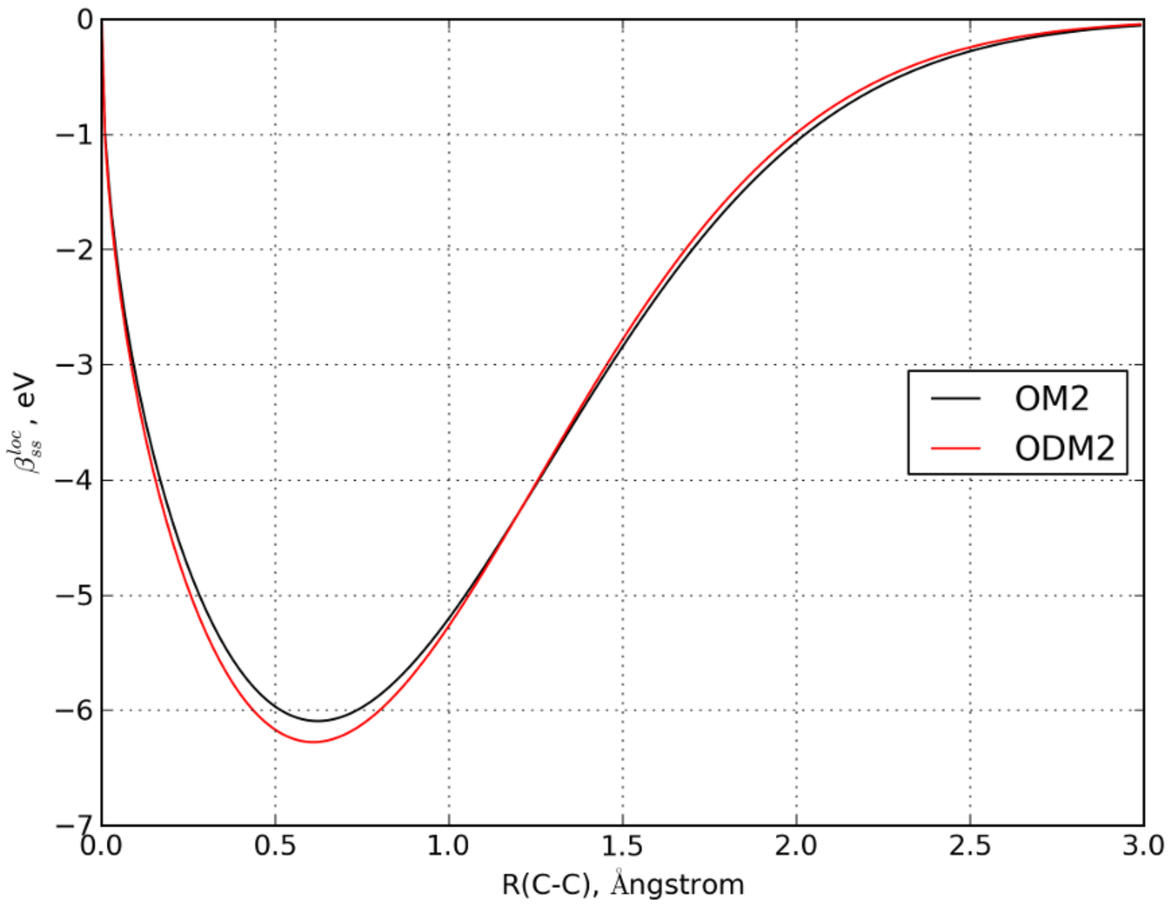

Figure S2: Comparison of *ss* local resonance integrals for the C−C pair calculated using standard OM2 and new ODM2 parameters.

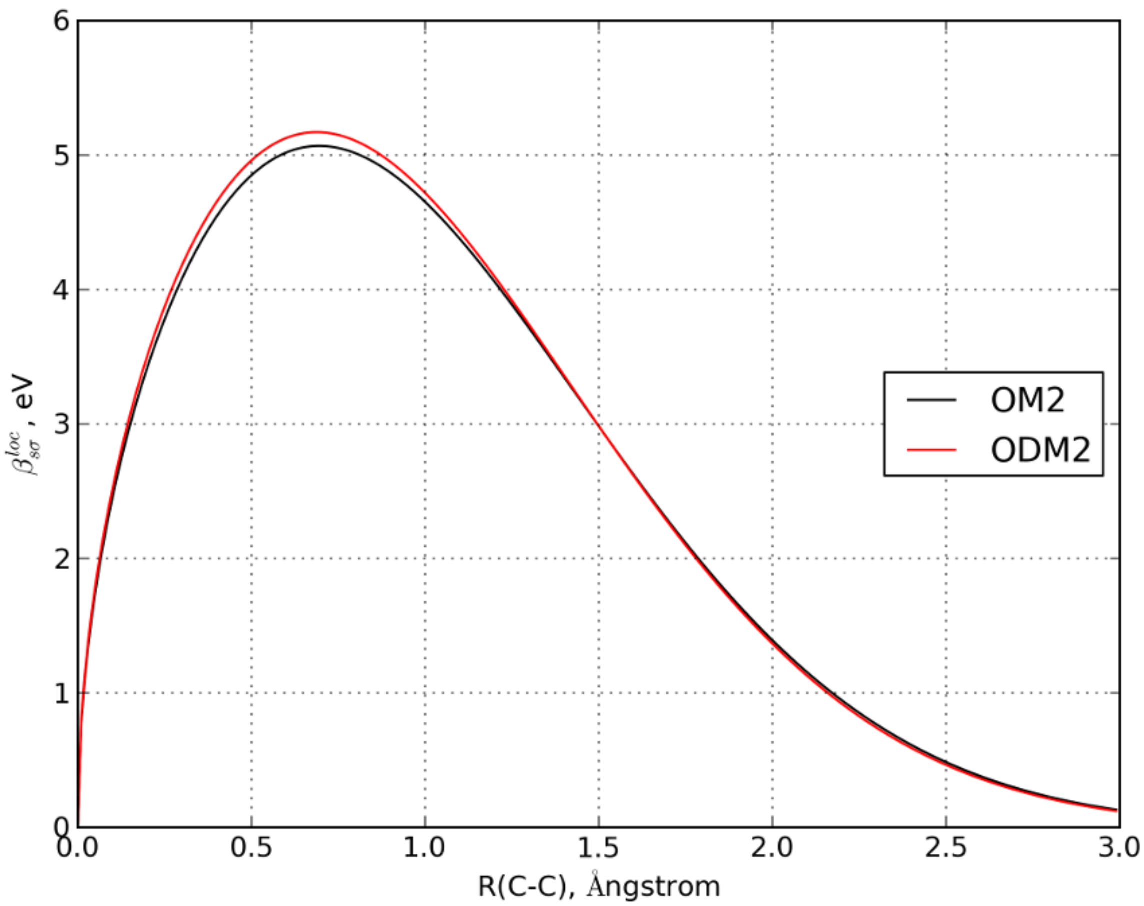

Figure S3: Comparison of $s\sigma$ local resonance integrals for the C−C pair calculated using standard OM2 and new ODM2 parameters.

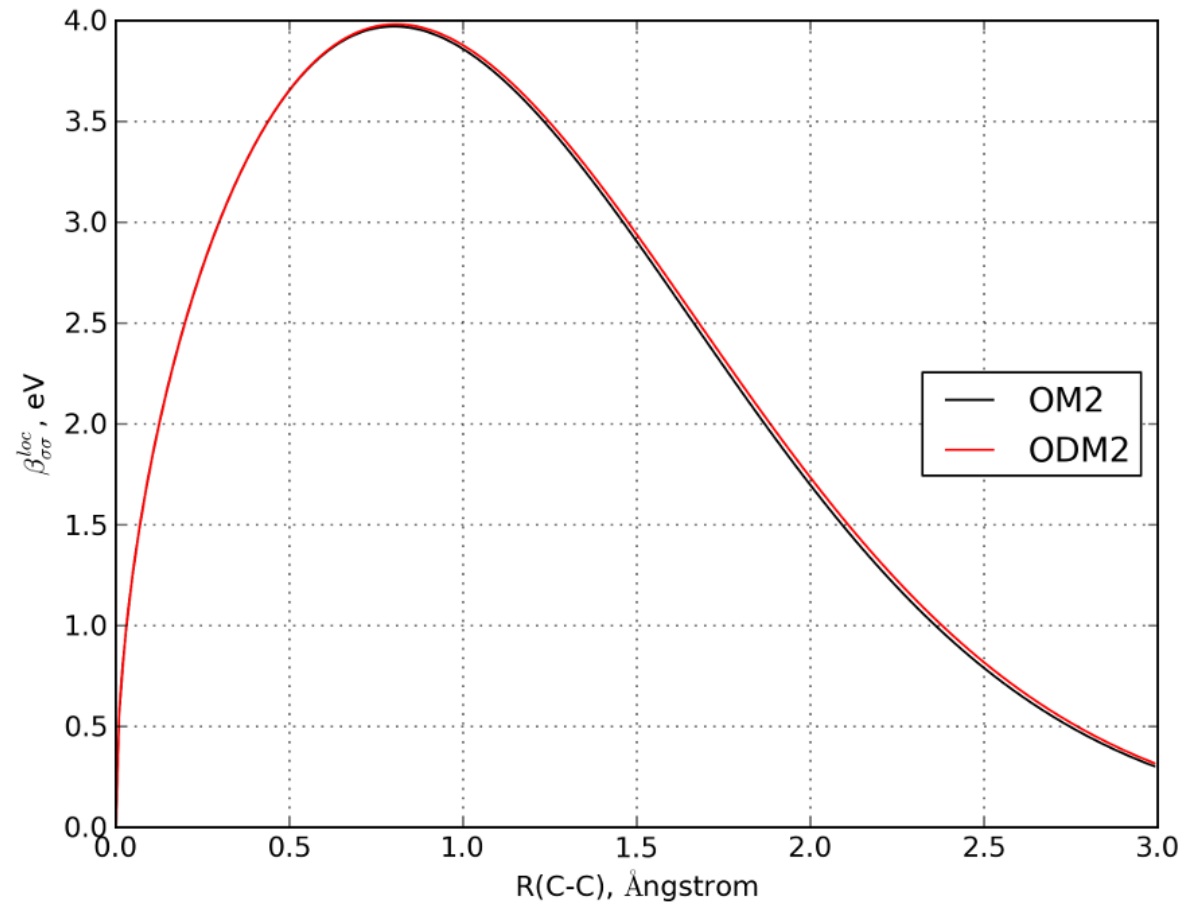

Figure S4: Comparison of $\sigma\sigma$ local resonance integrals for the C−C pair calculated using standard OM2 and new ODM2 parameters.

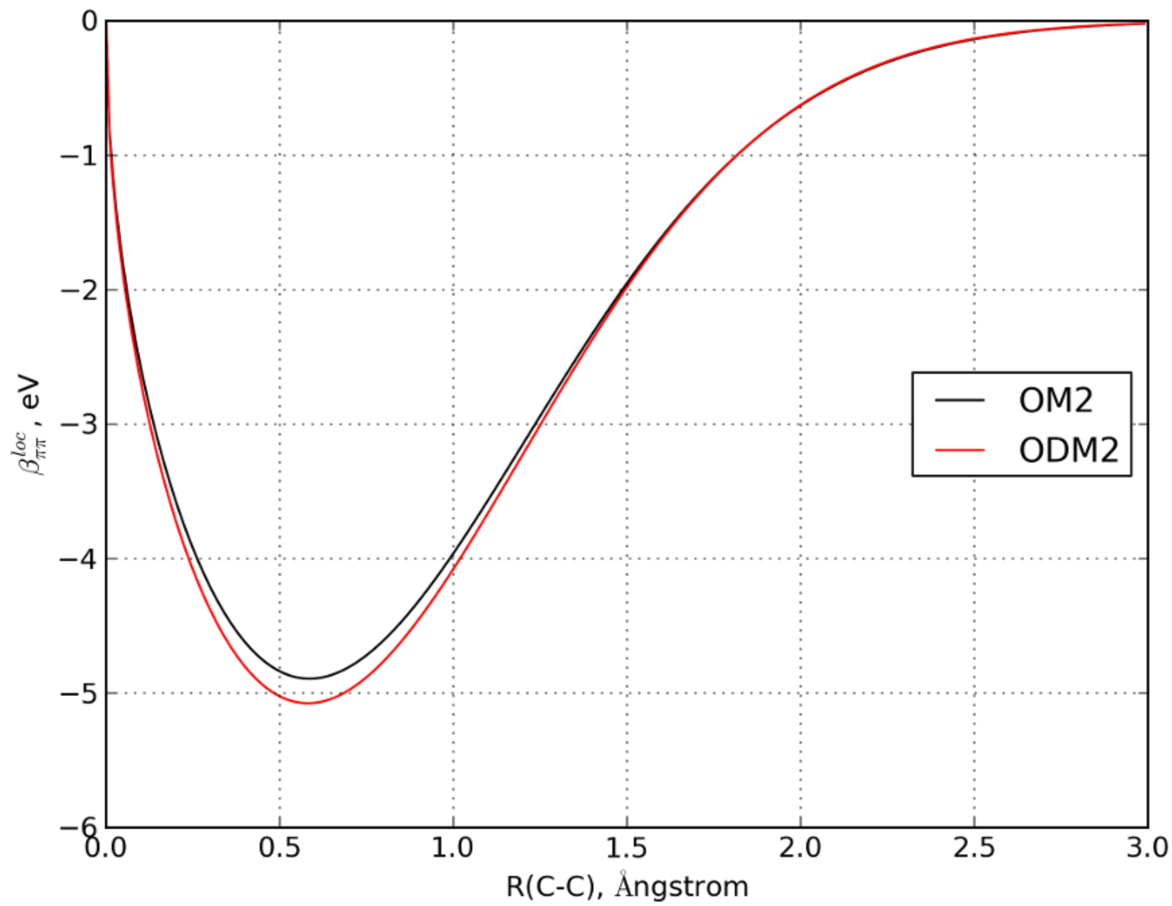

Figure S5: Comparison of $\pi\pi$ local resonance integrals for the C−C pair calculated using standard OM2 and new ODM2 parameters.

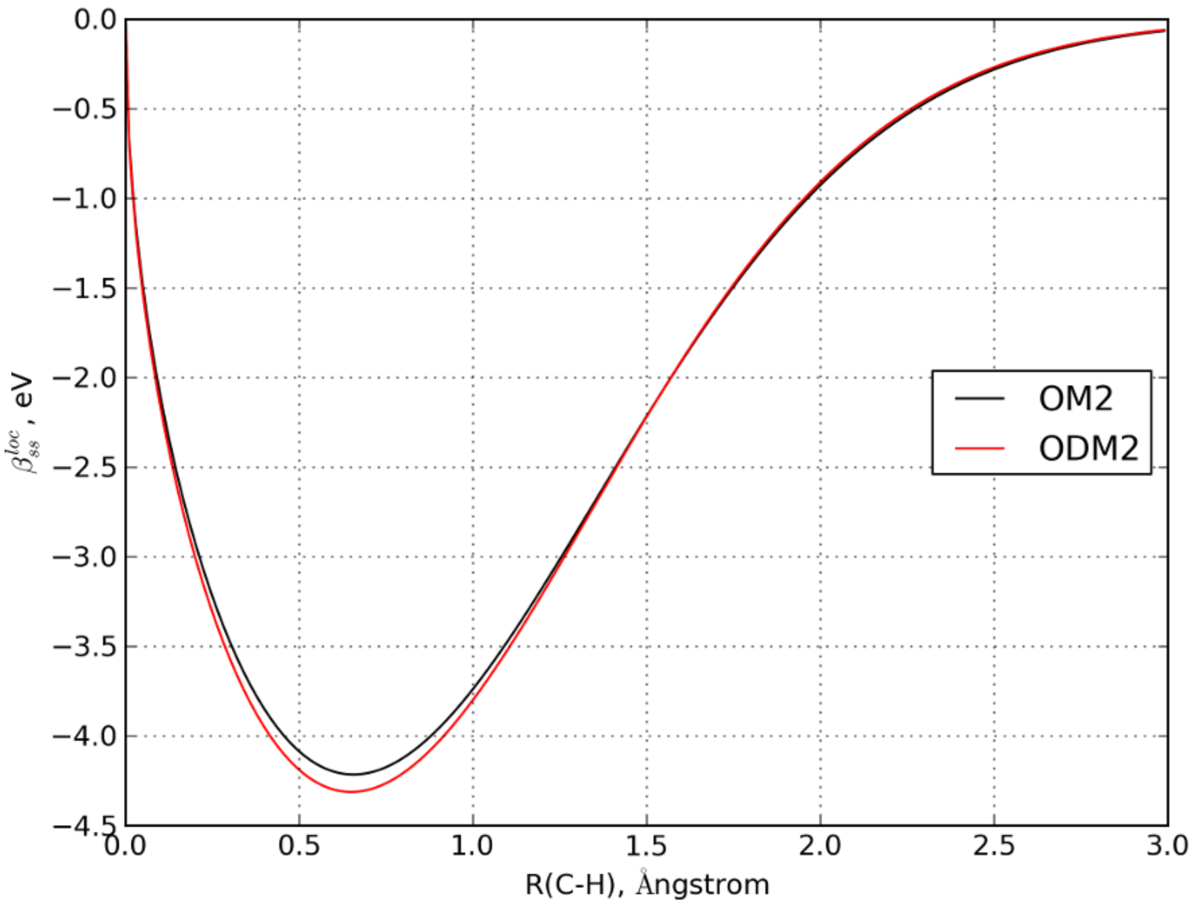

Figure S6: Comparison of ss local resonance integrals for the C−H pair calculated using standard OM2 and new ODM2 parameters.

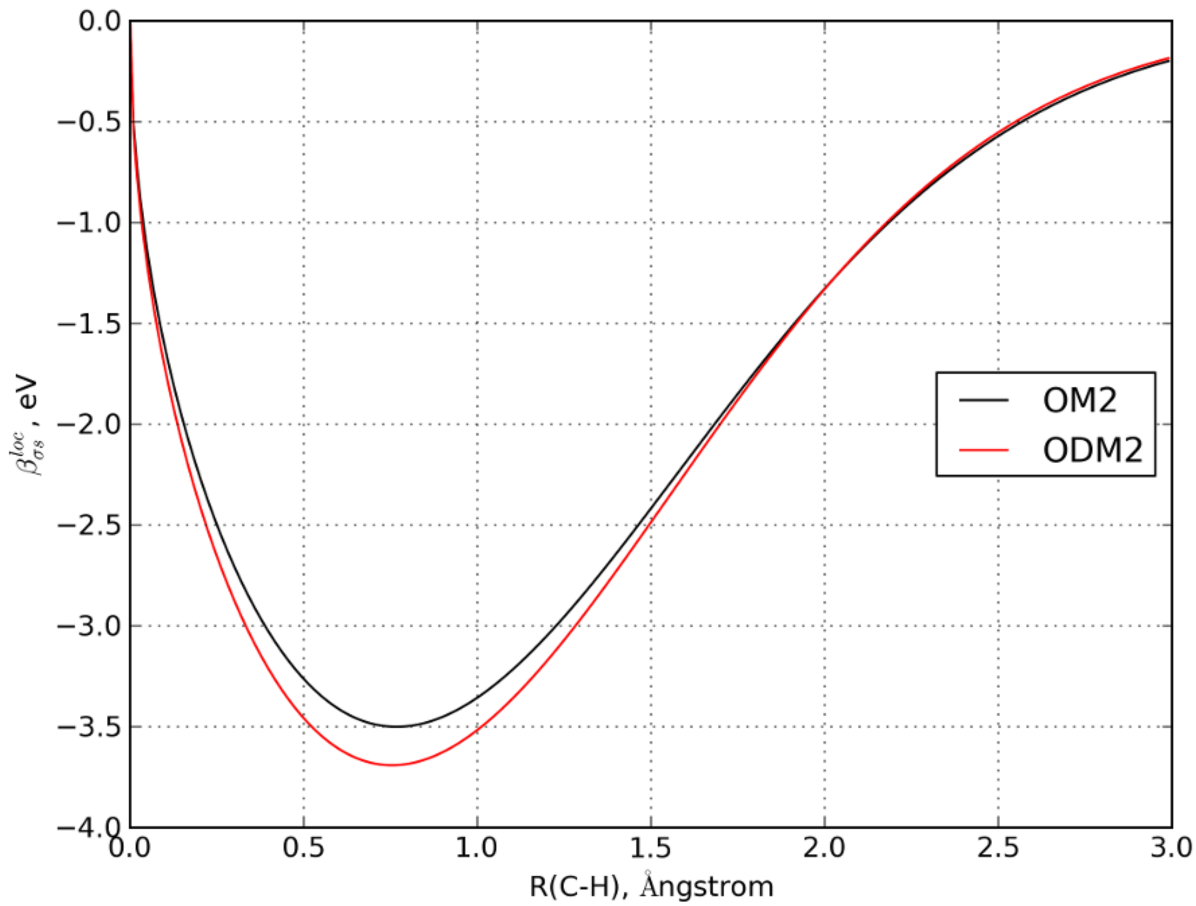

Figure S7: Comparison of σs local resonance integrals for the C−H pair calculated using standard OM2 and new ODM2 parameters.

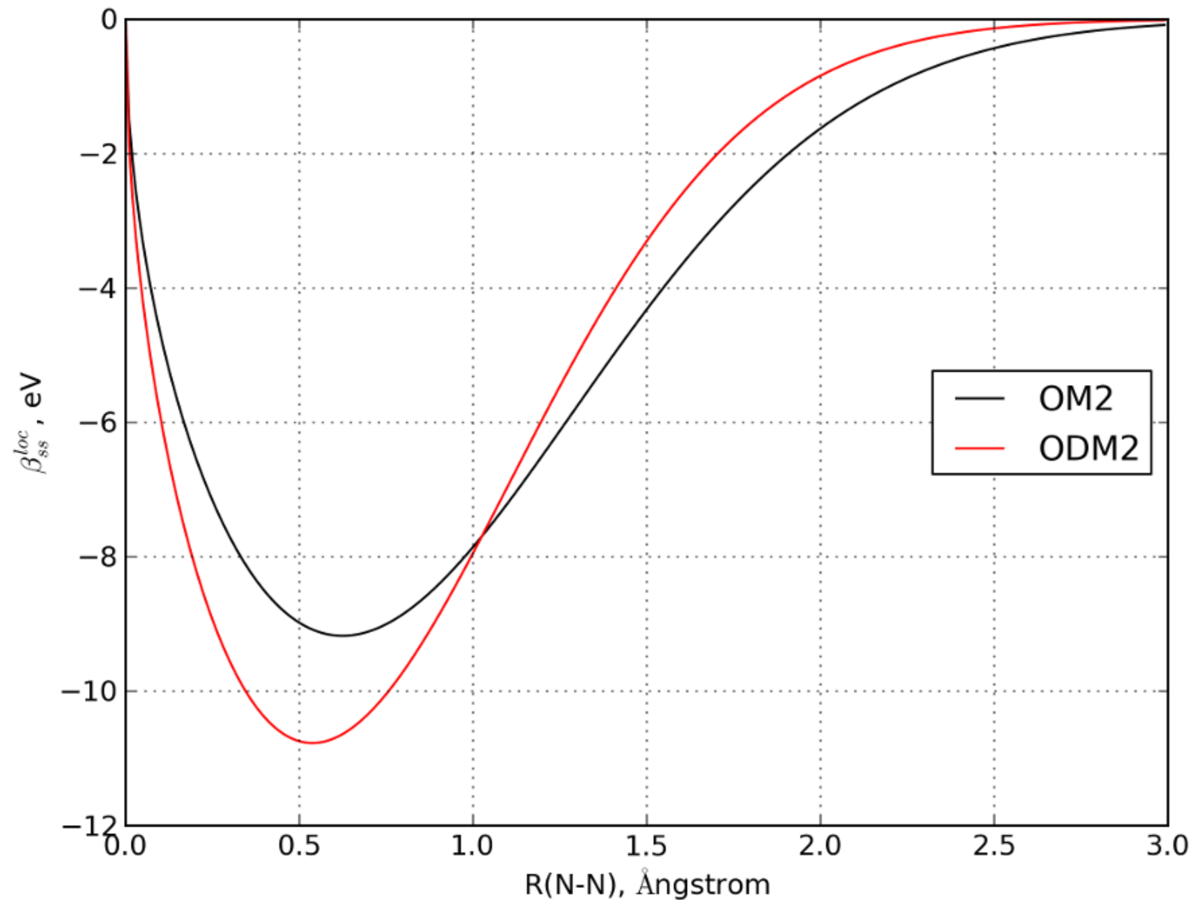

Figure S8: Comparison of ss local resonance integrals for the N−N pair calculated using standard OM2 and new ODM2 parameters.

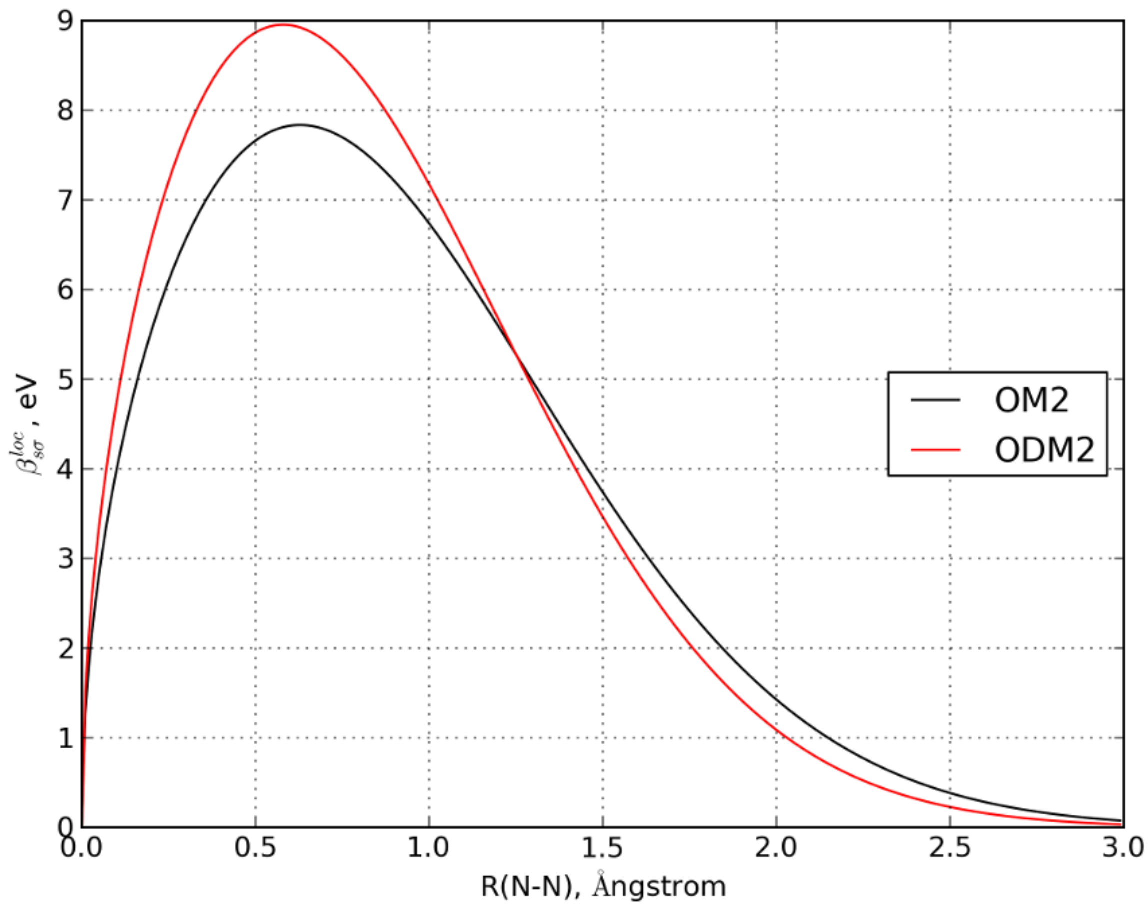

Figure S9: Comparison of $s\sigma$ local resonance integrals for the N−N pair calculated using standard OM2 and new ODM2 parameters.

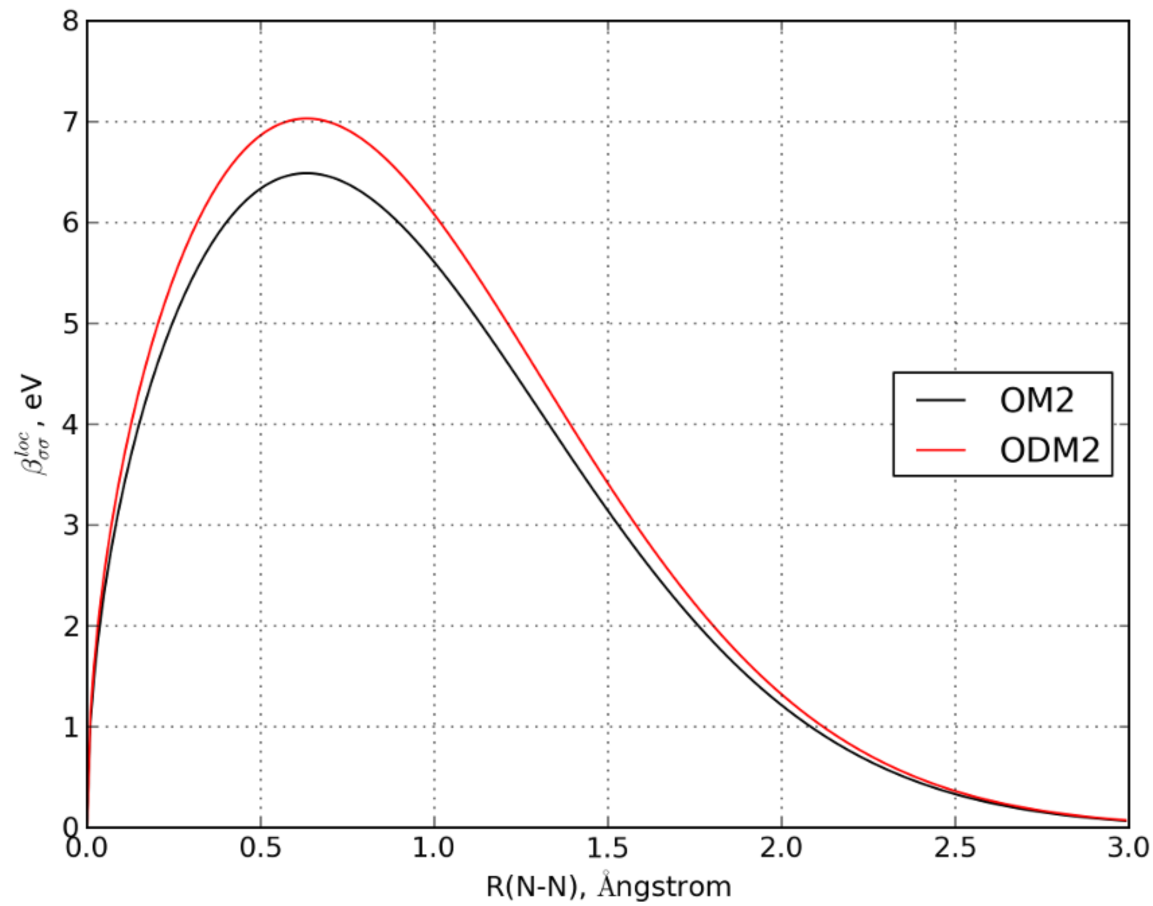

Figure S10: Comparison of $\sigma\sigma$ local resonance integrals for the N−N pair calculated using standard OM2 and new ODM2 parameters.

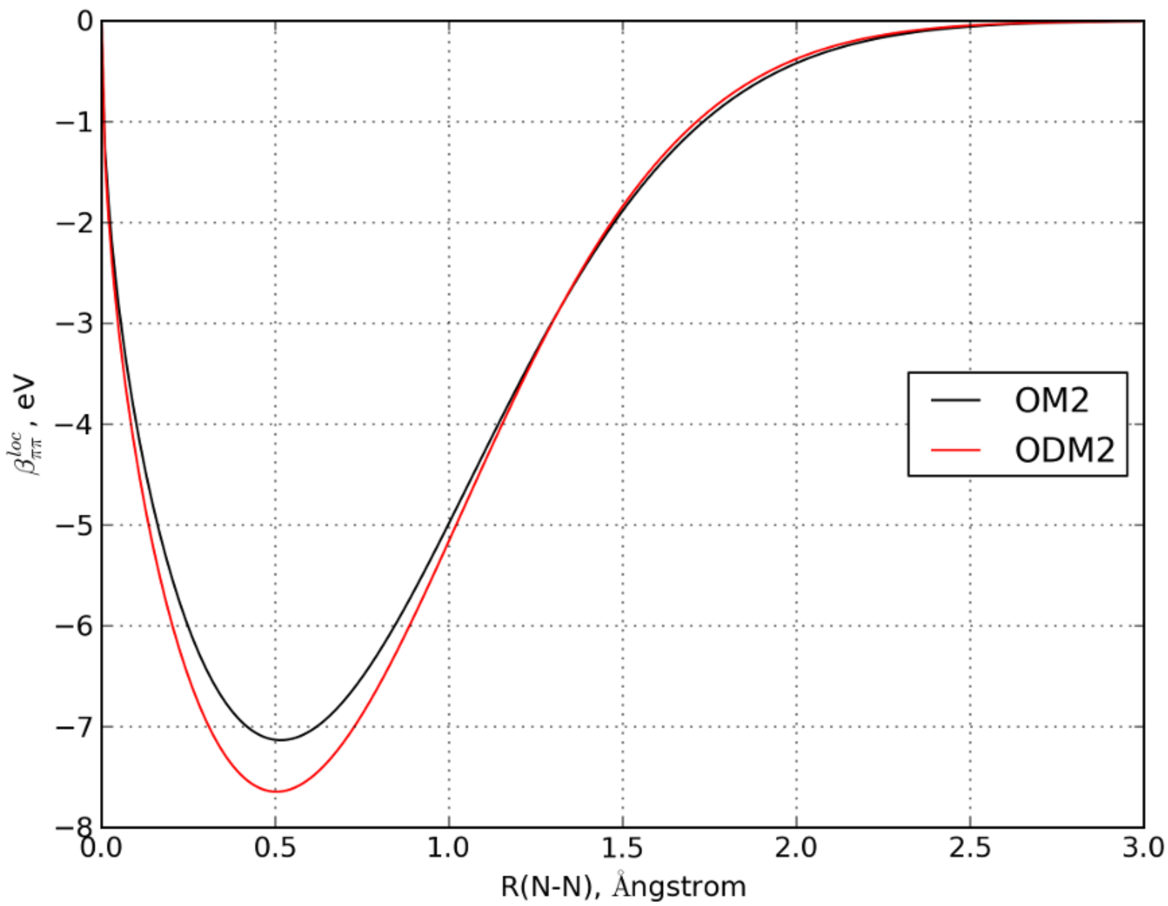

Figure S11: Comparison of $\pi\pi$ local resonance integrals for the N−N pair calculated using standard OM2 and new ODM2 parameters.

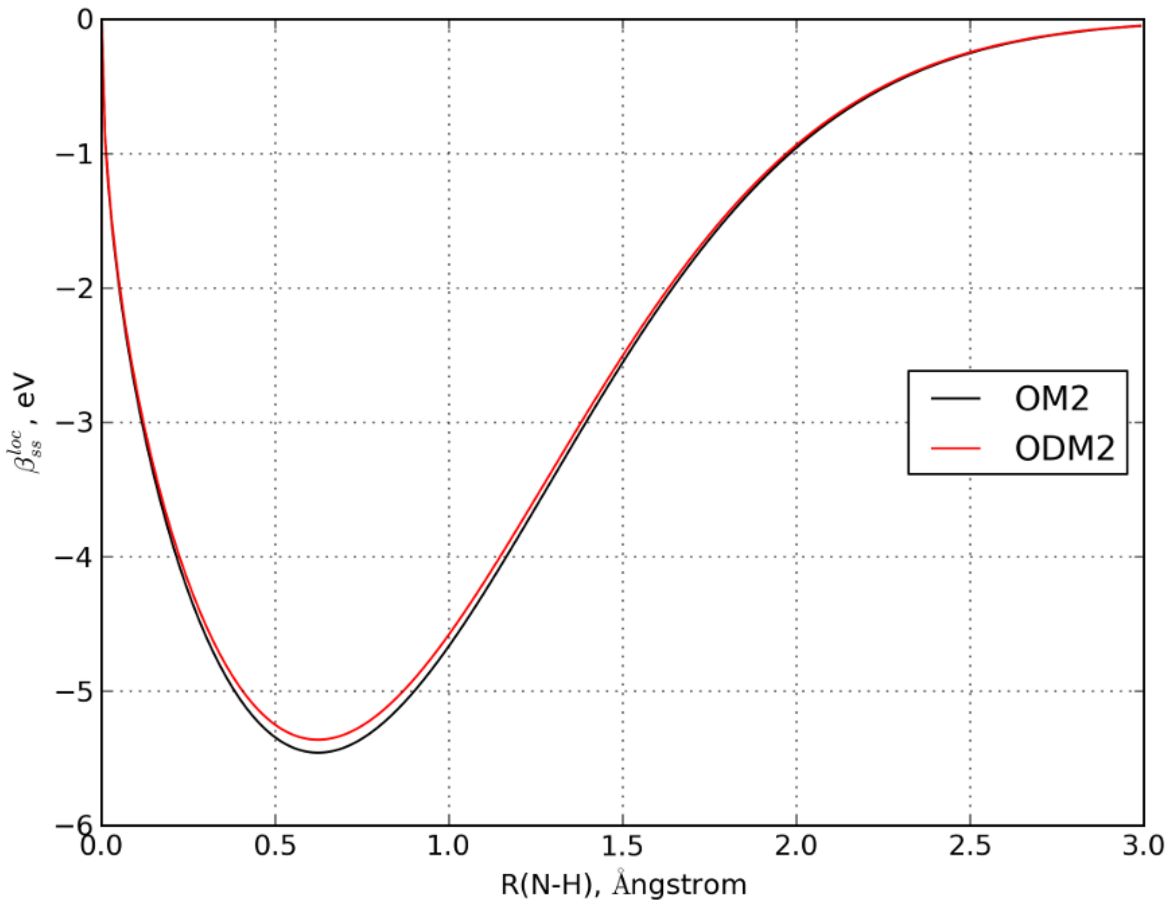

Figure S12: Comparison of *ss* local resonance integrals for the N−H pair calculated using standard OM2 and new ODM2 parameters.

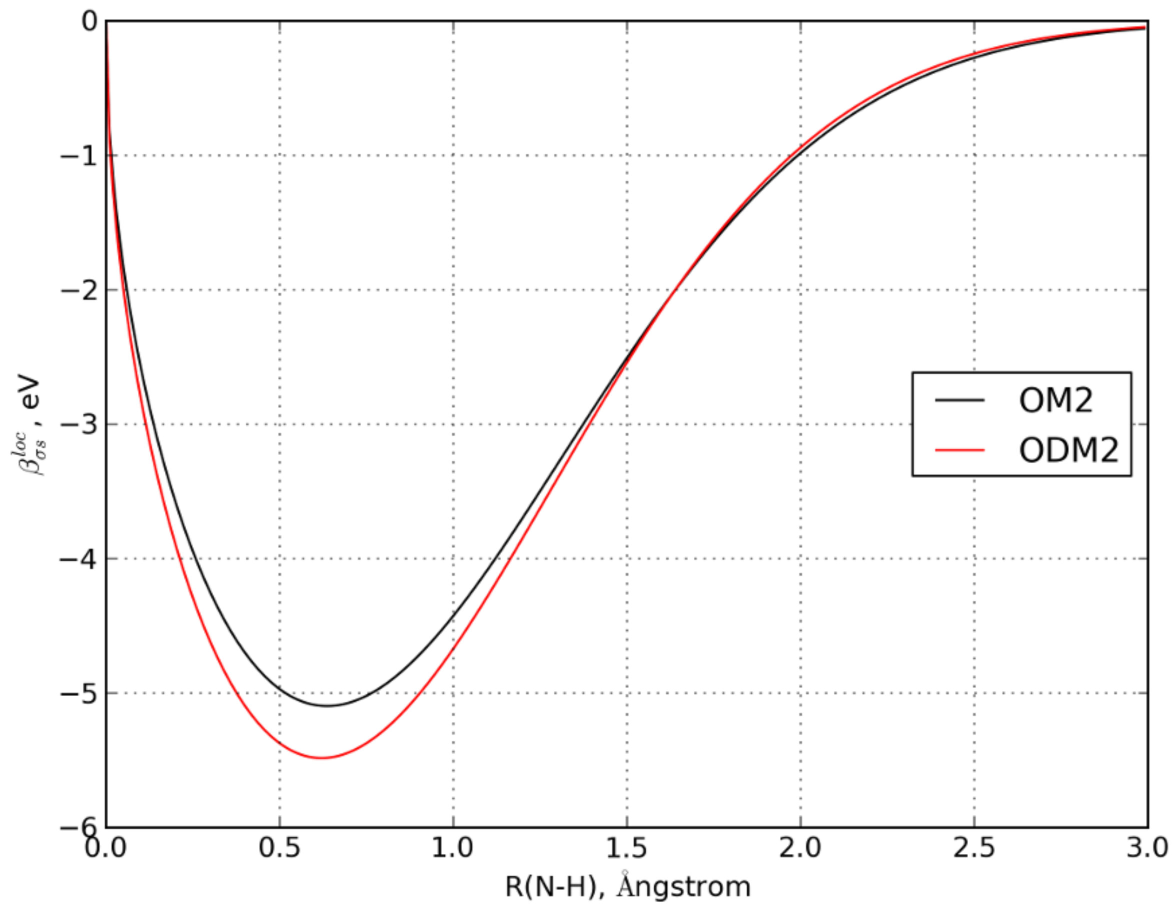

Figure S13: Comparison of σs local resonance integrals for the N−H pair calculated using standard OM2 and new ODM2 parameters.

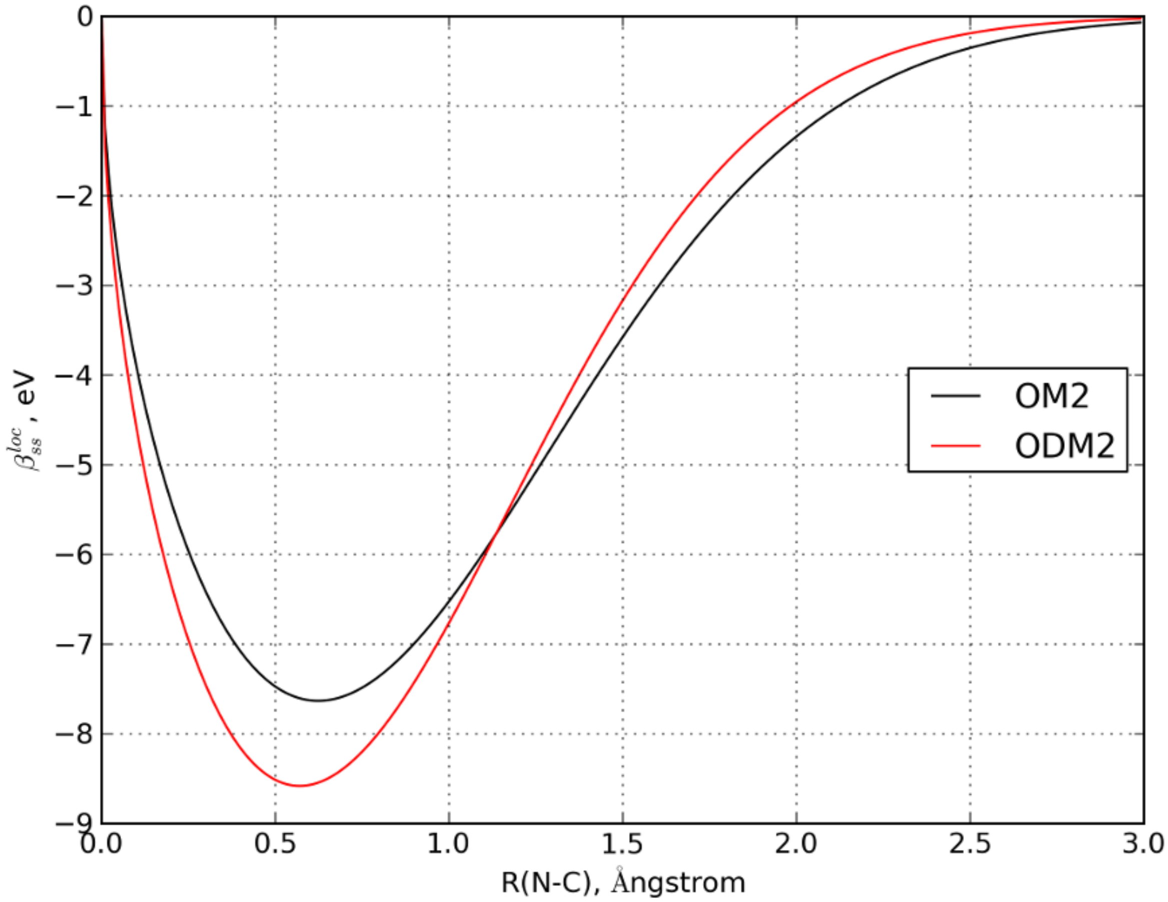

Figure S14: Comparison of *ss* local resonance integrals for the N−C pair calculated using standard OM2 and new ODM2 parameters.

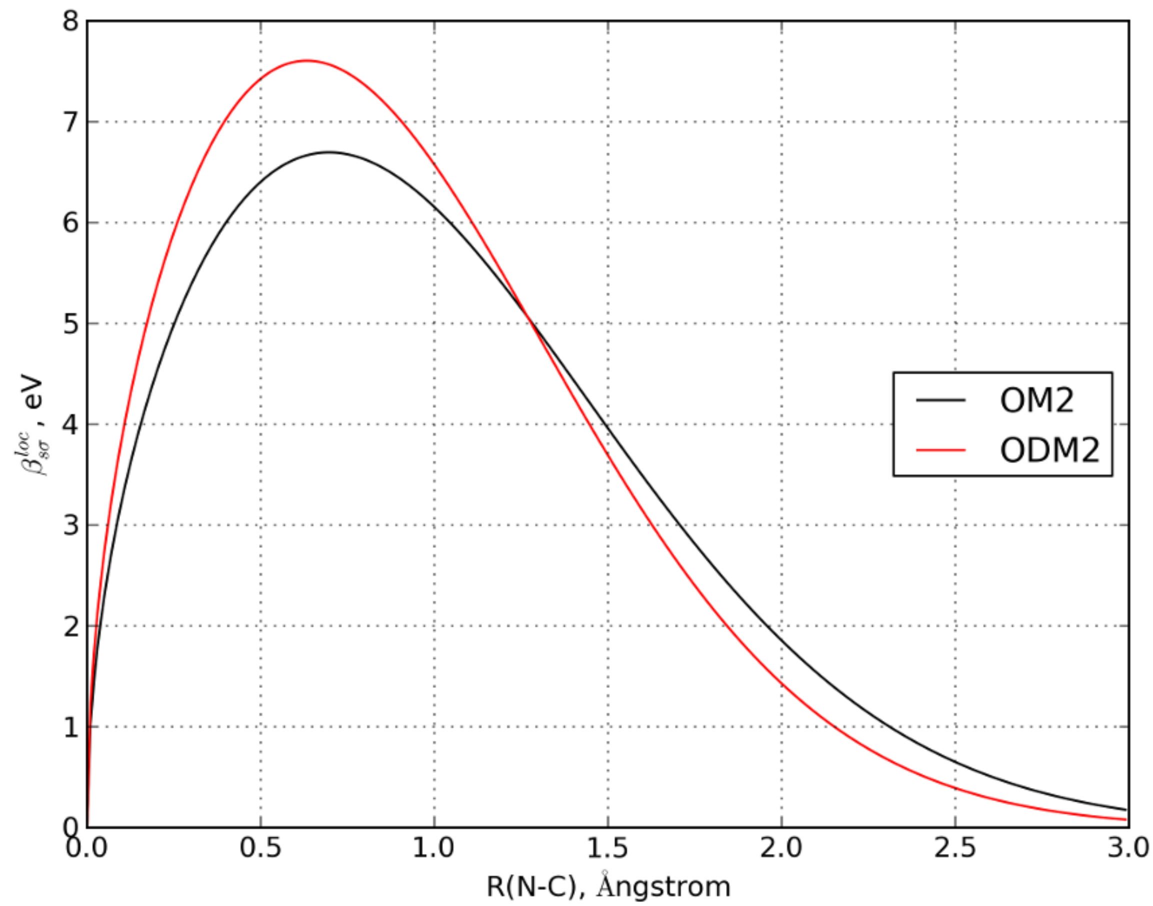

Figure S15: Comparison of $s\sigma$ local resonance integrals for the N−C pair calculated using standard OM2 and new ODM2 parameters.

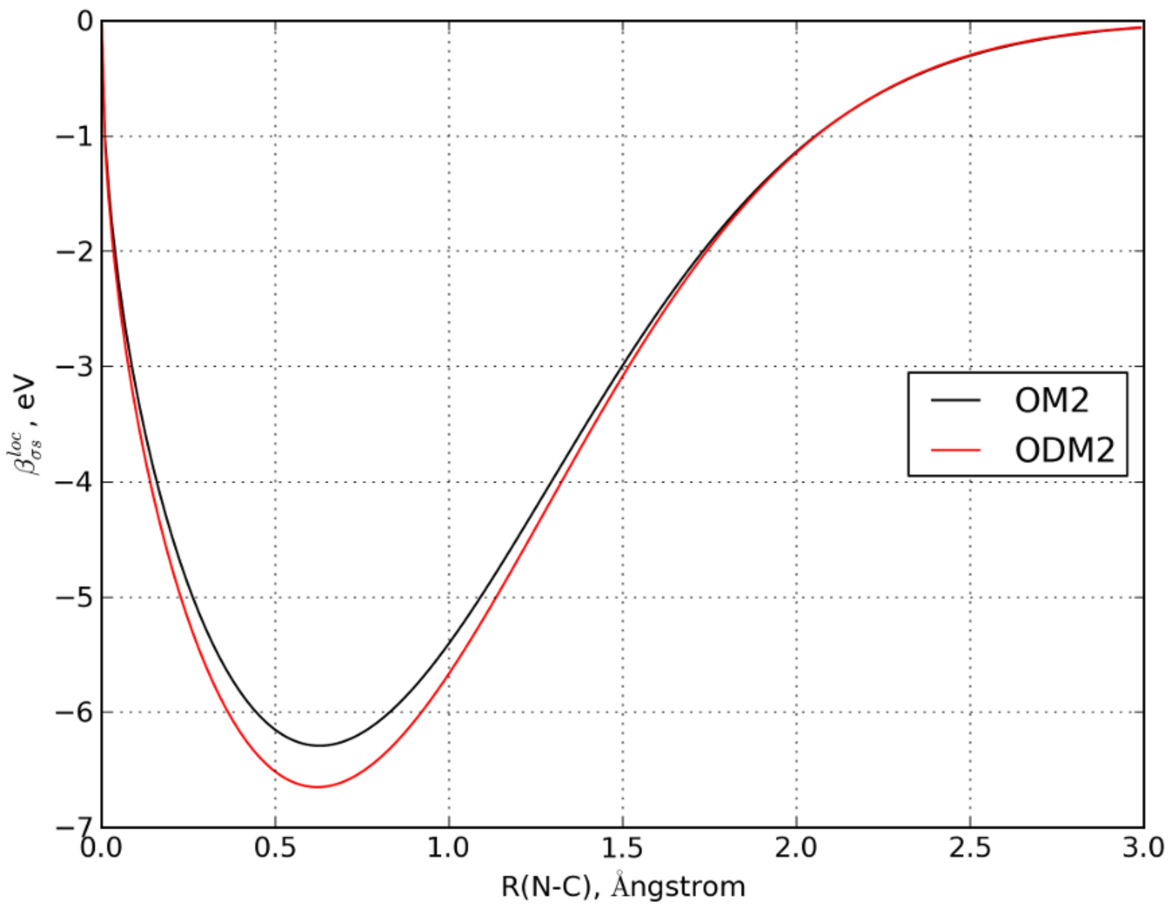

Figure S16: Comparison of σs local resonance integrals for the N−C pair calculated using standard OM2 and new ODM2 parameters.

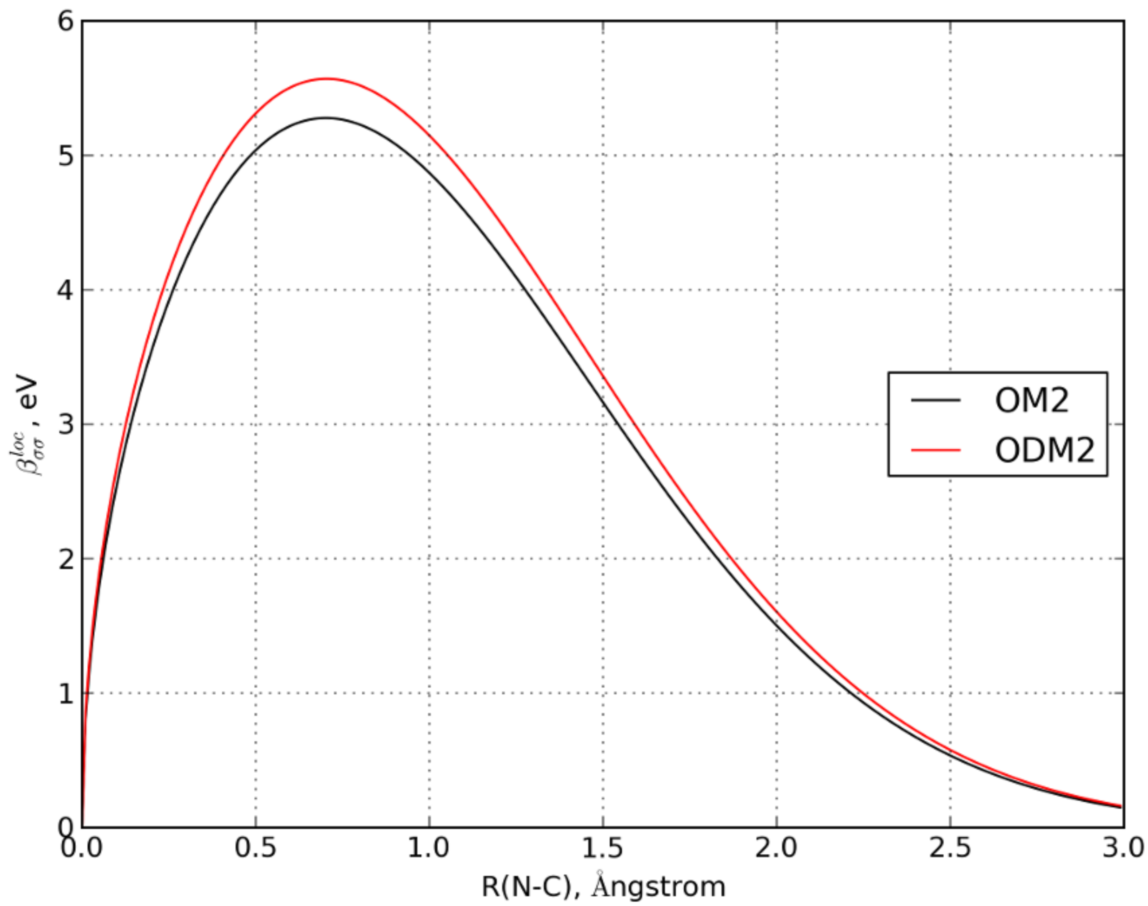

Figure S17: Comparison of $\sigma\sigma$ local resonance integrals for the N−C pair calculated using standard OM2 and new ODM2 parameters.

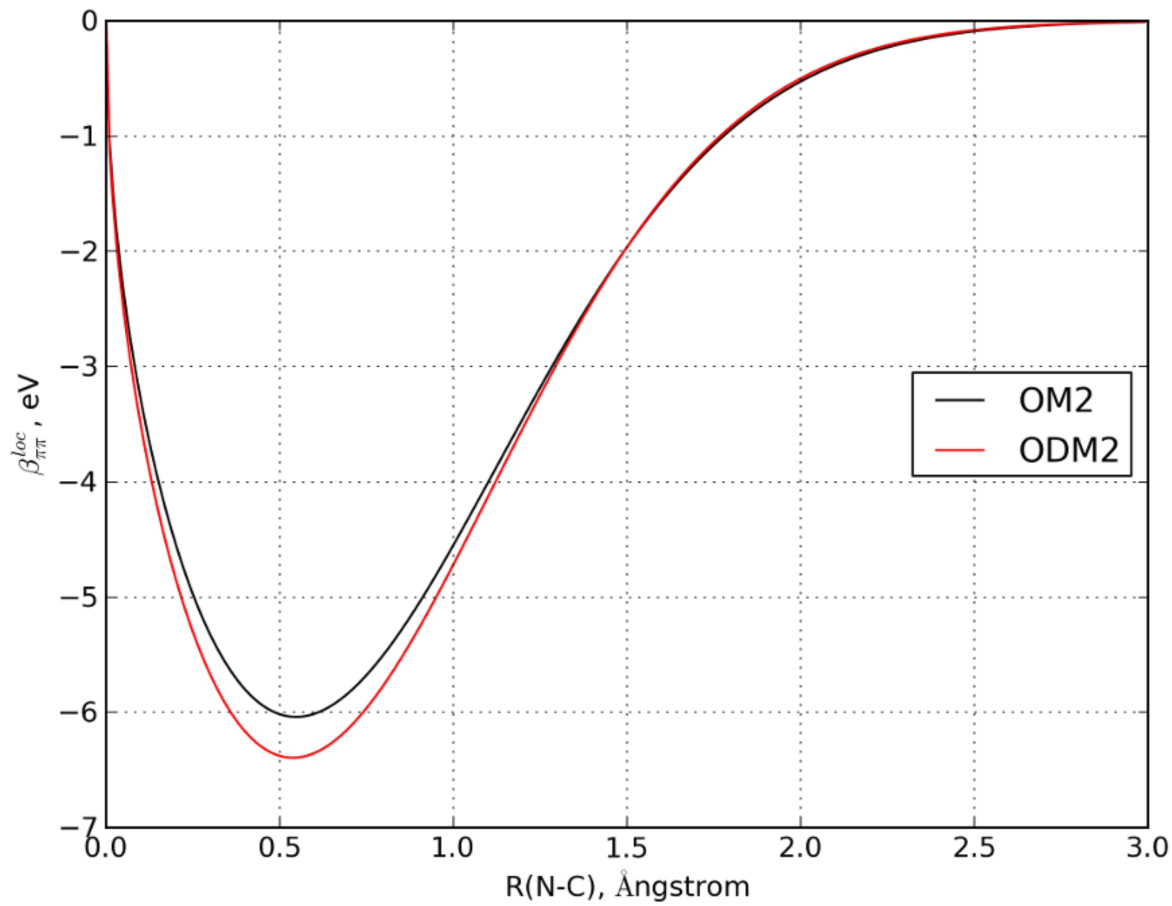

Figure S18: Comparison of $\pi\pi$ local resonance integrals for the N−C pair calculated using standard OM2 and new ODM2 parameters.

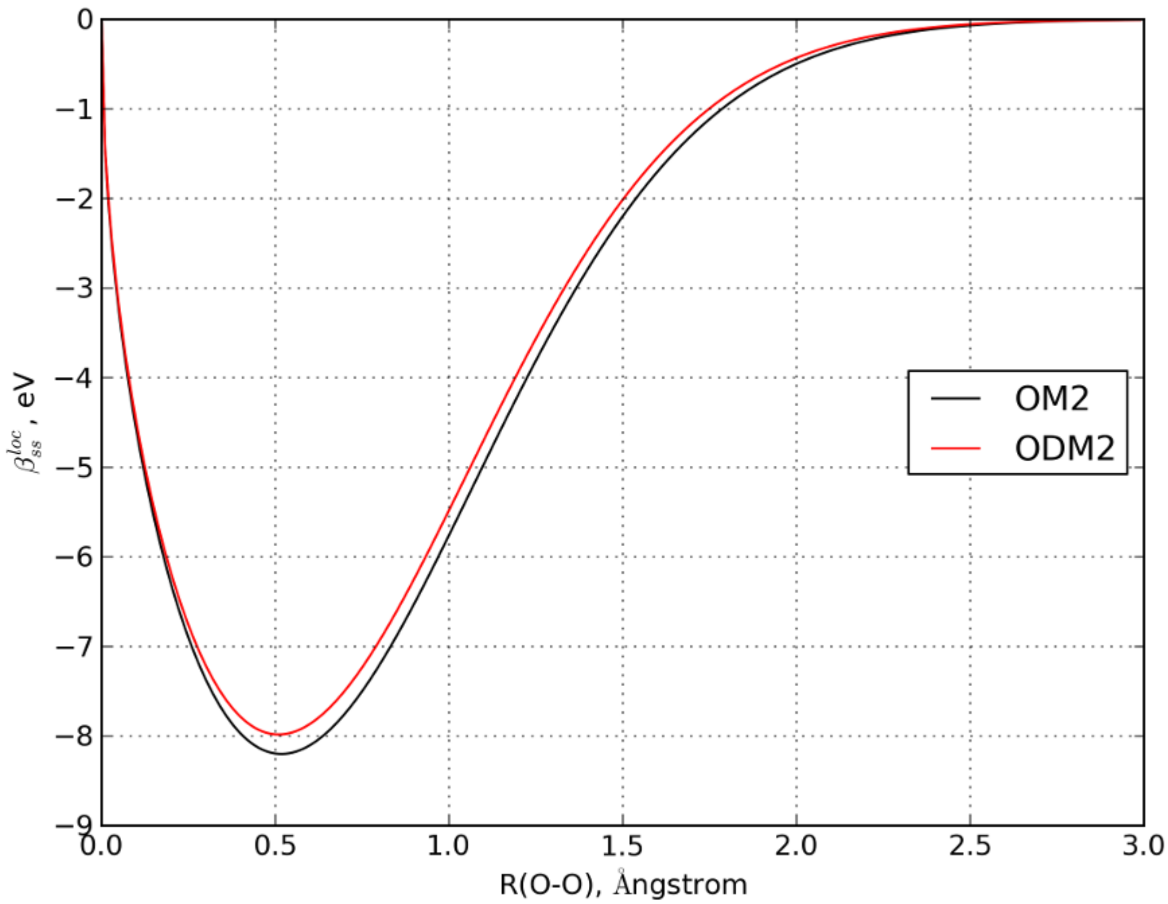

Figure S19: Comparison of *ss* local resonance integrals for the O−O pair calculated using standard OM2 and new ODM2 parameters.

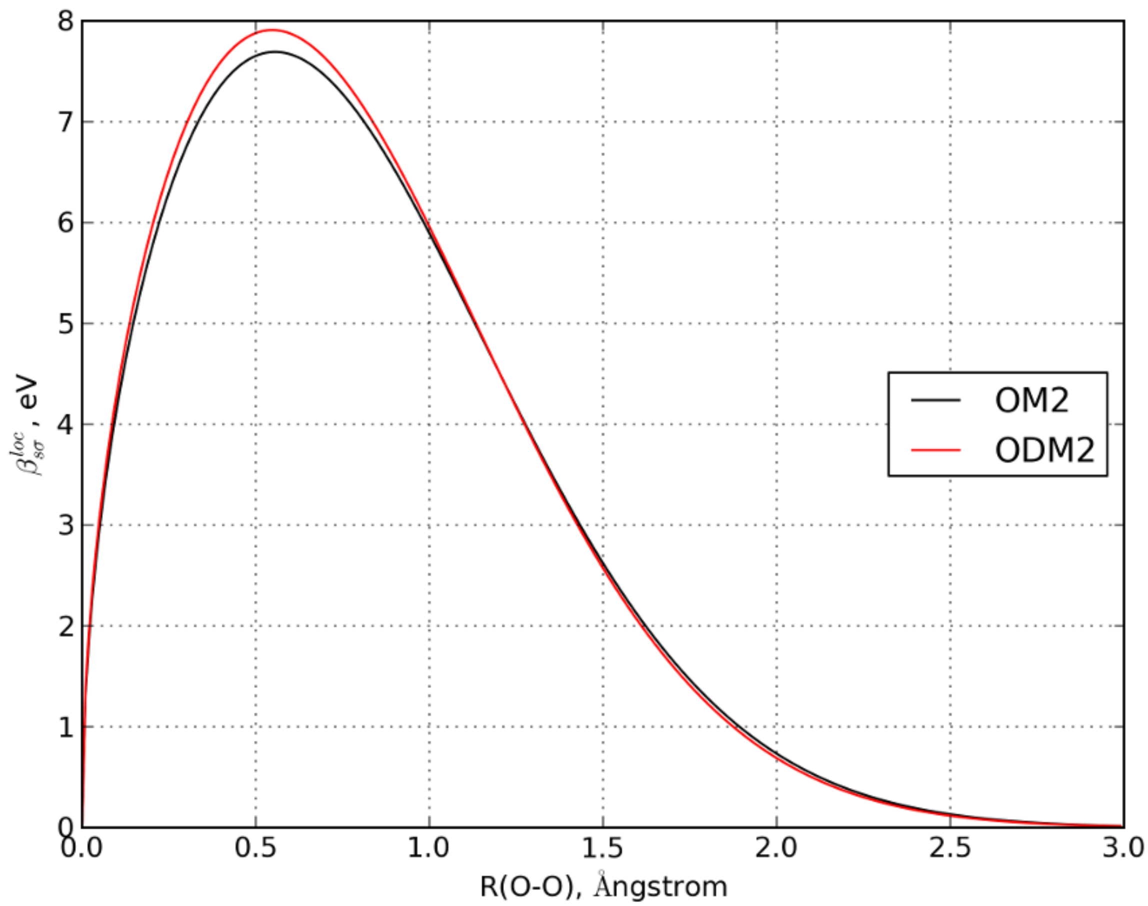

Figure S20: Comparison of $s\sigma$ local resonance integrals for the O−O pair calculated using standard OM2 and new ODM2 parameters.

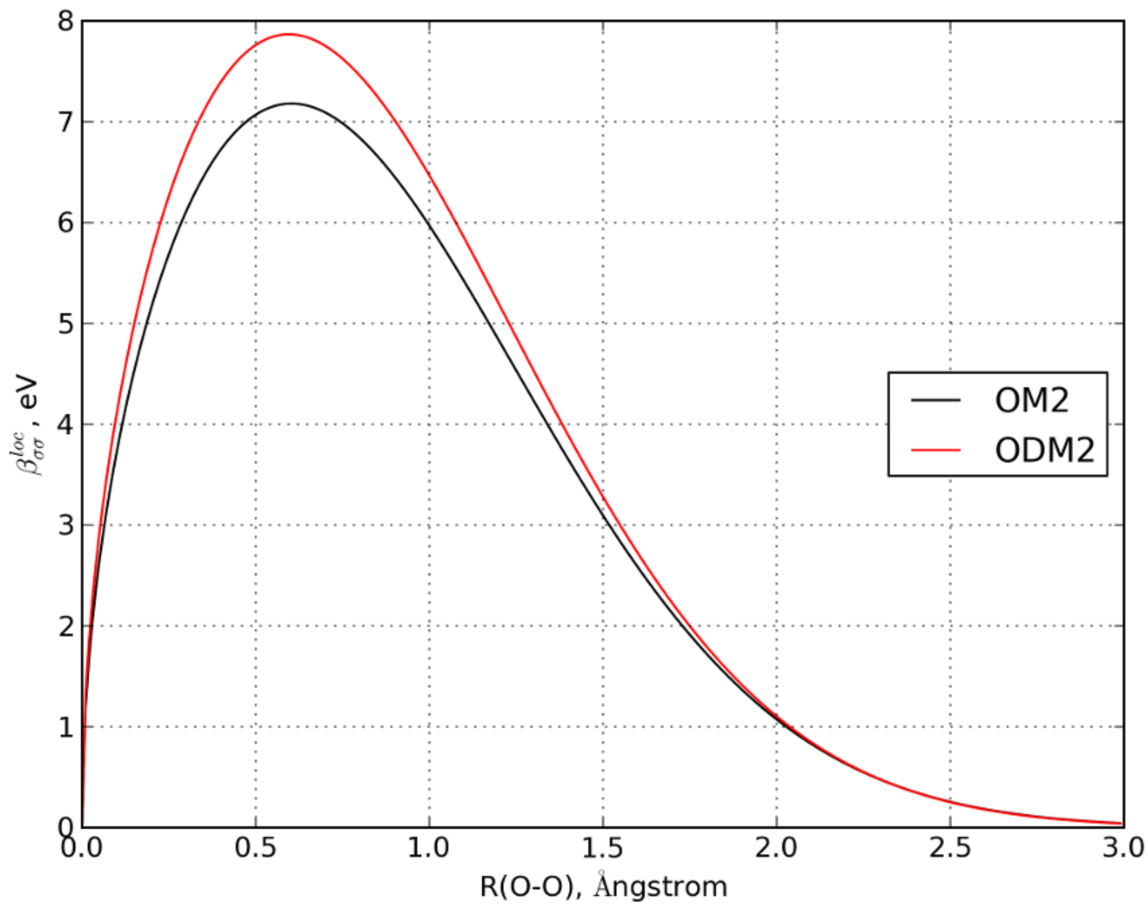

Figure S21: Comparison of $\sigma\sigma$ local resonance integrals for the O−O pair calculated using standard OM2 and new ODM2 parameters.

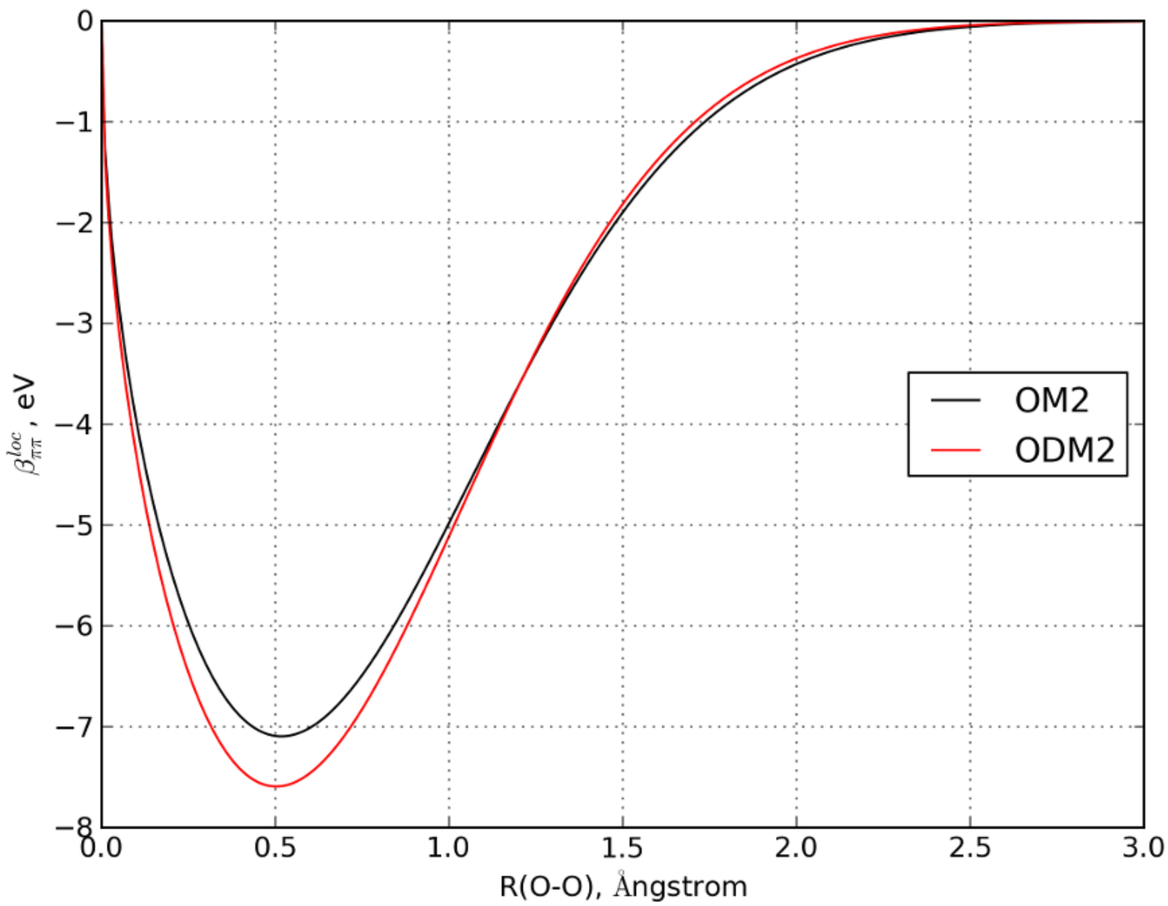

Figure S22: Comparison of $\pi\pi$ local resonance integrals for the O−O pair calculated using standard OM2 and new ODM2 parameters.

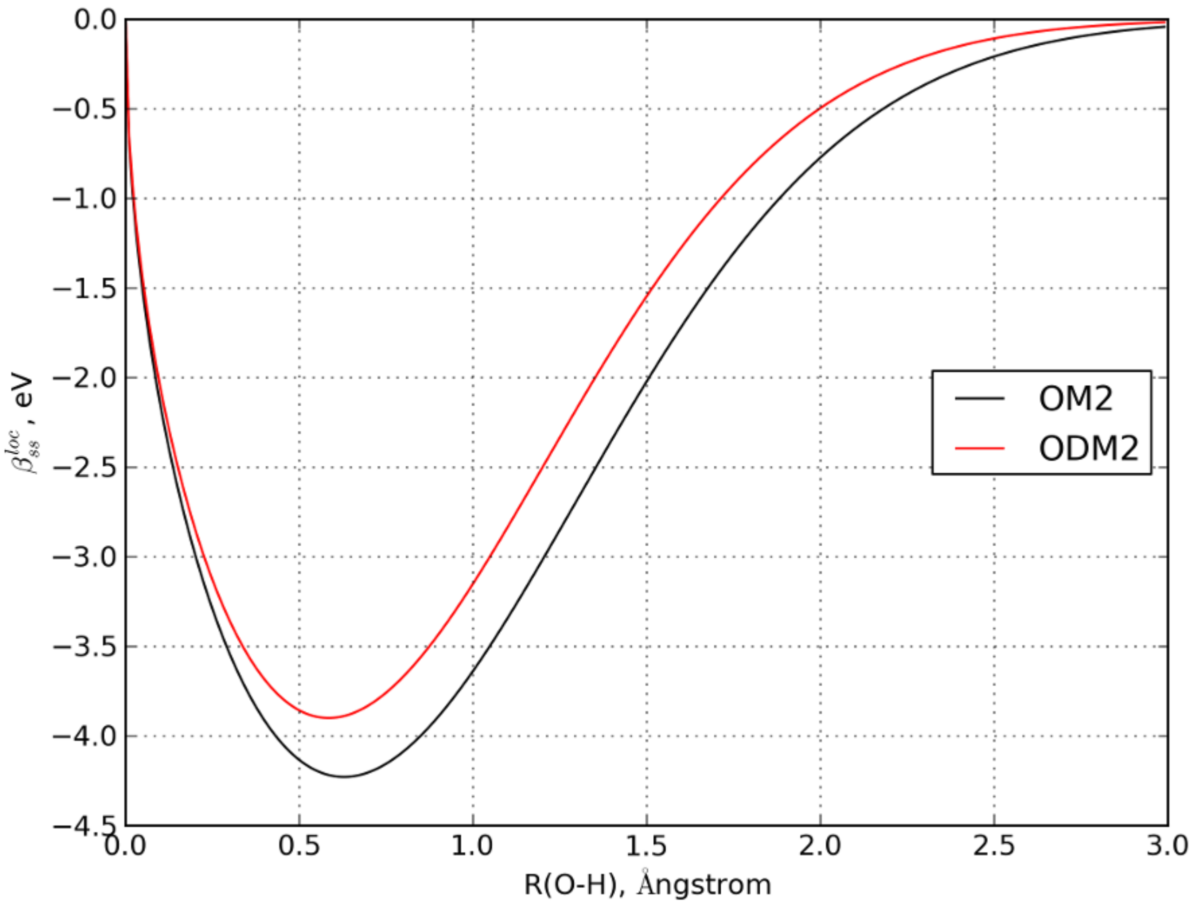

Figure S23: Comparison of *ss* local resonance integrals for the O−H pair calculated using standard OM2 and new ODM2 parameters.

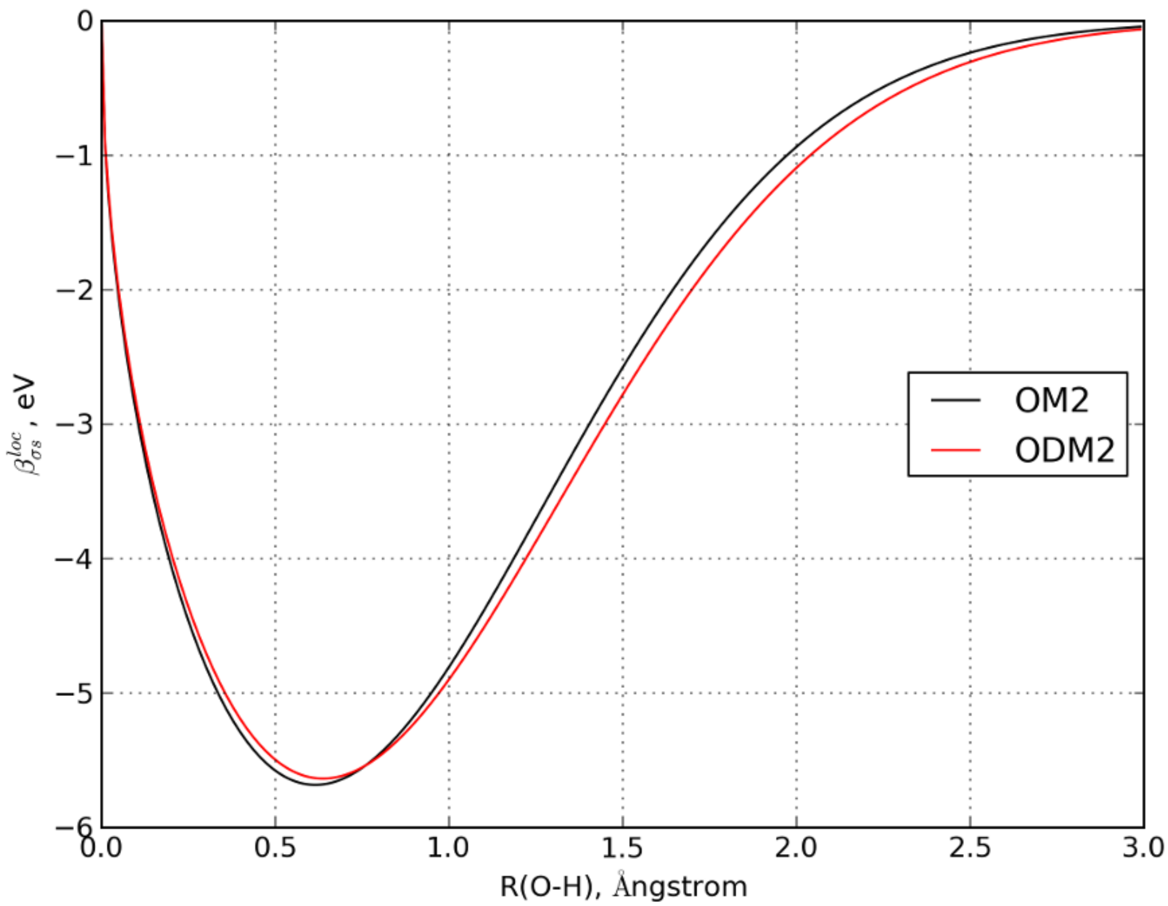

Figure S24: Comparison of σs local resonance integrals for the O−H pair calculated using standard OM2 and new ODM2 parameters.

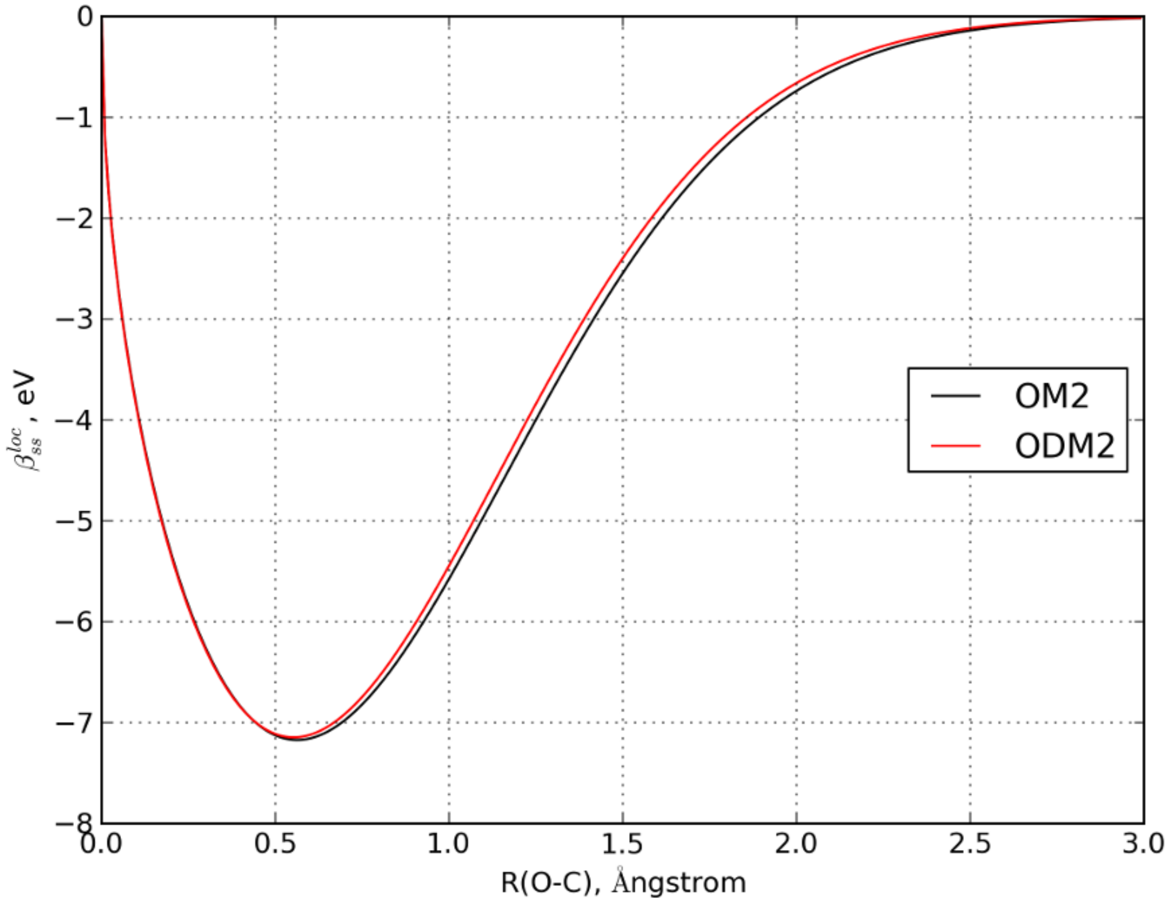

Figure S25: Comparison of ss local resonance integrals for the O−C pair calculated using standard OM2 and new ODM2 parameters.

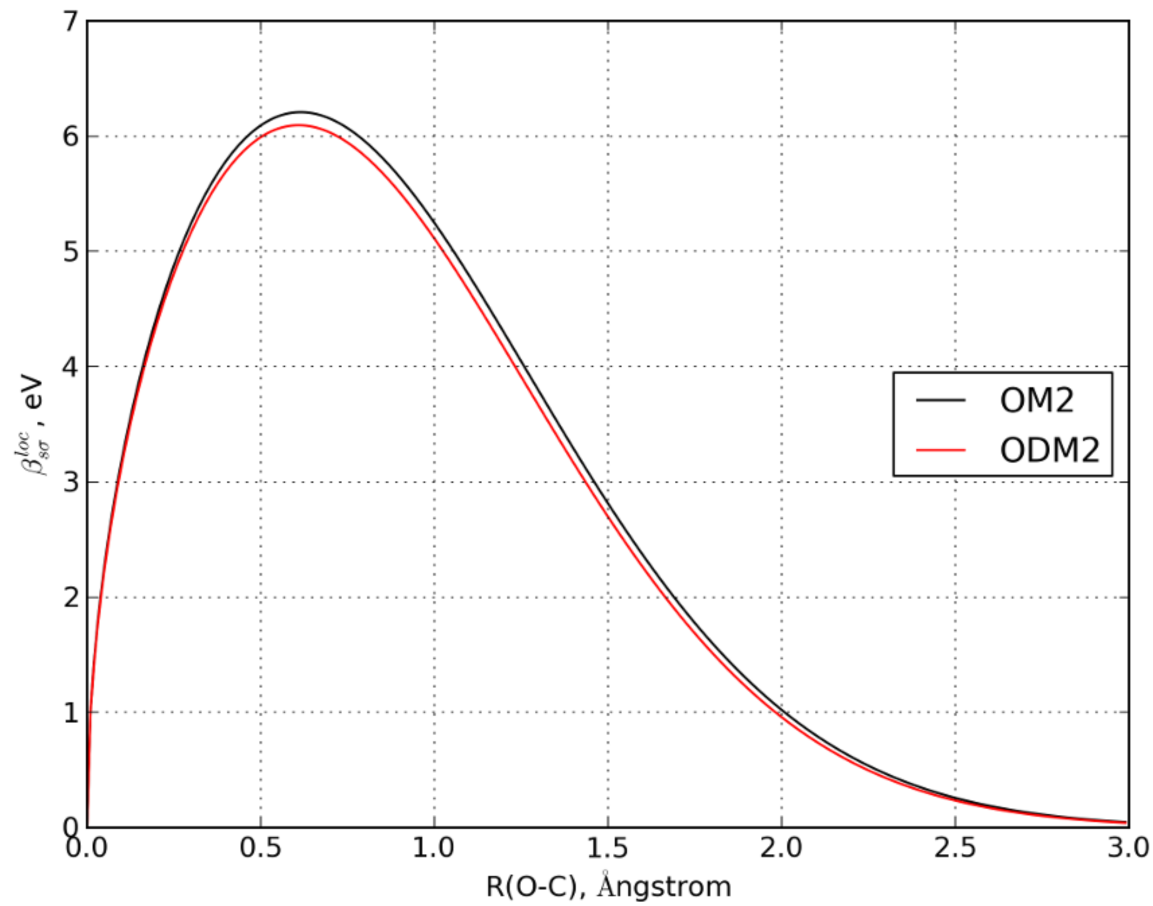

Figure S26: Comparison of $s\sigma$ local resonance integrals for the O−C pair calculated using standard OM2 and new ODM2 parameters.

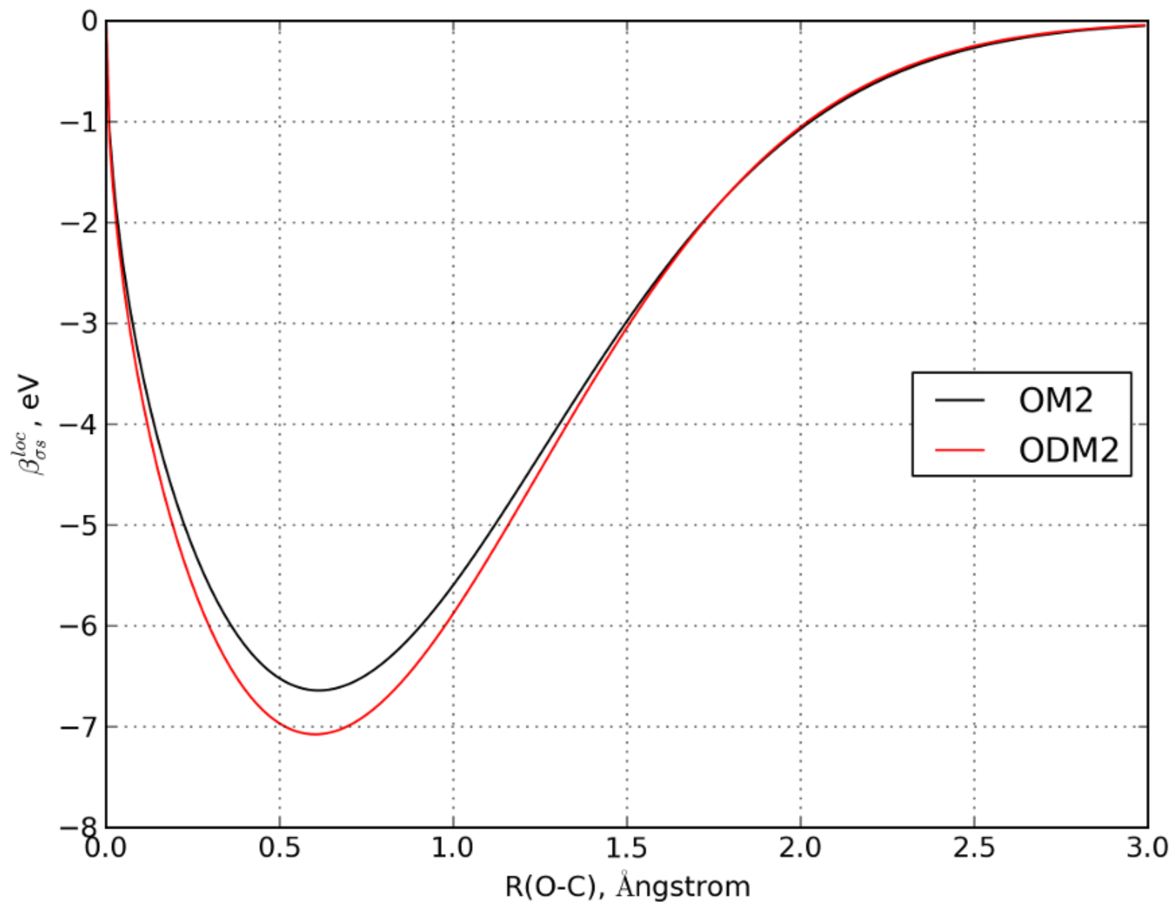

Figure S27: Comparison of σs local resonance integrals for the O−C pair calculated using standard OM2 and new ODM2 parameters.

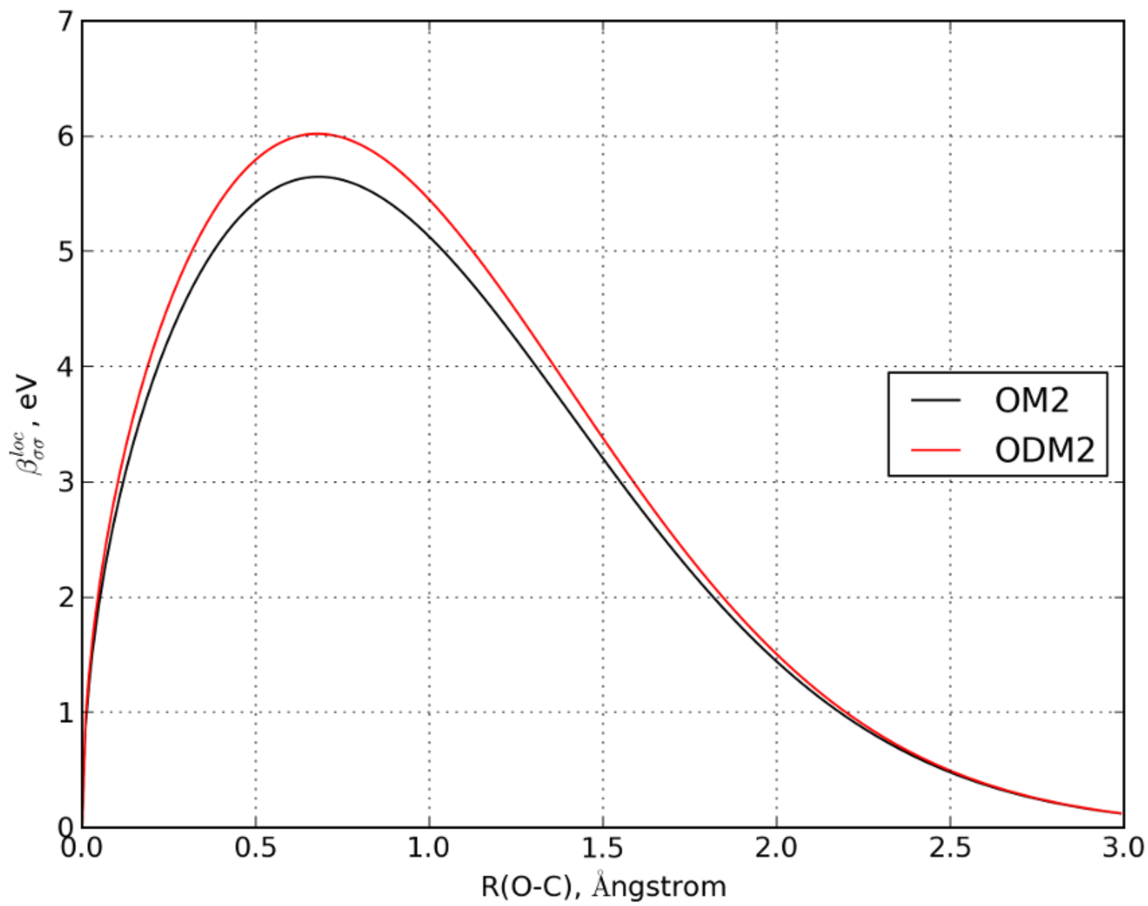

Figure S28: Comparison of $\sigma\sigma$ local resonance integrals for the O−C pair calculated using standard OM2 and new ODM2 parameters.

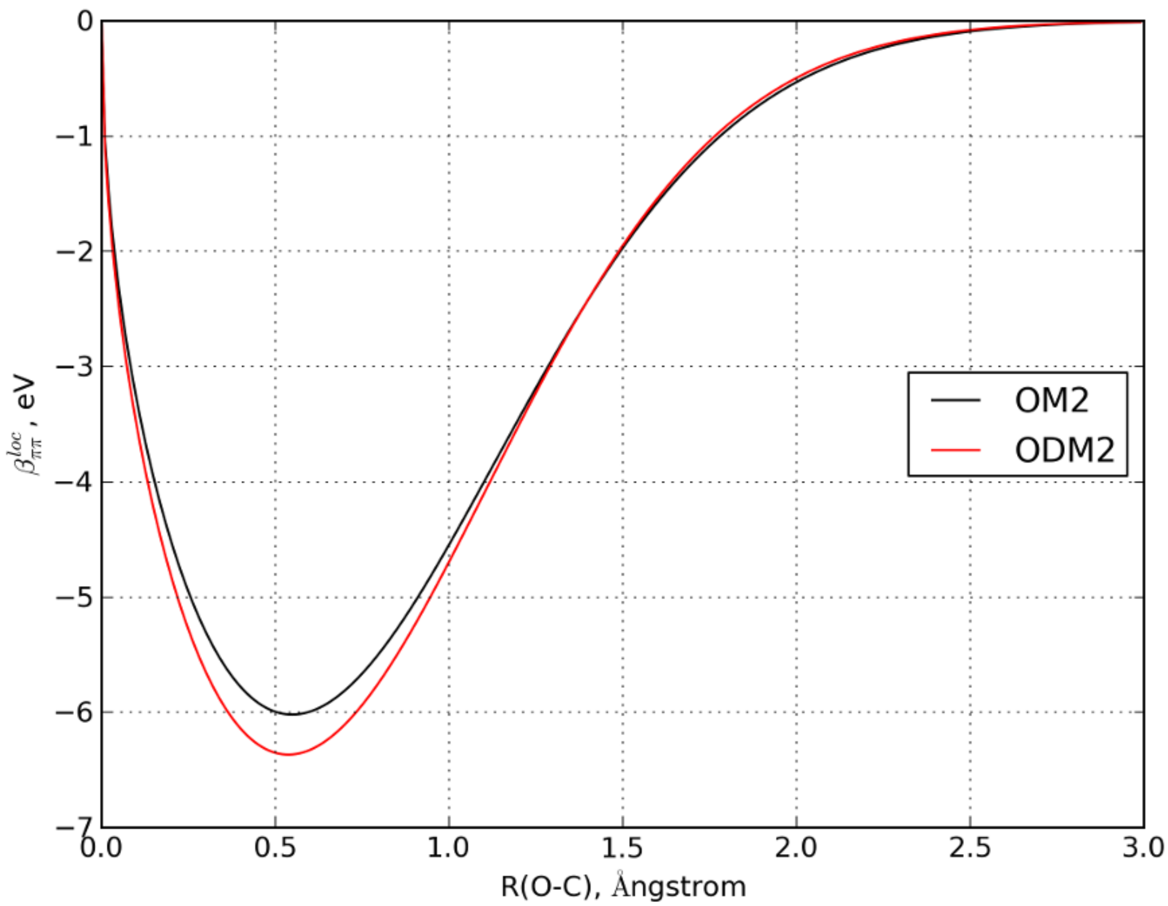

Figure S29: Comparison of $\pi\pi$ local resonance integrals for the O−C pair calculated using standard OM2 and new ODM2 parameters.

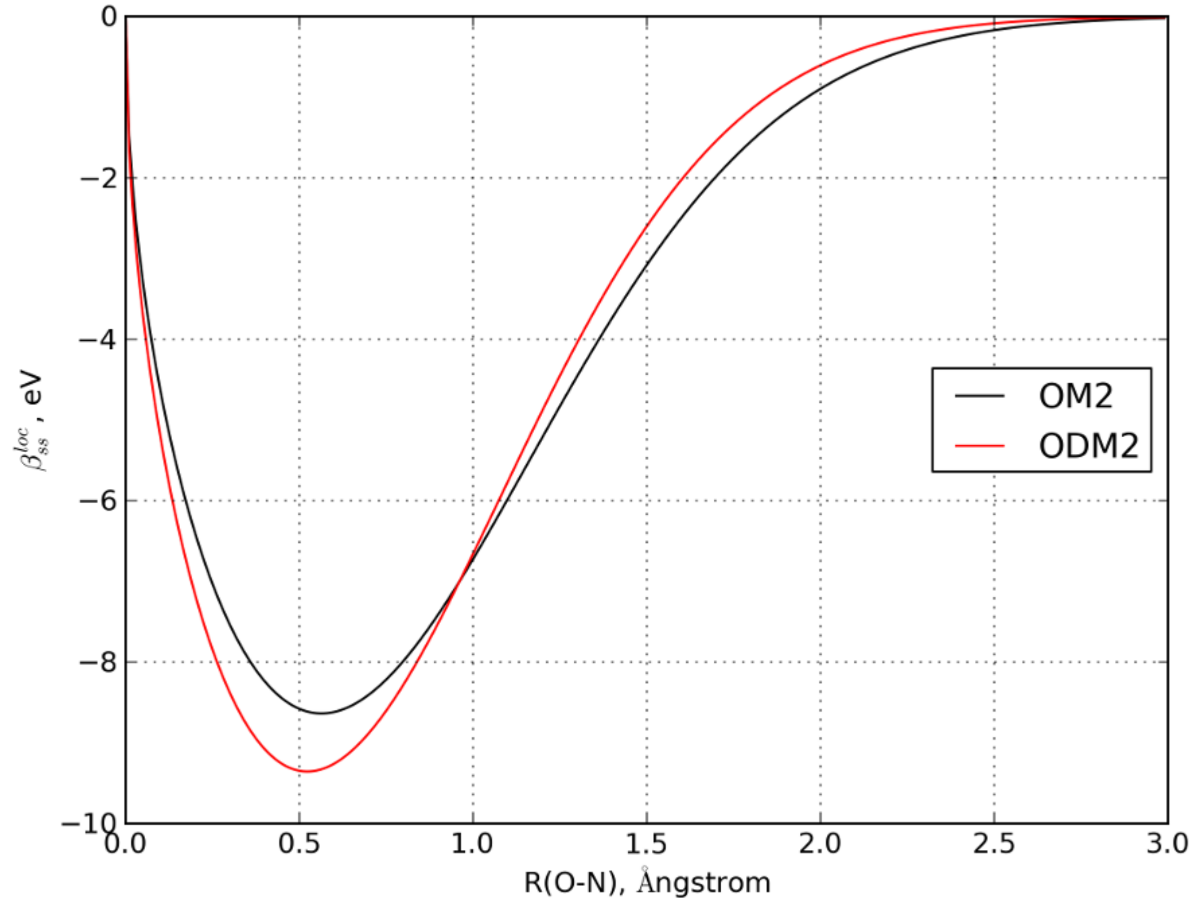

Figure S30: Comparison of *ss* local resonance integrals for the O−N pair calculated using standard OM2 and new ODM2 parameters.

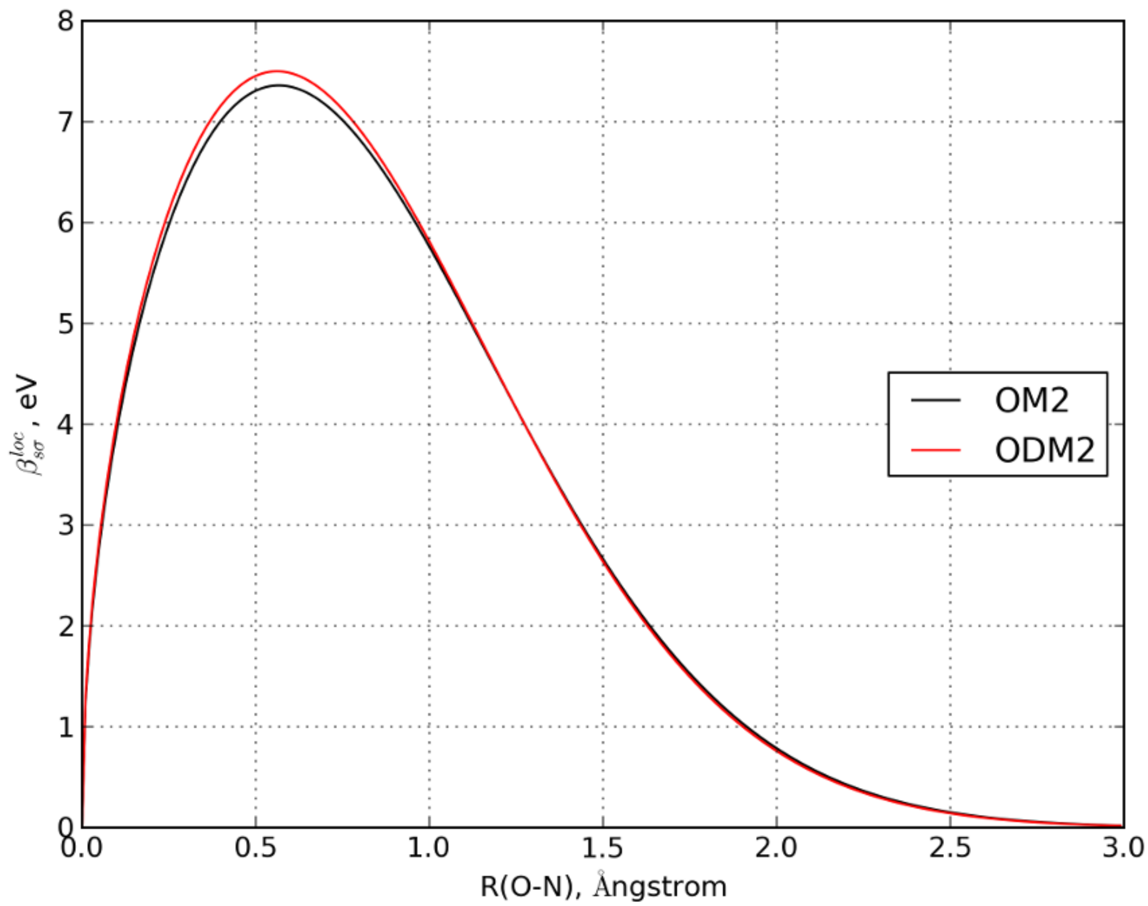

Figure S31: Comparison of $s\sigma$ local resonance integrals for the O−N pair calculated using standard OM2 and new ODM2 parameters.

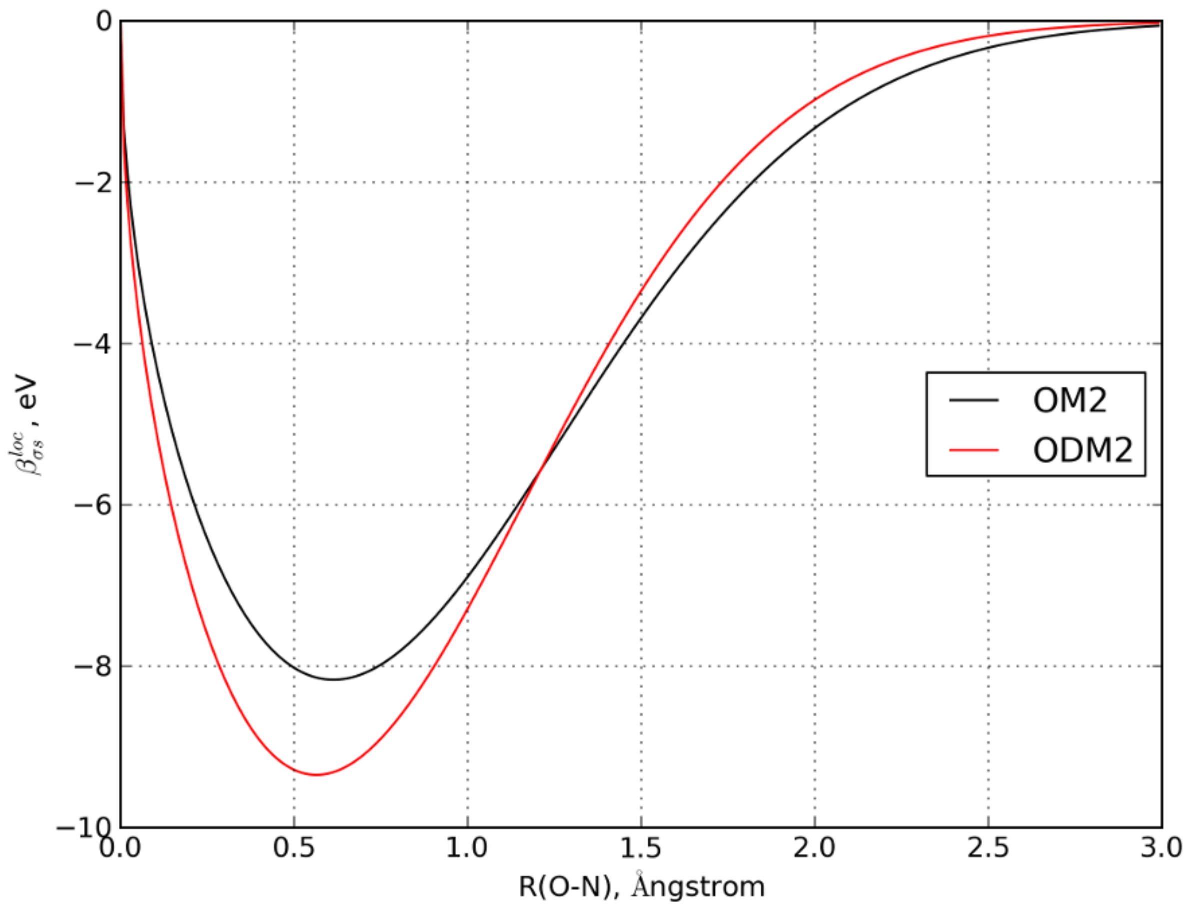

Figure S32: Comparison of σs local resonance integrals for the O−N pair calculated using standard OM2 and new ODM2 parameters.

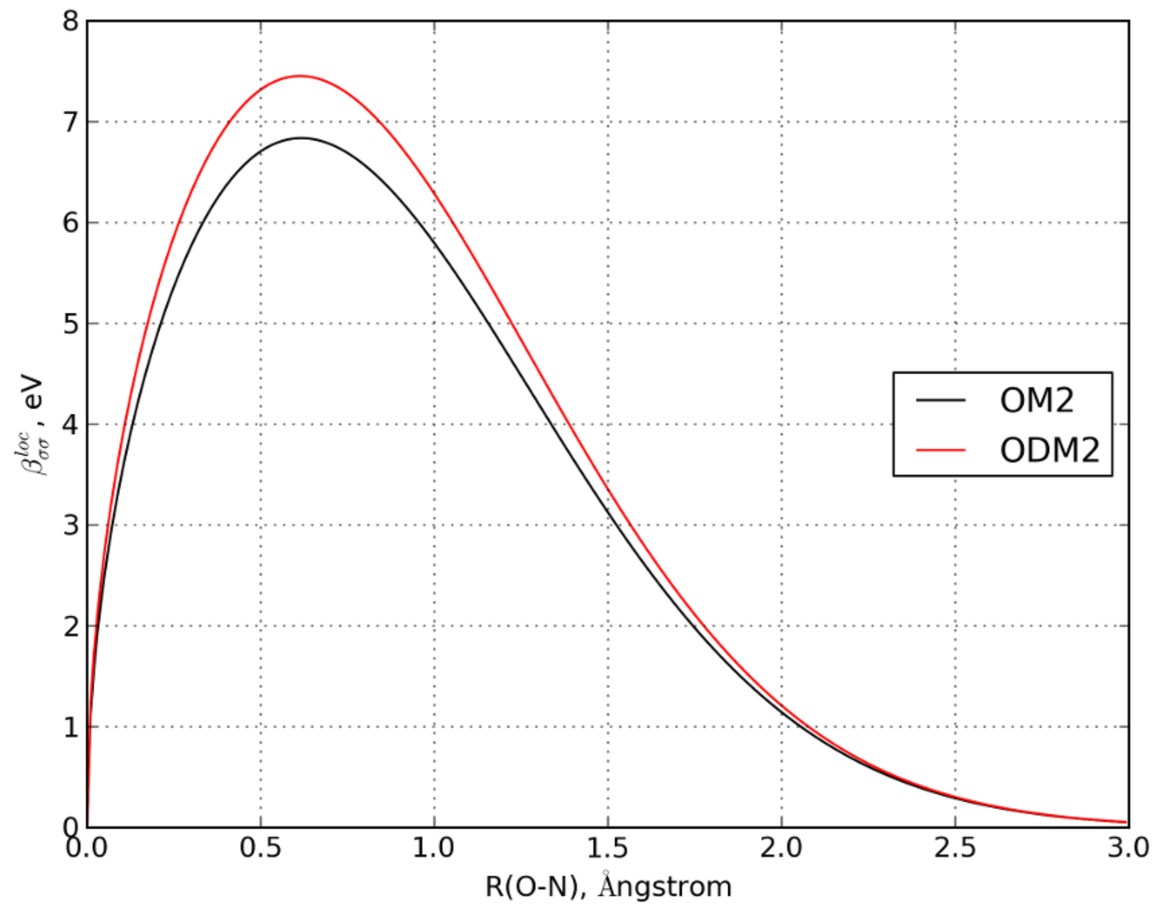

Figure S33: Comparison of $\sigma\sigma$ local resonance integrals for the O−N pair calculated using standard OM2 and new ODM2 parameters.

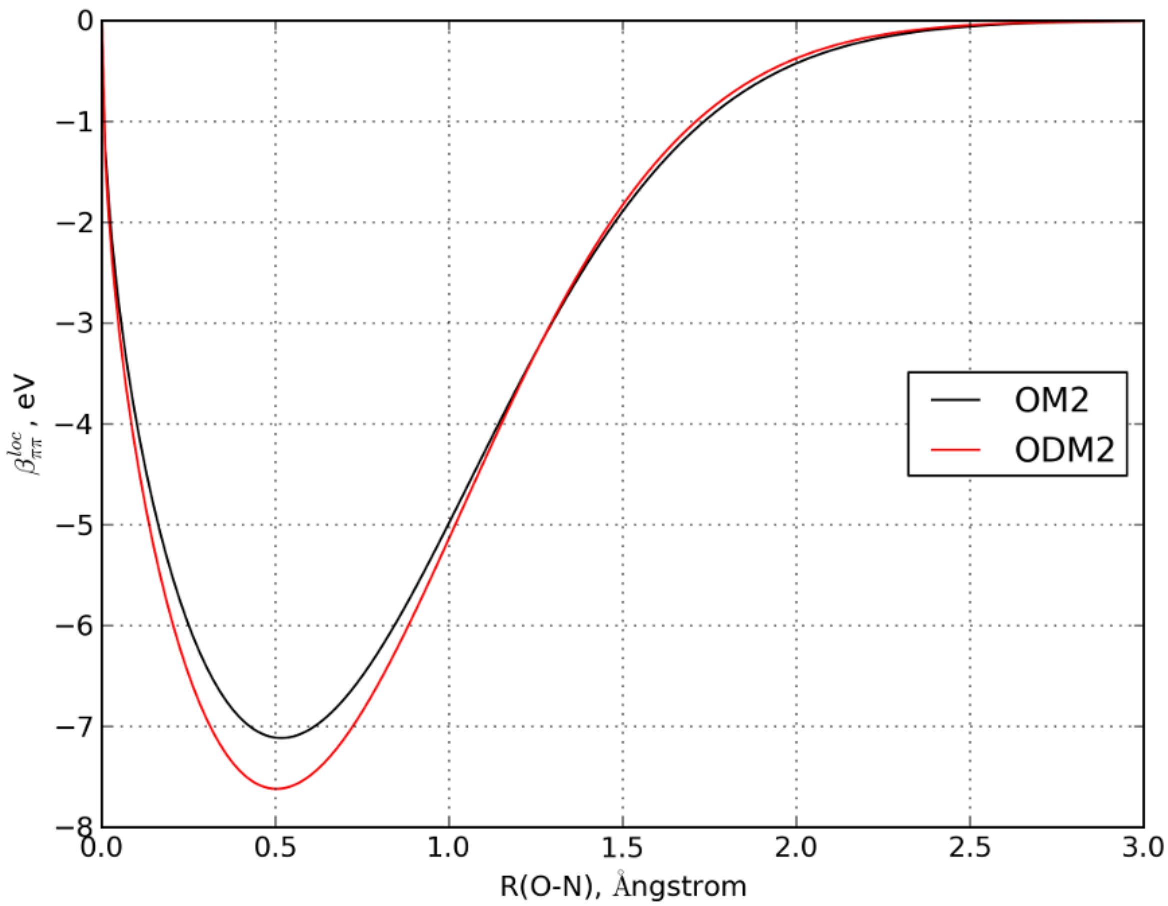

Figure S34: Comparison of $\pi\pi$ local resonance integrals for the O−N pair calculated using standard OM2 and new ODM2 parameters.

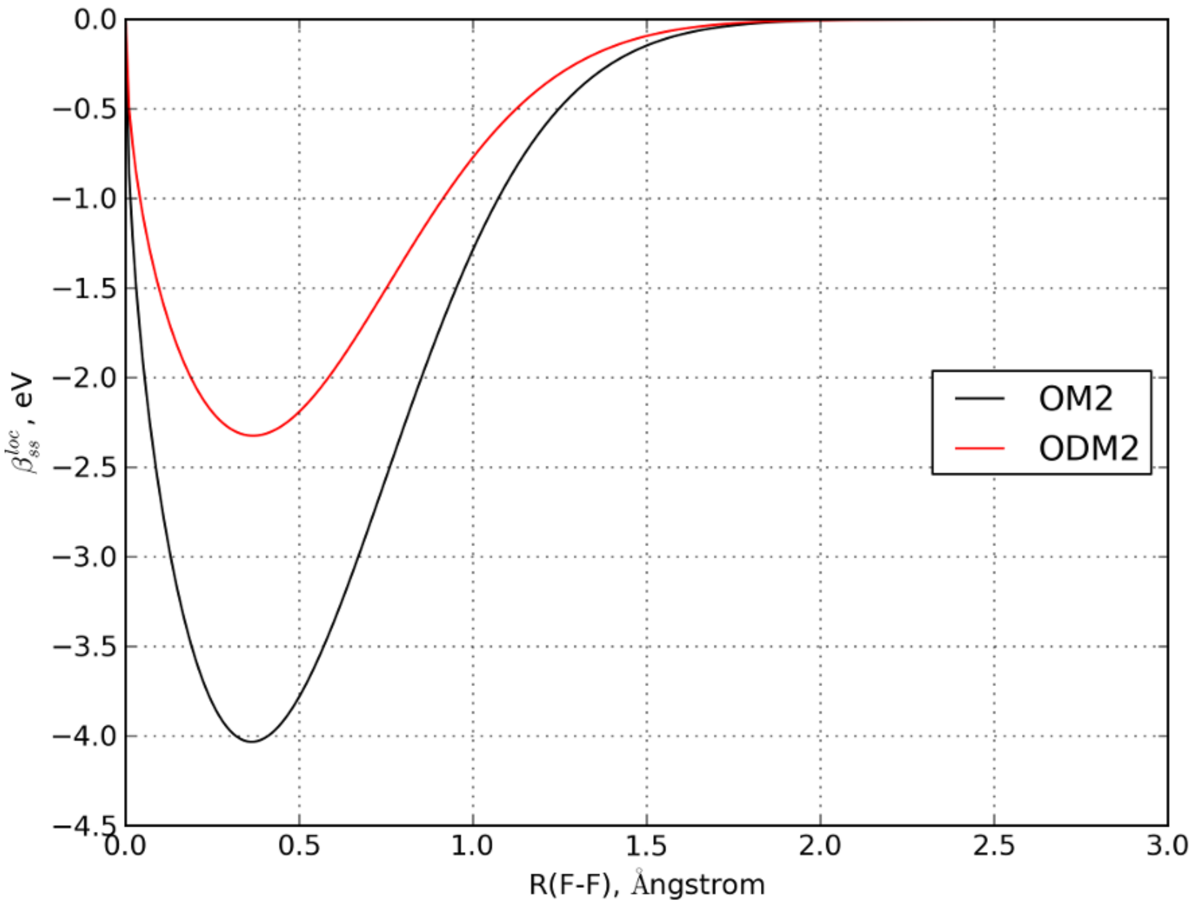

Figure S35: Comparison of ss local resonance integrals for the F−F pair calculated using standard OM2 and new ODM2 parameters.

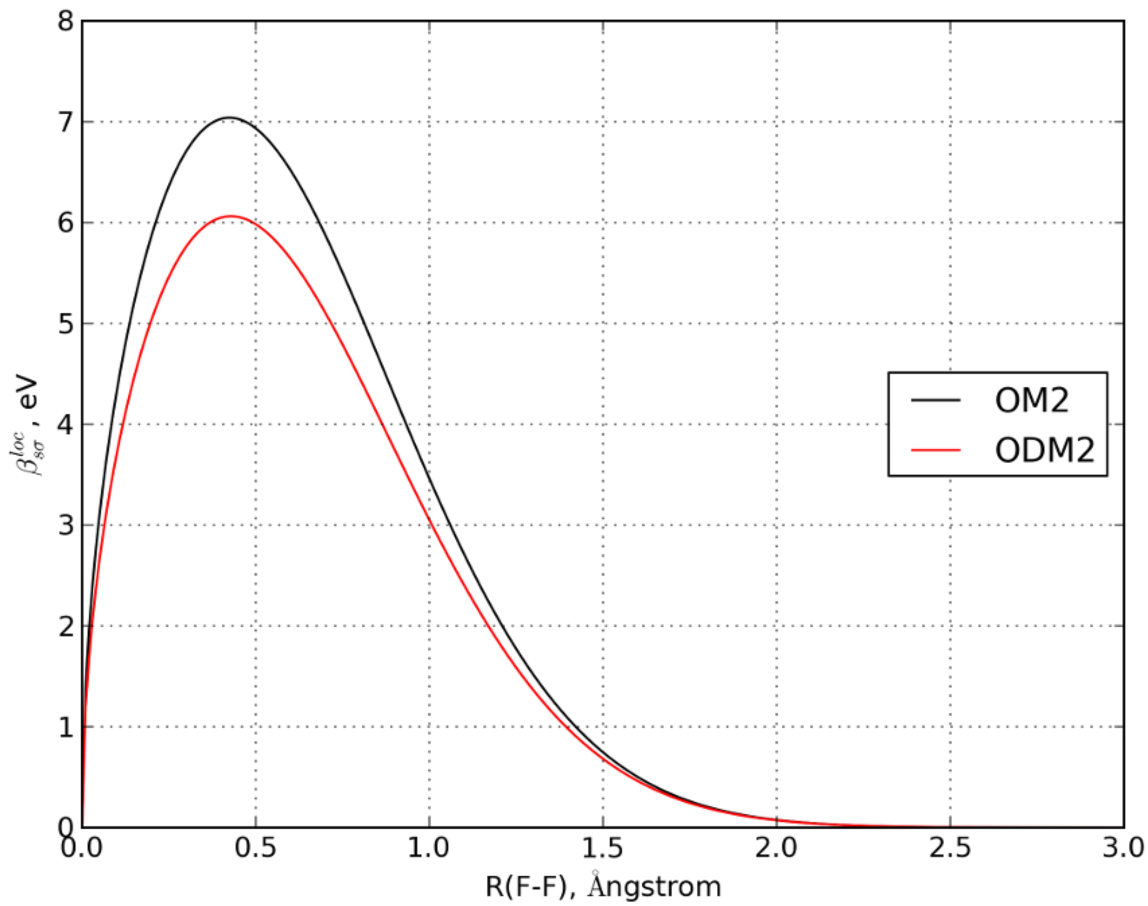

Figure S36: Comparison of $s\sigma$ local resonance integrals for the F−F pair calculated using standard OM2 and new ODM2 parameters.

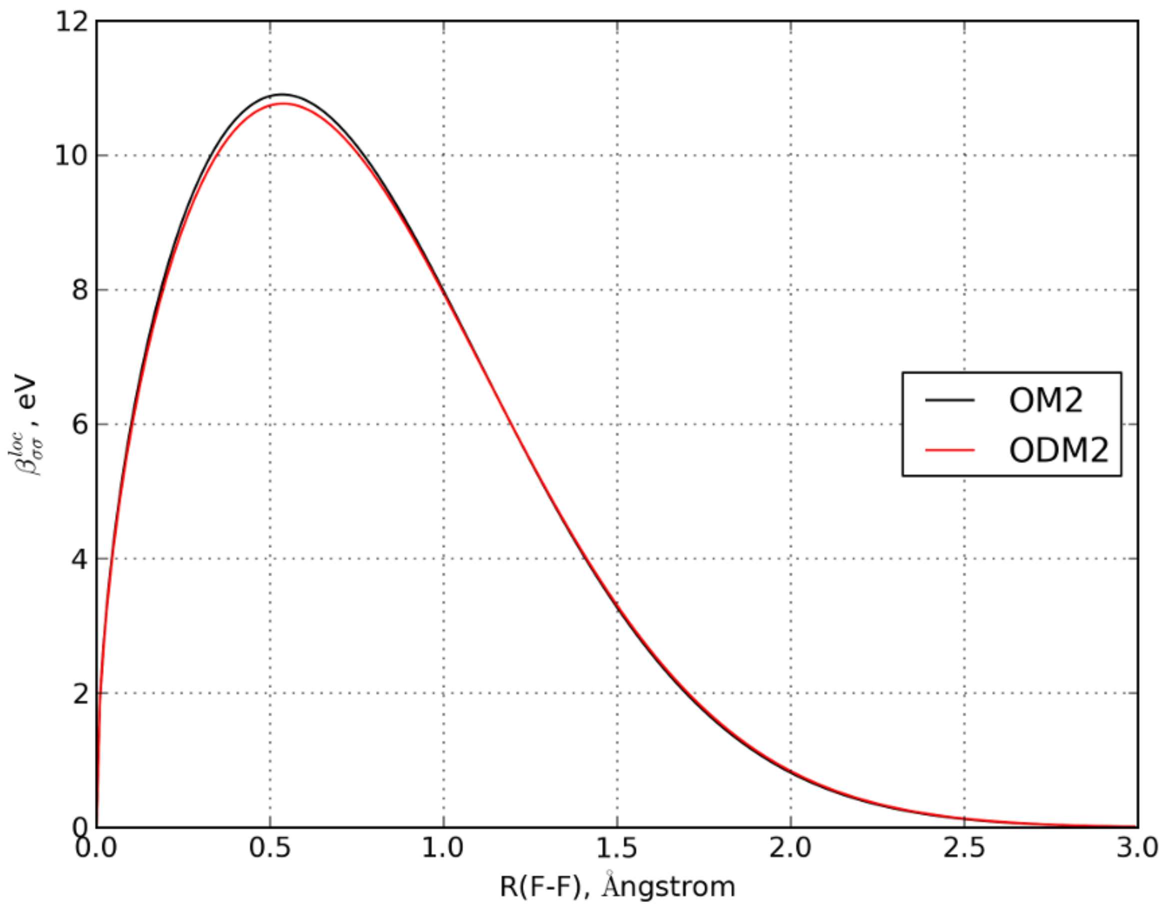

Figure S37: Comparison of $\sigma\sigma$ local resonance integrals for the F−F pair calculated using standard OM2 and new ODM2 parameters.

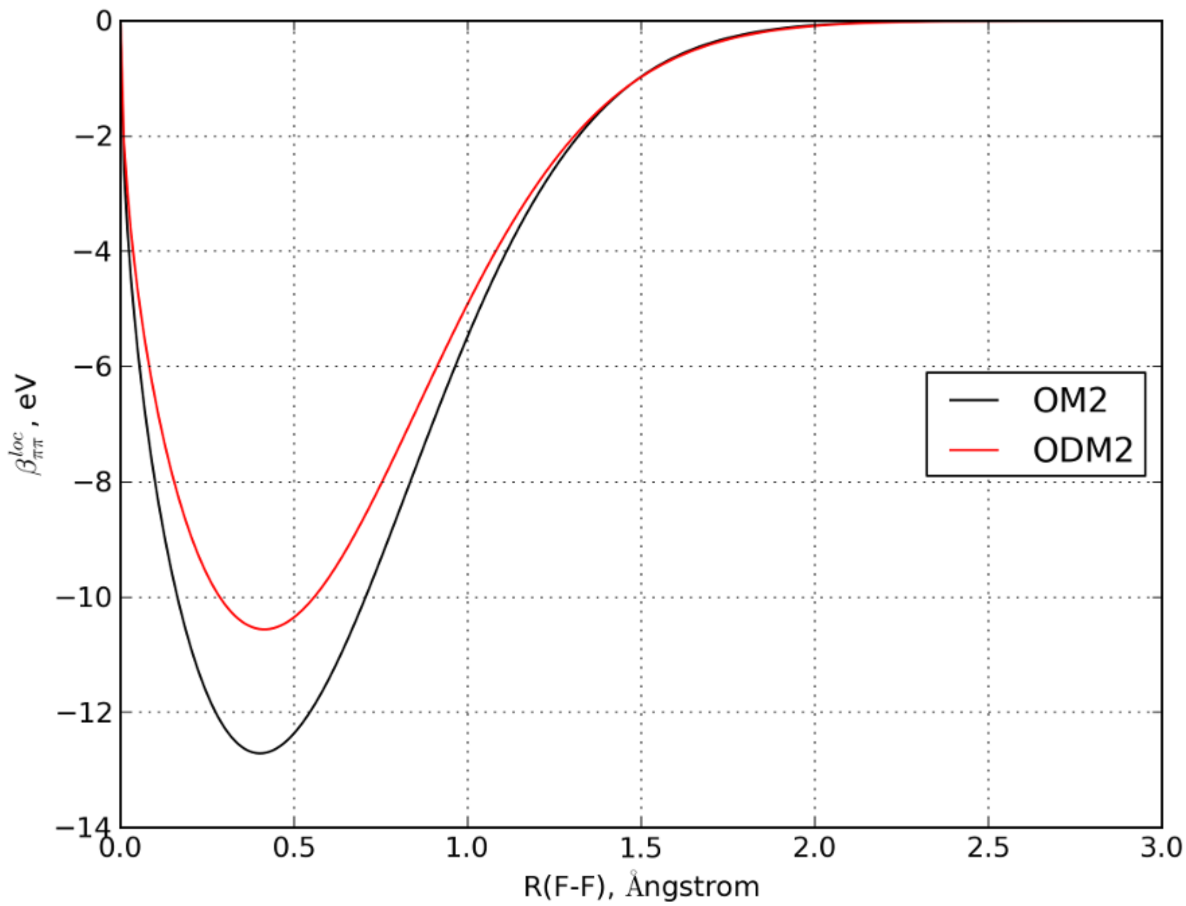

Figure S38: Comparison of $\pi\pi$ local resonance integrals for the F−F pair calculated using standard OM2 and new ODM2 parameters.

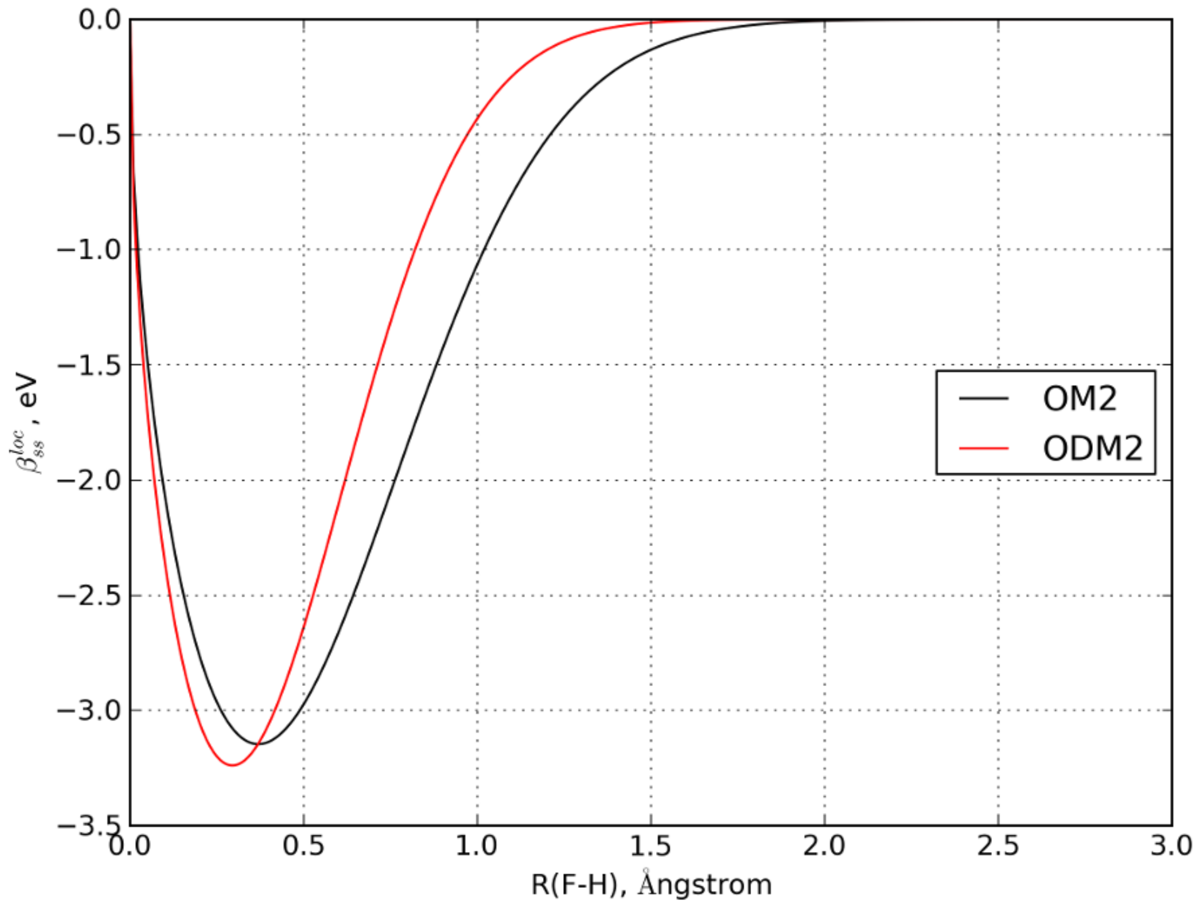

Figure S39: Comparison of ss local resonance integrals for the F−H pair calculated using standard OM2 and new ODM2 parameters.

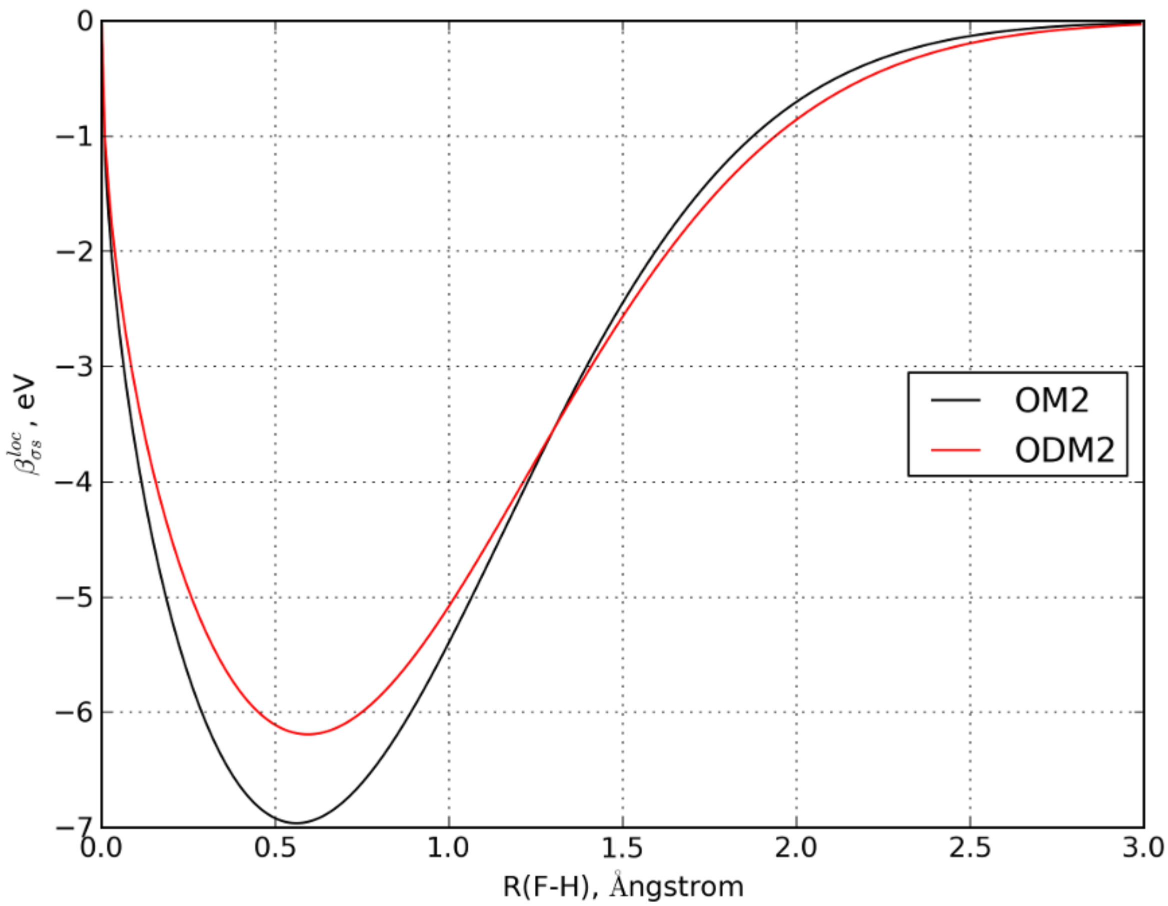

Figure S40: Comparison of σs local resonance integrals for the F−H pair calculated using standard OM2 and new ODM2 parameters.

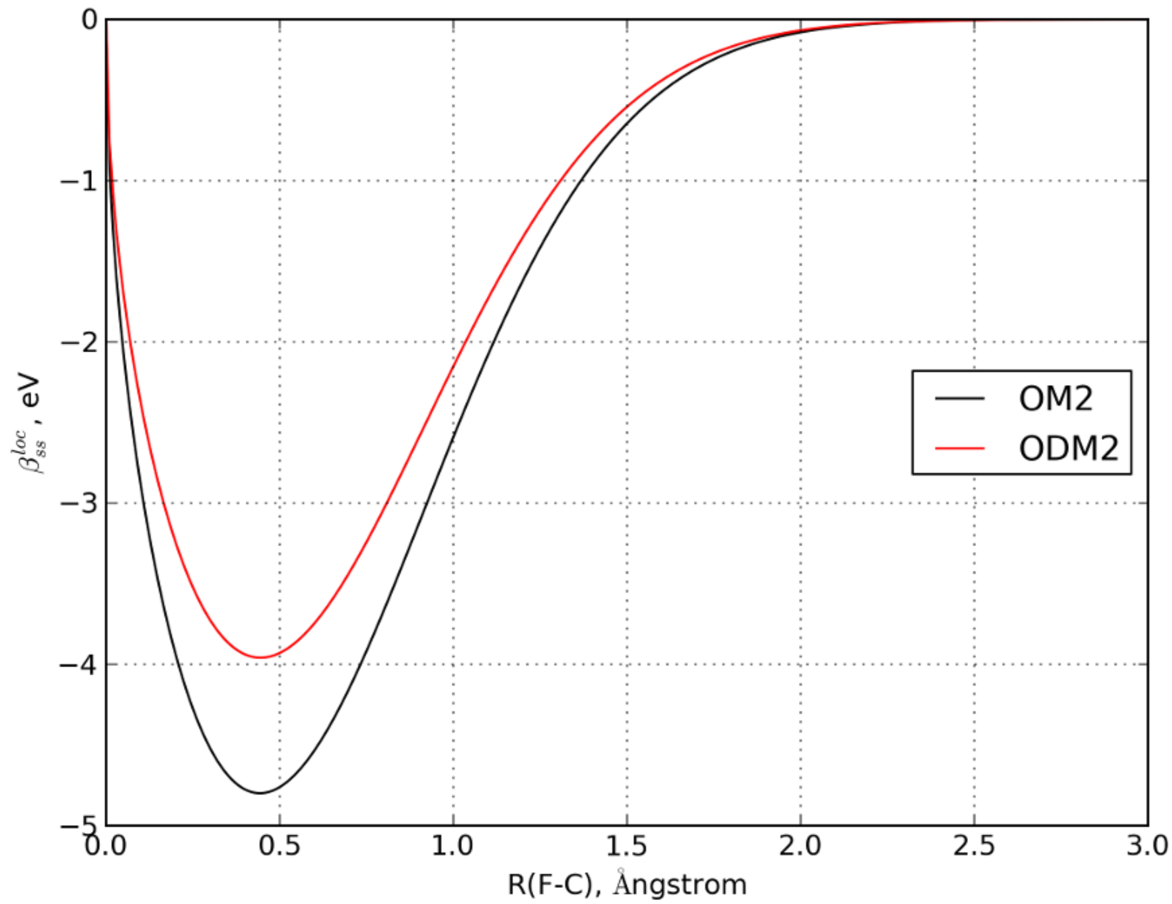

Figure S41: Comparison of ss local resonance integrals for the F−C pair calculated using standard OM2 and new ODM2 parameters.

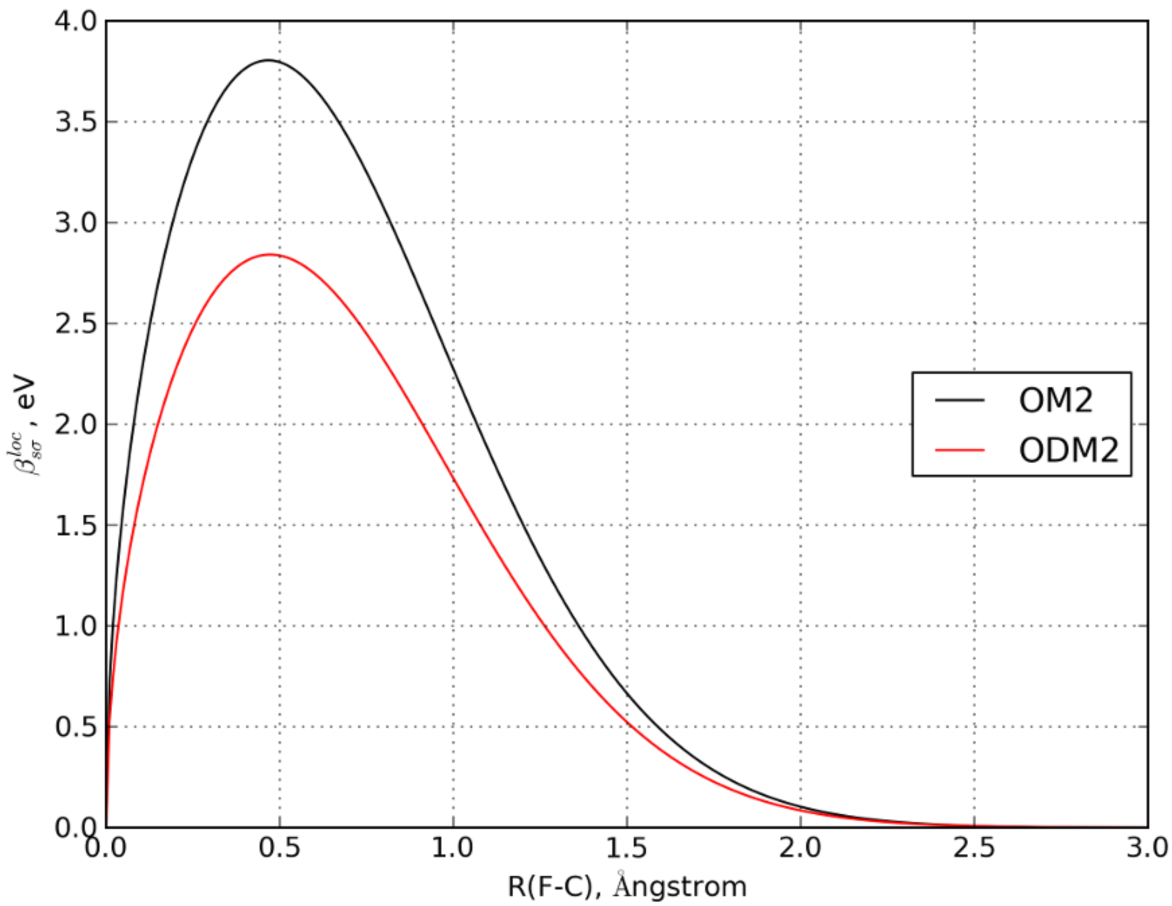

Figure S42: Comparison of $s\sigma$ local resonance integrals for the F−C pair calculated using standard OM2 and new ODM2 parameters.

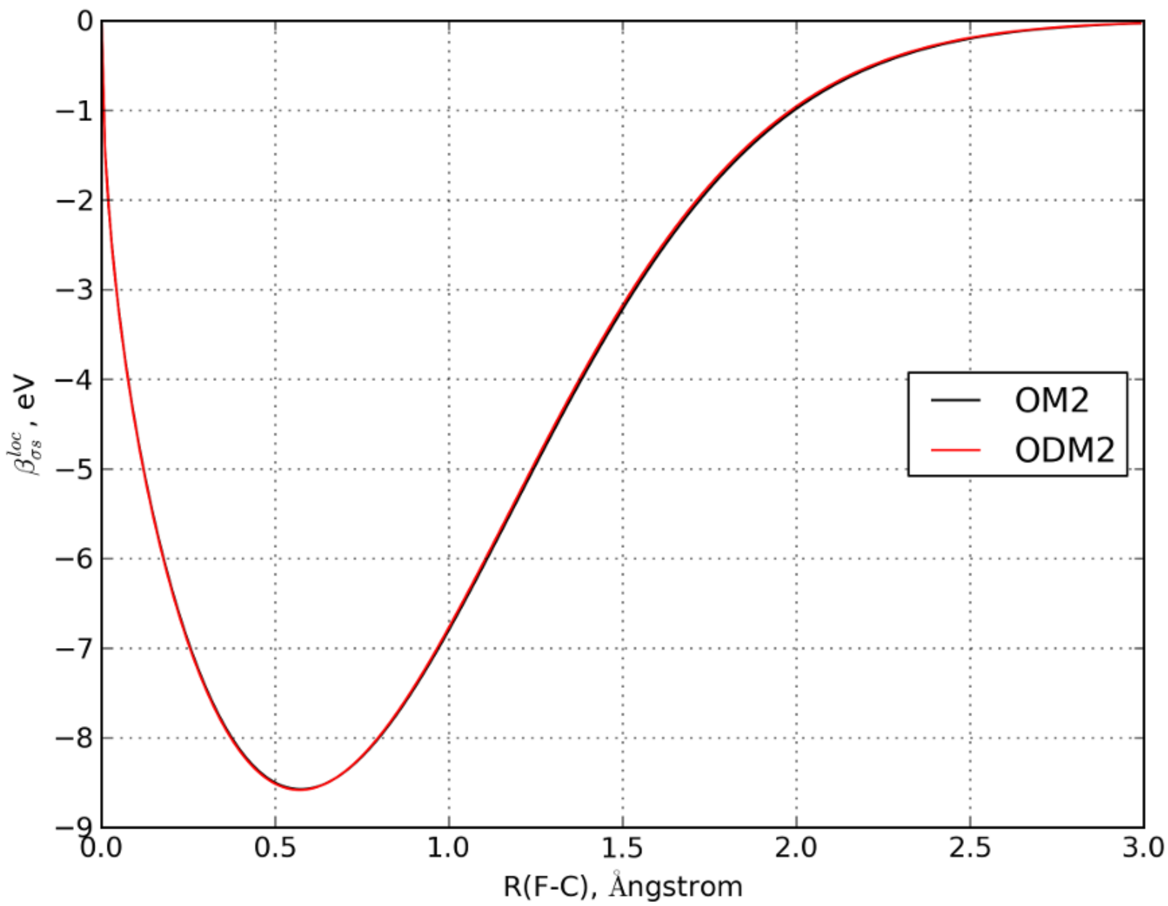

Figure S43: Comparison of σs local resonance integrals for the F−C pair calculated using standard OM2 and new ODM2 parameters.

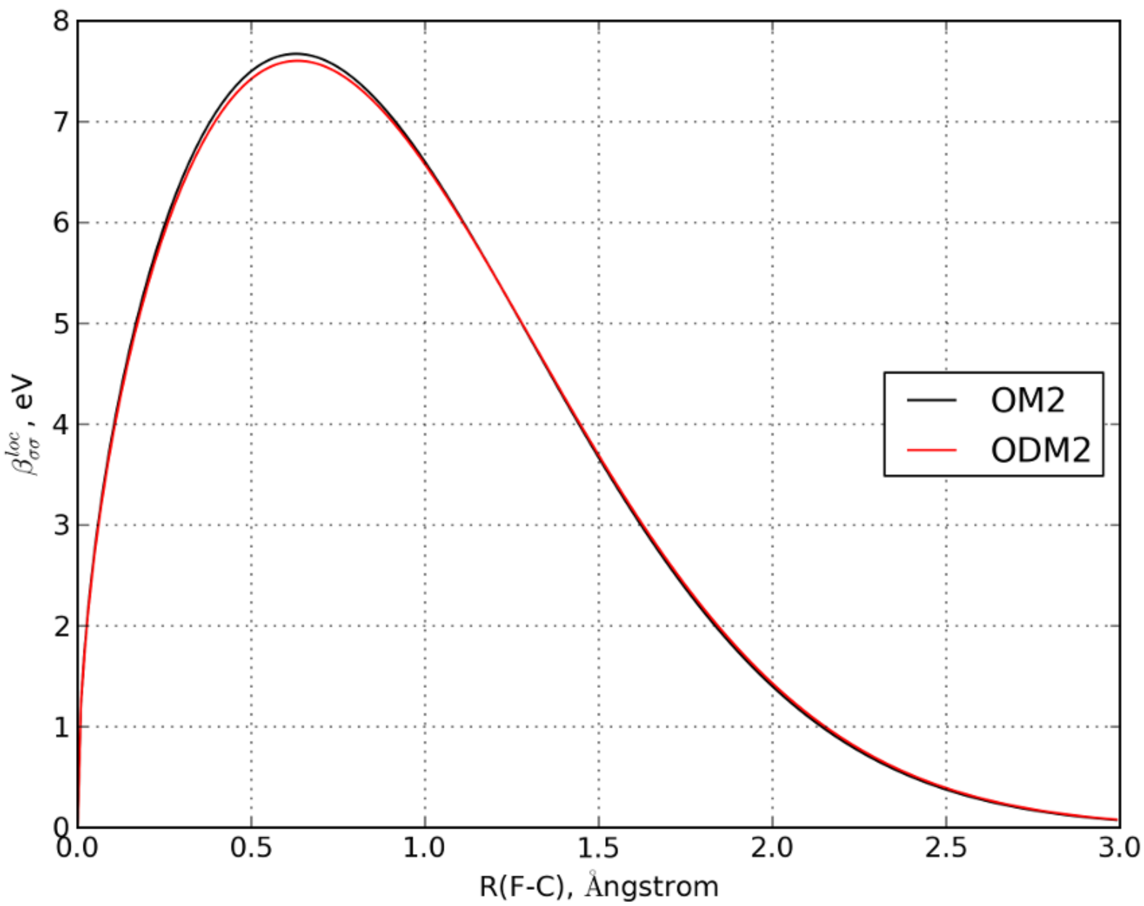

Figure S44: Comparison of $\sigma\sigma$ local resonance integrals for the F−C pair calculated using standard OM2 and new ODM2 parameters.

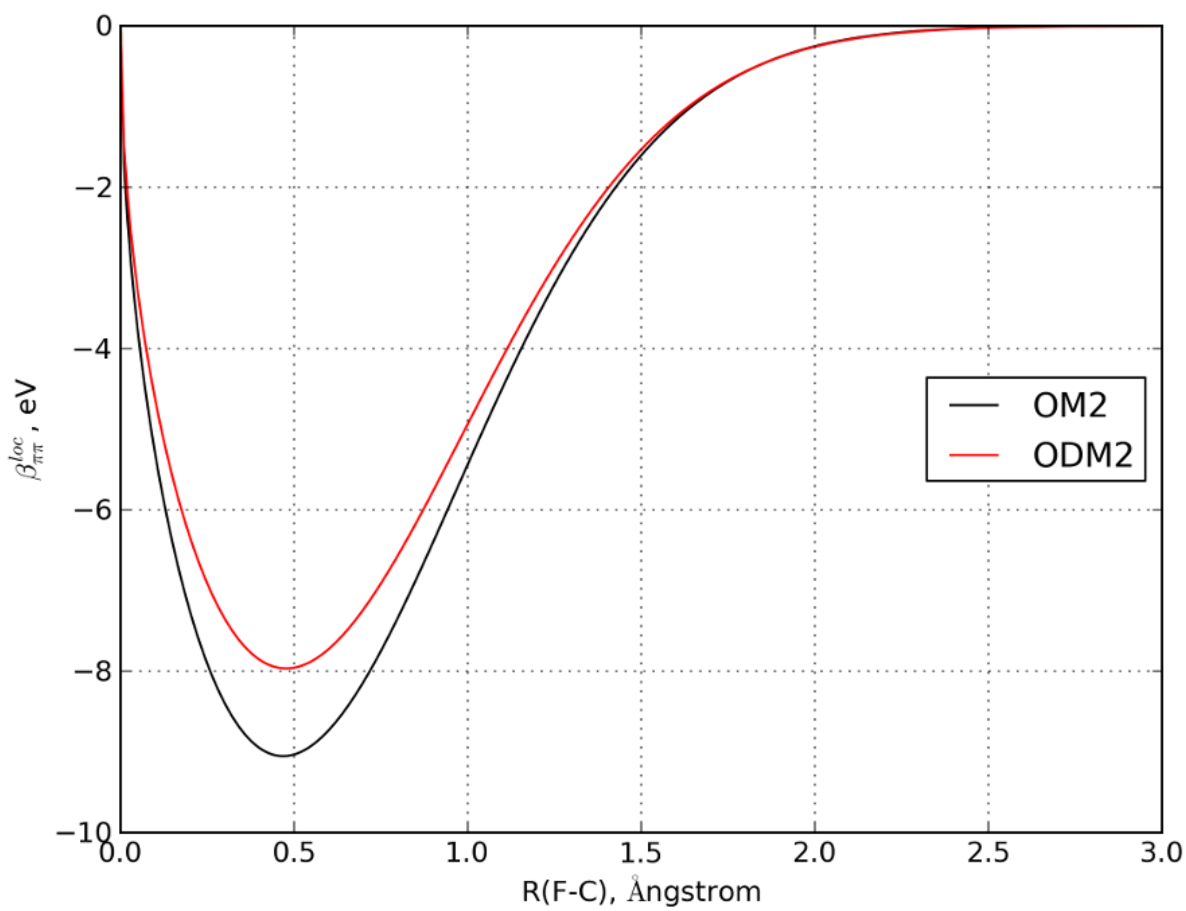

Figure S45: Comparison of $\pi\pi$ local resonance integrals for the F−C pair calculated using standard OM2 and new ODM2 parameters.

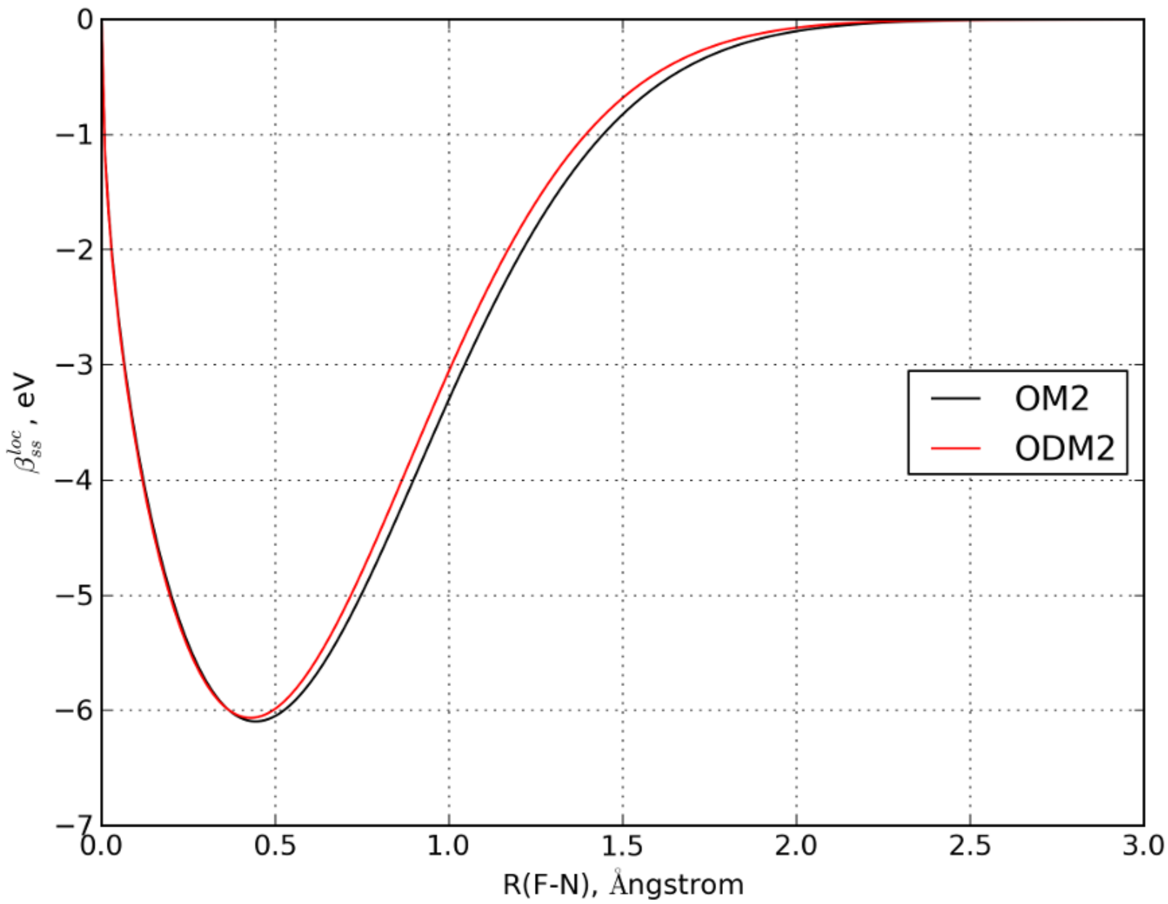

Figure S46: Comparison of *ss* local resonance integrals for the F−N pair calculated using standard OM2 and new ODM2 parameters.

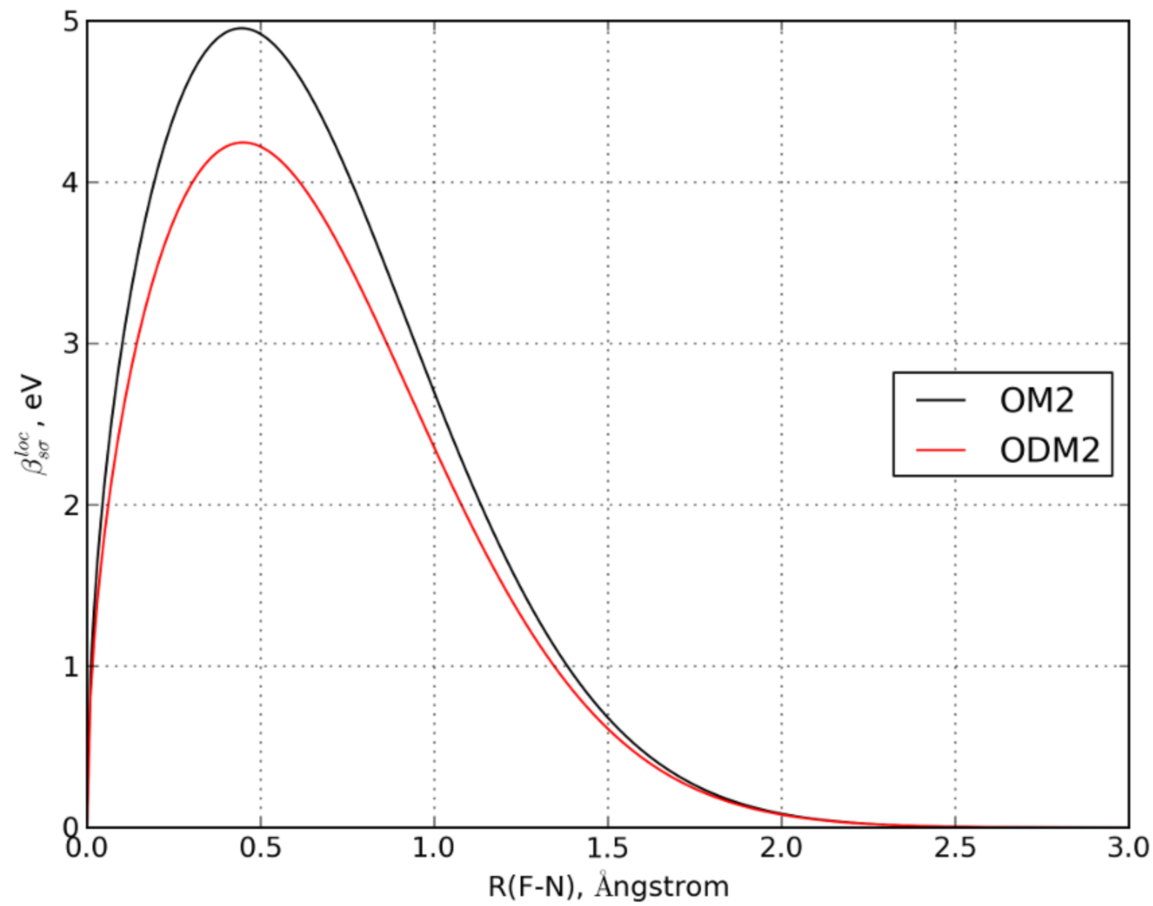

Figure S47: Comparison of $s\sigma$ local resonance integrals for the F−N pair calculated using standard OM2 and new ODM2 parameters.

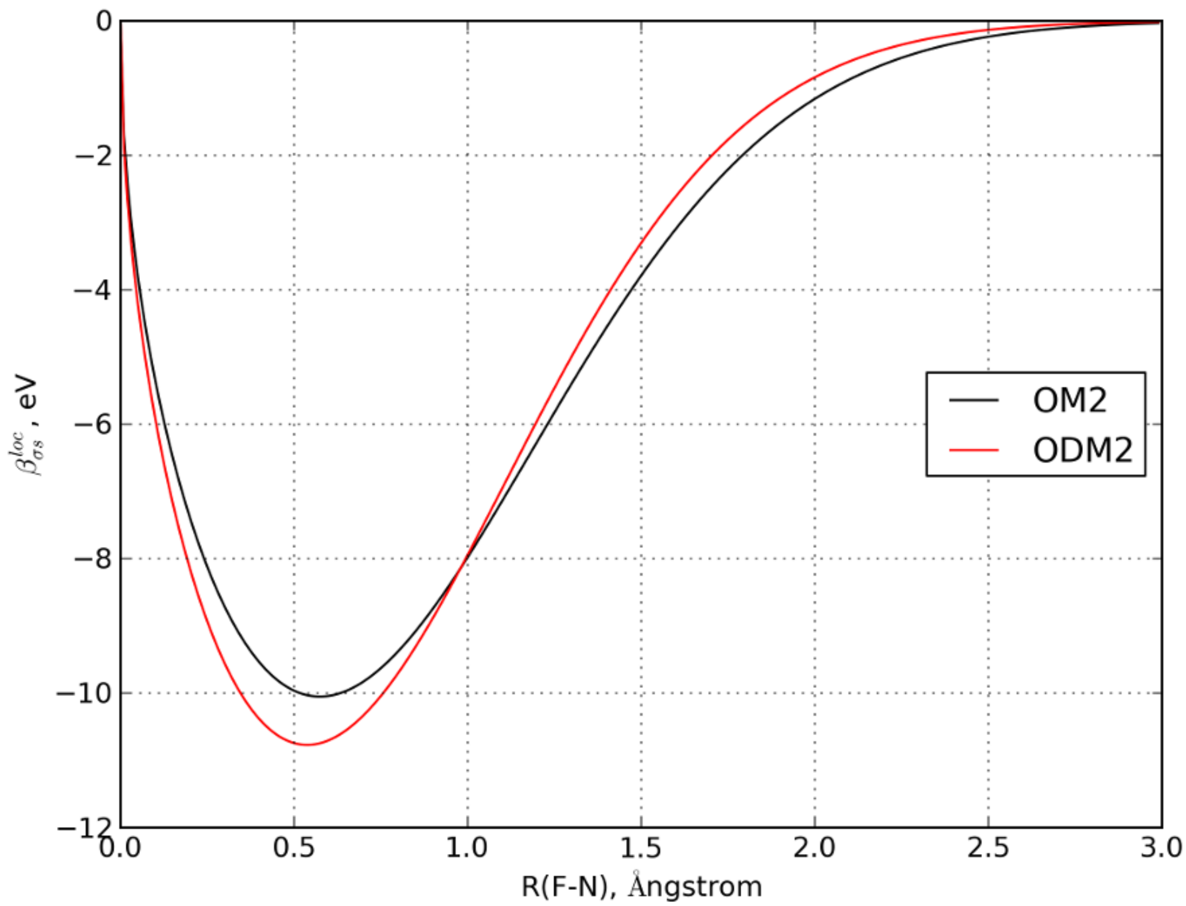

Figure S48: Comparison of σs local resonance integrals for the F−N pair calculated using standard OM2 and new ODM2 parameters.

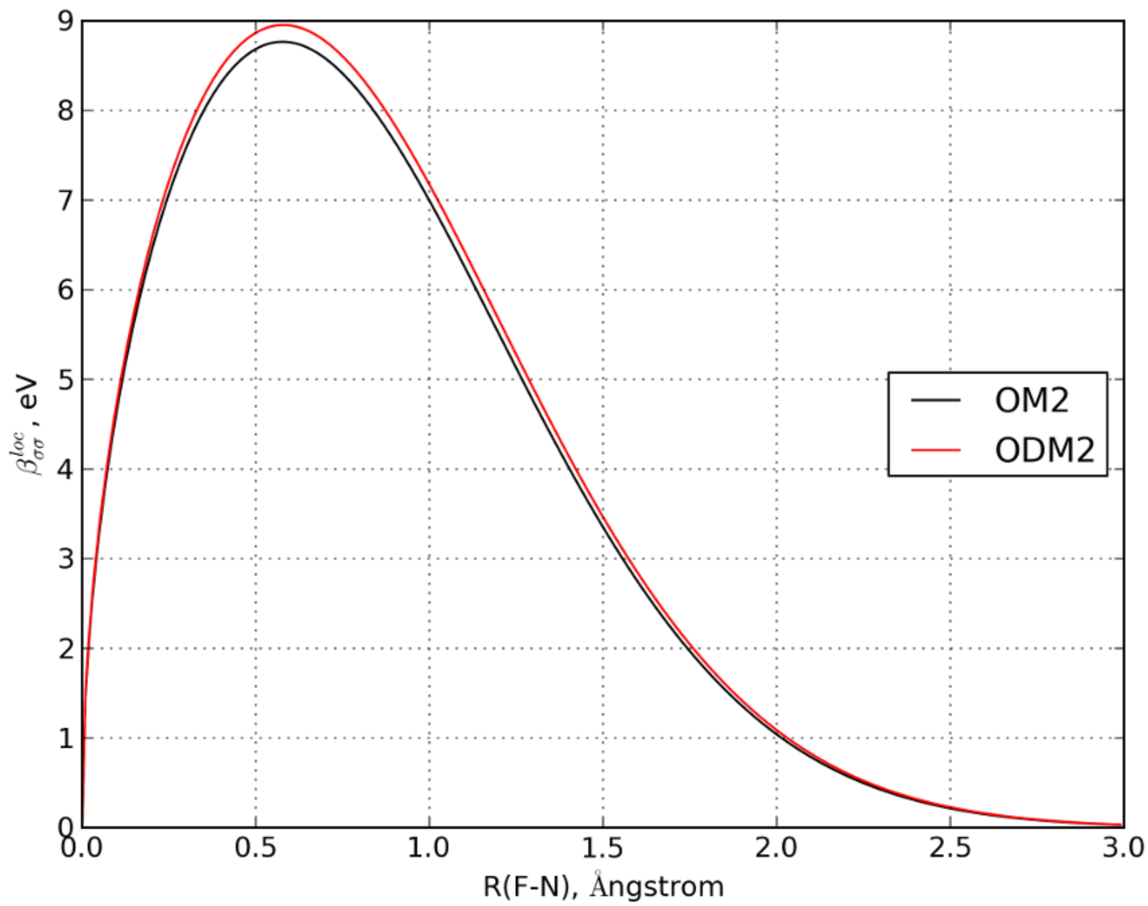

Figure S49: Comparison of $\sigma\sigma$ local resonance integrals for the F−N pair calculated using standard OM2 and new ODM2 parameters.

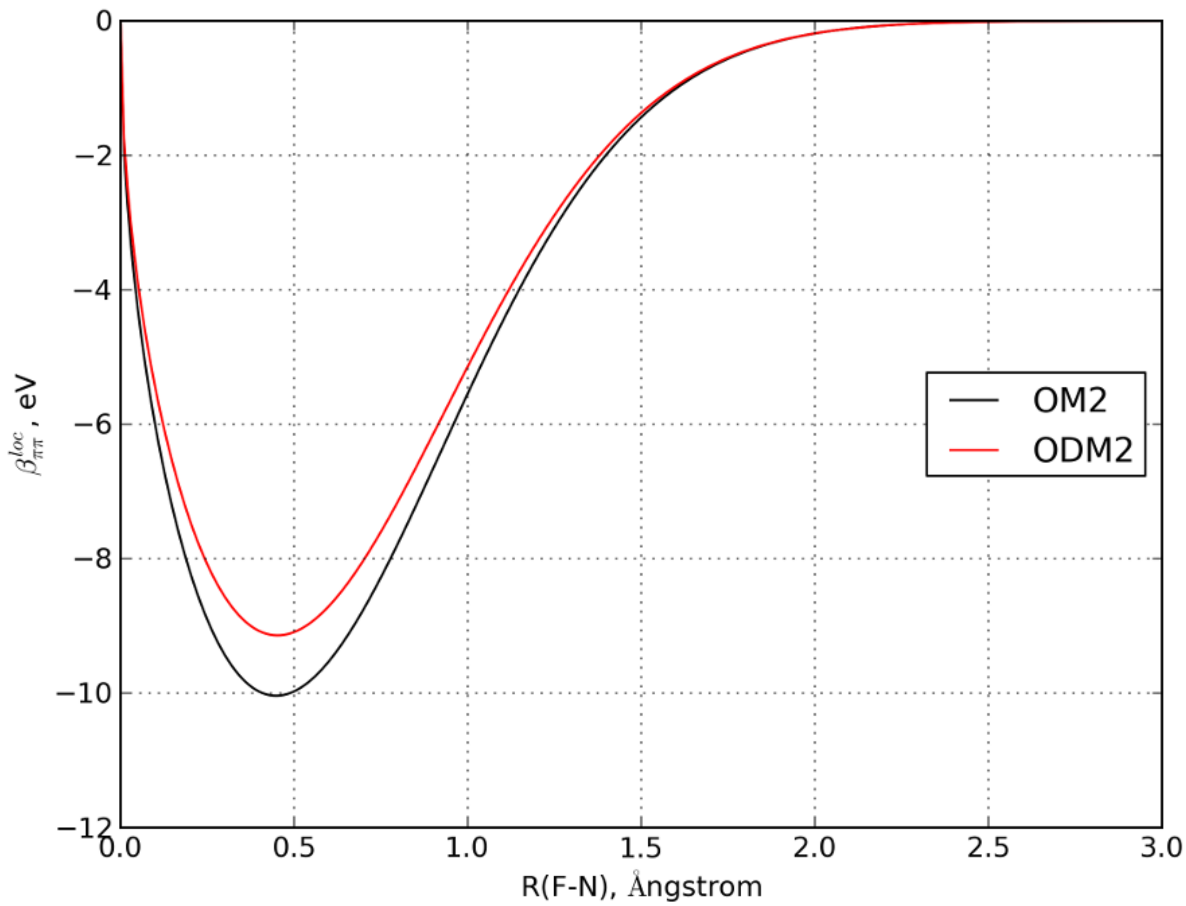

Figure S50: Comparison of $\pi\pi$ local resonance integrals for the F−N pair calculated using standard OM2 and new ODM2 parameters.

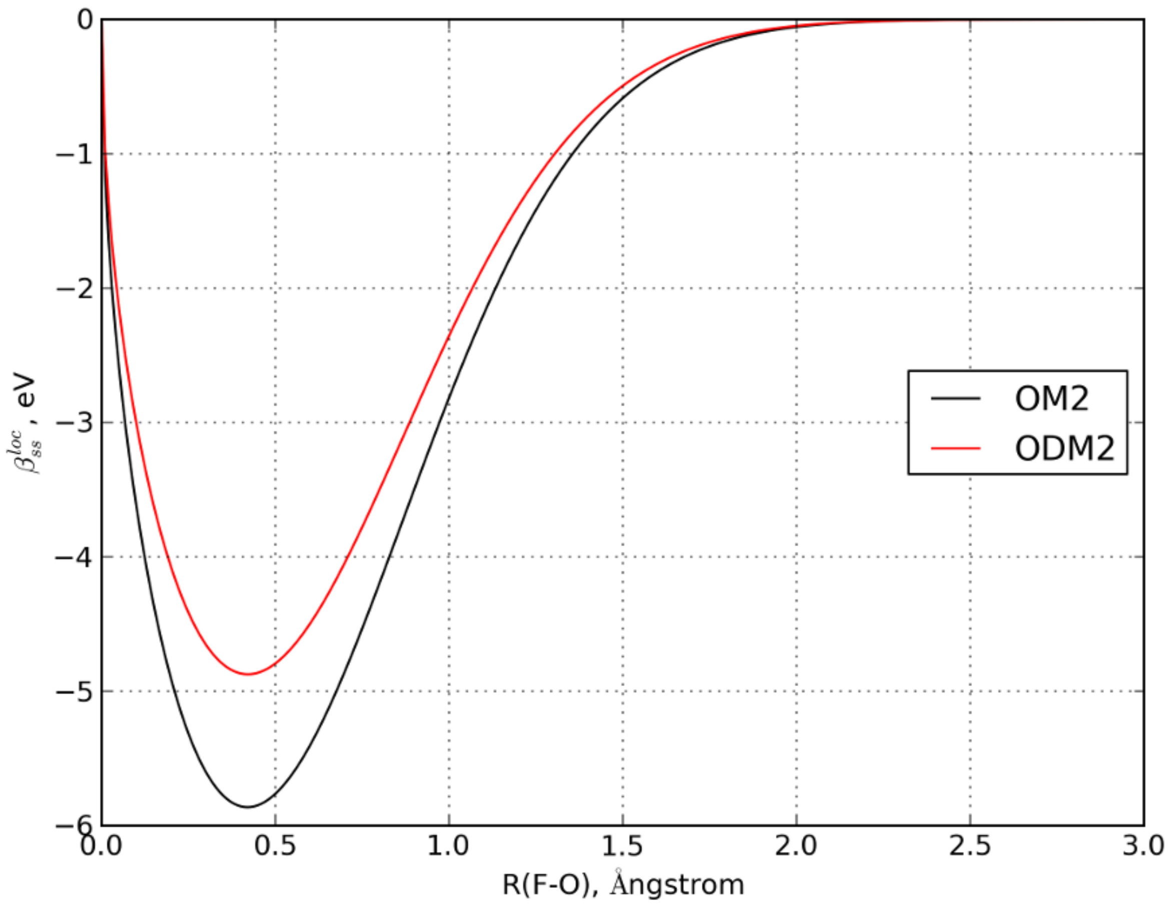

Figure S51: Comparison of *ss* local resonance integrals for the F−O pair calculated using standard OM2 and new ODM2 parameters.

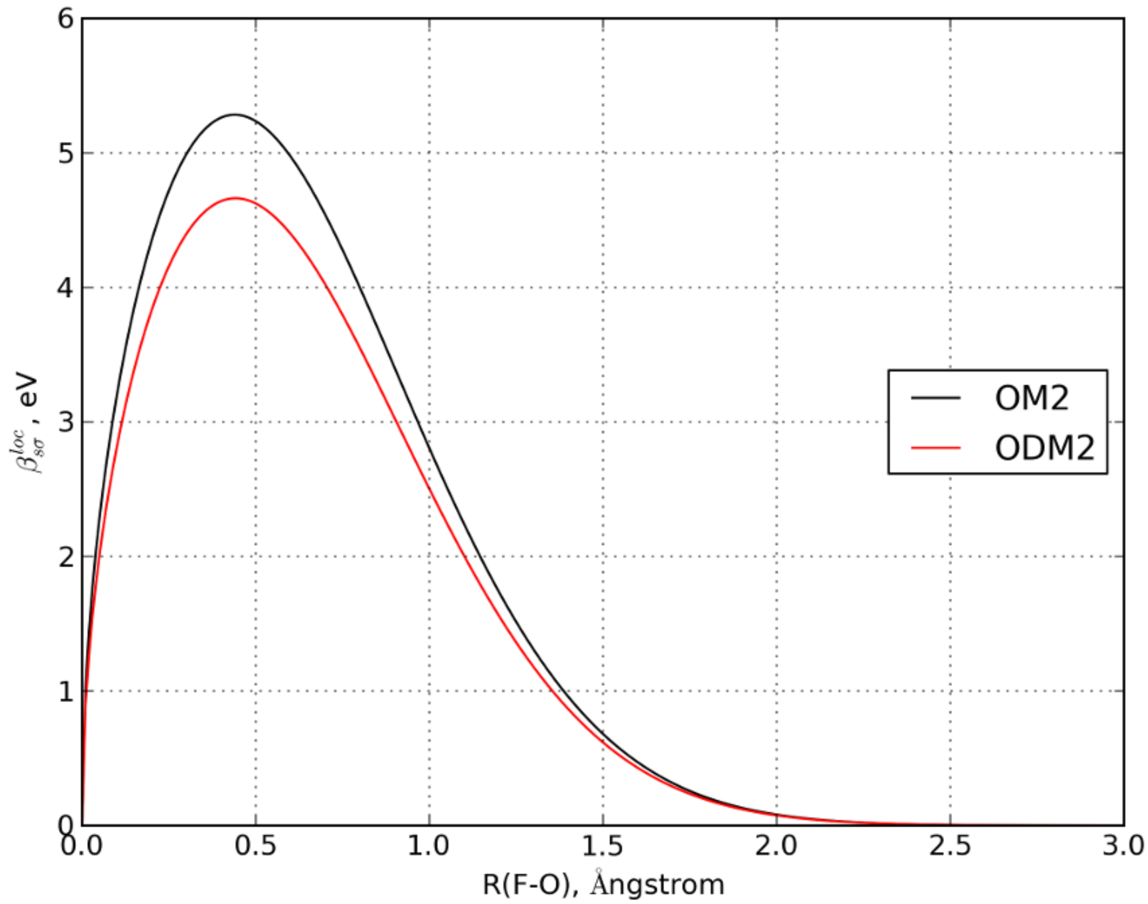

Figure S52: Comparison of $s\sigma$ local resonance integrals for the F−O pair calculated using standard OM2 and new ODM2 parameters.

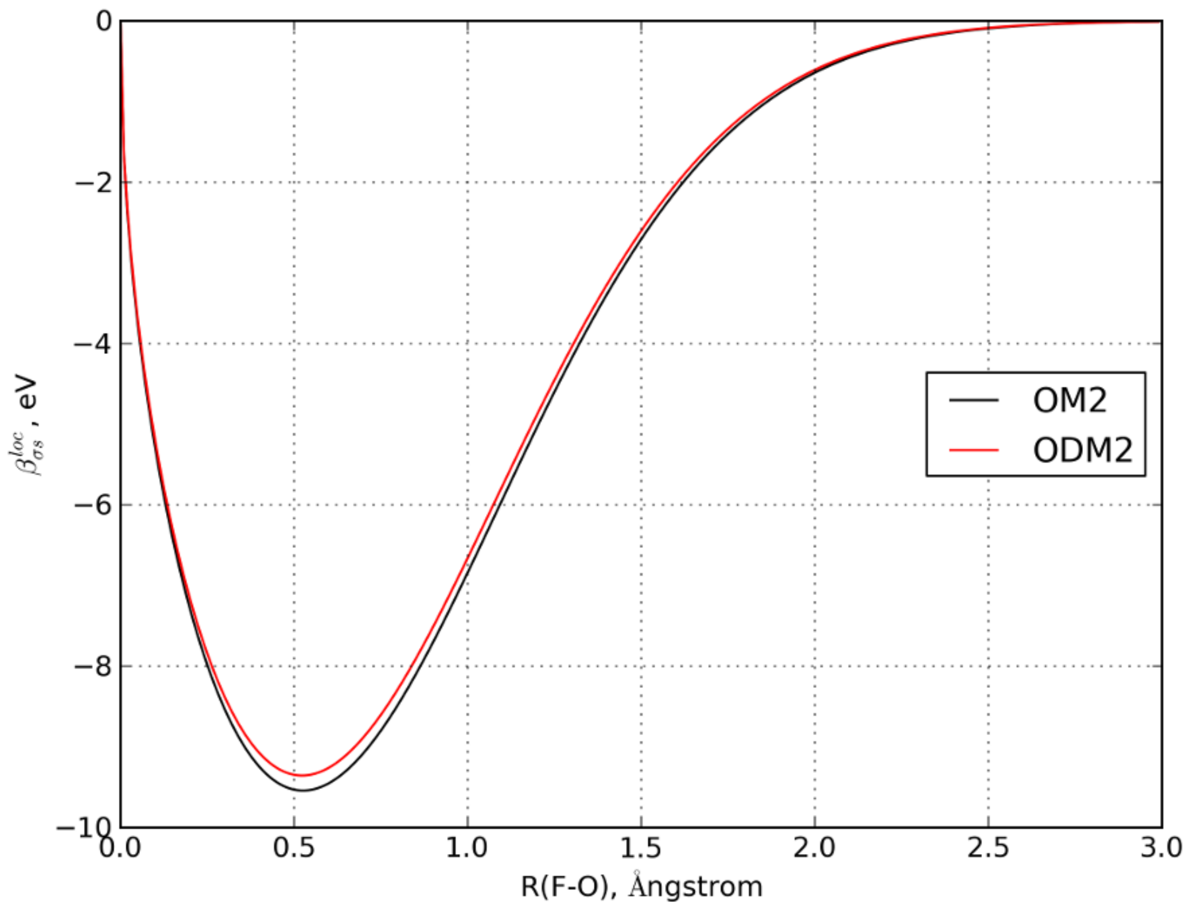

Figure S53: Comparison of σs local resonance integrals for the F−O pair calculated using standard OM2 and new ODM2 parameters.

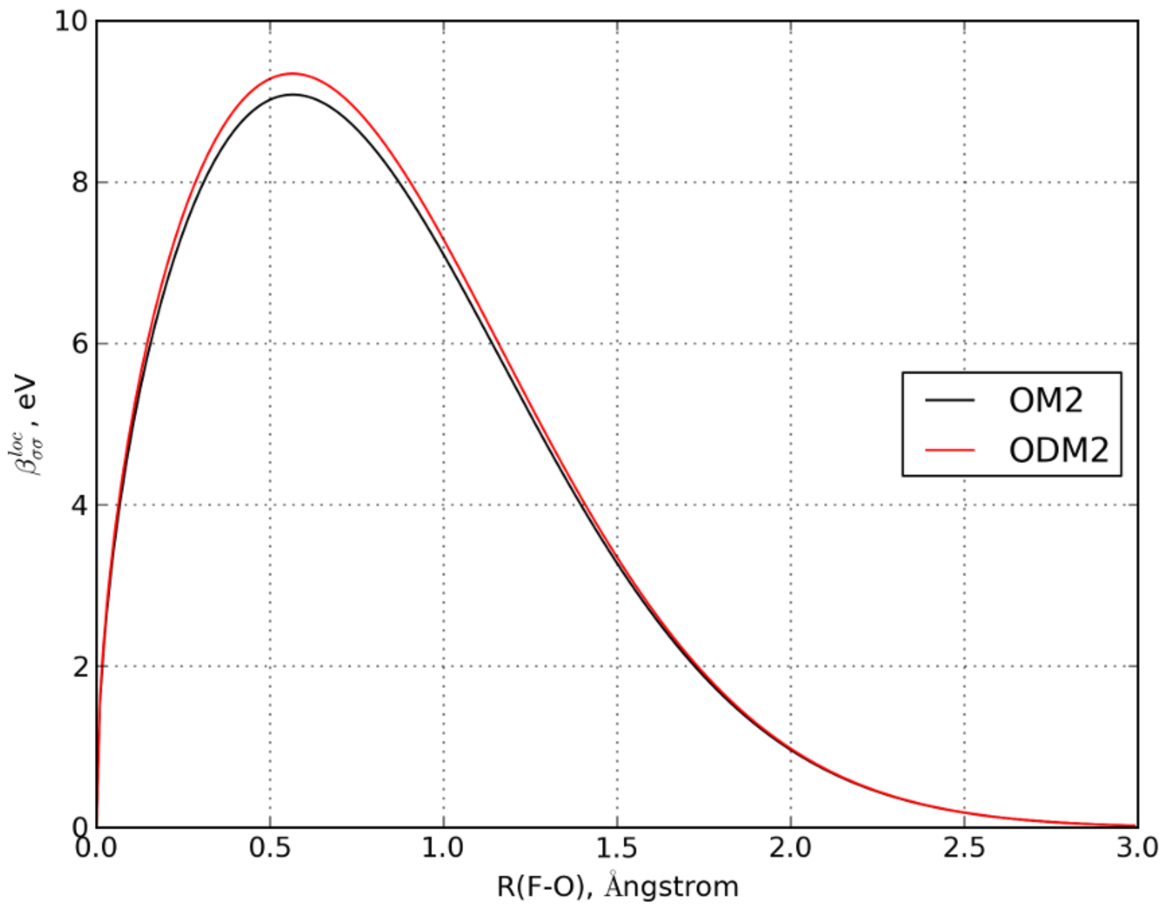

Figure S54: Comparison of $\sigma\sigma$ local resonance integrals for the F−O pair calculated using standard OM2 and new ODM2 parameters.

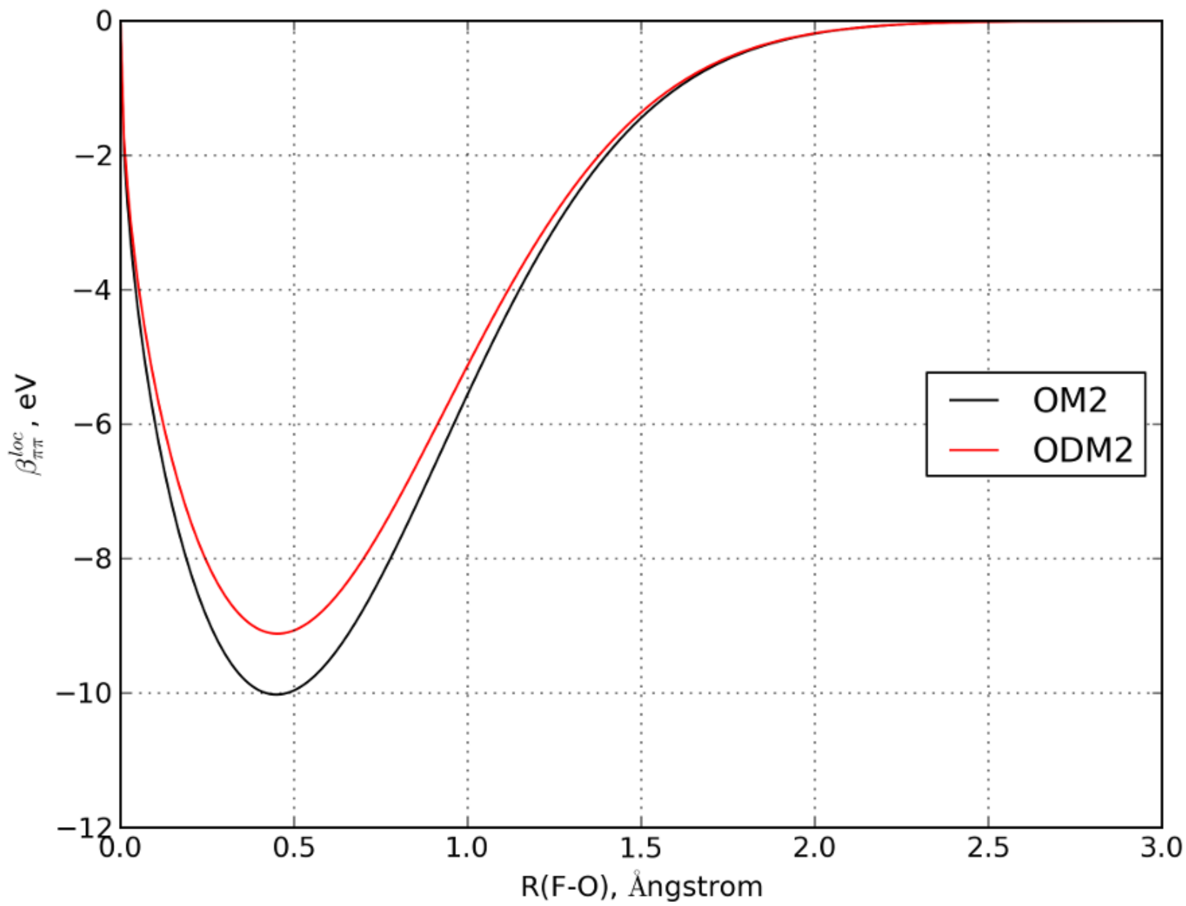

Figure S55: Comparison of $\pi\pi$ local resonance integrals for the F−O pair calculated using standard OM2 and new ODM2 parameters.

2.2 ODM3 vs OM3

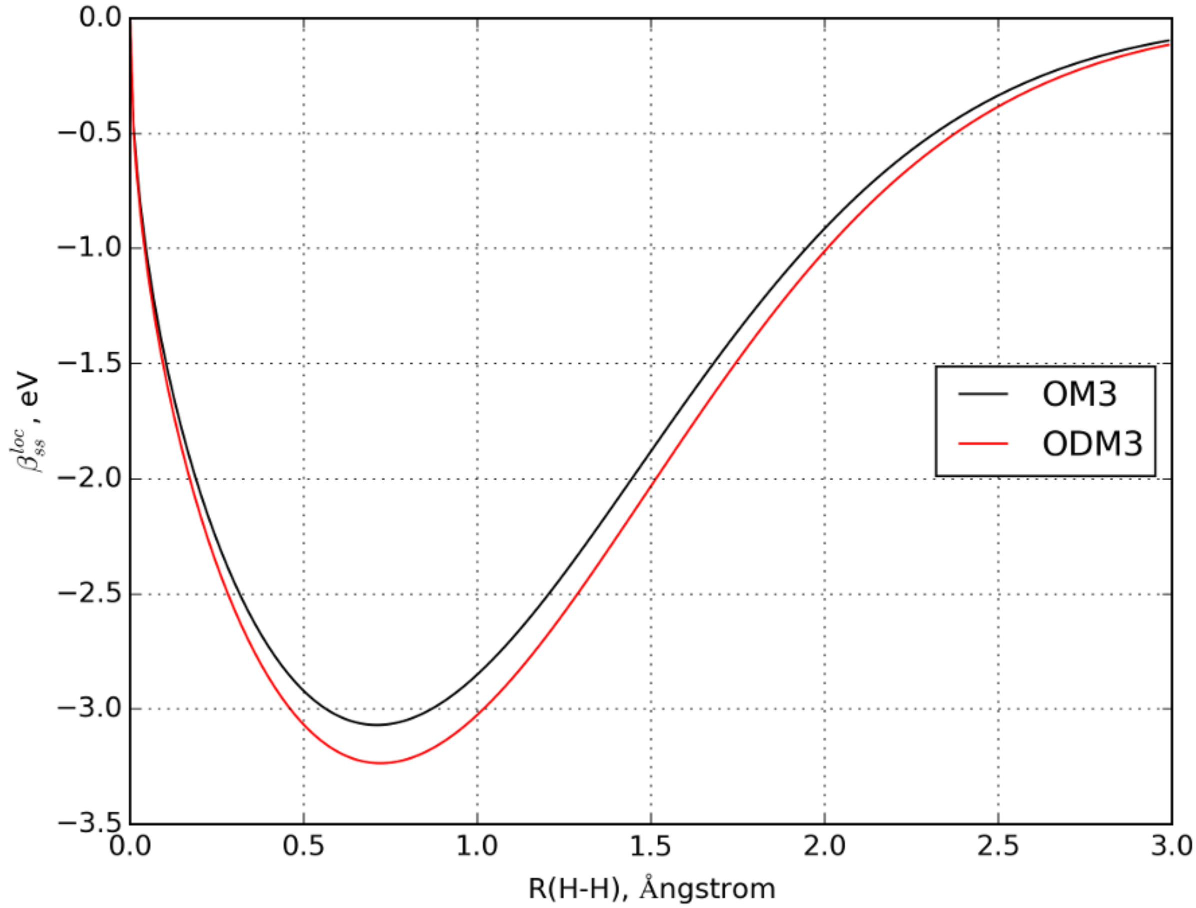

Figure S56: Comparison of ss local resonance integrals for the H−H pair calculated using standard OM3 and new ODM3 parameters.

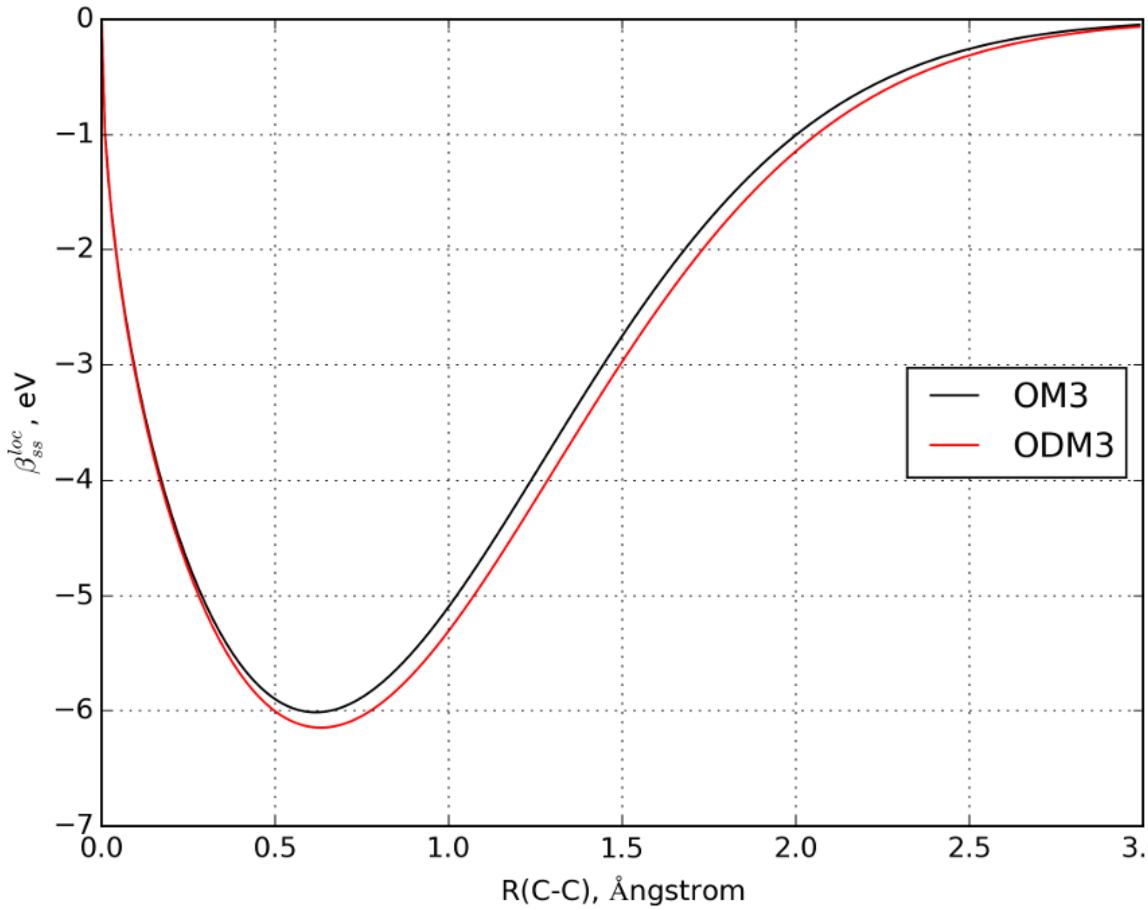

Figure S57: Comparison of *ss* local resonance integrals for the C−C pair calculated using standard OM3 and new ODM3 parameters.

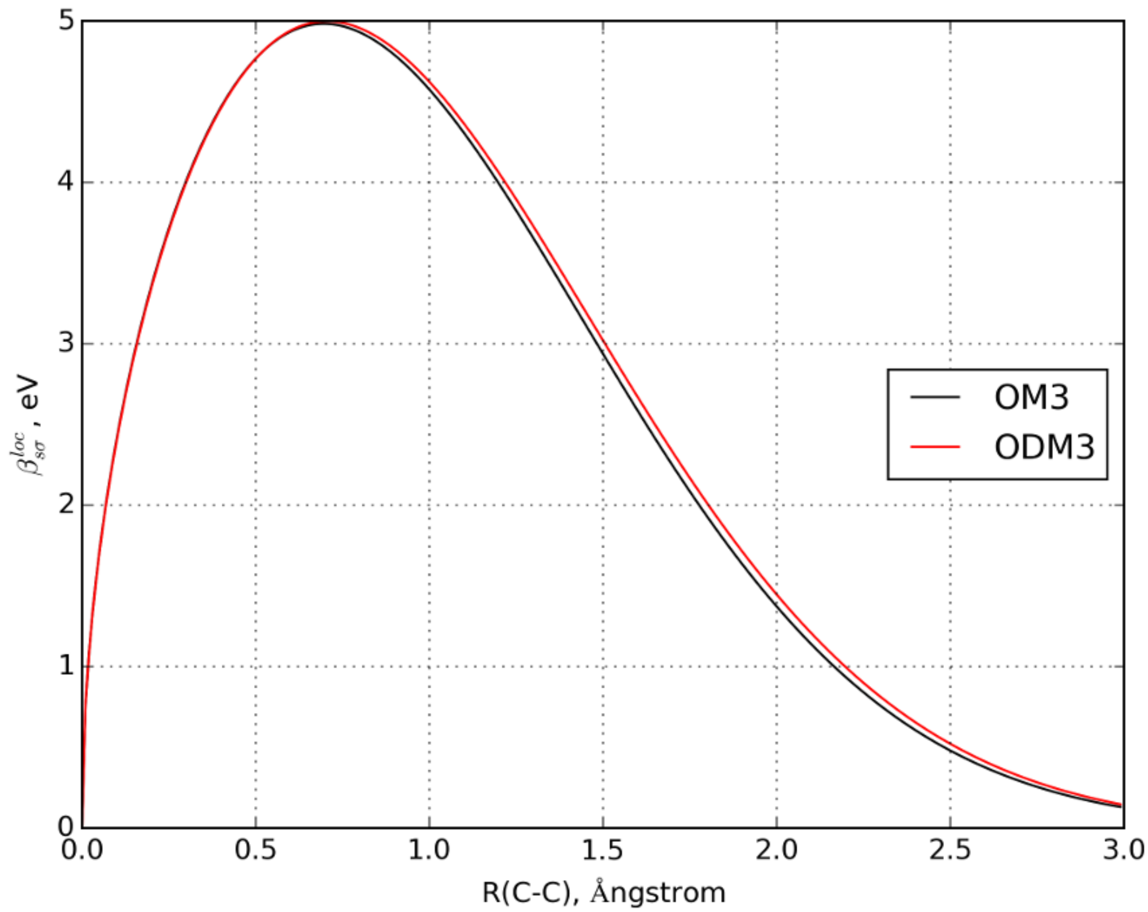

Figure S58: Comparison of $s\sigma$ local resonance integrals for the C−C pair calculated using standard OM3 and new ODM3 parameters.

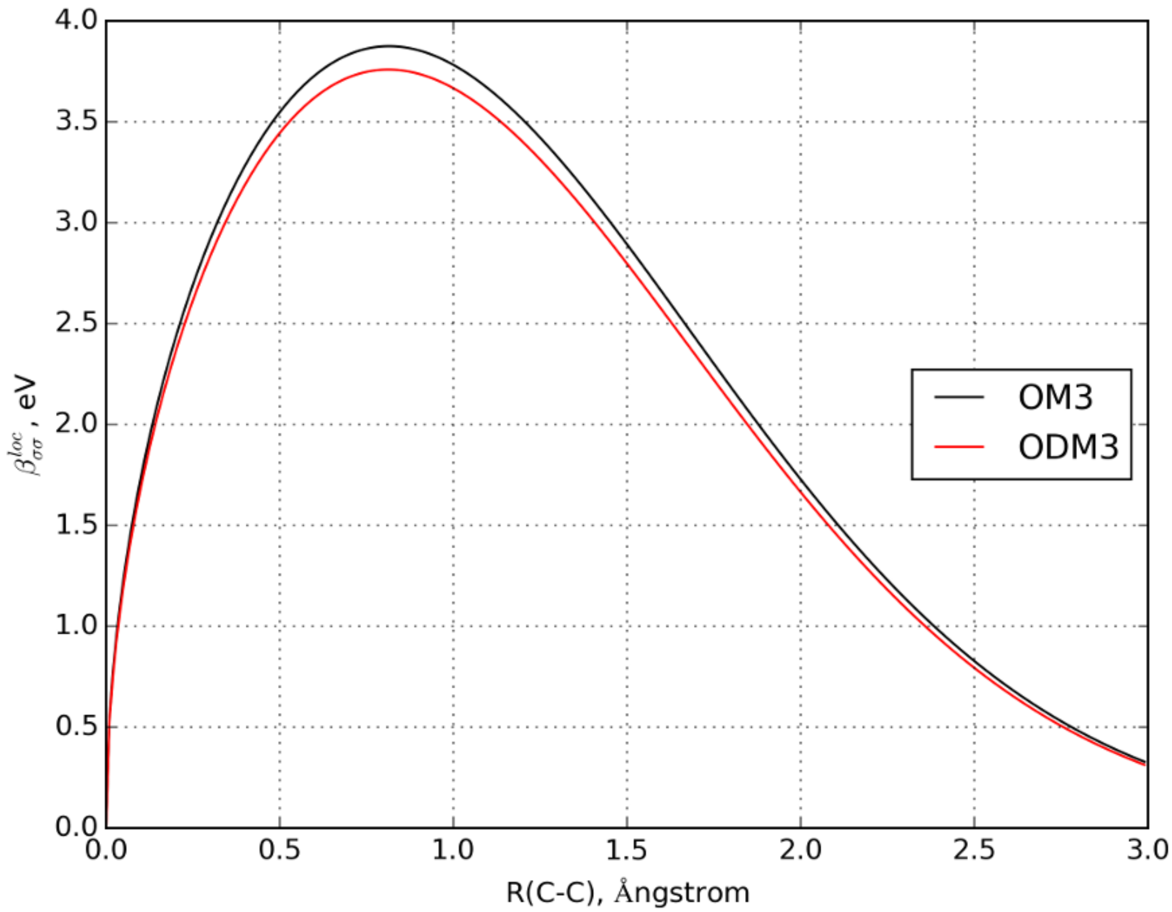

Figure S59: Comparison of $\sigma\sigma$ local resonance integrals for the C−C pair calculated using standard OM3 and new ODM3 parameters.

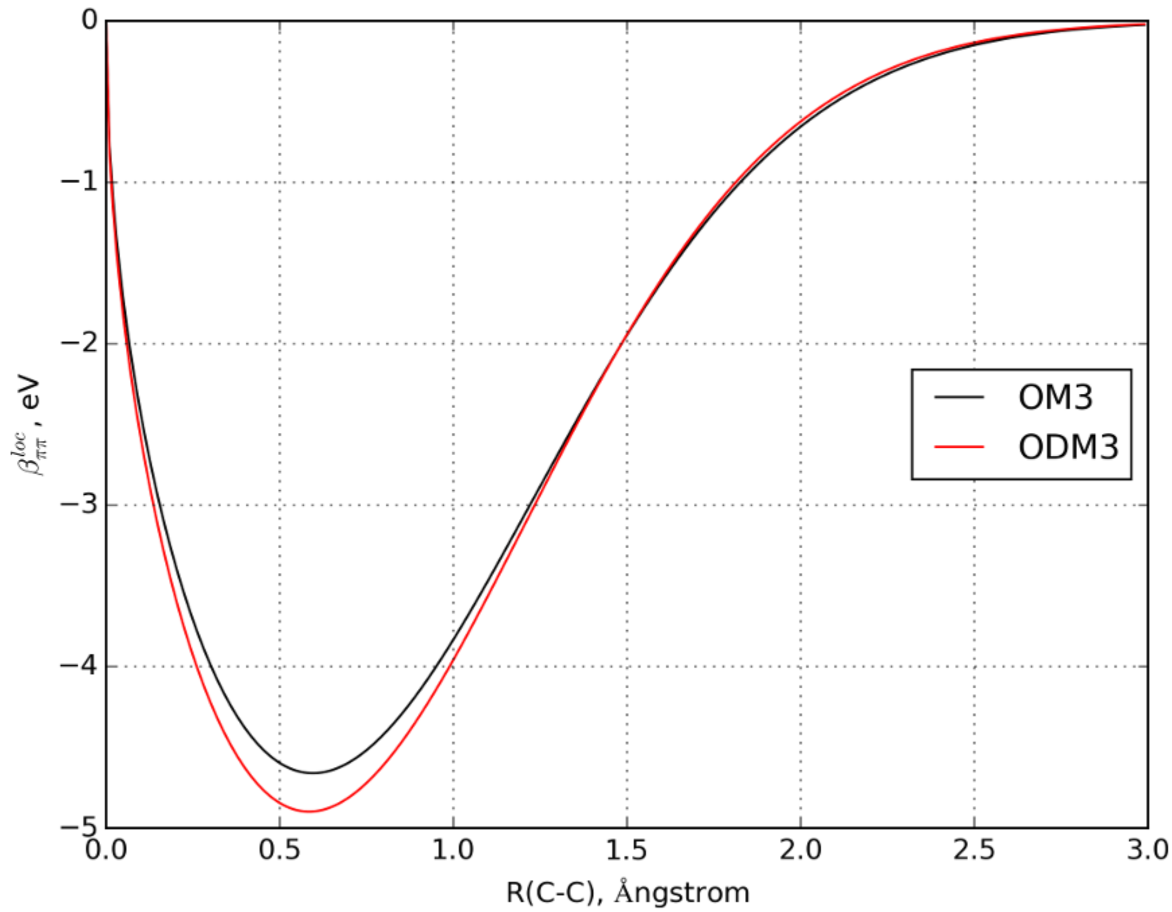

Figure S60: Comparison of $\pi\pi$ local resonance integrals for the C−C pair calculated using standard OM3 and new ODM3 parameters.

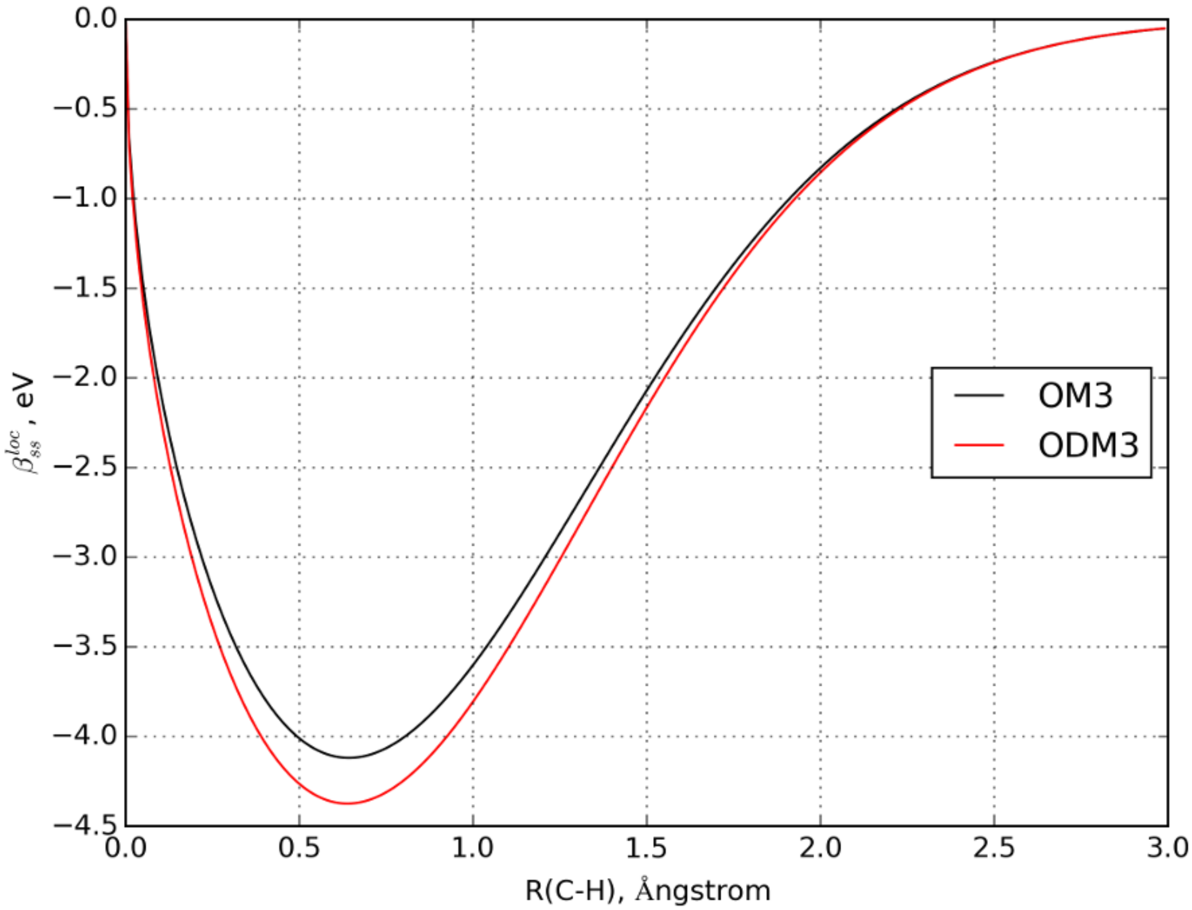

Figure S61: Comparison of *ss* local resonance integrals for the C−H pair calculated using standard OM3 and new ODM3 parameters.

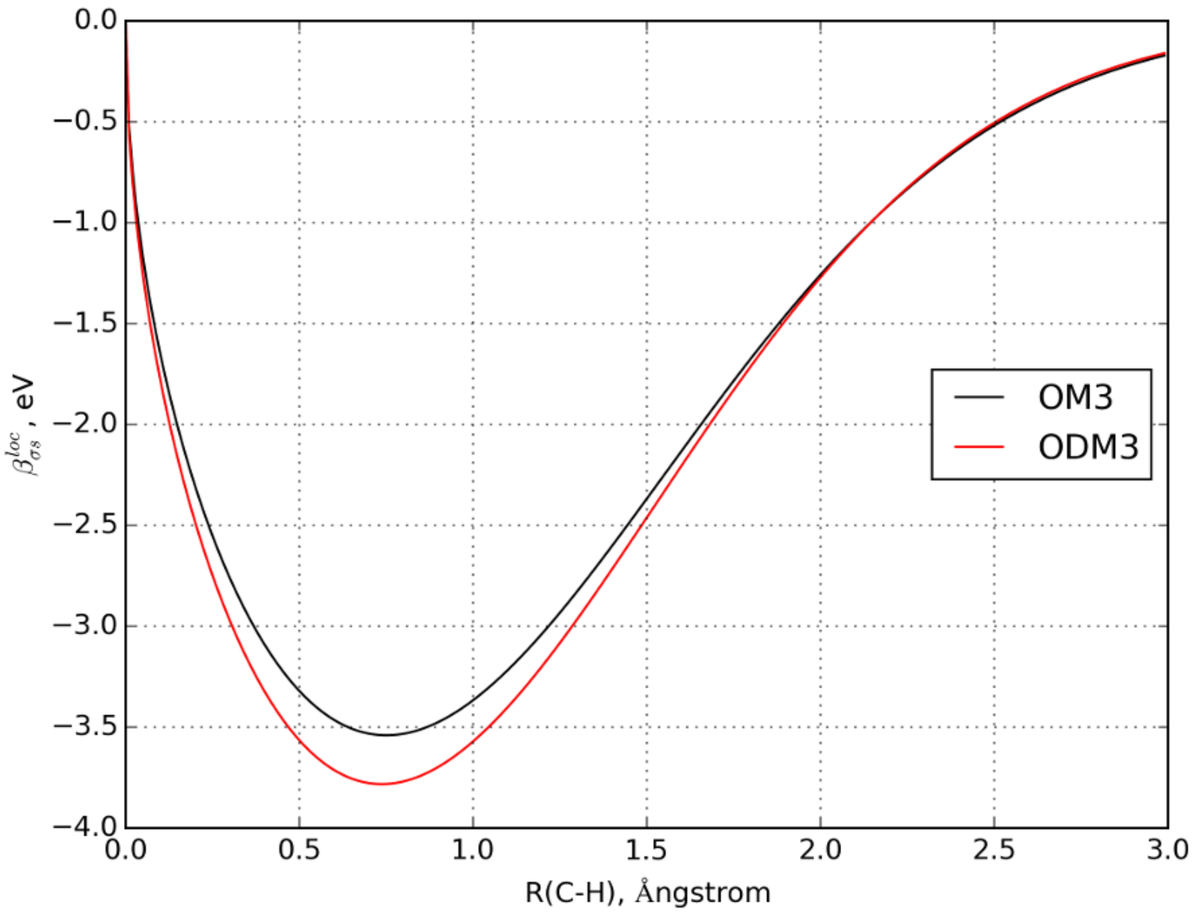

Figure S62: Comparison of σs local resonance integrals for the C−H pair calculated using standard OM3 and new ODM3 parameters.

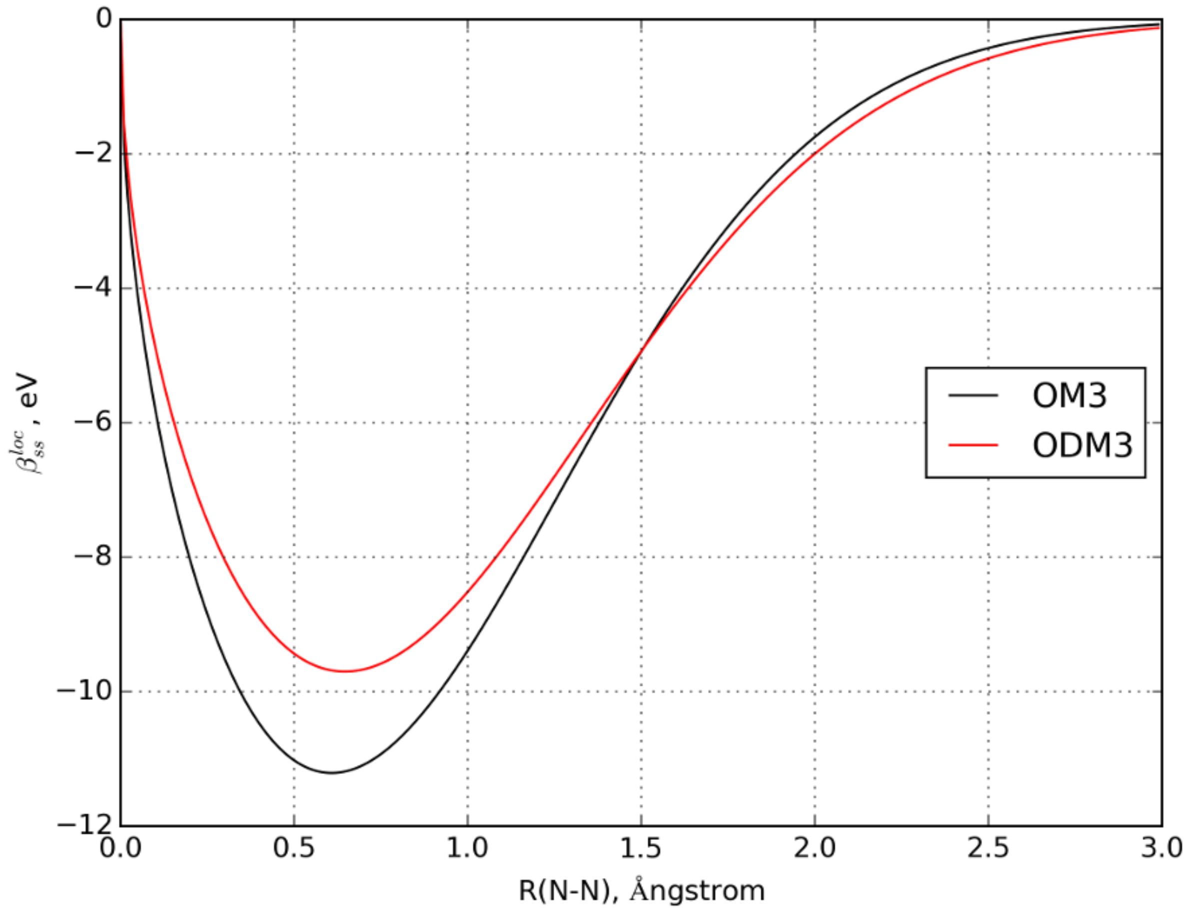

Figure S63: Comparison of ss local resonance integrals for the N−N pair calculated using standard OM3 and new ODM3 parameters.

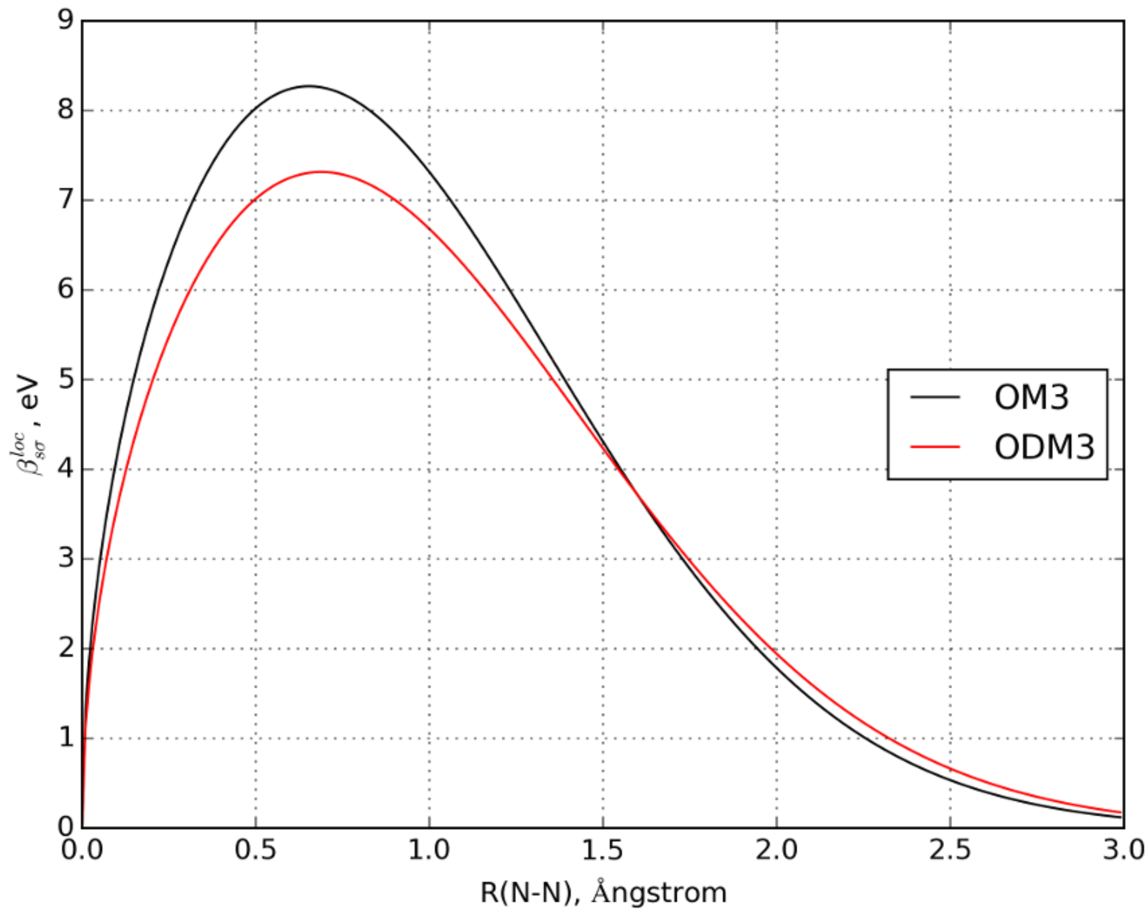

Figure S64: Comparison of $s\sigma$ local resonance integrals for the N−N pair calculated using standard OM3 and new ODM3 parameters.

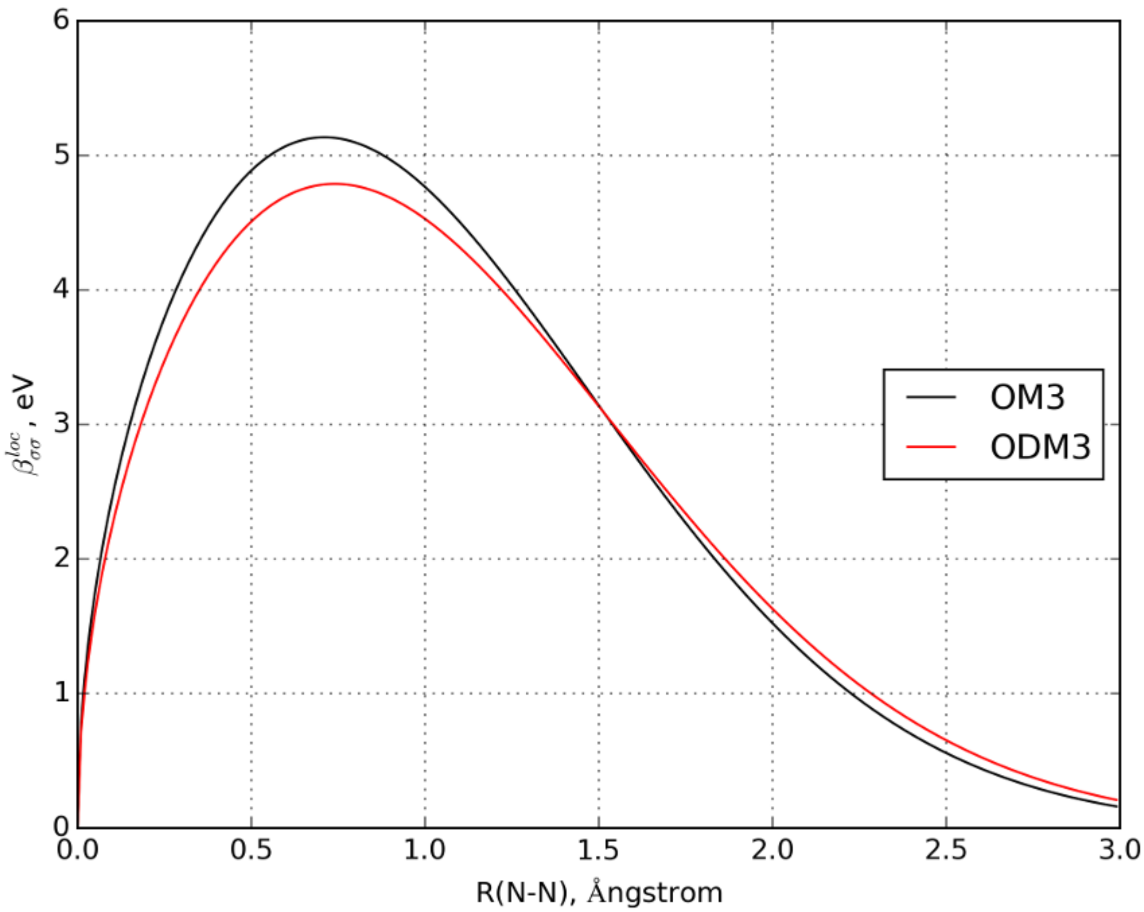

Figure S65: Comparison of $\sigma\sigma$ local resonance integrals for the N−N pair calculated using standard OM3 and new ODM3 parameters.

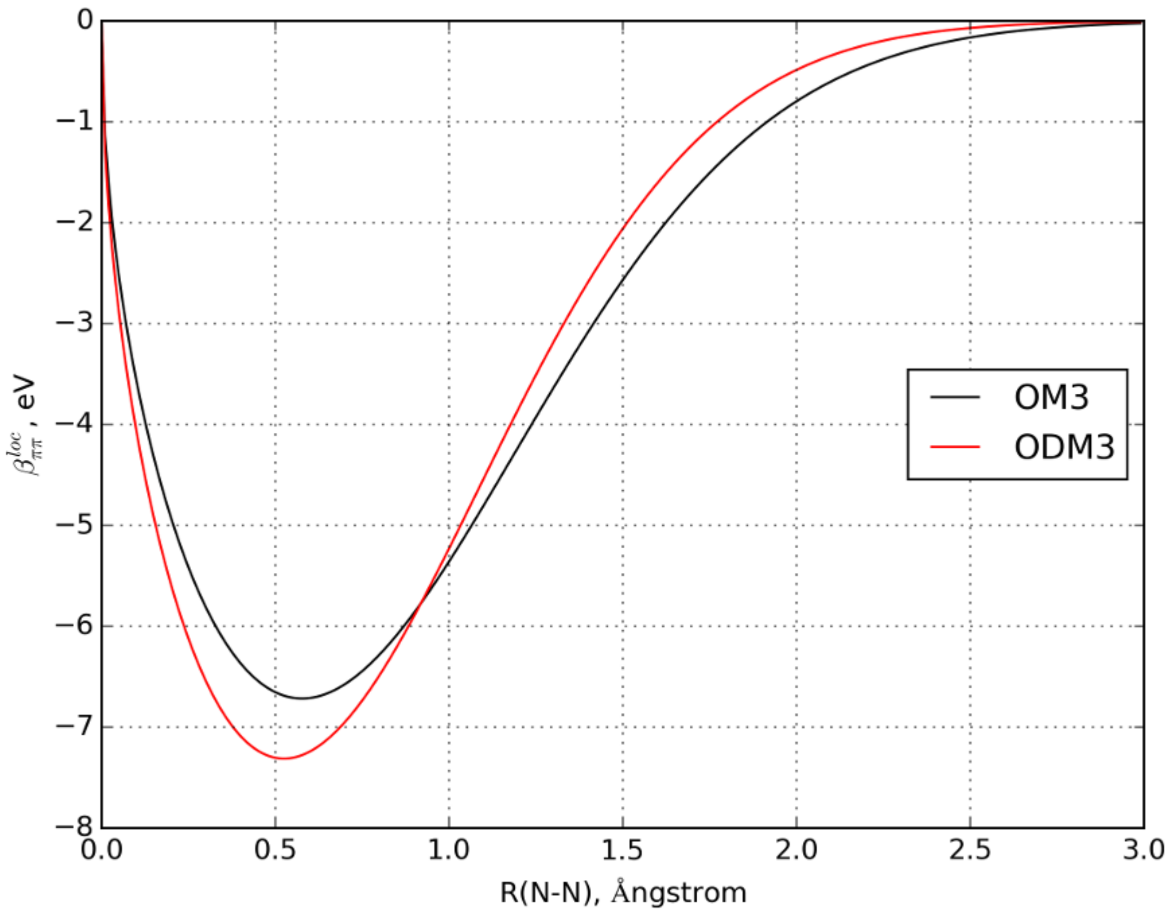

Figure S66: Comparison of $\pi\pi$ local resonance integrals for the N−N pair calculated using standard OM3 and new ODM3 parameters.

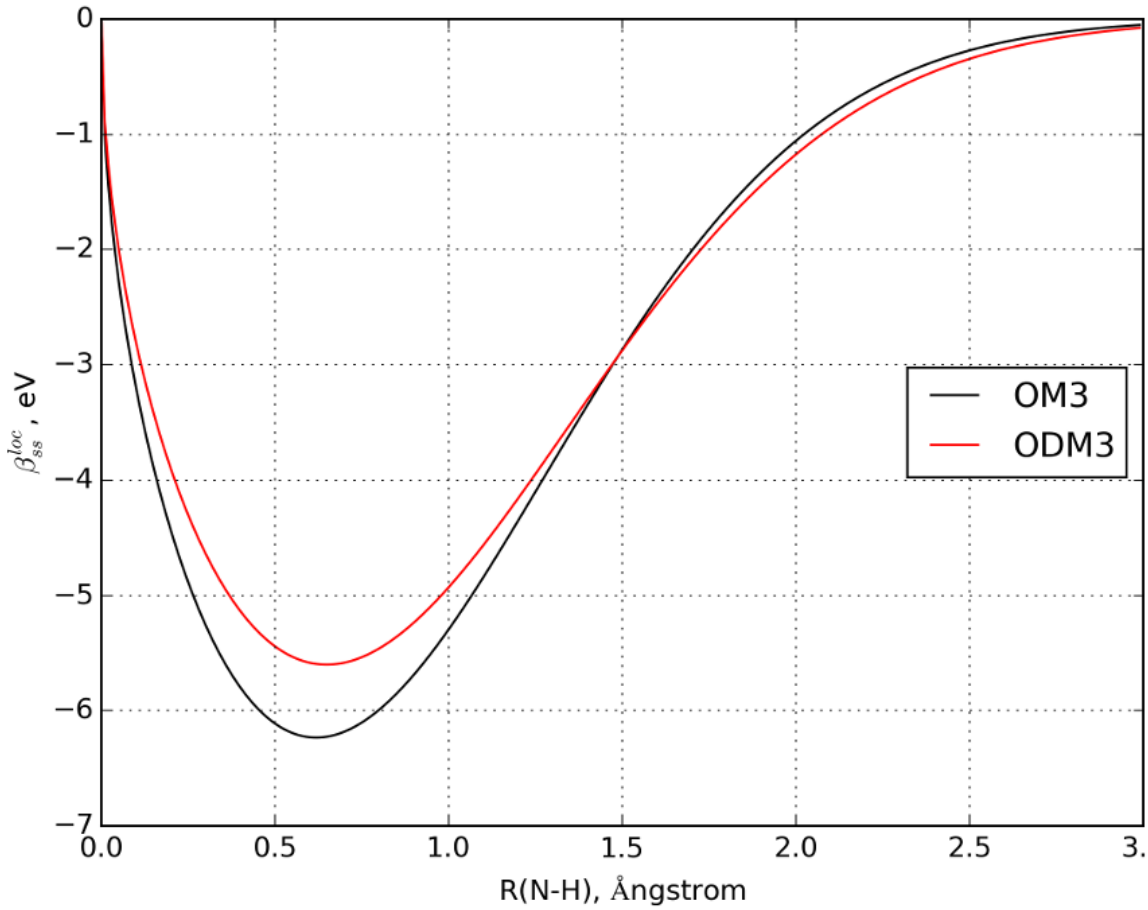

Figure S67: Comparison of *ss* local resonance integrals for the N−H pair calculated using standard OM3 and new ODM3 parameters.

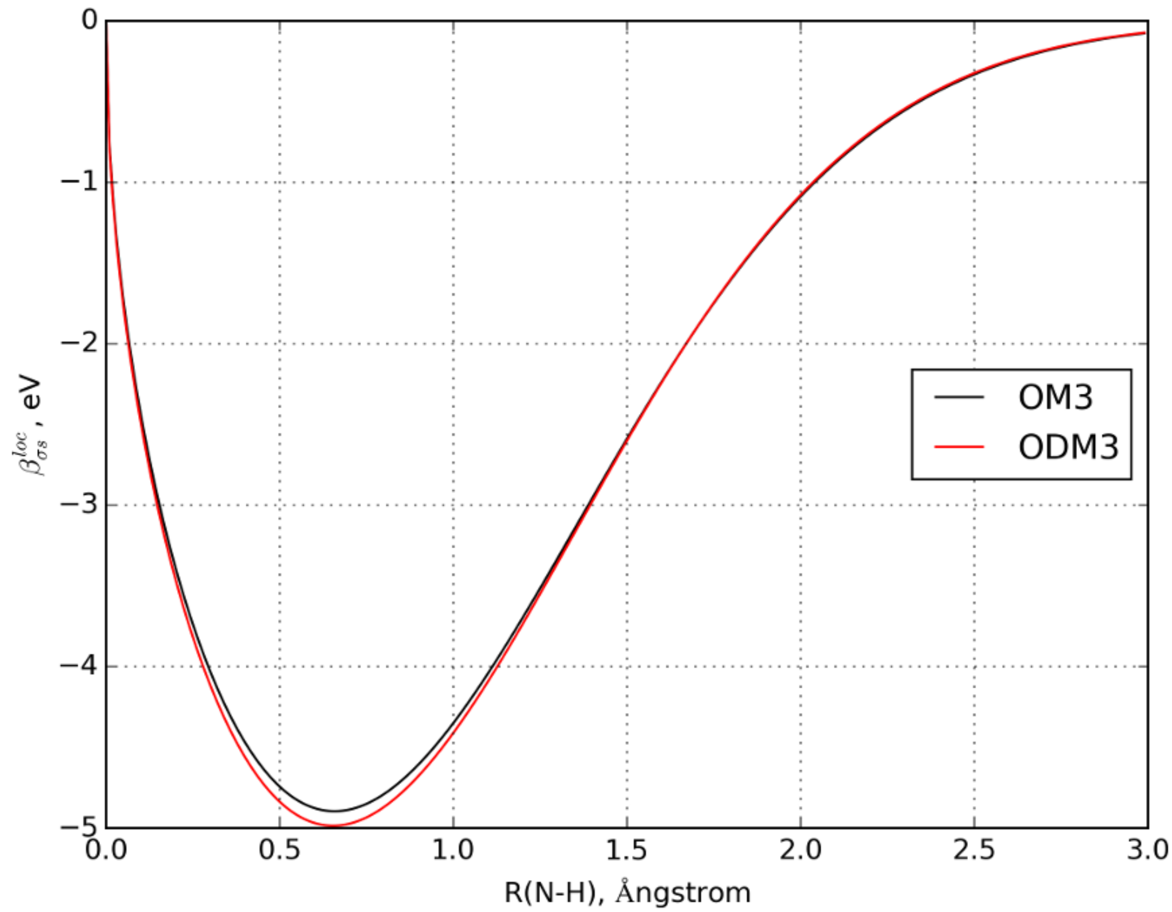

Figure S68: Comparison of σs local resonance integrals for the N−H pair calculated using standard OM3 and new ODM3 parameters.

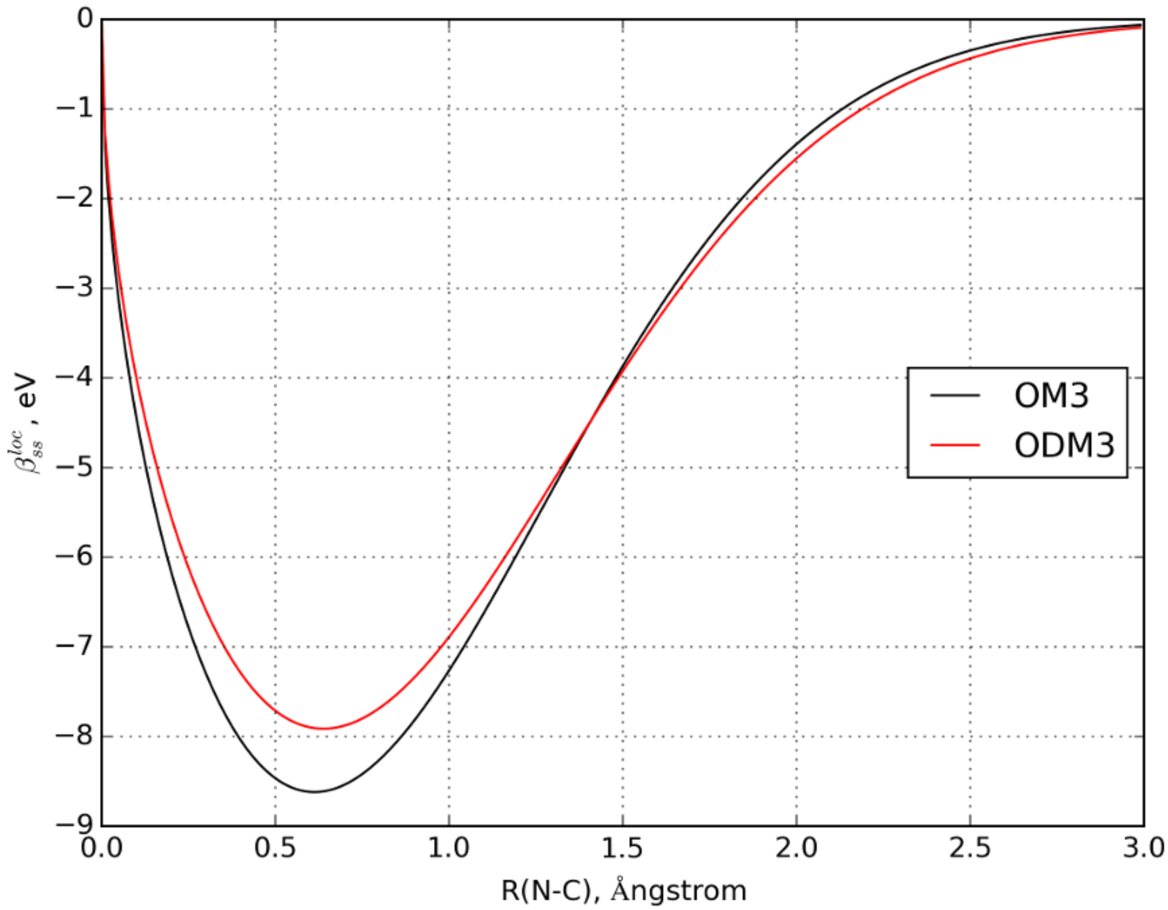

Figure S69: Comparison of *ss* local resonance integrals for the N−C pair calculated using standard OM3 and new ODM3 parameters.

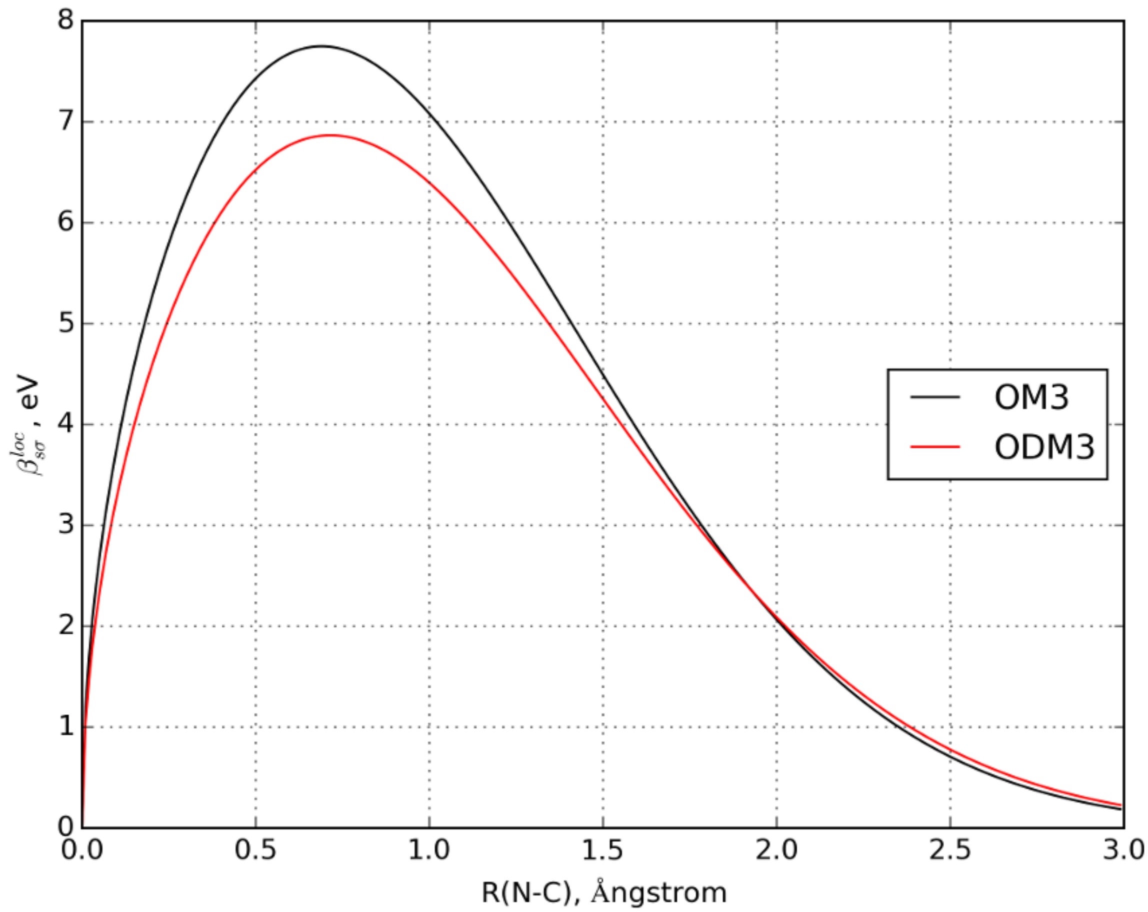

Figure S70: Comparison of $s\sigma$ local resonance integrals for the N−C pair calculated using standard OM3 and new ODM3 parameters.

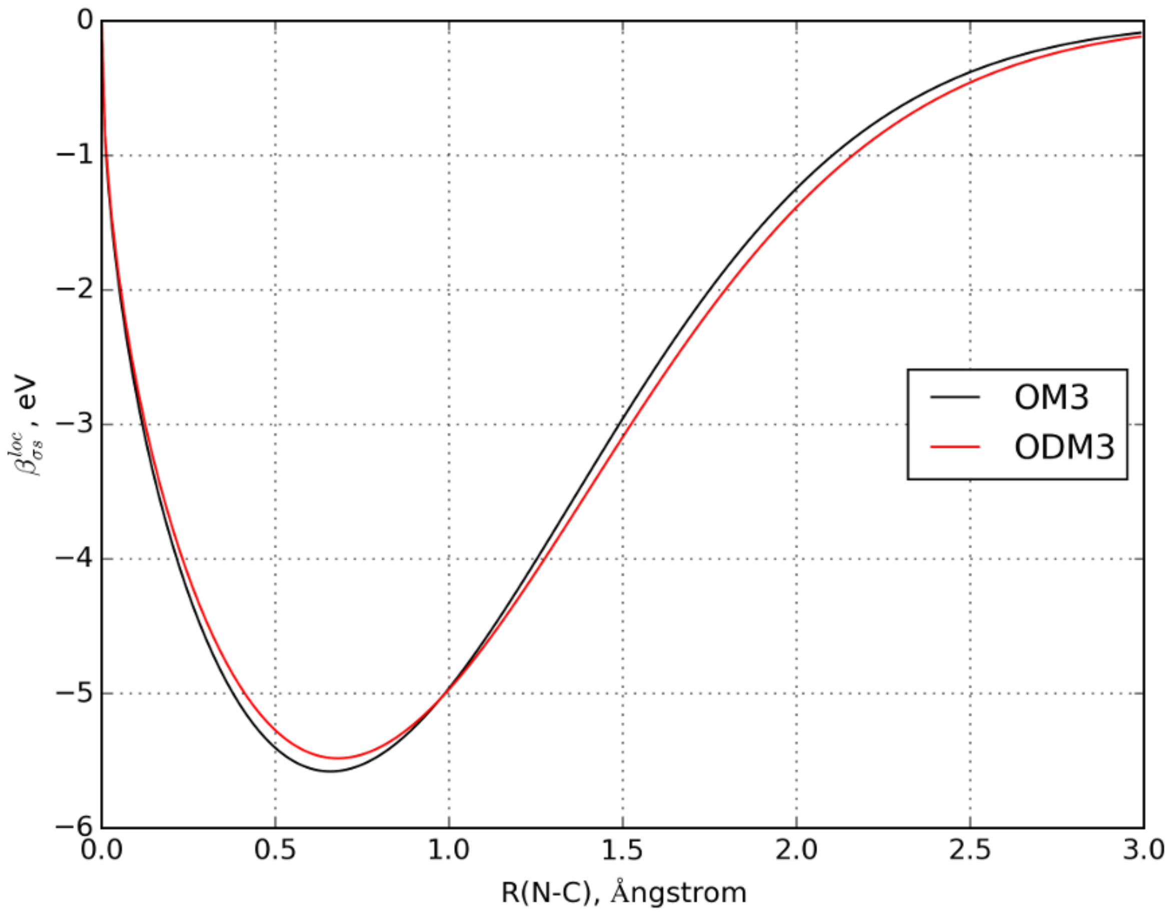

Figure S71: Comparison of σs local resonance integrals for the N−C pair calculated using standard OM3 and new ODM3 parameters.

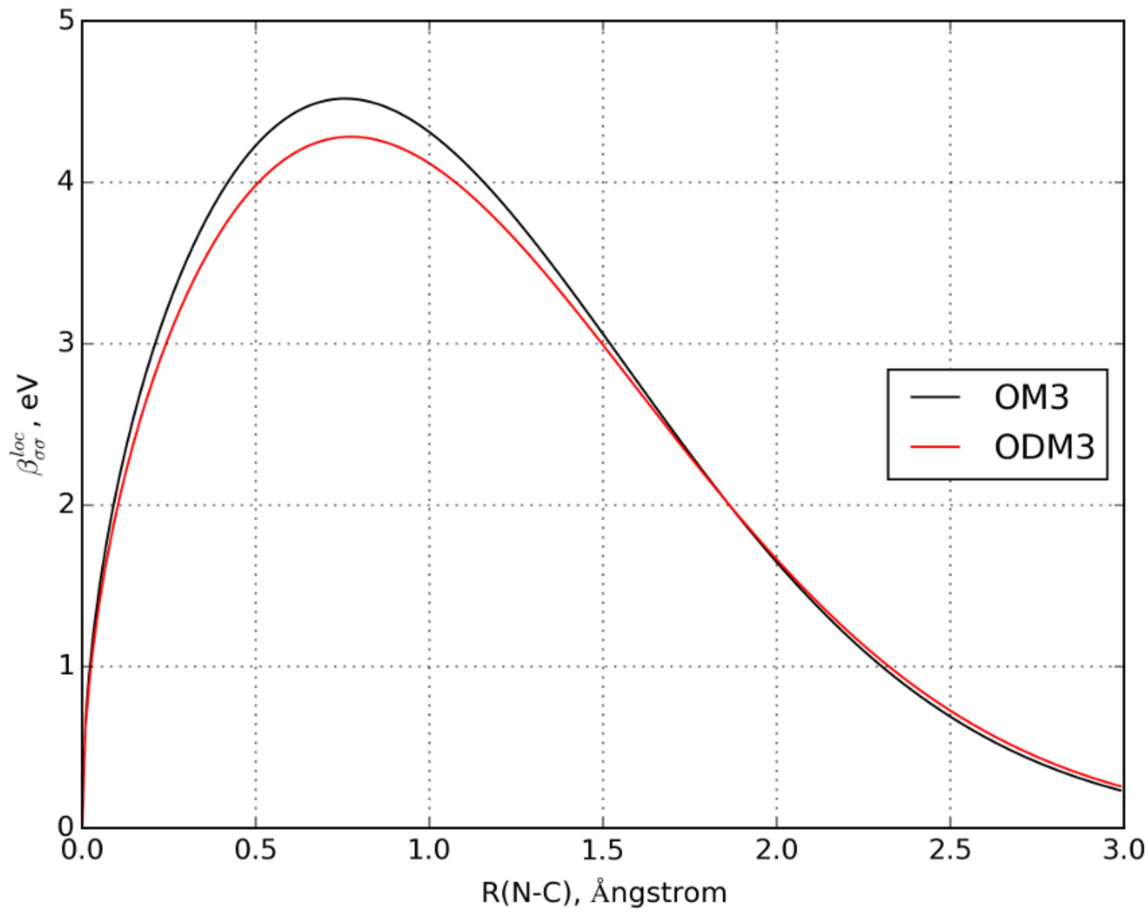

Figure S72: Comparison of $\sigma\sigma$ local resonance integrals for the N−C pair calculated using standard OM3 and new ODM3 parameters.

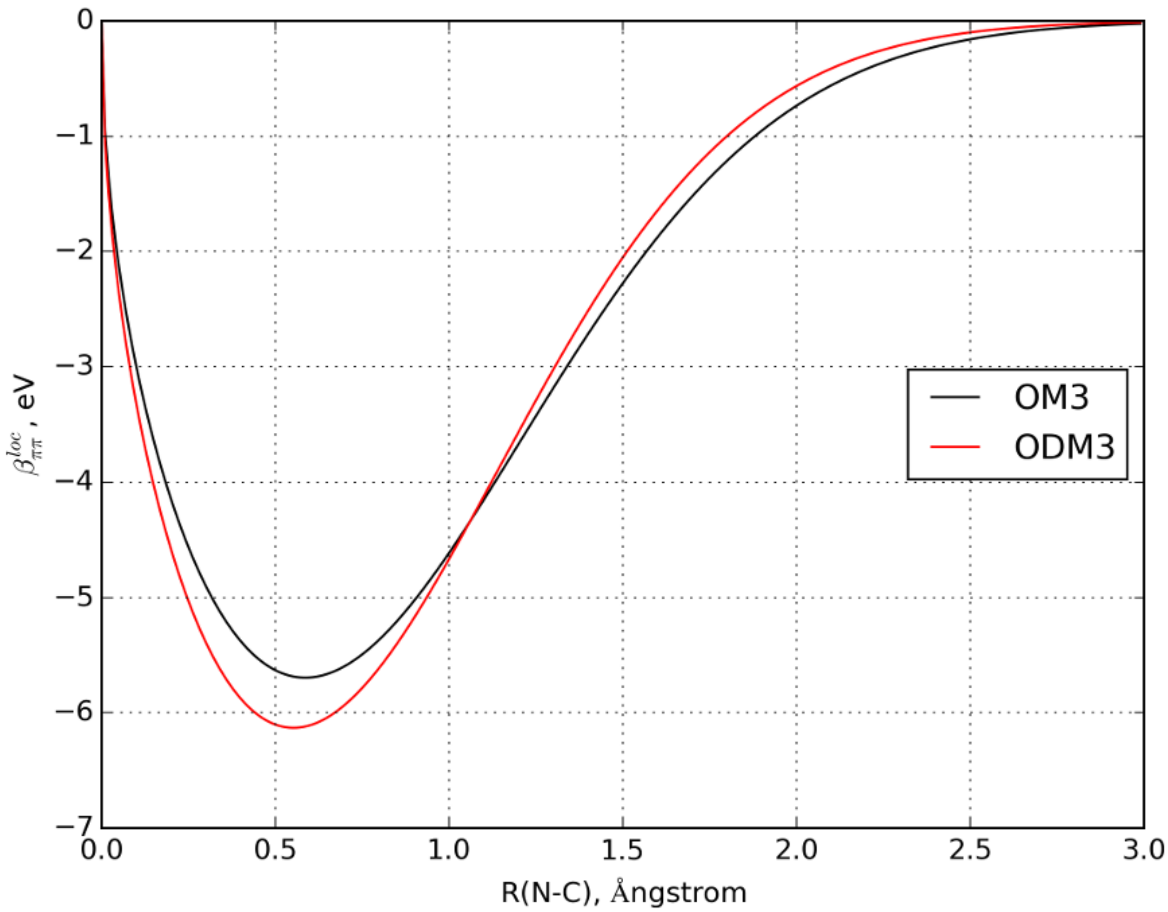

Figure S73: Comparison of $\pi\pi$ local resonance integrals for the N−C pair calculated using standard OM3 and new ODM3 parameters.

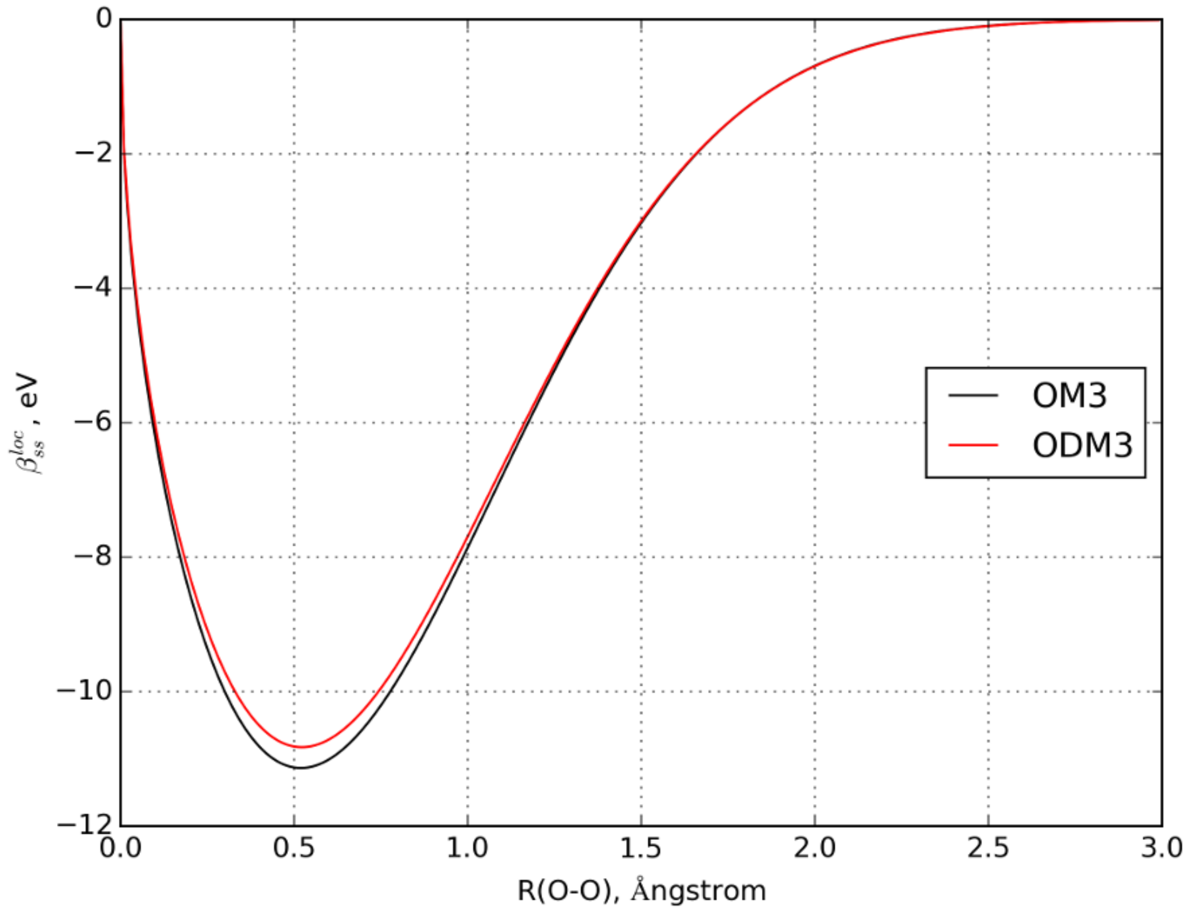

Figure S74: Comparison of *ss* local resonance integrals for the O−O pair calculated using standard OM3 and new ODM3 parameters.

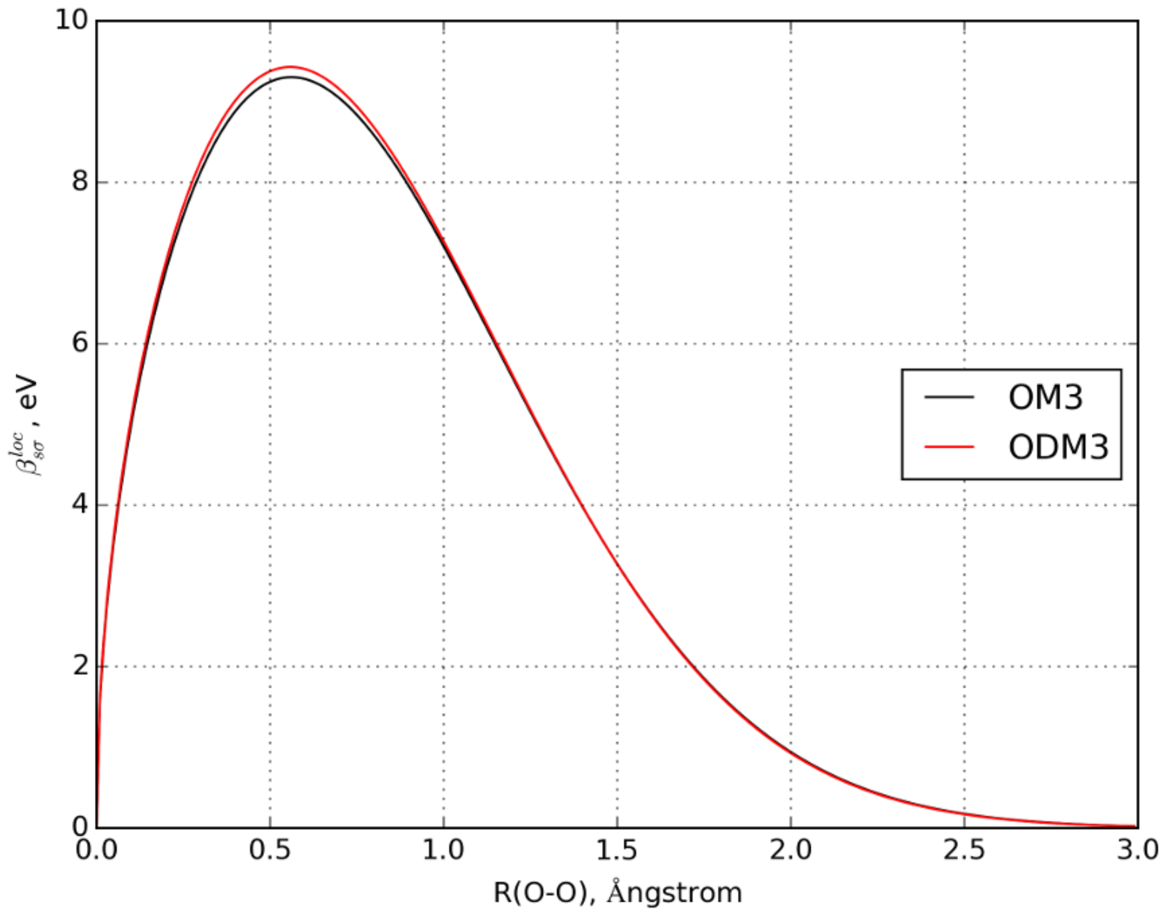

Figure S75: Comparison of $s\sigma$ local resonance integrals for the O−O pair calculated using standard OM3 and new ODM3 parameters.

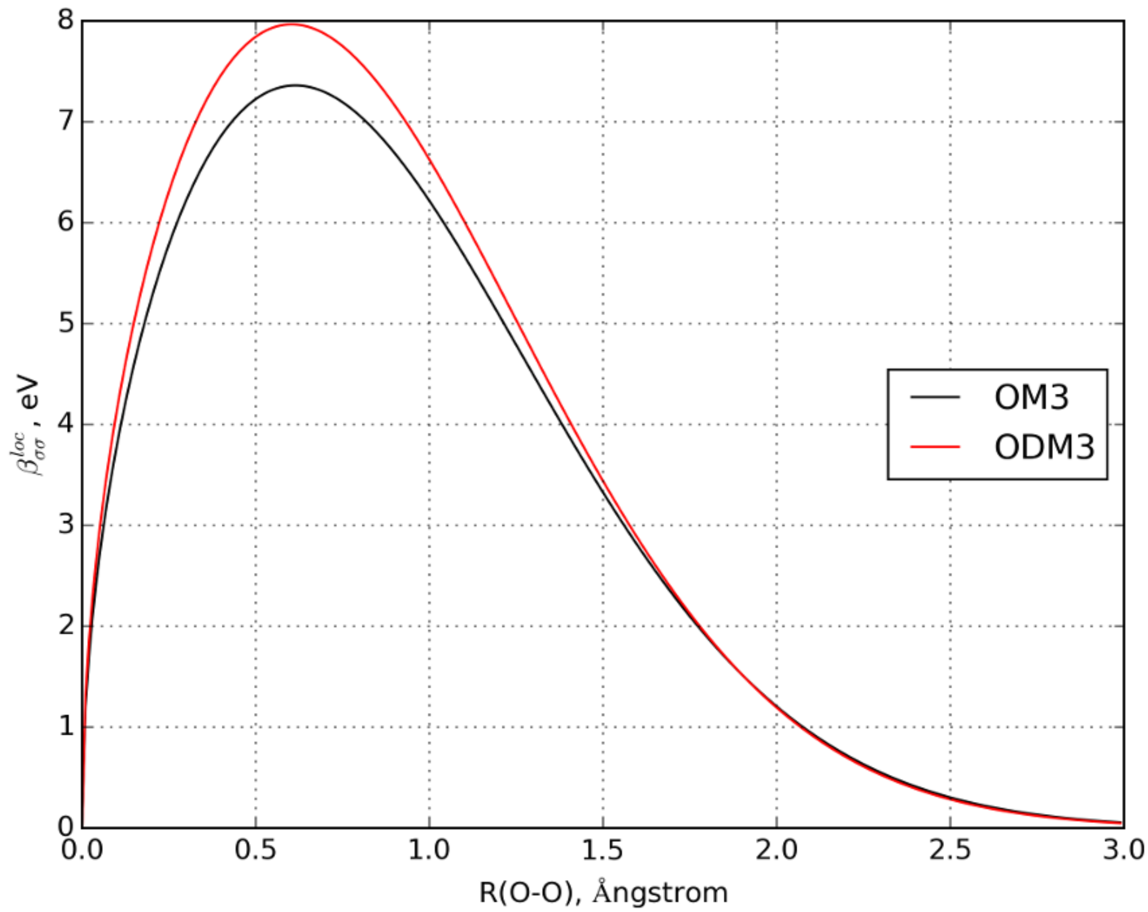

Figure S76: Comparison of $\sigma\sigma$ local resonance integrals for the O−O pair calculated using standard OM3 and new ODM3 parameters.

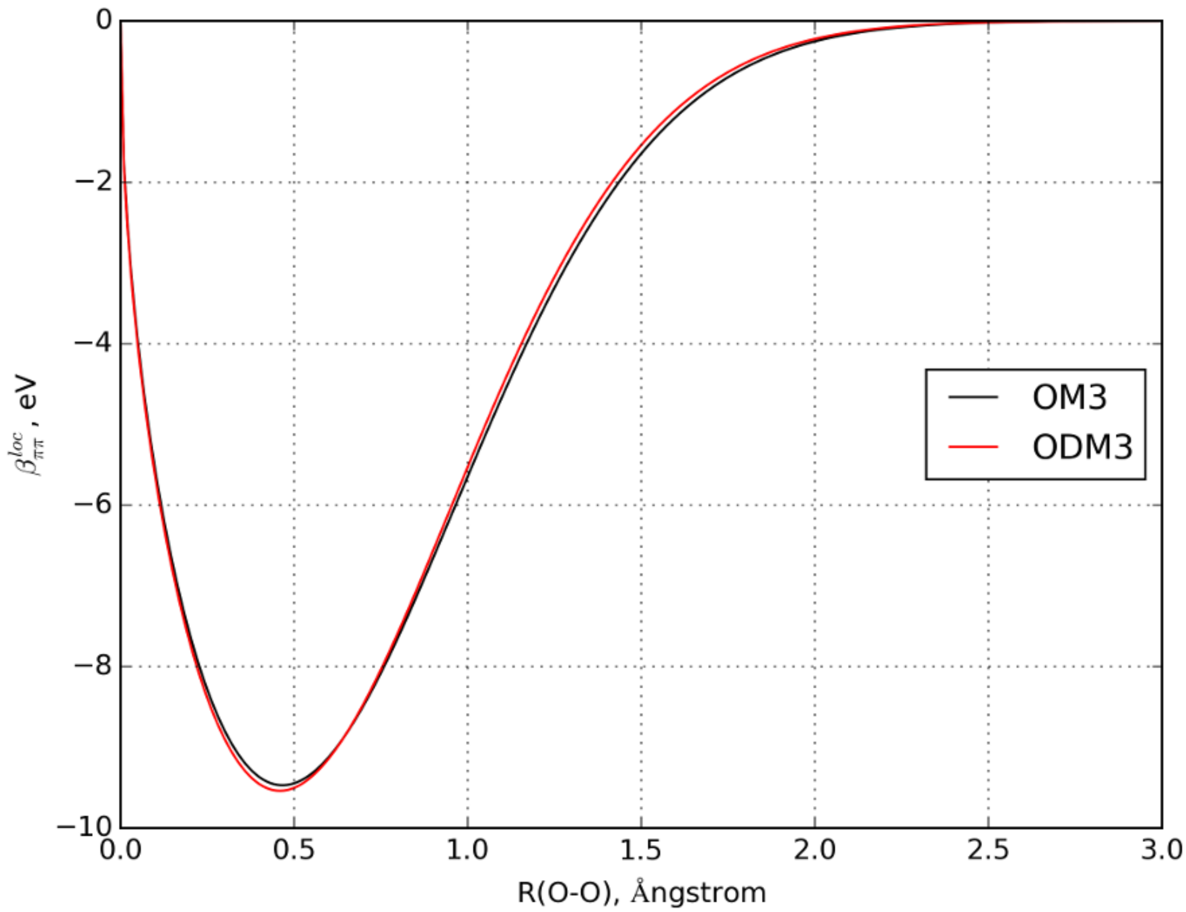

Figure S77: Comparison of $\pi\pi$ local resonance integrals for the O−O pair calculated using standard OM3 and new ODM3 parameters.

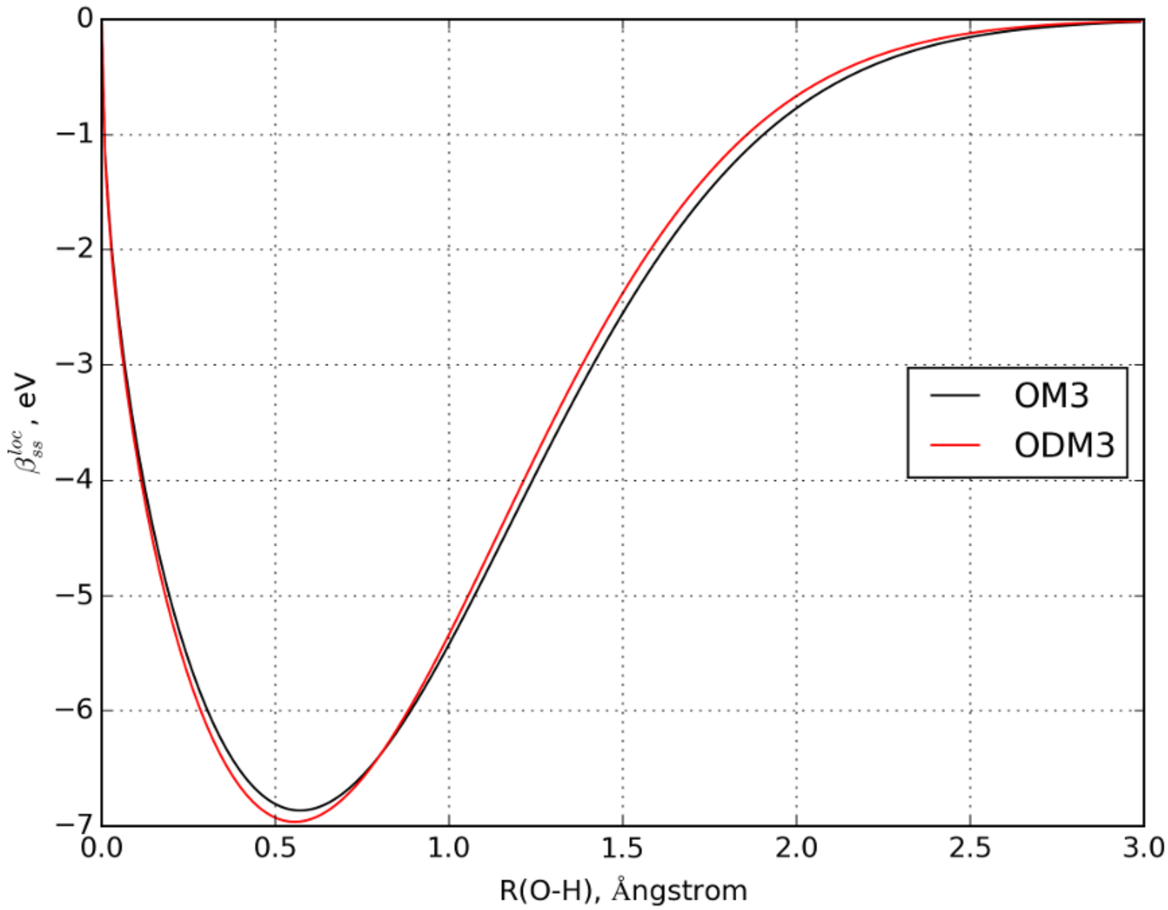

Figure S78: Comparison of *ss* local resonance integrals for the O−H pair calculated using standard OM3 and new ODM3 parameters.

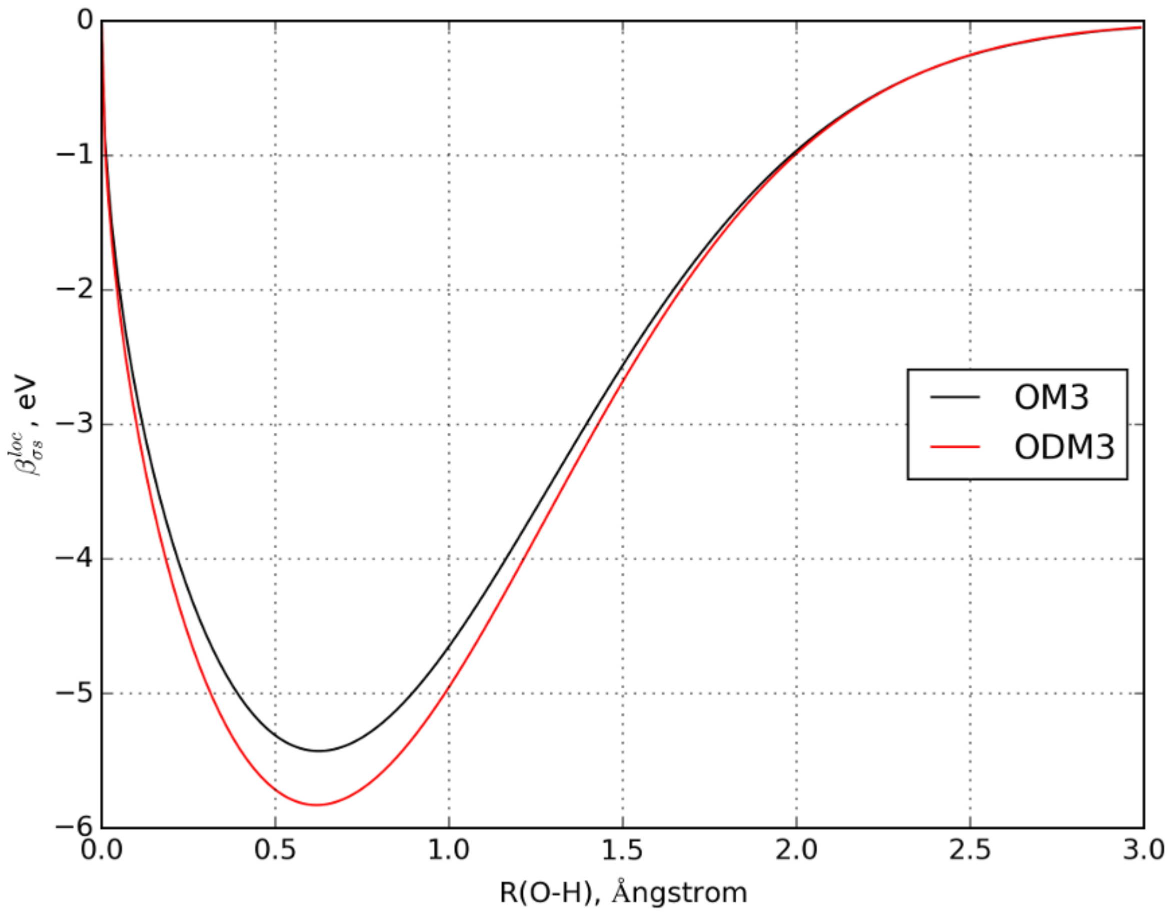

Figure S79: Comparison of σs local resonance integrals for the O−H pair calculated using standard OM3 and new ODM3 parameters.

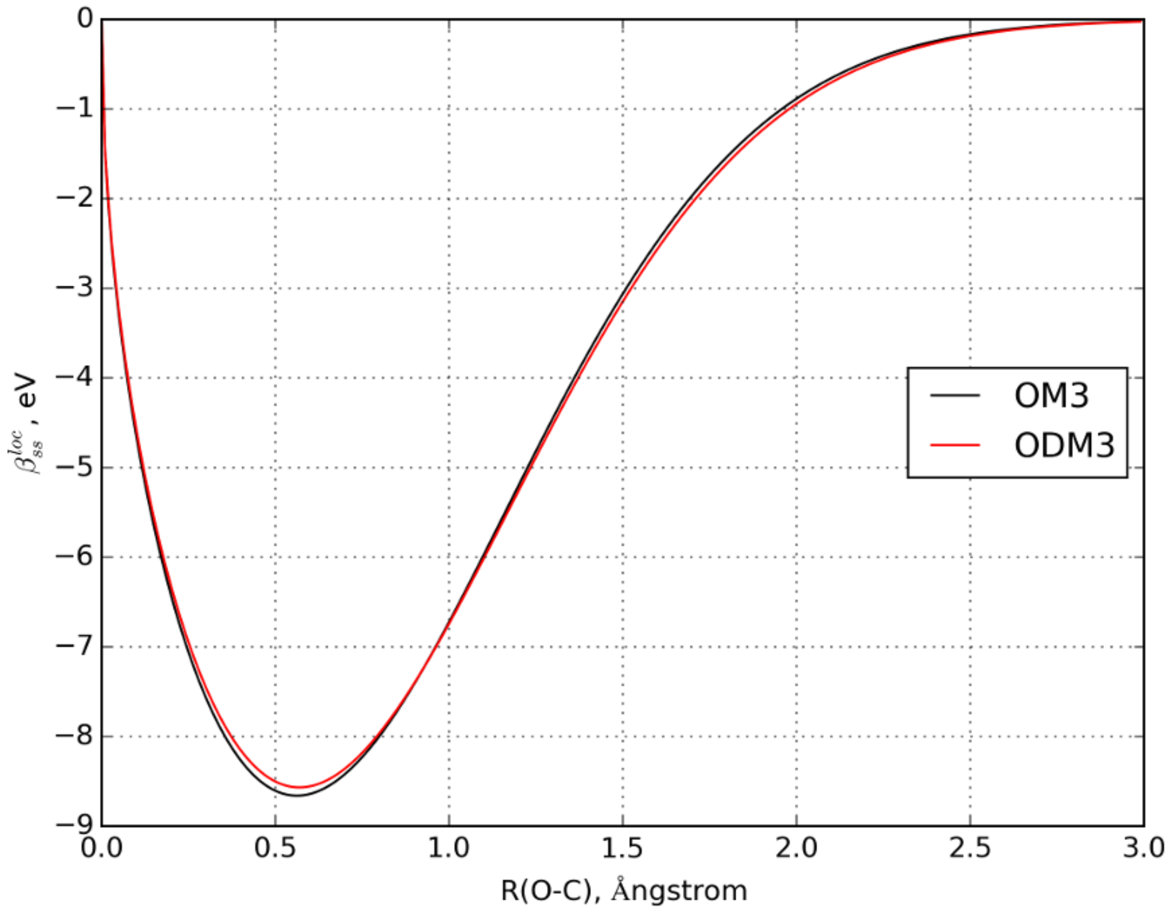

Figure S80: Comparison of *ss* local resonance integrals for the O−C pair calculated using standard OM3 and new ODM3 parameters.

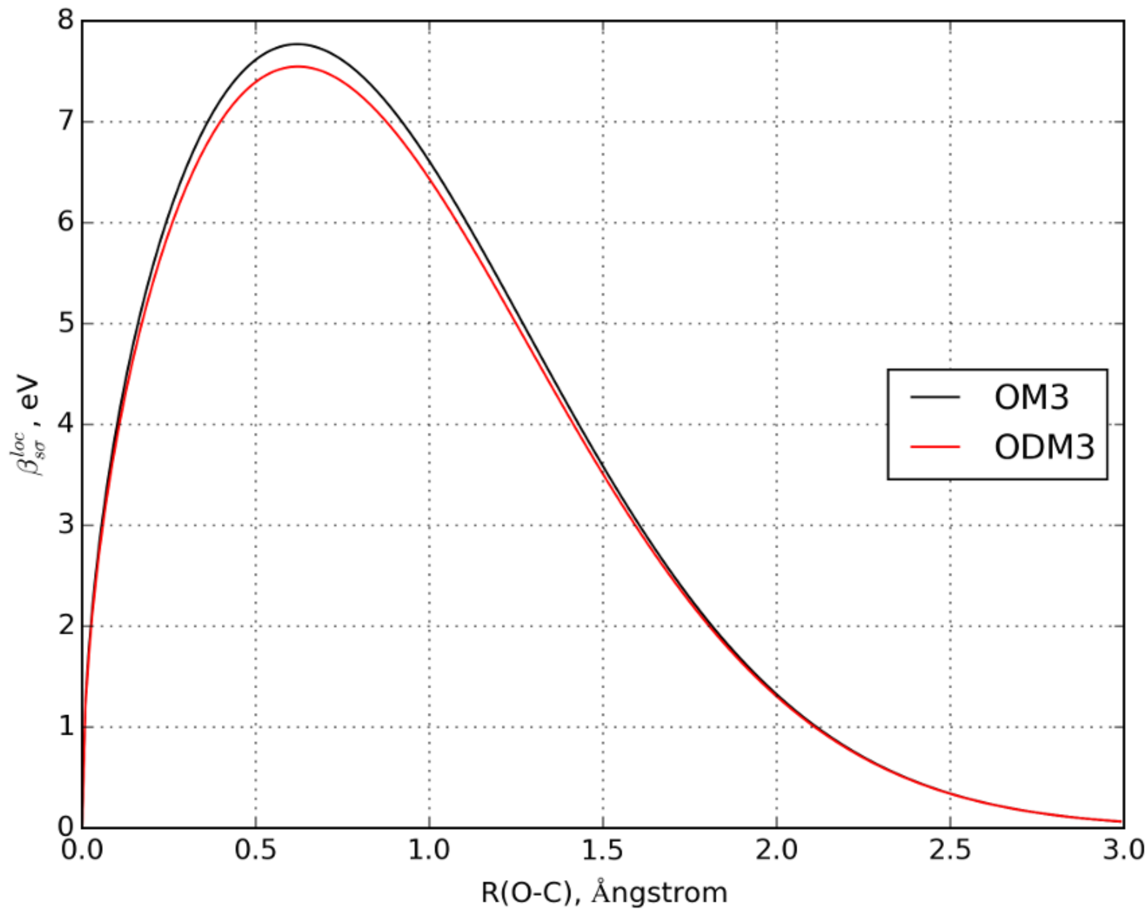

Figure S81: Comparison of $s\sigma$ local resonance integrals for the O−C pair calculated using standard OM3 and new ODM3 parameters.

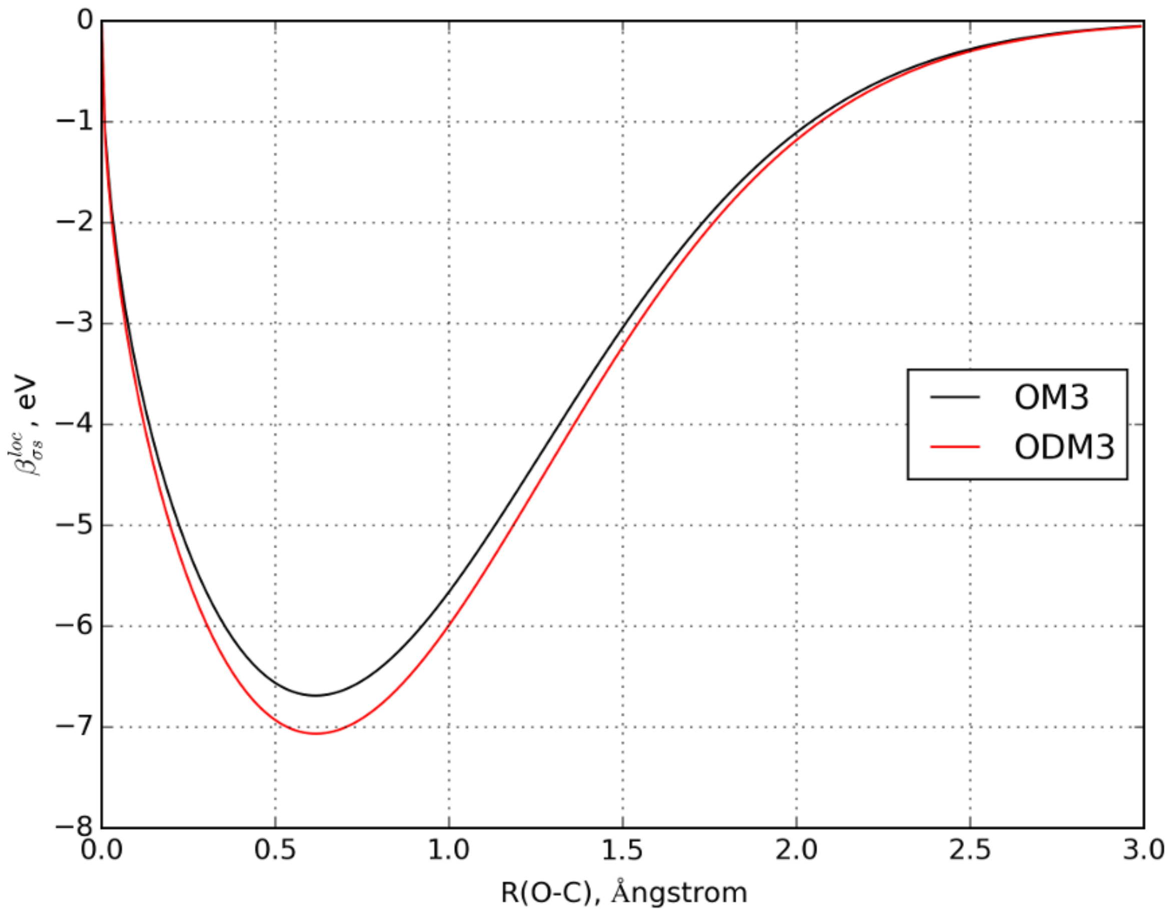

Figure S82: Comparison of σs local resonance integrals for the O−C pair calculated using standard OM3 and new ODM3 parameters.

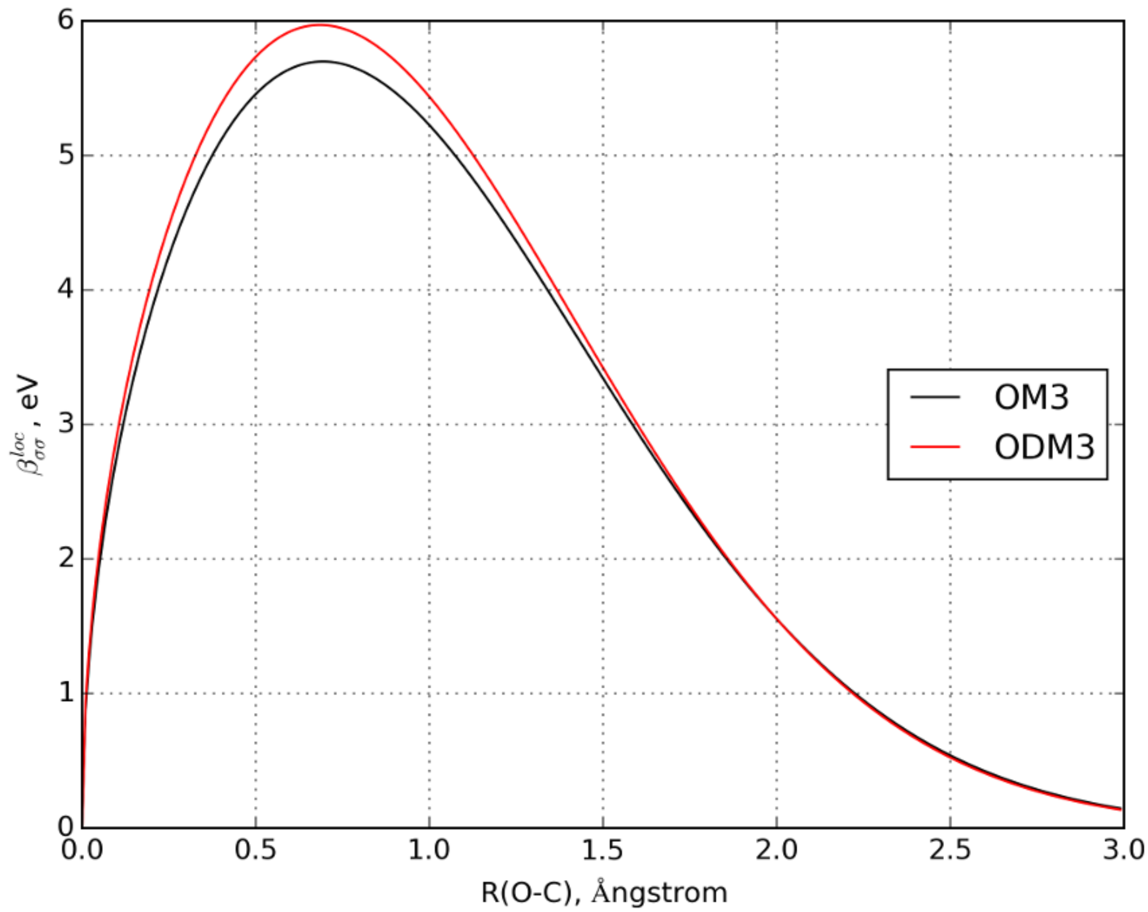

Figure S83: Comparison of $\sigma\sigma$ local resonance integrals for the O−C pair calculated using standard OM3 and new ODM3 parameters.

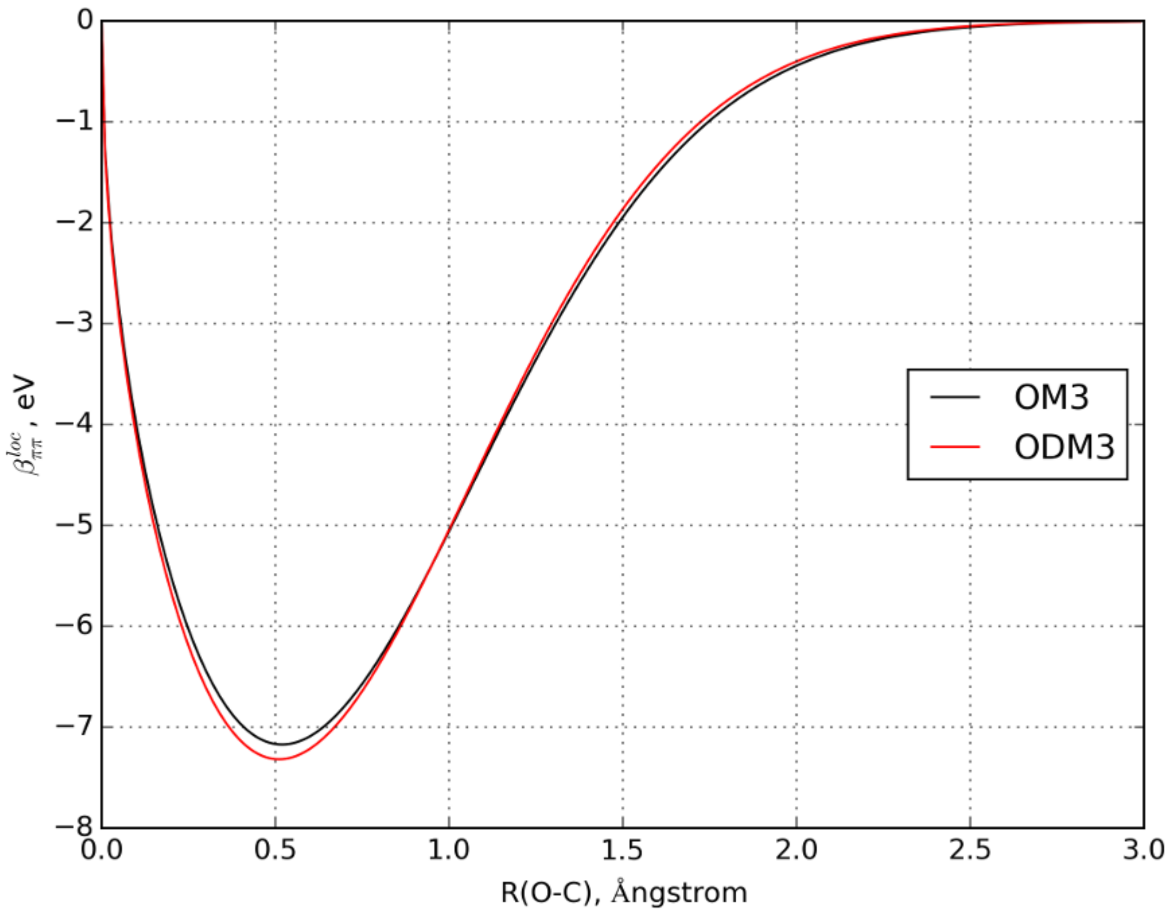

Figure S84: Comparison of $\pi\pi$ local resonance integrals for the O−C pair calculated using standard OM3 and new ODM3 parameters.

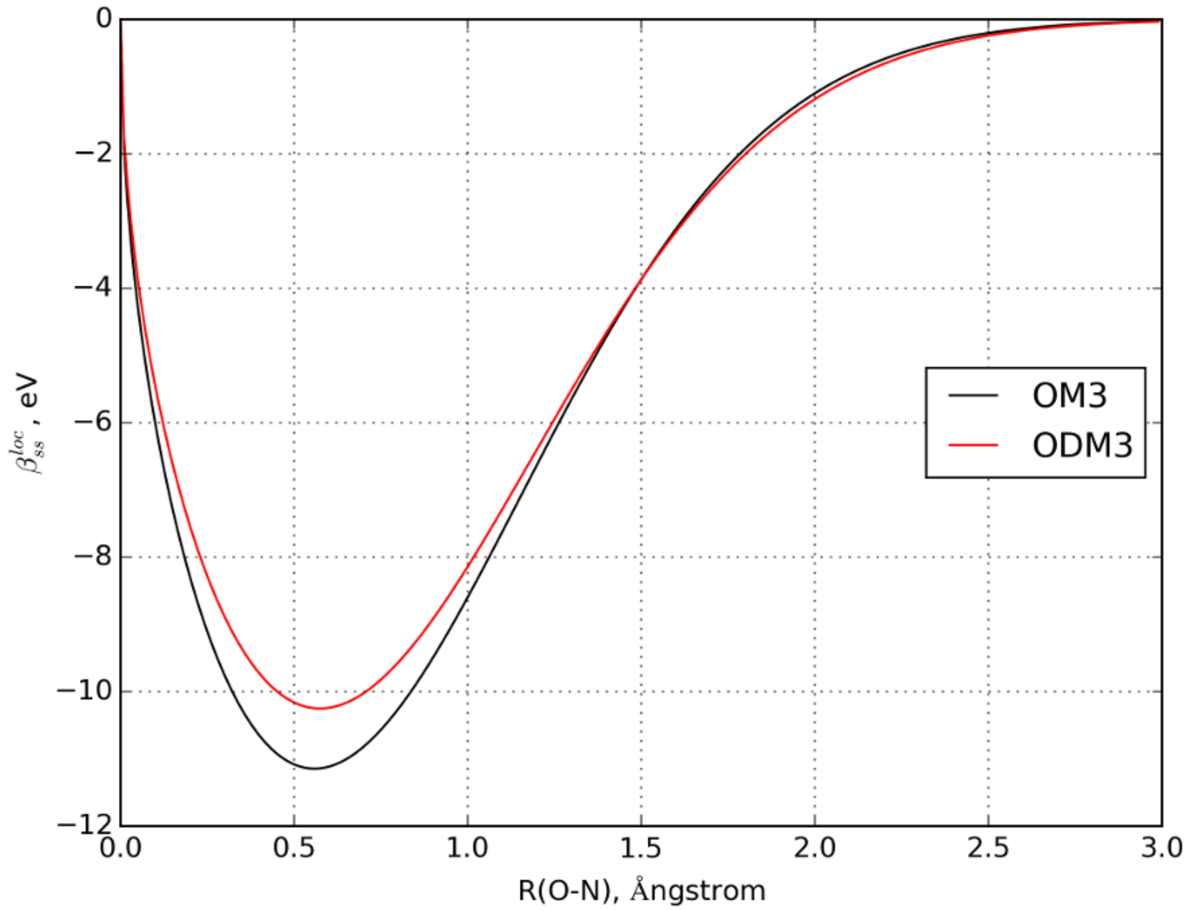

Figure S85: Comparison of ss local resonance integrals for the O−N pair calculated using standard OM3 and new ODM3 parameters.

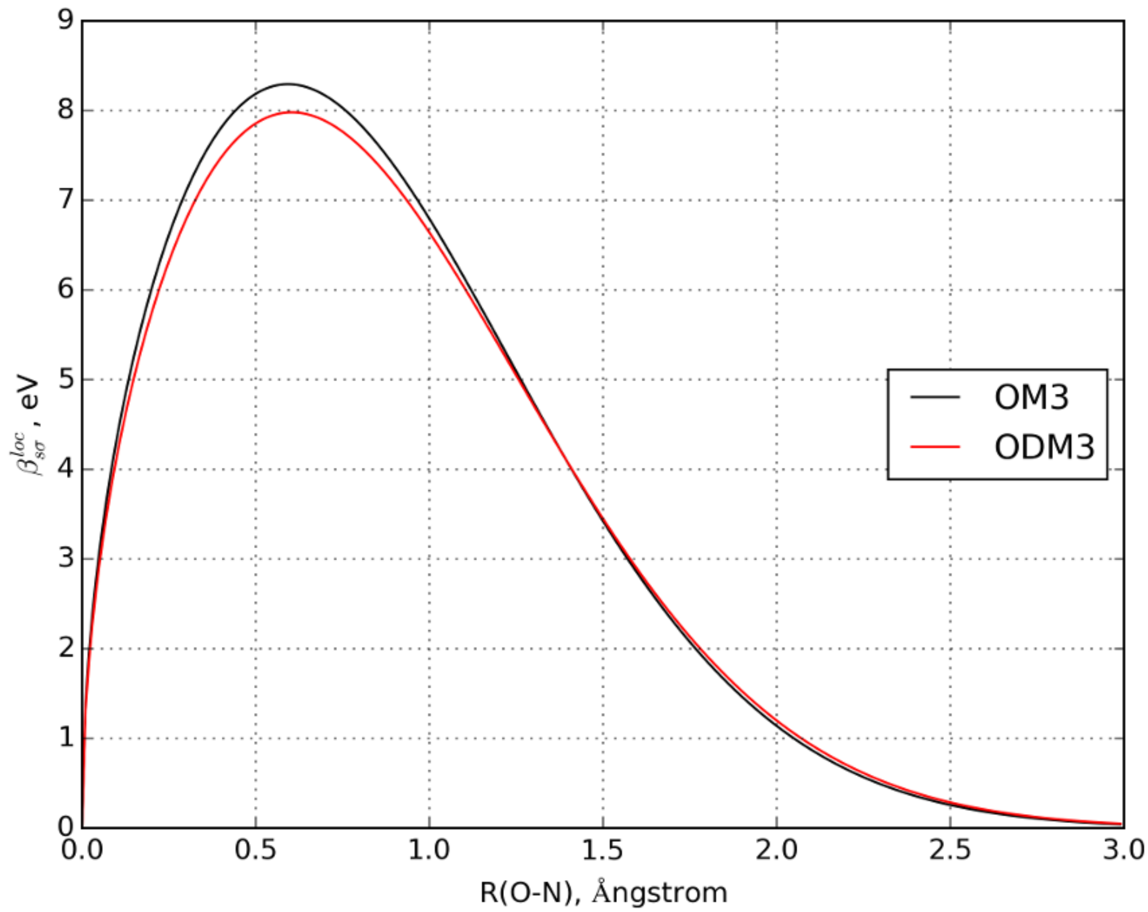

Figure S86: Comparison of $s\sigma$ local resonance integrals for the O−N pair calculated using standard OM3 and new ODM3 parameters.

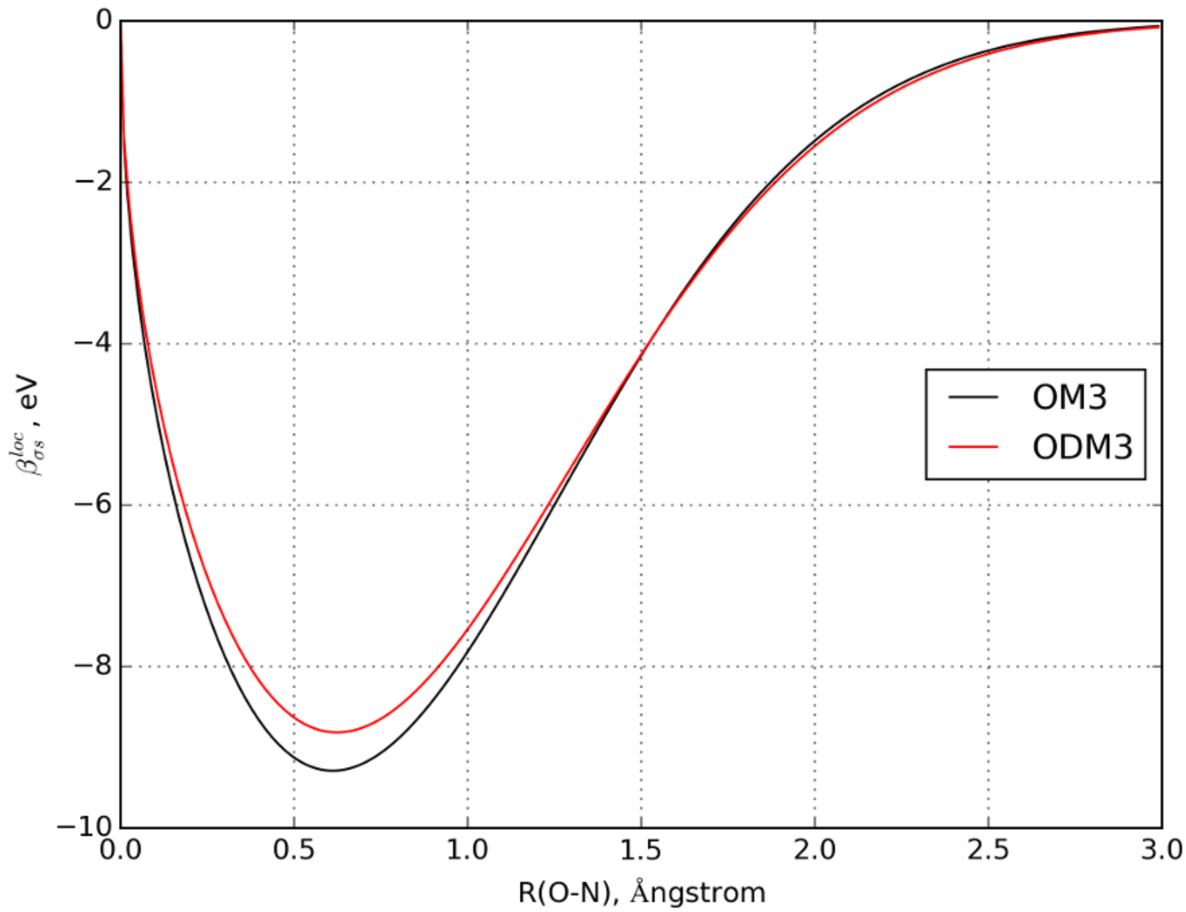

Figure S87: Comparison of σs local resonance integrals for the O−N pair calculated using standard OM3 and new ODM3 parameters.

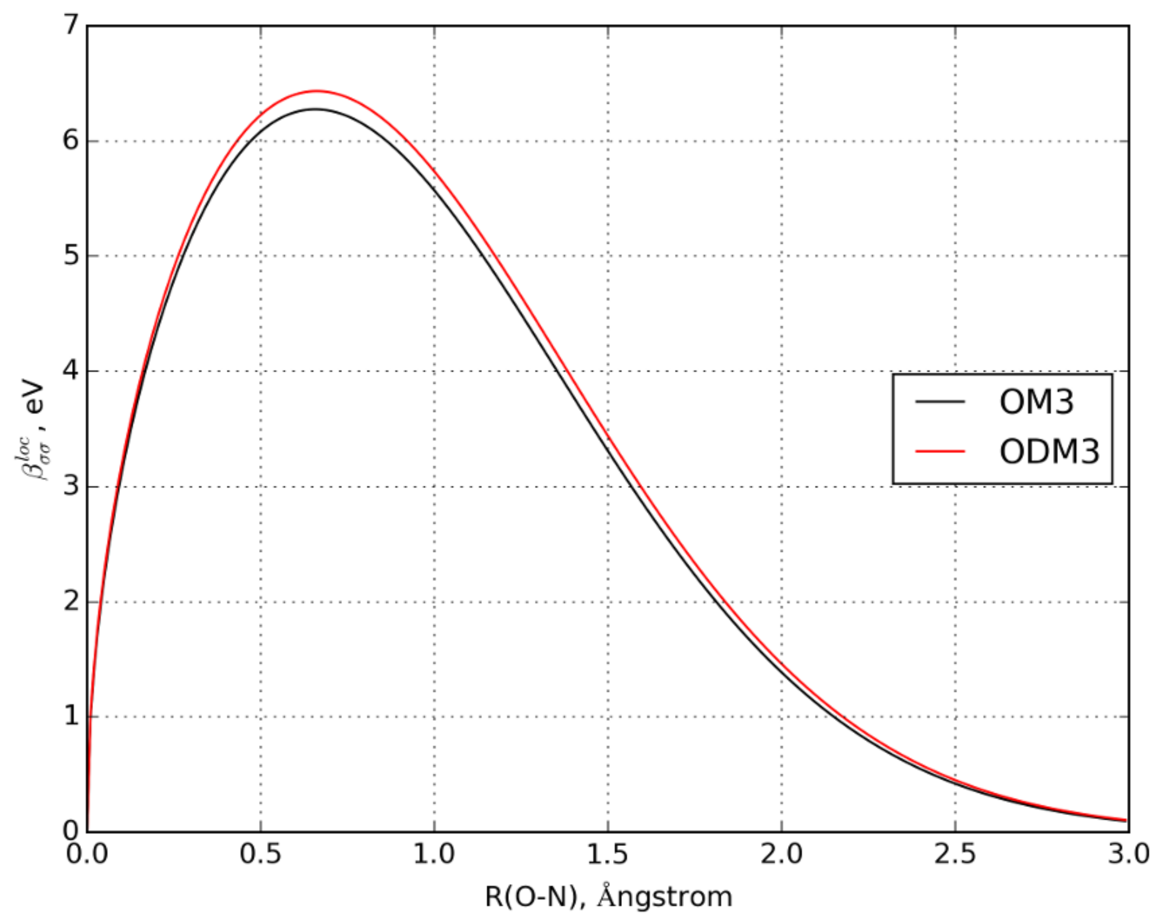

Figure S88: Comparison of $\sigma\sigma$ local resonance integrals for the O−N pair calculated using standard OM3 and new ODM3 parameters.

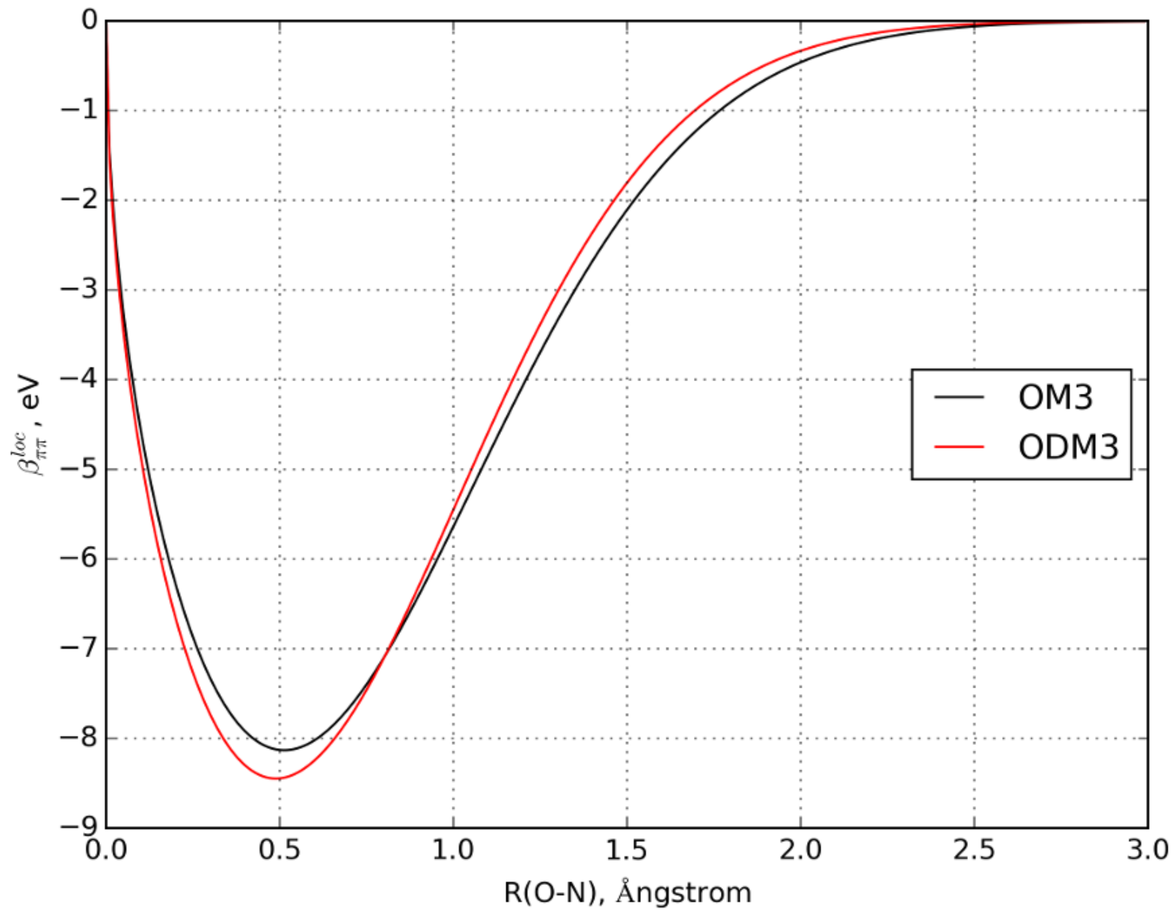

Figure S89: Comparison of $\pi\pi$ local resonance integrals for the O−N pair calculated using standard OM3 and new ODM3 parameters.

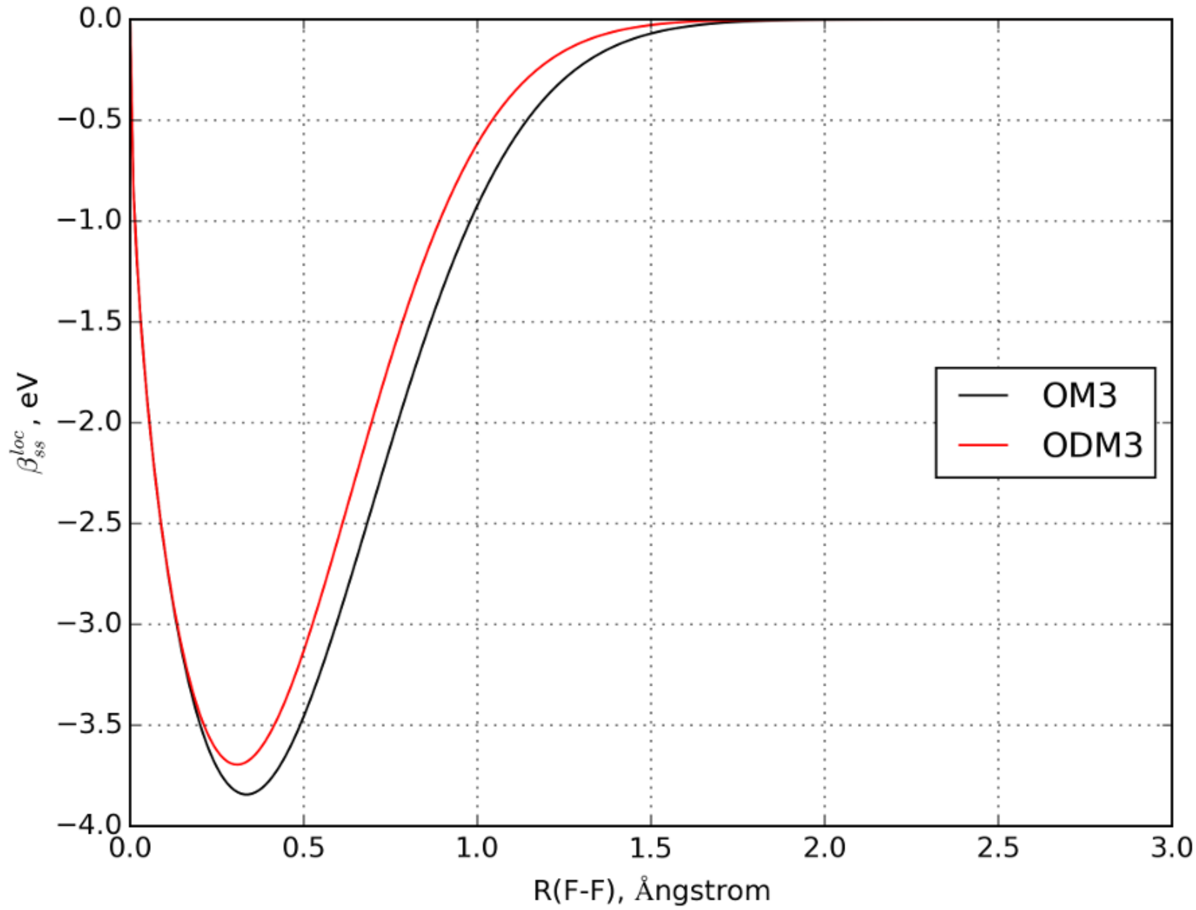

Figure S90: Comparison of *ss* local resonance integrals for the F−F pair calculated using standard OM3 and new ODM3 parameters.

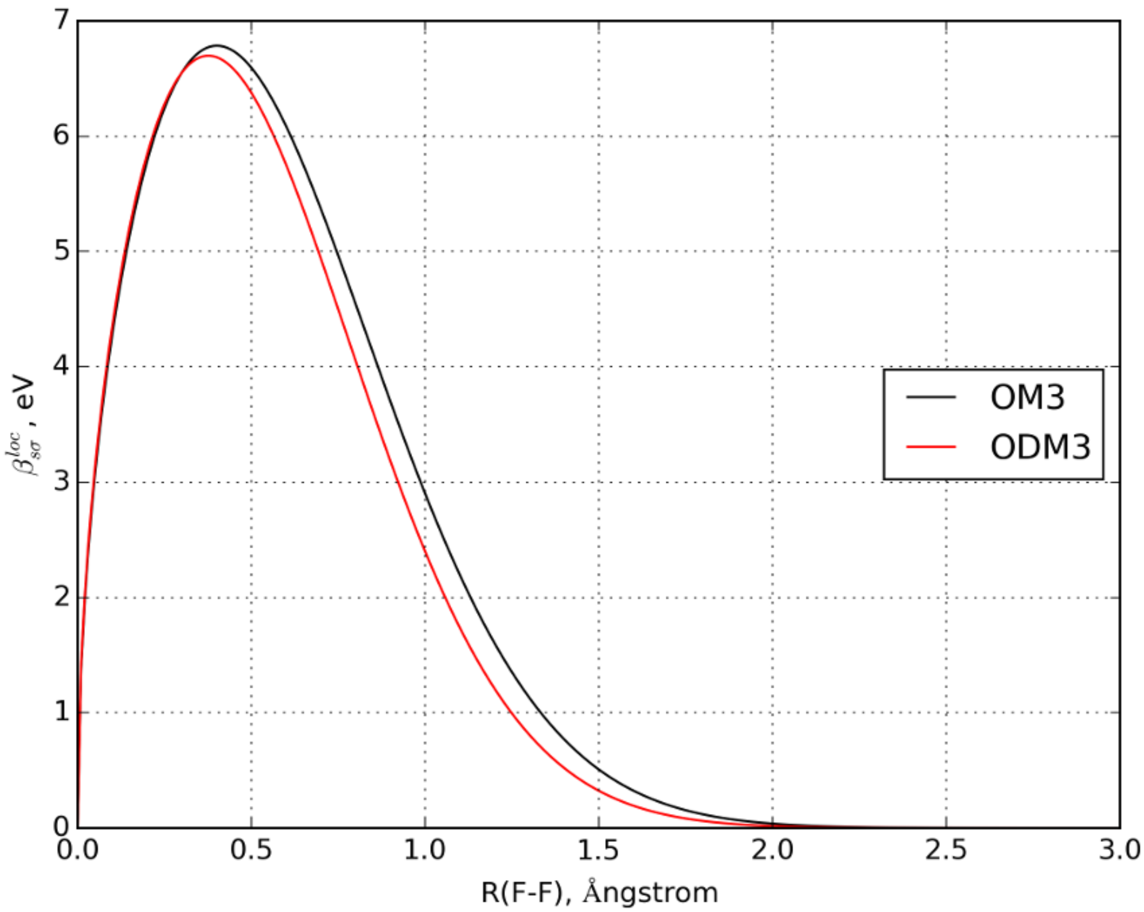

Figure S91: Comparison of $s\sigma$ local resonance integrals for the F−F pair calculated using standard OM3 and new ODM3 parameters.

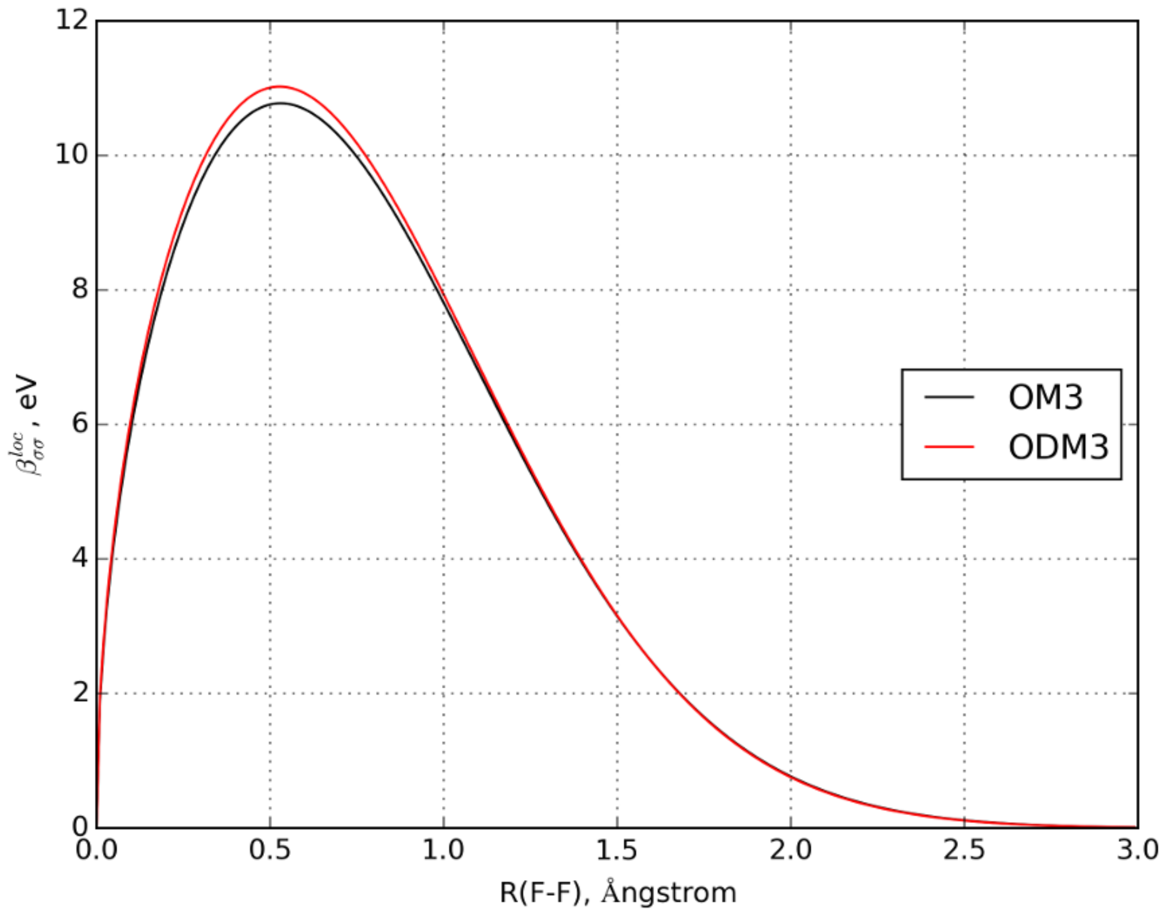

Figure S92: Comparison of $\sigma\sigma$ local resonance integrals for the F−F pair calculated using standard OM3 and new ODM3 parameters.

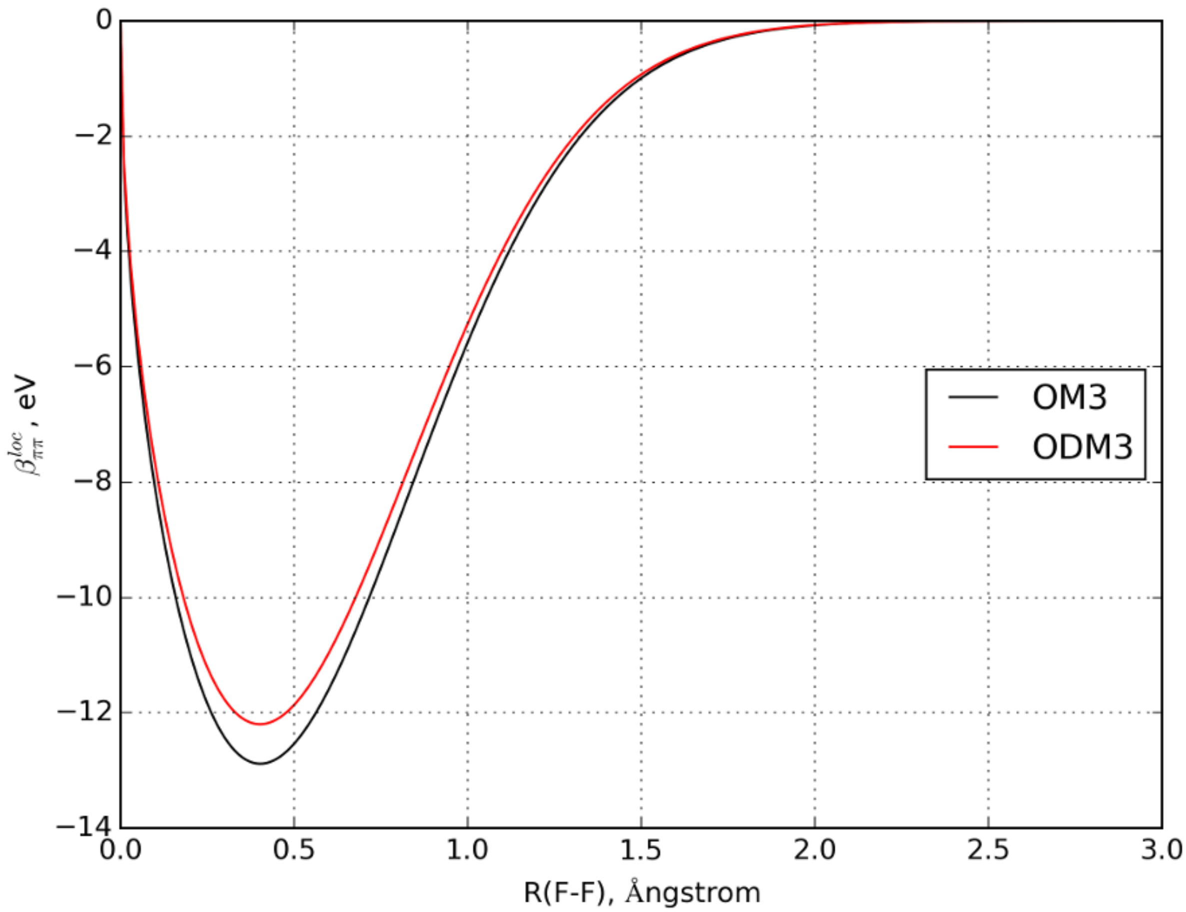

Figure S93: Comparison of $\pi\pi$ local resonance integrals for the F−F pair calculated using standard OM3 and new ODM3 parameters.

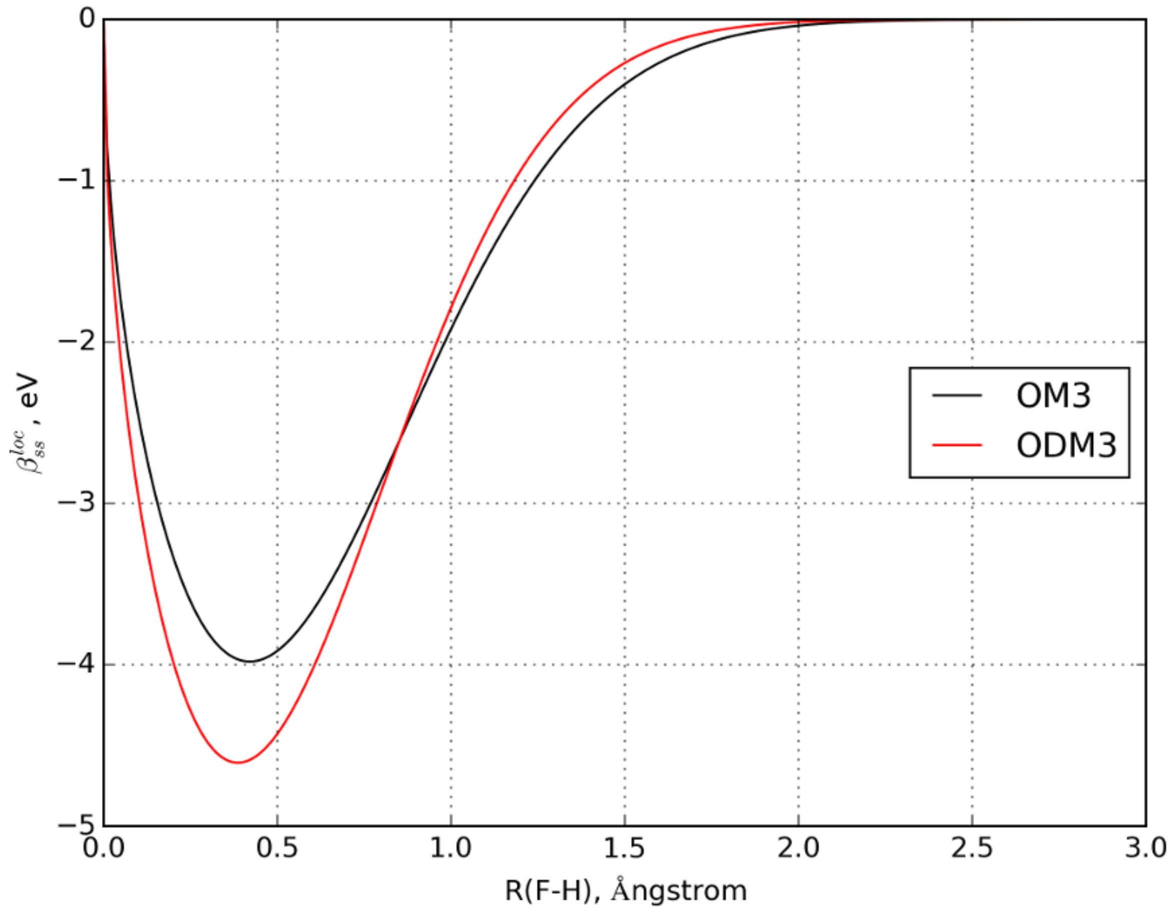

Figure S94: Comparison of ss local resonance integrals for the F−H pair calculated using standard OM3 and new ODM3 parameters.

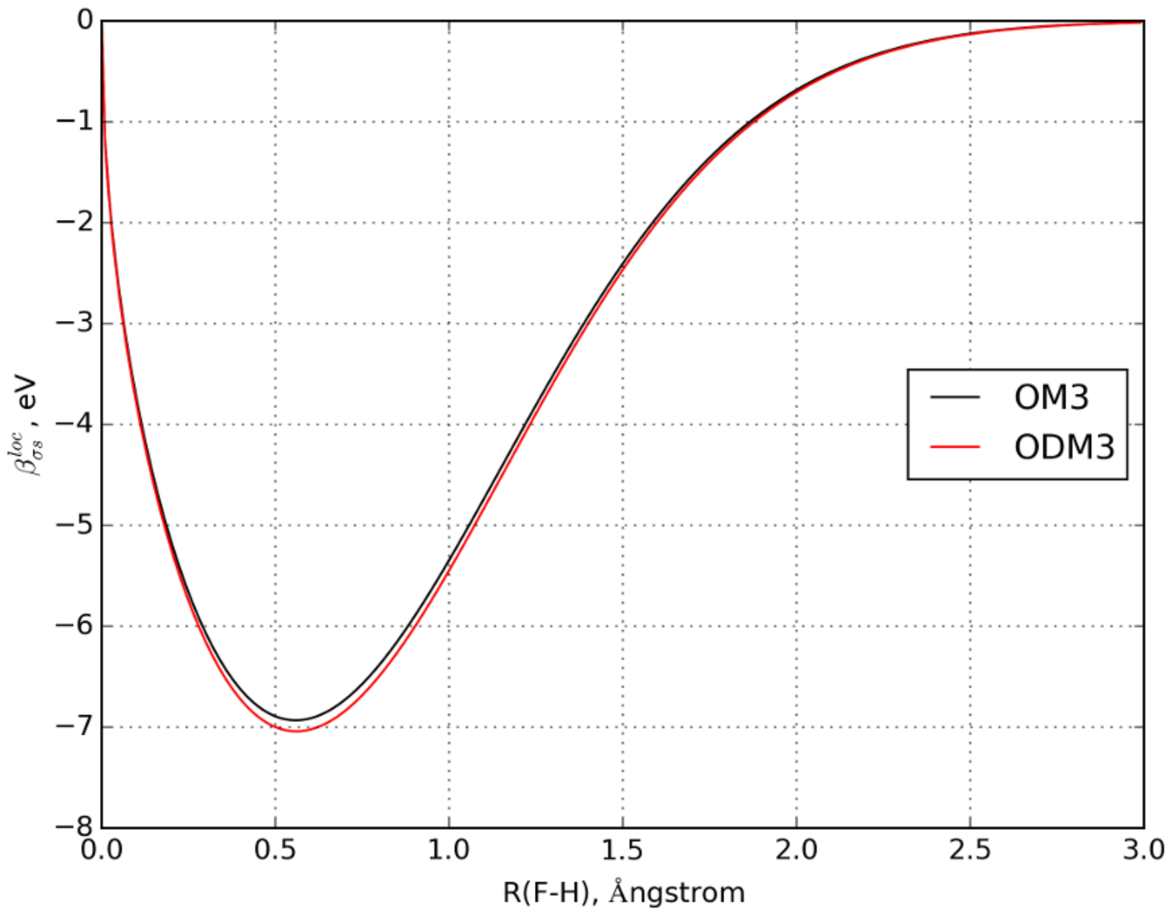

Figure S95: Comparison of σs local resonance integrals for the F−H pair calculated using standard OM3 and new ODM3 parameters.

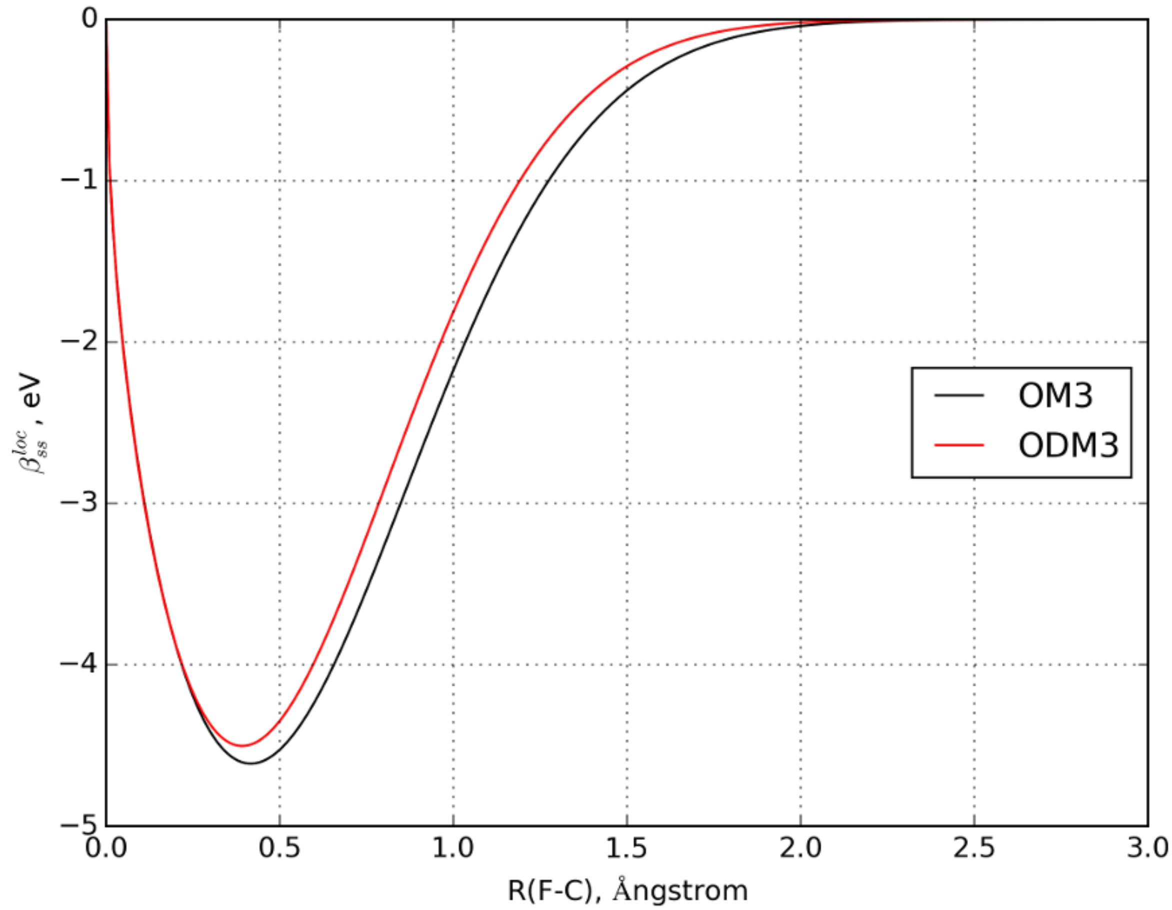

Figure S96: Comparison of ss local resonance integrals for the F−C pair calculated using standard OM3 and new ODM3 parameters.

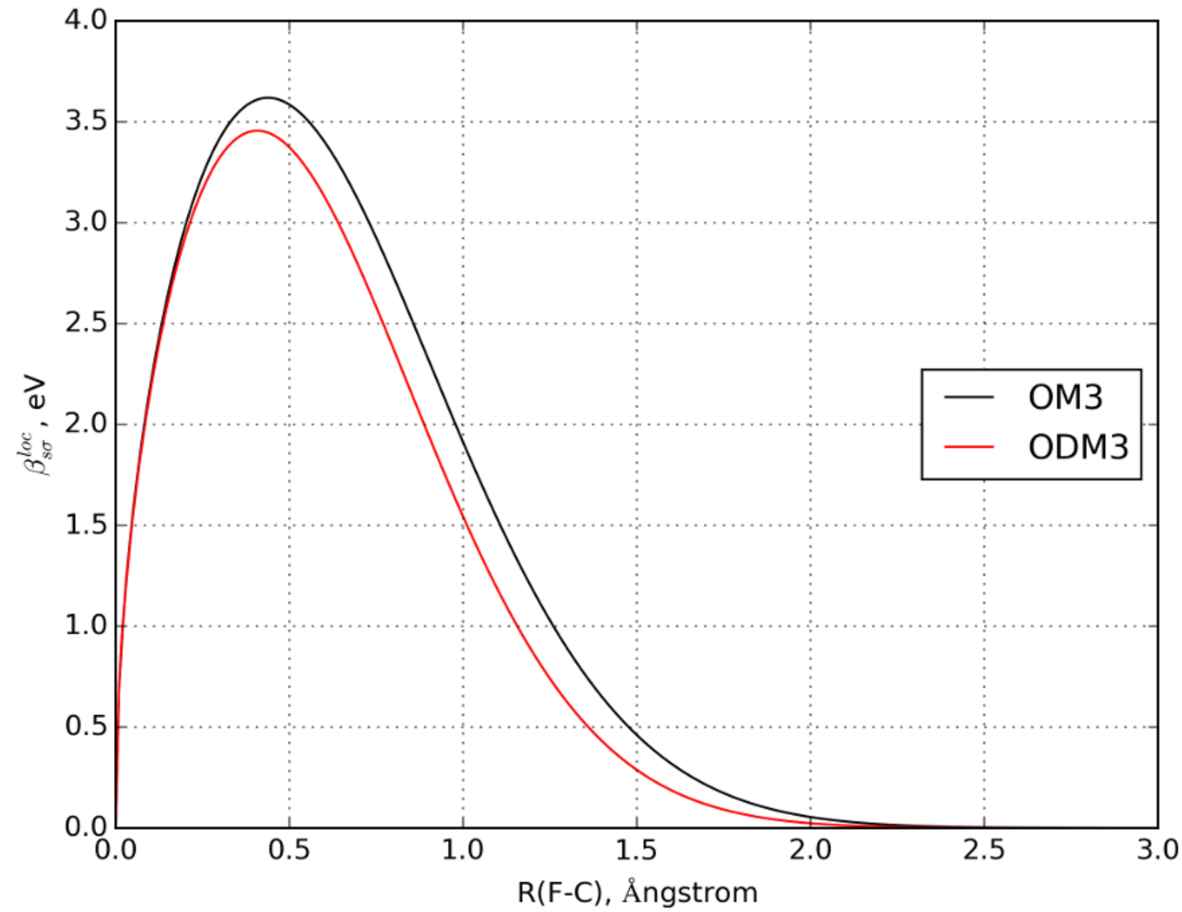

Figure S97: Comparison of $s\sigma$ local resonance integrals for the F−C pair calculated using standard OM3 and new ODM3 parameters.

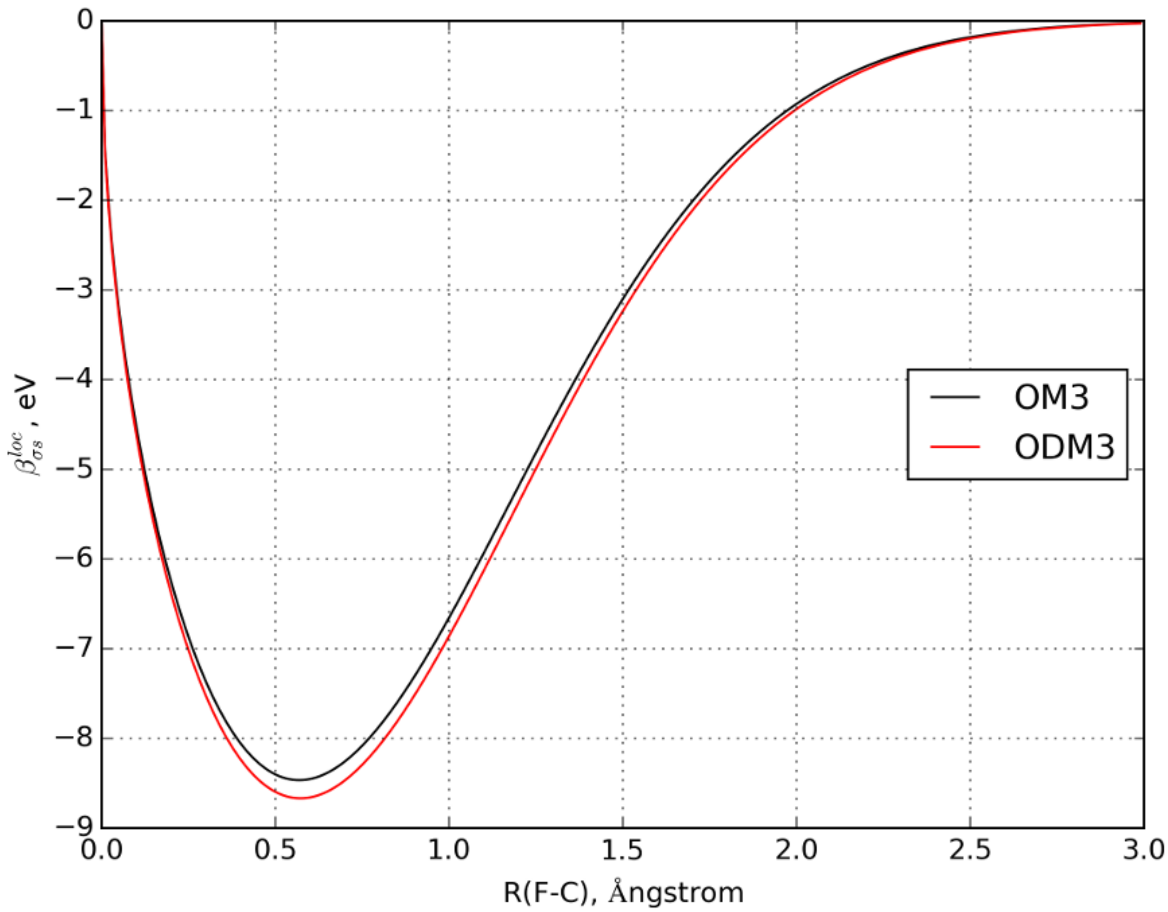

Figure S98: Comparison of σs local resonance integrals for the F−C pair calculated using standard OM3 and new ODM3 parameters.

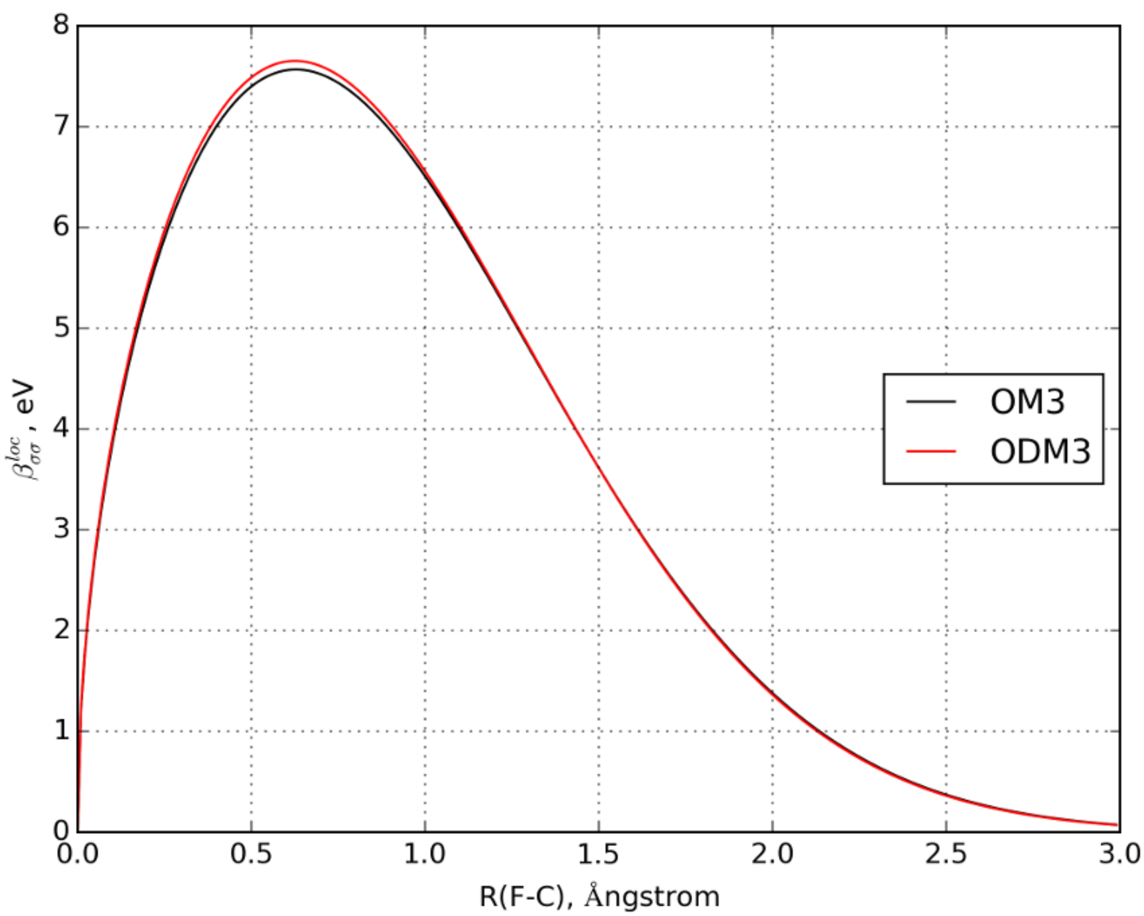

Figure S99: Comparison of $\sigma\sigma$ local resonance integrals for the F−C pair calculated using standard OM3 and new ODM3 parameters.

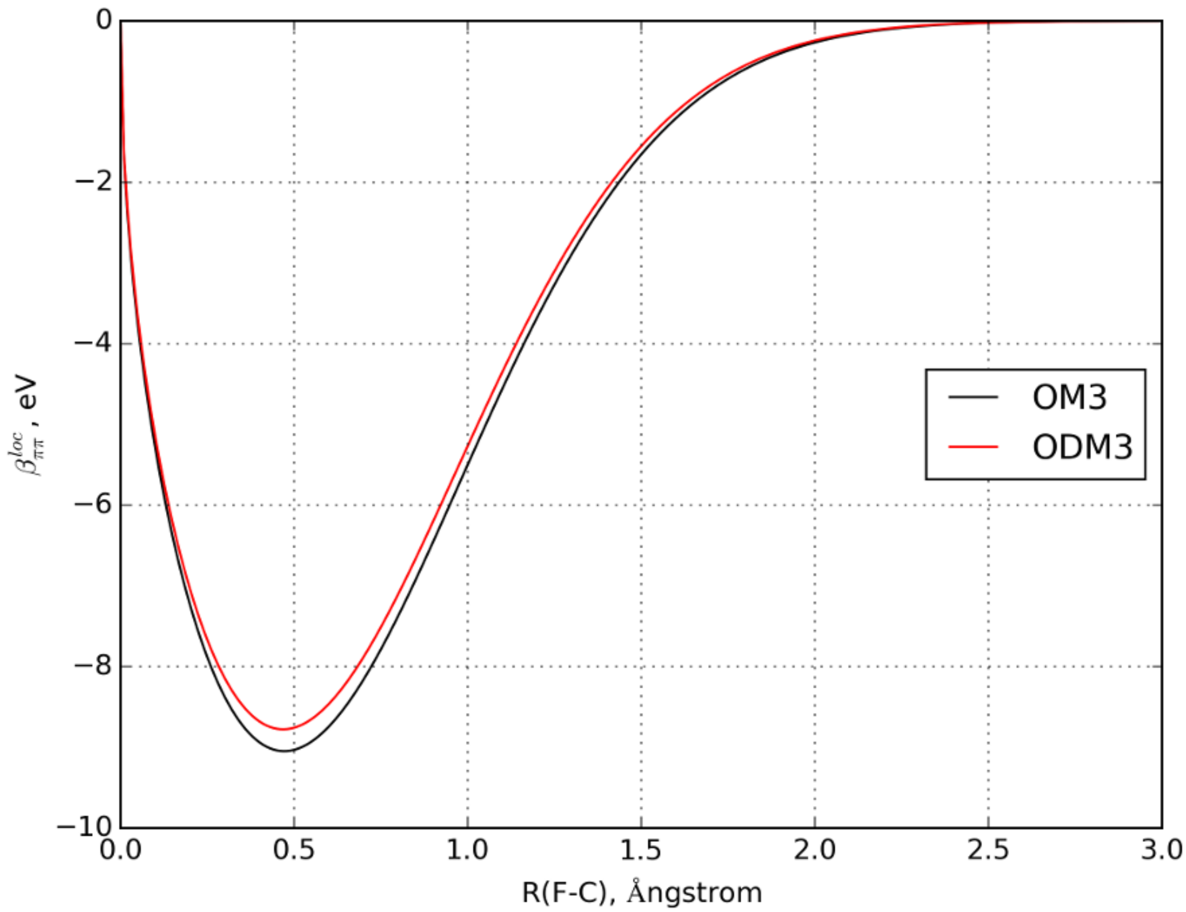

Figure S100: Comparison of $\pi\pi$ local resonance integrals for the F−C pair calculated using standard OM3 and new ODM3 parameters.

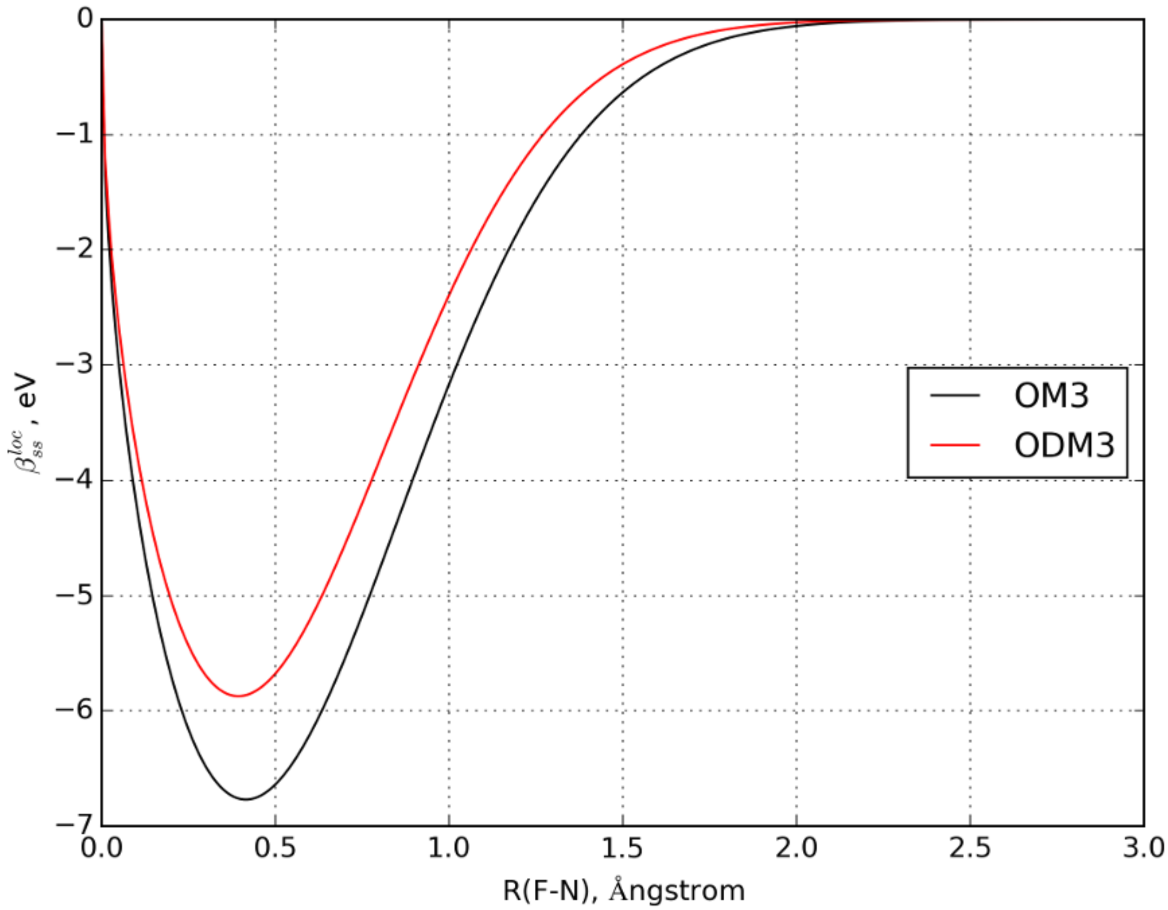

Figure S101: Comparison of *ss* local resonance integrals for the F−N pair calculated using standard OM3 and new ODM3 parameters.

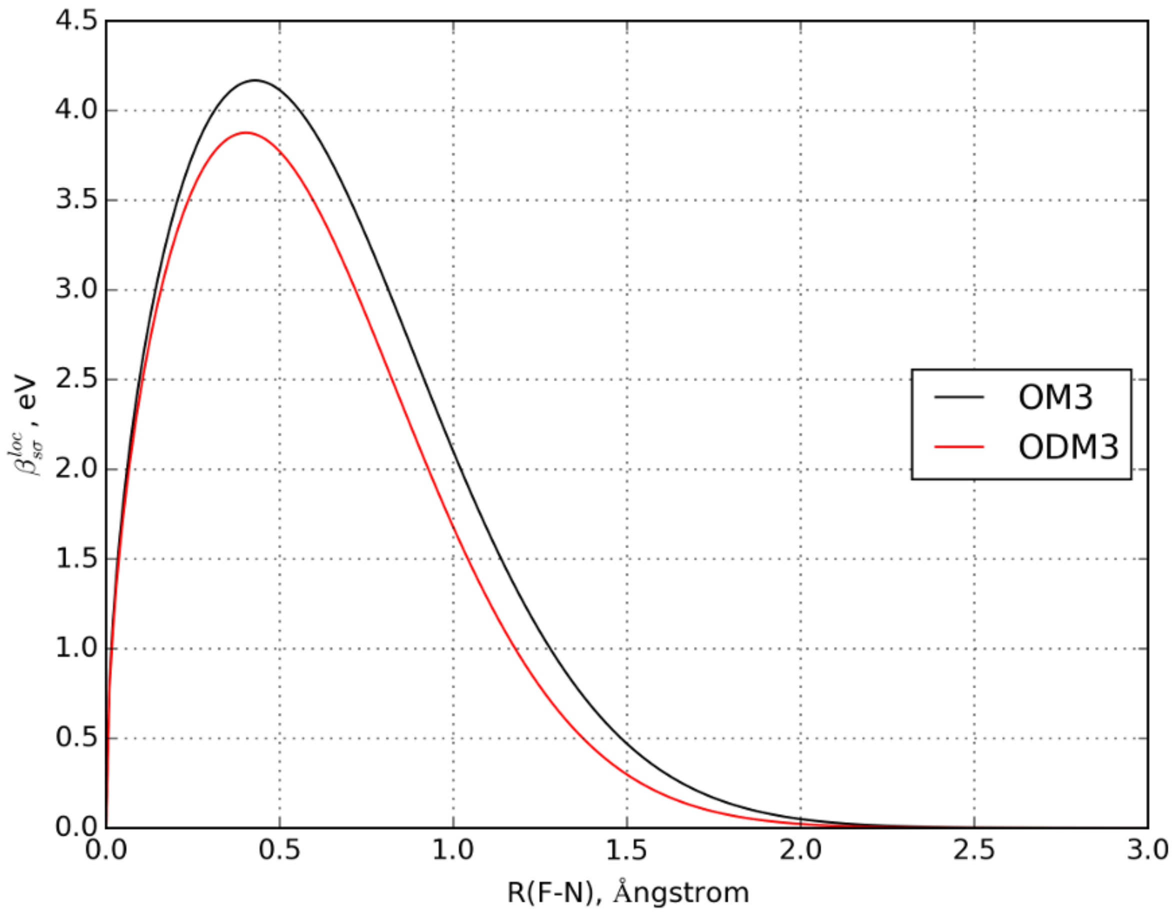

Figure S102: Comparison of $s\sigma$ local resonance integrals for the F−N pair calculated using standard OM3 and new ODM3 parameters.

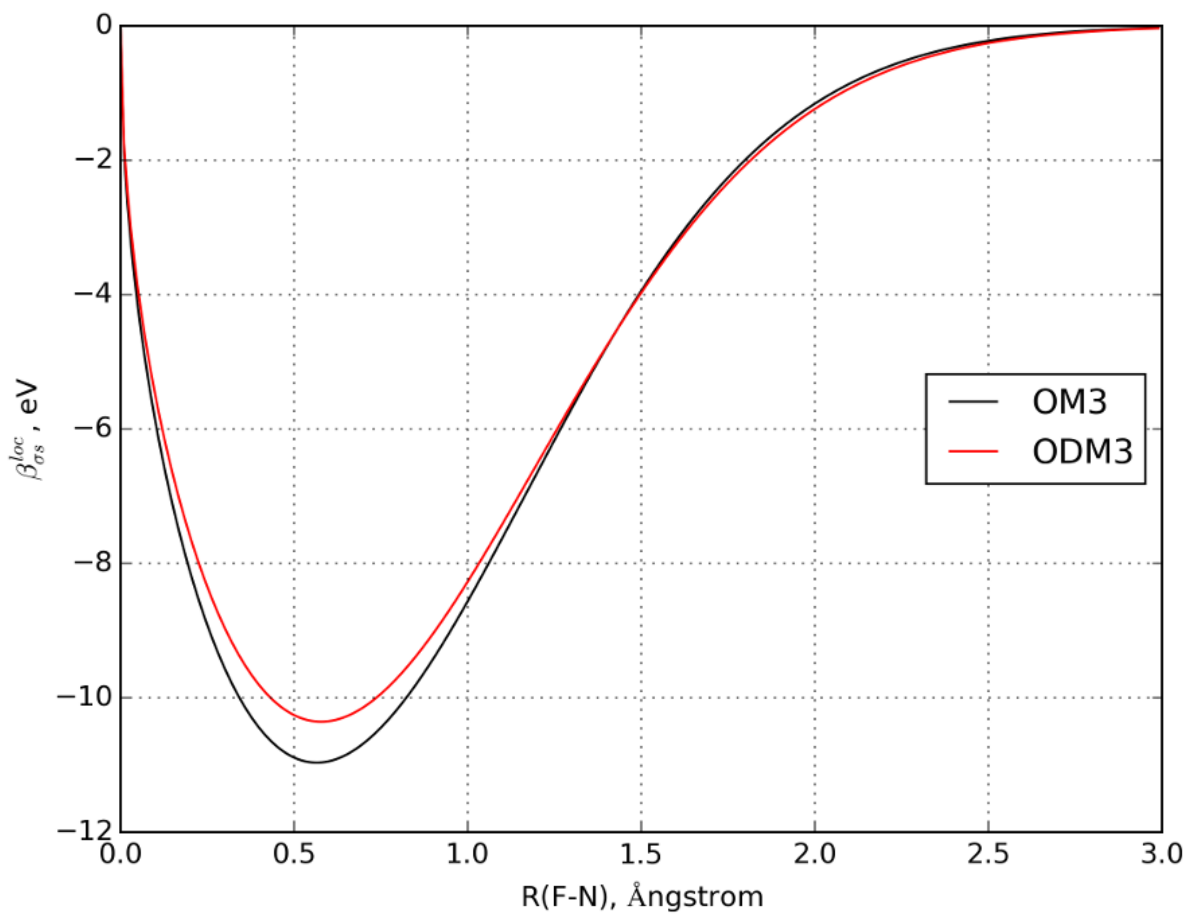

Figure S103: Comparison of σs local resonance integrals for the F−N pair calculated using standard OM3 and new ODM3 parameters.

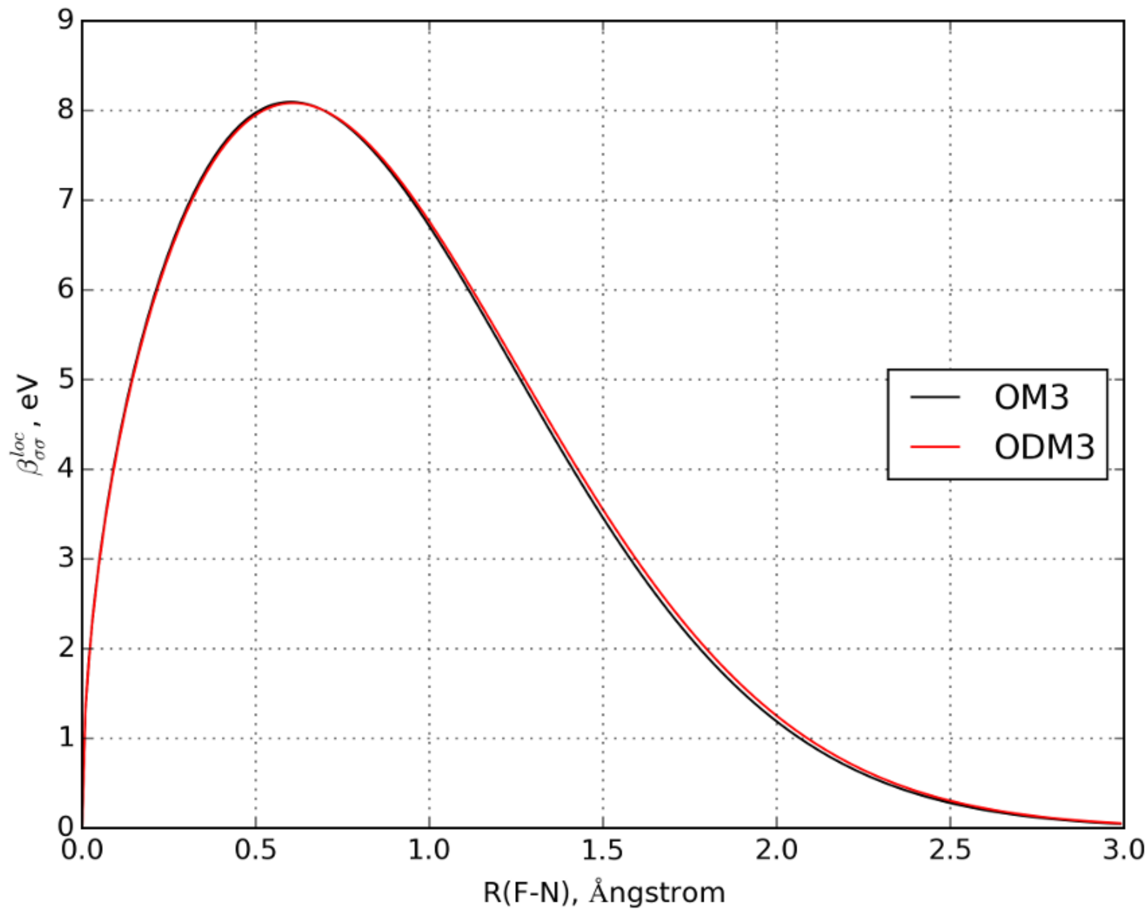

Figure S104: Comparison of $\sigma\sigma$ local resonance integrals for the F−N pair calculated using standard OM3 and new ODM3 parameters.

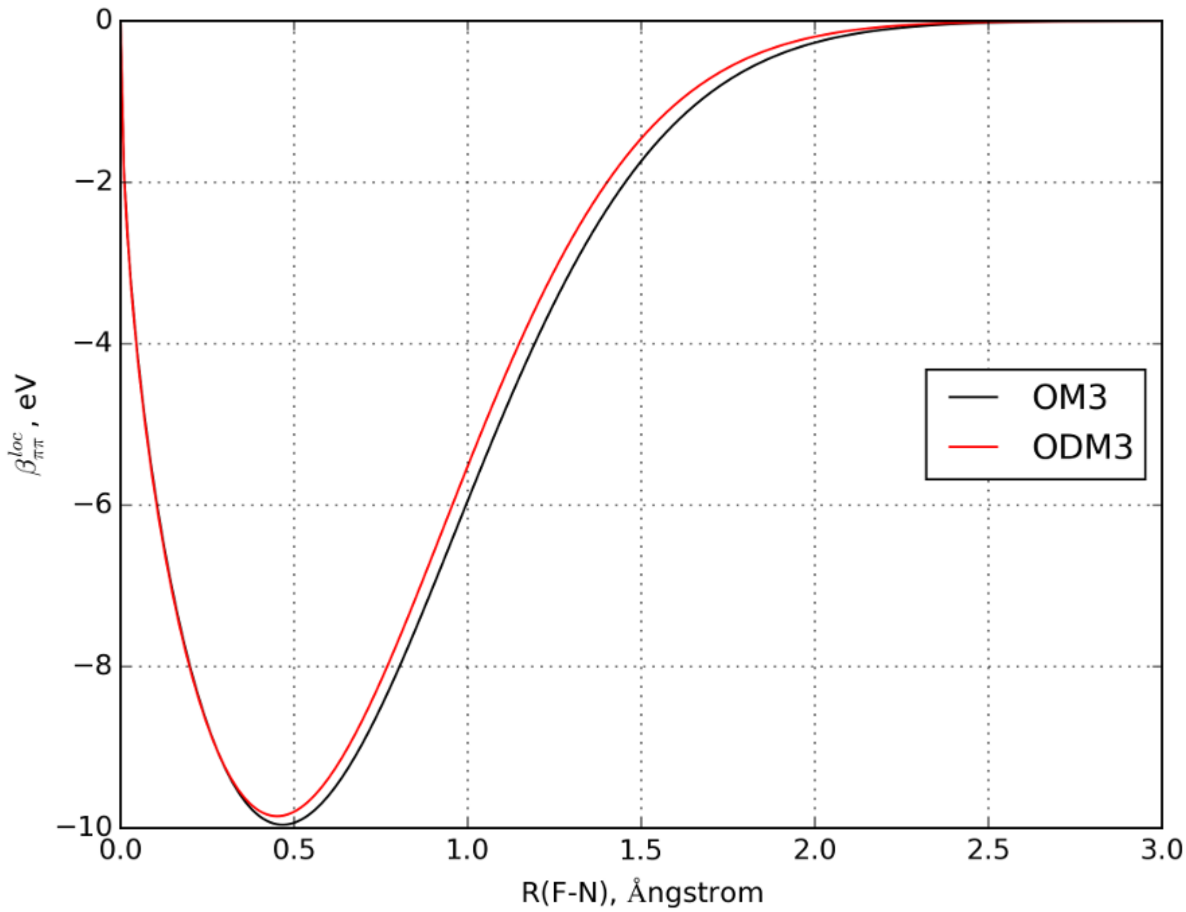

Figure S105: Comparison of $\pi\pi$ local resonance integrals for the F−N pair calculated using standard OM3 and new ODM3 parameters.

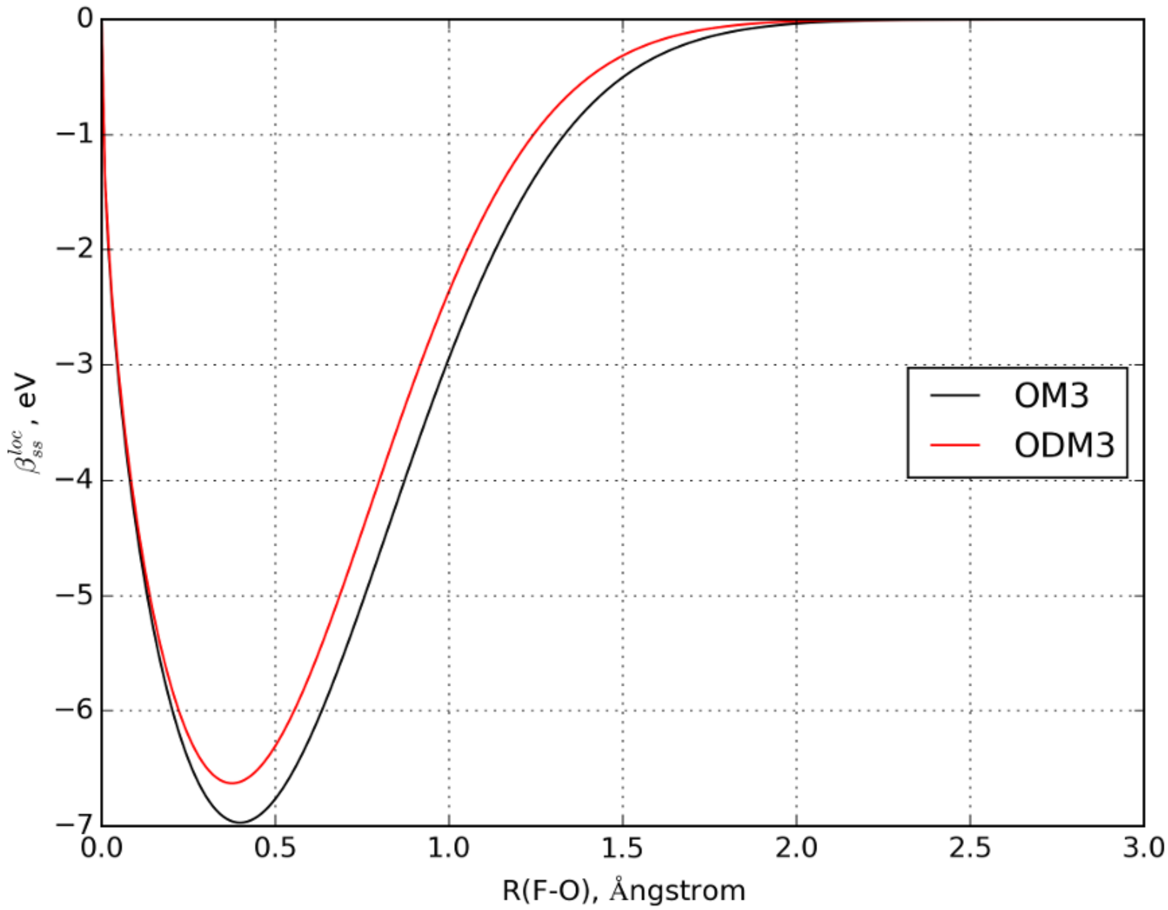

Figure S106: Comparison of *ss* local resonance integrals for the F−O pair calculated using standard OM3 and new ODM3 parameters.

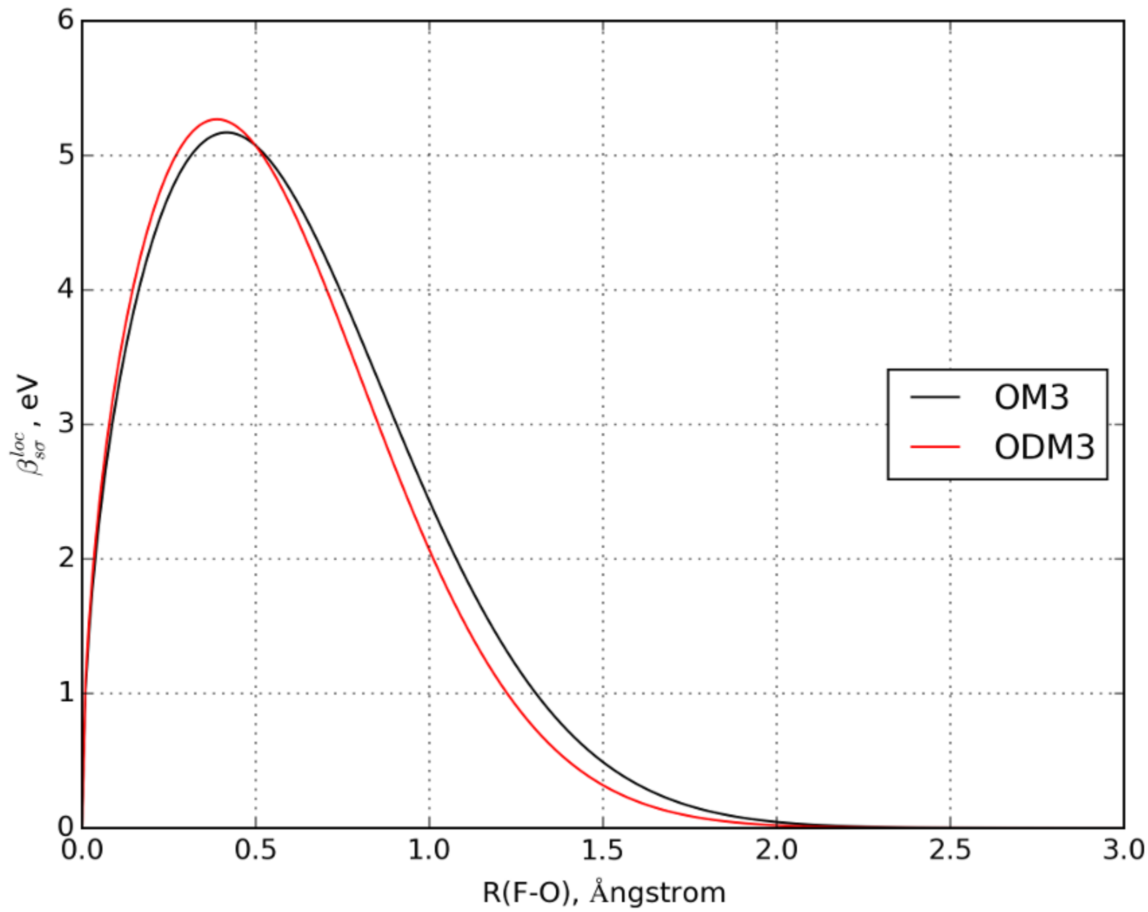

Figure S107: Comparison of $s\sigma$ local resonance integrals for the F−O pair calculated using standard OM3 and new ODM3 parameters.

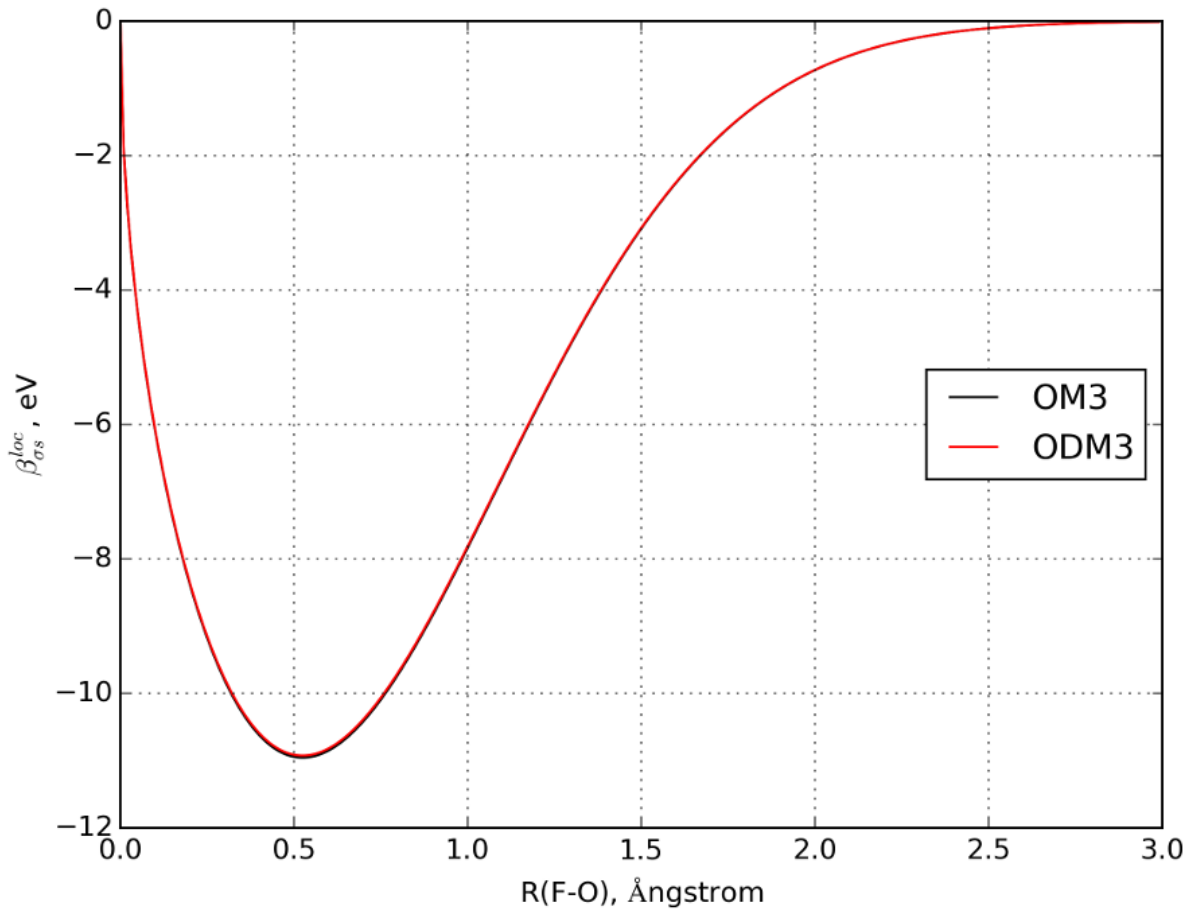

Figure S108: Comparison of σs local resonance integrals for the F−O pair calculated using standard OM3 and new ODM3 parameters.

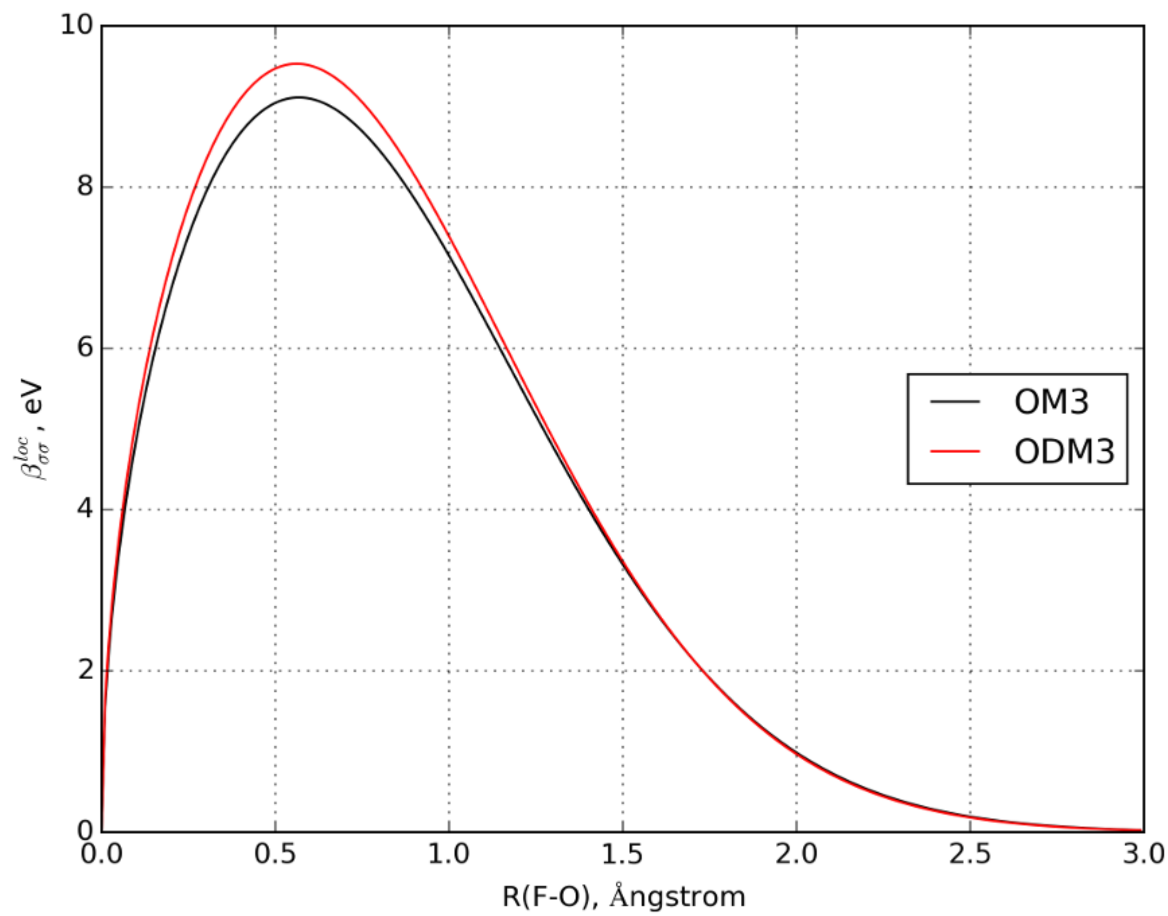

Figure S109: Comparison of $\sigma\sigma$ local resonance integrals for the F−O pair calculated using standard OM3 and new ODM3 parameters.

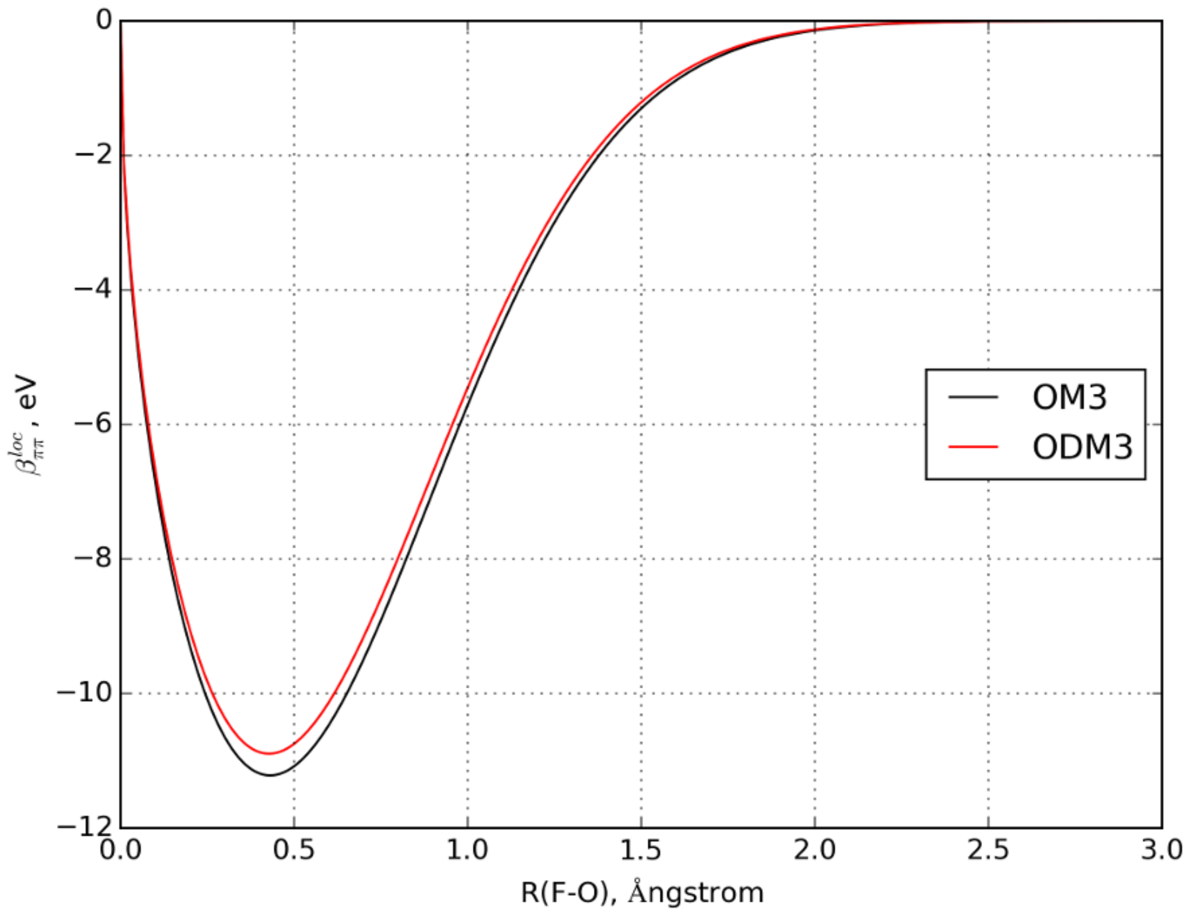

Figure S110: Comparison of $\pi\pi$ local resonance integrals for the F−O pair calculated using standard OM3 and new ODM3 parameters.

3 Tables with Additional Validation Results

Table S1: Mean Absolute Errors in Heats of Formation (kcal/mol), Bond Lengths (Å), Bond Angles (degree), Ionization Potentials (eV), and Dipole Moments (D) Calculated with the OMx, OMx-D3T, and ODMx Methods for the PDDG Set and Its Subsets

Subset	N	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Heats of Formation							
overall	622	3.55	7.72	3.14	3.68	10.73	3.12
CH	254	2.30	7.88	2.01	2.38	11.92	1.92
CHN	89	5.01	6.29	4.13	4.86	8.97	4.42
CHO	238	3.86	8.49	3.79	4.58	10.89	3.85
CHNO	41	6.24	5.29	4.32	3.96	6.22	3.50
Bond Lengths							
overall	153	0.014	0.014	0.014	0.018	0.017	0.014
CH	81	0.011	0.011	0.010	0.010	0.010	0.009
CHN	34	0.015	0.015	0.015	0.025	0.025	0.015
CHO	35	0.020	0.020	0.020	0.026	0.026	0.024
CHNO	3	0.027	0.027	0.026	0.044	0.044	0.039
C−H	38	0.010	0.010	0.010	0.013	0.013	0.011
C−C	52	0.010	0.010	0.010	0.010	0.010	0.010
C=C	15	0.009	0.009	0.008	0.009	0.009	0.008
C≡C	5	0.019	0.019	0.019	0.025	0.025	0.023
N−C	7	0.018	0.018	0.017	0.018	0.018	0.014
N−H	4	0.007	0.007	0.009	0.044	0.044	0.018
N≡C	5	0.017	0.017	0.018	0.046	0.046	0.022
O−H	6	0.037	0.037	0.035	0.058	0.057	0.057
O−C	7	0.018	0.018	0.017	0.022	0.022	0.021
O=C	9	0.015	0.015	0.021	0.019	0.018	0.015
Bond Angles							
overall	54	2.17	2.17	2.04	1.89	1.91	1.98
CH	20	1.37	1.40	1.36	0.91	1.00	1.00
CHN	12	1.30	1.28	1.23	1.33	1.31	1.54
CHO	21	3.08	3.07	2.82	2.76	2.75	2.86
∠CCH	16	1.02	1.03	1.05	0.96	1.01	1.13
∠CCC	13	1.78	1.82	1.74	1.19	1.26	1.25
∠OCH	3	3.03	3.04	3.33	3.02	3.03	3.09
∠COH	3	2.75	2.73	2.41	3.23	3.18	3.82
∠OCC	5	2.59	2.58	2.25	1.81	1.79	1.83
Ionization Potentials							
overall	98	0.31	0.31	0.27	0.51	0.52	0.49
CH	41	0.28	0.28	0.24	0.45	0.45	0.40
CHN	21	0.26	0.27	0.26	0.43	0.43	0.47
CHO	29	0.38	0.38	0.31	0.71	0.71	0.69
CHNO	4	0.29	0.29	0.31	0.28	0.29	0.25
Dipole Moments							
Overall	47	0.27	0.27	0.27	0.25	0.25	0.23
CH	10	0.11	0.11	0.10	0.11	0.11	0.11
CHN	14	0.25	0.25	0.21	0.30	0.30	0.32
CHO	20	0.34	0.34	0.39	0.27	0.27	0.24
CHNO	3	0.44	0.44	0.40	0.41	0.41	0.19

Table S2: Mean Absolute Errors in Heats of Formation (kcal/mol), Bond Lengths (Å), Bond Angles (degree), Ionization Potentials (eV), and Dipole Moments (D) Calculated with the OMx, OMx-D3T, and ODMx Methods for the PM7-CHNOF Set and Its Subsets

Subset	N	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Heats of Formation							
Overall	1168	4.85	11.07	4.71	4.83	15.07	4.28
DA	5	3.26	3.16	3.14	2.15	2.14	2.66
CH	310	4.16	14.25	4.15	3.63	20.12	3.50
CHN	214	5.43	9.23	5.03	5.69	14.15	5.20
CHO	373	4.22	11.48	4.46	5.18	14.42	4.16
CHF	32	3.50	6.11	4.70	2.44	6.16	2.27
CHNO	234	6.46	8.74	5.58	5.43	11.77	4.97
Bond Lengths							
Overall	175	0.015	0.015	0.015	0.019	0.019	0.017
DA	4	0.036	0.036	0.032	0.053	0.053	0.038
CH	74	0.011	0.011	0.010	0.011	0.011	0.010
CHN	31	0.014	0.014	0.014	0.020	0.020	0.013
CHO	31	0.016	0.016	0.017	0.021	0.021	0.019
CHF	18	0.016	0.016	0.015	0.020	0.020	0.017
CHNO	17	0.028	0.028	0.027	0.040	0.041	0.042
Bond Angles							
Overall	90	1.76	1.75	1.64	1.54	1.54	1.54
CH	32	0.90	0.92	0.83	0.49	0.53	0.47
CHN	20	1.44	1.43	1.32	1.35	1.32	1.45
CHO	20	2.33	2.33	1.99	1.98	1.98	1.93
CHF	11	1.47	1.47	1.37	1.11	1.11	1.05
CHNO	7	5.42	5.30	5.71	6.26	6.26	6.37
Ionization Potentials							
Overall	104	0.33	0.33	0.29	0.53	0.53	0.51
CH	36	0.25	0.25	0.21	0.47	0.47	0.42
CHN	18	0.28	0.28	0.31	0.42	0.43	0.46
CHO	29	0.44	0.44	0.36	0.77	0.78	0.74
CHF	14	0.34	0.34	0.33	0.29	0.29	0.33
CHNO	5	0.47	0.47	0.43	0.55	0.55	0.47
Dipole Moments							
Overall	58	0.24	0.24	0.27	0.22	0.22	0.21
CH	10	0.12	0.12	0.12	0.12	0.12	0.12
CHN	17	0.25	0.25	0.28	0.30	0.30	0.30
CHO	20	0.28	0.28	0.34	0.23	0.23	0.21
CHF	10	0.25	0.25	0.25	0.16	0.16	0.17

Table S3: Mean Absolute Errors in Atomization Enthalpies at 298 K (kcal/mol) Calculated with the OMx, OMx-D3T, and ODMx Methods for the C7H10O2 Set

Subset	N	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
overall	6095	6.30	6.30	6.22	7.67	7.68	7.50

Table S4: Mean Absolute Errors in Interaction Energies (kcal/mol) for the X40×10-CHNOF Set and Its Subsets at the Reference Geometries as Calculated with the OMx, OMx-D3T, and ODMx Methods

Subset	N	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Overall	100	1.62	1.38	1.37	1.89[a,b]	1.62[a,b]	1.87[a,b]
London Dispersion	10	0.29	0.17	0.17	0.41[a,b]	0.16[a,b]	0.23[a,b]
Induction	20	0.44	0.16	0.13	0.57	0.12	0.16
Dipole-Dipole Interaction	10	0.61	0.44	0.38	0.70	0.34	0.38
Stacking	20	3.07	2.71	2.74	2.90	2.59	2.45
Hydrogen Bonds	40	2.07	1.86	1.85	2.67	2.52	3.14
Scaled by 0.80	10	2.67	3.99	3.97	2.70	4.33	4.70
Scaled by 0.85	10	1.26	2.25	2.45	2.09	3.06	3.41
Scaled by 0.90	10	1.65	1.44	1.58	2.36	2.16	2.48
Scaled by 0.95	10	2.06	1.12	1.17	2.52	1.54	1.93
Near Equilibrium	10	2.16	1.09	0.96	2.47	1.26	1.58
Scaled by 1.05	10	2.10	1.17	1.04	2.29	1.18	1.41
Scaled by 1.10	10	1.96	1.15	1.04	2.06	1.12	1.30
Scaled by 1.25	10	1.39	0.89	0.84	1.36	0.80	0.89
Scaled by 1.50	10	0.72	0.50	0.49	0.64[a]	0.41[a]	0.50[a]
Scaled by 2.00	10	0.23	0.18	0.18	0.21[b]	0.16[b]	0.18[b]

[a] Dimer methane–F_2 scaled by 1.50 could not be converged at ODM3. [b] Dimer methane–F_2 scaled by 2.00 could not be converged at OM3, OM3-D3T, and ODM3.

Table S5: Mean Absolute Errors in Bond Lengths (Å) and Bond Angles (degree) Calculated with the OMx/MRCI, OMx-D3T/MRCI, and ODMx/MRCI Methods for the ExGeom Set and Its Subsets Relative to the CC2 Level of Theory

Subset	N	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Bond Lengths							
overall	543	0.018	0.018	0.018	0.021	0.021	0.018
singlet	377	0.018	0.018	0.018	0.022	0.022	0.019
triplet	166	0.018	0.018	0.016	0.019	0.019	0.017
C−C bonds	298	0.013	0.013	0.013	0.015	0.015	0.014
C−H bonds	75	0.011	0.011	0.010	0.017	0.017	0.015
C−O bonds	62	0.045	0.045	0.037	0.041	0.041	0.039
C−N bonds	68	0.023	0.023	0.023	0.032	0.032	0.026
N−H bonds	33	0.009	0.009	0.020	0.026	0.025	0.006
Bond Angles							
overall	287	1.99	2.00	1.92	2.00	2.01	2.04
singlet	187	1.99	2.01	1.96	2.05	2.07	2.15
triplet	100	1.98	1.98	1.85	1.90	1.91	1.83

4 Tables with Reference and Calculated Property Values for Individual Molecules in Benchmark Sets

Table S6: Benchmark Results for the CHNO Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Hydrogen	0.0[a]	−3.4	−3.5	−0.1	−0.0	−0.1	0.0
Methane	−17.9[b]	−19.3	−19.9	−19.3	−18.0	−19.1	−17.8
Ethane	−20.0[b]	−21.2	−23.0	−20.8	−20.8	−23.6	−20.0
Ethylene	12.5[b]	12.9	11.7	12.9	13.9	12.0	13.7
Acetylene	54.5[b]	54.2	53.6	53.9	54.7	53.7	54.2
Propane	−25.0[b]	−25.5	−28.7	−25.2	−25.4	−30.4	−24.8
Propene ecl	4.8[b]	4.7	2.3	4.8	5.0	1.1	5.0
Propyne	44.2[b]	44.5	42.9	44.3	44.1	41.5	44.3
Allene	45.5[b]	45.9	44.3	45.7	45.5	42.9	45.7
n-Butane	−30.0[b]	−30.1	−34.8	−29.9	−30.3	−37.5	−29.8
Isobutane	−32.1[b]	−31.8	−36.7	−31.9	−31.3	−38.8	−31.1
But-1-ene H-ecl	0.0[b]	0.1	−3.8	0.1	0.3	−5.7	0.3
trans-2-Butene	−2.7[b]	−3.8	−7.5	−3.7	−4.0	−9.8	−3.9
cis-2-Butene	−1.7[b]	−1.9	−5.8	−2.0	−2.2	−8.2	−2.3
Isobutene	−4.0[b]	−4.3	−8.2	−4.0	−3.9	−10.0	−3.6
1,2-Butadiene	38.8[b]	38.1	35.2	38.1	37.6	33.0	38.0
1,3-s-tr-Butadiene	26.3[b]	29.4	26.3	29.3	30.3	25.5	29.8
1-Butyne	39.5[b]	39.5	36.5	39.3	39.2	34.6	39.5
2-Butyne	34.8[b]	35.1	32.4	34.5	33.8	29.6	34.1
Vinylacetylene	73.0[c]	71.2	69.0	70.7	71.2	67.6	70.9
Butatriene	83.0[c]	81.9	79.8	81.1	80.7	77.3	80.8
n-Pentane	−35.1[b]	−34.7	−40.8	−34.7	−35.2	−44.6	−34.9
Neopentane	−40.2[b]	−39.6	−46.4	−40.2	−37.6	−48.1	−38.2
n-Hexane	−39.9[b]	−39.2	−46.9	−39.4	−40.0	−51.6	−39.9
tr-1,3-Pentadiene	18.2[b]	20.5	16.1	20.4	20.9	14.0	20.4
cis-1,3-Pentadiene	19.5[b]	22.4	17.8	22.1	22.8	15.6	22.1
1,4-Pentadiene	25.2[b]	26.9	22.4	25.1	26.8	19.7	24.5
Cyclopropane	12.7[b]	9.9	7.6	10.7	10.1	6.3	11.9
cis-Dimethylcyclopropane	1.3[d]	0.6	−5.0	1.1	0.1	−8.4	1.1
Cyclopropene	66.2[b]	67.4	65.7	66.9	65.5	62.8	65.6
1-Methylcyclopropene	58.2[b]	59.6	56.7	59.7	57.1	52.6	57.7
1,2-Dimethylcyclopropene	46.4[d]	51.8	47.7	52.5	48.9	42.5	49.9
Methylenecyclopropane	47.9[b]	45.0	42.0	45.4	43.7	39.1	44.7
Cyclobutane	6.8[b]	3.0	−1.0	2.4	2.9	−3.3	3.3
Cyclobutene plan	37.5[b]	41.3	38.2	40.2	40.8	35.8	40.0
1,2-Dimethylcyclobutene	19.8[d]	21.4	15.3	21.3	20.9	11.7	21.2
Methylenecyclobutane	29.0[b]	25.4	20.8	24.9	25.6	18.3	25.5
Cyclopentane envelope	−18.3[b]	−19.7	−25.5	−19.9	−20.8	−29.8	−20.3
Cyclopentene	8.1[b]	6.8	1.9	7.0	5.7	−2.0	6.0
Cyclopentadiene	32.1[b]	33.3	29.3	33.5	32.6	26.2	32.2
Cyclohexane chair (AMP)	−29.5[b]	−27.1	−35.0	−27.2	−28.5	−40.5	−28.5
Cyclohexene half-chair	−1.2[b]	0.4	−6.4	0.6	−1.1	−11.6	−0.9
1,3-Cyclohexadiene	25.4[b]	25.9	20.0	26.5	24.8	15.6	24.9
Benzene	19.7[b]	18.8	13.8	19.7	18.5	10.6	18.9
Toluene ecl	12.0[b]	9.5	2.9	9.7	9.6	−0.6	9.9
Ethylbenzene stag	7.1[b]	4.8	−3.5	5.4	5.0	−7.7	5.1
Styrene	35.3[b]	34.7	27.3	35.4	35.6	24.1	35.4
Cycloheptatriene	43.2[b]	46.7	39.8	46.7	46.1	35.4	45.8
Bicyclobutane	51.9[b]	62.0	59.0	61.7	59.9	55.2	61.4
Spirocyclopentane	44.3[b]	42.8	38.4	43.6	41.0	34.3	42.7
trans-Bicyclopropyl	30.9[b]	30.7	24.7	30.9	30.2	21.0	31.9
Bicyclo[2.1.0]pentane	37.8[c]	40.1	35.4	39.5	39.0	31.6	39.3
Norbornane	−13.1[b]	−12.5	−21.5	−13.3	−12.4	−26.3	−13.2
Norbornadiene	58.8[b]	51.8	44.8	51.4	52.0	41.1	50.6
Bicyclo[2.2.2]octane	−23.7[b]	−22.2	−33.6	−22.8	−23.4	−40.5	−23.9

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Table S6: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Naphthalene	35.9[b]	34.8	25.3	35.8	35.7	21.0	35.7
Adamantane	−32.2[b]	−30.4	−45.6	−31.5	−30.2	−53.1	−32.0
Cubane	148.7[b]	144.6	137.2	141.2	146.4	134.8	144.1
Nitrogen	0.0[a]	2.8	2.6	1.5	2.6	2.2	4.6
Ammonia	−11.0[b]	−5.9	−6.3	−12.0	−11.2	−12.0	−11.3
Methylamine	−5.5[b]	−4.1	−5.6	−6.3	−5.8	−8.1	−5.6
Dimethylamine	−4.4[b]	−5.1	−7.9	−4.2	−2.2	−6.5	−3.2
Trimethylamine	−5.7[b]	−8.0	−12.4	−4.5	−0.1	−6.7	−2.9
Ethylamine	−11.3[b]	−8.9	−11.7	−10.9	−12.1	−16.5	−11.9
n-Propylamine	−16.8[b]	−13.5	−17.8	−15.6	−16.9	−23.5	−16.8
Isopropylamine	−20.0[b]	−14.5	−18.9	−19.4	−17.4	−24.2	−18.3
tert-Butylamine	−28.9[b]	−22.3	−28.7	−27.4	−24.6	−34.3	−25.6
Aziridine	30.2[b]	36.3	34.3	36.0	35.4	32.3	38.0
Pyrrole	25.9[b]	33.7	30.2	35.6	32.0	26.3	33.9
Pyridine	33.6[b]	30.8	26.3	33.5	29.4	22.3	31.8
Pyridazine (1,2)	66.5[b]	48.4	44.3	55.3	51.1	44.6	56.0
Pyrimidine (1,3)	46.8[b]	44.5	40.4	48.0	41.9	35.4	43.8
Pyrazine (1,4)	46.9[b]	44.9	40.9	50.0	42.0	35.5	47.8
Aniline	20.8[b]	25.2	19.0	22.0	22.3	12.7	22.0
Hydrogen cyanide	32.3[e]	26.1	25.7	25.5	25.3	24.7	25.4
Acetonitrile	18.0[c]	17.5	16.2	17.3	15.3	13.2	15.3
Methylisocyanide	39.1[b]	38.3	36.9	37.6	26.7	24.4	21.8
Propionitrile	12.3[b]	12.3	9.6	12.1	10.2	6.0	10.5
Acrylonitrile	43.2[b]	45.6	43.6	45.3	43.7	40.5	43.6
Fumaronitrile	81.0[b]	79.7	76.9	79.7	75.2	70.8	75.8
Maleonitrile	81.3[b]	81.2	78.2	81.4	76.2	71.6	77.0
Dicyanoacetylene	126.5[b]	138.0	136.1	137.6	128.3	125.3	130.0
Cyanogen	73.3[b]	74.8	73.9	76.2	68.2	66.7	70.5
Benzonitrile	51.6[b]	49.7	43.7	50.1	48.0	38.6	48.3
Hydrazine	22.8[e]	18.5	17.4	17.6	16.5	14.7	17.2
Methylhydrazine	22.6[b]	18.2	15.8	18.7	20.1	16.5	20.1
1,1-Dimethylhydrazine	20.1[b]	14.8	10.8	17.8	21.4	15.4	19.6
1,2-Dimethylhydrazine	22.0[b]	17.1	13.2	20.6	22.8	16.9	22.0
trans-Azodiisopropane	8.6[b]	4.5	−4.5	0.6	5.8	−7.7	6.5
Hydrogen azide	70.3[c]	72.6	71.8	72.8	69.2	67.9	69.6
Oxygen Triplet	0.0[a]	2.0	1.9	3.9	−2.6	−2.8	0.4
Ozone	34.0[c]	37.9	37.5	39.7	48.7	48.1	52.8
Water	−57.8[b]	−56.5	−56.7	−58.9	−58.5	−58.8	−58.0
Methanol	−48.2[b]	−49.3	−50.3	−50.1	−49.8	−51.4	−49.7
Ethanol	−56.2[b]	−56.9	−59.1	−56.7	−57.2	−60.8	−56.6
Propanol	−61.0[b]	−61.9	−65.6	−61.9	−62.2	−67.9	−61.6
Isopropanol	−65.2[b]	−66.7	−70.5	−68.7	−67.2	−73.1	−67.5
tert-Butanol	−74.7[b]	−76.8	−82.4	−78.1	−75.9	−84.5	−76.1
Dimethylether	−44.0[b]	−45.6	−47.7	−45.9	−42.8	−46.2	−44.3
Diethylether	−60.3[b]	−61.1	−65.9	−60.2	−58.4	−65.7	−59.4
Oxirane	−12.6[b]	−13.3	−14.8	−10.1	−8.8	−11.2	−5.1
Furan	−8.3[b]	−2.9	−5.9	−3.4	−2.7	−7.4	−2.2
Phenol	−23.0[b]	−21.7	−27.2	−22.4	−23.6	−32.3	−23.2
Anisole plan	−16.2[b]	−16.0	−23.0	−16.3	−14.1	−25.0	−15.4
Hydrogen peroxide	−32.5[e]	−35.3	−35.8	−34.8	−36.9	−37.6	−36.1
Dimethylperoxide	−30.0[b]	−33.6	−36.0	−33.0	−29.0	−32.7	−30.4
Diethylperoxide	−46.1[b]	−52.6	−57.8	−49.5	−46.0	−53.8	−46.1
Carbon monoxide	−26.4[b]	−20.3	−20.5	−19.3	−21.5	−21.8	−17.5
Carbon dioxide	−94.1[b]	−80.5	−80.9	−81.8	−87.7	−88.4	−89.4
Carbon suboxide	−22.0[c]	−3.2	−4.4	−6.5	−16.9	−18.9	−16.2
Formaldehyde	−26.0[b]	−30.3	−30.9	−30.0	−31.9	−32.8	−32.3
Acetaldehyde free	−39.7[b]	−44.2	−45.8	−44.1	−46.5	−49.1	−46.7
Propionaldehyde ecl	−44.4[b]	−48.2	−51.3	−48.7	−50.5	−55.3	−50.5
Acetone ecl	−51.9[b]	−57.4	−60.4	−57.8	−59.3	−63.9	−59.3
Ketene	−11.4[b]	−5.1	−6.1	−6.5	−11.0	−12.6	−10.9
Acrolein free	−18.0[c]	−18.1	−20.3	−18.1	−19.1	−22.7	−19.8
Glyoxal	−50.7[b]	−59.1	−60.6	−58.5	−62.6	−65.0	−63.1
Biacetyl	−78.2[b]	−89.2	−93.4	−88.5	−91.6	−98.2	−90.5

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Table S6: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Acetylacetone	−91.0[b]	−99.2	−105.2	−99.8	−101.8	−111.0	−101.6
p-Quinone	−29.4[b]	−32.5	−37.9	−31.6	−32.9	−41.3	−32.0
Benzaldehyde	−8.8[b]	−14.5	−20.9	−13.6	−15.6	−25.6	−15.7
Formic acid (Z)	−90.5[b]	−86.9	−87.8	−88.0	−88.2	−89.7	−89.6
Acetic acid stag (Z)	−103.4[b]	−101.0	−103.0	−102.2	−102.7	−106.0	−103.8
Propionic acid C-ecl	−108.4[b]	−106.3	−109.8	−107.6	−107.5	−112.9	−108.4
Oxalic acid 4-ring	−173.0[b]	−165.0	−167.3	−166.7	−166.4	−170.2	−168.1
Benzoic acid	−70.3[b]	−71.1	−78.0	−71.2	−71.0	−81.8	−71.3
Methyl formiate (Z)	−85.0[b]	−81.4	−83.5	−82.1	−79.4	−82.6	−82.1
Methyl acetate ecl (Z)	−98.5[b]	−95.6	−98.8	−96.7	−93.8	−99.0	−96.7
Acetic anhydride ecl	−136.8[b]	−139.5	−143.9	−139.7	−138.8	−145.7	−142.3
Maleic anhydride	−95.2[b]	−87.1	−90.4	−87.4	−87.2	−92.5	−90.4
Formamide	−44.0[c]	−39.8	−41.1	−43.2	−46.3	−48.4	−48.5
Dimethylformamide	−45.8[b]	−43.5	−47.6	−39.4	−41.4	−47.7	−45.5
Nitrous oxide	19.6[e]	21.2	20.8	19.5	20.7	19.9	20.9
Dinitrotetroxide free	2.2[b]	13.2	11.5	8.7	9.5	6.7	4.6
Nitrous acid trans	−18.3[e]	−19.7	−20.3	−19.9	−26.8	−27.8	−25.8
Nitric acid	−32.1[e]	−33.6	−34.6	−35.9	−33.4	−35.1	−33.4
Methylnitrite	−15.9[b]	−16.8	−18.4	−17.4	−20.0	−22.6	−20.3
Nitromethane	−17.8[b]	−17.3	−19.1	−17.0	−15.7	−18.5	−13.5

a G.Pilcher and H.A.Skinner, in "The Chemistry of the Metal-Carbon Bond", edited by F.R.Hartley and S.Patai, Wiley, New York, 1982, pp. 43-90. b J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986. c S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988). d R.B. Turner, P. Goebel, B.J. Mallon, W. von E. Doering, J.F. Coburn Jr., and M. Pomerantz, J.Am.Chem.Soc. 90, 4315 (1968). See c in Table II, DT paper. e M.W.Chase, C.A.Davies, J.R.Downey, D.R.Frurip, R.A.McDonald, and A.N.Syverud, "JANAF Thermochemical Tables", 3rd edition, J.Phys.Chem.Ref.Data 14, Suppl.1 (1985).

Table S7: Benchmark Results for the CHNO Set. Ionization Potentials (eV)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Hydrogen	15.98[a]	15.68	15.68	15.64	15.65	15.65	15.67
Methane	14.00[a]	13.64	13.64	13.66	14.17	14.17	14.30
Ethane	12.10[b]	11.92	11.92	11.93	12.30	12.30	12.43
Ethylene	10.51[a]	10.74	10.74	10.53	11.05	11.05	10.87
Acetylene	11.40[a]	11.55	11.55	11.35	11.79	11.79	11.64
Propane	11.50[a]	11.39	11.39	11.36	11.69	11.69	11.82
Propene ecl	9.88[b]	9.99	9.99	9.81	10.28	10.29	10.16
Propyne	10.37[a]	10.64	10.64	10.47	10.88	10.88	10.78
Allene	10.07[c]	10.16	10.16	9.97	10.44	10.45	10.31
Isobutane	11.40[a]	11.06	11.07	10.96	11.41	11.41	11.53
1,3-s-tr-Butadiene	9.08[a]	9.32	9.32	9.10	9.61	9.61	9.43
Diacetylene	10.17[a]	10.30	10.30	10.06	10.47	10.47	10.29
Butatriene	9.15[d]	9.35	9.35	9.11	9.60	9.60	9.39
Neopentane	11.30[a]	10.82	10.82	10.70	11.31	11.31	11.31
Cyclopropane	11.00[b]	10.88	10.88	10.71	11.47	11.47	11.38
Cyclopropene	9.86[a]	9.84	9.84	9.70	10.13	10.13	10.06
Cyclobutane	11.00[c]	10.38	10.38	10.24	10.98	10.98	10.97
Cyclobutene plan	9.43[a]	9.65	9.64	9.49	9.93	9.93	9.82
Cyclopentene	9.18[a]	9.22	9.22	9.09	9.51	9.51	9.44
Cyclopentadiene	8.57[a]	8.82	8.82	8.63	9.10	9.10	8.97
Benzene	9.24[a]	9.59	9.59	9.41	9.91	9.91	9.76
Toluene ecl	8.82[b]	9.17	9.17	9.00	9.46	9.46	9.35
Naphthalene	8.15[a]	8.51	8.51	8.31	8.79	8.79	8.63
Nitrogen	15.60[b]	15.46	15.46	15.55	14.51	14.51	14.73
Ammonia	10.85[b]	10.67	10.67	10.84	11.23	11.23	11.30
Methylamine	9.45[c]	9.75	9.75	9.91	10.00	10.01	10.13
Dimethylamine	8.93[c]	9.23	9.23	9.41	9.24	9.25	9.38
Trimethylamine	8.54[c]	8.84	8.85	9.07	8.67	8.69	8.87
Aziridine	9.80[b]	10.13	10.13	10.19	10.39	10.39	10.41
Pyrrole	8.21[d]	8.46	8.47	8.27	8.65	8.65	8.49
Pyridine	9.67[e]	9.96	9.96	9.78	10.13	10.13	10.08
Hydrogen cyanide	13.60[b]	13.91	13.91	13.89	13.94	13.94	13.86
Acetonitrile	12.21[d]	12.50	12.50	12.52	12.63	12.63	12.67
Acrylonitrile	10.91[d]	10.88	10.88	10.80	11.09	11.09	11.06
Cyanoacetylene	11.60[c]	11.58	11.58	11.49	11.67	11.67	11.65
Cyanogen	13.36[d]	13.27	13.27	13.36	13.22	13.22	13.33
Ozone	12.75[c]	12.85	12.85	12.80	13.27	13.27	13.10
Water	12.62[b]	12.91	12.91	12.88	13.12	13.12	13.05
Methanol	10.96[a]	11.22	11.22	11.17	11.60	11.60	11.66
Dimethylether	10.04[a]	10.51	10.51	10.43	10.94	10.94	11.03
Oxirane	10.57[a]	11.31	11.31	11.21	11.79	11.79	11.84
Furan	8.88[a]	9.03	9.03	8.83	9.45	9.45	9.30
Carbon monoxide	14.01[a]	13.60	13.60	13.36	13.68	13.68	13.42
Carbon dioxide	13.78[a]	13.27	13.27	13.21	13.57	13.57	13.47
Formaldehyde	10.88[b]	11.03	11.03	10.91	11.26	11.26	11.25
Acetaldehyde free	10.21[a]	10.62	10.62	10.51	10.94	10.94	10.91
Acetone ecl	9.72[a]	10.31	10.31	10.19	10.67	10.67	10.58
Ketene	9.64[a]	9.75	9.75	9.59	9.97	9.97	9.82
Acrolein free	10.11[b]	10.59	10.59	10.47	10.87	10.87	10.83
trans-Glyoxal	10.59[a]	10.57	10.57	10.50	10.77	10.77	10.74
Formic acid (Z)	11.51[a]	11.72	11.72	11.65	12.12	12.12	12.09
Methyl formiate (Z)	11.02[a]	11.24	11.24	11.18	11.70	11.70	11.72

a J.W.Robinson (ed.), "Handbook of Spectroscopy", Vol.1, CRC Press, Baton Rouge, 1980. b D.W.Turner, C.Baker, A.D.Baker, and C.R.Brundle, "Molecular Photoelectron Spectroscopy", Wiley-Interscience, London, 1970. c Taken from the experimental data quoted in: M.J.S. Dewar, W.Thiel, J.Am.Chem.Soc. 99, 4907 (1977). d S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988). e From experimental data of dubious accuracy quoted in: J.J.P.Stewart, J.Comput.Chem. 10, 221 (1991). Original source: G.Dittmer and U.Niemann, Philips J.Res. 37, 1 (1982).

Table S8: Benchmark Results for the CHNO Set. Enthalpy Changes at 298 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Isobutane	−2.1[a]	−1.7	−1.9	−1.9	−1.0	−1.3	−1.3
trans-2-Butene	−2.7[a]	−3.9	−3.7	−3.8	−4.3	−4.1	−4.2
cis-2-Butene	−1.7[a]	−2.0	−2.0	−2.1	−2.5	−2.6	−2.6
cis-2-Butene	1.0[a]	1.8	1.7	1.7	1.8	1.5	1.6
Isobutene	−4.0[a]	−4.4	−4.5	−4.1	−4.2	−4.4	−3.9
2-Butyne	−4.7[a]	−4.4	−4.1	−4.8	−5.4	−4.9	−5.5
2-Methylbutane	−1.6[a]	−1.2	−1.6	−1.4	−0.3	−0.9	−0.7
Neopentane	−5.1[a]	−4.9	−5.6	−5.5	−2.5	−3.5	−3.4
cis-1,3-Pentadiene	1.3[a]	1.9	1.7	1.7	1.9	1.6	1.7
Isopropylamine	−3.2[a]	−1.0	−1.1	−3.8	−0.6	−0.7	−1.5
Methylisocyanide	21.1[a]	20.8	20.7	20.2	11.4	11.2	6.4
cis-Diimine	5.2[b]	−4.6	−4.6	−4.0	0.7	0.6	−2.7
Oxygen Singlet	22.5[c]	18.3	18.3	18.3	19.0	19.0	19.0
Isopropanol	−4.2[a]	−4.7	−4.9	−6.8	−5.0	−5.3	−5.9
Acetylacetone Enol	−4.0	5.2	5.5	3.6	4.6	5.0	4.9
Acetylacetone (TS)	6.9	5.8	6.1	3.1	4.6	5.0	4.9
Nitromethane	−1.9[a]	−0.6	−0.7	0.4	4.3	4.1	6.8

a J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986. b J.M.L.Martin and P.R.Taylor, Mol.Phys. 96, 681 (1999). c M.W.Chase, C.A.Davies, J.R.Downey, D.R.Frurip, R.A.McDonald, and A.N.Syverud, "JANAF Thermochemical Tables", 3rd edition, J.Phys.Chem.Ref.Data 14, Suppl.1 (1985).

Table S9: Benchmark Results for the CHNO Set. Activation Enthalpies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Ethane ecl	2.9[a]	2.8	2.8	2.3	2.4	2.5	2.0
Ethylene ort	65.0[b]	57.4	57.4	55.4	55.9	56.0	52.3
Propene stag	2.0[b]	0.8	0.8	0.1	0.7	0.7	0.0
n-Butane cis-Barrier	6.0[c]	5.1	4.9	5.0	5.0	4.7	5.0
But-1-ene C-ecl	0.4[c]	1.4	1.2	1.6	1.2	1.0	1.6
1,3-s-cis-Butadiene	3.8[b]	1.1	1.0	0.8	1.0	0.8	0.6
1,3-gauche-Butadiene	2.9[b]	0.9	0.8	1.1	0.8	0.6	1.0
1,3-Butadiene ort	6.0[b]	2.1	2.0	1.4	1.7	1.7	1.0
Cyclobutane plan	1.4[a]	0.0	0.0	0.0	0.0	0.0	0.0
Methylenecyclobutane plan	0.4[d]	0.0	0.0	0.0	0.0	0.0	−0.0
Cyclopentane planar	4.8[c]	2.6	2.7	2.8	1.9	2.0	2.3
Cyclopentene plan	0.7[e]	0.0	0.1	−0.4	0.0	0.0	−0.5
Cyclohexane twist (AMP)	4.8[c]	5.2	5.2	5.7	5.0	5.0	5.7
Cyclohexene plan	13.4[f]	11.9	12.1	12.0	9.8	10.2	10.4
Cyclohexadiene plan	3.2[g]	2.0	2.1	1.9	1.3	1.4	1.3
Toluene stag	0.1[c]	−0.0	−0.0	0.6	0.0	0.0	−0.6
Styrene plan	0.0[b]	0.2	0.2	−0.3	0.1	0.1	−0.4
Styrene ort	3.1[b]	0.8	0.9	0.7	0.7	0.9	0.6
Ammonia planar	5.8[h]	3.5	3.5	1.9	6.7	6.7	6.4
Methylamine ecl (TS rot)	2.0[i]	2.2	2.2	1.4	2.3	2.3	1.4
Methylamine planar (TS inv)	4.8[h]	3.6	3.6	2.3	4.2	4.2	3.3
Dimethylamine planar	4.4[h]	3.5	3.5	2.7	2.8	2.8	1.8
Trimethylamine planar (C3h inv)	6.0[h]	4.2	4.3	2.9	2.6	2.7	1.0
Trimethylamine (C3 inv)	6.0[h]	4.1	4.3	2.9	0.0	2.7	1.0
Aziridine planar (inv)	11.6[h]	13.4	13.4	11.8	11.5	11.5	9.0
Aniline planar	1.5[b]	0.5	0.6	−0.4	0.6	0.7	−0.1
Hydrazine trans	2.5[j]	8.0	8.0	5.8	1.8	1.8	−0.6
Hydrazine cis	8.3[j]	10.8	10.8	8.5	8.7	8.7	4.6
Methanol ecl	1.1[i]	1.8	1.8	1.2	1.6	1.6	0.9
Phenol plan	0.0[k]	0.0	0.0	−0.0	0.0	0.0	0.0
Phenol ort	3.5[b]	1.4	1.4	0.6	2.0	2.0	1.1
Anisole ort	3.0[l]	0.1	0.1	−0.1	0.5	0.5	0.2
Hydrogen peroxide cis	7.0[i]	8.5	8.5	8.4	10.5	10.5	10.1
Hydrogen peroxide trans	1.1[i]	2.5	2.5	0.4	1.1	1.1	0.2
Diethylperoxide	0.0[i]	3.2	3.4	2.6	1.4	1.6	1.0
Acetaldehyde ecl	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Acetaldehyde stag	1.1[c]	0.2	0.2	−0.3	0.3	0.3	−0.3
Propionaldehyde stag	1.5[c]	−0.8	−0.8	−0.8	−0.7	−0.6	−1.5
Acrolein s-trans	0.0	0.0	0.0	0.0	0.0	0.0	−0.0
Acrolein s-cis	1.7[b]	0.0	−0.0	0.1	−0.2	−0.2	0.1
Acrolein ort (TS rot)	4.7[m]	2.6	2.6	2.1	2.0	2.0	1.5
trans-Glyoxal	0.0[k]	0.0	0.0	0.0	0.8	0.8	0.5
cis-Glyoxal	4.8[n]	3.8	3.8	3.5	2.9	2.9	2.8
Glyoxal ort (TS)	5.9[n]	3.8	3.8	3.5	2.9	2.9	2.8
Biacetyl	0.0[i]	0.5	0.5	−0.5	0.9	0.9	0.5
Benzaldehyde ort	4.6[b]	3.6	3.7	3.1	3.3	3.3	2.6
Formic acid (E)	3.9[o]	6.1	6.1	7.9	6.2	6.2	6.5
Formic acid ort (TS)	12.4[o]	10.5	10.5	10.9	11.3	11.3	10.2
Acetic acid stag (E)	5.8[p]	5.6	5.6	6.5	5.8	5.7	6.2
Acetic acid stag ort (TS)	12.6[o]	10.1	10.1	9.4	10.9	10.8	9.6
Benzoic acid plan	0.0[k]	0.0	0.0	0.0	0.0	0.0	0.0
Benzoic acid ort	5.0[q]	4.0	4.1	3.4	3.5	3.6	2.7
Methyl formiate (E)	4.8[o]	4.0	4.1	5.0	4.1	4.2	4.3
Methyl formiate (Z) ECL	1.2[o]	−0.0	0.0	−0.5	0.1	0.2	−0.2
Methyl acetate ecl (E)	8.5[o]	5.1	4.8	6.3	5.9	5.6	6.6
Formamide plan	0.0[r]	0.0	0.0	0.0	0.0	0.0	0.0
Formamide rot	16.0[s]	13.7	13.7	12.6	14.9	14.9	12.6
Formamide rot LP cis	18.7[t]	16.7	16.7	14.8	17.8	17.8	15.4
Dinitrotetroxide plan	0.0[u]	0.1	0.1	0.0	0.1	0.1	−0.0
Dinitrotetroxide ort	2.9[u]	−0.1	−0.1	−0.3	−0.1	−0.1	−0.2

a Experimental data cited in: W.J. Hehre, L. Radom, P.v.R. Schleyer, and J.A. Pople, "Ab initio Molecular Orbital Theory", Wiley, New York, 1986. b Experimental conformational barriers cited in: M. Head-Gordon and J.A. Pople, J.Phys.Chem. 97, 1147 (1993) ; A.E. Dorigo, D.W. Pratt, and K.N. Houk, J.Am.Chem.Soc. 109, 6591 (1987). c Experimental data cited in: B.

Testa, "Grundlagen der Organischen Stereochemie", VCH, Weinheim, 1983. d M.E. Charro, J.C. Lopez, J.L. Alonso, G. Wlodarczak, and J. Demaison, J.Mol.Spectrosc. 162, 67 (1993). e W.D. Allen, A.G. Csaszar, and D.A. Horner, J.Am.Chem.Soc. 114, 6834 (1992), and literature cited therein. Cyclopentene. f V.E. Rivera-Gaines, S.J. Leibowitz, and J. Laane, J.Am.Chem.Soc. 113, 9735 (1991). g D. Autrey, J. Choo, and J. Laane, J.Phys.Chem.A 105, 10230 (2001). h A. Rauk, J.D. Andose, W.G. Frick, R. Tang, and K. Mislow, J.Am.Chem.Soc. 93, 6507 (1971). Inversions at nitrogen. i Taken from the experimental data quoted in: M.J.S. Dewar, W.Thiel, J.Am.Chem.Soc. 99, 4907 (1977). j V. Dyczmons, J.Phys.Chem.A 104, 8263 (2000). k J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986. l P.A. Kollman et al., J.Phys.Chem. 94, 4483 (1990). Anisole barrier. m Experimental data cited in: W.M.F. Fabian, J.Comput.Chem. 9, 369 (1988). n K.W. Butz, D.J. Krajnovich, and C.S. Parmenter, J.Chem.Phys. 93, 1557 (1990). Glyoxal internal rotation. o K.B. Wiberg and K.E. Laidig, J.Am.Chem.Soc. 109, 5935 (1987). p Experimental data cited in: A. St.-Amant, W. D. Cornell, P. A. Kollman, and T.A. Halgren, J.Comput.Chem. 16, 1483 (1995). q P.I. Nagy, D.A. Smith, G. Alagona and C. Ghio, J.Phys.Chem. 98, 486 (1994). r S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988). s K.B. Wiberg and P.R. Rablen, J.Am.Chem.Soc. 117, 2201 (1995). t K.B. Wiberg and C.M. Breneman, J.Am.Chem.Soc. 114, 831 (1992). u Y. Mo and Q. Zhang, Int.J.Quant.Chem. 56, 19 (1995). Computed and cited experimental data on N2O2 and N2O4.

Table S10: Benchmark Results for the FLUOR Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Fluorine	0.0[a]	0.6	0.5	−0.9	−1.7	−1.8	−1.3
Hydrogen fluoride	−65.1[a]	−63.3	−63.4	−68.6	−64.9	−65.0	−65.2
Methylfluoride	−56.0[a]	−60.4	−61.1	−58.6	−57.3	−58.5	−57.8
Difluoromethane	−108.1[b]	−110.9	−111.6	−109.4	−106.6	−107.8	−107.1
Trifluoromethane	−166.2[b]	−166.8	−167.6	−168.0	−162.0	−163.3	−162.4
Tetrafluoromethane	−223.1[b]	−220.5	−221.4	−227.1	−215.8	−217.3	−216.8
Fluoroethane	−63.0[c]	−67.5	−69.4	−66.1	−65.8	−68.8	−65.9
1,1-Difluoroethane	−118.8[b]	−121.8	−123.6	−121.5	−119.4	−122.4	−119.8
1,1,1-Trifluoroethane	−178.0[b]	−178.4	−180.4	−181.8	−176.3	−179.4	−176.9
Hexafluoroethane	−321.3[b]	−317.5	−319.7	−323.8	−310.5	−314.0	−311.6
i-Propylfluoride	−70.1[b]	−76.2	−79.4	−75.4	−75.1	−80.2	−75.3
Octafluorocyclobutane	−368.7[b]	−379.9	−384.6	−385.2	−372.9	−380.1	−373.8
Fluoroethene	−33.2[b]	−32.3	−33.5	−31.7	−32.2	−34.1	−32.6
1,2-Difluoroethene cis	−71.0[c]	−72.2	−73.5	−70.8	−71.7	−73.7	−72.2
1,2-Difluoroethene trans	−70.0[c]	−74.3	−75.6	−72.6	−72.7	−74.8	−73.4
1,1-Difluoroethene	−80.1[b]	−78.4	−79.6	−79.7	−79.9	−81.9	−80.1
Trifluoroethene	−117.2[b]	−116.4	−117.7	−116.3	−115.9	−118.0	−116.3
Tetrafluoroethene	−157.5[b]	−156.3	−157.7	−158.2	−155.9	−158.2	−156.5
Fluorobenzene	−27.7[b]	−27.3	−32.3	−26.7	−28.0	−35.9	−27.9
1,2-Difluorobenzene	−70.2[b]	−69.1	−74.1	−68.7	−69.9	−77.9	−70.0
1,3-Difluorobenzene	−73.9[b]	−72.9	−78.0	−72.5	−74.0	−82.0	−74.0
1,4-Difluorobenzene	−73.3[b]	−72.6	−77.6	−72.2	−73.5	−81.5	−73.8
Pentafluorobenzene	−192.8[b]	−191.8	−197.1	−192.1	−192.7	−201.0	−192.7
Hexafluorobenzene	−228.3[b]	−228.4	−233.7	−228.3	−228.8	−237.2	−228.6
Fluoroacetylene	25.1[d]	26.9	26.2	26.8	23.9	22.9	24.1
Difluoroacetylene	1.4[d]	4.4	3.8	3.9	−2.6	−3.7	−3.8
Hypofluorous acid	−23.5[a]	−19.6	−19.8	−18.7	−20.3	−20.7	−20.0
Fluoroethanol gauche	−100.0[c]	−100.7	−103.1	−101.1	−100.1	−103.8	−101.1
1,1,1-Trifluoroethanol	−212.3[a]	−209.2	−211.6	−212.4	−206.4	−210.2	−206.7
Trifluoromethylhypofluorite	−182.8[a]	−174.0	−175.3	−176.9	−166.3	−168.4	−168.7
Difluorine monoxide	5.9[a]	5.3	5.1	7.0	7.2	6.7	8.1
Formyl fluoride	−90.0[a]	−86.3	−86.9	−85.3	−88.2	−89.2	−89.8
Acetyl fluoride	−105.7[b]	−100.0	−101.6	−100.2	−103.0	−105.7	−104.4
Carbonyl fluoride	−145.9[e]	−136.5	−137.1	−137.9	−138.7	−139.7	−141.0
Trifluoroacetic acid trans	−246.5[b]	−242.3	−244.6	−245.8	−239.7	−243.3	−240.4
p-Fluorobenzoic acid	−118.2[b]	−116.9	−123.9	−117.4	−117.4	−128.3	−117.8
Trifluoroamine	−29.8[b]	−30.1	−30.7	−26.5	−35.9	−36.9	−37.1
(Z)-Difluorodiazene	16.4[a]	13.5	12.8	17.6	11.7	10.5	8.1
(E)-Difluorodiazene	19.4[a]	22.7	22.0	24.0	22.4	21.3	21.0
Tetrafluorohydrazine gauche	−8.0[c]	−6.3	−7.7	−1.3	−6.4	−8.6	−16.0
Fluorocyanide	8.6[a]	1.9	1.5	1.9	−1.5	−2.2	−2.4
Trifluoroacetonitrile	−119.0[b]	−125.5	−127.0	−127.8	−125.1	−127.5	−123.5
Fluorocarbene	34.2[f]	24.9	24.6	25.1	24.4	23.9	26.4
Difluorocarbene	−43.8[g]	−57.8	−58.1	−55.8	−55.7	−56.3	−50.0
Nitrosyl fluoride	−15.7[a]	−10.4	−10.7	−9.5	−21.6	−22.2	−21.3
Nitryl fluoride	−26.0[a]	−25.7	−26.4	−25.4	−29.3	−30.4	−28.9
Fluorine nitrate	2.5[b]	2.6	1.5	1.1	4.3	2.5	3.3
Nitrosyl trifluoride	−39.0[a]	−50.0	−51.0	−42.4	−50.7	−52.3	−49.0

a M.W.Chase, C.A.Davies, J.R.Downey, D.R.Frurip, R.A.McDonald, and A.N.Syverud, "JANAF Thermochemical Tables", 3rd edition, J.Phys.Chem.Ref.Data 14, Suppl.1 (1985). b J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986. c S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988). d S.Parthiban, J.M.L.Martin, and J.F.Liebman, Mol.Phys. 100, 453 (2002). e N.L.Haworth, M.H.Smith, G.B.Bacskay, and J.C.Mackie, J.Phys.Chem.A 104, 7600 (2000). f J.C.Poutsma, J.A.Paulimo, and R.R.Squires, J.Phys.Chem.A 101, 5327 (1997). g J.Demaison, L.Margules, J.M.L.Martin, and J.E.Boggs, Phys.Chem.Chem.Phys. 4, 3282 (2002).

Table S11: Benchmark Results for the FLUOR Set. Ionization Potentials (eV)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Fluorine	15.83[a]	16.32	16.32	16.12	16.36	16.36	16.71
Hydrogen fluoride	16.03[a]	16.45	16.45	16.32	17.03	17.03	17.28
Methylfluoride	13.31[a]	13.07	13.07	13.11	13.41	13.41	13.67
Difluoromethane	13.17[a]	12.98	12.98	13.02	13.23	13.23	13.54
Trifluoromethane	14.67[a]	14.17	14.17	14.19	14.45	14.45	14.78
Tetrafluoromethane	16.23[a]	16.27	16.27	16.26	16.89	16.89	17.24
Fluoroethane	12.43[a]	12.01	12.01	12.02	12.28	12.28	12.47
1,1-Difluoroethane	12.80[a]	12.30	12.30	12.28	12.69	12.69	12.91
1,1,1-Trifluoroethane	13.80[a]	13.23	13.23	13.21	13.78	13.78	13.98
Hexafluoroethane	14.60[a]	13.67	13.67	13.69	13.92	13.91	14.22
Fluoroethene	10.58[a]	10.59	10.59	10.44	10.85	10.85	10.81
1,2-Difluoroethene cis	10.43[a]	10.38	10.38	10.27	10.56	10.56	10.63
1,2-Difluoroethene trans	10.38[a]	10.43	10.43	10.32	10.61	10.61	10.68
1,1-Difluoroethene	10.72[a]	10.62	10.62	10.49	10.84	10.84	10.86
Trifluoroethene	10.53[a]	10.40	10.40	10.30	10.53	10.53	10.66
Tetrafluoroethene	10.52[a]	10.38	10.38	10.29	10.45	10.45	10.63
Fluorobenzene	9.19[a]	9.58	9.58	9.43	9.85	9.85	9.79
1,2-Difluorobenzene	9.68[a]	9.71	9.71	9.57	9.92	9.92	9.91
1,3-Difluorobenzene	9.68[a]	9.79	9.79	9.65	10.02	10.02	10.00
1,4-Difluorobenzene	9.15[a]	9.58	9.58	9.45	9.80	9.80	9.81
Hexafluorobenzene	10.12[a]	10.50	10.50	10.40	10.60	10.60	10.69
Fluoroacetylene	11.30[a]	11.33	11.33	11.21	11.52	11.52	11.51
Hypofluorous acid	13.00[a]	13.23	13.23	13.17	13.44	13.44	13.49
1,1,1-Trifluoroethanol	11.74[a]	12.04	12.04	11.99	12.34	12.34	12.42
Trifluoromethylhypofluorite	13.64[a]	14.01	14.01	13.94	14.20	14.20	14.36
Difluorine monoxide	13.26[a]	13.56	13.56	13.50	13.78	13.78	13.93
Acetyl fluoride	11.80[a]	11.86	11.86	11.77	12.30	12.30	12.31
Carbonyl fluoride	13.60[a]	13.39	13.39	13.31	13.86	13.86	13.90
Hexafluoroacetone	12.09[a]	12.03	12.03	11.95	12.16	12.16	12.24
Trifluoroamine	13.73[a]	13.29	13.29	13.44	13.68	13.68	13.99
(E)-Difluorodiazene	12.80[b]	12.47	12.47	12.63	12.45	12.45	12.72
Tetrafluorohydrazine gauche	12.84[a]	12.87	12.87	12.95	12.59	12.59	13.01
Difluorodiazacyclopropane	11.78[a]	11.41	11.41	11.44	11.58	11.58	11.62
Hexafluorodimethyldiimine cis	11.35[a]	11.20	11.20	11.06	10.98	10.99	11.14
2,4,6-Trifluorotriazine	12.00[a]	12.29	12.29	12.20	12.15	12.15	12.21
Pentafluoropyridine	10.27[a]	10.59	10.59	10.48	10.65	10.65	10.67
Difluorocarbene	12.27[a]	12.18	12.18	11.99	12.12	12.12	12.14
Nitrosyl fluoride	12.94[a]	12.80	12.80	12.82	13.00	13.00	13.04
Nitryl fluoride	13.51[a]	13.69	13.69	13.68	14.08	14.08	13.91

a Taken from the experimental data quoted in: M.J.S. Dewar, H.S. Rzepa, J.Am.Chem.Soc. 100, 58 (1978). b S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988).

Table S12: Benchmark Results for the RADICALS71 Subset of the OVS7-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
CH Doublet	142.5[a]	140.0	139.9	136.0	138.1	137.9	134.7
CH2+ Doublet C2v	331.0[b]	322.5	322.2	312.8	324.9	324.5	315.9
Carbene Triplet C2v	93.7[a]	91.9	91.6	89.6	90.3	89.8	88.7
Carbene Singlet C2v	102.8[a]	103.9	103.7	98.4	101.3	100.8	96.9
Methyl radical C3v	35.0[c]	33.7	33.3	31.8	35.2	34.5	33.0
Ethyl radical C1	28.9[c]	24.8	23.3	23.9	24.6	22.3	23.7
n-Propyl radical C1	23.9[d]	20.7	17.9	19.7	20.3	15.9	19.1
i-Propyl radical C1	21.5[c]	14.3	11.6	14.1	13.4	9.0	13.2
n-Butyl radical C1	18.0[b]	16.3	12.0	15.3	15.4	9.2	14.3
sec-Butyl radical C1	16.1[a]	9.9	5.7	9.5	8.8	2.3	7.8
i-Butyl radical C1	16.0[b]	14.7	10.2	13.4	14.9	8.0	13.4
tert-Butyl radical C1	12.3[c]	3.2	−1.1	3.6	2.4	−4.2	2.9
Ethylene radical cation D2	254.8[b]	244.8	243.6	238.9	251.5	249.6	246.3
Vinyl radical Cs	71.6[c]	67.4	66.6	66.5	66.4	64.9	66.1
Acetylene radical cation linear D2h	317.4[b]	312.4	311.8	306.0	318.1	317.1	312.5
Allyl radical C2v	40.8[c]	42.9	40.8	41.9	43.6	40.2	42.1
Propargyl radical C2v	81.0[d]	87.9	86.5	86.1	87.4	85.3	85.9
Propen-2-yl radical ecl Cs	58.1[b]	53.0	51.1	53.4	51.6	48.5	52.3
Cyclopropenyl radical Cs	105.0[b]	108.4	107.1	107.8	103.9	101.6	104.9
Cyclopropyl radical Cs	66.9[b]	62.4	60.4	62.6	60.2	56.9	61.9
Cyclopentadienyl radical C2v	58.0[b]	65.3	61.7	64.1	65.1	59.3	62.8
Phenyl radical C2v	81.2[e]	71.5	67.0	72.9	70.4	63.2	72.4
Phenoxy radical C2v	12.9[d]	12.5	7.3	12.6	12.6	4.4	12.3
Benzyl radical C2v	48.4[c]	54.1	47.9	53.8	54.6	44.9	53.5
Amidyl radical (NH2) C2v	45.1[c]	47.8	47.5	41.1	39.3	38.9	35.4
NH2+ triplet C2v	302.0[b]	299.0	298.8	295.6	292.2	291.8	288.4
Ammonia radical cation D3h	223.2[b]	216.6	216.2	214.6	214.4	213.7	213.7
Aminomethyl radical	38.0[b]	29.3	28.2	28.0	25.2	23.3	27.3
Cyanide radical	104.9[a]	111.6	111.4	109.8	102.7	102.3	101.1
Cyanomethyl radical C2v	58.1[c]	64.1	63.0	62.9	62.1	60.4	61.1
Azidyl radical (N3) Cs	99.0[f]	100.0	99.5	102.8	100.8	99.9	101.7
Hydroxyl radical	9.4[c]	5.3	5.3	4.0	4.3	4.2	3.1
OH+ triplet	309.1[b]	301.9	301.8	297.8	301.8	301.6	296.5
Water radical cation C2v	233.0[b]	227.5	227.3	223.3	227.0	226.7	225.1
Formyl radical (HCO) Cs	10.0[c]	0.1	−0.3	−0.2	−4.4	−4.9	−3.1
Methoxy radical (CH3O) C1	4.1[c]	0.4	−0.4	1.3	1.3	−0.0	1.8
Hydroxymethyl radical (CH2OH)	−4.1[c]	−10.8	−11.5	−11.7	−12.2	−13.5	−11.3
HO2 radical Cs	2.5[b]	−4.3	−4.6	−2.9	−4.2	−4.7	−2.1
Acetyl radical (CH3CO) C1	−2.4[c]	−16.1	−17.3	−14.7	−19.9	−21.9	−17.6
Cyanate radical (NCO) linear	37.0[b]	39.7	39.2	39.7	34.3	33.5	32.2
Nitric oxide (NO)	21.6[f]	24.5	24.4	24.1	15.2	14.9	15.6
Nitrogen dioxide (NO2) C2v	7.9[f]	5.1	4.7	3.5	−1.5	−2.2	−1.3

a L.A.Curtiss, K.Raghavachari, P.C.Redfern, and J.A.Pople, J.Chem.Phys. 106, 1063 (1997). b S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988). c J. Berkowitz, G. B. Ellison, and D. Gutman, J.Phys.Chem. 98, 2744 (1994). d W. Tsang, "Heats of Formation of Organic Free Radicals by Kinetic Methods" in: Energetics of Organic Free Radicals, J.A.M. Simoes, A. Greenberg, J.F. Liebman (eds.), Blackie Academic and Professional, London, 1996, pp. 22-58. e G3 values derived from the data in: L.A.Curtiss, K.Raghavachari, P.C.Redfern, V.Rassolov, and J.A.Pople, J.Chem.Phys. 112, 7374 (2000). f M.W.Chase, C.A.Davies, J.R.Downey, D.R.Frurip, R.A.McDonald, and A.N.Syverud, "JANAF Thermochemical Tables", 3rd edition, J.Phys.Chem.Ref.Data 14, Suppl.1 (1985).

Table S13: Benchmark Results for the RADICALS71 Subset of the OVS7-CHNOF Set. Ionization Potentials (eV)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
CH Doublet	10.64[a]	9.92	9.92	9.56	9.91	9.91	9.55
Methyl radical C3v	9.84[a]	9.81	9.81	9.53	10.12	10.12	9.88
Ethyl radical C1	8.51[a]	8.59	8.59	8.39	8.95	8.95	8.75
n-Propyl radical C1	8.43[a]	8.55	8.55	8.32	8.81	8.81	8.63
i-Propyl radical C1	7.69[a]	7.88	7.88	7.72	8.21	8.22	8.02
n-Butyl radical C1	8.50[a]	8.48	8.48	8.24	8.82	8.94	8.74
sec-Butyl radical C1	7.59[a]	7.83	7.83	7.66	8.12	8.12	7.87
i-Butyl radical C1	8.31[a]	8.55	8.55	8.30	8.85	8.86	8.67
tert-Butyl radical C1	6.92[a]	7.47	7.48	7.31	7.70	7.71	7.52
Vinyl radical Cs	9.45[a]	9.31	9.31	9.14	9.68	9.68	9.49
Allyl radical C2v	8.13[a]	8.07	8.07	7.81	8.35	8.35	8.13
Propargyl radical C2v	8.34[a]	8.42	8.42	8.15	8.64	8.64	8.41
Cyclopropenyl radical Cs	6.60[b]	7.84	7.84	7.63	8.15	8.15	7.91
Cyclopropyl radical Cs	8.05[a]	9.06	9.06	8.87	9.48	9.49	9.26
Cyclopentadienyl radical C2v	8.69[a]	8.73	8.73	8.51	9.02	9.02	8.85
Phenyl radical C2v	9.20[a]	9.19	9.19	8.92	9.68	9.68	9.48
Phenoxy radical C2v	8.84[a]	8.59	8.59	8.44	8.86	8.87	8.72
Benzyl radical C2v	7.20[a]	7.34	7.34	7.09	7.61	7.61	7.41
Amidyl radical (NH2) C2v	12.45[a]	12.43	12.43	12.61	12.54	12.54	12.48
Ammonia radical cation D3h	23.50[a]	22.01	22.01	22.25	21.96	21.96	21.92
Cyanide radical	14.17[a]	14.16	14.16	14.02	14.05	14.05	13.91
Formyl radical (HCO) Cs	9.31[a]	9.61	9.61	9.41	9.68	9.68	9.47
HO2 radical Cs	11.53[a]	12.21	12.21	12.14	12.42	12.42	12.33
Nitric oxide (NO)	9.25[a]	10.35	10.35	10.31	10.05	10.05	10.07
Nitrogen dioxide (NO2) C2v	9.80[a]	11.48	11.48	11.33	11.37	11.37	11.23

a V.N.Kondratev (ed.), "Dissociation Energies of Chemical Bonds, Ionization Potentials, and Electron Affinities", Nauka, Moscow, 1974 (in Russian). b S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988).

Table S14: Benchmark Results for the RADICALS71 Subset of the OVS7-CHNOF Set. Enthalpy Changes at 298 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Carbene Triplet linear	5.5[a]	5.1	5.1	4.8	7.9	7.9	6.7
Carbene Singlet C2v	9.1[b]	12.0	12.0	8.9	11.0	11.0	8.2
Carbene Singlet linear	28.2[a]	21.6	21.6	24.6	25.4	25.4	27.1
Amidyl radical (NH2) linear	34.4[c]	39.1	39.1	36.9	40.4	40.5	39.8

a M.E.Jacox, "Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules", J.Phys.Chem.Ref.Data Monograph No. 3 (1994). b L.A.Curtiss, K.Raghavachari, P.C.Redfern, and J.A.Pople, J.Chem.Phys. 106, 1063 (1997). c S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988).

Table S15: Benchmark Results for the ANIONS24 Subset of the OVS7-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
H-	33.2[a]	56.7	56.7	60.4	61.1	61.1	63.7
CH3-	33.2[b]	48.9	48.5	50.0	41.3	40.5	44.1
CH3CH2-	35.1[b]	36.6	35.1	38.6	30.3	27.9	34.1
HCC-	65.5[b]	61.9	61.4	67.5	61.7	60.9	68.3
CH2CH-	52.8[b]	52.7	51.8	56.1	47.9	46.4	52.6
c-C5H5-	19.6[b]	28.2	24.6	32.2	20.9	15.2	23.0
C6H5-	54.7[b]	44.9	40.4	50.4	41.6	34.4	47.5
NH2-	27.0[b]	51.6	51.4	41.4	39.8	39.4	37.6
CH3NH-	32.0[b]	31.9	30.8	27.1	25.6	23.8	24.5
(CH3)2N-	26.1[b]	17.4	15.1	15.7	17.1	13.4	14.6
C4H4N-	18.9[b]	25.5	22.4	30.6	20.9	15.9	25.5
NC-	17.7[b]	23.5	23.2	24.3	15.7	15.3	17.3
CH2CN-	25.1[b]	37.9	36.8	38.3	32.7	30.9	31.9
OH-	−32.7[b]	−24.2	−24.2	−23.8	−29.0	−29.2	−26.3
CH3O-	−33.2[b]	−46.1	−46.9	−42.4	−51.1	−52.4	−48.6
C2H5O-	−44.5[b]	−52.7	−54.6	−49.9	−58.1	−61.2	−56.3
C6H5O-	−39.4[b]	−39.2	−44.3	−36.1	−46.2	−54.4	−43.3
HCOO-	−110.9[b]	−111.8	−112.4	−109.0	−118.7	−119.8	−118.1
CH3COO-	−120.5[b]	−121.9	−123.6	−120.5	−127.6	−130.5	−127.0
C6H5COO-	−97.3[b]	−99.8	−106.4	−96.6	−103.7	−114.0	−101.9
HOO-	−22.5[b]	−27.5	−27.7	−25.2	−33.9	−34.4	−29.1
HCO-	1.9[b]	−22.8	−23.1	−18.4	−28.5	−29.0	−22.2
NO2-	−45.2[b]	−51.1	−51.5	−50.5	−55.6	−56.3	−52.6
CH2NO2-	−27.2[b]	−36.5	−37.9	−33.4	−37.4	−39.7	−27.8

a M.W.Chase, C.A.Davies, J.R.Downey, D.R.Frurip, R.A.McDonald, and A.N.Syverud, "JANAF Thermochemical Tables", 3rd edition, J.Phys.Chem.Ref.Data 14, Suppl.1 (1985). b S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988).

Table S16: Benchmark Results for the CATIONS41 Subset of the OVS7-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
H+	365.7[a]	343.8	343.8	340.1	339.4	339.4	336.8
CH+	387.8[b]	366.9	366.8	354.7	364.7	364.5	353.0
CH3+ methyl D3h	261.3[b]	255.7	255.3	248.1	262.4	261.6	255.0
C2H3+ nonclassical C2v	265.9[b]	280.4	279.6	272.5	282.2	280.8	276.7
C2H5+ nonclassical C2v	215.6[b]	222.9	221.4	216.7	227.7	225.4	223.9
C3H3+ cyclopropenyl C2v	257.0[b]	259.4	258.0	253.8	262.2	260.0	258.3
HCCCH2+ propargyl C2v	282.0[b]	276.4	275.1	269.6	280.9	278.7	275.2
C3H5+ allyl C2v	226.0[b]	223.7	221.5	217.8	230.7	227.3	225.5
C3H7+ 2-propyl C2v	190.9[b]	185.1	182.4	179.8	190.0	185.6	186.5
C3H7+ 1-propyl (29) Cs	211.0[b]	206.6	203.8	200.5	212.3	207.9	208.3
C4H7+ methylallyl Cs	207.9[c]	199.3	195.8	194.3	205.7	200.4	201.9
C4H9+ n-butyl sec Cs	183.0[b]	176.8	172.7	171.9	182.1	175.6	179.0
C4H9+ tert-butyl C3h	165.8[b]	158.2	153.9	155.0	163.5	156.8	162.4
C6H5+ phenyl C2v	269.3[b]	254.5	250.1	249.1	262.6	255.5	259.8
C6H5CH2+ benzyl Cs	215.0[b]	214.6	208.4	210.2	221.7	212.0	217.8
NH2+ triplet C2v	302.0[b]	299.0	298.8	295.6	292.2	291.8	288.4
CH2NH2+ C2v	179.4[d]	174.9	173.7	172.9	173.4	171.6	175.4
HCNH+ linear	226.0[b]	221.6	221.0	214.9	211.4	210.5	209.4
CH3CNH+ C3v	195.0[b]	201.5	199.9	193.3	190.8	188.2	187.9
C5H5NH+ pyridinium C2v	178.0[b]	175.0	170.1	175.0	176.6	168.9	179.4
OH+ triplet	309.1[b]	301.9	301.8	297.8	301.8	301.6	296.5
CHO+ formyl linear	197.3[b]	194.8	194.5	190.8	192.6	192.0	190.3
CH3CHOH+ Cs	139.0[b]	138.8	136.9	135.7	144.0	141.0	143.4
CH3CO+ acetyl C3v	156.0[b]	162.3	161.0	157.3	160.6	158.6	158.2
H3O+ C3v	141.0[b]	142.9	142.5	139.0	141.7	141.1	146.2
CH3OH2+ Cs	136.0[b]	142.4	141.0	137.3	146.6	144.5	147.7
(CH3)2OH+ Cs	130.0[b]	141.8	139.1	136.3	151.2	147.1	149.8
C4H5O+ furan C-prot Cs	165.0[b]	161.5	158.2	156.1	170.6	165.3	167.5
OCOH+ Cs	141.0[b]	150.8	150.2	145.5	148.5	147.5	145.1
H2COH+ Cs	169.3[e]	166.4	165.7	162.3	172.4	171.2	171.0
HC(OH)2+ Cs	96.0[b]	100.2	99.0	96.4	106.0	104.2	104.9
NO+	235.3[b]	259.8	259.7	258.4	243.6	243.3	244.8
NO2+ linear	233.0[b]	239.7	239.3	234.2	230.8	230.1	229.0

a J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986. b S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988). c J.C. Traeger, J.Phys.Chem. 90, 4114 (1986). d G. de Oliveira, J.M.L.Martin, I.K.C.Silwal, and J.F.Liebman, J.Comp.Chem. 22, 1297 (2001). e J.C. Traeger and J.L. Holmes, J.Phys.Chem. 97, 3453 (1993).

Table S17: Benchmark Results for the CATIONS41 Subset of the OVS7-CHNOF Set. Enthalpy Changes at 298 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
HCCCH2+ propargyl C2v	27.0[a]	17.0	17.1	15.8	18.7	18.8	16.9
C3H7+ 1-propyl (29) Cs	20.1[a]	21.4	21.4	20.7	22.3	22.2	21.7
C4H9+ tert-butyl C3h	−17.2[a]	−18.6	−18.8	−16.8	−18.6	−18.8	−16.6
NH2+ singlet C2v	30.1[b]	26.0	26.0	26.7	26.1	26.0	24.7
OH+ singlet	50.5[b]	35.5	35.5	35.5	35.5	35.5	35.5

a S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988). b M.E.Jacox, "Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules", J.Phys.Chem.Ref.Data Monograph No. 3 (1994).

Table S18: Benchmark Results for the BIGMOL20 Subset of the OVS7-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Tetrahydro-2H-pyran	−53.4[a]	−53.1	−59.6	−54.5	−51.7	−61.8	−53.8
Maleic anhydride	−95.2[a]	−87.1	−90.4	−87.4	−87.2	−92.5	−90.4
Cyclohexanone	−54.0[a]	−59.9	−67.6	−60.0	−62.1	−73.7	−61.8
Benzoquinone	−29.4[a]	−32.5	−37.9	−31.6	−32.9	−41.3	−32.0
Hydroquinone	−63.4[a]	−60.6	−66.7	−63.2	−64.6	−74.2	−64.4
2-Methoxytetrahydropyran	−95.5[a]	−97.2	−106.1	−99.2	−90.3	−103.6	−95.2
Naphthalene	35.9[a]	34.8	25.3	35.8	35.7	21.0	35.7
2-Aminobenzoic acid	−70.7[a]	−68.6	−77.0	−73.1	−70.8	−83.6	−71.2
1-Naphthol	−7.1[a]	−5.1	−15.3	−5.5	−5.5	−21.3	−5.3
2-Naphthol	−7.2[a]	−5.9	−16.0	−6.6	−6.6	−22.2	−6.6
1,4-Naphthoquinone	−26.5[a]	−32.7	−42.7	−31.5	−31.8	−47.3	−30.9
Isophthalic acid	−166.4[a]	−159.5	−168.5	−160.8	−159.4	−173.2	−160.5
Terephthalic acid	−171.6[a]	−159.5	−168.4	−160.7	−159.2	−173.0	−160.2
1-Naphthoic acid	−53.3[a]	−55.2	−67.0	−55.3	−52.8	−71.0	−53.3
2-Naphthoic acid	−55.6[a]	−55.1	−66.7	−55.3	−53.9	−71.7	−54.6
Anthracene	55.2[a]	55.5	41.4	56.4	57.5	35.8	57.0
Phenanthrene	49.6[b]	46.8	32.4	48.0	49.1	27.0	48.8
9,10-Anthraquinone	−22.8[a]	−32.7	−47.5	−31.4	−30.4	−53.0	−29.5
9,10-Phenanthraquinone	−33.3[a]	−23.6	−38.5	−21.6	−21.6	−44.4	−20.7
5,12-Naphthacenequinone	−8.1[a]	−17.5	−36.9	−16.2	−14.0	−43.6	−13.6

a J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986. b S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988).

Table S19: Benchmark Results for the ISOMERS44 Subset of the OVS7-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
n-Pentane	−35.1[a]	−34.7	−40.8	−34.7	−35.2	−44.6	−34.9
2-Methylbutane	−36.7[a]	−35.9	−42.4	−36.1	−35.5	−45.4	−35.5
Neopentane	−40.2[a]	−39.6	−46.4	−40.2	−37.6	−48.1	−38.2
n-Hexane	−39.9[a]	−39.2	−46.9	−39.4	−40.0	−51.6	−39.9
3-Methylpentane	−41.1[a]	−39.9	−48.2	−40.2	−39.5	−52.0	−39.9
2-Methylpentane	−41.8[a]	−40.4	−48.5	−40.9	−40.3	−52.5	−40.6
2,3-Dimethylbutane	−42.6[a]	−41.1	−49.7	−41.7	−39.8	−52.8	−40.4
2,2-Dimethylbutane	−44.5[a]	−42.8	−51.6	−43.4	−40.7	−54.0	−41.5
But-1-ene H-ecl	0.0[a]	0.1	−3.8	0.1	0.3	−5.7	0.3
cis-2-Butene	−1.7[a]	−1.9	−5.8	−2.0	−2.2	−8.2	−2.3
trans-2-Butene	−2.7[a]	−3.8	−7.5	−3.7	−4.0	−9.8	−3.9
Isobutene	−4.0[a]	−4.3	−8.2	−4.0	−3.9	−10.0	−3.6
1-Butyne	39.5[a]	39.5	36.5	39.3	39.2	34.6	39.5
2-Butyne	34.8[a]	35.1	32.4	34.5	33.8	29.6	34.1
Cyclooctatetraene	70.7[a]	75.2	67.2	74.3	73.9	61.6	72.1
Dimethylamine	−4.4[a]	−5.1	−7.9	−4.2	−2.2	−6.5	−3.2
Ethylamine	−11.3[a]	−8.9	−11.7	−10.9	−12.1	−16.5	−11.9
Acetonitrile	18.0[b]	17.5	16.2	17.3	15.3	13.2	15.3
Methylisocyanide	39.1[a]	38.3	36.9	37.6	26.7	24.4	21.8
Propanol	−61.0[a]	−61.9	−65.6	−61.9	−62.2	−67.9	−61.6
Isopropanol	−65.2[a]	−66.7	−70.5	−68.7	−67.2	−73.1	−67.5
n-Butanol	−65.7[a]	−66.4	−71.6	−68.0	−67.6	−75.5	−67.9
Isobutanol	−67.8[a]	−67.5	−73.0	−69.6	−68.1	−76.7	−68.5
2-Butanol	−70.0[a]	−71.2	−76.6	−73.4	−71.7	−80.0	−72.2
tert-Butanol	−74.7[a]	−76.8	−82.4	−78.1	−75.9	−84.5	−76.1
Dimethylether	−44.0[a]	−45.6	−47.7	−45.9	−42.8	−46.2	−44.3
Ethanol	−56.2[a]	−56.9	−59.1	−56.7	−57.2	−60.8	−56.6

a J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986. b S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988).

Table S20: Benchmark Results for the ISOMERS44 Subset of the OVS7-CHNOF Set. Enthalpy Changes at 298 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
2-Methylbutane	−1.6	−1.2	−1.6	−1.4	−0.3	−0.9	−0.7
Neopentane	−5.1[a]	−4.9	−5.6	−5.5	−2.5	−3.5	−3.4
3-Methylpentane	−1.2[a]	−0.6	−1.3	−0.8	0.5	−0.4	0.0
2-Methylpentane	−1.8[a]	−1.2	−1.7	−1.5	−0.3	−0.9	−0.7
2,3-Dimethylbutane	−2.7[a]	−1.9	−2.8	−2.3	0.2	−1.1	−0.5
2,2-Dimethylbutane	−4.5[a]	−3.5	−4.7	−4.0	−0.7	−2.3	−1.5
cis-2-Butene	−1.7[a]	−2.0	−2.0	−2.1	−2.5	−2.6	−2.6
trans-2-Butene	−2.7[a]	−3.9	−3.7	−3.8	−4.3	−4.1	−4.2
Isobutene	−4.0[a]	−4.4	−4.5	−4.1	−4.2	−4.4	−3.9
2-Butyne	−4.7[a]	−4.4	−4.1	−4.8	−5.4	−4.9	−5.5
Ethylamine	−6.9[a]	−3.7	−3.8	−6.7	−9.8	−10.0	−8.7
Methylisocyanide	21.1[a]	20.8	20.7	20.2	11.4	11.2	6.4
Isopropanol	−4.2[a]	−4.7	−4.9	−6.8	−5.0	−5.3	−5.9
Isobutanol	−2.1[a]	−1.1	−1.5	−1.6	−0.5	−1.2	−0.7
2-Butanol	−4.3[a]	−4.8	−5.0	−5.4	−4.2	−4.4	−4.3
tert-Butanol	−9.0[a]	−10.4	−10.8	−10.1	−8.3	−8.9	−8.3
Ethanol	−12.2[a]	−11.3	−11.4	−10.8	−14.5	−14.6	−12.3

a J.B.Pedley, R.D.Naylor, and S.P.Kirby, ”Thermochemical Data of Organic Compounds”, 2nd ed., Chapman and Hall, London, 1986.

Table S21: Benchmark Results for the CONFORMERS30 Subset of the OVS7-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Propane tr/tr	−25.0[a]	−25.5	−28.7	−25.2	−25.4	−30.4	−24.8
Biphenyl	43.6[b]	39.0	27.0	40.1	40.1	21.8	40.0
n-Butane	−30.0[a]	−30.1	−34.8	−29.9	−30.3	−37.5	−29.8
Cyclohexane chair	−29.5[a]	−27.1	−35.0	−27.2	−28.5	−40.5	−28.5
Methylcyclohexane eq	−37.0[b]	−33.9	−43.7	−34.7	−34.8	−49.5	−35.6
1,4-tr-Dimethylcyclohexane ee	−44.1[a]	−40.8	−52.4	−42.2	−41.1	−58.5	−42.6
Dimethylether tr/tr	−44.0[a]	−45.6	−47.7	−45.9	−42.8	−46.2	−44.3
2-Methoxytetrahydropyran ax	−95.5[a]	−97.2	−106.1	−99.2	−90.3	−103.6	−95.2
Aminocyclohexane eq	−25.0[b]	−17.3	−26.5	−22.8	−21.2	−35.1	−22.9
N-Methylpiperidine eq	−12.0[b]	−10.1	−19.2	−9.2	−4.8	−18.4	−8.8
4-Methylpiperidine eq	−19.0[b]	−13.5	−22.7	−15.5	−13.5	−27.4	−15.2

a J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986. b S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988).

Table S22: Benchmark Results for the CONFORMERS30 Subset of the OVS7-CHNOF Set. Enthalpy Changes at 298 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Propane tr/cis	3.7[a]	2.7	2.7	2.2	2.3	2.4	2.0
Propane cis/cis	8.8[a]	5.6	5.6	4.7	4.9	4.9	4.0
n-Butane cis	6.0[b]	5.1	4.9	5.0	5.0	4.7	5.0
n-Butane gauche	0.8[c]	0.8	0.7	0.9	0.9	0.7	0.9
Cyclohexane boat	5.5[b]	6.1	6.2	6.2	5.7	5.7	6.0
Cyclohexane twist	4.8[b]	5.2	5.2	5.7	5.0	5.0	5.7
Methylcyclohexane ax	1.7[b]	1.8	1.5	2.1	1.8	1.4	2.2
t-Butyl-Cyclohexane ax	4.8[b]	5.6	5.1	6.0	5.1	4.5	5.6
1,4-tr-Dimethylcyclohexane aa	3.6	3.6	2.9	4.3	3.7	2.9	4.4
Dimethylether tr/cis	2.7[a]	2.0	2.0	1.5	1.8	1.8	1.2
Dimethylether cis/cis	7.0[a]	3.2	3.3	2.2	3.0	3.1	1.8
Dihydroxymethane g+g-	3.5[d]	2.7	2.7	2.7	3.5	3.4	3.0
Dihydroxymethane aa	9.2[d]	8.8	8.8	10.7	10.0	10.0	10.2
2-Methoxytetrahydropyran eq	1.1[e]	3.0	3.0	2.9	3.6	3.6	2.1
Aminocyclohexane ax	1.4[e]	1.8	1.7	0.4	2.0	1.8	1.8
N-Methylpiperidine ax	3.1[e]	1.3	1.0	4.0	0.6	0.2	1.4
4-Methylpiperidine ax	1.9[b]	1.7	1.4	2.1	1.9	1.5	2.3

a J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986. b Experimental data cited in: B. Testa, "Grundlagen der Organischen Stereochemie", VCH, Weinheim, 1983. c Experimental data cited in: T.A. Halgren and R.B. Nachbar, J.Comput.Chem. 17, 587 (1996). d U. Salzner and P.v.R. Schleyer, J.Am.Chem.Soc. 115, 10231 (1993). e Experimental data cited in: A. St.-Amant, W. D. Cornell, P. A. Kollman, and T.A. Halgren, J.Comput.Chem. 16, 1483 (1995).

Table S23: Benchmark Results for the FLUORINE91 Subset of the OVS7-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
2: CH3F	−56.9[a]	−60.4	−61.1	−58.6	−57.3	−58.5	−57.8
3: CH2F2	−108.4[a]	−110.9	−111.6	−109.4	−106.6	−107.8	−107.1
4: CHF3	−167.1[a]	−166.8	−167.6	−168.0	−162.0	−163.3	−162.4
5: CF4	−223.9[a]	−220.5	−221.4	−227.1	−215.8	−217.3	−216.8
7: CH2F	−7.7[a]	−13.6	−14.1	−12.6	−13.1	−13.9	−13.3
8: CHF2	−58.6[a]	−68.0	−68.6	−66.9	−67.5	−68.4	−66.0
9: CF3	−112.2[a]	−123.2	−123.8	−124.1	−122.6	−123.6	−120.0
11: CHF	34.8[a]	24.9	24.6	25.1	24.4	23.9	26.4
12: CF2	−46.6[a]	−57.8	−58.1	−55.8	−55.7	−56.3	−50.0
14: CF	58.0[a]	52.3	52.2	55.4	52.7	52.4	57.2
16: CHFO	−92.0[a]	−86.3	−86.9	−85.3	−88.2	−89.2	−89.8
17: CF2O	−145.7[a]	−136.5	−137.1	−137.9	−138.7	−139.7	−141.0
19: CFO	−42.7[a]	−50.7	−51.1	−48.6	−54.5	−55.1	−52.7
21: CH2FOH	−101.9[a]	−103.2	−104.2	−103.0	−100.6	−102.3	−101.8
22: CHF2OH	−161.6[a]	−162.5	−163.7	−163.8	−157.8	−159.7	−159.9
23: CF3OH	−218.3[a]	−215.1	−216.3	−219.6	−209.8	−211.8	−212.4
24: CH3OF	−21.5[a]	−22.1	−23.2	−20.8	−19.8	−21.5	−20.1
25: CH2FOF	−71.2[a]	−71.3	−72.5	−69.3	−66.4	−68.3	−67.9
26: CHF2OF	−123.9[a]	−123.5	−124.7	−123.5	−117.0	−119.0	−119.1
27: CF3OF	−178.0[a]	−174.0	−175.3	−176.9	−166.3	−168.4	−168.7
29: CH2FO	−48.9[a]	−49.9	−50.8	−49.1	−47.0	−48.4	−49.4
30: CHF2O	−98.0[a]	−99.0	−99.9	−99.5	−93.2	−94.6	−96.5
31: CF3O	−151.2[a]	−150.5	−151.4	−153.4	−143.8	−145.3	−147.4
33: CHFOH	−53.0[a]	−64.2	−65.1	−63.1	−63.2	−64.6	−61.4
34: CF2OH	−108.7[a]	−122.6	−123.5	−122.4	−120.3	−121.7	−118.3
35: CH2OF	26.1[a]	−17.0	−17.8	−14.4	−12.0	−13.4	−13.5
36: CHFOF	−15.3[a]	−28.8	−29.7	−24.7	−24.6	−26.0	−18.9
38: CF3OOH	−193.1[a]	−193.9	−195.5	−196.7	−185.7	−188.3	−188.0
40: CF3OO	−152.9[a]	−157.5	−158.9	−159.7	−147.8	−150.0	−148.3
42: FCOOH	−146.9[a]	−136.4	−137.3	−137.5	−137.1	−138.7	−139.6
44: FCOO-B2	−86.5[a]	−70.0	−70.7	−68.7	−66.5	−67.7	−71.7
46: CF2OHOH	−212.3[a]	−210.6	−212.2	−211.7	−203.5	−206.1	−207.8
48: OCF2OH	−146.9[a]	−145.5	−146.8	−147.6	−139.1	−141.2	−144.3
50: CH3CH2F	−65.7[a]	−67.5	−69.4	−66.1	−65.8	−68.8	−65.9
51: CH2FCH2F	−107.3[a]	−111.3	−113.1	−108.7	−106.9	−109.9	−108.4
52: CH3CHF2	−121.3[a]	−121.8	−123.6	−121.5	−119.4	−122.4	−119.8
53: CHF2CH2F	−161.1[a]	−164.1	−166.0	−162.7	−159.0	−162.1	−160.3
54: CH3CF3	−181.3[a]	−178.4	−180.4	−181.8	−176.3	−179.4	−176.9
55: CHF2CHF2	−212.5[a]	−213.2	−215.2	−212.8	−206.0	−209.2	−207.3
56: CH2FCF3	−219.0[a]	−217.3	−219.3	−219.4	−212.3	−215.5	−213.5
60: CH2FCH2	−14.7[a]	−20.7	−22.2	−20.6	−19.2	−21.7	−21.2
61: CH3CHF	−18.2[a]	−25.9	−27.4	−24.8	−27.1	−29.5	−26.4
62: CH2FCHF	−58.1[a]	−68.8	−70.3	−66.5	−67.5	−70.0	−68.0
63: CHF2CH2	−68.3[a]	−72.6	−74.1	−73.4	−70.0	−72.5	−72.1
64: CH3CF2	−71.9[a]	−81.9	−83.4	−81.3	−83.2	−85.7	−81.1
65: CH2FCF2	−110.0[a]	−121.4	−123.0	−119.5	−119.5	−122.1	−118.7
66: CHF2CHF	−110.6[a]	−119.2	−120.8	−117.9	−115.8	−118.4	−116.7
67: CF3CH2	−127.3[a]	−127.3	−129.0	−131.5	−124.3	−126.9	−126.7
68: CF3CHF	−168.3[a]	−172.1	−173.8	−174.1	−168.8	−171.5	−169.4
69: CHF2CF2	−160.3[a]	−169.9	−171.6	−169.4	−165.9	−168.6	−165.5
72: CH2CHF	−34.4[a]	−32.3	−33.5	−31.7	−32.2	−34.1	−32.6
73: CHFCHF-Z	−73.8[a]	−74.3	−75.6	−72.6	−72.7	−74.8	−73.4
74: CHFCHF-E	−74.5[a]	−72.2	−73.5	−70.8	−71.7	−73.7	−72.2
75: CH2CF2	−84.5[a]	−78.4	−79.6	−79.7	−79.9	−81.9	−80.1
76: CHFCF2	−120.1[a]	−116.4	−117.7	−116.3	−115.9	−118.0	−116.3
77: CF2CF2	−162.3[a]	−158.5	−159.8	−158.9	−155.9	−158.2	−156.5
79: CH2FCH	40.7[a]	30.9	29.7	29.5	30.2	28.2	28.4
81: CF3CH	−58.2[a]	−60.9	−62.2	−66.4	−57.8	−60.0	−60.6
82: CH3CF	17.9[a]	−3.9	−5.1	−2.2	−3.8	−5.8	0.7
83: CH2FCF	−21.7[a]	−41.9	−43.1	−39.0	−38.4	−40.4	−35.1
84: CHF2CF	−67.7[a]	−87.4	−88.7	−85.3	−82.7	−84.8	−79.2
85: CF3CF	−124.0[a]	−138.8	−140.2	−139.4	−133.1	−135.4	−129.5

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Table S23: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
87: CHFCH-Z	28.7[a]	27.1	26.2	27.6	26.9	25.4	26.3
88: CHFCH-E	28.3[a]	28.4	27.5	28.6	27.7	26.2	27.2
89: CH2CF	26.0[a]	20.2	19.3	21.3	17.2	15.7	19.4
90: CHFCF-Z	−10.8[a]	−16.7	−17.7	−14.1	−18.4	−20.0	−16.2
91: CHFCF-E	−10.4[a]	−17.0	−17.9	−14.5	−18.1	−19.7	−15.9
92: CF2CH	−18.7[a]	−14.9	−15.8	−16.0	−16.3	−17.8	−16.6
93: CF2CF	−54.0[a]	−56.9	−57.8	−55.3	−58.7	−60.3	−56.3
95: CH2FC	78.8[a]	65.1	64.1	65.8	66.5	64.8	66.0
96: CHF2C	36.1[a]	22.0	21.0	21.6	25.3	23.6	24.3
97: CF3C	−18.4[a]	−26.5	−27.6	−30.0	−21.9	−23.7	−23.3
99: HCCF	24.8[a]	26.9	26.2	26.8	23.9	22.9	24.1
100: FCCF	0.0[a]	4.4	3.8	3.9	−2.6	−3.7	−3.8
102: CHFC	71.5[a]	58.6	57.8	59.1	61.0	59.8	61.2
103: CF2C	30.4[a]	22.2	21.4	22.1	26.5	25.3	26.7
105: CCF	109.3[a]	94.0	93.5	95.7	97.7	96.9	101.0
107: CHFCO	−38.8[a]	−37.8	−38.8	−38.6	−42.5	−44.1	−42.5
108: CF2CO	−75.0[a]	−96.6	−97.7	−95.5	−93.5	−95.3	−88.3
110: CFCO	19.3[a]	−7.8	−8.5	−5.8	−7.3	−8.6	−2.2
112: CH2FCHO	−80.2[a]	−87.8	−89.4	−86.6	−87.8	−90.5	−88.9
113: CHF2CHO	−130.4[a]	−135.7	−137.5	−135.7	−133.6	−136.4	−135.0
114: CF3CHO	−186.5[a]	−188.1	−189.9	−191.3	−186.3	−189.2	−187.7
115: CH3CFO	−105.8[a]	−100.0	−101.6	−100.2	−103.0	−105.7	−104.4
116: CH2FCFO	−143.6[a]	−139.2	−140.9	−138.0	−139.7	−142.4	−141.6
117: CHF2CFO	−190.7[a]	−187.1	−188.9	−186.7	−186.2	−189.0	−187.6
118: CF3CFO	−246.3[a]	−238.5	−240.3	−241.8	−237.3	−240.3	−239.3
120: CH2FCO	−41.9[a]	−57.4	−58.7	−55.1	−58.7	−60.9	−56.6
121: CHF2CO	−90.3[a]	−105.9	−107.2	−104.2	−105.7	−107.9	−103.4
122: CF3CO	−145.6[a]	−158.3	−159.7	−159.6	−157.5	−159.8	−155.1
125: C3F6	−277.6[a]	−272.8	−275.6	−276.8	−269.4	−273.8	−270.3

a N.L.Haworth, M.H.Smith, G.B.Bacskay, and J.C.Mackie, J.Phys.Chem.A 104, 7600 (2000).

Table S24: Benchmark Results for the G2 Subset of the G2G3-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
CH radical, doublet, C0v	142.5[a]	140.0	139.9	136.0	138.1	137.9	134.7
Triplet methylene (CH2), C2v, 3-B1	93.7[a]	91.9	91.6	89.6	90.3	89.8	88.7
Singlet methylene (CH2), C2v, 1-A1	102.8[a]	103.9	103.7	98.4	101.3	100.8	96.9
Methyl radical (CH3), D3h	35.0[a]	33.7	33.3	31.8	35.2	34.5	32.3
Methane (CH4), Td	−17.9[a]	−19.3	−19.9	−19.3	−18.0	−19.1	−17.8
NH, triplet, C0v	85.2[a]	85.4	85.3	80.7	79.8	79.6	76.2
NH2 radical, C2v, 2-B1	45.1[a]	47.8	47.5	41.1	39.3	38.9	35.4
Ammonia (NH3), C3v	−11.0[a]	−5.9	−6.3	−12.0	−11.2	−12.0	−11.3
OH radical, C0v	9.4[a]	5.3	5.3	4.0	4.3	4.2	3.1
Water (H2O), C2v	−57.8[a]	−56.5	−56.7	−58.9	−58.5	−58.8	−58.0
Hydrogen fluoride (HF), C0v	−65.1[a]	−63.3	−63.4	−68.6	−64.9	−65.0	−65.2
Acetylene (C2H2), D0h	54.2[a]	54.2	53.6	53.9	54.7	53.7	54.2
Ethylene (H2C=CH2), D2h	12.5[a]	12.9	11.7	12.9	13.9	12.0	13.7
Ethane (H3C-CH3), D3d	−20.1[a]	−21.2	−23.0	−20.8	−20.8	−23.6	−20.0
Cyano radical (CN), C0v, 2-Sigma+	104.9[a]	111.6	111.4	109.8	102.7	102.3	101.1
Hydrogen cyanide (HCN), C0v	31.5[a]	26.1	25.7	25.5	25.3	24.7	25.4
Carbon monoxide (CO), C0v	−26.4[a]	−20.3	−20.5	−19.3	−21.5	−21.8	−17.5
HCO radical, bent, Cs	10.0[a]	0.1	−0.3	−0.2	−4.4	−4.9	−3.1
Formaldehyde (H2C=O), C2v	−26.0[a]	−30.3	−30.9	−30.0	−31.9	−32.8	−32.3
Methanol (CH3-OH), Cs	−48.0[a]	−49.3	−50.3	−50.1	−49.8	−51.4	−49.7
N2 molecule, D0h	0.0[a]	2.8	2.6	1.5	2.6	2.2	4.6
Hydrazine (H2N-NH2), C2	22.8[a]	18.5	17.4	17.6	16.5	14.7	16.6
NO radical, C0v, 2-Pi	21.6[a]	24.5	24.4	24.1	15.2	14.9	15.6
O2 molecule, D0h, triplet	0.0[a]	2.0	1.9	3.9	−2.6	−2.8	0.4
Hydrogen peroxide (HO-OH), C2	−32.5[a]	−35.3	−35.8	−34.8	−36.9	−37.6	−36.0
F2 molecule, D0h	0.0[a]	0.6	0.5	−0.9	−1.7	−1.8	−1.3
Carbon dioxide (CO2), D0h	−94.1[a]	−80.5	−80.9	−81.8	−87.7	−88.4	−89.4
CF4, Td	−223.0[a]	−220.5	−221.4	−227.1	−215.8	−217.3	−216.8
COF2, C2v	−152.7[a]	−136.5	−137.1	−137.9	−138.7	−139.7	−141.0
N2O, Cs	19.6[a]	21.2	20.8	19.5	20.7	19.9	20.9
NF3, C3v	−31.6[a]	−30.1	−30.7	−26.5	−35.9	−36.9	−37.1
O3 (ozone), C2v	34.1[a]	37.9	37.5	39.7	48.7	48.1	52.8
F2O, C2v	5.9[a]	5.3	5.1	7.0	7.2	6.7	8.1
C2F4 (F2C=CF2), D2h	−157.4[a]	−156.3	−157.7	−158.2	−155.9	−158.2	−156.5
CF3CN, C3v	−118.4[a]	−125.5	−127.0	−127.8	−125.1	−127.5	−123.5
Propyne (C3H4), C3v	44.2[a]	44.5	42.9	44.3	44.1	41.5	44.3
Allene (C3H4), D2d	45.5[a]	45.9	44.3	45.7	45.5	42.9	45.7
Cyclopropene (C3H4), C2v	66.2[a]	67.4	65.7	66.9	65.5	62.8	65.6
Propene (C3H6), Cs	4.8[a]	4.7	2.3	4.8	5.0	1.1	5.0
Cyclopropane (C3H6), D3h	12.7[a]	9.9	7.6	10.7	10.1	6.3	11.9
Propane (C3H8), C2v	−25.0[a]	−25.5	−28.7	−25.2	−25.4	−30.4	−24.8
Trans-1,3-butadiene (C4H6), C2h	26.3[a]	29.4	26.3	29.3	30.3	25.5	29.8
2-Butyne (C4H6), D3h, eclipsed	34.8[a]	35.1	32.4	35.1	33.8	29.6	34.6
Methylenecyclopropane (C4H6), C2v	47.9[a]	45.0	42.0	45.4	43.7	39.1	44.7
Bicyclo[1.1.0]butane (C4H6), C2v	51.9[a]	62.0	59.0	61.7	59.9	55.2	61.4
Cyclobutene (C4H6), C2v	37.4[a]	41.3	38.2	40.2	40.8	35.8	40.0
Cyclobutane (C4H8), D2d	6.8[a]	3.0	−1.0	2.4	2.9	−3.3	3.3
Isobutene (C4H8), C2v	−4.0[a]	−4.3	−8.2	−4.0	−3.9	−10.0	−3.6
Trans-butane (C4H10), C2h	−30.0[a]	−30.1	−34.8	−29.9	−30.3	−37.5	−29.8
Isobutane (C4H10), C3v	−32.1[a]	−31.8	−36.7	−31.9	−31.3	−38.8	−31.1
Spiropentane (C5H8), D2d	44.3[a]	42.8	38.4	43.6	41.0	34.3	42.7
Benzene (C6H6), D6h	19.7[a]	18.8	13.8	19.7	18.5	10.6	18.9
Difluoromethane (H2CF2), C2v	−107.7[a]	−110.9	−111.6	−109.4	−106.6	−107.8	−107.1
Trifluoromethane (HCF3), C3v	−166.6[a]	−166.8	−167.6	−168.0	−162.0	−163.3	−162.4
Methylamine (H3C-NH2), Cs	−5.5[a]	−4.1	−5.6	−6.3	−5.8	−8.1	−5.6
Acetonitrile (CH3-CN), C3v	18.0[a]	17.5	16.2	17.3	15.3	13.2	15.3
Nitromethane (CH3-NO2), Cs	−17.8[a]	−17.3	−19.1	−17.0	−15.7	−18.5	−13.5
Methylnitrite (CH3-O-N=O), NOCH trans, ONOC cis, Cs	−15.9[a]	−23.4	−25.1	−22.8	−25.9	−28.7	−25.9
Formic acid (HCOOH), HOCO cis, Cs	−90.5[a]	−86.9	−87.8	−88.0	−88.2	−89.7	−89.6
Methyl formate (HCOOCH3), OCOC cis, Cs	−85.0[a]	−81.4	−83.5	−82.1	−79.4	−82.6	−82.1
Acetamide (CH3CONH2), C1	−57.0[a]	−50.7	−53.2	−55.6	−57.4	−61.4	−59.1
Aziridine (cyclic CH2-NH-CH2 ring), Cs	30.2[a]	36.3	34.3	36.0	35.4	32.3	38.0

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Table S24: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Cyanogen (NCCN), D0h	73.3[a]	74.8	73.9	76.2	68.2	66.7	70.5
Dimethylamine, (CH3)2NH, Cs	−4.4[a]	−5.1	−7.9	−4.2	−2.2	−6.5	−3.2
Trans-ethylamine (CH3-CH2-NH2), Cs	−11.3[a]	−8.9	−11.7	−10.9	−12.1	−16.5	−11.9
Ketene (H2C=C=O), C2v	−11.4[a]	−5.1	−6.1	−6.5	−11.0	−12.6	−10.9
Oxirane (cyclic CH2-O-CH2), C2v	−12.6[a]	−13.3	−14.8	−10.1	−8.8	−11.2	−5.1
Acetaldehyde (CH3CHO), Cs	−39.7[a]	−44.2	−45.8	−44.1	−46.5	−49.1	−46.7
Glyoxal (O=CH-CH=O), trans, C2h	−50.7[a]	−59.1	−60.6	−58.5	−61.8	−64.2	−62.6
Ethanol (CH3CH2OH), trans, Cs	−56.2[a]	−56.9	−59.1	−56.7	−57.2	−60.8	−56.6
Dimethyl ether (CH3-O-CH3), C2v	−44.0[a]	−45.6	−47.7	−45.9	−42.8	−46.2	−44.3
Vinyl fluoride (H2C=CHF), Cs	−33.2[a]	−32.3	−33.5	−31.7	−32.2	−34.1	−32.6
Acrylonitrile (H2C=CHCN), Cs	43.2[a]	45.6	43.6	45.3	43.7	40.5	43.6
Acetone (CH3-CO-CH3), C2v	−51.9[a]	−57.4	−60.4	−57.8	−59.3	−63.9	−59.3
Acetic acid (CH3COOH), single bonds trans, Cs	−103.4[a]	−101.0	−103.0	−102.2	−102.7	−106.0	−103.8
Acetyl fluoride (CH3COF), HCCO cis, Cs	−105.7[a]	−100.0	−101.6	−100.2	−103.0	−105.7	−104.4
Isopropanol, (CH3)2CH-OH, gauche isomer, C1	−65.2[a]	−66.3	−70.1	−67.0	−66.6	−72.5	−66.5
Methyl ethyl ether (CH3-CH2-O-CH3), trans, Cs	−51.7[a]	−53.4	−56.8	−53.0	−50.6	−56.0	−51.9
Trimethyl amine, (CH3)3N, C3v	−5.7[a]	−8.0	−12.4	−4.5	−0.1	−6.7	−2.9
Furan (cyclic C4H4O), C2v	−8.3[a]	−2.9	−5.9	−3.4	−2.7	−7.4	−2.2
Pyrrole (planar cyclic C4H4NH), C2v	25.9[a]	33.7	30.2	35.6	32.0	26.3	33.9
Pyridine (cyclic C5H5N), C2v	33.6[a]	30.8	26.3	33.5	29.4	22.3	31.8
H2 molecule, D0h	0.0[a]	−3.4	−3.5	−0.1	−0.0	−0.1	0.0
CCH radical, C0v	135.1[a]	139.6	139.1	149.2	141.1	140.4	141.9
C2H3 radical, Cs, 2-A'	71.6[a]	67.4	66.6	66.5	66.4	64.9	66.1
CH3CO radical, HCCO cis, Cs, 2-A'	−2.4[a]	−16.0	−17.2	−15.3	−19.9	−21.9	−17.6
H2COH radical, C1	−4.1[a]	−10.8	−11.5	−11.7	−12.2	−13.5	−11.3
CH3O radical, Cs, 2-A'	4.1[a]	0.4	−0.4	1.3	1.3	−0.0	1.7
CH3CH2O radical, Cs, 2-A"	−3.7[a]	−5.6	−7.6	−6.4	−5.2	−8.3	−6.4
C2H5 radical, staggered, Cs, 2-A'	28.9[a]	24.8	23.3	23.9	24.6	22.3	23.7
(CH3)2CH radical, Cs, 2-A'	21.5[a]	14.3	11.6	14.1	13.4	9.0	13.2
t-Butyl radical, (CH3)3C, C3v	12.3[a]	3.2	−1.1	3.6	2.4	−4.2	2.9
NO2 radical, C2v, 2-A1	7.9[a]	5.1	4.7	3.5	−1.5	−2.2	−1.3

a L.A.Curtiss, K.Raghavachari, P.C.Redfern, and J.A.Pople, J.Chem.Phys. 106, 1063 (1997).

Table S25: Benchmark Results for the G3 Subset of the G2G3-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Methylallene C1	38.8[a]	38.1	35.2	38.1	37.6	33.0	38.0
C5H8 (Isoprene) C1	18.0[a]	21.4	16.6	21.7	22.6	15.2	21.9
Cyclopentane twist C2v	−18.3[a]	−19.7	−25.5	−19.3	−20.8	−29.8	−19.7
n-Pentane C2v	−35.1[a]	−34.7	−40.8	−34.7	−35.2	−44.6	−34.9
Neopentane Td	−40.2[a]	−39.6	−46.4	−40.2	−37.6	−48.1	−38.2
1,3-Cyclohexadiene C2	25.4[a]	25.9	20.0	26.5	24.8	15.6	24.9
1,4-Cyclohexadiene D2h	25.0[a]	26.8	21.0	26.8	24.8	15.8	24.6
Cyclohexane chair D3d	−29.5[a]	−27.1	−35.0	−27.2	−28.5	−40.5	−28.5
n-Hexane C2h	−39.9[a]	−39.2	−46.9	−39.4	−40.0	−51.6	−39.9
3-Methylpentane Cs	−41.1[a]	−39.9	−48.2	−40.2	−39.5	−52.0	−39.9
Toluene stag Cs	12.0[a]	9.5	2.9	10.3	9.6	−0.6	9.3
n-Heptane C2v	−44.9[a]	−43.8	−53.0	−44.2	−44.8	−58.7	−45.0
Cyclooctatetraene C2v	70.7[a]	75.2	67.2	74.3	73.9	61.6	72.1
n-Octane C2h	−49.9[a]	−48.3	−59.0	−48.9	−49.7	−65.8	−50.1
Naphthalene D2h	35.9[a]	34.8	25.3	35.8	35.7	21.0	35.7
Azulene Cs	69.1[a]	83.4	74.0	82.7	82.5	68.1	81.6
Z-Methylacetate Cs	−98.4[a]	−95.6	−98.8	−96.7	−93.8	−99.0	−96.7
tert-Butanol Cs	−74.7[a]	−76.8	−82.4	−78.1	−75.9	−84.5	−76.1
Anilin Cs	20.8[a]	25.2	19.0	22.0	22.3	12.7	22.0
Phenol (planar) Cs	−23.0[a]	−21.7	−27.2	−22.4	−23.6	−32.3	−23.2
Divinylether Cs	−3.3[a]	4.5	1.2	3.9	4.6	−0.6	2.9
Tetrahydrofuran C2	−44.0[a]	−47.9	−52.5	−48.9	−46.3	−53.5	−47.3
Cyclopentanone C2	−45.9[a]	−55.0	−60.6	−54.7	−57.5	−66.1	−56.9
Benzoquinone D2h	−29.4[a]	−32.5	−37.9	−31.6	−32.9	−41.3	−32.0
Pyrimidine C2v	46.8[a]	44.5	40.4	48.0	41.9	35.4	43.8
N==C-CH2-CH2-C==N 1,2-Dicyanoethane C2h	50.1[a]	47.7	44.0	47.3	43.4	37.7	43.4
Pyrazin D2h	46.9[a]	44.9	40.9	50.0	42.0	35.5	47.8
CH3-C(=O)-C==CH (Acetylacetylene) Cs	15.6[a]	11.2	8.5	10.9	9.8	5.5	10.2
CH3-CH=CH-CHO (Crotonaldehyd) Cs	−24.0[a]	−27.9	−31.5	−27.9	−29.5	−35.1	−30.0
Acetic anhydride C2	−136.8[a]	−139.5	−143.9	−139.7	−138.8	−145.7	−142.3
(CH3)2CH-CN (Isobutanenitrile) Cs	5.6[a]	5.1	0.8	4.6	3.5	−3.1	3.6
Methylethylketone Cs	−57.1[a]	−61.8	−66.2	−62.7	−63.4	−70.3	−64.0
2-Methylpropionaldehyde Cs	−51.6[a]	−56.0	−60.7	−56.2	−57.1	−64.3	−57.5
1,4-Dioxane C2h	−75.5[a]	−76.5	−81.8	−79.3	−72.4	−80.5	−76.3
Tetrahydropyrrole Cs	−0.8[a]	0.8	−4.4	−0.7	1.5	−6.6	−0.3
Nitro-s-butane C1	−39.1[a]	−36.2	−42.9	−38.0	−34.8	−44.9	−33.7
Diethylether C2v	−60.3[a]	−61.1	−65.9	−60.2	−58.4	−65.7	−59.4
CH3-CH(OCH3)2 (Acetal) C1	−93.1[a]	−96.4	−102.2	−97.6	−88.7	−97.5	−93.1
t-Butylamine Cs	−28.9[a]	−22.3	−28.7	−27.4	−24.6	−34.3	−25.6
N-Methylpyrrole Cs	24.6[a]	31.1	26.0	36.4	33.5	25.6	34.2
Tetrahydropyran Cs	−53.4[a]	−53.1	−59.6	−54.5	−51.7	−61.8	−53.8
Diethylketone C2v	−61.6[a]	−66.0	−71.9	−66.9	−67.5	−76.7	−67.9
Isopropylacetate C1	−115.1[a]	−113.7	−120.2	−114.2	−111.3	−121.1	−113.8
Perhydropyridine (Piperidine) Cs	−11.3[a]	−6.7	−14.1	−5.7	−7.2	−18.5	−8.2
t-Butylmethylether Cs	−67.8[a]	−70.5	−77.9	−72.0	−66.1	−77.2	−68.3
1,3-Difluorobenzene C2v	−73.9[a]	−72.9	−78.0	−72.5	−74.0	−82.0	−74.0
1,4-Difluorobenzene D2h	−73.3[a]	−72.6	−77.6	−72.2	−73.5	−81.5	−73.8
Fluorobenzene C2v	−27.7[a]	−27.3	−32.3	−26.7	−28.0	−35.9	−27.9
Diisopropylether C2	−76.3[a]	−77.7	−86.2	−78.1	−74.1	−86.8	−76.2
C2F6 D3d	−321.3[a]	−317.5	−319.7	−323.8	−310.5	−314.0	−311.6
CF3 C2v	−111.3[a]	−123.2	−123.8	−124.1	−122.6	−123.6	−120.0
Phenyl radical C2v	81.2[a]	71.5	67.0	72.9	70.4	63.2	72.4

a G3 values derived from the data in: L.A.Curtiss, K.Raghavachari, P.C.Redfern, V.Rassolov, and J.A.Pople, J.Chem.Phys. 112, 7374 (2000).

Table S26: Benchmark Results for the ALKANES28 Subset of the G2G3-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Methane	−17.8[a]	−19.3	−19.9	−19.3	−18.0	−19.1	−17.8
Ethane	−20.0[a]	−21.2	−23.0	−20.8	−20.8	−23.6	−20.0
Propane	−25.0[a]	−25.5	−28.7	−25.2	−25.4	−30.4	−24.8
n-Butane	−30.0[a]	−30.1	−34.8	−29.9	−30.3	−37.5	−29.8
n-Pentane	−35.1[a]	−34.7	−40.8	−34.7	−35.2	−44.6	−34.9
n-Hexane	−39.9[a]	−39.2	−46.9	−39.4	−40.0	−51.6	−39.9
n-Heptane	−44.9[a]	−43.8	−53.0	−44.2	−44.8	−58.7	−45.0
n-Octane	−49.9[a]	−48.3	−59.0	−48.9	−49.7	−65.8	−50.1
n-Nonane	−54.5[a]	−52.9	−65.1	−53.7	−54.5	−72.9	−55.1
n-Decane	−59.6[a]	−57.5	−71.2	−58.4	−59.3	−79.9	−60.2
n-Undecane	−64.8[a]	−62.0	−77.3	−63.2	−64.2	−87.0	−65.3
n-Dodecane	−69.2[a]	−66.6	−83.4	−67.9	−69.0	−94.1	−70.4
n-Tridecane	−74.5[b]	−71.1	−89.4	−72.7	−73.8	−101.2	−75.4
n-Tetradecane	−79.4[b]	−75.7	−95.5	−77.4	−78.7	−108.3	−80.5
n-Pentadecane	−84.8[b]	−80.3	−101.6	−82.1	−83.5	−115.3	−85.6
n-Hexadecane	−89.6[a]	−84.8	−107.7	−86.9	−88.4	−122.4	−90.6
2-Methylpropane	−32.1[a]	−31.8	−36.7	−31.9	−31.3	−38.8	−31.1
2-Methylbutane	−36.7[a]	−35.9	−42.4	−36.1	−35.5	−45.4	−35.5
2-Methylpentane	−41.8[a]	−40.4	−48.5	−40.9	−40.3	−52.5	−40.6
2-Methylhexane	−46.5[a]	−45.0	−54.6	−45.6	−45.1	−59.6	−45.7
2-Methylheptane	−51.5[a]	−49.5	−60.7	−50.4	−50.0	−66.7	−50.8
2-Methylnonane	−62.1[a]	−58.7	−72.9	−59.9	−59.6	−80.9	−61.0

a J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986. b P.C.Redfern, P.Zapol, L.A.Curtiss, and K.Raghavachari, J.Phys.Chem.A 104, 5850 (2000).

Table S27: Benchmark Results for the ALKANES28 Subset of the G2G3-CHNOF Set. Enthalpy Changes at 298 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
2-Methylpropane	−2.1[a]	−1.7	−1.9	−1.9	−1.0	−1.3	−1.3
2-Methylbutane	−1.6[a]	−1.2	−1.6	−1.4	−0.3	−0.9	−0.7
2-Methylpentane	−1.8[a]	−1.2	−1.7	−1.5	−0.3	−0.9	−0.7
2-Methylhexane	−1.6[a]	−1.2	−1.7	−1.5	−0.3	−0.9	−0.7
2-Methylheptane	−1.6[a]	−1.2	−1.7	−1.5	−0.3	−0.9	−0.7
2-Methylnonane	−2.5[a]	−1.2	−1.7	−1.5	−0.3	−0.9	−0.7

a J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986.

Table S28: Benchmark Results for the TAE140 Subset of the W4-11-CHNOF Set. Atomization Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
The OMx and OMx-D3T energies are uncorrected atomization enthalpies at 298 K							
h2	109.5[a]	106.3	106.4	108.2	104.0	104.1	109.1
ch2-trip	190.7[a]	182.9	183.1	194.3	184.8	185.2	195.3
ch3	307.9[a]	293.3	293.7	310.6	291.9	292.7	309.3
ch4	420.4[a]	398.5	399.2	422.7	397.3	398.4	420.8
c2h6	713.1[a]	674.8	676.6	713.4	674.4	677.3	712.0
propane	1007.9[a]	953.8	957.0	1007.2	953.7	958.7	1005.8
ch2-sing	181.5[a]	170.2	170.5	184.4	172.6	173.1	185.5
ch	84.2[a]	82.8	82.9	90.3	84.6	84.8	91.5
c2h5f	721.5[a]	687.5	689.3	721.0	685.1	688.1	719.7
ch3nh2	582.3[a]	546.8	548.2	582.2	547.3	549.7	580.2
ch3f	423.0[a]	405.8	406.5	424.3	402.2	403.3	422.8
propene	861.6[a]	819.9	822.3	861.0	819.6	823.4	860.2
nh3	298.0[a]	273.1	273.6	296.6	278.0	278.7	296.5
ethanol	811.2[a]	768.1	770.3	808.5	767.7	771.3	807.3
ch3nh	474.6[a]	449.3	450.4	477.2	451.4	453.3	479.1
c2h4	564.1[a]	537.2	538.4	563.7	536.0	537.9	562.4
methanol	513.5[a]	486.3	487.3	512.8	485.9	487.6	511.7
nh2	182.6[a]	169.2	169.5	185.7	176.6	177.1	191.0
nh	83.1[a]	79.7	79.8	88.2	84.9	85.1	92.7
ch2nh2	482.3[a]	461.5	462.6	488.6	464.7	466.6	488.0
h2o	233.0[a]	219.9	220.1	231.8	220.0	220.4	230.0
hf	141.6[a]	132.6	132.6	144.0	135.2	135.3	139.9
ch2ch	446.1[a]	430.2	431.1	450.3	431.4	432.8	450.6
oh	107.2[a]	106.1	106.2	111.1	106.5	106.6	112.0
propyne	705.6[a]	675.2	676.8	704.3	675.4	678.0	704.1
acetaldehyde	677.9[a]	652.8	654.4	681.3	654.9	657.5	683.8
allene	704.1[a]	675.2	676.8	703.9	675.5	678.1	703.7
c2h3f	573.9[a]	548.4	549.6	570.3	548.2	550.2	570.9
oxirane	651.5[a]	622.3	623.8	648.4	617.5	620.0	642.6
ch2f2	437.7[a]	420.5	421.3	435.4	416.4	417.7	433.1
ch2c	359.9[a]	359.7	360.4	373.5	359.4	360.5	371.5
n2h4	438.3[a]	408.8	409.9	439.4	411.0	412.9	439.9
ch2nh	439.4[a]	418.2	419.1	441.2	421.4	422.9	441.4
acetic	804.0[a]	768.3	770.4	799.1	767.9	771.2	799.4
c2h2	405.5[a]	390.9	391.5	405.5	390.5	391.5	405.5
h2co	374.7[a]	364.4	364.9	377.4	365.5	366.4	379.7
h2cn	343.7[a]	333.0	333.6	347.0	334.1	335.1	347.7
t-hcoh	322.5[a]	323.9	324.4	338.4	322.2	323.1	331.5
c-hcoh	317.6[a]	322.5	323.1	335.0	316.0	316.9	324.4
ketene	533.5[a]	508.8	509.8	525.8	514.1	515.7	530.6
formic	501.9[a]	477.6	478.5	494.6	477.0	478.5	495.1
hcnh	336.2[a]	326.1	326.7	343.1	334.6	335.6	348.2
glyoxal	635.1[a]	622.9	624.4	640.4	625.2	627.6	644.2
hcof	403.7[a]	383.9	384.5	392.7	385.9	386.9	398.0
cf4	478.8[a]	463.5	464.4	478.9	461.3	462.8	468.9
hccf	398.5[a]	384.4	385.0	394.9	387.5	388.5	398.0
hcn	313.4[a]	309.6	310.0	319.2	307.8	308.4	318.8
hnc	298.2[a]	292.0	292.5	306.0	305.8	306.5	321.7
cch	266.2[a]	254.0	254.4	263.1	256.5	257.2	263.4
hco	279.4[a]	281.2	281.5	287.7	284.6	285.1	290.0
co	259.7[a]	248.2	248.4	248.5	248.3	248.6	247.0
oxirene	456.1[a]	439.4	440.4	453.9	439.5	441.1	453.1
f2co	420.6[a]	400.9	401.5	408.1	403.5	404.5	412.4
hocn	410.1[a]	392.8	393.5	404.3	392.8	393.9	407.3
hooh	269.1[a]	254.6	255.0	266.3	253.8	254.6	265.6
t-n2h2	296.5[a]	286.3	286.9	303.6	298.6	299.7	309.4
hnco	434.7[a]	399.7	400.4	415.5	407.5	408.7	425.0
c-n2h2	291.1[a]	289.5	290.1	305.7	296.4	297.4	307.4
cf2	258.8[a]	264.2	264.5	264.9	263.6	264.1	259.7
co2	390.1[a]	366.5	366.9	372.1	372.6	373.3	380.9
fccf	386.1[a]	373.1	373.8	379.5	379.8	380.9	386.6

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Table S28: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
dioxirane	410.0[a]	398.6	399.4	404.3	383.6	384.9	393.6
cf	132.7[a]	137.3	137.4	135.0	137.1	137.3	133.5
nccn	502.0[a]	492.5	493.5	499.9	493.1	494.7	504.0
n2	228.5[a]	223.2	223.4	227.5	213.6	214.0	222.8
n2h	224.9[a]	230.2	230.6	239.5	233.3	233.9	240.3
hoo	175.5[a]	173.4	173.6	178.4	170.2	170.6	174.9
hcno	365.0[a]	349.7	350.4	365.1	352.0	353.2	363.1
honc	350.1[a]	340.9	341.7	355.8	348.9	350.1	371.3
hno	205.9[a]	204.0	204.3	214.4	213.8	214.3	220.6
hof	158.7[a]	148.2	148.4	153.5	145.9	146.2	152.0
c-hono	312.2[a]	304.8	305.4	316.4	309.1	310.2	319.6
t-hono	312.6[a]	300.2	300.9	310.0	306.2	307.3	317.1
hnnn	331.8[a]	316.9	317.7	326.9	301.4	302.7	325.4
cn	181.3[a]	172.2	172.4	176.7	179.6	180.0	185.3
no	152.7[a]	147.7	147.8	150.4	156.2	156.5	159.2
n2o	270.8[a]	259.6	260.1	268.2	248.6	249.4	264.9
c-hooo	233.1[a]	227.6	228.1	234.0	220.0	221.0	226.2
o2	120.8[a]	115.7	115.8	116.0	121.6	121.8	120.4
f2	39.0[a]	35.1	35.2	37.7	33.0	33.1	32.8
t-hooo	233.3[a]	221.9	222.4	229.1	219.3	220.2	225.7
no2	227.9[a]	225.0	225.4	231.5	229.4	230.1	236.4
of	53.1[a]	48.0	48.1	47.6	46.9	47.1	47.5
c2	147.0[a]	145.4	145.6	150.6	123.5	124.0	124.8
f2o	93.8[a]	91.0	91.3	91.9	86.4	86.8	87.8
fo2	134.7[a]	115.1	115.4	116.0	116.6	117.1	119.0
foof	152.4[a]	143.1	143.6	144.8	133.7	134.6	137.8
o3	147.4[a]	139.6	140.0	141.9	129.5	130.0	128.9
The OMx and OMx-D3T energies are corrected by excluding ZPVE and thermal contributions							
h2	109.5[a]	110.9	111.0	108.2	108.9	109.0	109.1
ch2-trip	190.7[a]	191.5	191.8	194.3	193.6	194.0	195.3
ch3	307.9[a]	308.3	308.7	310.6	306.5	307.3	309.3
ch4	420.4[a]	421.7	422.4	422.7	420.2	421.3	420.8
c2h6	713.1[a]	712.4	714.2	713.4	711.5	714.4	712.0
propane	1007.9[a]	1005.6	1008.8	1007.2	1004.8	1009.8	1005.8
ch2-sing	181.5[a]	178.5	178.8	184.4	181.0	181.5	185.5
ch	84.2[a]	86.0	86.2	90.3	88.0	88.2	91.5
c2h5f	721.5[a]	721.2	723.0	721.0	718.4	721.4	719.7
ch3nh2	582.3[a]	578.6	580.0	582.2	578.4	580.7	580.2
ch3f	423.0[a]	425.3	426.0	424.3	421.5	422.6	422.8
propene	861.6[a]	859.7	862.2	861.0	859.0	862.8	860.2
nh3	298.0[a]	290.4	290.9	296.6	294.9	295.6	296.5
ethanol	811.2[a]	807.0	809.2	808.5	806.7	810.3	807.3
ch3nh	474.6[a]	473.9	475.0	477.2	475.5	477.4	479.1
c2h4	564.1[a]	562.8	563.9	563.7	561.3	563.3	562.4
methanol	513.5[a]	511.0	512.0	512.8	510.9	512.6	511.7
nh2	182.6[a]	178.7	178.9	185.7	186.1	186.6	191.0
nh	83.1[a]	83.4	83.5	88.2	88.8	88.9	92.7
ch2nh2	482.3[a]	485.9	487.1	488.6	488.9	490.8	488.0
h2o	233.0[a]	229.4	229.6	231.8	230.4	230.7	230.0
hf	141.6[a]	137.1	137.2	144.0	139.9	140.0	139.9
ch2ch	446.1[a]	448.6	449.5	450.3	449.8	451.3	450.6
oh	107.2[a]	109.9	110.0	111.1	110.7	110.8	112.0
propyne	705.6[a]	703.1	704.7	704.3	703.2	705.8	704.1
acetaldehyde	677.9[a]	680.5	682.1	681.3	682.5	685.1	683.8
allene	704.1[a]	702.8	704.5	703.9	702.9	705.5	703.7
c2h3f	573.9[a]	570.1	571.3	570.3	569.7	571.7	570.9
oxirane	651.5[a]	650.4	651.9	648.4	645.5	648.0	642.6
ch2f2	437.7[a]	436.0	436.8	435.4	431.8	433.1	433.1
ch2c	359.9[a]	372.5	373.2	373.5	372.1	373.3	371.5
n2h4	438.3[a]	434.7	435.9	439.4	436.2	438.0	439.9
ch2nh	439.4[a]	438.0	438.9	441.2	440.8	442.3	441.4
acetic	804.0[a]	797.3	799.4	799.1	797.1	800.5	799.4
c2h2	405.5[a]	404.7	405.3	405.5	404.4	405.4	405.5
h2co	374.7[a]	377.5	378.0	377.4	378.7	379.6	379.7
h2cn	343.7[a]	345.8	346.5	347.0	346.6	347.7	347.7

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Table S28: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
t-hcoh	322.5[a]	335.8	336.4	338.4	334.7	335.6	331.5
c-hcoh	317.6[a]	334.3	334.9	335.0	328.2	329.1	324.4
ketene	533.5[a]	524.5	525.4	525.8	529.9	531.5	530.6
formic	501.9[a]	492.9	493.8	494.6	492.8	494.3	495.1
hcnh	336.2[a]	338.7	339.3	343.1	346.8	347.9	348.2
glyoxal	635.1[a]	640.7	642.1	640.4	642.6	645.0	644.2
hcof	403.7[a]	393.6	394.2	392.7	395.7	396.7	398.0
cf4	478.8[a]	470.3	471.2	478.9	468.1	469.6	468.9
hccf	398.5[a]	394.3	395.0	394.9	397.6	398.7	398.0
hcn	313.4[a]	318.3	318.7	319.2	316.2	316.9	318.8
hnc	298.2[a]	300.1	300.5	306.0	314.0	314.7	321.7
cch	266.2[a]	261.0	261.4	263.1	275.2	275.9	263.4
hco	279.4[a]	287.5	287.9	287.7	291.2	291.8	290.0
co	259.7[a]	250.6	250.8	248.5	250.8	251.1	247.0
oxirene	456.1[a]	454.0	454.9	453.9	454.4	455.9	453.1
f2co	420.6[a]	406.6	407.3	408.1	409.4	410.5	412.4
hocn	410.1[a]	402.7	403.4	404.3	402.8	403.9	407.3
hooh	269.1[a]	266.5	267.0	266.3	266.4	267.2	265.6
t-n2h2	296.5[a]	300.0	300.7	303.6	312.1	313.1	309.4
hnco	434.7[a]	409.4	410.1	415.5	417.1	418.2	425.0
c-n2h2	291.1[a]	303.1	303.7	305.7	309.6	310.6	307.4
cf2	258.8[a]	267.1	267.4	264.9	266.4	267.0	259.7
co2	390.1[a]	371.5	371.9	372.1	377.9	378.6	380.9
fccf	386.1[a]	378.5	379.2	379.5	385.1	386.2	386.6
dioxirane	410.0[a]	414.3	415.2	404.3	399.1	400.5	393.6
cf	132.7[a]	138.6	138.7	135.0	138.4	138.6	133.5
nccn	502.0[a]	501.2	502.1	499.9	501.3	502.9	504.0
n2	228.5[a]	226.1	226.3	227.5	216.2	216.5	222.8
n2h	224.9[a]	236.7	237.1	239.5	239.3	240.0	240.3
hoo	175.5[a]	179.9	180.2	178.4	177.0	177.4	174.9
hcno	365.0[a]	359.6	360.3	365.1	361.6	362.8	363.1
honc	350.1[a]	350.3	351.1	355.8	358.5	359.7	371.3
hno	205.9[a]	211.0	211.3	214.4	220.8	221.4	220.6
hof	158.7[a]	154.6	154.8	153.5	152.6	153.0	152.0
c-hono	312.2[a]	314.0	314.6	316.4	318.6	319.7	319.6
t-hono	312.6[a]	309.2	309.8	310.0	315.6	316.6	317.1
hnnn	331.8[a]	326.6	327.4	326.9	310.5	311.8	325.4
cn	181.3[a]	174.7	175.0	176.7	182.1	182.5	185.3
no	152.7[a]	149.9	150.0	150.4	158.4	158.7	159.2
n2o	270.8[a]	264.3	264.8	268.2	253.0	253.8	264.9
c-hooo	233.1[a]	235.9	236.4	234.0	228.6	229.5	226.2
o2	120.8[a]	117.6	117.7	116.0	123.5	123.7	120.4
f2	39.0[a]	36.5	36.6	37.7	34.3	34.4	32.8
t-hooo	233.3[a]	230.2	230.7	229.1	227.8	228.6	225.7
no2	227.9[a]	228.7	229.2	231.5	233.2	233.9	236.4
of	53.1[a]	49.3	49.4	47.6	48.1	48.3	47.5
c2	147.0[a]	147.7	148.0	150.6	125.7	126.2	124.8
f2o	93.8[a]	93.7	94.0	91.9	88.9	89.3	87.8
fo2	134.7[a]	118.0	118.3	116.0	119.3	119.9	119.0
foof	152.4[a]	147.5	148.0	144.8	137.7	138.6	137.8
o3	147.4[a]	143.2	143.5	141.9	132.9	133.5	128.9

a A.Karton, S.Daon, J.M.Martin, Chem.Phys.Lett. 510, 165 (2011).

Table S29: Benchmark Results for the BDE99 Subset of the W4-11-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
The OMx and OMx-D3T energies are uncorrected atomization enthalpies at 298 K							
F–OOF→F+OOF	17.6[a]	28.0	28.2	28.8	17.1	17.5	18.8
FO–OF→FO+OF	46.2[a]	47.0	47.4	49.7	39.8	40.3	42.8
O–OF→O+OF	81.7[a]	67.1	67.3	68.5	69.6	70.0	71.5
OO–F→OO+F	13.9[a]	−0.6	−0.4	0.1	−5.0	−4.7	−1.5
F–OF→F+OF	40.7[a]	43.0	43.1	44.4	39.4	39.7	40.3
H–OF→H+OF	105.6[a]	100.2	100.3	105.9	98.9	99.1	104.5
HO–F→HO+F	51.5[a]	42.1	42.2	42.4	39.4	39.6	40.1
ON–O→ON+O	75.1[a]	77.3	77.6	81.0	73.2	73.6	77.2
N–NO→N+NO	118.1[a]	111.9	112.2	117.8	92.4	93.0	105.7
NN–O→NN+O	42.4[a]	36.4	36.7	40.7	35.0	35.5	42.0
trans-H–ONO→trans-H+ONO	84.8[a]	75.3	75.5	78.5	76.9	77.2	80.8
trans-HO–NO→trans-HO+NO	52.7[a]	46.4	46.8	48.4	43.6	44.2	46.0
H–NC→H+NC	116.8[a]	119.8	120.0	129.3	126.2	126.5	136.4
HN–C→HN+C	215.1[a]	212.3	212.6	217.7	220.9	221.4	229.0
HO–NC→HO+NC	61.6[a]	62.6	63.0	68.0	62.7	63.5	74.0
HN–CO→HN+CO	91.9[a]	71.8	72.2	78.7	74.3	75.0	85.3
HC–NO→HC+NO	128.0[a]	119.3	119.7	124.4	111.2	111.9	112.5
H–NO→H+NO	53.1[a]	56.3	56.5	64.0	57.6	57.9	61.4
HN–O→HN+O	122.8[a]	124.3	124.5	126.2	128.8	129.2	127.9
H3C–OH→H3C+OH	98.4[a]	86.9	87.3	91.1	87.5	88.3	90.4
trans-HC–OH→trans-HC+OH	131.1[a]	135.0	135.3	136.9	131.1	131.7	128.1
trans-HCO–H→trans-HCO+H	43.0[a]	42.7	42.9	50.6	37.7	38.0	41.6
H(O=)C–OH→H(O=)C+OH	115.3[a]	90.3	90.8	95.7	85.9	86.7	93.2
H2C=C–O→H2C=C+O	173.5[a]	149.1	149.4	152.3	154.8	155.2	159.0
H2C–C=O→H2C+C=O	83.0[a]	77.7	78.2	82.9	81.1	82.0	88.2
H(O=)C–C(=O)H→H(O=)C+C(=O)H	76.3[a]	60.5	61.3	65.0	56.1	57.3	64.2
H3C–C(=O)H→H3C+C(=O)H	90.6[a]	78.3	79.1	83.0	78.3	79.6	84.5
F2C–O→F2C+O	161.8[a]	136.7	137.0	143.2	139.9	140.4	152.7
F–C(=O)H→F+C(=O)H	124.3[a]	102.7	103.0	105.0	101.3	101.7	108.0
H–C(=O)H→H+C(=O)H	95.2[a]	83.2	83.4	89.7	80.9	81.2	89.7
H2C–O→H2C+O	183.9[a]	181.5	181.8	183.1	180.7	181.2	184.3
H–CO→H+CO	19.7[a]	33.0	33.1	39.2	36.3	36.6	43.0
HC–O→HC+O	195.2[a]	198.4	198.6	197.4	200.0	200.3	198.5
OC–O→OC+O	130.4[a]	118.3	118.5	123.5	124.4	124.8	133.9
H2N–CH2→H2N+CH2	108.9[a]	109.4	110.0	108.5	103.3	104.3	101.6
H–N(-H)CH2→H+N(-H)CH2	42.8[a]	43.3	43.5	47.4	43.3	43.7	46.6
H3C–NH→H3C+NH	83.7[a]	76.3	76.9	78.4	74.6	75.5	77.1
H–CH2NH→H+CH2NH	35.2[a]	31.1	31.3	36.0	30.0	30.4	37.7
H–CH2NH2→H+CH2NH2	100.0[a]	85.3	85.6	93.7	82.6	83.1	92.2
H3C(H-)N–H→H3C(H-)N+H	107.7[a]	97.5	97.8	105.1	95.9	96.3	101.1
H–C(H)=NH→H+C(H)=NH	103.2[a]	92.1	92.4	98.1	86.9	87.3	93.1
HN–CH→HN+CH	168.9[a]	163.7	164.0	164.6	165.0	165.6	164.0
H–NCH→H+NCH	22.8[a]	16.5	16.8	23.9	26.8	27.2	29.4
H–CN→H+CN	132.1[a]	137.4	137.6	142.5	128.1	128.4	133.5
HC–N→HC+N	229.2[a]	226.8	227.1	228.9	223.2	223.6	227.3
NC–CN→NC+CN	139.3[a]	148.1	148.7	146.5	133.8	134.7	133.4
trans-HOO–O→trans-HOO+O	57.8[a]	48.5	48.8	50.7	49.1	49.6	50.8
trans-HO–OO→trans-HO+OO	5.3[a]	0.0	0.4	2.0	−8.7	−8.2	−6.7
trans-H–OOO→trans-H+OOO	85.9[a]	82.3	82.4	87.3	89.9	90.2	96.8
OO–O→OO+O	26.6[a]	23.9	24.1	25.9	7.9	8.3	8.4
HOO–H→HOO+H	93.6[a]	81.2	81.4	87.9	83.6	83.9	90.7
HO–OH→HO+OH	54.7[a]	42.3	42.6	44.0	40.8	41.3	41.6
HO–O→HO+O	68.3[a]	67.2	67.4	67.3	63.7	64.0	62.9
H–OO→H+OO	54.7[a]	57.7	57.8	62.4	48.6	48.9	54.5
HO–H→HO+H	125.8[a]	113.7	113.8	120.7	113.5	113.7	118.0
HN–NN→HN+NN	20.2[a]	14.1	14.6	11.1	2.9	3.7	9.9
H2N–NH2→H2N+NH2	73.1[a]	70.4	71.0	68.1	57.7	58.7	57.9
trans-HN–NH→trans-HN+NH	130.3[a]	126.9	127.3	127.1	128.8	129.4	124.0
HN–N→HN+N	141.8[a]	150.5	150.8	151.3	148.3	148.8	147.5
H2N–H→H2N+H	115.4[a]	103.9	104.1	110.9	101.4	101.7	105.5
HN–H→HN+H	99.5[a]	89.5	89.6	97.4	91.7	92.0	98.3

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Table S29: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
H2CC–CH2→H2CC+CH2	153.4[a]	132.6	133.3	136.0	131.3	132.3	136.8
HCC–CH3→HCC+CH3	131.6[a]	127.9	128.6	130.6	127.0	128.1	131.4
H2C=(H)C–CH3→H2C=(H)C+CH3	107.6[a]	96.4	97.5	100.1	96.3	97.9	100.4
H2C=(H)C–F→H2C=(H)C+F	127.8[a]	118.2	118.5	120.1	116.8	117.3	120.3
H3C–CH3→H3C+CH3	97.3[a]	88.3	89.1	92.3	90.6	91.9	93.4
H2C–CH2→H2C+CH2	182.6[a]	171.4	172.1	175.0	166.4	167.5	171.7
H2C=C–H→H2C=C+H	86.2[a]	70.5	70.7	76.7	72.0	72.3	79.0
H–C(H)=CH→H+C(H)=CH	40.6[a]	39.3	39.6	44.8	40.9	41.3	45.1
H2C–C→H2C+C	169.2[a]	176.8	177.2	179.2	174.6	175.3	176.2
HCC–F→HCC+F	132.3[a]	130.4	130.6	131.8	131.0	131.3	134.6
HC–CF→HC+CF	181.5[a]	164.4	164.7	169.6	165.8	166.4	173.0
HCC–H→HCC+H	139.4[a]	136.9	137.1	142.4	134.0	134.3	142.1
HC–CH→HC+CH	237.1[a]	225.4	225.8	224.9	221.3	221.8	222.5
H3C–F→H3C+F	115.1[a]	112.5	112.8	113.7	110.2	110.6	113.5
H3C–H→H3C+H	112.5[a]	105.3	105.5	112.1	105.4	105.7	111.5
H2C–H→H2C+H	117.1[a]	110.4	110.6	116.2	107.1	107.5	114.0
HC–H→HC+H	106.5[a]	100.1	100.2	104.0	100.2	100.4	103.9
FC–F→FC+F	126.1[a]	127.0	127.1	129.8	126.5	126.8	126.3
The OM*x* and OM*x*-D3T energies are corrected by excluding ZPVE and thermal contributions							
F–OOF→F+OOF	17.6[a]	29.5	29.7	28.8	18.4	18.7	18.8
FO–OF→FO+OF	46.2[a]	48.8	49.2	49.7	41.5	42.0	42.8
O–OF→O+OF	81.7[a]	68.7	68.9	68.5	71.2	71.6	71.5
OO–F→OO+F	13.9[a]	0.4	0.6	0.1	−4.2	−3.9	−1.5
F–OF→F+OF	40.7[a]	44.4	44.6	44.4	40.8	41.1	40.3
H–OF→H+OF	105.6[a]	105.3	105.4	105.9	104.5	104.7	104.5
HO–F→HO+F	51.5[a]	44.7	44.8	42.4	41.9	42.2	40.1
ON–O→ON+O	75.1[a]	78.9	79.1	81.0	74.7	75.2	77.2
N–NO→N+NO	118.1[a]	114.4	114.7	117.8	94.5	95.1	105.7
NN–O→NN+O	42.4[a]	38.2	38.5	40.7	36.7	37.2	42.0
trans-H–ONO→trans-H+ONO	84.8[a]	80.4	80.6	78.5	82.4	82.7	80.8
trans-HO–NO→trans-HO+NO	52.7[a]	49.4	49.8	48.4	46.5	47.1	46.0
H–NC→H+NC	116.8[a]	125.3	125.5	129.3	131.9	132.3	136.4
HN–C→HN+C	215.1[a]	216.7	217.0	217.7	225.2	225.8	229.0
HO–NC→HO+NC	61.6[a]	65.7	66.1	68.0	65.8	66.5	74.0
HN–CO→HN+CO	91.9[a]	75.4	75.8	78.7	77.5	78.2	85.3
HC–NO→HC+NO	128.0[a]	123.7	124.2	124.4	115.2	115.9	112.5
H–NO→H+NO	53.1[a]	61.1	61.3	64.0	62.4	62.7	61.4
HN–O→HN+O	122.8[a]	127.6	127.8	126.2	132.1	132.5	127.9
H3C–OH→H3C+OH	98.4[a]	92.8	93.3	91.1	93.8	94.5	90.4
trans-HC–OH→trans-HC+OH	131.1[a]	139.9	140.2	136.9	136.1	136.6	128.1
trans-HCO–H→trans-HCO+H	43.0[a]	48.3	48.5	50.6	43.5	43.8	41.6
H(O=)C–OH→H(O=)C+OH	115.3[a]	95.5	96.0	95.7	90.9	91.7	93.2
H2C=C–O→H2C=C+O	173.5[a]	152.0	152.3	152.3	157.8	158.3	159.0
H2C–C=O→H2C+C=O	83.0[a]	82.3	82.9	82.9	85.6	86.5	88.2
H(O=)C–C(=O)H→H(O=)C+C(=O)H	76.3[a]	65.7	66.4	65.0	60.1	61.4	64.2
H3C–C(=O)H→H3C+C(=O)H	90.6[a]	84.7	85.6	83.0	84.8	86.1	84.5
F2C–O→F2C+O	161.8[a]	139.5	139.8	143.2	143.0	143.5	152.7
F–C(=O)H→F+C(=O)H	124.3[a]	106.1	106.3	105.0	104.5	104.9	108.0
H–C(=O)H→H+C(=O)H	95.2[a]	89.9	90.2	89.7	87.5	87.9	89.7
H2C–O→H2C+O	183.9[a]	186.0	186.2	183.1	185.2	185.7	184.3
H–CO→H+CO	19.7[a]	36.9	37.1	39.2	40.4	40.7	43.0
HC–O→HC+O	195.2[a]	201.5	201.7	197.4	203.2	203.6	198.5
OC–O→OC+O	130.4[a]	120.9	121.1	123.5	127.1	127.5	133.9
H2N–CH2→H2N+CH2	108.9[a]	115.8	116.4	108.5	109.2	110.2	101.6
H–N(-H)CH2→H+N(-H)CH2	42.8[a]	47.9	48.2	47.4	48.1	48.5	46.6
H3C–NH→H3C+NH	83.7[a]	82.2	82.8	78.4	80.3	81.2	77.1
H–CH2NH→H+CH2NH	35.2[a]	35.9	36.1	36.0	34.7	35.1	37.7
H–CH2NH2→H+CH2NH2	100.0[a]	92.7	92.9	93.7	89.5	89.9	92.2
H3C(H-)N–H→H3C(H-)N+H	107.7[a]	104.7	105.0	105.1	102.8	103.3	101.1
H–C(H)=NH→H+C(H)=NH	103.2[a]	99.3	99.6	98.1	94.0	94.4	93.1
HN–CH→HN+CH	168.9[a]	169.3	169.7	164.6	170.1	170.7	164.0
H–NCH→H+NCH	22.8[a]	20.4	20.6	23.9	30.6	31.0	29.4
H–CN→H+CN	132.1[a]	143.6	143.8	142.5	134.2	134.4	133.5
HC–N→HC+N	229.2[a]	232.3	232.6	228.9	228.2	228.7	227.3
NC–CN→NC+CN	139.3[a]	151.7	152.2	146.5	137.1	138.0	133.4

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Table S29: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
trans-HOO–O→trans-HOO+O	57.8[a]	50.3	50.6	50.7	50.8	51.2	50.8
trans-HO–OO→trans-HO+OO	5.3[a]	2.7	3.0	2.0	−6.4	−5.9	−6.7
trans-H–OOO→trans-H+OOO	85.9[a]	87.0	87.2	87.3	94.8	95.1	96.8
OO–O→OO+O	26.6[a]	25.6	25.8	25.9	9.4	9.8	8.4
HOO–H→HOO+H	93.6[a]	86.6	86.8	87.9	89.5	89.7	90.7
HO–OH→HO+OH	54.7[a]	46.7	47.0	44.0	45.1	45.6	41.6
HO–O→HO+O	68.3[a]	70.0	70.2	67.3	66.3	66.6	62.9
H–OO→H+OO	54.7[a]	62.3	62.4	62.4	53.4	53.7	54.5
HO–H→HO+H	125.8[a]	119.5	119.6	120.7	119.7	119.9	118.0
HN–NN→HN+NN	20.2[a]	17.2	17.7	11.1	5.5	6.3	9.9
H2N–NH2→H2N+NH2	73.1[a]	77.4	78.0	68.1	63.9	64.9	57.9
trans-HN–NH→trans-HN+NH	130.3[a]	133.3	133.7	127.1	134.6	135.2	124.0
HN–N→HN+N	141.8[a]	153.4	153.7	151.3	150.6	151.0	147.5
H2N–H→H2N+H	115.4[a]	111.8	111.9	110.9	108.8	109.1	105.5
HN–H→HN+H	99.5[a]	95.3	95.4	97.4	97.4	97.6	98.3
H2CC–CH2→H2CC+CH2	153.4[a]	138.9	139.5	136.0	137.2	138.2	136.8
HCC–CH3→HCC+CH3	131.6[a]	133.8	134.5	130.6	121.5	122.6	131.4
H2C=(H)C–CH3→H2C=(H)C+CH3	107.6[a]	102.9	103.9	100.1	102.6	104.3	100.4
H2C=(H)C–F→H2C=(H)C+F	127.8[a]	121.5	121.8	120.1	119.9	120.4	120.3
H3C–CH3→H3C+CH3	97.3[a]	95.9	96.8	92.3	98.5	99.8	93.4
H2C–CH2→H2C+CH2	182.6[a]	179.8	180.4	175.0	174.2	175.3	171.7
H2C=C–H→H2C=C+H	86.2[a]	76.2	76.3	76.7	77.7	78.0	79.0
H–C(H)=CH→H+C(H)=CH	40.6[a]	43.9	44.2	44.8	45.4	45.9	45.1
H2C–C→H2C+C	169.2[a]	181.0	181.4	179.2	178.6	179.3	176.2
HCC–F→HCC+F	132.3[a]	133.3	133.5	131.8	122.5	122.8	134.6
HC–CF→HC+CF	181.5[a]	169.7	170.1	169.6	171.2	171.8	173.0
HCC–H→HCC+H	139.4[a]	143.7	143.9	142.4	129.2	129.5	142.1
HC–CH→HC+CH	237.1[a]	232.7	233.0	224.9	228.4	229.0	222.5
H3C–F→H3C+F	115.1[a]	117.1	117.3	113.7	114.9	115.3	113.5
H3C–H→H3C+H	112.5[a]	113.5	113.7	112.1	113.7	114.0	111.5
H2C–H→H2C+H	117.1[a]	116.8	117.0	116.2	112.9	113.3	114.0
HC–H→HC+H	106.5[a]	105.5	105.6	104.0	105.5	105.8	103.9
FC–F→FC+F	126.1[a]	128.5	128.7	129.8	128.0	128.3	126.3

a A.Karton, S.Daon, J.M.Martin, Chem.Phys.Lett. 510, 165 (2011).

Table S30: Benchmark Results for the HAT707 Subset of the W4-11-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
The OMx and OMx-D3T energies are uncorrected atomization enthalpies at 298 K							
H+CH3F→HF+CH3	−26.6[a]	−20.0	−19.9	−30.3	−25.0	−24.7	−26.4
H+FOOF→HF+FOO	−124.0[a]	−104.6	−104.5	−115.2	−118.1	−117.8	−121.0
H+FOOF→OH+FOF	−48.6[a]	−54.1	−53.9	−58.2	−59.2	−58.9	−62.0
H+FOO→OH+OF	−25.6[a]	−39.1	−38.9	−42.7	−36.8	−36.6	−40.5
H+FOO→HF+O2	−127.7[a]	−133.2	−133.1	−143.9	−140.2	−140.0	−141.4
H+FOF→HF+OF	−100.9[a]	−89.6	−89.5	−99.7	−95.8	−95.6	−99.5
H+FOF→OH+F2	−52.5[a]	−50.3	−50.2	−56.8	−53.1	−52.9	−56.9
H+HOF→OH+HF	−90.2[a]	−90.5	−90.4	−101.6	−95.8	−95.7	−99.8
H+OF→HF+O	−88.6[a]	−84.6	−84.5	−96.5	−88.3	−88.2	−92.4
H+OF→OH+F	−54.1[a]	−58.1	−58.1	−63.5	−59.5	−59.5	−64.5
H+O2N→OH+NO	−32.1[a]	−28.8	−28.7	−30.1	−33.3	−33.0	−34.8
H+O2N→NH+O2	24.0[a]	29.6	29.8	27.3	22.9	23.2	23.2
H+N2O→OH+N2	−64.8[a]	−69.7	−69.5	−70.4	−71.5	−71.2	−69.9
H+N2O→NH+NO	35.0[a]	32.2	32.4	29.6	7.5	7.9	13.0
H+trans-HONO→OH+HNO	−0.5[a]	−9.9	−9.7	−15.5	−14.0	−13.7	−15.4
H+trans-HONO→NH+HO2	54.0[a]	47.2	47.4	43.4	51.1	51.5	49.5
H+HNCO→NH+HCO	72.2[a]	38.8	39.1	39.5	38.0	38.4	42.3
H+HNCO→CH+HNO	144.6[a]	113.0	113.2	110.8	109.1	109.5	112.9
H+HNCO→OH+HCN	14.1[a]	−16.0	−15.8	−14.8	−6.7	−6.4	−5.8
H+HNO→NH+OH	15.6[a]	18.2	18.3	15.1	22.4	22.6	15.9
H+NO→NH+O	69.7[a]	68.0	68.0	62.2	71.3	71.3	66.5
H+NO→OH+N	45.5[a]	41.6	41.6	39.3	49.7	49.8	47.2
H+oxirene→OH+C2H2	−56.7[a]	−57.6	−57.4	−62.8	−57.4	−57.0	−64.3
H+oxirane→OH+C2H4	−19.8[a]	−21.0	−20.8	−26.3	−24.9	−24.6	−31.8
H+methanol→OH+CH4	−14.1[a]	−18.4	−18.1	−21.0	−17.9	−17.4	−21.0
H+trans-HCOH→CH+H2O	5.3[a]	21.2	21.4	16.3	17.6	17.9	10.1
H+trans-HCOH→OH+CH2	24.5[a]	34.9	35.0	32.9	31.0	31.3	24.2
H+formic acid→OH+trans-HCOH	72.2[a]	47.6	47.9	45.1	48.2	48.7	51.6
H+formic acid→H2O+HCO	−10.5[a]	−23.4	−23.1	−25.0	−27.6	−27.0	−24.8
H+formic acid→CH+H2O2	148.6[a]	140.3	140.6	138.0	138.5	139.1	138.1
H+ketene→OH+CH2C	66.3[a]	43.0	43.2	41.2	48.3	48.6	47.1
H+ketene→CH+H2CO	74.6[a]	61.7	62.0	58.1	64.0	64.5	59.4
H+glyoxal→OH+oxirene	71.8[a]	77.4	77.8	75.4	79.2	79.9	79.1
H+glyoxal→CH+formic acid	49.0[a]	62.5	62.9	55.6	63.6	64.3	57.5
H+acetaldehyde→CH+methanol	80.1[a]	83.7	84.2	78.2	84.3	85.0	80.6
H+acetaldehyde→OH+C2H4	6.6[a]	9.5	9.8	6.5	12.4	12.9	9.4
H+F2CO→OH+CF2	54.6[a]	30.5	30.8	32.1	33.4	33.8	40.7
H+F2CO→CH+FOF	242.6[a]	227.1	227.4	225.8	232.5	232.9	233.1
H+HFCO→HF+HCO	−17.3[a]	−29.8	−29.6	−39.0	−33.9	−33.6	−31.8
H+H2CO→OH+CH2 ($^3B_1$)	76.7[a]	75.4	75.6	71.9	74.2	74.5	72.4
H+H2CO→CH+H2O	57.5[a]	61.7	62.0	55.3	60.8	61.2	58.2
H+HCO→OH+CH	88.0[a]	92.3	92.4	86.3	93.5	93.7	86.5
H+CO2→OH+CO	23.2[a]	12.2	12.3	12.4	17.9	18.2	21.9
H+CO2→CH+O2	185.1[a]	168.0	168.2	165.8	166.4	166.7	168.9
H+CO→CH+O	175.5[a]	165.4	165.5	158.3	163.6	163.7	155.5
H+CO→OH+C	152.5[a]	142.1	142.2	137.4	141.8	141.9	135.0
H+HCN→NH+CH	146.1[a]	147.1	147.3	140.7	138.2	138.5	134.6
H+CN→CH+N	97.1[a]	89.4	89.5	86.4	95.0	95.2	93.8
H+CN→NH+C	98.2[a]	92.5	92.6	88.5	94.7	94.9	92.6
H+trans-HO3→OH+HO2	−49.4[a]	−57.6	−57.4	−60.4	−57.3	−57.1	−61.2
H+O3→OH+O2	−80.6[a]	−82.2	−82.1	−85.2	−98.6	−98.4	−103.6
H+H2O2→OH+H2O	−71.1[a]	−71.4	−71.3	−76.6	−72.7	−72.4	−76.4
H+HO2→2OH	−38.9[a]	−38.9	−38.8	−43.9	−42.8	−42.6	−49.0
H+H2O→OH+H2	16.3[a]	7.4	7.5	12.5	9.5	9.7	8.9
H+trans-H2N2→NH+NH2	30.9[a]	37.4	37.6	29.7	37.1	37.5	25.7
H+propyne→CH+C2H4	57.3[a]	55.2	55.5	50.4	54.8	55.3	50.2
H+propene→CH+C2H6	64.3[a]	62.3	62.9	57.2	60.5	61.3	56.7
H+C2H3F→HF+C2H3	−13.8[a]	−14.4	−14.1	−24.0	−18.4	−18.0	−19.5
H+C2H3F→CH+CH3F	66.7[a]	59.8	60.2	55.8	61.4	62.0	56.6
H+C2H4→CH+CH4	59.5[a]	55.9	56.3	50.7	54.1	54.7	50.1
H+C2H3→CH+CH3	54.0[a]	54.2	54.5	49.4	54.8	55.3	49.8

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Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
H+C2F2→CH+CF2	43.1[a]	26.1	26.3	24.3	31.6	31.9	35.3
H+HCCF→HF+C2H	−9.3[a]	−2.2	−2.1	−12.2	−4.2	−4.0	−5.2
H+C2H2→CH+CH2	130.6[a]	125.3	125.5	120.9	121.1	121.4	118.6
H+CF2→CH+F2	135.5[a]	146.3	146.4	136.9	146.0	146.2	135.5
H+CF2→HF+CF	−15.6[a]	−5.6	−5.5	−14.2	−8.7	−8.5	−13.6
H+CH2 ($^3B_1$)→CH+H2	−3.0[a]	−6.2	−6.1	−4.1	−3.8	−3.7	−5.2
H+CF→HF+C	−8.9[a]	4.7	4.8	−9.0	1.9	2.0	−6.4
H+CF→CH+F	48.5[a]	54.5	54.5	44.8	52.5	52.5	42.0
H+F2→HF+F	−102.6[a]	−97.5	−97.4	−106.4	−102.2	−102.2	−107.1
H+O2→OH+O	13.6[a]	9.6	9.6	4.8	15.1	15.2	8.5
H+N2→NH+N	145.4[a]	143.5	143.5	139.3	128.7	128.8	130.1
C+CH3F→CF+CH3	−17.6[a]	−24.7	−24.6	−21.4	−26.9	−26.7	−20.0
C+FOOF→CF+FOO	−115.1[a]	−109.3	−109.2	−106.3	−120.0	−119.9	−114.6
C+FOOF→CO+FOF	−201.1[a]	−196.1	−196.0	−195.7	−200.9	−200.8	−197.0
C+FOO→CO+OF	−178.1[a]	−181.1	−181.1	−180.1	−178.6	−178.6	−175.5
C+FOO→CF+O2	−118.8[a]	−137.9	−137.8	−135.0	−142.1	−142.0	−135.0
C+FOF→CF+OF	−92.0[a]	−94.3	−94.3	−90.7	−97.7	−97.6	−93.1
C+FOF→CO+F2	−205.0[a]	−192.3	−192.3	−194.3	−194.9	−194.9	−191.9
C+HOF→CO+HF	−242.7[a]	−232.6	−232.6	−239.1	−237.6	−237.6	−234.8
C+OF→CF+O	−79.7[a]	−89.3	−89.3	−87.5	−90.1	−90.2	−86.0
C+OF→CO+F	−206.7[a]	−200.2	−200.3	−201.0	−201.3	−201.4	−199.5
C+O2N→CO+NO	−184.6[a]	−170.9	−170.8	−167.5	−175.1	−174.9	−169.8
C+O2N→CN+O2	−74.3[a]	−62.9	−62.8	−61.1	−71.8	−71.7	−69.4
C+N2O→CO+N2	−217.4[a]	−211.8	−211.7	−207.8	−213.3	−213.1	−205.0
C+N2O→CN+NO	−63.2[a]	−60.3	−60.2	−58.9	−87.2	−87.1	−79.6
C+trans-HONO→CO+HNO	−153.0[a]	−152.0	−151.9	−153.0	−155.8	−155.6	−150.5
C+trans-HONO→CN+HO2	−44.2[a]	−45.3	−45.2	−45.1	−43.6	−43.4	−43.1
C+HNCO→CN+HCO	−26.0[a]	−53.7	−53.5	−48.9	−56.7	−56.5	−50.3
C+HNCO→CO+HCN	−138.4[a]	−158.1	−157.9	−152.2	−148.5	−148.3	−140.8
C+HNO→CN+OH	−82.7[a]	−74.3	−74.3	−73.4	−72.3	−72.3	−76.7
C+NO→CN+O	−28.6[a]	−24.5	−24.6	−26.2	−23.5	−23.6	−26.1
C+NO→CO+N	−107.0[a]	−100.5	−100.5	−98.1	−92.1	−92.1	−87.8
C+oxirene→CO+C2H2	−209.2[a]	−199.7	−199.6	−200.2	−199.2	−199.0	−199.4
C+oxirane→CO+C2H4	−172.3[a]	−163.1	−163.0	−163.8	−166.7	−166.5	−166.8
C+methanol→CO+CH4	−166.7[a]	−160.5	−160.3	−158.4	−159.6	−159.4	−156.1
C+trans-HCOH→CO+CH2	−128.0[a]	−107.2	−107.1	−104.5	−110.8	−110.7	−110.8
C+formic acid→CO+trans-HCOH	−80.3[a]	−94.4	−94.2	−92.3	−93.5	−93.2	−83.4
C+ketene→CO+CH2C	−86.2[a]	−99.1	−99.0	−96.2	−93.5	−93.3	−87.9
C+glyoxal→CO+oxirene	−80.7[a]	−64.7	−64.4	−62.0	−62.6	−62.0	−55.9
C+acetaldehyde→CO+C2H4	−146.0[a]	−132.6	−132.4	−130.9	−129.4	−129.0	−125.6
C+F2CO→CO+CF2	−97.9[a]	−111.6	−111.4	−105.4	−108.4	−108.2	−94.3
C+HFCO→CF+HCO	−8.4[a]	−34.5	−34.4	−30.1	−35.8	−35.6	−25.4
C+H2CO→CO+CH2 ($^3B_1$)	−75.8[a]	−66.7	−66.6	−65.5	−67.6	−67.4	−62.7
C+HCO→CO+CH	−64.5[a]	−49.8	−49.7	−51.1	−48.3	−48.2	−48.5
C+CO2→CO+CO	−129.3[a]	−129.9	−129.9	−125.0	−123.9	−123.8	−113.1
C+HCN→CN+CH	47.9[a]	54.6	54.7	52.2	43.5	43.6	42.1
C+O3→CO+O2	−233.1[a]	−224.3	−224.2	−222.6	−240.4	−240.3	−238.6
C+H2O2→CO+H2O	−223.6[a]	−213.5	−213.4	−214.1	−214.5	−214.4	−211.4
C+HO2→CO+OH	−191.4[a]	−181.0	−181.0	−181.3	−184.5	−184.5	−184.0
C+H2O→CO+H2	−136.2[a]	−134.7	−134.7	−124.9	−132.2	−132.3	−126.1
C+trans-H2N2→CN+NH2	−67.4[a]	−55.1	−55.0	−58.8	−57.6	−57.4	−66.9
C+C2H3F→CF+C2H3	−4.9[a]	−19.1	−18.9	−15.0	−20.3	−20.0	−13.1
C+HCCF→CF+C2H	−0.4[a]	−6.9	−6.8	−3.3	−6.1	−6.0	1.2
C+CF2→2*CF	−6.7[a]	−10.3	−10.3	−5.2	−10.6	−10.5	−7.2
C+F2→CF+F	−93.7[a]	−102.1	−102.2	−97.4	−104.1	−104.2	−100.7
C+O2→CO+O	−138.9[a]	−132.5	−132.5	−132.6	−126.7	−126.8	−126.6
C+N2→CN+N	47.1[a]	51.0	50.9	50.9	34.0	33.9	37.6
N+FOOF→NO+FOF	−94.2[a]	−95.6	−95.5	−97.6	−108.9	−108.7	−109.2
N+FOO→NO+OF	−71.1[a]	−80.6	−80.6	−82.0	−86.5	−86.5	−87.7
N+FOF→NO+F2	−98.0[a]	−91.8	−91.8	−96.2	−102.8	−102.8	−104.1
N+HOF→NO+HF	−135.7[a]	−132.1	−132.1	−141.0	−145.5	−145.5	−147.0
N+OF→NO+F	−99.7[a]	−99.7	−99.7	−102.9	−109.2	−109.3	−111.7
N+O2N→NO+NO	−77.6[a]	−70.4	−70.3	−69.4	−83.0	−82.8	−82.0
N+O2N→N2+O2	−121.4[a]	−113.9	−113.8	−112.0	−105.8	−105.7	−106.9
N+N2O→NO+N2	−110.4[a]	−111.3	−111.2	−109.7	−121.2	−121.0	−117.1

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Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
N+trans-HONO→NO+HNO	−46.0[a]	−51.4	−51.3	−54.9	−63.7	−63.5	−62.7
N+trans-HONO→N2+HO2	−91.4[a]	−96.3	−96.1	−95.9	−77.6	−77.3	−80.6
N+HNCO→N2+HCO	−73.2[a]	−104.6	−104.5	−99.8	−90.7	−90.4	−87.8
N+HNCO→CN+HNO	47.5[a]	23.5	23.7	24.4	14.1	14.3	19.1
N+HNCO→NO+HCN	−31.4[a]	−57.6	−57.4	−54.1	−56.4	−56.2	−53.0
N+HNO→N2+OH	−129.8[a]	−125.3	−125.2	−124.2	−106.3	−106.2	−114.2
N+NO→N2+O	−75.7[a]	−75.5	−75.5	−77.1	−57.4	−57.5	−63.7
N+oxirene→NO+C2H2	−102.2[a]	−99.2	−99.0	−102.1	−107.1	−106.9	−111.5
N+oxirane→NO+C2H4	−65.3[a]	−62.6	−62.4	−65.6	−74.6	−74.4	−79.0
N+methanol→NO+CH4	−59.7[a]	−60.0	−59.8	−60.3	−67.6	−67.3	−68.2
N+trans-HCOH→CN+H2O	−91.8[a]	−68.2	−68.1	−70.1	−77.4	−77.3	−83.7
N+trans-HCOH→NO+CH2	−21.0[a]	−6.7	−6.6	−6.4	−18.7	−18.6	−23.0
N+formic acid→NO+trans-HCOH	26.7[a]	6.1	6.3	5.8	−1.5	−1.1	4.4
N+formic acid→CN+H2O2	51.5[a]	50.9	51.1	51.6	43.5	43.9	44.3
N+ketene→NO+CH2C	20.8[a]	1.4	1.5	1.9	−1.4	−1.2	−0.1
N+ketene→CN+H2CO	−22.6[a]	−27.8	−27.6	−28.2	−31.0	−30.7	−34.4
N+glyoxal→NO+oxirene	26.3[a]	35.8	36.2	36.1	29.5	30.1	31.9
N+glyoxal→CN+formic acid	−48.1[a]	−26.9	−26.6	−30.8	−31.4	−30.9	−36.3
N+acetaldehyde→CN+methanol	−17.0[a]	−5.7	−5.3	−8.1	−10.7	−10.2	−13.2
N+acetaldehyde→NO+C2H4	−39.0[a]	−32.1	−31.8	−32.8	−37.3	−36.9	−37.8
N+F2CO→NO+CF2	9.1[a]	−11.0	−10.9	−7.3	−16.3	−16.1	−6.5
N+F2CO→CN+FOF	145.5[a]	137.7	137.8	139.4	137.4	137.7	139.3
N+H2CO→NO+CH2 ($^3B_1$)	31.2[a]	33.8	33.9	32.6	24.5	24.7	25.1
N+H2CO→CN+H2O	−39.7[a]	−27.7	−27.6	−31.1	−34.2	−34.0	−35.6
N+HCO→NO+CH	42.5[a]	50.7	50.8	47.0	43.8	43.9	39.3
N+CO2→NO+CO	−22.3[a]	−29.4	−29.3	−26.9	−31.8	−31.7	−25.3
N+CO2→CN+O2	88.0[a]	78.6	78.7	79.4	71.4	71.5	75.1
N+CO→CN+O	78.4[a]	76.0	76.0	71.9	68.6	68.5	61.7
N+CO→NO+C	107.0[a]	100.5	100.5	98.1	92.1	92.1	87.8
N+HCN→N2+CH	0.7[a]	3.7	3.7	1.4	9.5	9.6	4.5
N+CN→N2+C	−47.1[a]	−51.0	−50.9	−50.9	−34.0	−33.9	−37.6
N+trans-HO3→NO+HO2	−95.0[a]	−99.2	−99.1	−99.7	−107.0	−106.9	−108.4
N+O3→NO+O2	−126.1[a]	−123.8	−123.7	−124.5	−148.3	−148.2	−150.8
N+H2O2→NO+H2O	−116.6[a]	−113.0	−112.9	−116.0	−122.4	−122.3	−123.6
N+HO2→NO+OH	−84.4[a]	−80.4	−80.4	−83.2	−92.5	−92.4	−96.2
N+H2O→NO+H2	−29.3[a]	−34.2	−34.2	−26.8	−40.2	−40.2	−38.3
N+trans-H2N2→N2+NH2	−114.5[a]	−106.1	−105.9	−109.6	−91.6	−91.4	−104.5
N+propyne→CN+C2H4	−39.8[a]	−34.2	−34.0	−36.0	−40.2	−39.9	−43.6
N+propene→CN+C2H6	−32.9[a]	−27.1	−26.7	−29.1	−34.5	−33.9	−37.1
N+C2H3F→CN+CH3F	−30.4[a]	−29.6	−29.3	−30.6	−33.6	−33.2	−37.2
N+C2H4→CN+CH4	−37.7[a]	−33.5	−33.2	−35.7	−41.0	−40.5	−43.7
N+C2H3→CN+CH3	−43.1[a]	−35.3	−35.1	−37.0	−40.2	−39.9	−44.0
N+C2F2→CN+CF2	−54.0[a]	−63.3	−63.2	−62.1	−63.4	−63.3	−58.5
N+C2H2→CN+CH2	33.4[a]	35.9	36.0	34.5	26.1	26.3	24.8
N+CF2→CN+F2	38.4[a]	56.9	56.9	50.5	51.0	51.0	41.7
N+CH2 ($^3B_1$)→CN+H2	−100.1[a]	−95.6	−95.7	−90.5	−98.8	−98.9	−99.0
N+CF→CN+F	−48.6[a]	−34.9	−35.0	−41.6	−42.5	−42.7	−51.8
N+O2→NO+O	−31.9[a]	−32.0	−32.0	−34.5	−34.6	−34.7	−38.7
O+CH3F→OF+CH3	62.0[a]	64.5	64.7	66.1	63.3	63.5	66.0
O+FOOF→OF+FOO	−35.4[a]	−20.0	−19.9	−18.8	−29.8	−29.7	−28.7
O+FOOF→O2+FOF	−62.2[a]	−63.6	−63.5	−63.1	−74.3	−74.1	−70.5
O+FOO→O2+OF	−39.2[a]	−48.6	−48.6	−47.5	−51.9	−51.8	−49.0
O+FOF→OF+OF	−12.4[a]	−5.0	−5.0	−3.2	−7.5	−7.4	−7.2
O+FOF→O2+F2	−66.1[a]	−59.9	−59.8	−61.7	−68.2	−68.1	−65.4
O+HOF→O2+HF	−103.8[a]	−100.1	−100.1	−106.5	−110.9	−110.9	−108.3
O+OF→O2+F	−67.8[a]	−67.7	−67.7	−68.4	−74.6	−74.7	−72.9
O+O2N→O2+NO	−45.7[a]	−38.4	−38.3	−34.9	−48.4	−48.2	−43.3
O+trans-HONO→O2+HNO	−14.1[a]	−19.5	−19.3	−20.4	−29.1	−28.9	−23.9
O+trans-HONO→NO+HO2	−15.6[a]	−20.8	−20.6	−18.8	−20.1	−19.8	−17.0
O+HNCO→NO+HCO	2.6[a]	−29.2	−28.9	−22.7	−33.3	−32.9	−24.2
O+HNCO→CO+HNO	−30.9[a]	−52.5	−52.3	−47.5	−54.5	−54.2	−42.6
O+HNCO→O2+HCN	0.5[a]	−25.6	−25.4	−19.6	−21.8	−21.5	−14.3
O+HNO→NO+OH	−54.1[a]	−49.8	−49.7	−47.1	−48.9	−48.7	−50.6
O+NO→O2+N	31.9[a]	32.0	32.0	34.5	34.6	34.7	38.7
O+oxirene→O2+C2H2	−70.3[a]	−67.2	−67.0	−67.6	−72.5	−72.2	−72.8

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Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
O+oxirane→O2+C2H4	−33.4[a]	−30.6	−30.4	−31.2	−40.0	−39.7	−40.2
O+methanol→O2+CH4	−27.7[a]	−28.0	−27.8	−25.8	−33.0	−32.6	−29.5
O+trans-HCOH→CO+H2O	−170.2[a]	−144.2	−144.1	−142.0	−146.0	−145.8	−145.4
O+trans-HCOH→O2+CH2	10.9[a]	25.3	25.4	28.1	15.9	16.1	15.8
O+formic acid→O2+trans-HCOH	58.6[a]	38.1	38.3	40.3	33.2	33.6	43.2
O+formic acid→CO+H2O2	−26.9[a]	−25.1	−24.9	−20.3	−25.1	−24.6	−17.4
O+ketene→O2+CH2C	52.7[a]	33.4	33.6	36.4	33.2	33.4	38.6
O+ketene→CO+H2CO	−100.9[a]	−103.8	−103.5	−100.1	−99.6	−99.2	−96.1
O+glyoxal→O2+oxirene	58.2[a]	67.8	68.2	70.6	64.1	64.7	70.6
O+glyoxal→CO+formic acid	−126.5[a]	−102.9	−102.6	−102.7	−100.0	−99.4	−98.0
O+acetaldehyde→CO+methanol	−95.4[a]	−81.7	−81.3	−80.0	−79.3	−78.7	−74.9
O+acetaldehyde→O2+C2H4	−7.1[a]	−0.1	0.2	1.7	−2.7	−2.3	0.9
O+F2CO→O2+CF2	41.0[a]	20.9	21.1	27.2	18.3	18.6	32.2
O+F2CO→CO+FOF	67.1[a]	61.7	61.9	67.6	68.8	69.1	77.6
O+HFCO→OF+HCO	71.2[a]	54.7	54.9	57.4	54.4	54.6	60.5
O+H2CO→O2+CH2 ($^3B_1$)	63.1[a]	65.8	65.9	67.1	59.1	59.4	63.9
O+H2CO→CO+H2O	−118.0[a]	−103.7	−103.5	−103.0	−102.8	−102.5	−97.3
O+HCO→O2+CH	74.4[a]	82.7	82.8	81.5	78.4	78.5	78.0
O+CO2→O2+CO	9.6[a]	2.6	2.7	7.6	2.8	3.0	13.4
O+CO→O2+C	138.9[a]	132.5	132.5	132.6	126.7	126.8	126.6
O+HCN→NO+CH	76.5[a]	79.1	79.2	78.5	67.0	67.1	68.2
O+CN→CO+N	−78.4[a]	−76.0	−76.0	−71.9	−68.6	−68.5	−61.7
O+CN→NO+C	28.6[a]	24.5	24.6	26.2	23.5	23.6	26.1
O+trans-HO3→O2+HO2	−63.1[a]	−67.2	−67.1	−65.2	−72.4	−72.2	−69.6
O+O3→O2+O2	−94.2[a]	−91.8	−91.7	−90.1	−113.7	−113.5	−112.0
O+H2O2→O2+H2O	−84.7[a]	−81.0	−80.9	−81.5	−87.8	−87.6	−84.9
O+HO2→O2+OH	−52.5[a]	−48.5	−48.4	−48.7	−57.9	−57.8	−57.5
O+H2O→O2+H2	2.7[a]	−2.2	−2.2	7.7	−5.5	−5.5	0.5
O+trans-H2N2→NO+NH2	−38.8[a]	−30.6	−30.4	−32.5	−34.2	−33.9	−40.8
O+propyne→CO+C2H4	−118.2[a]	−110.2	−110.0	−107.9	−108.8	−108.5	−105.3
O+propene→CO+C2H6	−111.2[a]	−103.1	−102.6	−101.0	−103.1	−102.4	−98.8
O+C2H3F→OF+C2H3	74.7[a]	70.2	70.4	72.5	69.8	70.2	72.8
O+C2H3F→CO+CH3F	−108.8[a]	−105.6	−105.3	−102.5	−102.3	−101.7	−98.9
O+C2H4→CO+CH4	−116.0[a]	−109.6	−109.2	−107.5	−109.6	−109.0	−105.4
O+C2H3→CO+CH3	−121.5[a]	−111.3	−111.0	−108.9	−108.8	−108.4	−105.7
O+C2F2→CO+CF2	−132.4[a]	−139.3	−139.2	−133.9	−132.0	−131.8	−120.2
O+HCCF→OF+C2H	79.2[a]	82.4	82.5	84.2	84.0	84.2	87.1
O+C2H2→CO+CH2	−45.0[a]	−40.2	−40.0	−37.4	−42.5	−42.3	−36.9
O+CF2→CO+F2	−40.0[a]	−19.1	−19.1	−21.3	−17.7	−17.6	−20.0
O+CF2→OF+CF	73.0[a]	78.9	79.0	82.3	79.6	79.7	78.8
O+CH2 ($^3B_1$)→CO+H2	−178.5[a]	−171.7	−171.6	−162.4	−167.5	−167.4	−160.7
O+CF→OF+C	79.7[a]	89.3	89.3	87.5	90.1	90.2	86.0
O+CF→CO+F	−127.0[a]	−110.9	−111.0	−113.5	−111.2	−111.2	−113.5
O+F2→OF+F	−14.0[a]	−12.9	−12.9	−9.9	−13.9	−14.0	−14.7
O+N2→NO+N	75.7[a]	75.5	75.5	77.1	57.4	57.5	63.7
F+CH3F→F2+CH3	76.0[a]	77.4	77.6	76.0	77.2	77.5	80.7
F+FOOF→F2+FOO	−21.4[a]	−7.1	−7.0	−8.9	−15.9	−15.7	−13.9
F+FOOF→OF+FOF	5.5[a]	4.1	4.2	5.3	0.4	0.6	2.5
F+FOO→OF+OF	28.6[a]	19.1	19.2	20.9	22.7	22.9	24.0
F+FOO→F2+O2	−25.1[a]	−35.7	−35.6	−37.6	−38.0	−37.8	−34.3
F+FOF→F2+OF	1.7[a]	7.9	7.9	6.7	6.4	6.6	7.6
F+HOF→OF+HF	−36.1[a]	−32.4	−32.3	−38.1	−36.3	−36.2	−35.3
F+OF→F2+O	14.0[a]	12.9	12.9	9.9	13.9	14.0	14.7
F+O2N→OF+NO	22.1[a]	29.3	29.4	33.5	26.2	26.5	29.7
F+N2O→OF+N2	−10.7[a]	−11.6	−11.4	−6.9	−12.0	−11.7	−5.5
F+trans-HONO→OF+HNO	53.7[a]	48.2	48.4	48.0	45.5	45.8	49.0
F+HNCO→CF+HNO	96.1[a]	58.5	58.7	66.0	56.6	57.0	70.9
F+HNCO→OF+HCN	68.2[a]	42.1	42.3	48.7	52.8	53.1	58.7
F+NO→OF+N	99.7[a]	99.7	99.7	102.9	109.2	109.3	111.7
F+oxirene→OF+C2H2	−2.5[a]	0.5	0.7	0.8	2.1	2.5	0.1
F+oxirane→OF+C2H4	34.4[a]	37.1	37.3	37.2	34.6	34.9	32.7
F+methanol→OF+CH4	40.0[a]	39.7	40.0	42.5	41.7	42.1	43.4
F+trans-HCOH→CF+H2O	−43.2[a]	−33.3	−33.1	−28.5	−34.9	−34.6	−31.9
F+trans-HCOH→OF+CH2	78.7[a]	93.0	93.1	96.4	90.5	90.8	88.7
F+formic acid→OF+trans-HCOH	126.3[a]	105.8	106.0	108.6	107.8	108.2	116.1

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Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
F+formic acid→CF+H2O2	100.1[a]	85.8	86.1	93.2	86.1	86.6	96.1
F+ketene→OF+CH2C	120.5[a]	101.1	101.3	104.7	107.8	108.1	111.6
F+ketene→CF+H2CO	26.1[a]	7.2	7.5	13.4	11.6	12.0	17.4
F+glyoxal→OF+oxirene	126.0[a]	135.5	135.9	139.0	138.7	139.4	143.6
F+glyoxal→CF+formic acid	0.5[a]	8.0	8.4	10.8	11.2	11.8	15.5
F+acetaldehyde→CF+methanol	31.6[a]	29.2	29.7	33.5	31.8	32.5	38.6
F+acetaldehyde→OF+C2H4	60.7[a]	67.6	67.9	70.1	71.9	72.4	73.9
F+F2CO→OF+CF2	108.8[a]	88.6	88.9	95.6	92.9	93.3	105.2
F+F2CO→CF+FOF	194.1[a]	172.6	172.9	181.1	180.0	180.4	191.1
F+HFCO→F2+HCO	85.3[a]	67.6	67.8	67.3	68.3	68.6	75.3
F+H2CO→OF+CH2 ($^3B_1$)	130.8[a]	133.5	133.7	135.5	133.7	134.0	136.8
F+H2CO→CF+H2O	9.0[a]	7.2	7.4	10.5	8.4	8.7	16.2
F+HCO→OF+CH	142.1[a]	150.4	150.5	149.9	153.0	153.2	151.0
F+CO2→OF+CO	77.3[a]	70.3	70.4	75.9	77.4	77.7	86.4
F+CO2→CF+O2	136.6[a]	113.5	113.7	121.0	114.0	114.2	127.0
F+CO→CF+O	127.0[a]	110.9	111.0	113.5	111.2	111.2	113.5
F+CO→OF+C	206.7[a]	200.2	200.3	201.0	201.3	201.4	199.5
F+CN→CF+N	48.6[a]	34.9	35.0	41.6	42.5	42.7	51.8
F+trans-HO3→OF+HO2	4.7[a]	0.5	0.7	3.1	2.2	2.4	3.3
F+O3→OF+O2	−26.5[a]	−24.1	−24.0	−21.7	−39.1	−38.9	−39.1
F+H2O2→OF+H2O	−17.0[a]	−13.3	−13.2	−13.1	−13.1	−12.9	−11.9
F+H2O→OF+H2	70.4[a]	65.5	65.6	76.1	69.1	69.2	73.4
F+propyne→CF+C2H4	8.8[a]	0.7	1.0	5.6	2.4	2.8	8.2
F+propene→CF+C2H6	15.8[a]	7.8	8.3	12.5	8.1	8.8	14.8
F+C2H3F→F2+C2H3	88.8[a]	83.1	83.3	82.4	83.8	84.2	87.5
F+C2H3F→CF+CH3F	18.2[a]	5.3	5.7	11.0	8.9	9.5	14.6
F+C2H4→CF+CH4	11.0[a]	1.4	1.8	6.0	1.6	2.2	8.1
F+C2H3→CF+CH3	5.5[a]	−0.3	−0.0	4.6	2.4	2.8	7.8
F+C2F2→CF+CF2	−5.4[a]	−28.4	−28.2	−20.4	−20.9	−20.6	−6.6
F+HCCF→F2+C2H	93.3[a]	95.3	95.4	94.1	98.0	98.2	101.8
F+C2H2→CF+CH2	82.1[a]	70.8	71.0	76.1	68.6	68.9	76.6
F+CF2→F2+CF	87.0[a]	91.8	91.9	92.2	93.5	93.7	93.5
F+CH2 ($^3B_1$)→CF+H2	−51.5[a]	−60.7	−60.6	−48.9	−56.3	−56.2	−47.2
F+CF→F2+C	93.7[a]	102.1	102.2	97.4	104.1	104.2	100.7
F+O2→OF+O	67.8[a]	67.7	67.7	68.4	74.6	74.7	72.9
OH+CH3F→HOF+CH3	63.6[a]	70.5	70.6	71.3	70.9	71.0	73.4
OH+FOOF→HOF+FOO	−33.8[a]	−14.1	−14.0	−13.6	−22.3	−22.2	−21.2
OH+FOOF→HO2+FOF	−9.7[a]	−15.2	−15.1	−14.4	−16.4	−16.3	−13.0
OH+FOO→HO2+OF	13.3[a]	−0.2	−0.1	1.2	5.9	6.0	8.5
OH+FOO→HOF+O2	−37.5[a]	−42.7	−42.7	−42.3	−44.4	−44.3	−41.6
OH+FOF→HOF+OF	−10.7[a]	0.9	0.9	2.0	0.1	0.1	0.3
OH+FOF→HO2+F2	−13.6[a]	−11.4	−11.4	−13.0	−10.3	−10.3	−7.9
OH+HOF→HO2+HF	−51.3[a]	−51.6	−51.6	−57.8	−53.0	−53.1	−50.8
OH+OF→HOF+O	1.6[a]	5.9	5.9	5.2	7.6	7.5	7.4
OH+OF→HO2+F	−15.2[a]	−19.2	−19.3	−19.7	−16.8	−16.9	−15.4
OH+O2N→HO2+NO	6.8[a]	10.1	10.1	13.8	9.5	9.6	14.2
OH+O2N→HNO+O2	8.4[a]	11.4	11.4	12.2	0.5	0.6	7.3
OH+N2O→HO2+N2	−26.0[a]	−30.8	−30.7	−26.6	−28.7	−28.6	−20.9
OH+N2O→HNO+NO	19.4[a]	14.0	14.1	14.5	−14.9	−14.7	−2.9
OH+trans-HONO→HO2+HNO	38.4[a]	29.0	29.1	28.3	28.8	28.9	33.6
OH+HNCO→HCO+HNO	56.6[a]	20.7	20.8	24.5	15.6	15.8	26.4
OH+HNCO→HO2+HCN	53.0[a]	22.9	23.0	29.0	36.0	36.2	43.2
OH+NO→HNO+O	54.1[a]	49.8	49.7	47.1	48.9	48.7	50.6
OH+NO→HO2+N	84.4[a]	80.4	80.4	83.2	92.5	92.4	96.2
OH+oxirene→HO2+C2H2	−17.8[a]	−18.8	−18.6	−18.9	−14.7	−14.4	−15.3
OH+oxirane→HO2+C2H4	19.1[a]	17.9	18.0	17.5	17.8	18.0	17.3
OH+methanol→HO2+CH4	24.8[a]	20.5	20.7	22.9	24.9	25.2	28.0
OH+trans-HCOH→HCO+H2O	−82.7[a]	−71.1	−71.0	−70.1	−75.9	−75.8	−76.4
OH+trans-HCOH→HO2+CH2	63.4[a]	73.7	73.8	76.8	73.8	73.9	73.3
OH+formic acid→HO2+trans-HCO	111.1[a]	86.5	86.7	88.9	91.0	91.3	100.7
OH+formic acid→HCO+H2O2	60.6[a]	48.0	48.2	51.7	45.1	45.4	51.6
OH+ketene→HO2+CH2C	105.2[a]	81.9	82.0	85.0	91.0	91.2	96.1
OH+ketene→HCO+H2CO	−13.4[a]	−30.6	−30.5	−28.2	−29.5	−29.2	−27.1
OH+glyoxal→HO2+oxirene	110.7[a]	116.2	116.6	119.3	122.0	122.5	128.1
OH+glyoxal→HCO+formic acid	−39.0[a]	−29.8	−29.5	−30.7	−29.8	−29.4	−29.0

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Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
OH+acetaldehyde→HCO+methanol	−7.8[a]	−8.6	−8.2	−8.1	−9.2	−8.7	−5.9
OH+acetaldehyde→HO2+C2H4	45.4[a]	48.3	48.6	50.4	55.1	55.5	58.4
OH+F2CO→HO2+CF2	93.5[a]	69.4	69.5	75.9	76.2	76.4	89.7
OH+F2CO→HCO+FOF	154.6[a]	134.8	134.9	139.5	139.0	139.2	146.6
OH+HFCO→HOF+HCO	72.9[a]	60.7	60.8	62.6	61.9	62.1	68.0
OH+H2CO→HO2+CH2 ($^3B_1$)	115.6[a]	114.2	114.3	115.8	117.0	117.1	121.4
OH+H2CO→HCO+H2O	−30.5[a]	−30.6	−30.5	−31.0	−32.6	−32.5	−28.3
OH+HCO→HO2+CH	126.9[a]	131.2	131.2	130.2	136.3	136.3	135.5
OH+CO2→HO2+CO	62.1[a]	51.0	51.1	56.2	60.7	60.8	70.9
OH+CO2→HCO+O2	97.1[a]	75.7	75.8	79.5	73.0	73.0	82.4
OH+CO→HCO+O	87.5[a]	73.1	73.1	71.9	70.2	70.0	69.0
OH+CO→HO2+C	191.4[a]	181.0	181.0	181.3	184.5	184.5	184.0
OH+HCN→HNO+CH	130.5[a]	128.9	129.0	125.6	115.9	115.9	118.7
OH+CN→HCO+N	9.1[a]	−2.9	−2.9	0.1	1.5	1.5	7.3
OH+CN→HNO+C	82.7[a]	74.3	74.3	73.4	72.3	72.3	76.7
OH+trans-HO3→HO2+HO2	−10.6[a]	−18.7	−18.7	−16.5	−14.6	−14.5	−12.2
OH+O3→HO2+O2	−41.7[a]	−43.3	−43.3	−41.4	−55.8	−55.8	−54.5
OH+H2O2→HO2+H2O	−32.2[a]	−32.5	−32.5	−32.8	−29.9	−29.8	−27.4
OH+H2O→HO2+H2	55.2[a]	46.3	46.3	56.4	52.3	52.3	58.0
OH+trans-H2N2→HNO+NH2	15.3[a]	19.2	19.3	14.6	14.7	14.9	9.7
OH+propyne→HCO+C2H4	−30.7[a]	−37.1	−36.9	−36.0	−38.7	−38.4	−36.3
OH+propene→HCO+C2H6	−23.7[a]	−30.0	−29.6	−29.1	−33.0	−32.4	−29.8
OH+C2H3F→HOF+C2H3	76.4[a]	76.1	76.3	77.7	77.4	77.7	80.2
OH+C2H3F→HCO+CH3F	−21.3[a]	−32.5	−32.2	−30.6	−32.1	−31.7	−29.9
OH+C2H4→HCO+CH4	−28.5[a]	−36.4	−36.1	−35.6	−39.4	−39.0	−36.4
OH+C2H3→HCO+CH3	−34.0[a]	−38.1	−38.0	−36.9	−38.7	−38.4	−36.7
OH+C2F2→HCO+CF2	−44.9[a]	−66.2	−66.1	−62.0	−61.9	−61.8	−51.2
OH+HCCF→HOF+C2H	80.9[a]	88.3	88.4	89.4	91.6	91.7	94.6
OH+C2H2→HCO+CH2	42.6[a]	33.0	33.1	34.6	27.6	27.8	32.1
OH+CF2→HCO+F2	47.5[a]	54.0	54.0	50.6	52.5	52.5	49.0
OH+CF2→HOF+CF	74.6[a]	84.9	84.9	87.5	87.1	87.2	86.2
OH+CH2 ($^3B_1$)→HCO+H2	−91.0[a]	−98.5	−98.5	−90.5	−97.3	−97.4	−91.7
OH+CF→HOF+C	81.3[a]	95.2	95.2	92.7	97.7	97.7	93.4
OH+CF→HCO+F	−39.5[a]	−37.8	−37.9	−41.6	−41.0	−41.2	−44.5
OH+F2→HOF+F	−12.4[a]	−6.9	−7.0	−4.7	−6.4	−6.5	−7.3
OH+O2→HO2+O	52.5[a]	48.5	48.4	48.7	57.9	57.8	57.5
OH+N2→HNO+N	129.8[a]	125.3	125.2	124.2	106.3	106.2	114.2
OF+CH3F→FOF+CH3	74.4[a]	69.6	69.6	69.3	70.8	70.9	73.1
OF+FOOF→FOF+FOO	−23.1[a]	−15.0	−14.9	−15.6	−22.3	−22.3	−21.5
OF+FOO→FOF+O2	−26.8[a]	−43.6	−43.6	−44.3	−44.4	−44.4	−41.8
OF+FOF→FOO+F2	−26.9[a]	−11.2	−11.2	−14.2	−16.3	−16.3	−16.4
OF+HOF→FOO+HF	−64.6[a]	−51.5	−51.5	−59.0	−59.0	−59.0	−59.3
OF+OF→FOF+O	12.4[a]	5.0	5.0	3.2	7.5	7.4	7.2
OF+OF→FOO+F	−28.6[a]	−19.1	−19.2	−20.9	−22.7	−22.9	−24.0
OF+O2N→FOO+NO	−6.5[a]	10.2	10.3	12.6	3.5	3.6	5.7
OF+N2O→FOO+N2	−39.3[a]	−30.7	−30.6	−27.8	−34.7	−34.5	−29.4
OF+trans-HONO→FOO+HNO	25.1[a]	29.2	29.2	27.1	22.8	22.9	25.1
OF+HNCO→FOO+HCN	39.7[a]	23.1	23.2	27.8	30.1	30.3	34.7
OF+NO→FOO+N	71.1[a]	80.6	80.6	82.0	86.5	86.5	87.7
OF+oxirene→FOO+C2H2	−31.1[a]	−18.6	−18.5	−20.1	−20.6	−20.4	−23.8
OF+oxirane→FOO+C2H4	5.8[a]	18.0	18.1	16.3	11.9	12.1	8.7
OF+methanol→FOO+CH4	11.4[a]	20.7	20.8	21.6	19.0	19.2	19.5
OF+trans-HCOH→FOO+CH2	50.1[a]	73.9	74.0	75.5	67.8	67.9	64.7
OF+formic acid→FOO+trans-HCO	97.8[a]	86.7	86.9	87.7	85.1	85.4	92.1
OF+ketene→FOO+CH2C	91.9[a]	82.0	82.1	83.8	85.1	85.2	87.6
OF+glyoxal→FOO+oxirene	97.4[a]	116.4	116.7	118.1	116.0	116.5	119.6
OF+acetaldehyde→FOO+C2H4	32.1[a]	48.5	48.7	49.2	49.2	49.5	49.9
OF+F2CO→FOO+CF2	80.2[a]	69.6	69.7	74.7	70.2	70.4	81.2
OF+HFCO→FOF+HCO	83.6[a]	59.8	59.9	60.6	61.9	62.0	67.7
OF+H2CO→FOO+CH2 ($^3B_1$)	102.3[a]	114.4	114.5	114.6	111.0	111.2	112.9
OF+HCO→FOO+CH	113.6[a]	131.4	131.4	129.0	130.3	130.3	127.0
OF+CO2→FOO+CO	48.8[a]	51.2	51.2	55.0	54.7	54.8	62.4
OF+CO→FOO+C	178.1[a]	181.1	181.1	180.1	178.6	178.6	175.5
OF+trans-HO3→FOO+HO2	−23.9[a]	−18.6	−18.5	−17.7	−20.5	−20.4	−20.7
OF+O3→FOO+O2	−55.0[a]	−43.2	−43.1	−42.6	−61.8	−61.7	−63.0

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Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
OF+H2O2→FOO+H2O	-45.5^a	−32.4	−32.3	−34.0	−35.8	−35.8	−35.9
OF+H2O→FOO+H2	41.8^a	46.5	46.4	55.2	46.4	46.3	49.5
OF+C2H3F→FOF+C2H3	87.1^a	75.2	75.4	75.7	77.3	77.6	80.0
OF+HCCF→FOF+C2H	91.6^a	87.4	87.5	87.4	91.6	91.6	94.3
OF+CF2→FOF+CF	85.4^a	84.0	84.0	85.5	87.1	87.1	85.9
OF+CF→FOF+C	92.0^a	94.3	94.3	90.7	97.7	97.6	93.1
OF+F2→FOF+F	-1.7^a	−7.9	−7.9	−6.7	−6.4	−6.6	−7.6
OF+O2→FOO+O	39.2^a	48.6	48.6	47.5	51.9	51.8	49.0
The OMx and OMx-D3T energies are corrected by excluding ZPVE and thermal contributions							
H+CH3F→HF+CH3	-26.6^a	−20.1	−19.9	−30.3	−25.0	−24.7	−26.4
H+FOOF→HF+FOO	-124.0^a	−107.7	−107.5	−115.2	−121.5	−121.3	−121.0
H+FOOF→OH+FOF	-48.6^a	−56.1	−56.0	−58.2	−61.9	−61.6	−62.0
H+FOO→OH+OF	-25.6^a	−41.2	−41.1	−42.7	−39.4	−39.2	−40.5
H+FOO→HF+O2	-127.7^a	−136.8	−136.6	−143.9	−144.1	−143.9	−141.4
H+FOF→HF+OF	-100.9^a	−92.7	−92.6	−99.7	−99.1	−98.9	−99.5
H+FOF→OH+F2	-52.5^a	−52.7	−52.6	−56.8	−56.0	−55.9	−56.9
H+HOF→OH+HF	-90.2^a	−92.5	−92.4	−101.6	−98.0	−97.9	−99.8
H+OF→HF+O	-88.6^a	−87.8	−87.8	−96.5	−91.8	−91.7	−92.4
H+OF→OH+F	-54.1^a	−60.6	−60.6	−63.5	−62.6	−62.5	−64.5
H+O2N→OH+NO	-32.1^a	−31.0	−30.8	−30.1	−35.9	−35.6	−34.8
H+O2N→NH+O2	24.0^a	27.8	28.0	27.3	20.9	21.2	23.2
H+N2O→OH+N2	-64.8^a	−71.7	−71.5	−70.4	−73.9	−73.6	−69.9
H+N2O→NH+NO	35.0^a	31.0	31.3	29.6	5.8	6.1	13.0
H+trans-HONO→OH+HNO	-0.5^a	−11.7	−11.5	−15.5	−15.9	−15.6	−15.4
H+trans-HONO→NH+HO2	54.0^a	45.9	46.2	43.4	49.9	50.3	49.5
H+HNCO→NH+HCO	72.2^a	38.5	38.7	39.5	37.1	37.5	42.3
H+HNCO→CH+HNO	144.6^a	112.4	112.6	110.8	108.2	108.6	112.9
H+HNCO→OH+HCN	14.1^a	−18.9	−18.6	−14.8	−9.8	−9.4	−5.8
H+HNO→NH+OH	15.6^a	17.7	17.8	15.1	21.4	21.7	15.9
H+NO→NH+O	69.7^a	66.5	66.5	62.2	69.7	69.7	66.5
H+NO→OH+N	45.5^a	40.0	40.0	39.3	47.8	47.9	47.2
H+oxirene→OH+C2H2	-56.7^a	−60.6	−60.4	−62.8	−60.7	−60.3	−64.3
H+oxirane→OH+C2H4	-19.8^a	−22.2	−22.0	−26.3	−26.4	−26.1	−31.8
H+methanol→OH+CH4	-14.1^a	−20.7	−20.4	−21.0	−19.9	−19.5	−21.0
H+trans-HCOH→CH+H2O	5.3^a	20.4	20.6	16.3	16.4	16.7	10.1
H+trans-HCOH→OH+CH2	24.5^a	34.5	34.6	32.9	30.5	30.8	24.2
H+formic acid→OH+trans-HCOH	72.2^a	47.1	47.4	45.1	47.4	47.9	51.6
H+formic acid→H2O+HCO	-10.5^a	−24.0	−23.7	−25.0	−28.8	−28.2	−24.8
H+formic acid→CH+H2O2	148.6^a	140.3	140.6	138.0	138.4	138.9	138.1
H+ketene→OH+CH2C	66.3^a	42.1	42.3	41.2	47.1	47.5	47.1
H+ketene→CH+H2CO	74.6^a	61.0	61.3	58.1	63.2	63.7	59.4
H+glyoxal→OH+oxirene	71.8^a	76.8	77.2	75.4	77.6	78.3	79.1
H+glyoxal→CH+formic acid	49.0^a	61.8	62.2	55.6	61.8	62.4	57.5
H+acetaldehyde→CH+methanol	80.1^a	83.5	84.0	78.2	83.6	84.3	80.6
H+acetaldehyde→OH+C2H4	6.6^a	7.9	8.2	6.5	10.5	11.1	9.4
H+F2CO→OH+CF2	54.6^a	29.6	29.9	32.1	32.3	32.7	40.7
H+F2CO→CH+FOF	242.6^a	226.9	227.1	225.8	232.5	232.9	233.1
H+HFCO→HF+HCO	-17.3^a	−31.1	−30.9	−39.0	−35.4	−35.1	−31.8
H+H2CO→OH+CH2 ($^3B_1$)	76.7^a	76.1	76.3	71.9	74.5	74.9	72.4
H+H2CO→CH+H2O	57.5^a	62.0	62.2	55.3	60.3	60.7	58.2
H+HCO→OH+CH	88.0^a	91.6	91.7	86.3	92.6	92.8	86.5
H+CO2→OH+CO	23.2^a	11.0	11.1	12.4	16.5	16.7	21.9
H+CO2→CH+O2	185.1^a	167.9	168.0	165.8	166.4	166.7	168.9
H+CO→CH+O	175.5^a	164.6	164.6	158.3	162.8	162.9	155.5
H+CO→OH+C	152.5^a	140.7	140.8	137.4	140.1	140.3	135.0
H+HCN→NH+CH	146.1^a	148.9	149.1	140.7	139.5	139.7	134.6
H+CN→CH+N	97.1^a	88.7	88.8	86.4	94.1	94.2	93.8
H+CN→NH+C	98.2^a	91.4	91.5	88.5	93.3	93.5	92.6
H+trans-HO3→OH+HO2	-49.4^a	−59.6	−59.4	−60.4	−59.9	−59.6	−61.2
H+O3→OH+O2	-80.6^a	−84.3	−84.2	−85.2	−101.3	−101.0	−103.6
H+H2O2→OH+H2O	-71.1^a	−72.8	−72.6	−76.6	−74.6	−74.4	−76.4
H+HO2→2OH	-38.9^a	−39.9	−39.8	−43.9	−44.4	−44.2	−49.0
H+H2O→OH+H2	16.3^a	8.6	8.7	12.5	10.8	10.9	8.9
H+trans-H2N2→NH+NH2	30.9^a	38.0	38.2	29.7	37.2	37.6	25.7
H+propyne→CH+C2H4	57.3^a	54.3	54.6	50.4	53.8	54.3	50.2

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Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
H+propene→CH+C2H6	64.3[a]	61.3	61.8	57.2	59.4	60.2	56.7
H+C2H3F→HF+C2H3	−13.8[a]	−15.7	−15.4	−24.0	−20.0	−19.6	−19.5
H+C2H3F→CH+CH3F	66.7[a]	58.7	59.1	55.8	60.3	60.9	56.6
H+C2H4→CH+CH4	59.5[a]	55.0	55.4	50.7	53.1	53.8	50.1
H+C2H3→CH+CH3	54.0[a]	54.3	54.6	49.4	55.3	55.8	49.8
H+C2F2→CH+CF2	43.1[a]	25.4	25.6	24.3	30.7	31.0	35.3
H+HCCF→HF+C2H	−9.3[a]	−3.8	−3.7	−12.2	−17.4	−17.2	−5.2
H+C2H2→CH+CH2	130.6[a]	127.2	127.4	120.9	122.8	123.2	118.6
H+CF2→CH+F2	135.5[a]	144.6	144.7	136.9	144.2	144.3	135.5
H+CF2→HF+CF	−15.6[a]	−8.6	−8.5	−14.2	−11.9	−11.7	−13.6
H+CH2 ($^3B_1$)→CH+H2	−3.0[a]	−5.4	−5.4	−4.1	−3.4	−3.2	−5.2
H+CF→HF+C	−8.9[a]	1.5	1.5	−9.0	−1.5	−1.4	−6.4
H+CF→CH+F	48.5[a]	52.6	52.6	44.8	50.4	50.4	42.0
H+F2→HF+F	−102.6[a]	−100.7	−100.6	−106.4	−105.6	−105.6	−107.1
H+O2→OH+O	13.6[a]	7.7	7.7	4.8	12.9	12.9	8.5
H+N2→NH+N	145.4[a]	142.7	142.8	139.3	127.5	127.6	130.1
C+CH3F→CF+CH3	−17.6[a]	−21.5	−21.4	−21.4	−23.5	−23.3	−20.0
C+FOOF→CF+FOO	−115.1[a]	−109.1	−109.0	−106.3	−120.0	−119.9	−114.6
C+FOOF→CO+FOF	−201.1[a]	−196.9	−196.8	−195.7	−202.0	−201.9	−197.0
C+FOO→CO+OF	−178.1[a]	−182.0	−181.9	−180.1	−179.6	−179.5	−175.5
C+FOO→CF+O2	−118.8[a]	−138.2	−138.2	−135.0	−142.6	−142.5	−135.0
C+FOF→CF+OF	−92.0[a]	−94.2	−94.2	−90.7	−97.6	−97.6	−93.1
C+FOF→CO+F2	−205.0[a]	−193.4	−193.4	−194.3	−196.2	−196.2	−191.9
C+HOF→CO+HF	−242.7[a]	−233.2	−233.2	−239.1	−238.1	−238.2	−234.8
C+OF→CF+O	−79.7[a]	−89.3	−89.3	−87.5	−90.3	−90.4	−86.0
C+OF→CO+F	−206.7[a]	−201.3	−201.4	−201.0	−202.7	−202.8	−199.5
C+O2N→CO+NO	−184.6[a]	−171.7	−171.6	−167.5	−176.0	−175.9	−169.8
C+O2N→CN+O2	−74.3[a]	−63.6	−63.5	−61.1	−72.4	−72.3	−69.4
C+N2O→CO+N2	−217.4[a]	−212.4	−212.3	−207.8	−214.0	−213.9	−205.0
C+N2O→CN+NO	−63.2[a]	−60.3	−60.2	−58.9	−87.5	−87.4	−79.6
C+trans-HONO→CO+HNO	−153.0[a]	−152.4	−152.3	−153.0	−156.1	−155.9	−150.5
C+trans-HONO→CN+HO2	−44.2[a]	−45.4	−45.3	−45.1	−43.4	−43.3	−43.1
C+HNCO→CN+HCO	−26.0[a]	−52.9	−52.7	−48.9	−56.2	−56.0	−50.3
C+HNCO→CO+HCN	−138.4[a]	−159.6	−159.4	−152.2	−150.0	−149.7	−140.8
C+HNO→CN+OH	−82.7[a]	−73.7	−73.6	−73.4	−71.9	−71.8	−76.7
C+NO→CN+O	−28.6[a]	−24.9	−24.9	−26.2	−23.7	−23.8	−26.1
C+NO→CO+N	−107.0[a]	−100.8	−100.8	−98.1	−92.4	−92.4	−87.8
C+oxirene→CO+C2H2	−209.2[a]	−201.4	−201.2	−200.2	−200.8	−200.6	−199.4
C+oxirane→CO+C2H4	−172.3[a]	−162.9	−162.8	−163.8	−166.6	−166.4	−166.8
C+methanol→CO+CH4	−166.7[a]	−161.4	−161.2	−158.4	−160.0	−159.8	−156.1
C+trans-HCOH→CO+CH2	−128.0[a]	−106.3	−106.2	−104.5	−109.6	−109.5	−110.8
C+formic acid→CO+trans-HCOH	−80.3[a]	−93.6	−93.4	−92.3	−92.7	−92.4	−83.4
C+ketene→CO+CH2C	−86.2[a]	−98.6	−98.5	−96.2	−93.0	−92.8	−87.9
C+glyoxal→CO+oxirene	−80.7[a]	−63.9	−63.6	−62.0	−62.6	−62.0	−55.9
C+acetaldehyde→CO+C2H4	−146.0[a]	−132.9	−132.6	−130.9	−129.6	−129.2	−125.6
C+F2CO→CO+CF2	−97.9[a]	−111.1	−111.0	−105.4	−107.8	−107.6	−94.3
C+HFCO→CF+HCO	−8.4[a]	−32.6	−32.4	−30.1	−33.9	−33.7	−25.4
C+H2CO→CO+CH2 ($^3B_1$)	−75.8[a]	−64.7	−64.5	−65.5	−65.6	−65.4	−62.7
C+HCO→CO+CH	−64.5[a]	−49.1	−49.1	−51.1	−47.6	−47.5	−48.5
C+CO2→CO+CO	−129.3[a]	−129.8	−129.7	−125.0	−123.7	−123.6	−113.1
C+HCN→CN+CH	47.9[a]	57.6	57.6	52.2	46.2	46.2	42.1
C+O3→CO+O2	−233.1[a]	−225.0	−225.0	−222.6	−241.4	−241.3	−238.6
C+H2O2→CO+H2O	−223.6[a]	−213.5	−213.4	−214.1	−214.8	−214.7	−211.4
C+HO2→CO+OH	−191.4[a]	−180.6	−180.6	−181.3	−184.5	−184.5	−184.0
C+H2O→CO+H2	−136.2[a]	−132.1	−132.1	−124.9	−129.3	−129.4	−126.1
C+trans-H2N2→CN+NH2	−67.4[a]	−53.4	−53.2	−58.8	−56.1	−55.9	−66.9
C+C2H3F→CF+C2H3	−4.9[a]	−17.1	−16.9	−15.0	−18.5	−18.2	−13.1
C+HCCF→CF+C2H	−0.4[a]	−5.3	−5.2	−3.3	−15.9	−15.9	1.2
C+CF2→2*CF	−6.7[a]	−10.1	−10.0	−5.2	−10.4	−10.3	−7.2
C+F2→CF+F	−93.7[a]	−102.1	−102.2	−97.4	−104.1	−104.2	−100.7
C+O2→CO+O	−138.9[a]	−133.0	−133.1	−132.6	−127.3	−127.3	−126.6
C+N2→CN+N	47.1[a]	51.4	51.3	50.9	34.1	34.1	37.6
N+FOOF→NO+FOF	−94.2[a]	−96.1	−96.0	−97.6	−109.6	−109.5	−109.2
N+FOO→NO+OF	−71.1[a]	−81.2	−81.1	−82.0	−87.2	−87.1	−87.7
N+FOF→NO+F2	−98.0[a]	−92.6	−92.6	−96.2	−103.8	−103.8	−104.1

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Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
N+HOF→NO+HF	−135.7[a]	−132.4	−132.4	−141.0	−145.8	−145.7	−147.0
N+OF→NO+F	−99.7[a]	−100.6	−100.6	−102.9	−110.3	−110.4	−111.7
N+O2N→NO+NO	−77.6[a]	−71.0	−70.9	−69.4	−83.7	−83.5	−82.0
N+O2N→N2+O2	−121.4[a]	−114.9	−114.8	−112.0	−106.6	−106.4	−106.9
N+N2O→NO+N2	−110.4[a]	−111.7	−111.5	−109.7	−121.7	−121.5	−117.1
N+trans-HONO→NO+HNO	−46.0[a]	−51.6	−51.5	−54.9	−63.7	−63.5	−62.7
N+trans-HONO→N2+HO2	−91.4[a]	−96.8	−96.6	−95.9	−77.6	−77.4	−80.6
N+HNCO→N2+HCO	−73.2[a]	−104.2	−104.1	−99.8	−90.4	−90.1	−87.8
N+HNCO→CN+HNO	47.5[a]	23.6	23.8	24.4	14.1	14.4	19.1
N+HNCO→NO+HCN	−31.4[a]	−58.8	−58.7	−54.1	−57.6	−57.3	−53.0
N+HNO→N2+OH	−129.8[a]	−125.0	−125.0	−124.2	−106.0	−105.9	−114.2
N+NO→N2+O	−75.7[a]	−76.2	−76.3	−77.1	−57.8	−57.9	−63.7
N+oxirene→NO+C2H2	−102.2[a]	−100.6	−100.4	−102.1	−108.5	−108.2	−111.5
N+oxirane→NO+C2H4	−65.3[a]	−62.2	−62.0	−65.6	−74.2	−73.9	−79.0
N+methanol→NO+CH4	−59.7[a]	−60.6	−60.4	−60.3	−67.7	−67.3	−68.2
N+trans-HCOH→CN+H2O	−91.8[a]	−68.3	−68.2	−70.1	−77.7	−77.6	−83.7
N+trans-HCOH→NO+CH2	−21.0[a]	−5.5	−5.4	−6.4	−17.2	−17.1	−23.0
N+formic acid→NO+trans-HCOH	26.7[a]	7.2	7.4	5.8	−0.3	0.0	4.4
N+formic acid→CN+H2O2	51.5[a]	51.6	51.8	51.6	44.3	44.7	44.3
N+ketene→NO+CH2C	20.8[a]	2.1	2.3	1.9	−0.6	−0.4	−0.1
N+ketene→CN+H2CO	−22.6[a]	−27.7	−27.5	−28.2	−30.9	−30.6	−34.4
N+glyoxal→NO+oxirene	26.3[a]	36.8	37.2	36.1	29.8	30.4	31.9
N+glyoxal→CN+formic acid	−48.1[a]	−26.9	−26.6	−30.8	−32.3	−31.8	−36.3
N+acetaldehyde→CN+methanol	−17.0[a]	−5.2	−4.8	−8.1	−10.5	−9.9	−13.2
N+acetaldehyde→NO+C2H4	−39.0[a]	−32.1	−31.8	−32.8	−37.2	−36.8	−37.8
N+F2CO→NO+CF2	9.1[a]	−10.3	−10.2	−7.3	−15.5	−15.2	−6.5
N+F2CO→CN+FOF	145.5[a]	138.2	138.3	139.4	138.4	138.7	139.3
N+H2CO→NO+CH2 ($^3B_1$)	31.2[a]	36.1	36.2	32.6	26.8	27.0	25.1
N+H2CO→CN+H2O	−39.7[a]	−26.7	−26.6	−31.1	−33.7	−33.5	−35.6
N+HCO→NO+CH	42.5[a]	51.6	51.7	47.0	44.8	44.9	39.3
N+CO2→NO+CO	−22.3[a]	−29.0	−28.9	−26.9	−31.3	−31.1	−25.3
N+CO2→CN+O2	88.0[a]	79.2	79.2	79.4	72.3	72.4	75.1
N+CO→CN+O	78.4[a]	75.9	75.8	71.9	68.7	68.6	61.7
N+CO→NO+C	107.0[a]	100.8	100.8	98.1	92.4	92.4	87.8
N+HCN→N2+CH	0.7[a]	6.2	6.3	1.4	12.0	12.1	4.5
N+CN→N2+C	−47.1[a]	−51.4	−51.3	−50.9	−34.1	−34.1	−37.6
N+trans-HO3→NO+HO2	−95.0[a]	−99.5	−99.4	−99.7	−107.6	−107.5	−108.4
N+O3→NO+O2	−126.1[a]	−124.3	−124.2	−124.5	−149.0	−148.9	−150.8
N+H2O2→NO+H2O	−116.6[a]	−112.7	−112.6	−116.0	−122.4	−122.2	−123.6
N+HO2→NO+OH	−84.4[a]	−79.9	−79.8	−83.2	−92.1	−92.1	−96.2
N+H2O→NO+H2	−29.3[a]	−31.4	−31.4	−26.8	−37.0	−37.0	−38.3
N+trans-H2N2→N2+NH2	−114.5[a]	−104.7	−104.6	−109.6	−90.3	−90.0	−104.5
N+propyne→CN+C2H4	−39.8[a]	−34.4	−34.2	−36.0	−40.2	−40.0	−43.6
N+propene→CN+C2H6	−32.9[a]	−27.4	−27.0	−29.1	−34.6	−34.0	−37.1
N+C2H3F→CN+CH3F	−30.4[a]	−30.0	−29.7	−30.6	−33.8	−33.4	−37.2
N+C2H4→CN+CH4	−37.7[a]	−33.7	−33.4	−35.7	−40.9	−40.5	−43.7
N+C2H3→CN+CH3	−43.1[a]	−34.4	−34.2	−37.0	−38.7	−38.4	−44.0
N+C2F2→CN+CF2	−54.0[a]	−63.3	−63.2	−62.1	−63.4	−63.2	−58.5
N+C2H2→CN+CH2	33.4[a]	38.5	38.6	34.5	28.8	29.0	24.8
N+CF2→CN+F2	38.4[a]	55.9	55.9	50.5	50.1	50.1	41.7
N+CH2 ($^3B_1$)→CN+H2	−100.1[a]	−94.1	−94.2	−90.5	−97.4	−97.5	−99.0
N+CF→CN+F	−48.6[a]	−36.1	−36.2	−41.6	−43.7	−43.8	−51.8
N+O2→NO+O	−31.9[a]	−32.3	−32.3	−34.5	−34.9	−34.9	−38.7
O+CH3F→OF+CH3	62.0[a]	67.8	67.9	66.1	66.8	67.1	66.0
O+FOOF→OF+FOO	−35.4[a]	−19.8	−19.7	−18.8	−29.7	−29.6	−28.7
O+FOOF→O2+FOF	−62.2[a]	−63.8	−63.7	−63.1	−74.7	−74.5	−70.5
O+FOO→O2+OF	−39.2[a]	−48.9	−48.8	−47.5	−52.3	−52.2	−49.0
O+FOF→OF+OF	−12.4[a]	−4.9	−4.8	−3.2	−7.3	−7.2	−7.2
O+FOF→O2+F2	−66.1[a]	−60.4	−60.3	−61.7	−68.9	−68.8	−65.4
O+HOF→O2+HF	−103.8[a]	−100.1	−100.1	−106.5	−110.9	−110.8	−108.3
O+OF→O2+F	−67.8[a]	−68.3	−68.3	−68.4	−75.4	−75.5	−72.9
O+O2N→O2+NO	−45.7[a]	−38.7	−38.6	−34.9	−48.8	−48.6	−43.3
O+trans-HONO→O2+HNO	−14.1[a]	−19.4	−19.2	−20.4	−28.8	−28.5	−23.9
O+trans-HONO→NO+HO2	−15.6[a]	−20.6	−20.4	−18.8	−19.8	−19.5	−17.0
O+HNCO→NO+HCO	2.6[a]	−28.0	−27.8	−22.7	−32.6	−32.2	−24.2

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Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
O+HNCO→CO+HNO	−30.9[a]	−52.2	−52.0	−47.5	−54.6	−54.3	−42.6
O+HNCO→O2+HCN	0.5[a]	−26.6	−26.4	−19.6	−22.7	−22.4	−14.3
O+HNO→NO+OH	−54.1[a]	−48.8	−48.7	−47.1	−48.2	−48.1	−50.6
O+NO→O2+N	31.9[a]	32.3	32.3	34.5	34.9	34.9	38.7
O+oxirene→O2+C2H2	−70.3[a]	−68.3	−68.1	−67.6	−73.6	−73.2	−72.8
O+oxirane→O2+C2H4	−33.4[a]	−29.9	−29.7	−31.2	−39.3	−39.0	−40.2
O+methanol→O2+CH4	−27.7[a]	−28.4	−28.1	−25.8	−32.8	−32.4	−29.5
O+trans-HCOH→CO+H2O	−170.2[a]	−144.2	−144.0	−142.0	−146.4	−146.2	−145.4
O+trans-HCOH→O2+CH2	10.9[a]	26.8	26.9	28.1	17.7	17.9	15.8
O+formic acid→O2+trans-HCOH	58.6[a]	39.4	39.7	40.3	34.6	35.0	43.2
O+formic acid→CO+H2O2	−26.9[a]	−24.3	−24.0	−20.3	−24.4	−23.9	−17.4
O+ketene→O2+CH2C	52.7[a]	34.4	34.6	36.4	34.3	34.5	38.6
O+ketene→CO+H2CO	−100.9[a]	−103.6	−103.4	−100.1	−99.6	−99.2	−96.1
O+glyoxal→O2+oxirene	58.2[a]	69.1	69.5	70.6	64.7	65.3	70.6
O+glyoxal→CO+formic acid	−126.5[a]	−102.8	−102.4	−102.7	−101.0	−100.4	−98.0
O+acetaldehyde→CO+methanol	−95.4[a]	−81.1	−80.6	−80.0	−79.2	−78.6	−74.9
O+acetaldehyde→O2+C2H4	−7.1[a]	0.2	0.5	1.7	−2.4	−1.9	0.9
O+F2CO→O2+CF2	41.0[a]	21.9	22.1	27.2	19.4	19.7	32.2
O+F2CO→CO+FOF	67.1[a]	62.3	62.5	67.6	69.7	70.0	77.6
O+HFCO→OF+HCO	71.2[a]	56.7	56.9	57.4	56.4	56.6	60.5
O+H2CO→O2+CH2 ($^3B_1$)	63.1[a]	68.4	68.5	67.1	61.6	61.9	63.9
O+H2CO→CO+H2O	−118.0[a]	−102.6	−102.4	−103.0	−102.4	−102.2	−97.3
O+HCO→O2+CH	74.4[a]	83.9	84.0	81.5	79.7	79.8	78.0
O+CO2→O2+CO	9.6[a]	3.3	3.4	7.6	3.6	3.8	13.4
O+CO→O2+C	138.9[a]	133.0	133.1	132.6	127.3	127.3	126.6
O+HCN→NO+CH	76.5[a]	82.4	82.6	78.5	69.8	70.0	68.2
O+CN→CO+N	−78.4[a]	−75.9	−75.8	−71.9	−68.7	−68.6	−61.7
O+CN→NO+C	28.6[a]	24.9	24.9	26.2	23.7	23.8	26.1
O+trans-HO3→O2+HO2	−63.1[a]	−67.3	−67.1	−65.2	−72.7	−72.5	−69.6
O+O3→O2+O2	−94.2[a]	−92.0	−91.9	−90.1	−114.1	−114.0	−112.0
O+H2O2→O2+H2O	−84.7[a]	−80.5	−80.3	−81.5	−87.5	−87.3	−84.9
O+HO2→O2+OH	−52.5[a]	−47.6	−47.5	−48.7	−57.2	−57.1	−57.5
O+H2O→O2+H2	2.7[a]	0.9	0.9	7.7	−2.1	−2.0	0.5
O+trans-H2N2→NO+NH2	−38.8[a]	−28.5	−28.3	−32.5	−32.5	−32.1	−40.8
O+propyne→CO+C2H4	−118.2[a]	−110.3	−110.0	−107.9	−108.9	−108.6	−105.3
O+propene→CO+C2H6	−111.2[a]	−103.3	−102.8	−101.0	−103.4	−102.7	−98.8
O+C2H3F→OF+C2H3	74.7[a]	72.2	72.4	72.5	71.8	72.1	72.8
O+C2H3F→CO+CH3F	−108.8[a]	−105.9	−105.5	−102.5	−102.5	−102.0	−98.9
O+C2H4→CO+CH4	−116.0[a]	−109.6	−109.3	−107.5	−109.6	−109.1	−105.4
O+C2H3→CO+CH3	−121.5[a]	−110.3	−110.0	−108.9	−107.5	−107.1	−105.7
O+C2F2→CO+CF2	−132.4[a]	−139.2	−139.1	−133.9	−132.1	−131.9	−120.2
O+HCCF→OF+C2H	79.2[a]	84.0	84.1	84.2	74.4	74.5	87.1
O+C2H2→CO+CH2	−45.0[a]	−37.4	−37.2	−37.4	−39.9	−39.7	−36.9
O+CF2→CO+F2	−40.0[a]	−20.0	−19.9	−21.3	−18.6	−18.5	−20.0
O+CF2→OF+CF	73.0[a]	79.2	79.3	82.3	79.9	80.0	78.8
O+CH2 ($^3B_1$)→CO+H2	−178.5[a]	−170.0	−170.0	−162.4	−166.2	−166.1	−160.7
O+CF→OF+C	79.7[a]	89.3	89.3	87.5	90.3	90.4	86.0
O+CF→CO+F	−127.0[a]	−112.0	−112.1	−113.5	−112.4	−112.4	−113.5
O+F2→OF+F	−14.0[a]	−12.8	−12.8	−9.9	−13.8	−13.9	−14.7
O+N2→NO+N	75.7[a]	76.2	76.3	77.1	57.8	57.9	63.7
F+CH3F→F2+CH3	76.0[a]	80.6	80.7	76.0	80.7	80.9	80.7
F+FOOF→F2+FOO	−21.4[a]	−7.0	−6.9	−8.9	−15.9	−15.7	−13.9
F+FOOF→OF+FOF	5.5[a]	4.4	4.6	5.3	0.7	0.9	2.5
F+FOO→OF+OF	28.6[a]	19.4	19.5	20.9	23.1	23.3	24.0
F+FOO→F2+O2	−25.1[a]	−36.1	−36.0	−37.6	−38.5	−38.3	−34.3
F+FOF→F2+OF	1.7[a]	7.9	8.0	6.7	6.5	6.6	7.6
F+HOF→OF+HF	−36.1[a]	−31.9	−31.8	−38.1	−35.4	−35.3	−35.3
F+OF→F2+O	14.0[a]	12.8	12.8	9.9	13.8	13.9	14.7
F+O2N→OF+NO	22.1[a]	29.6	29.7	33.5	26.6	26.9	29.7
F+N2O→OF+N2	−10.7[a]	−11.1	−10.9	−6.9	−11.4	−11.1	−5.5
F+trans-HONO→OF+HNO	53.7[a]	48.9	49.1	48.0	46.6	46.9	49.0
F+HNCO→CF+HNO	96.1[a]	59.8	60.0	66.0	57.8	58.2	70.9
F+HNCO→OF+HCN	68.2[a]	41.7	41.9	48.7	52.7	53.1	58.7
F+NO→OF+N	99.7[a]	100.6	100.6	102.9	110.3	110.4	111.7
F+oxirene→OF+C2H2	−2.5[a]	−0.1	0.2	0.8	1.9	2.2	0.1

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Table S30: … *continued from previous page* …

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
F+oxirane→OF+C2H4	34.4[a]	38.4	38.6	37.2	36.1	36.5	32.7
F+methanol→OF+CH4	40.0[a]	39.9	40.2	42.5	42.7	43.1	43.4
F+trans-HCOH→CF+H2O	−43.2[a]	−32.2	−32.0	−28.5	−34.1	−33.8	−31.9
F+trans-HCOH→OF+CH2	78.7[a]	95.0	95.2	96.4	93.1	93.3	88.7
F+formic acid→OF+trans-HCOH	126.3[a]	107.7	108.0	108.6	110.0	110.4	116.1
F+formic acid→CF+H2O2	100.1[a]	87.7	88.1	93.2	88.0	88.5	96.1
F+ketene→OF+CH2C	120.5[a]	102.7	102.9	104.7	109.7	110.0	111.6
F+ketene→CF+H2CO	26.1[a]	8.4	8.7	13.4	12.8	13.3	17.4
F+glyoxal→OF+oxirene	126.0[a]	137.4	137.8	139.0	140.1	140.8	143.6
F+glyoxal→CF+formic acid	0.5[a]	9.2	9.6	10.8	11.4	12.0	15.5
F+acetaldehyde→CF+methanol	31.6[a]	31.0	31.4	33.5	33.2	33.9	38.6
F+acetaldehyde→OF+C2H4	60.7[a]	68.4	68.8	70.1	73.1	73.6	73.9
F+F2CO→OF+CF2	108.8[a]	90.2	90.4	95.6	94.9	95.2	105.2
F+F2CO→CF+FOF	194.1[a]	174.3	174.6	181.1	182.1	182.5	191.1
F+HFCO→F2+HCO	85.3[a]	69.6	69.7	67.3	70.2	70.5	75.3
F+H2CO→OF+CH2 ($^3B_1$)	130.8[a]	136.7	136.8	135.5	137.1	137.4	136.8
F+H2CO→CF+H2O	9.0[a]	9.5	9.7	10.5	9.9	10.3	16.2
F+HCO→OF+CH	142.1[a]	152.2	152.3	149.9	155.1	155.3	151.0
F+CO2→OF+CO	77.3[a]	71.6	71.7	75.9	79.0	79.3	86.4
F+CO2→CF+O2	136.6[a]	115.3	115.4	121.0	116.0	116.2	127.0
F+CO→CF+O	127.0[a]	112.0	112.1	113.5	112.4	112.4	113.5
F+CO→OF+C	206.7[a]	201.3	201.4	201.0	202.7	202.8	199.5
F+CN→CF+N	48.6[a]	36.1	36.2	41.6	43.7	43.8	51.8
F+trans-HO3→OF+HO2	4.7[a]	1.0	1.2	3.1	2.7	2.9	3.3
F+O3→OF+O2	−26.5[a]	−23.7	−23.6	−21.7	−38.7	−38.5	−39.1
F+H2O2→OF+H2O	−17.0[a]	−12.2	−12.0	−13.1	−12.1	−11.8	−11.9
F+H2O→OF+H2	70.4[a]	69.2	69.2	76.1	73.4	73.4	73.4
F+propyne→CF+C2H4	8.8[a]	1.7	2.0	5.6	3.4	3.8	8.2
F+propene→CF+C2H6	15.8[a]	8.7	9.2	12.5	9.0	9.8	14.8
F+C2H3F→F2+C2H3	88.8[a]	85.0	85.2	82.4	85.6	86.0	87.5
F+C2H3F→CF+CH3F	18.2[a]	6.1	6.5	11.0	9.9	10.5	14.6
F+C2H4→CF+CH4	11.0[a]	2.4	2.8	6.0	2.7	3.3	8.1
F+C2H3→CF+CH3	5.5[a]	1.7	2.0	4.6	4.9	5.4	7.8
F+C2F2→CF+CF2	−5.4[a]	−27.2	−27.0	−20.4	−19.7	−19.4	−6.6
F+HCCF→F2+C2H	93.3[a]	96.9	97.0	94.1	88.2	88.4	101.8
F+C2H2→CF+CH2	82.1[a]	74.6	74.8	76.1	72.4	72.8	76.6
F+CF2→F2+CF	87.0[a]	92.0	92.1	92.2	93.8	93.9	93.5
F+CH2 ($^3B_1$)→CF+H2	−51.5[a]	−58.0	−57.9	−48.9	−53.8	−53.7	−47.2
F+CF→F2+C	93.7[a]	102.1	102.2	97.4	104.1	104.2	100.7
F+O2→OF+O	67.8[a]	68.3	68.3	68.4	75.4	75.5	72.9
OH+CH3F→HOF+CH3	63.6[a]	72.4	72.5	71.3	73.0	73.2	73.4
OH+FOOF→HOF+FOO	−33.8[a]	−15.2	−15.1	−13.6	−23.5	−23.4	−21.2
OH+FOOF→HO2+FOF	−9.7[a]	−16.2	−16.2	−14.4	−17.5	−17.4	−13.0
OH+FOO→HO2+OF	13.3[a]	−1.3	−1.3	1.2	4.9	5.0	8.5
OH+FOO→HOF+O2	−37.5[a]	−44.3	−44.3	−42.3	−46.1	−46.0	−41.6
OH+FOF→HOF+OF	−10.7[a]	−0.3	−0.3	2.0	−1.1	−1.1	0.3
OH+FOF→HO2+F2	−13.6[a]	−12.8	−12.8	−13.0	−11.7	−11.7	−7.9
OH+HOF→HO2+HF	−51.3[a]	−52.6	−52.6	−57.8	−53.6	−53.7	−50.8
OH+OF→HOF+O	1.6[a]	4.6	4.6	5.2	6.2	6.1	7.4
OH+OF→HO2+F	−15.2[a]	−20.7	−20.8	−19.7	−18.2	−18.3	−15.4
OH+O2N→HO2+NO	6.8[a]	8.9	9.0	13.8	8.4	8.6	14.2
OH+O2N→HNO+O2	8.4[a]	10.1	10.1	12.2	−0.6	−0.5	7.3
OH+N2O→HO2+N2	−26.0[a]	−31.8	−31.7	−26.6	−29.6	−29.4	−20.9
OH+N2O→HNO+NO	19.4[a]	13.3	13.4	14.5	−15.6	−15.5	−2.9
OH+trans-HONO→HO2+HNO	38.4[a]	28.2	28.3	28.3	28.4	28.6	33.6
OH+HNCO→HCO+HNO	56.6[a]	20.8	20.9	24.5	15.6	15.8	26.4
OH+HNCO→HO2+HCN	53.0[a]	21.0	21.2	29.0	34.5	34.7	43.2
OH+NO→HNO+O	54.1[a]	48.8	48.7	47.1	48.2	48.1	50.6
OH+NO→HO2+N	84.4[a]	79.9	79.8	83.2	92.1	92.1	96.2
OH+oxirene→HO2+C2H2	−17.8[a]	−20.7	−20.6	−18.9	−16.3	−16.1	−15.3
OH+oxirane→HO2+C2H4	19.1[a]	17.7	17.8	17.5	17.9	18.1	17.3
OH+methanol→HO2+CH4	24.8[a]	19.2	19.4	22.9	24.5	24.7	28.0
OH+trans-HCOH→HCO+H2O	−82.7[a]	−71.2	−71.1	−70.1	−76.2	−76.1	−76.4
OH+trans-HCOH→HO2+CH2	63.4[a]	74.4	74.4	76.8	74.9	75.0	73.3
OH+formic acid→HO2+trans-HCO	111.1[a]	87.0	87.2	88.9	91.8	92.1	100.7

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Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
OH+formic acid→HCO+H2O2	60.6[a]	48.7	48.9	51.7	45.8	46.2	51.6
OH+ketene→HO2+CH2C	105.2[a]	82.0	82.1	85.0	91.5	91.6	96.1
OH+ketene→HCO+H2CO	−13.4[a]	−30.6	−30.4	−28.2	−29.4	−29.1	−27.1
OH+glyoxal→HO2+oxirene	110.7[a]	116.7	117.0	119.3	121.9	122.4	128.1
OH+glyoxal→HCO+formic acid	−39.0[a]	−29.8	−29.5	−30.7	−30.8	−30.3	−29.0
OH+acetaldehyde→HCO+methanol	−7.8[a]	−8.1	−7.7	−8.1	−9.0	−8.5	−5.9
OH+acetaldehyde→HO2+C2H4	45.4[a]	47.8	48.0	50.4	54.9	55.2	58.4
OH+F2CO→HO2+CF2	93.5[a]	69.5	69.7	75.9	76.7	76.9	89.7
OH+F2CO→HCO+FOF	154.6[a]	135.3	135.4	139.5	139.9	140.1	146.6
OH+HFCO→HOF+HCO	72.9[a]	61.4	61.5	62.6	62.6	62.8	68.0
OH+H2CO→HO2+CH2 ($^3B_1$)	115.6[a]	116.0	116.1	115.8	118.9	119.0	121.4
OH+H2CO→HCO+H2O	−30.5[a]	−29.6	−29.5	−31.0	−32.2	−32.1	−28.3
OH+HCO→HO2+CH	126.9[a]	131.5	131.5	130.2	136.9	137.0	135.5
OH+CO2→HO2+CO	62.1[a]	50.9	50.9	56.2	60.8	60.9	70.9
OH+CO2→HCO+O2	97.1[a]	76.3	76.3	79.5	73.8	73.9	82.4
OH+CO→HCO+O	87.5[a]	73.0	72.9	71.9	70.2	70.1	69.0
OH+CO→HO2+C	191.4[a]	180.6	180.6	181.3	184.5	184.5	184.0
OH+HCN→HNO+CH	130.5[a]	131.2	131.2	125.6	118.0	118.1	118.7
OH+CN→HCO+N	9.1[a]	−2.9	−2.9	0.1	1.5	1.5	7.3
OH+CN→HNO+C	82.7[a]	73.7	73.6	73.4	71.9	71.8	76.7
OH+trans-HO3→HO2+HO2	−10.6[a]	−19.7	−19.6	−16.5	−15.5	−15.4	−12.2
OH+O3→HO2+O2	−41.7[a]	−44.4	−44.4	−41.4	−56.9	−56.9	−54.5
OH+H2O2→HO2+H2O	−32.2[a]	−32.9	−32.8	−32.8	−30.3	−30.2	−27.4
OH+H2O→HO2+H2	55.2[a]	48.5	48.5	56.4	55.2	55.1	58.0
OH+trans-H2N2→HNO+NH2	15.3[a]	20.3	20.4	14.6	15.8	15.9	9.7
OH+propyne→HCO+C2H4	−30.7[a]	−37.3	−37.1	−36.0	−38.7	−38.5	−36.3
OH+propene→HCO+C2H6	−23.7[a]	−30.3	−29.9	−29.1	−33.1	−32.6	−29.8
OH+C2H3F→HOF+C2H3	76.4[a]	76.8	77.0	77.7	78.0	78.3	80.2
OH+C2H3F→HCO+CH3F	−21.3[a]	−32.9	−32.6	−30.6	−32.3	−31.9	−29.9
OH+C2H4→HCO+CH4	−28.5[a]	−36.6	−36.3	−35.6	−39.4	−39.0	−36.4
OH+C2H3→HCO+CH3	−34.0[a]	−37.3	−37.1	−36.9	−37.3	−37.0	−36.7
OH+C2F2→HCO+CF2	−44.9[a]	−66.2	−66.1	−62.0	−61.9	−61.8	−51.2
OH+HCCF→HOF+C2H	80.9[a]	88.7	88.7	89.4	80.6	80.6	94.6
OH+C2H2→HCO+CH2	42.6[a]	35.6	35.7	34.6	30.3	30.4	32.1
OH+CF2→HCO+F2	47.5[a]	53.0	53.0	50.6	51.6	51.6	49.0
OH+CF2→HOF+CF	74.6[a]	83.8	83.9	87.5	86.1	86.2	86.2
OH+CH2 ($^3B_1$)→HCO+H2	−91.0[a]	−97.0	−97.1	−90.5	−95.9	−96.0	−91.7
OH+CF→HOF+C	81.3[a]	93.9	93.9	92.7	96.5	96.5	93.4
OH+CF→HCO+F	−39.5[a]	−39.0	−39.1	−41.6	−42.2	−42.4	−44.5
OH+F2→HOF+F	−12.4[a]	−8.2	−8.3	−4.7	−7.6	−7.7	−7.3
OH+O2→HO2+O	52.5[a]	47.6	47.5	48.7	57.2	57.1	57.5
OH+N2→HNO+N	129.8[a]	125.0	125.0	124.2	106.0	105.9	114.2
OF+CH3F→FOF+CH3	74.4[a]	72.7	72.7	69.3	74.2	74.3	73.1
OF+FOOF→FOF+FOO	−23.1[a]	−14.9	−14.9	−15.6	−22.4	−22.3	−21.5
OF+FOO→FOF+O2	−26.8[a]	−44.0	−44.0	−44.3	−45.0	−45.0	−41.8
OF+FOF→FOO+F2	−26.9[a]	−11.4	−11.5	−14.2	−16.6	−16.6	−16.4
OF+HOF→FOO+HF	−64.6[a]	−51.2	−51.3	−59.0	−58.6	−58.6	−59.3
OF+OF→FOF+O	12.4[a]	−44.4	−44.6	3.2	−40.8	−41.1	7.2
OF+OF→FOO+F	−28.6[a]	−68.7	−68.9	−20.9	−71.2	−71.6	−24.0
OF+O2N→FOO+NO	−6.5[a]	10.2	10.3	12.6	3.5	3.6	5.7
OF+N2O→FOO+N2	−39.3[a]	−30.5	−30.4	−27.8	−34.5	−34.4	−29.4
OF+trans-HONO→FOO+HNO	25.1[a]	29.6	29.6	27.1	23.5	23.6	25.1
OF+HNCO→FOO+HCN	39.7[a]	22.4	22.5	27.8	29.6	29.8	34.7
OF+NO→FOO+N	71.1[a]	81.2	81.1	82.0	87.2	87.1	87.7
OF+oxirene→FOO+C2H2	−31.1[a]	−19.4	−19.3	−20.1	−21.3	−21.1	−23.8
OF+oxirane→FOO+C2H4	5.8[a]	19.0	19.1	16.3	13.0	13.2	8.7
OF+methanol→FOO+CH4	11.4[a]	20.6	20.7	21.6	19.5	19.8	19.5
OF+trans-HCOH→FOO+CH2	50.1[a]	75.7	75.7	75.5	70.0	70.0	64.7
OF+formic acid→FOO+trans-HCO	97.8[a]	88.4	88.5	87.7	86.9	87.1	92.1
OF+ketene→FOO+CH2C	91.9[a]	83.3	83.4	83.8	86.6	86.7	87.6
OF+glyoxal→FOO+oxirene	97.4[a]	118.0	118.4	118.1	117.0	117.5	119.6
OF+acetaldehyde→FOO+C2H4	32.1[a]	49.1	49.3	49.2	50.0	50.3	49.9
OF+F2CO→FOO+CF2	80.2[a]	70.9	71.0	74.7	71.7	71.9	81.2
OF+HFCO→FOF+HCO	83.6[a]	61.7	61.7	60.6	63.7	63.9	67.7
OF+H2CO→FOO+CH2 ($^3B_1$)	102.3[a]	117.3	117.4	114.6	113.9	114.1	112.9

... *continued on next page* ...

Table S30: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
OF+HCO→FOO+CH	113.6[a]	132.8	132.8	129.0	132.0	132.0	127.0
OF+CO2→FOO+CO	48.8[a]	52.2	52.2	55.0	55.9	56.0	62.4
OF+CO→FOO+C	178.1[a]	182.0	181.9	180.1	179.6	179.5	175.5
OF+trans-HO3→FOO+HO2	−23.9[a]	−18.3	−18.3	−17.7	−20.4	−20.4	−20.7
OF+O3→FOO+O2	−55.0[a]	−43.1	−43.1	−42.6	−61.8	−61.8	−63.0
OF+H2O2→FOO+H2O	−45.5[a]	−31.5	−31.5	−34.0	−35.2	−35.1	−35.9
OF+H2O→FOO+H2	41.8[a]	49.8	49.8	55.2	50.2	50.1	49.5
OF+C2H3F→FOF+C2H3	87.1[a]	77.1	77.2	75.7	79.1	79.4	80.0
OF+HCCF→FOF+C2H	91.6[a]	88.9	89.0	87.4	81.7	81.7	94.3
OF+CF2→FOF+CF	85.4[a]	84.1	84.1	85.5	87.2	87.3	85.9
OF+CF→FOF+C	92.0[a]	94.2	94.2	90.7	97.6	97.6	93.1
OF+F2→FOF+F	−1.7[a]	−7.9	−8.0	−6.7	−6.5	−6.6	−7.6
OF+O2→FOO+O	39.2[a]	48.9	48.8	47.5	52.3	52.2	49.0

a A.Karton, S.Daon, J.M.Martin, Chem.Phys.Lett. 510, 165 (2011).

Table S31: Benchmark Results for the ISOMER20 Subset of the W4-11-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
The OMx and OMx-D3T energies are uncorrected atomization enthalpies at 298 K							
trans-HONO→cis-HONO	0.4[a]	−4.6	−4.6	−6.4	−2.9	−2.9	−2.5
HCN→HNC	15.2[a]	17.6	17.5	13.2	2.0	1.9	−2.9
HNCO→HOCN	24.7[a]	6.9	6.9	11.2	14.8	14.8	17.6
HNCO→HONC	84.6[a]	58.8	58.8	59.7	58.6	58.6	53.7
HNCO→HCNO	69.8[a]	50.0	50.0	50.4	55.5	55.5	61.9
HOCN→HONC	59.9[a]	51.9	51.9	48.6	43.9	43.8	36.1
HOCN→HCNO	45.1[a]	43.1	43.1	39.2	40.7	40.7	44.2
HCNO→HONC	14.8[a]	8.8	8.8	9.4	3.1	3.1	−8.1
formaldehyde→trans-HCOH	52.2[a]	40.5	40.5	39.0	43.2	43.3	48.1
trans-HCOH→cis-HCOH	4.8[a]	1.3	1.3	3.3	6.2	6.2	7.1
HCCH→H2CC	45.6[a]	31.3	31.2	32.0	31.1	31.0	33.9
trans-HO3→cis-HO3	0.2[a]	−5.7	−5.7	−4.9	−0.7	−0.8	−0.5
trans-H2N2→cis-H2N2	5.4[a]	−3.2	−3.2	−2.1	2.3	2.2	2.0
propyne→allene	1.5[a]	−0.0	−0.1	0.4	−0.0	−0.1	0.4
formic acid→dioxirane	91.9[a]	79.0	79.1	90.2	93.4	93.5	101.5
ketene→oxirene	77.4[a]	69.4	69.4	72.0	74.6	74.6	77.5
acetaldehyde→oxirane	26.3[a]	30.5	30.6	32.9	37.3	37.5	41.2
H2CN→HN=CH	7.5[a]	6.9	6.9	3.9	−0.5	−0.5	−0.6
H2NCH2→H3CNH	7.7[a]	12.2	12.2	11.4	13.3	13.3	8.9
The OMx and OMx-D3T energies are corrected by excluding ZPVE and thermal contributions							
trans-HONO→cis-HONO	0.4[a]	−4.8	−4.8	−6.4	−3.0	−3.1	−2.5
HCN→HNC	15.2[a]	18.3	18.2	13.2	2.2	2.2	−2.9
HNCO→HOCN	24.7[a]	6.6	6.7	11.2	14.3	14.3	17.6
HNCO→HONC	84.6[a]	59.0	59.0	59.7	58.6	58.5	53.7
HNCO→HCNO	69.8[a]	49.7	49.7	50.4	55.4	55.5	61.9
HOCN→HONC	59.9[a]	52.4	52.4	48.6	44.3	44.2	36.1
HOCN→HCNO	45.1[a]	43.1	43.1	39.2	41.2	41.2	44.2
HCNO→HONC	14.8[a]	9.3	9.3	9.4	3.1	3.1	−8.1
formaldehyde→trans-HCOH	52.2[a]	41.6	41.6	39.0	44.0	44.0	48.1
trans-HCOH→cis-HCOH	4.8[a]	1.5	1.5	3.3	6.5	6.5	7.1
HCCH→H2CC	45.6[a]	32.3	32.2	32.0	32.3	32.1	33.9
trans-HO3→cis-HO3	0.2[a]	−5.7	−5.7	−4.9	−0.8	−0.8	−0.5
trans-H2N2→cis-H2N2	5.4[a]	−3.1	−3.1	−2.1	2.5	2.5	2.0
propyne→allene	1.5[a]	0.3	0.2	0.4	0.3	0.2	0.4
formic acid→dioxirane	91.9[a]	78.5	78.6	90.2	93.7	93.8	101.5
ketene→oxirene	77.4[a]	70.5	70.5	72.0	75.6	75.6	77.5
acetaldehyde→oxirane	26.3[a]	30.1	30.2	32.9	37.0	37.1	41.2
H2CN→HN=CH	7.5[a]	7.1	7.2	3.9	−0.2	−0.2	−0.6
H2NCH2→H3CNH	7.7[a]	12.1	12.1	11.4	13.4	13.4	8.9

a A.Karton, S.Daon, J.M.Martin, Chem.Phys.Lett. 510, 165 (2011).

Table S32: Benchmark Results for the SN13 Subset of the W4-11-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
The OMx and OMx-D3T energies are uncorrected atomization enthalpies at 298 K							
CH3F+H→F+CH4	2.5[a]	7.3	7.3	1.6	4.8	4.9	2.0
CH2F2+H→F+CH3F	14.7[a]	14.7	14.7	11.1	14.3	14.4	10.3
CH3F+CH3→F+C2H6	17.8[a]	24.3	23.7	21.4	19.6	18.7	20.1
CH2F2+CH3→F+C2H5F	24.0[a]	26.3	25.7	25.0	23.2	22.3	22.6
C2H5F+CH3→F+propane	21.5[a]	26.9	26.0	24.3	23.3	22.1	23.2
CH3F+NH2→F+CH3NH2	23.2[a]	28.2	27.7	27.7	31.5	30.7	33.6
CH3F+NH→F+CH3NH	31.4[a]	36.2	35.9	35.3	35.7	35.1	36.4
CH3F+OH→F+CH3OH	16.7[a]	25.7	25.4	22.6	22.7	22.3	23.0
CH3F+HCO→F+CH3COH	24.5[a]	34.2	33.7	30.7	31.9	31.0	29.0
CH3+FHCO→F+CH3COH	33.8[a]	24.4	23.9	22.0	23.0	22.1	23.5
FHCO+H→F+H2CO	29.1[a]	19.6	19.6	15.3	20.4	20.5	18.3
F2CO+H→F+FHCO	16.9[a]	16.9	17.0	15.3	17.6	17.6	14.4
FHCO+HCO→F+glyoxal	48.1[a]	42.2	41.7	40.0	45.3	44.4	43.8
The OMx and OMx-D3T energies are corrected by excluding ZPVE and thermal contributions							
CH3F+H→F+CH4	2.5[a]	3.6	3.6	1.6	1.3	1.3	2.0
CH2F2+H→F+CH3F	14.7[a]	10.7	10.7	11.1	10.4	10.5	10.3
CH3F+CH3→F+C2H6	17.8[a]	21.2	20.5	21.4	16.4	15.5	20.1
CH2F2+CH3→F+C2H5F	24.0[a]	23.1	22.5	25.0	19.9	19.0	22.6
C2H5F+CH3→F+propane	21.5[a]	23.8	22.9	24.3	20.1	18.8	23.2
CH3F+NH2→F+CH3NH2	23.2[a]	25.4	24.9	27.7	29.2	28.5	33.6
CH3F+NH→F+CH3NH	31.4[a]	34.8	34.5	35.3	34.7	34.1	36.4
CH3F+OH→F+CH3OH	16.7[a]	24.3	24.0	22.6	21.2	20.8	23.0
CH3F+HCO→F+CH3COH	24.5[a]	32.3	31.7	30.7	30.2	29.3	29.0
CH3+FHCO→F+CH3COH	33.8[a]	21.3	20.7	22.0	19.7	18.9	23.5
FHCO+H→F+H2CO	29.1[a]	16.1	16.1	15.3	17.0	17.1	18.3
F2CO+H→F+FHCO	16.9[a]	13.1	13.1	15.3	13.7	13.7	14.4
FHCO+HCO→F+glyoxal	48.1[a]	40.4	39.9	40.0	44.4	43.5	43.8

a A.Karton, S.Daon, J.M.Martin, Chem.Phys.Lett. 510, 165 (2011).

Table S33: Benchmark Results for the MB08–165 Subset of the GMTKN30-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
The OMx and OMx-D3T energies are uncorrected atomization enthalpies at 298 K							
001	129.0[a]	112.3	113.4	133.0	114.1	115.5	125.7
069	201.2[a]	152.7	154.7	206.1	190.2	193.1	214.5
075	32.6[a]	20.8	22.4	2.5	30.6	32.9	37.8
079	139.5[a]	124.7	126.0	141.6	133.7	135.5	139.3
082	−120.4[a]	−98.5	−97.2	−124.7	−95.8	−93.8	−111.8
084	−18.3[a]	−15.9	−15.4	−23.6	−15.9	−15.2	−20.0
085	−117.7[a]	−96.4	−96.8	−146.8	−108.8	−109.8	−142.0
090	−109.0[a]	−106.0	−105.4	−107.2	−103.8	−103.2	−108.3
099	67.9[a]	59.7	60.8	65.0	58.8	60.3	65.4
101	20.5[a]	5.2	6.4	23.7	8.9	10.6	15.5
103	−171.7[a]	−93.2	−91.7	−130.8	−100.0	−97.6	−126.5
105	−107.3[a]	−107.8	−106.4	−128.5	−97.7	−95.6	−114.8
107	−124.8[a]	−114.6	−112.4	−103.0	−97.4	−94.0	−97.5
109	−8.5[a]	−25.0	−23.8	−3.0	−9.1	−7.3	0.1
111	−362.4[a]	−333.9	−333.2	−406.2	−315.3	−314.4	−375.2
115	−67.9[a]	−62.7	−61.3	−68.9	−59.1	−57.0	−75.4
117	−25.5[a]	−0.8	−0.5	−46.1	−5.5	−5.2	−26.8
123	−125.6[a]	−140.6	−138.4	−126.8	−122.2	−118.9	−121.2
129	−570.6[a]	−472.6	−472.8	−633.0	−503.9	−504.5	−606.0
139	−266.7[a]	−231.1	−229.5	−249.2	−215.8	−213.5	−242.6
143	−192.4[a]	−163.1	−161.7	−192.5	−147.7	−145.5	−167.6
151	−225.2[a]	−219.4	−218.7	−263.5	−209.9	−209.2	−247.5
152	59.2[a]	42.5	44.3	58.1	62.9	65.4	66.4
157	−240.7[a]	−217.8	−217.7	−270.4	−231.3	−231.2	−267.3
164	52.3[a]	41.7	43.5	62.1	64.0	66.5	71.5
The OMx and OMx-D3T energies are corrected by excluding ZPVE and thermal contributions							
001	129.0[a]	122.7	123.9	133.0	125.5	126.9	125.7
069	201.2[a]	177.4	180.7	206.1	212.5	217.9	214.5
075	32.6[a]	14.4	16.0	2.5	25.4	27.7	37.8
079	139.5[a]	132.9	134.3	141.6	133.4	143.6	139.3
082	−120.4[a]	−112.6	−111.2	−124.7	−108.7	−106.6	−111.8
084	−18.3[a]	−20.1	−19.6	−23.6	−19.6	−18.9	−20.0
085	−117.7[a]	−129.6	−123.3	−146.8	−142.6	−140.0	−142.0
090	−109.0[a]	−110.9	−107.8	−107.2	−110.0	−106.2	−108.3
099	67.9[a]	62.6	63.7	65.0	62.9	64.5	65.4
101	20.5[a]	12.9	13.6	23.7	14.7	18.3	15.5
103	−171.7[a]	−116.6	−115.0	−130.8	−120.2	−117.8	−126.5
105	−107.3[a]	−122.0	−120.6	−128.5	−110.5	−108.4	−114.8
107	−124.8[a]	−104.8	−102.5	−103.0	−88.4	−84.9	−97.5
109	−8.5[a]	−10.2	−9.0	−3.0	3.3	6.3	0.1
111	−362.4[a]	−379.1	−378.3	−406.2	−356.0	−355.1	−375.2
115	−67.9[a]	−63.3	−61.9	−68.9	−64.1	−57.2	−75.4
117	−25.5[a]	−26.8	−26.5	−46.1	−31.0	−28.2	−26.8
123	−125.6[a]	−130.6	−128.4	−126.8	−112.3	−108.9	−121.2
129	−570.6[a]	−579.7	−579.8	−633.0	−601.6	−602.3	−606.0
139	−266.7[a]	−244.5	−242.9	−249.2	−228.8	−226.5	−242.6
143	−192.4[a]	−178.1	−176.7	−192.5	−161.0	−158.8	−167.6
151	−225.2[a]	−245.5	−244.9	−263.5	−237.2	−234.0	−247.5
152	59.2[a]	48.3	50.0	58.1	70.3	72.9	66.4
157	−240.7[a]	−254.6	−254.5	−270.4	−264.7	−264.7	−267.3
164	52.3[a]	48.7	50.5	62.1	70.9	73.5	71.5

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; M.Korth and S.Grimme, J.Chem.Theory Comput. 5, 993-1003 (2010).

Table S34: Benchmark Results for the W4–08 Subset of the GMTKN30-CHNOF Set. Atomization Energies at 0 K (kcal/mol). The OMx and OMx-D3T Energies Are Corrected by Excluding ZPVE and Thermal Contributions

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
c2h6	713.1[a]	712.4	714.2	713.4	711.5	714.4	712.0
h2cn	343.8[a]	345.8	346.5	347.0	346.6	347.7	347.7
nccn	502.0[a]	501.2	502.1	499.9	501.3	502.9	504.0
ch2nh2	482.3[a]	485.9	487.1	488.6	488.9	490.8	488.0
ch3nh	474.6[a]	473.9	475.0	477.2	475.5	477.4	479.1
ch3nh2	582.3[a]	578.6	580.0	582.2	578.4	580.7	580.2
cf2	258.8[a]	267.1	267.4	264.9	266.4	267.0	259.7
n2h	224.9[a]	236.7	237.1	239.5	239.3	240.0	240.3
n2h2	296.5[a]	300.0	300.7	303.6	312.1	313.1	309.4
n2h4	438.3[a]	434.7	435.9	439.4	436.2	438.0	439.9
fo2	134.7[a]	118.0	118.3	116.0	119.3	119.9	119.0
foof	152.4[a]	147.5	148.0	144.8	137.7	138.6	137.8
h2	109.5[a]	109.0	109.1	106.5	107.6	107.7	108.4
oh	107.2[a]	109.9	110.0	111.1	110.7	110.8	112.0
hf	141.6[a]	137.2	137.2	144.0	139.9	140.0	139.9
h2o	233.0[a]	229.4	229.6	231.8	230.4	230.7	230.0
ch	84.2[a]	86.0	86.2	90.3	88.0	88.2	91.5
ch2	190.7[a]	191.5	191.8	194.3	193.6	194.0	195.3
ch3	307.9[a]	308.3	308.7	310.6	305.8	306.6	309.3
ch4	420.4[a]	421.7	422.4	422.7	420.2	421.3	420.8
c2h	266.2[a]	261.0	284.3	263.1	275.2	275.9	263.4
c2h2	405.5[a]	404.7	405.3	405.5	404.4	405.4	405.5
nh3	298.0[a]	291.7	292.1	297.9	296.0	296.7	297.5
c2	147.0[a]	147.7	148.0	150.6	125.7	126.2	124.8
n2	228.5[a]	226.1	226.3	227.5	216.2	216.5	222.8
co	259.7[a]	250.6	250.8	248.5	250.8	251.1	247.0
cn	181.3[a]	174.7	175.0	176.7	182.1	182.5	185.3
no	152.8[a]	149.5	149.6	150.1	157.7	158.0	159.0
o2	120.8[a]	117.7	117.8	116.1	123.5	123.7	120.4
of	53.1[a]	49.3	49.4	47.6	48.1	48.3	47.5
f2	39.0[a]	37.3	37.4	38.5	35.6	35.8	34.2
nh	83.1[a]	83.4	83.5	88.2	88.8	89.0	92.7
nh2	182.6[a]	178.7	178.9	185.7	186.1	186.6	191.0
hcn	313.4[a]	318.3	318.7	319.2	316.2	316.9	318.8
hof	158.7[a]	154.6	154.8	153.5	152.6	153.0	152.0
cf	132.7[a]	138.4	138.5	134.7	138.3	138.6	133.2
ch2c	359.9[a]	372.5	373.2	373.5	372.1	373.3	371.5
ch2ch	446.1[a]	448.6	449.5	450.3	449.8	451.3	450.6
c2h4	564.1[a]	562.8	563.9	563.7	561.3	563.3	562.4
ch2nh	439.4[a]	438.0	438.9	441.2	440.8	442.3	441.4
hco	279.4[a]	287.5	287.9	287.7	291.2	291.8	290.0
ch2o	374.7[a]	377.5	378.0	377.4	378.7	379.6	379.7
co2	390.1[a]	371.5	371.9	372.1	377.9	378.6	380.9
hno	205.9[a]	211.0	211.3	214.4	220.8	221.4	220.6
no2	227.9[a]	228.7	229.2	231.5	233.2	233.9	236.4
n2o	270.9[a]	264.3	264.8	268.2	253.0	253.8	264.9
o3	147.4[a]	143.2	143.5	141.9	132.9	133.5	128.9
hoo	175.5[a]	179.9	180.2	178.4	177.0	177.4	174.9
h2o2	269.1[a]	266.5	267.0	266.3	266.4	267.2	265.6
f2o	93.8[a]	93.7	94.0	91.9	88.9	89.3	87.8

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; A.Karton, A.Tarnopolsky, J.F.Lamere, G.C.Schatz, and J.M.L.Martin, J.Phys.Chem.A 112, 12868 (2008).

Table S35: Benchmark Results for the G21IP Subset of the GMTKN30-CHNOF Set. Ionization Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
H→H+	314.9[a]	291.7	291.7	288.0	287.3	287.3	284.7
C→C+	259.6[a]	230.9	230.9	221.6	227.7	227.7	218.1
N→N+	335.3[a]	314.3	314.3	316.7	309.4	309.4	307.5
O→O+	313.8[a]	309.7	309.7	306.7	309.1	309.1	302.5
F→F+	401.7[a]	393.4	393.4	388.2	398.8	398.8	403.9
CH4→CH4+	296.3[a]	284.9	284.9	284.8	288.2	288.2	289.2
NH3→NH3+	235.7[a]	221.9	221.9	226.8	225.6	225.6	226.2
OH→OH+	300.9[a]	298.6	298.6	296.7	301.4	301.4	298.0
H2O→H2O+	292.6[a]	284.0	284.0	283.4	286.2	286.2	285.2
HF→HF+	371.3[a]	362.5	362.5	360.9	374.8	374.8	380.1
C2H2→C2H2+	264.6[a]	258.4	258.4	253.7	264.3	264.3	260.6
C2H4→C2H4+	243.7[a]	232.9	232.9	228.3	239.1	239.2	235.4
CO→CO+	323.0[a]	314.5	314.5	308.6	313.5	313.5	307.5
N2→N2+	359.4[a]	355.4	355.4	357.7	334.7	334.7	339.1
O2→O2+	277.7[a]	298.1	298.1	293.0	288.9	288.9	285.2

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; L.A.Curtiss, K.Raghavachari, G.W.Trucks, and J.A.Pople, J.Chem.Phys. 94, 7221 (1991).

Table S36: Benchmark Results for the G21EA Subset of the GMTKN30-CHNOF Set. Electron Affinities (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
C- → C	29.2[a]	18.3	18.3	9.0	15.1	15.1	5.5
O- → O	33.7[a]	28.1	28.1	25.2	27.6	27.6	20.9
F- → F	78.4[a]	70.4	70.4	65.1	75.7	75.7	80.8
CH- → CH	27.9[a]	18.0	18.0	9.6	18.1	18.1	9.5
CH2- → CH2	13.4[a]	3.2	3.2	−1.5	7.0	7.0	1.7
CH3- → CH3	1.2[a]	−16.8	−16.8	−20.9	−8.8	−8.7	−14.5
NH- → NH	8.3[a]	−8.9	−8.9	−6.3	−9.6	−9.6	−11.6
NH2- → NH2	16.8[a]	−3.8	−3.8	−0.7	−0.5	−0.5	−2.6
OH- → OH	41.7[a]	29.4	29.4	27.5	33.6	33.6	29.5
O2- → O2	9.5[a]	18.9	18.9	16.4	17.0	17.0	13.0
NO- → NO	−0.2[a]	13.2	13.2	13.0	10.0	10.0	6.7
CN- → CN	89.5[a]	88.4	88.4	85.8	88.0	88.0	84.3

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; L.A.Curtiss, K.Raghavachari, G.W.Trucks, and J.A.Pople, J.Chem.Phys. 94, 7221 (1991).

Table S37: Benchmark Results for the PA Subset of the GMTKN30-CHNOF Set. Proton Affinities (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
$C2H4 + H+ \rightarrow C2H5+$	167.8[a]	152.6	152.8	160.8	149.4	149.8	154.3
$C4H6 + H+ \rightarrow C4H7+$	193.4[a]	197.0	197.3	205.6	191.3	191.8	198.1
$C6H8 + H+ \rightarrow C6H9+$	209.7[a]	212.3	212.7	221.2	206.2	206.7	213.2
$C8H10 + H+ \rightarrow C8H11+$	219.7[a]	221.6	221.9	230.6	215.3	215.8	222.3
$NH3 + H+ \rightarrow NH4+$	211.9[a]	221.4	221.6	221.3	213.3	213.7	215.0
$H2O + H+ \rightarrow H3O+$	171.6[a]	167.6	167.8	172.3	165.7	166.0	165.8
$C2H2 + H+ \rightarrow C2H3+$	157.4[a]	134.0	134.2	142.4	134.0	134.4	139.1
$H2 + H+ \rightarrow H3+$	106.3[a]	47.9	48.0	40.1	69.4	69.6	65.2

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010).

Table S38: Benchmark Results for the SIE11 Subset of the GMTKN30-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
[(NH3)2]+ → NH3 + [NH3]+	35.3[a]	27.3	28.1	27.8	30.9	32.1	35.0
[(H2O)2]+ → H2O + [H2O]+	37.2[a]	31.2	31.7	31.8	30.5	31.3	30.0
[C4H10]+ → C2H5 + [C2H5]+	35.3[a]	52.7	54.6	56.4	44.0	46.7	46.9
[(CH3)2CO]+ → CH3 + [CH3CO]+	22.6[a]	28.6	29.8	29.5	22.4	24.3	23.5
C2H4 ... F2 → C2H4 + F2	1.1[a]	−0.3	0.0	0.0	−0.5	−0.1	−0.1

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010).

Table S39: Benchmark Results for the BHPERI Subset of the GMTKN30-CHNOF Set. Barriers at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
[cyclobutene]‡	35.3[a]	41.9	41.7	43.1	42.2	41.9	43.6
[cis-1,3,5-hexatriene]‡	30.9[a]	38.2	37.4	38.6	36.3	35.1	37.7
[o-xylylene]‡	28.3[a]	43.3	43.3	43.0	42.1	42.0	42.7
[1,3-pentadiene]‡	39.6[a]	34.3	33.8	35.4	33.7	32.8	35.6
[1,3-cyclopentadiene]‡	28.2[a]	42.0	42.1	42.1	37.0	37.1	38.4
[1,5-hexadiene]‡	35.6[a]	41.2	40.1	40.6	42.9	41.3	42.9
[1,3-butadiene + C2H4]‡	22.1[a]	28.5	25.4	26.1	28.6	24.2	26.5
[1,3-cyclopentadiene + C2H4]‡	18.3[a]	27.7	24.5	24.3	28.4	23.8	25.2
[1,3-cyclopentadiene]‡	9.8[a]	29.4	25.0	24.6	30.5	24.5	26.0
[cis-triscyclopropacyclohexane]‡	23.6[a]	38.2	38.3	38.2	38.4	38.6	38.2
[N2O + C2H4]‡	26.3[a]	23.0	21.4	25.4	15.6	13.3	21.2
[N3H + C2H4]‡	18.1[a]	22.3	20.4	20.5	12.5	9.8	14.0
[N2CH2 + C2H4]‡	12.2[a]	16.4	14.4	13.9	13.1	10.2	12.5
[HCNO + C2H4]‡	11.1[a]	11.6	9.9	12.4	10.9	8.4	10.3
[HCNNH + C2H4]‡	5.3[a]	7.4	5.5	4.9	5.9	3.1	4.7
[HCNCH2 + C2H4]‡	4.0[a]	8.3	6.2	6.4	10.3	7.4	9.5
[H2COHN + C2H4]‡	11.5[a]	18.8	16.7	17.2	19.5	16.4	16.5
[H2CNHNH + C2H4]‡	4.0[a]	14.6	12.2	12.8	10.9	7.4	8.3
[H2CNHCH2 + C2H4]‡	−1.4[a]	11.1	8.7	7.2	11.2	7.9	7.1
[1,3-cyclopentadiene + C2H4]‡	15.0[a]	28.8	25.5	25.3	29.2	24.5	26.0
[furane + C2H4]‡	19.8[a]	24.8	22.1	22.3	26.2	22.3	23.8
[pyrrole + C2H4]‡	25.4[a]	34.6	31.6	30.5	34.3	30.0	32.7

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010).

Table S40: Benchmark Results for the BH76 Subset of the GMTKN30-CHNOF Set. Barriers at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
H + N2O → OH + N2	18.1[a]	−1.3	−1.7	−4.7	−4.3	−4.8	−4.8
H + N2O ← OH + N2	83.2[a]	68.5	67.9	65.7	68.8	67.9	65.8
H + FH → HF + H	42.2[a]	−1.2	−1.4	−9.1	1.7	1.5	−5.3
H + FH ← HF + H	42.2[a]	−1.2	−1.4	−9.1	1.7	1.5	−5.3
H + CH3F → HF + CH3	30.4[a]	10.1	9.9	5.0	14.5	14.2	10.2
H + CH3F ← HF + CH3	57.0[a]	30.1	29.7	35.3	39.5	38.9	36.6
H + F2 → HF + F	2.3[a]	3.6	3.5	0.5	6.6	6.3	3.2
H + F2 ← HF + F	106.2[a]	99.9	99.7	105.5	106.6	106.4	108.0
F- + CH3F → CH3F + F-	−0.3[a]	13.7	13.4	14.3	18.0	17.5	16.2
F- + CH3F ← CH3F + F-	−0.3[a]	13.7	13.4	14.3	18.0	17.5	16.2
F-...CH3F → FCH3...F-	13.4[a]	22.5	22.5	23.6	26.1	26.1	25.0
F-...CH3F ← FCH3...F-	13.4[a]	22.5	22.5	23.6	26.1	26.1	25.0
OH- + CH3F → CH3OH + F-	−2.8[a]	11.4	10.8	11.8	11.7	10.8	6.7
OH- + CH3F ← CH3OH + F-	17.3[a]	26.6	26.2	26.7	31.1	30.5	34.9
OH-...CH3F → HOCH3...F-	11.0[a]	20.7	20.6	21.7	20.8	20.5	16.7
OH-...CH3F ← HOCH3...F-	47.2[a]	57.2	57.2	61.0	63.4	63.4	66.0
H + N2 → HN2	14.7[a]	2.5	2.2	2.4	−7.0	−7.4	−5.7
H + N2 ← HN2	10.7[a]	9.5	9.4	14.4	13.4	13.2	12.0
H + CO → HCO	3.2[a]	−1.8	−2.1	−2.7	−0.8	−1.3	−1.7
H + CO ← HCO	22.7[a]	31.5	31.4	36.8	36.0	35.7	41.7
H + C2H4 → C2H5	1.7[a]	4.2	3.7	3.8	4.8	4.0	4.3
H + C2H4 ← C2H5	41.8[a]	43.5	43.3	48.4	45.6	45.3	50.1
CH3 + C2H4 → C3H7	6.8[a]	10.5	9.3	8.9	10.3	8.6	9.1
CH3 + C2H4 ← C3H7	33.0[a]	35.0	34.9	36.2	37.7	37.6	38.5
HNC → HCN	48.2[a]	89.8	89.8	93.0	76.9	76.9	82.6
HNC ← HCN	33.1[a]	72.1	72.2	79.6	75.1	75.1	85.5
OH + H2 → H2O + H	5.1[a]	5.2	4.9	−0.0	2.7	2.2	3.1
OH + H2 ← H2O + H	21.2[a]	12.6	12.4	12.5	12.2	11.9	12.0
CH3 + H2 → CH4 + H	12.1[a]	5.2	4.7	1.2	0.7	−0.1	−1.0
CH3 + H2 ← CH4 + H	15.3[a]	4.2	3.8	5.1	2.1	1.5	1.3
OH + CH4 → H2O + CH3	6.7[a]	2.9	2.3	−0.2	3.7	3.0	5.2
OH + CH4 ← H2O + CH3	19.6[a]	11.3	10.7	8.4	11.9	11.0	11.8
H + H2 → H2 + H	9.6[a]	1.3	1.0	1.4	−5.1	−5.6	−6.8
H + H2 ← H2 + H	9.6[a]	1.3	1.0	1.4	−5.1	−5.6	−6.8
OH + NH3 → H2O + NH2	3.2[a]	8.9	8.4	8.2	4.3	3.5	4.1
OH + NH3 ← H2O + NH2	12.7[a]	17.3	16.7	16.4	15.3	14.5	15.6
OH + C2H6 → H2O + C2H5	3.4[a]	0.7	0.1	−2.6	1.9	1.0	3.1
OH + C2H6 ← H2O + C2H5	19.9[a]	16.2	15.4	12.9	17.9	16.7	17.4
F + H2 → HF + H	1.8[a]	4.8	4.6	3.6	7.0	6.8	5.9
F + H2 ← HF + H	33.4[a]	31.0	30.9	39.5	38.2	38.0	36.7
O + CH4 → OH + CH3	13.7[a]	2.5	2.2	1.2	2.4	1.9	3.8
O + CH4 ← OH + CH3	8.1[a]	3.4	2.9	0.2	3.4	2.7	4.2
H + OH → H2 + O	10.7[a]	1.2	1.0	−0.3	−0.1	−0.5	−0.2
H + OH ← H2 + O	13.1[a]	1.4	1.2	−3.2	−2.6	−2.9	−3.0
NH2 + CH3 → NH + CH4	8.0[a]	7.8	7.2	7.3	2.9	1.9	3.8
NH2 + CH3 ← NH + CH4	22.4[a]	23.6	22.9	21.9	16.6	15.7	16.9
NH2 + C2H5 → NHC2H6	7.5[a]	11.1	10.1	10.6	6.7	5.4	7.6
NH2 + C2H5 ← NHC2H6	18.3[a]	19.8	19.0	18.2	12.5	11.5	13.0
C2H6 + NH2 → C2H5 + NH3	10.4[a]	14.7	13.9	13.6	9.5	8.2	10.6
C2H6 + NH2 ← C2H5 + NH3	17.4[a]	21.9	20.9	20.9	14.4	13.0	13.4
NH2 + CH4 → NH3 + CH3	14.5[a]	18.2	17.5	17.2	12.9	11.8	14.2
NH2 + CH4 ← NH3 + CH3	17.8[a]	18.3	17.6	17.6	10.0	8.9	9.3
s-trans-cis-C5H8 → s-trans-cis-C5H8	38.4[a]	34.7	34.2	35.7	33.8	33.0	35.7
s-trans-cis-C5H8 ← s-trans-cis-C5H8	38.4[a]	34.7	34.2	35.7	33.8	33.0	35.7

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; Y.Zhao, B.J.Lynch, D.G.Truhlar, J.Phys.Chem.A 108, 2715 (2004) ; Y.Zhao, N.Gonzalez-Garcia, and D.G.Truhlar, J.Phys.Chem.A 109, 2012 (2005).

Table S41: Benchmark Results for the BH76RC Subset of the GMTKN30-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
H + N2O → OH + N2	−65.1[a]	−69.8	−69.6	−70.4	−73.0	−72.7	−70.6
H + CH3F → HF + CH3	−26.6[a]	−20.0	−19.8	−30.3	−25.0	−24.7	−26.4
H + F2 → HF + F	−103.9[a]	−96.2	−96.2	−105.0	−100.1	−100.0	−104.8
OH- + CH3F → CH3OH + F-	−20.1[a]	−15.2	−15.4	−14.9	−19.4	−19.7	−28.2
OH-...CH3F → HOCH3...F-	−36.2[a]	−36.5	−36.6	−39.3	−42.6	−42.9	−49.3
H + N2 → HN2	4.0[a]	−7.1	−7.3	−12.0	−20.3	−20.6	−17.7
H + CO → HCO	−19.5[a]	−33.3	−33.4	−39.5	−36.7	−37.0	−43.4
H + C2H4 → C2H5	−40.0[a]	−39.3	−39.6	−44.6	−40.8	−41.2	−45.8
CH3 + C2H4 → C3H7	−26.1[a]	−24.5	−25.6	−27.2	−27.3	−29.0	−29.4
HNC → HCN	−15.1[a]	−17.7	−17.6	−13.3	−1.9	−1.8	3.0
OH + H2 → H2O + H	−16.1[a]	−7.4	−7.5	−12.5	−9.6	−9.7	−9.0
CH3 + H2 → CH4 + H	−3.2[a]	1.1	0.9	−3.9	−1.4	−1.6	−2.4
OH + CH4 → H2O + CH3	−12.9[a]	−8.5	−8.4	−8.6	−8.2	−8.0	−6.6
OH + NH3 → H2O + NH2	−9.5[a]	−8.3	−8.3	−8.2	−11.0	−11.0	−11.5
OH + C2H6 → H2O + C2H5	−16.5[a]	−15.5	−15.3	−15.5	−16.0	−15.7	−14.3
F + H2 → HF + H	−31.6[a]	−26.2	−26.2	−35.8	−31.2	−31.2	−30.8
O + CH4 → OH + CH3	5.6[a]	−0.8	−0.7	1.0	−1.0	−0.8	−0.4
H + OH → H2 + O	−2.4[a]	−0.2	−0.2	2.9	2.4	2.5	2.8
NH2 + CH3 → NH + CH4	−14.4[a]	−15.7	−15.8	−14.6	−13.7	−13.8	−13.1
NH2 + C2H5 → NHC2H6	−10.8[a]	−8.7	−8.9	−7.6	−5.9	−6.1	−5.4
C2H6 + NH2 → C2H5 + NH3	−7.0[a]	−7.2	−7.0	−7.4	−4.9	−4.7	−2.8
NH2 + CH4 → NH3 + CH3	−3.3[a]	−0.1	−0.1	−0.4	2.9	2.9	4.9

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; Y.Zhao, B.J.Lynch, D.G.Truhlar, J.Phys.Chem.A 108, 2715 (2004) ; Y.Zhao, N.Gonzalez-Garcia, and D.G.Truhlar, J.Phys.Chem.A 109, 2012 (2005).

Table S42: Benchmark Results for the RSE43 Subset of the GMTKN30-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
(C6H5)CH2	−15.2[a]	−8.9	−8.7	−9.1	−8.6	−8.4	−8.5
CH2CCN	1.9[a]	1.8	2.0	1.8	−1.0	−0.6	1.8
CH2CF	6.8[a]	−1.3	−1.2	−0.9	−4.6	−4.5	−1.5
CH3CF2CH2	0.1[a]	−3.4	−3.2	−3.1	−2.6	−2.4	−2.7
CF3CH2	1.4[a]	−2.3	−2.2	−2.0	−1.3	−1.1	−1.4
CH2FCH2	−1.3[a]	−4.1	−4.0	−3.8	−3.6	−3.5	−3.9
HOCH2CH2	−1.8[a]	−6.3	−6.2	−6.3	−7.0	−6.8	−6.9
CH2CHCH2	−17.5[a]	−15.1	−15.0	−15.4	−14.9	−14.8	−14.9
CH2CHO	−10.0[a]	−8.3	−8.2	−8.7	−6.9	−6.8	−6.9
CH2CN	−8.6[a]	−7.3	−7.3	−7.3	−8.2	−8.1	−6.7
CH2CONH2	−6.3[a]	−5.3	−5.1	−5.6	−4.5	−4.3	−4.0
CH3NHCOCH2	−6.3[a]	−5.2	−5.0	−5.5	−4.3	−4.1	−3.9
CH2COOCH3	−6.6[a]	−5.0	−4.9	−5.6	−4.5	−4.4	−4.3
CH2COOH	−6.4[a]	−4.9	−4.8	−5.4	−4.5	−4.3	−4.3
(CH2CHCH2)CH2	−3.0[a]	−6.1	−5.9	−6.1	−6.6	−6.3	−6.4
CH2F	−3.9[a]	−6.7	−6.7	−6.6	−9.2	−9.2	−7.8
CH2NH2	−12.0[a]	−20.0	−19.9	−18.4	−22.8	−22.7	−19.1
CH2NH+3	4.7[a]	−3.7	−3.6	−3.5	−4.9	−4.7	−3.5
CH3NHCH2	−12.6[a]	−18.7	−18.6	−16.8	−22.3	−22.1	−19.1
CH2NHCHO	−11.1[a]	−16.2	−16.1	−14.9	−17.2	−17.1	−13.9
CH2NHOH	−8.6[a]	−15.4	−15.3	−13.2	−17.2	−17.0	−13.5
(CH3)2NCH2	−12.8[a]	−17.6	−17.3	−15.3	−21.8	−21.4	−18.5
CH2NO2	−3.3[a]	−6.3	−6.2	−7.3	−4.7	−4.6	−3.2
CF3OCH2	−3.9[a]	−10.0	−9.9	−9.5	−10.7	−10.5	−8.7
CH3OCH2	−2.7[a]	−8.1	−8.0	−7.5	−8.6	−8.4	−7.5
CH2OCHO	−5.9[a]	−10.5	−10.4	−9.7	−10.4	−10.3	−8.9
CH3COOCH2	−6.2[a]	−9.9	−9.7	−8.9	−10.2	−10.0	−8.5
CH2OH	−4.2[a]	−9.7	−9.7	−9.3	−10.7	−10.7	−9.9
H2NCHCN	−22.5[a]	−27.1	−26.9	−25.0	−28.6	−28.4	−24.6
H2NCHCONH2	−24.1[a]	−29.7	−29.4	−27.6	−29.7	−29.4	−25.8
H2NCHCOOH	−25.4[a]	−31.7	−31.5	−30.2	−33.1	−32.8	−29.5
H2CCCH	−13.1[a]	−11.0	−11.0	−11.3	−11.2	−11.1	−11.1
(CH3)3C	−6.4[a]	−17.5	−17.1	−16.4	−19.4	−18.8	−18.1
(CH3)3CCH2	−2.3[a]	−6.4	−6.1	−6.3	−6.7	−6.3	−6.5

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; F.Neese, T.Schwabe, S.Kossmann, B.Schirmer, and S.Grimme, J.Chem.Theory Comput. 5, 3060 (2009).

Table S43: Benchmark Results for the O3ADD6 Subset of the GMTKN30-CHNOF Set. Relative Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
o3_c2h2_vdw	−1.9[a]	−1.3	−2.0	−2.0	−1.1	−2.0	−1.9
o3_c2h2_ts	7.7[a]	−3.8	−4.8	−2.8	3.6	1.9	3.1
o3_c2h2_add	−63.8[a]	−35.9	−36.9	−81.3	−19.2	−20.6	−78.9
o3_c2h4_vdw	−1.9[a]	−1.6	−2.5	−2.5	−1.0	−2.2	−2.1
o3_c2h4_ts	3.4[a]	−5.0	−6.4	−4.9	2.0	−0.0	0.7
o3_c2h4_add	−57.1[a]	−81.9	−82.9	−83.5	−71.1	−72.7	−77.2

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; Y.Zhao, O.Tishchenko, J.R.Gour, W.Li, J.J.Lutz, P.Piecuch, and D.J.Truhlar, J.Phys.Chem.A 113, 5786 (2009).

Table S44: Benchmark Results for the G2RC Subset of the GMTKN30-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
$CO2 + H2 \rightarrow HCOOH$	−2.0[a]	−5.5	−5.9	−15.1	−1.3	−2.0	−6.2
$CH3CHO \rightarrow CO + CH4$	−2.5[a]	6.7	7.5	10.9	10.2	11.4	16.9
$CO + H2O \rightarrow CO2 + H2$	−7.0[a]	−5.0	−5.1	−0.3	−8.5	−8.6	−13.1
$CH3CN + H2O \rightarrow CH3CONH2$	−20.1[a]	−11.7	−12.7	−18.0	−17.8	−19.3	−21.0
$C2H2 + HF \rightarrow CH2CHF$	−25.4[a]	−25.0	−25.6	−21.2	−22.8	−23.7	−25.8
$H2CO + H2 \rightarrow CH3OH$	−29.2[a]	−15.7	−16.1	−27.4	−16.9	−17.5	−23.3
$C2H2 + C2H4 \rightarrow C4H8$	−32.7[a]	−26.5	−27.9	−30.7	−28.7	−30.8	−31.8
$N2 + 3H2 \rightarrow 2NH3$	−38.9[a]	−7.2	−7.7	−44.2	−36.2	−37.0	−46.5
$C2H2 + H2 \rightarrow C2H4$	−48.4[a]	−40.8	−41.3	−50.8	−42.4	−43.3	−48.7
$CO + 3H2 \rightarrow H2O + CH4$	−64.8[a]	−52.3	−52.8	−82.5	−58.6	−59.5	−78.0
$OF2 + H2 \rightarrow F2 + H2O$	−68.7[a]	−59.0	−58.9	−70.7	−64.9	−64.9	−68.3
$N2O + H2 \rightarrow N2 + H2O$	−80.7[a]	−77.6	−77.5	−83.1	−81.2	−81.0	−79.4
$C2H4 + CH2 \rightarrow C3H6$	−109.1[a]	−107.5	−108.4	−108.1	−105.7	−107.1	−105.9
$H2 + F2 \rightarrow 2HF$	−134.3[a]	−123.9	−123.9	−141.7	−132.6	−132.6	−137.2
$3C2H2 \rightarrow C6H6$	−151.6[a]	−148.1	−151.2	−153.8	−149.4	−154.3	−154.2

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; L.A.Curtiss, K.Raghavachari, P.C.Redfern, and J.A.Pople, J.Chem.Phys. 106, 1063 (1997).

Table S45: Benchmark Results for the ISO34 Subset of the GMTKN30-CHNOF Set. Relative Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
propyne → allene	1.6[a]	−0.2	−0.3	0.1	−0.2	−0.3	0.2
propyne → cyclopropene	21.9[a]	22.5	22.5	22.6	20.8	20.6	20.9
propylene → cyclopropane	7.2[a]	4.8	4.8	4.6	5.0	5.0	6.1
trans-2-butene → cis-2-butene	1.0[a]	2.1	2.0	2.6	2.1	1.9	2.7
isobutylene → trans-2-butene	0.9[a]	1.4	1.7	1.0	0.6	1.0	0.2
trans-2-butene → 1-butene	2.6[a]	3.8	3.7	3.8	4.4	4.2	4.3
1,3-butadiene → cyclobutene	11.2[a]	12.0	12.0	10.6	10.5	10.4	9.8
cyclopentene → ethenylcyclopropane	22.9[a]	22.1	22.6	23.0	23.5	24.2	24.9
piperylene → 1,4-pentadiene	6.9[a]	5.5	5.3	5.6	5.6	5.5	5.6
neopentane → pentane	3.6[a]	7.0	7.8	6.9	4.1	5.2	4.4
tetramethylbutane → octane	1.9[a]	8.0	10.9	7.7	1.0	5.1	1.5
toluene → norbornadiene	47.0[a]	44.2	43.7	43.2	44.1	43.4	42.6
ethenylbenzene → cyclooctatetraene	36.0[a]	46.0	45.7	45.7	42.6	42.2	42.8
acetonitrile → isocyanomethane	24.2[a]	22.2	22.2	21.8	12.6	12.5	7.4
ethanamine → dimethylamine	7.3[a]	3.2	3.2	5.9	10.0	10.0	9.4
N-methylmethanimine → aziridine	10.8[a]	22.7	22.8	20.3	20.3	20.3	23.5
ethylenediamine → 1,2-dimethylhydrazine	27.0[a]	15.5	15.8	22.4	27.0	27.4	26.8
pyrrolidine → cyclobutanamine	11.2[a]	12.2	12.4	10.5	6.7	6.9	7.6
pyrimidine → pyrazine	4.6[a]	0.2	0.2	1.8	−0.8	−0.8	4.1
pyrazine → pyridazine	20.2[a]	7.4	7.4	8.4	9.1	9.0	7.3
2-methylpyridine → 4-methylpyridine	0.9[a]	−1.0	−1.1	0.3	−0.1	−0.1	−0.1
aniline → 2-methylpyridine	3.2[a]	−2.3	−2.1	1.8	−1.6	−1.4	0.7
cyclohexanamine → 2-methylpiperidine	5.3[a]	3.8	3.9	7.1	7.6	7.7	7.5
ethanol → methoxymethane	12.5[a]	10.7	10.8	11.3	14.1	14.2	12.4
acetaldehyde → oxirane	26.5[a]	30.3	30.4	32.5	36.9	37.1	40.8
acetic acid → methyl formate	18.2[a]	21.6	21.7	20.8	24.3	24.3	21.7
ethylene glycol → methyl peroxide	64.2[a]	58.0	58.4	59.7	62.5	63.2	61.8
acetone → oxetane	31.2[a]	41.4	41.4	39.0	44.4	44.4	42.1
oxolane → ethoxyethene	11.9[a]	19.1	19.3	19.9	19.3	19.7	19.9
N-methylacetamide → dimethylformamide	9.5[a]	8.9	8.7	14.0	13.2	12.9	12.1
oxolan-2-one → ethenyl acetate	14.1[a]	16.8	17.4	18.4	16.7	17.6	17.5
oxan-2-one → acetylacetone	7.1[a]	−11.5	−11.2	−9.6	−15.8	−15.3	−12.4
hexanoic acid → methyl pivalate	5.6[a]	1.1	0.6	1.1	7.7	7.0	6.1
2-methylphenol → phenylmethanol	7.3[a]	5.2	5.3	4.7	5.1	5.3	3.9

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; S.Grimme, M.Steinmetz, and M.Korth, J.Org.Chem. 72, 2118 (2007) ; M.P.Repasky, J.Chandrasekhar, and W.L.Jorgensen, J.Comput.Chem. 23, 1601 (2002) ; K.W.Sattelmeyer, J.Tirado-Rives, and W.L.Jorgensen, J.Phys.Chem.A 110, 13551 (2006).

Table S46: Benchmark Results for the ISOL22 Subset of the GMTKN30-CHNOF Set. Relative Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
i2p	40.6[a]	32.6	38.0	37.9	30.5	37.9	36.0
i3p	11.7[a]	10.2	10.0	10.6	1.9	1.7	4.6
i5p	34.9[a]	33.1	34.7	35.6	37.2	39.7	39.0
i6p	25.9[a]	8.7	8.6	4.7	−1.9	−1.8	1.0
i7p	18.8[a]	17.5	20.3	19.9	16.0	19.9	18.7
i8p	18.3[a]	26.9	22.2	21.0	19.9	14.0	16.7
i9p	22.3[a]	22.3	23.6	22.7	19.3	21.1	20.2
i10p	7.9[a]	5.6	6.4	4.7	6.2	7.5	4.1
i11p	38.1[a]	64.6	64.8	66.6	67.6	67.8	69.9
i12p	1.0[a]	2.5	2.5	1.6	3.2	3.1	0.4
i13p	35.1[a]	27.6	28.0	34.2	37.8	38.4	37.5
i14p	5.2[a]	7.6	8.4	8.2	9.2	10.3	5.7
i15p	3.9[a]	9.4	10.4	15.7	9.5	11.0	15.8
i16p	22.6[a]	17.9	17.7	18.5	19.7	19.6	19.0
i17p	11.1[a]	10.3	11.0	11.5	10.2	11.2	11.2
i18p	26.1[a]	29.9	31.5	32.8	28.0	30.1	29.9
i20p	4.5[a]	3.2	2.8	3.7	4.7	4.3	3.3
i22p	0.5[a]	−0.4	2.7	3.7	0.4	4.5	4.6

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 7, 291 (2011) ; R.Huenerbein, B.Schirmer, J.Moellmann, and S.Grimme, Phys.Chem.Chem.Phys. 12, 6940 (2010).

Table S47: Benchmark Results for the DC9 Subset of the GMTKN30-CHNOF Set. Relative Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
2-pyridone → 2-hydroxypyridine	−1.0[a]	−1.7	−1.6	−0.8	1.0	1.2	3.3
[C20]cage → [C20]bowl	−13.3[a]	−106.9	−104.2	−115.0	−106.9	−102.2	−104.9
hepta-1,2,3,5,6-hexaene → hepta-1,3,5-triyne	−14.3[a]	−14.3	−14.2	−15.0	−14.1	−14.1	−15.5
2 tetramethyl-ethen → octamethylcylobutane	−19.2[a]	−14.9	−22.4	−22.1	−7.5	−17.6	−15.0
(CH)12 isomerization	−19.5[a]	−34.2	−35.3	−35.0	−32.4	−34.2	−31.8
carbo-[3]-oxacarbon isomerization	−26.9[a]	−80.1	−80.5	−83.2	−66.8	−67.3	−65.5
N2CH2 + C2H4 → (CH2)3N2	−38.1[a]	−46.7	−48.4	−49.0	−50.5	−53.2	−50.0

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010).

Table S48: Benchmark Results for the DARC Subset of the GMTKN30-CHNOF Set. Relative Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
ethene + butadiene	−43.8[a]	−40.0	−42.6	−44.0	−43.5	−47.3	−46.5
ethyne + butadiene	−59.3[a]	−57.1	−59.2	−60.0	−60.2	−63.4	−62.4
ethene + cyclopentadiene	−30.0[a]	−26.3	−29.2	−31.1	−25.9	−30.1	−29.9
ethyne + cyclopentadiene	−33.1[a]	−36.0	−38.4	−39.9	−35.3	−38.9	−38.9
ethene + cyclohexadiene	−36.5[a]	−34.6	−37.9	−39.1	−34.8	−39.5	−38.8
ethyne + cyclohexadiene	−48.2[a]	−51.3	−54.1	−54.9	−50.3	−54.5	−54.2
furane + maleine (endo-product)	−14.4[a]	−31.6	−35.6	−35.8	−26.7	−32.3	−31.8
furane + maleine (exo-product)	−16.2[a]	−32.5	−36.2	−36.8	−27.6	−32.8	−32.9
furane + maleinimide (endo-product)	−17.2[a]	−32.0	−36.0	−36.7	−28.6	−34.4	−33.6
furane + maleinimide (exo-product)	−19.2[a]	−33.4	−37.2	−38.2	−30.1	−35.5	−35.0
cyclopentadiene + maleine (endo-product)	−31.6[a]	−37.9	−42.3	−42.9	−34.6	−40.7	−39.4
cyclopentadiene + maleine (exo-product)	−32.1[a]	−38.9	−43.1	−43.9	−35.6	−41.5	−40.6
cyclopentadiene + maleinimide (endo-product)	−34.1[a]	−37.9	−42.4	−43.5	−36.2	−42.5	−40.9
cyclopentadiene + maleinimide (exo-product)	−34.4[a]	−38.9	−43.3	−44.5	−37.2	−43.3	−42.1

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; E.R.Johnson, P.Mori-Sanchez, A.J.Cohen, and W.J.Yang, J.Chem.Phys. 129, 204112 (2008).

Table S49: Benchmark Results for the BSR36 Subset of the GMTKN30-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
The OMx and OMx-D3T energies are uncorrected atomization enthalpies at 298 K							
2,3-dimethylbutane + 4 CH4 → 5 C2H6	9.8[a]	13.4	15.9	14.8	9.0	12.4	11.4
2-methylpentane + 4 CH4 → 5 C2H6	9.7[a]	12.6	14.6	14.3	9.4	12.0	11.8
2,2-dimethylbutane + 4 CH4 → 5 C2H6	11.4[a]	16.2	18.9	17.7	10.7	14.3	13.2
3-methylpentane + 4 CH4 → 5 C2H6	9.0[a]	11.6	13.8	13.1	8.2	11.1	10.6
hexane + 4 CH4 → 5 C2H6	8.7[a]	11.0	12.5	12.6	8.9	10.8	11.1
heptane + 5 CH4 → 6 C2H6	10.9[a]	13.7	15.6	15.8	11.1	13.5	14.0
2,4-dimethylpentane + 5 CH4 → 6 C2H6	13.1[a]	16.9	19.9	19.1	11.9	15.8	15.2
2-methylhexane + 5 CH4 → 6 C2H6	11.9[a]	15.4	17.8	17.5	11.6	14.7	14.7
2,2-dimethylpentane + 5 CH4 → 6 C2H6	13.5[a]	19.1	22.2	21.0	13.0	17.2	16.2
2,3-dimethylpentane + 5 CH4 → 6 C2H6	11.4[a]	15.4	18.6	17.3	10.4	14.7	13.4
2,2,3-trimethylbutane + 5 CH4 → 6 C2H6	13.0[a]	19.5	23.3	21.4	12.1	17.3	15.4
3,3-dimethylpentane + 5 CH4 → 6 C2H6	12.8[a]	17.3	21.0	19.3	10.8	15.7	14.0
3-methylhexane + 5 CH4 → 6 C2H6	11.2[a]	14.5	17.1	16.5	10.6	14.0	13.6
3-ethylpentane + 5 CH4 → 6 C2H6	10.2[a]	13.9	16.7	16.0	9.9	13.6	13.0
tetramethylbutane + 6 CH4 → 7 C2H6	15.1[a]	24.7	30.0	27.1	13.9	21.1	18.1
cyclopentane + 5 CH4 → 5 C2H6	2.4[a]	11.2	11.5	10.5	7.4	7.8	7.0
cyclohexane + 6 CH4 → 6 C2H6	10.7[a]	16.9	18.2	17.2	13.0	14.7	14.0
methylcyclopentane + 6 CH4 → 6 C2H6	6.3[a]	16.4	17.4	16.3	11.5	12.8	12.0
methylcyclohexane + 7 CH4 → 7 C2H6	14.9[a]	22.3	24.4	23.3	17.0	19.7	19.0
1,1-dimethylcyclopentane + 7 CH4 → 7 C2H6	10.7[a]	23.3	25.5	23.5	15.6	18.6	16.9
cis-1,3-dimethylcyclopentane + 7 CH4 → 7 C2H6	10.1[a]	21.7	23.4	22.2	15.8	18.0	17.1
cis-1,2-dimethylcyclopentane + 7 CH4 → 7 C2H6	9.1[a]	20.0	22.2	20.2	13.4	16.2	14.5
trans-1,2-dimethylcyclopentane + 7 CH4 → 7 C2H6	10.5[a]	21.5	23.4	22.1	15.3	17.8	16.8
trans-1,3-dimethylcyclopentane + 7 CH4 → 7 C2H6	9.8[a]	22.0	23.8	22.5	16.0	18.3	17.4
spiro[4.5]decane + 12 CH4 → 11 C2H6	19.3[a]	37.0	40.9	37.5	25.6	30.7	27.9
bicyclo[3.3.2]decane + 12 CH4 → 11 C2H6	9.7[a]	15.0	19.5	15.3	8.2	14.2	9.3
decahydroazulene + 12 CH4 → 11 C2H6	15.2[a]	29.7	33.2	30.8	21.4	25.9	23.8
trans-decalin + 12 CH4 → 11 C2H6	26.1[a]	39.4	43.0	41.0	29.9	34.8	33.5
cis-decalin + 12 CH4 → 11 C2H6	23.4[a]	36.8	40.9	37.9	27.0	32.4	29.9
dicyclohexyl + 14 CH4 → 13 C2H6	28.0[a]	42.4	47.6	44.8	31.4	38.2	36.1
hexylcyclohexane + 12 CH4 → 12 C2H6	25.4[a]	35.3	39.7	38.6	27.2	32.9	32.5
adamantane + 14 CH4 → 12 C2H6	27.6[a]	50.6	54.0	49.4	36.8	41.4	37.8
1,3-dimethyladamantane + 16 CH4 → 14 C2H6	39.6[a]	66.2	71.9	66.6	47.4	55.0	51.1
2,2-dimethyladamantane + 16 CH4 → 14 C2H6	32.4[a]	59.1	65.3	59.1	40.5	48.8	43.5
1,3,5,7-tetramethyladamantane + 18 CH4 → 16 C2H6	51.4[a]	81.5	89.7	83.7	57.9	68.6	64.4
diamantane + 22 CH4 → 18 C2H6	47.1[a]	85.3	91.2	83.4	62.2	69.9	64.0
The OMx and OMx-D3T energies are corrected by excluding ZPVE and thermal contributions							
2,3-dimethylbutane + 4 CH4 → 5 C2H6	9.8[a]	12.1	14.7	14.8	7.8	11.2	11.4
2-methylpentane + 4 CH4 → 5 C2H6	9.7[a]	11.6	13.5	14.3	8.4	11.0	11.8
2,2-dimethylbutane + 4 CH4 → 5 C2H6	11.4[a]	14.9	17.6	17.7	9.3	13.0	13.2
3-methylpentane + 4 CH4 → 5 C2H6	9.0[a]	10.6	12.7	13.1	7.2	10.0	10.6
hexane + 4 CH4 → 5 C2H6	8.7[a]	10.1	11.6	12.6	8.0	10.0	11.1
heptane + 5 CH4 → 6 C2H6	10.9[a]	12.6	14.5	15.8	10.1	12.5	14.0
2,4-dimethylpentane + 5 CH4 → 6 C2H6	13.1[a]	15.4	18.4	19.1	10.4	14.4	15.2
2-methylhexane + 5 CH4 → 6 C2H6	11.9[a]	14.1	16.5	17.5	10.4	13.5	14.7
2,2-dimethylpentane + 5 CH4 → 6 C2H6	13.5[a]	17.5	20.7	21.0	11.4	15.6	16.2
2,3-dimethylpentane + 5 CH4 → 6 C2H6	11.4[a]	13.9	17.2	17.3	8.9	13.2	13.4
2,2,3-trimethylbutane + 5 CH4 → 6 C2H6	13.0[a]	17.9	21.7	21.4	10.3	15.5	15.4
3,3-dimethylpentane + 5 CH4 → 6 C2H6	12.8[a]	15.8	19.5	19.3	9.2	14.1	14.0
3-methylhexane + 5 CH4 → 6 C2H6	11.2[a]	13.2	15.8	16.5	9.3	12.7	13.6
3-ethylpentane + 5 CH4 → 6 C2H6	10.2[a]	12.6	15.4	16.0	8.6	12.3	13.0
tetramethylbutane + 6 CH4 → 7 C2H6	15.1[a]	22.7	28.0	27.1	11.5	18.8	18.1
cyclopentane + 5 CH4 → 5 C2H6	2.4[a]	8.0	8.3	10.5	4.2	4.7	7.0
cyclohexane + 6 CH4 → 6 C2H6	10.7[a]	14.4	15.7	17.2	10.5	12.3	14.0
methylcyclopentane + 6 CH4 → 6 C2H6	6.3[a]	12.8	13.9	16.3	7.9	9.2	12.0
methylcyclohexane + 7 CH4 → 7 C2H6	14.9[a]	19.4	21.4	23.3	14.1	16.8	19.0
1,1-dimethylcyclopentane + 7 CH4 → 7 C2H6	10.7[a]	19.3	21.5	23.5	11.5	14.5	16.9
cis-1,3-dimethylcyclopentane + 7 CH4 → 7 C2H6	10.1[a]	18.5	19.6	22.2	12.5	14.1	17.1
cis-1,2-dimethylcyclopentane + 7 CH4 → 7 C2H6	9.1[a]	16.7	18.9	20.2	10.1	13.0	14.5
trans-1,2-dimethylcyclopentane + 7 CH4 → 7 C2H6	10.5[a]	17.6	19.5	22.1	12.0	14.5	16.8
trans-1,3-dimethylcyclopentane + 7 CH4 → 7 C2H6	9.8[a]	18.8	20.5	22.5	12.8	15.0	17.4

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Table S49: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
spiro[4.5]decane + 12 CH4 → 11 C2H6	19.3[a]	31.3	35.2	37.5	19.9	25.1	27.9
bicyclo[3.3.2]decane + 12 CH4 → 11 C2H6	9.7[a]	9.3	14.1	15.3	2.8	8.8	9.3
decahydroazulene + 12 CH4 → 11 C2H6	15.2[a]	24.1	27.7	30.8	15.8	20.4	23.8
trans-decalin + 12 CH4 → 11 C2H6	26.1[a]	34.0	37.7	41.0	24.6	29.5	33.5
cis-decalin + 12 CH4 → 11 C2H6	23.4[a]	31.4	35.5	37.9	21.7	27.1	29.9
dicyclohexyl + 14 CH4 → 13 C2H6	28.0[a]	36.6	41.8	44.8	25.7	32.5	36.1
hexylcyclohexane + 12 CH4 → 12 C2H6	25.4[a]	31.2	35.7	38.6	23.3	29.0	32.5
adamantane + 14 CH4 → 12 C2H6	27.6[a]	43.1	46.5	49.4	29.4	34.0	37.8
1,3-dimethyladamantane + 16 CH4 → 14 C2H6	39.6[a]	57.8	63.5	66.6	38.9	46.5	51.1
2,2-dimethyladamantane + 16 CH4 → 14 C2H6	32.4[a]	50.9	57.1	59.1	32.0	40.4	43.5
1,3,5,7-tetramethyladamantane + 18 CH4 → 16 C2H6	51.4[a]	72.2	80.3	83.7	48.2	59.0	64.4
diamantane + 22 CH4 → 18 C2H6	47.1[a]	72.9	78.8	83.4	49.8	57.6	64.0

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 7, 291 (2011) ; H.Krieg, and S.Grimme, Mol.Phys. 108, 2655 (2010).

Table S50: Benchmark Results for the IDISP Subset of the GMTKN30-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
2 anthracene → anthracene dimer	−9.0[a]	−18.3	−28.9	−29.1	−17.9	−31.5	−30.6
2 p-xylene → [2.2]-paracyclophane + 2 H2	−58.5[a]	−52.1	−45.2	−62.6	−54.8	−45.8	−56.8
n-octane → iso-octane	−1.9[a]	−8.1	−11.1	−7.9	−0.5	−4.8	−1.1
[C14H30]folded → [C14H30]linear	8.2[a]	−0.5	−6.5	−0.2	11.8	3.4	10.9
[C22H46]folded → [C22H46]linear	−3.1[a]	−6.4	−4.2	−5.2	−7.0	−4.3	−5.7
n-undecane → 2,2,3,3,4,4-hexamethyl-pentane	0.4[a]	−9.8	−0.6	−3.3	−15.2	−3.5	−7.1

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 7, 291 (2011) ; T.Schwabe and S.Grimme, Phys.Chem.Chem.Phys. 9, 3397 (2007).

Table S51: Benchmark Results for the WATER27 Subset of the GMTKN30-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
[H2O]2	5.0[a]	4.0	4.4	4.5	4.5	5.0	4.6
[H2O]3 cyclic	15.8[a]	12.0	13.2	13.7	13.1	14.8	13.2
[H2O]4 cyclic	27.4[a]	22.9	24.8	26.0	26.6	29.3	27.0
[H2O]5 cyclic	35.9[a]	30.6	33.0	34.4	36.2	39.5	36.6
[H2O]6 prism	46.0[a]	36.9	41.4	43.3	41.1	47.1	42.9
[H2O]6 cage	45.8[a]	36.1	40.4	42.4	40.7	46.5	42.5
[H2O]6 book	45.3[a]	37.3	40.8	42.7	43.2	48.1	44.3
[H2O]6 cyclic	44.3[a]	38.8	41.7	43.0	46.2	50.1	46.3
[H2O]8 cube (D2d)	72.6[a]	58.0	64.8	68.2	66.1	75.3	69.3
[H2O]8 cube (S4)	72.6[a]	58.0	64.8	68.3	66.1	75.2	69.2
[H2O]20 dodecahedron	200.1[a] 198.6[b]	160.1	177.4	186.1	188.8	211.6	196.8
[H2O]20 fused cubes	212.6[a] 208.0[b]	164.1	186.3	195.3	181.7	211.3	193.3
[H2O]20 face-sharing	215.0[a] 208.0[b]	166.6	188.0	196.9	187.4	215.9	198.6
[H2O]20 edge-sharing	217.9[a] 209.7[b]	167.3	188.3	197.1	188.6	216.3	198.6
H3O+[H2O]	33.5[a]	35.2	35.7	35.0	43.0	43.8	42.7
H3O+[H2O]2	56.9[a]	56.2	57.3	56.2	65.5	67.0	64.6
H3O+[H2O]3	76.5[a]	74.2	75.8	75.3	83.5	85.8	82.8
H3O+[H2O]6 (3D)	117.8[a]	107.3	112.2	114.5	118.5	125.1	120.7
H3O+[H2O]2 (2D)	114.9[a]	110.2	113.9	114.6	124.4	129.4	125.3
OH-[H2O]	26.6[a]	34.9	35.3	36.6	41.4	41.9	42.9
OH-[H2O]2	48.4[a]	53.6	54.4	56.1	61.0	62.3	62.3
OH-[H2O]3	67.6[a]	70.1	71.6	74.2	78.3	80.5	80.2
OH-[H2O]4 (C4)	84.8[a]	82.4	85.3	88.0	88.6	92.7	90.7
OH-[H2O]4 (Cs)	84.8[a]	82.0	85.4	88.0	89.7	94.4	92.4
OH-[H2O]5	100.7[a]	92.9	97.6	100.7	98.1	104.6	100.8
OH-[H2O]6	115.7[a]	104.7	110.6	114.6	111.3	119.4	115.3
[H2O]8 cube (S4) - H3O+[H2O]6 [OH-]	28.5[a]	20.3	21.1	20.0	−0.0	1.0	4.6

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; V.S.Bryantsev, M.S.Diallo, A.C.T.van Duin, and W.A.Goddard III, J.Chem.Theory Comput. 5, 1016 (2009).

Table S52: Benchmark Results for the S22 Subset of the GMTKN30-CHNOF Set. Dissociation Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
01	3.2[a]	2.0	2.5	2.5	2.1	2.8	2.7
02	5.0[a]	4.2	4.5	4.8	4.5	5.1	4.7
03	18.8[a]	13.6	14.8	15.6	11.5	13.3	12.9
04	16.1[a]	13.0	14.3	15.1	11.7	13.5	13.8
05	20.7[a]	17.5	19.5	19.6	16.2	18.7	18.7
06	17.0[a]	11.0	13.4	13.2	11.3	14.3	16.1
07	16.7[a]	11.1	13.6	13.4	11.4	14.5	16.3
08	0.5[a]	−0.1	0.5	0.5	−0.1	0.5	0.5
09	1.5[a]	0.4	1.5	1.4	−0.2	1.2	1.0
10	1.4[a]	0.2	1.4	1.4	−0.1	1.4	1.3
11	2.6[a]	−1.1	2.4	2.8	−1.0	3.2	3.4
12	4.2[a]	0.9	4.4	5.1	0.6	4.9	5.3
13	9.7[a]	4.3	9.1	9.3	3.9	9.8	9.7
14	4.6[a]	−1.6	3.2	3.7	−1.4	4.5	4.5
15	11.7[a]	4.0	10.6	11.1	3.3	11.5	11.2
16	1.5[a]	1.1	1.6	1.6	0.6	1.3	1.2
17	3.3[a]	2.3	3.5	3.4	1.9	3.4	3.1
18	2.3[a]	1.3	2.5	2.6	0.8	2.3	2.3
19	4.5[a]	3.1	4.5	4.5	1.7	3.6	3.3
20	2.7[a]	0.7	2.8	2.7	−0.1	2.5	2.4
21	5.6[a]	2.4	5.2	5.0	1.2	4.6	4.2
22	7.1[a]	3.9	6.2	6.2	3.3	6.1	5.7

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 7, 291 (2011) ; P.Jurecka, J.Sponer, J.Cerny, and P.Hobza, Phys.Chem.Chem.Phys. 8, 1985 (2006) ; T.Takatani, E.G.Hohenstein, M.Malagoli, M.S.Marshall, and C.D.Sherrill, J.Chem.Phys. 132, 144104 (2010).

Table S53: Benchmark Results for the ADIM6 Subset of the GMTKN30-CHNOF Set. Dissociation Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
(ethane)2 $\rightarrow$ 2 ethane	1.3[a]	0.0	1.2	1.2	−0.3	1.2	1.1
(propane)2 $\rightarrow$ 2 propane	2.0[a]	0.1	1.9	1.9	−0.5	1.7	1.6
(butane)2 $\rightarrow$ 2 butane	2.8[a]	0.2	2.8	2.8	−0.6	2.6	2.4
(pentane)2 $\rightarrow$ 2 pentane	3.7[a]	0.3	3.7	3.6	−0.8	3.3	3.1
(hexane)2 $\rightarrow$ 2 hexane	4.6[a]	0.4	4.6	4.5	−1.0	4.2	3.9
(heptane)2 $\rightarrow$ 2 heptane	5.6[a]	0.2	5.3	5.1	−1.5	4.6	4.2

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 7, 291 (2011) ; S.Tsuzuki, K.Honda, T.Uchimaru, and M.Mikami, J.Chem.Phys. 124, 114304 (2006) ; H.Krieg and S.Grimme, Mol.Phys. 108, 2655 (2010).

Table S54: Benchmark Results for the PCONF Subset of the GMTKN30-CHNOF Set. Relative Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
444	0.1[a]	0.3	2.0	1.5	−0.2	2.0	1.7
357	0.9[a]	1.4	2.0	1.8	1.4	2.1	1.7
366	1.1[a]	−1.3	1.8	0.6	−0.2	3.6	3.1
215	0.8[a]	1.1	2.4	1.8	0.4	2.1	1.7
300	1.3[a]	−1.8	0.9	0.9	−1.5	1.9	1.5
114	1.9[a]	3.1	3.7	2.5	3.1	3.7	3.1
412	2.4[a]	1.2	1.6	1.5	0.0	0.6	0.4
691	2.1[a]	−0.3	2.4	2.6	−0.1	3.4	3.4
470	2.5[a]	1.1	2.8	1.7	0.9	3.1	1.7
224	2.0[a]	2.2	3.4	1.8	1.5	3.1	2.5

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; D.Reha, H.Valdes, J.Vondrasek, P.Hobza, A.Abu-Riziq, B.Crews, and M.S.de Vries, Chem.-Eur.J. 11, 6803 (2005).

Table S55: Benchmark Results for the ACONF Subset of the GMTKN30-CHNOF Set. Relative Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
B_G	0.6[a]	0.9	0.7	1.1	1.0	0.8	1.2
P_TG	0.6[a]	0.8	0.6	0.9	1.0	0.7	1.1
P_GG	1.0[a]	2.0	1.5	2.2	2.4	1.8	2.6
P_GX	2.8[a]	3.3	2.9	3.4	3.3	2.7	3.5
H_gtt	0.6[a]	0.8	0.6	0.9	1.0	0.7	1.1
H_tgt	0.6[a]	0.7	0.5	0.8	0.9	0.7	1.0
H_tgg	0.9[a]	1.9	1.3	2.1	2.4	1.6	2.6
H_gtg	1.2[a]	1.6	1.2	1.8	1.9	1.4	2.2
H_g+t+g-	1.3[a]	1.7	1.3	2.0	2.0	1.5	2.3
H_ggg	1.2[a]	2.9	2.1	3.2	3.7	2.6	3.9
H_g+x-t+	2.6[a]	3.1	2.6	3.2	3.2	2.6	3.3
H_t+g+x-	2.7[a]	3.1	2.7	3.2	3.2	2.6	3.4
H_g+x-g-	3.3[a]	3.8	3.1	4.0	4.0	3.1	4.2
H_x+g-g-	3.1[a]	4.3	3.5	4.4	4.6	3.4	4.7
H_x+g-x+	4.9[a]	6.1	5.3	6.2	6.1	4.9	6.2

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; D.Gruzman, A.Karton, and J.M.L.Martin, J.Phys.Chem.A 113, 11974 (2009).

Table S56: Benchmark Results for the SCONF Subset of the GMTKN30-CHNOF Set. Relative Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
C2	0.8[a]	0.2	0.1	0.2	0.4	0.3	0.4
C3	2.6[a]	1.3	1.7	3.8	1.8	2.4	2.5
C4	3.4[a]	1.3	1.6	3.9	2.1	2.6	2.7
C5	4.9[a]	5.3	5.7	6.4	5.7	6.3	6.1
C6	5.2[a]	5.0	5.4	5.8	5.2	5.9	5.4
C7	4.5[a]	2.1	2.3	4.4	3.0	3.4	3.2
C8	4.7[a]	2.6	2.8	5.1	3.7	4.1	4.1
C9	6.7[a]	5.7	6.2	6.8	6.3	7.2	6.3
C10	6.8[a]	4.4	4.9	6.2	5.4	6.3	5.6
C11	6.1[a]	3.3	3.6	5.9	4.8	5.4	5.2
C12	6.0[a]	2.8	3.2	5.3	4.2	4.8	4.5
C13	6.2[a]	5.0	5.2	6.3	6.8	7.1	6.7
C14	6.8[a]	4.5	4.9	6.2	5.5	6.1	5.8
C15	6.7[a]	3.6	3.9	5.6	5.0	5.5	5.3
G2	0.3[a]	−0.4	−0.5	−0.7	−0.5	−0.6	−0.6
G3	5.9[a]	3.4	2.2	−1.9	1.8	−0.0	0.1
G4	5.3[a]	5.0	3.7	−0.6	1.9	0.1	0.2

a L.Goerigk and S.Grimme, J.Chem.Theory Comput. 6, 107 (2010) ; G.I.Csonka, A.D.French, G.P.Johnson, and C.A.Stortz, J.Chem.Theory Comput. 5, 679 (2009).

Table S57: Benchmark Results for the MGAE109/11 Subset of the CE345-CHNOF Set. Atomization Energies at 0 K (kcal/mol). The OMx and OMx-D3T Energies Are Corrected by Excluding ZPVE and Thermal Contributions

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
C2F4	591.1[a]	578.6	580.0	581.6	580.3	582.5	581.2
C2H2	405.5[a]	404.5	405.2	405.3	404.1	405.2	405.2
C2H4	563.7[a]	562.8	564.0	563.7	561.3	563.3	562.4
C2H4O	651.1[a]	650.5	652.0	648.4	645.4	647.9	642.4
C2H5	603.9[a]	606.3	607.7	608.3	606.2	608.5	608.2
C2H5O	699.0[a]	698.0	699.9	698.9	696.1	699.2	698.0
C2H5OCH3	1095.6[a]	1092.9	1096.4	1094.9	1089.5	1094.9	1092.6
C2H6	713.0[a]	712.4	714.2	713.4	711.5	714.3	712.0
C3H4_all	703.5[a]	702.8	704.4	703.9	702.8	705.4	703.6
C3H4_cyc	683.0[a]	680.2	681.9	681.5	682.0	684.7	682.9
C3H4_pro	705.1[a]	702.8	704.4	704.0	702.8	705.4	703.7
C3H6	853.7[a]	855.7	858.0	856.2	854.5	858.3	853.9
C3H8	1007.1[a]	1005.5	1008.7	1007.1	1004.7	1009.7	1005.7
C4H10_anti	1301.7[a]	1298.7	1303.3	1301.0	1298.0	1305.3	1299.7
C4H10_iso	1303.4[a]	1300.9	1305.8	1303.4	1299.3	1306.9	1301.3
C4H4O	994.3[a]	986.6	989.5	988.0	984.9	989.6	985.7
C4H5N	1071.9[a]	1061.9	1065.5	1061.5	1059.1	1064.9	1060.5
C4H6_bic	987.6[a]	975.7	978.7	977.1	976.7	981.5	976.4
C4H6_cyc	1002.0[a]	996.7	999.8	999.2	996.6	1001.6	998.9
C4H6_tra	1012.7[a]	1008.4	1011.5	1009.9	1006.8	1011.7	1008.8
C4H6_yne	1004.5[a]	1000.9	1003.6	1002.4	1001.3	1005.5	1002.0
C4H8_cyc	1149.4[a]	1148.3	1152.4	1151.2	1147.5	1153.9	1149.3
C4H8_iso	1159.0[a]	1158.0	1161.9	1159.4	1156.7	1162.9	1158.2
C4H9_t	1199.7[a]	1207.0	1211.3	1208.7	1207.2	1213.8	1208.5
C5H5N	1238.1[a]	1239.3	1243.8	1237.7	1238.1	1245.3	1237.7
C5H8_spi	1284.7[a]	1285.1	1289.5	1286.1	1285.5	1292.3	1285.5
C6H6	1368.1[a]	1367.6	1372.6	1368.0	1366.7	1374.7	1368.0
CCH	265.3[a]	283.8	284.2	263.0	275.0	275.7	263.2
CF3CN	641.2[a]	644.6	646.1	647.9	641.8	644.3	643.0
CF4	477.9[a]	469.6	470.5	478.4	467.7	469.2	468.5
CH	84.2[a]	86.0	86.1	90.3	88.0	88.2	91.5
CH2_1A1	181.5[a]	178.4	178.7	184.4	181.0	181.4	185.5
CH2_3B1	190.8[a]	191.5	191.8	194.4	193.6	194.0	195.4
CH2CH	446.1[a]	448.7	449.6	450.3	449.9	451.3	450.6
CH2OH	410.1[a]	413.5	414.3	415.1	414.3	415.5	413.9
CH3	307.9[a]	308.3	308.7	310.6	305.8	306.6	309.3
CH3CH2OH	810.8[a]	806.9	809.1	808.4	806.5	810.1	807.1
CH3CHCH2	860.9[a]	859.7	862.1	860.9	858.9	862.7	860.1
CH3CHCH3	901.0[a]	906.0	908.7	907.9	906.7	911.0	908.3
CH3CHO	677.4[a]	680.3	681.9	681.1	682.3	684.9	683.6
CH3CN	616.0[a]	615.5	616.9	616.4	613.8	616.0	617.5
CH3CO	582.0[a]	594.6	595.8	593.6	597.2	599.9	595.5
CH3COCH3	978.5[a]	983.8	986.8	984.8	984.4	989.1	985.9
CH3COOH	803.7[a]	797.8	799.9	798.9	797.4	800.8	799.2
CH3NH2	582.3[a]	578.7	580.2	582.4	578.4	580.8	580.3
CH3NO2	601.8[a]	597.2	599.0	599.7	591.9	594.8	591.6
CH3OCH3	798.5[a]	796.9	799.1	799.0	793.6	797.1	796.5
CH3OH	513.5[a]	510.9	511.9	512.7	510.8	512.4	511.5
CH4	420.4[a]	421.7	422.4	422.7	420.2	421.3	420.8
CHF3	458.7[a]	452.4	453.2	455.0	449.2	450.5	450.0
CN	181.4[a]	174.6	174.8	176.5	181.6	181.9	185.2
CO	259.7[a]	250.4	250.5	248.2	250.5	250.8	246.7
CO2	390.2[a]	370.7	371.2	371.2	377.1	377.8	380.1
F2	39.0[a]	37.7	37.8	39.0	36.4	36.5	35.0
H2	109.5[a]	110.9	111.0	108.2	108.9	109.0	109.1
H2CCO	532.7[a]	524.2	525.2	525.5	529.6	531.2	530.3
H2CO	374.7[a]	377.3	377.9	377.2	378.5	379.5	379.5
H2O	233.0[a]	229.4	229.6	231.8	230.3	230.7	229.9
HCN	313.4[a]	318.2	318.6	319.0	315.7	316.4	318.6
HCO	279.4[a]	287.6	287.9	287.7	291.3	291.9	290.1
HCOCOH	634.0[a]	640.3	641.8	640.0	642.2	644.5	643.8

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Table S57: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
HCOOCH3	785.9[a]	775.9	778.0	778.3	773.3	776.6	777.7
HCOOH	501.5[a]	492.7	493.6	494.3	492.5	494.0	494.8
HF	141.6[a]	137.1	137.2	144.0	139.9	140.0	139.8
HOOH	269.0[a]	267.1	267.5	266.8	266.9	267.7	266.2
N2	228.5[a]	226.1	226.3	227.6	215.2	215.6	222.5
NF3	205.7[a]	204.0	204.5	200.5	208.8	209.7	210.8
NH	83.1[a]	83.4	83.5	88.2	88.7	88.9	92.7
NH2	182.6[a]	178.7	179.0	185.7	186.1	186.5	191.0
NH2NH2	438.6[a]	435.3	436.5	439.9	436.1	437.9	439.7
NH3	298.0[a]	291.9	292.4	298.2	296.0	296.7	297.6
NO	152.8[a]	149.8	150.0	150.4	158.3	158.6	159.2
O2	120.8[a]	117.0	117.1	115.4	123.7	123.9	120.6
OH	107.2[a]	109.9	109.9	111.1	110.6	110.7	111.9

a Y. Zhao, N.E. Schultz, and D.G. Truhlar, J.Chem.Theory Comput. 2, 364-382 (2006) ; R. Peverati and D.G. Truhlar, J.Chem.Phys. 135, 191102 (2011).

Table S58: Benchmark Results for the IsoL6/11 Subset of the CE345-CHNOF Set. Relative Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
10-product	6.8[a]	5.6	6.4	4.7	6.2	7.5	4.1
13-product	33.5[a]	27.6	28.0	34.2	37.8	38.4	37.5
14-product	5.3[a]	7.6	8.4	8.2	9.2	10.3	5.7
20-product	4.7[a]	3.2	2.8	3.7	4.7	4.3	3.3
3-product	9.8[a]	10.2	10.0	10.6	1.9	1.7	4.6
9-product	21.8[a]	22.3	23.6	22.7	19.3	21.1	20.2

a S. Luo, Y. Zhao, and D.G. Truhlar, Phys.Chem.Chem.Phys. 13, 13683-13689 (2011).

Table S59: Benchmark Results for the IP21 Subset of the CE345-CHNOF Set. Ionization Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
C $\rightarrow$ C+ + e-	259.7[a]	230.9	230.9	221.6	227.7	227.7	218.1
O $\rightarrow$ O+ + e-	313.7[a]	309.7	309.7	306.7	309.1	309.1	302.5
O2 $\rightarrow$ O2+ + e-	278.9[a]	296.7	296.7	291.8	288.7	288.7	285.1
OH $\rightarrow$ OH+ + e-	298.9[a]	296.6	296.6	294.4	297.7	297.7	294.2

a Y. Zhao, N.E. Schultz, and D.G. Truhlar, J.Chem.Theory Comput. 2, 364-382 (2006) ; Y. Zhao, N.E. Schultz, and D.G. Truhlar, J.Chem.Phys. 123, 161103 (2005) ; Y. Zhao and D.G. Truhlar, J.Phys.Chem.A 109, 5656-5667 (2005) ; B.J. Lynch, Y. Zhao, and D.G. Truhlar,

Table S60: Benchmark Results for the EA13/03 Subset of the CE345-CHNOF Set. Electron Affinities (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
C + e- → C-	29.2[a]	18.3	18.3	9.0	15.1	15.1	5.5
O + e- → O-	33.8[a]	28.1	28.1	25.2	27.6	27.6	20.9
O2 + e- → O2-	10.8[a]	20.6	20.6	18.0	18.5	18.5	14.6
OH + e- → OH-	42.3[a]	29.4	29.4	27.5	33.6	33.6	29.5

a Y. Zhao, N.E. Schultz, and D.G. Truhlar, J.Chem.Theory Comput. 2, 364-382 (2006) ; Y. Zhao, N.E. Schultz, and D.G. Truhlar, J.Chem.Phys. 123, 161103 (2005) ; Y. Zhao and D.G. Truhlar, J.Phys.Chem.A 109, 5656-5667 (2005) ; B.J. Lynch, Y. Zhao, and D.G. Truhlar,

Table S61: Benchmark Results for the PA8/06 Subset of the CE345-CHNOF Set. Proton Affinities (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
C2H2 + H+ → C2H3+	156.6[a]	133.3	133.5	141.8	133.3	133.7	138.5
H2 + H+ → H3+	105.9[a]	42.8	42.9	34.6	65.1	65.3	60.0
H2O + H+ → H3O+	171.8[a]	167.7	167.9	172.6	165.9	166.2	166.2
NH3 + H+ → NH4+	211.9[a]	221.5	221.8	221.5	213.5	213.9	215.0

a Y. Zhao and D.G. Truhlar, J.Phys.Chem.A 110, 10478-10486 (2006).

Table S62: Benchmark Results for the ABDE12 Subset of the CE345-CHNOF Set. Dissociation Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
CH3-CH3 → CH3 + CH3	97.4[a]	96.3	97.1	92.6	100.2	101.5	93.8
CH3-OCH3 → CH3 + OCH3	89.8[a]	85.5	86.4	84.9	85.0	86.4	83.9
C2H5-CH3 → C2H5 + CH3	95.9[a]	91.2	92.5	88.6	93.1	94.9	88.6
C2H5-H → C2H5 + H	108.9[a]	106.2	106.5	105.3	105.4	105.9	103.9
C2H5-OCH3 → C2H5 + OCH3	95.3[a]	83.4	84.6	83.1	80.6	82.4	81.0
C2H5-OH → C2H5 + OH	100.3[a]	91.2	91.9	89.5	90.4	91.5	87.7
(CH3)2HC-CH3 → (CH3)2HC + CH3	95.0[a]	86.9	88.6	85.3	87.3	89.8	84.2
(CH3)2HC-OCH3 → (CH3)2HC + OCH3	91.5[a]	80.7	82.4	81.8	76.9	79.3	78.6
(CH3)3C-CH3 → (CH3)3C + CH3	93.7[a]	83.7	85.8	83.1	82.6	85.7	80.9
(CH3)3C-H → (CH3)3C + H	103.9[a]	94.3	94.9	95.2	92.7	93.6	93.3
(CH3)3C-OCH3 → (CH3)3C + OCH3	89.3[a]	78.8	80.5	81.1	73.9	77.1	76.7
(CH3)3C-OH → (CH3)3C + OH	115.0[a]	89.9	91.2	90.9	87.0	88.9	86.6

a Y. Zhao, N.E. Schultz, and D.G. Truhlar, J.Chem.Theory Comput. 2, 364-382 (2006) ; Y. Zhao and D.G. Truhlar, J.Chem.Phys. 125, 194101 (2006) ; E.I. Izgorodina, M.L. Coote, and L.J. Radom, J.Phys.Chem.A 109, 7558-7566 (2005) ; R. Peverati, Y. Zhao, and D.G. Truhlar,

Table S63: Benchmark Results for the HC7/11 Subset of the CE345-CHNOF Set. Reaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
D3d-octahedrane → (CH)12 #22-isomer	14.3[a]	22.3	22.3	21.7	20.6	20.9	18.7
D3d-octahedrane → (CH)12 #31-isomer	25.0[a]	36.1	36.6	37.1	34.6	35.7	34.0
(CH3)3CC(CH3)3 → n-C8H18	1.9[a]	7.8	10.8	7.6	0.2	4.5	0.8
n-C6H14 + 4 CH4 → 5 C2H6	9.8[a]	10.8	12.2	12.3	8.6	10.5	10.8
n-C8H18 + 6 CH4 → 7 C2H6	14.8[a]	16.2	18.4	18.6	13.0	15.9	16.4
adamantane → 3 C2H4 + 2 C2H2	194.0[a]	175.3	185.8	191.3	178.2	193.5	192.6
bicycle[2.2.2]octane → 3 C2H4 + C2H2	127.2[a]	112.5	119.7	123.7	116.3	126.9	125.9

a R. Peverati, Y. Zhao, and D.G. Truhlar, J.Phys.Chem.Lett. 2, 1991-1997 (2011).

Table S64: Benchmark Results for the πTC13 Subset of the CE345-CHNOF Set. Proton Affinities (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
C10H12 + H+ → C10H13+	225.9[a]	227.9	228.3	237.1	221.3	221.8	228.4
C2H4 + H+ → C2H5+	167.8[a]	151.7	151.9	160.0	148.4	148.8	153.3
C4H6 + H+ → C4H7+	193.4[a]	197.1	197.4	205.7	191.1	191.6	198.0
C6H8 + H+ → C6H9+	209.7[a]	212.4	212.7	221.3	206.0	206.6	213.1
C8H10 + H+ → C8H11+	219.7[a]	221.7	222.0	230.7	215.1	215.7	222.2
C9H10NH + H+ → C9H10NH2+	241.0[a]	241.8	242.2	247.8	234.3	234.9	240.4
CH2NH + H+ → CH2NH2+	214.5[a]	213.7	214.0	218.2	208.6	209.0	213.1
C3H4NH + H+ → C3H4NH2+	226.2[a]	227.1	227.5	232.2	221.1	221.6	226.6
C5H6NH + H+ → C5H6NH2+	233.4[a]	234.3	234.7	239.8	227.6	228.1	233.3
C7H8NH + H+ → C7H8NH2+	238.2[a]	238.8	239.2	244.6	231.6	232.2	237.6

a Y. Zhao, N.E. Schultz, and D.G. Truhlar, J.Chem.Phys. 123, 161103 (2005) ; Y. Zhao and D.G. Truhlar, J.Phys.Chem.A 110, 10478-10486 (2006) ; Y. Zhao, and D.G. Truhlar, J.Chem.Phys. 125, 194101 (2006).

Table S65: Benchmark Results for the πTC13 Subset of the CE345-CHNOF Set. Relative Energies at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
H2C=C=CH2 → HCC-CH3	-1.4^{a}	-0.5	-0.4	-0.9	-0.6	-0.6	-1.0
H2C=CCC=CH2 → HCC-CC-CH3	-8.8^{a}	-8.4	-8.4	-9.0	-8.8	-8.7	-9.6
H2C=CCCCC=CH2 → HCC-CC-CC-CH3	-14.3^{a}	-15.6	-15.6	-16.4	-16.1	-16.0	-17.4

a Y. Zhao, N.E. Schultz, and D.G. Truhlar, J.Chem.Phys. 123, 161103 (2005) ; Y. Zhao and D.G. Truhlar, J.Phys.Chem.A 110, 10478-10486 (2006) ; Y. Zhao, and D.G. Truhlar, J.Chem.Phys. 125, 194101 (2006).

Table S66: Benchmark Results for the HTBH38/08 Subset of the CE345-CHNOF Set. Barriers at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
TS C2H5 + NH2	7.5[a]	11.1	10.1	10.6	6.7	5.4	7.6
TS C2H5 + NH2	18.3[a]	19.8	19.0	18.2	12.5	11.5	13.0
TS CH3 + H2	12.1[a]	5.2	4.7	1.2	0.7	−0.1	−1.0
TS CH3 + H2	15.3[a]	4.2	3.8	5.1	2.1	1.5	1.3
TS CH3 + NH2	8.0[a]	7.8	7.2	7.3	2.9	1.9	3.8
TS CH3 + NH2	22.4[a]	23.6	22.9	21.9	16.6	15.7	16.9
TS F + H2	1.4[a]	4.8	4.6	3.6	7.0	6.8	5.9
TS F + H2	33.4[a]	31.0	30.9	39.5	38.2	38.0	36.7
TS H + HO	10.5[a]	1.2	1.0	−0.3	−0.1	−0.5	−0.2
TS H + HO	12.9[a]	1.4	1.2	−3.2	−2.6	−2.9	−3.0
TS H + H2	9.6[a]	1.3	1.0	1.4	−5.1	−5.6	−6.8
TS NH2 + CH4	14.5[a]	18.2	17.5	17.2	12.9	11.8	14.2
TS NH2 + CH4	17.8[a]	18.3	17.6	17.6	10.0	8.9	9.3
TS NH2 + C2H6	10.4[a]	14.7	13.9	13.6	9.5	8.2	10.6
TS NH2 + C2H6	17.4[a]	21.9	20.9	20.9	14.4	13.0	13.4
TS O + CH4	13.5[a]	2.5	2.2	1.2	2.4	1.9	3.8
TS O + CH4	7.9[a]	3.4	2.9	0.2	3.4	2.7	4.2
TS OH + H2	4.9[a]	5.2	4.9	−0.0	2.7	2.2	3.1
TS OH + H2	21.2[a]	12.6	12.4	12.5	12.2	11.9	12.0
TS OH + NH3	3.0[a]	8.9	8.4	8.2	4.3	3.5	4.1
TS OH + NH3	12.7[a]	17.3	16.7	16.4	15.3	14.5	15.6
TS OH + CH4	6.5[a]	2.9	2.3	−0.2	3.7	3.0	5.2
TS OH + CH4	19.6[a]	11.3	10.7	8.4	11.9	11.0	11.8
TS OH + C2H6	3.2[a]	0.7	0.1	−2.6	1.9	1.0	3.1
TS OH + C2H6	19.9[a]	16.2	15.4	12.9	17.9	16.7	17.4
TS s-t-C5H8 → c-C5H8	38.4[a]	34.7	34.2	35.7	33.8	33.0	35.7

a Y. Zhao, N.E. Schultz, and D.G. Truhlar, J.Chem.Theory Comput. 2, 364-382 (2006) ; Y. Zhao, B.J. Lynch, and D.G. Truhlar, Phys.Chem.Chem.Phys. 7, 43-52 (2005) ; Y. Zhao, N. Gonzalez-Garcia, and D.G. Truhlar, J.Phys.Chem.A 109, 2012-2018 (2005) ;

Table S67: Benchmark Results for the NHTBH38/08 Subset of the CE345-CHNOF Set. Barriers at 0 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
TS CH3 + C2H4	6.8[a]	10.5	9.3	8.9	10.3	8.6	9.1
TS CH3 + C2H4	33.0[a]	35.0	34.9	36.2	37.7	37.6	38.5
TS F- + CH3F	−0.3[a]	13.7	13.4	14.3	18.0	17.5	16.2
TS F- + CH3F	13.4[a]	22.5	22.5	23.6	26.1	26.1	25.0
TS H + N2	14.4[a]	2.5	2.2	2.4	−7.0	−7.4	−5.7
TS H + N2	10.6[a]	9.5	9.4	14.4	13.4	13.2	12.0
TS H + CO	3.2[a]	−1.8	−2.1	−2.7	−0.8	−1.3	−1.7
TS H + CO	22.7[a]	31.5	31.4	36.8	36.0	35.7	41.7
TS H + F2	2.3[a]	3.6	3.5	0.5	6.6	6.3	3.2
TS H + F2	105.8[a]	99.9	99.7	105.5	106.6	106.4	108.0
TS H + FH	42.2[a]	−1.2	−1.4	−9.1	1.7	1.5	−5.3
TS H + N2O	17.1[a]	−1.3	−1.7	−4.7	−4.3	−4.8	−4.8
TS H + N2O	82.3[a]	68.5	67.9	65.7	68.8	67.9	65.8
TS H + C2H4	1.7[a]	4.2	3.7	3.8	4.8	4.0	4.3
TS H + C2H4	41.8[a]	43.5	43.3	48.4	45.6	45.3	50.1
TS H + FCH3	30.4[a]	10.1	9.9	5.0	14.5	14.2	10.2
TS H + FCH3	57.0[a]	30.1	29.7	35.3	39.5	38.9	36.6
TS HCN	48.1[a]	89.8	89.8	93.0	76.9	76.9	82.6
TS HCN	32.8[a]	72.1	72.2	79.6	75.1	75.1	85.5
TS OH- + CH3F	−2.4[a]	11.4	10.8	11.8	11.7	10.8	6.7
TS OH- + CH3F	17.7[a]	26.6	26.2	26.7	31.1	30.5	34.9
TS OH- + CH3F	11.0[a]	20.7	20.6	21.7	20.8	20.5	16.7
TS OH- + CH3F	47.2[a]	57.2	57.2	61.0	63.4	63.4	66.0

a Y. Zhao, N.E. Schultz, and D.G. Truhlar, J.Chem.Theory Comput. 2, 364-382 (2006) ; Y. Zhao, B.J. Lynch, and D.G. Truhlar, Phys.Chem.Chem.Phys. 7, 43-52 (2005) ; Y. Zhao, N. Gonzalez-Garcia, and D.G. Truhlar, J.Phys.Chem.A 109, 2012-2018 (2005) ;

Table S68: Benchmark Results for the NCCE31/05 Subset of the CE345-CHNOF Set. Dissociation Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
C2H2-C2H2	1.3[a]	1.0	1.5	1.5	0.6	1.3	1.2
C2H4-C2H4	1.4[a]	0.4	1.5	1.4	−0.1	1.3	1.1
C2H4-F2	1.1[a]	−0.3	−0.0	−0.0	−0.6	−0.1	−0.1
CH4-CH4	0.5[a]	−0.1	0.5	0.5	−0.2	0.5	0.5
H2O-H2O	5.0[a]	4.0	4.3	4.5	4.4	4.9	4.6
HCONH2-HCONH2	14.9[a]	11.9	13.3	13.6	10.7	12.5	11.9
HCOOH-HCOOH	16.1[a]	12.6	13.8	14.5	11.0	12.7	12.1
HF-HF	4.6[a]	1.6	1.8	2.3	−0.1	0.2	0.2
NH3-NH3	3.1[a]	2.0	2.5	2.5	2.3	2.9	3.1
NH3-H2O	6.4[a]	4.5	5.0	4.4	5.7	6.4	6.7
P-C6H6-C6H6	2.8[a]	−1.7	1.2	1.6	−2.2	1.2	1.5
S-C6H6-C6H6	1.8[a]	−2.1	0.4	0.8	−2.4	0.5	0.8
T-C6H6-C6H6	2.7[a]	0.2	2.1	2.1	−1.2	1.2	1.2

a Y. Zhao and D.G. Truhlar, J.Phys.Chem.A 109, 5656-5667 (2005) ; Y. Zhao and D.G. Truhlar, J.Chem.Theory Comput. 1, 415-432 (2005).

Table S69: Benchmark Results for the PDDG Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
01.zt Hydrogen	0.0[a]	−3.4	−3.5	−0.1	−0.0	−0.1	0.0
02.zt Methane	−17.9[b]	−19.3	−19.9	−19.3	−18.0	−19.1	−17.8
03.zt Ethane	−20.0[c]	−21.2	−23.0	−20.8	−20.8	−23.6	−20.0
04.zt n-Propane	−25.0[c]	−25.5	−28.7	−25.2	−25.4	−30.4	−24.8
05.zt n-Butane	−30.0[c]	−30.1	−34.8	−29.9	−30.3	−37.5	−29.8
06.zt n-Pentane	−35.1[c]	−34.7	−40.8	−34.7	−35.2	−44.6	−34.9
07.zt n-Hexane	−40.0[c]	−39.2	−46.9	−39.4	−40.0	−51.6	−39.9
08.zt n-Heptane	−44.9[c]	−43.8	−53.0	−44.2	−44.8	−58.7	−45.0
09.zt n-Octane	−49.8[c]	−48.3	−59.0	−48.9	−49.7	−65.8	−50.1
10.zt n-Nonane	−54.8[c]	−52.9	−65.1	−53.7	−54.5	−72.9	−55.1
11.zt n-Decane	−59.6[b]	−57.5	−71.2	−58.4	−59.3	−79.9	−60.2
12.zt 2-Methylpropane	−32.1[c]	−31.8	−36.7	−31.9	−31.3	−38.8	−31.1
13.zt 2,2-Dimethylpropane	−40.1[c]	−39.6	−46.4	−40.2	−37.6	−48.1	−38.2
14.zt 2-Methylbutane	−36.9[c]	−35.9	−42.4	−36.1	−35.5	−45.4	−35.5
15.zt 2,2-Dimethylbutane	−44.5[b]	−42.8	−51.6	−43.4	−40.7	−54.0	−41.5
16.zt 2-Methylpentane	−41.8[b]	−40.4	−48.5	−40.9	−40.3	−52.5	−40.6
17.zt 3-Methylpentane	−41.1[b]	−39.9	−48.2	−40.2	−39.5	−52.0	−39.9
18.zt 2,3-Dimethylbutan	−42.5[d]	−41.1	−49.7	−41.7	−39.8	−52.8	−40.4
19.zt 2,2,3-Trimethylbutane	−49.0[d]	−47.5	−58.6	−48.5	−44.4	−60.9	−45.8
20.zt 3-Ethylpentane	−45.2[b]	−42.6	−53.0	−43.0	−42.3	−57.8	−42.8
21.zt 2,2,3,3-Tetramethylbutane	−53.9[c]	−53.4	−67.1	−54.9	−48.1	−68.3	−50.9
22.zt 2-Methylhexane	−46.5[b]	−45.0	−54.6	−45.6	−45.1	−59.6	−45.7
23.zt 3-Methylhexane	−45.7[b]	−44.4	−54.3	−45.0	−44.4	−59.1	−45.0
24.zt 2,2-Dimethylpentane	−49.2[b]	−47.3	−57.7	−48.2	−45.5	−61.1	−46.6
25.zt 3,3-Dimethylpentane	−48.1[b]	−45.7	−56.5	−46.3	−43.5	−59.6	−44.4
26.zt 2,3-Dimethylpentane	−47.3[b]	−44.7	−55.2	−45.5	−43.5	−59.1	−44.5
27.zt 2,4-Dimethylpentane	−48.2[b]	−46.1	−56.3	−47.1	−45.3	−60.6	−46.5
28.zt 2-Methylheptane	−51.5[b]	−49.5	−60.7	−50.4	−50.0	−66.7	−50.8
29.zt 3-Methylheptane	−50.8[b]	−49.0	−60.4	−49.8	−49.2	−66.3	−50.1
30.zt 4-Methylheptane	−50.7[b]	−48.9	−60.4	−49.8	−49.2	−66.3	−50.1
31.zt 3-Ethylhexane	−50.4[b]	−47.1	−59.2	−47.8	−47.1	−64.9	−48.0
32.zt 2,2-Dimethylhexane	−53.7[b]	−51.8	−63.8	−53.0	−50.3	−68.2	−51.7
33.zt 2,3-Dimethylhexane	−51.1[b]	−49.3	−61.3	−50.3	−48.3	−66.2	−49.6
34.zt 2,4-Dimethylhexane	−52.4[b]	−50.1	−62.1	−51.3	−49.4	−67.2	−50.9
35.zt 2,5-Dimethylhexane	−53.2[b]	−50.7	−62.4	−51.8	−50.2	−67.6	−51.5
36.zt 3,3-Dimethylhexane	−52.6[b]	−50.2	−62.6	−51.1	−48.3	−66.7	−49.6
37.zt 3,4-Dimethylhexane	−50.9[b]	−48.1	−60.3	−48.9	−47.0	−65.2	−48.2
38.zt 3-Ethyl-2-methylpentane	−50.4[b]	−47.4	−60.1	−48.3	−46.1	−64.8	−47.4
39.zt 3-Ethyl-3-methylpentane	−51.4[b]	−48.7	−61.8	−49.7	−46.3	−65.6	−47.7
40.zt 2,2,3-Trimethylpentane	−52.6[b]	−51.3	−64.3	−52.6	−48.3	−67.5	−50.1
41.zt 2,2,4-Trimethylpentane	−53.5[b]	−51.6	−64.2	−53.2	−49.4	−68.1	−51.4
42.zt 2,3,3-Trimethylpentane	−51.7[b]	−50.2	−63.3	−51.2	−46.9	−66.4	−48.5
43.zt 2,3,4-Trimethylpentane	−51.9[b]	−49.6	−62.4	−50.8	−47.6	−66.5	−49.1
44.zt 3,3-Diethylpentane	−55.6[c]	−51.4	−66.8	−52.7	−48.8	−71.3	−50.7
45.zt 2,2,3,3-Tetramethylpentane	−56.7[b]	−55.9	−71.7	−57.4	−50.4	−73.6	−52.8
46.zt 2,2,3,4-Tetramethylpentane	−56.6[b]	−53.5	−67.3	−53.5	−50.7	−70.6	−50.2
47.zt 2,2,4,4-Tetramethylpentane	−57.8[b]	−54.7	−70.0	−56.9	−50.8	−73.2	−53.5
48.zt 2,3,3,4-Tetramethylpentane	−56.4[b]	−51.5	−67.1	−52.9	−47.1	−70.1	−49.2
49.zt Ethylene	12.4[b]	12.9	11.7	12.9	13.9	12.0	13.7
50.zt Propene	4.9[b]	5.5	3.1	4.9	5.6	1.8	5.0
51.zt 1-Butene	−0.2[b]	0.1	−3.8	0.2	0.3	−5.7	0.3
52.zt 1-Pentene	−5.3[b]	−4.6	−9.9	−4.7	−4.6	−12.8	−4.8
53.zt 1-Hexene	−9.9[b]	−9.1	−16.0	−9.4	−9.4	−19.9	−9.9
54.zt 1-Heptene	−14.8[b]	−13.7	−22.1	−14.2	−14.2	−27.0	−14.9
55.zt 1-Octene	−19.4[b]	−18.3	−28.2	−18.9	−19.1	−34.0	−20.0
56.zt 1-Nonene	−25.0[e]	−22.8	−34.2	−23.7	−23.9	−41.1	−25.1
57.zt 1-Decene	−29.8[f]	−27.4	−40.3	−28.4	−28.7	−48.2	−30.2
58.zt trans-2-Butene	−3.0[b]	−3.8	−7.5	−3.7	−4.0	−9.8	−3.9
59.zt cis-2-Butene	−1.9[b]	−1.9	−5.8	−2.0	−2.2	−8.2	−2.3
60.zt cis-2-Pentane	−7.0[b]	−6.9	−12.4	−7.1	−7.2	−15.6	−7.3
61.zt trans-2-Pentene	−7.9[b]	−8.3	−13.5	−8.3	−8.6	−16.6	−8.6
62.zt cis-2-Hexene	−12.5[b]	−11.6	−18.2	−11.1	−12.1	−22.3	−11.6

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Table S69: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
63.zt trans-2-Hexene	−12.9[b]	−13.0	−19.7	−13.1	−13.5	−23.7	−13.8
64.zt cis-3-Hexene	−11.4[b]	−11.0	−17.9	−11.3	−11.3	−21.9	−11.7
65.zt trans-3-Hexene	−13.0[b]	−12.8	−19.5	−12.9	−13.2	−23.4	−13.3
66.zt 2-Methylpropene	−4.3[b]	−3.1	−7.0	−3.9	−2.9	−9.0	−3.8
67.zt 2-Methyl-2-butene	−10.1[b]	−11.6	−17.2	−11.5	−11.4	−19.9	−11.3
68.zt 2-Methyl-1-butene	−8.6[b]	−8.7	−14.3	−8.4	−8.2	−16.8	−8.0
69.zt 3-Methyl-1-butene	−6.6[b]	−6.5	−12.2	−6.9	−5.6	−14.2	−6.1
70.zt 2,3-Dimethyl-2-butene	−16.4[b]	−19.8	−27.2	−19.7	−18.9	−30.2	−18.9
71.zt 2,3-Dimethyl-1-butene	−15.2[b]	−14.8	−22.3	−14.9	−13.5	−25.0	−13.9
72.zt 2-Methyl-1-pentene	−14.2[b]	−13.4	−20.6	−13.4	−13.1	−23.9	−13.2
73.zt 3-Methyl-1-pentene	−11.8[b]	−9.3	−16.9	−9.7	−8.4	−19.8	−9.0
74.zt 4-Methyl-1-pentene	−12.2[b]	−10.4	−17.7	−10.9	−9.8	−20.8	−10.6
75.zt 2-Methyl-2-pentene	−16.0[b]	−15.7	−22.9	−15.5	−15.6	−26.5	−15.4
76.zt cis-3-Methyl-2-pentene	−14.9[b]	−15.8	−23.2	−15.8	−15.5	−26.7	−15.6
77.zt trans-3-Methyl-2-pentene	−15.1[b]	−16.0	−23.3	−16.0	−15.7	−26.8	−15.8
78.zt cis-4-Methyl-2-pentene	−13.7[b]	−13.1	−19.9	−13.4	−12.7	−23.8	−13.1
79.zt trans-4-Methyl-2-pentene	−14.7[b]	−13.5	−20.7	−13.7	−13.0	−23.9	−13.4
80.zt 2-Ethyl-1-butene	−13.4[b]	−13.2	−20.5	−13.0	−12.4	−23.5	−12.4
81.zt 3,3-Dimethyl-1-butene	−14.5[b]	−13.1	−20.9	−14.3	−10.6	−22.3	−12.1
82.zt 5-Methyl-1-hexene	−15.7[b]	−14.9	−23.8	−15.7	−14.6	−27.9	−15.7
83.zt 3-Methyl-trans-3-hexene	−18.4[b]	−20.7	−29.5	−21.0	−20.6	−33.9	−20.9
84.zt 3-Methyl-cis-3-hexene	−19.0[b]	−20.5	−29.4	−20.7	−20.3	−33.7	−20.6
85.zt 2,4-Dimethyl-1-pentene	−20.0[b]	−19.2	−28.6	−19.9	−18.3	−32.3	−19.2
86.zt 4,4-Dimethyl-1-pentene	−19.4[b]	−17.9	−27.7	−19.2	−15.7	−30.2	−17.5
87.zt 2,4-Dimethyl-2-pentene	−21.2[b]	−22.4	−31.4	−22.8	−21.6	−35.1	−22.1
88.zt 4,4-Dimethyl-trans-2-pentene	−21.2[b]	−21.7	−31.0	−22.6	−19.6	−33.6	−20.9
89.zt 4,4-Dimethyl-cis-2-pentene	−17.4[b]	−18.0	−27.7	−18.6	−15.9	−30.4	−16.9
90.zt 3-Methyl-2-ethyl-1-butene	−19.0[b]	−19.2	−28.7	−19.6	−17.7	−31.9	−18.4
91.zt 2,3,3-Trimethyl-1-butene	−20.4[b]	−21.4	−31.3	−22.0	−18.1	−32.9	−19.1
92.zt 2,2-Dimethyl-cis-3-hexene	−21.3[b]	−22.7	−34.0	−23.6	−20.6	−37.5	−21.9
93.zt 2,2-Dimethyl-trans-3-hexene	−25.7[b]	−26.3	−37.1	−27.3	−24.2	−40.5	−25.7
94.zt 2-Methyl-3-ethyl-1-pentene	−24.0[b]	−23.6	−35.2	−24.6	−22.2	−39.4	−23.7
95.zt 2,4,4-Trimethyl-1-pentene	−26.4[b]	−25.8	−37.7	−27.1	−23.2	−40.7	−25.1
96.zt 2,4,4-Trimethyl-2-pentene	−25.1[b]	−27.2	−38.7	−28.0	−24.6	−41.7	−25.8
97.zt Allene	45.6[b]	45.9	44.3	45.7	45.5	42.9	45.7
98.zt 1,2-Butadiene	38.8[b]	38.1	35.2	38.1	37.6	33.0	38.0
99.zt 1,2-Pentadiene	33.6[b]	33.3	29.0	33.2	32.8	26.0	33.1
100.zt 2,3-Pentadiene	31.8[b]	30.4	26.2	30.5	29.5	23.0	30.2
101.zt 3-Methyl-1,2-butadiene	30.9[g]	29.4	24.9	29.5	29.3	22.4	29.9
102.zt trans-Dimethyl butatriene	63.3[h]	64.2	59.5	63.8	62.4	55.1	63.3
103.zt 1,3-Butadiene	26.1[b]	29.4	26.3	29.3	30.3	25.5	29.8
104.zt 1, trans-3-Pentadiene	18.1[b]	20.5	16.1	20.4	20.9	14.0	20.4
105.zt 1, cis-3-Pentadiene	19.1[b]	21.4	16.9	21.5	21.8	14.7	21.4
106.zt 1,4-Pentadiene	25.2[b]	26.0	21.4	25.8	26.3	19.3	25.5
107.zt cis-1,3,5-Hexatriene	41.1[i]	44.8	39.7	44.5	45.8	37.9	44.7
108.zt 1,5-Hexadiene	20.1[b]	21.0	14.9	20.6	21.2	11.9	20.2
109.zt Isoprene	18.1[b]	21.4	16.6	21.7	22.6	15.2	21.9
110.zt 2,3-Dimethyl-1,3-butadiene	10.8[b]	12.6	6.0	12.8	13.9	4.0	13.7
111.zt 4-Methyl-1,3-pentadiene	11.4[j]	12.6	6.4	12.8	13.3	3.8	13.1
112.zt Acetylene	54.3[b]	54.2	53.6	53.9	54.7	53.7	54.2
113.zt Propyne	44.4[b]	44.5	42.9	44.3	44.1	41.5	44.3
114.zt 1-Butyne	39.5[b]	39.5	36.5	39.3	39.2	34.6	39.5
115.zt 1-Pentyne	34.4[k]	34.6	30.1	34.3	34.2	27.4	34.4
116.zt 1-Hexyne	29.2[k]	30.0	24.1	29.5	29.4	20.3	29.4
117.zt 1-Heptyne	24.8[k]	25.5	18.0	24.8	24.6	13.3	24.3
118.zt 1-Octyne	19.3[k]	20.9	11.9	20.0	19.8	6.2	19.2
119.zt 1-Nonyne	14.9[k]	16.3	5.8	15.3	14.9	−0.9	14.2
120.zt 1-Decyne	10.0[f]	11.8	−0.2	10.5	10.1	−8.0	9.1
121.zt 2-Butyne	34.7[b]	35.1	32.4	35.1	33.8	29.6	34.6
122.zt 2-Pentyne	30.7[k]	30.0	26.0	30.1	28.9	22.6	29.9
123.zt 2-Hexyne	25.7[k]	25.1	19.6	24.4	23.9	15.4	24.1
124.zt 3-Hexyne	25.2[k]	25.0	19.5	24.6	24.0	15.6	25.1
125.zt 3-Methyl-1-butyne	32.6[d]	32.4	27.8	32.0	32.9	25.8	33.0

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Table S69: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
126.zt 3,3-Dimethylbutyne	25.6[l]	23.8	17.2	23.1	25.9	16.0	25.5
127.zt 2-Heptyne	20.3[m]	20.6	13.6	19.7	19.1	8.3	19.1
128.zt 1,3-Butadiyne	113.0[d]	118.0	116.6	116.8	116.1	113.7	115.9
129.zt 3-Heptyne	19.8[m]	20.1	13.1	20.0	18.9	8.3	19.9
130.zt 2-Octyne	15.2[m]	16.0	7.5	15.0	14.2	1.3	14.0
131.zt 3-Octyne	14.9[m]	15.6	7.1	15.3	14.1	1.3	14.8
132.zt 4-Octyne	14.4[m]	15.2	6.7	15.0	13.9	1.1	14.7
133.zt 1-Buten-3-yne	72.8[d]	71.2	69.0	70.7	71.2	67.6	70.9
134.zt 1-Pentyne-cis-3-ene	61.1[n]	62.7	58.9	62.4	62.3	56.4	62.3
135.zt 1-Pentyne-trans-3-ene	61.4[n]	61.8	58.2	61.3	61.5	55.9	61.3
136.zt 3-Methyl-1-butyne-3-ene	61.8[o]	61.8	58.1	61.6	62.1	56.3	62.2
137.zt Benzene	19.8[b]	18.8	13.8	19.7	18.5	10.6	18.9
138.zt Naphthalene	36.0[b]	34.8	25.3	35.8	35.7	21.0	35.7
139.zt Anthracene	55.2[b]	55.5	41.4	56.4	57.5	35.8	57.0
140.zt Biphenyl	43.5[b]	39.0	27.0	40.1	40.2	21.9	40.1
141.zt Azulene	73.5[b]	83.4	74.0	82.7	82.5	68.1	81.6
142.zt Indene	39.1[b]	37.5	29.1	38.2	37.5	24.4	37.3
143.zt Biphenylene	100.5[f]	103.7	93.3	105.4	103.2	87.1	104.4
144.zt Toluene	12.0[b]	9.5	2.9	9.7	9.6	−0.6	9.9
145.zt Ethylbenzene	7.2[b]	4.8	−3.5	5.4	5.0	−7.7	5.1
146.zt Styrene	35.3[b]	34.7	27.3	35.4	35.8	24.1	35.4
147.zt Phenylacetylene	78.2[d]	75.3	69.0	75.6	75.6	65.7	75.9
148.zt Cumene	0.9[d]	−1.5	−11.8	−1.2	−0.5	−16.1	−0.9
149.zt n-Propylbenzene	1.9[d]	0.1	−9.8	0.5	0.1	−14.9	−0.1
150.zt a-Methylstyrene	27.0[d]	25.8	16.5	26.5	27.1	13.0	27.0
151.zt b-cis-Methylstyrene	29.0[d]	27.7	18.4	28.2	28.1	14.0	27.8
152.zt b-trans-Methylstyrene	28.0[d]	25.9	17.1	26.5	26.4	12.8	26.1
153.zt o-Xylene	4.6[b]	0.3	−8.1	0.9	1.3	−11.7	1.4
154.zt m-Xylene	4.1[b]	0.2	−7.9	−0.3	0.7	−11.9	0.9
155.zt p-Xylene	4.3[b]	0.3	−7.8	0.9	0.8	−11.8	−0.2
156.zt 1-Methyl-2-ethylbenzene	0.4[b]	−3.7	−14.0	−3.2	−2.5	−18.3	−2.7
157.zt 1-Methyl-3-ethylbenzene	−0.4[b]	−4.5	−14.4	−4.6	−3.9	−19.0	−3.9
158.zt 1-Methyl-4-ethylbenzene	−0.8[b]	−4.4	−14.3	−4.5	−3.8	−18.9	−3.8
159.zt 1,2,4-Trimethylbenzene	−3.3[b]	−8.8	−18.9	−9.0	−7.5	−22.9	−7.6
160.zt 1,2,3-Trimethylbenzene	−2.3[b]	−7.6	−17.9	−7.0	−5.8	−21.6	−5.7
161.zt Mesitylene	−3.8[b]	−9.0	−18.8	−9.8	−8.1	−23.1	−8.7
162.zt Indane	14.4[b]	9.9	0.3	10.3	9.3	−5.1	9.6
163.zt Cyclopropane	12.7[b]	9.9	7.6	10.7	10.1	6.3	11.9
164.zt Cyclobutane	6.8[b]	3.0	−1.0	2.4	2.9	−3.3	3.3
165.zt Cyclopentane	−18.4[b]	−19.7	−25.5	−19.9	−20.8	−29.8	−20.3
166.zt Cyclohexane	−29.5[b]	−27.0	−34.9	−27.2	−28.4	−40.5	−28.4
167.zt Cycloheptane	−28.2[b]	−23.7	−33.7	−24.1	−26.4	−41.5	−26.6
168.zt Cyclooctane	−29.7[b]	−23.8	−35.8	−25.0	−27.8	−45.6	−29.0
169.zt Cyclononane	−31.7[b]	−25.6	−39.9	−27.1	−29.3	−50.4	−31.1
170.zt Methylcyclopropane	5.5[e]	4.9	1.0	5.4	4.6	−1.4	6.0
171.zt Methylcyclopentane	−25.3[b]	−26.7	−34.4	−26.8	−27.5	−39.1	−27.0
172.zt ax-Methylcyclohexane	−35.2[p]	−32.2	−42.2	−32.6	−33.0	−48.1	−33.4
173.zt Ethylcyclopropane	1.1[q]	0.1	−5.3	0.5	−0.3	−8.6	0.9
174.zt Ethylcyclopentane	−30.3[b]	−31.1	−40.5	−31.4	−32.0	−46.1	−31.8
175.zt Propylcyclopentane	−35.4[b]	−35.7	−46.6	−36.2	−36.8	−53.2	−36.9
176.zt Butylcyclopentane	−40.2[d]	−40.2	−52.7	−40.9	−41.6	−60.3	−42.0
177.zt Ethylcyclohexane	−41.0[b]	−38.0	−49.5	−38.9	−38.9	−56.2	−40.0
178.zt n-Propylcyclohexane	−46.2[b]	−41.4	−54.7	−42.5	−42.5	−62.4	−43.7
179.zt Methylenecyclopropane	47.9[b]	45.0	42.0	45.4	43.7	39.1	44.7
180.zt Methylenecyclobutane	29.1[c]	25.4	20.8	24.9	25.6	18.3	25.5
181.zt Methylenecyclopentane	3.0[c]	−1.3	−8.0	−1.2	−1.9	−12.0	−1.6
182.zt 1,2,3-Trimethylenecyclopropane	94.6[r]	112.4	108.2	112.9	109.5	102.9	109.8
183.zt 1,2-Dimethylenecyclobutane	48.8[h]	48.2	42.8	47.9	48.9	40.5	48.7
184.zt 3-(2-Propylidenen)- 1,4-pentadiene	30.9[h]	30.7	21.3	30.3	33.1	19.0	31.9
185.zt cis-1,2-Dimethylcyclopropane	1.3[k]	0.6	−5.0	1.1	0.1	−8.4	1.1
186.zt Ethylcyclobutane	−6.3[h]	−8.8	−16.1	−9.8	−8.8	−19.9	−9.0
187.zt cis-1,2-Dimethylcyclopentane	−30.9[b]	−31.7	−41.6	−32.1	−31.9	−46.6	−31.8
188.zt trans-1,2-Dimethylcyclopentane	−32.7[b]	−33.7	−43.3	−34.9	−34.0	−48.3	−34.4

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Table S69: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
189.zt cis-1,3-Dimethylcyclopentane	-32.5^{b}	−33.7	−43.1	−34.2	−34.1	−48.2	−34.8
190.zt trans-1,3-Dimethylcyclopentane	-31.9^{b}	−33.8	−43.2	−34.3	−34.1	−48.3	−34.3
191.zt cis-1,2-Dimethylcyclohexane	-41.1^{b}	−38.2	−50.3	−39.1	−38.1	−56.3	−39.3
192.zt trans-1,2-Dimethylcyclohexane	-43.0^{b}	−40.0	−51.8	−41.3	−40.0	−57.7	−41.5
193.zt cis-1,3-Dimethylcyclohexane	-44.1^{b}	−40.7	−52.4	−42.1	−41.1	−58.5	−42.6
194.zt trans-1,3-Dimethylcyclohexane	-42.2^{b}	−39.0	−50.9	−40.1	−39.2	−57.0	−40.5
195.zt cis-1,4-Dimethylcyclohexane	-42.2^{b}	−39.0	−51.0	−40.1	−39.3	−57.1	−40.5
196.zt trans-1,4-Dimethylcyclohexane	-44.1^{b}	−40.8	−52.4	−42.2	−41.1	−58.5	−42.6
197.zt cis-cis-1,3,5- Trimethylcyclohexane	-50.7^{b}	−47.5	−61.0	−49.6	−47.3	−67.4	−49.7
198.zt cis-trans-1,3,5- Trimethylcyclohexane	-49.4^{d}	−45.8	−59.6	−47.5	−45.4	−66.0	−47.5
199.zt 1,1-Dimethylcyclopropane	-2.0^{s}	−1.8	−7.3	−1.3	−1.6	−10.2	−0.8
200.zt 1,1-Dimethylcyclopentane	-33.0^{b}	−35.1	−44.9	−35.8	−34.4	−49.1	−34.8
201.zt 1,1-Dimethylcyclohexane	-43.2^{b}	−40.5	−52.7	−41.7	−39.6	−57.8	−41.1
202.zt Vinylcyclopropane	30.4^{h}	29.8	25.3	30.2	30.1	23.1	31.0
203.zt 1,3-Cycloheptadiene	22.6^{b}	27.0	19.1	27.2	24.8	12.8	24.9
204.zt Cyclooctatetraene	71.1^{b}	75.2	67.2	74.3	73.9	61.6	72.1
205.zt Cyclopropene	66.2^{b}	67.4	65.7	66.9	65.5	62.8	65.6
206.zt Cyclobutene	37.5^{b}	41.3	38.2	40.2	40.8	35.8	40.0
207.zt Cyclopentene	8.2^{b}	6.8	1.9	7.0	5.7	−2.0	6.0
208.zt Cyclohexene	-1.1^{b}	0.4	−6.4	0.6	−1.1	−11.6	−0.9
209.zt Cyclooctene	-6.5^{b}	2.0	−9.2	1.5	−0.8	−17.6	−1.4
210.zt 1-Methylcyclopropene	58.2^{b}	59.6	56.7	59.7	57.1	52.6	57.7
211.zt 1,2-Dimethylcyclopropene	46.4^{k}	51.8	47.7	52.5	48.9	42.5	49.9
212.zt cis-1-Methyl-2- vinylcyclopropane	24.6^{h}	25.4	19.1	25.6	25.4	15.9	25.8
213.zt 3,4-Dimethylenecyclobutene	80.4^{h}	90.8	86.4	90.9	90.6	83.7	90.6
214.zt 1,2,3,4,5-Pentamethyl cyclopentadiene	-5.9^{h}	−10.3	−23.4	−11.4	−8.7	−28.2	−9.2
215.zt 1-Methylcyclopentene	-0.6^{b}	−2.9	−9.3	−2.6	−3.7	−13.7	−3.3
216.zt 3-Methylcyclopentene	2.0^{b}	−0.2	−6.8	−0.3	−0.7	−10.9	−0.9
217.zt 4-Methylcyclopentene	3.5^{b}	−0.4	−7.1	−0.6	−1.1	−11.3	−1.3
218.zt 1-Ethylcyclohexene	-15.2^{b}	−13.6	−23.9	−13.7	−14.5	−30.0	−14.7
219.zt 1,3,5-Cycloheptatriene	43.9^{b}	46.7	39.8	46.7	46.1	35.4	45.8
220.zt 1,3-Cyclopentadiene	31.9^{b}	33.3	29.3	33.5	32.6	26.2	32.2
221.zt Fulvene	53.6^{h}	56.9	52.1	57.3	57.4	49.9	56.9
222.zt 1,3-Cyclohexadiene	25.4^{b}	25.9	20.0	26.5	24.8	15.6	24.9
223.zt Bullvalene	79.8^{f}	84.5	73.3	85.5	83.5	66.5	84.3
224.zt Bicyclobutane	51.9^{b}	62.0	59.0	61.7	59.9	55.2	61.4
225.zt Spiropentane	44.2^{b}	42.8	38.4	43.6	41.0	34.3	42.7
226.zt Bicyclopropyl	30.9^{b}	30.5	24.4	31.1	30.1	20.7	32.2
227.zt Bicyclo[2.1.0]pentane	37.3^{k}	40.1	35.4	39.5	39.0	31.6	39.3
228.zt Norbornane	-12.4^{q}	−12.5	−21.5	−13.3	−12.4	−26.3	−13.2
229.zt Norbornadiene	58.6^{c}	51.8	44.9	51.5	52.1	41.1	50.7
230.zt Bicyclo[2.2.2]octane	-23.6^{c}	−22.0	−33.3	−22.1	−23.3	−40.4	−23.3
231.zt 1,4-Dimethylnorbornane	-30.6^{t}	−29.9	−43.1	−31.6	−27.9	−47.5	−29.9
232.zt 2,3-Dimethylnorbornane	-25.7^{t}	−25.2	−38.5	−27.0	−24.1	−43.9	−26.2
233.zt Bicyclo[2.2.0]hexane	29.8^{u}	24.6	17.9	22.8	24.7	14.5	24.0
234.zt cis-Bicyclo[4.2.0]octane	-6.4^{b}	−5.0	−15.8	−6.2	−6.1	−22.4	−6.7
235.zt cis-Bicyclo[3.3.0]octane	-22.2^{c}	−26.1	−36.8	−26.5	−27.1	−43.2	−27.0
236.zt trans-Bicyclo[3.3.0]octane	-15.9^{c}	−14.1	−24.8	−15.1	−15.5	−31.6	−16.1
237.zt cis-Bicyclo[4.3.0]nonane	-30.4^{b}	−29.1	−42.3	−30.0	−30.4	−50.1	−31.1
238.zt trans-Bicyclo[4.3.0]nonane	-31.4^{b}	−25.3	−38.2	−26.1	−26.8	−46.1	−27.4
239.zt cis-Bicyclo[4.4.0]decane	-40.4^{c}	−35.9	−51.5	−37.4	−37.0	−60.2	−39.0
240.zt trans-Bicyclo[4.4.0]decane	-43.5^{c}	−38.5	−53.6	−40.5	−39.8	−62.3	−42.3
241.zt Cubane	148.7^{b}	144.6	137.2	141.2	146.4	134.8	144.1
242.zt Adamantane	-31.9^{c}	−30.4	−45.6	−31.5	−30.2	−53.1	−32.0
243.zt Diamantane	-34.9^{v}	−35.3	−58.3	−38.1	−33.5	−67.6	−37.8
244.zt Bicyclo[3.1.0]hexane	9.1^{b}	8.9	2.3	9.5	7.6	−2.6	8.8
245.zt Bicyclo[4.1.0]heptane	0.3^{b}	4.3	−4.4	4.7	2.4	−10.9	3.2
246.zt Bicyclo[5.1.0]octane	-3.9^{b}	5.5	−5.4	5.5	2.9	−13.4	3.3
247.zt Bicyclo[6.1.0]nonane	-7.4^{b}	5.1	−8.0	4.6	1.9	−17.6	1.7
248.zt Bicyclo[1.1.1]pentane	49.6^{u}	63.5	58.7	60.6	61.2	53.7	59.8
249.zt Bicyclo[2.1.1]hexane	15.3^{u}	20.5	13.6	18.6	20.1	9.4	18.8
250.zt Cyclodecane	-36.9^{c}	−28.5	−45.0	−30.3	−32.2	−56.5	−34.7
251.zt Cyclododecane	-54.6^{c}	−39.8	−60.4	−43.0	−43.4	−73.3	−47.4

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Table S69: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
252.zt eq-Methylcyclohexane	−37.0[c]	−33.9	−43.7	−34.7	−34.8	−49.5	−35.6
253.zt Protoadamantane	−20.5[c]	−21.1	−36.3	−22.2	−21.2	−43.9	−22.7
254.zt tri-tert-Butylmethane	−56.2[w]	−49.7	−75.9	−52.6	−41.3	−79.2	−46.1
b01.zt Nitrogen	0.0[a]	2.8	2.6	1.5	2.6	2.2	4.6
b02.zt Ammonia	−11.0[x]	−5.9	−6.3	−12.0	−11.2	−12.0	−11.3
b03.zt Methylamine	−5.5[b]	−4.1	−5.6	−6.3	−5.8	−8.1	−5.6
b04.zt Ethylamine	−11.3[b]	−8.6	−11.3	−11.9	−11.1	−15.5	−11.3
b05.zt n-Propylamine	−16.8[b]	−13.5	−17.7	−16.9	−16.1	−22.7	−16.5
b06.zt n-Butylamine	−22.7[c]	−18.0	−23.7	−21.6	−20.9	−29.7	−21.5
b07.zt Dimethylamine	−4.4[b]	−5.1	−7.9	−4.2	−2.2	−6.5	−3.2
b08.zt Trimethylamine	−5.7[c]	−8.0	−12.4	−4.5	−0.1	−6.7	−2.9
b09.zt Isopropylamine	−20.0[c]	−14.5	−18.9	−19.4	−17.4	−24.2	−18.3
b10.zt sec-Butylamine	−25.4[c]	−19.4	−25.5	−23.1	−22.7	−32.0	−23.3
b11.zt tert-Butylamine	−28.9[c]	−22.3	−28.7	−27.4	−24.6	−34.3	−25.6
b12.zt Diethylamine	−17.3[c]	−14.7	−20.3	−15.9	−13.8	−22.3	−15.5
b13.zt Triethylamine	−22.1[c]	−18.0	−27.5	−17.9	−14.9	−29.4	−18.9
b14.zt Diisopropylamine	−34.4[e]	−25.3	−34.9	−28.3	−25.2	−39.3	−27.8
b15.zt Hydrocyanic acid	32.3[y]	26.1	25.7	25.5	25.3	24.7	25.4
b16.zt Acetonitrile	17.7[z]	17.5	16.2	17.3	15.3	13.2	15.3
b17.zt Propionitrile	12.3[c]	12.3	9.6	12.1	10.2	6.0	10.5
b18.zt n-Propyl cyanide	8.1[c]	7.5	3.3	7.1	5.3	−1.1	5.4
b19.zt Isopropyl cyanide	5.6[c]	5.1	0.8	4.6	3.5	−3.1	3.6
b20.zt Cyanogen	73.3[c]	74.8	73.9	76.2	68.2	66.7	70.5
b21.zt Malononitrile	63.6[a1]	56.6	54.4	56.9	51.7	48.2	52.3
b22.zt Acrylonitrile	43.2[c]	45.6	43.6	45.3	43.7	40.5	43.6
b23.zt E-2-Butenedinitrile	81.3[b]	79.7	76.9	79.7	75.2	70.8	75.8
b24.zt Tricyanoethylene	124.4[b]	119.1	115.1	120.1	111.4	105.4	113.5
b25.zt Dicyanacetylene	127.5[y]	138.0	136.1	137.6	128.3	125.3	130.0
b26.zt Hydrazine	22.8[y]	18.5	17.4	17.6	16.5	14.7	17.2
b27.zt Methylhydrazine	22.6[b]	18.2	15.8	18.7	20.1	16.5	20.1
b28.zt 1,2-Dimethylhydrazine	22.0[c]	17.5	13.9	19.6	23.2	17.6	22.1
b29.zt 1,1-Dimethylhydrazine	20.1[c]	14.8	10.8	17.8	27.0	15.4	22.2
b30.zt 2,3-Diazabutadiene	58.0[e]	55.7	53.4	57.4	55.7	52.2	56.4
b31.zt Tetramethyltetrazene	64.7[c]	55.2	47.0	60.3	74.0	61.9	68.2
b32.zt Azidomethylbenzene	99.5[f]	91.3	82.7	94.2	93.0	80.0	92.8
b33.zt Methyl azide	67.0[e]	67.0	65.1	68.7	67.8	64.9	68.6
b34.zt Isocyanomethane	39.1[c]	38.3	36.9	37.6	26.7	24.4	21.8
b35.zt trans-Diazene	36.0[e]	37.2	36.6	35.3	26.4	25.4	31.6
b36.zt Azoisopropane	8.6[c]	4.6	−4.7	2.0	6.0	−7.9	7.4
b37.zt Ethylenediamine	−4.1[f]	3.4	−0.5	−3.6	−1.6	−7.5	−2.9
b38.zt Methyleneimine	16.0[b1]	20.9	20.0	18.5	16.1	14.6	16.2
b39.zt Guanidine	8.0[e]	31.9	29.2	17.7	20.8	16.6	14.6
b40.zt Aziridine	30.2[c]	36.3	34.3	36.0	35.4	32.3	38.0
b41.zt Pryrrolidine	−0.8[c]	0.0	−4.4	−0.7	0.4	−7.8	−0.5
b42.zt Piperidine	−11.3[c]	−6.6	−13.9	−8.2	−6.3	−17.5	−8.2
b43.zt Cyclopentyl azide	52.8[e]	58.2	49.8	60.4	59.3	46.8	59.7
b44.zt Cyclohexyl azide	36.9[e]	51.0	40.9	52.7	52.3	37.3	51.4
b45.zt Diazirine	63.9[c1]	87.4	86.4	89.3	80.2	78.5	91.8
b46.zt Pyrrole	25.9[c]	33.7	30.2	35.6	32.0	26.3	33.9
b47.zt Tetrazole	80.0[c]	70.7	68.3	75.2	73.5	69.6	74.0
b48.zt [1,1'-Biphenyl]-2-amine	44.1[f]	45.1	31.4	41.9	44.1	23.4	43.1
b49.zt Dipropyldiazene	12.3[c]	8.0	−0.7	6.0	9.3	−4.2	12.1
b50.zt Pyridine	33.5[c]	30.8	26.3	33.5	29.4	22.3	31.8
b51.zt Pyridazine	66.5[c]	48.4	44.3	55.3	51.1	44.6	56.0
b52.zt Pyrimidine	46.8[c]	44.5	40.4	48.0	41.9	35.4	43.8
b53.zt Pyrazine	46.9[c]	44.9	40.9	50.0	42.0	35.5	47.8
b54.zt 2-Methylpyridine	23.7[c]	22.6	16.6	23.9	20.9	11.5	23.0
b55.zt 3-Methylpyridine	25.4[c]	21.2	15.2	23.4	20.3	10.8	22.1
b56.zt 4-Methylpyridine	24.8[c]	21.2	15.1	23.2	20.4	10.9	21.9
b57.zt 2,3-Dimethylpyridine	16.3[b]	13.4	5.5	14.6	12.3	0.2	14.3
b58.zt 2,4-Dimethylpyridine	15.3[b]	13.1	5.5	13.6	11.9	0.1	13.1
b59.zt 2,5-Dimethylpyridine	15.9[b]	13.3	5.7	13.9	11.9	0.2	12.9
b60.zt 2,6-Dimethylpyridine	14.0[b]	14.5	6.9	14.3	12.4	0.7	13.2
b61.zt 3,4-Dimethylpyridine	16.7[b]	11.8	3.8	14.3	11.7	−0.5	13.8

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Table S69: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
b62.zt 3,5-Dimethylpyridine	17.4^{b}	11.7	4.0	13.8	11.1	−0.7	12.9
b63.zt Benzotriazole	80.2^{f}	76.8	69.9	80.7	77.9	67.0	79.2
b64.zt Indole	37.4^{c}	48.5	40.6	49.0	47.0	34.8	47.5
b65.zt Aniline	20.8^{c}	25.2	19.0	22.0	22.3	12.7	22.0
b66.zt Phenyl cyanide	51.5^{c}	49.7	43.7	50.1	48.0	38.6	48.3
b67.zt Phenylhydrazine	48.5^{c}	47.9	40.5	49.5	48.9	37.5	49.0
b68.zt Cyclobutylamine	9.8^{c}	11.9	6.7	7.8	8.4	0.4	8.0
b69.zt Cyclopentyamine	-13.1^{c}	−9.9	−17.0	−14.6	−13.8	−24.6	−14.2
b70.zt Cyclohexylamine	-25.1^{c}	−17.3	−26.5	−22.8	−21.2	−35.1	−22.9
b71.zt Isobutylamine	18.4^{f}	22.4	19.0	18.9	19.3	14.0	20.6
b72.zt Quinuclidine	-1.0^{c}	2.3	−8.5	6.4	7.3	−9.1	5.4
b73.zt 2-Methylpiperidine	-20.2^{c}	−13.3	−22.4	−16.5	−13.3	−27.0	−16.1
b74.zt Quinoline	47.9^{d1}	48.7	39.7	50.4	48.0	34.1	49.7
b75.zt Isoquinoline	48.9^{d1}	46.9	37.9	49.8	46.7	32.7	48.4
b76.zt Quinoxaline	57.4^{e1}	64.7	56.3	67.8	61.9	48.8	66.8
b77.zt Acridine	65.5^{f1}	71.7	58.2	72.0	71.6	50.9	72.7
b78.zt Phenazine	80.9^{g1}	90.1	77.3	90.9	87.1	67.4	91.7
b79.zt 3,4-Benzoquinoline	57.5^{d1}	60.3	46.5	62.2	61.0	39.9	61.9
b80.zt 5,6-Benzoquinoline	55.9^{h1}	60.6	46.8	62.4	61.2	40.0	62.7
b81.zt 7,8-Benzoquinoline	59.9^{f1}	59.3	45.6	61.0	59.8	38.8	61.3
b82.zt Carbazole	50.1^{i1}	58.7	46.3	58.0	57.6	38.6	57.1
b83.zt Benzimidazole	43.4^{j1}	57.5	50.2	57.6	56.6	45.1	57.2
b84.zt Indazole	58.1^{j1}	64.4	57.0	68.0	65.5	54.0	68.0
b85.zt Pyrazole	42.9^{j1}	47.8	44.6	52.0	49.3	44.3	52.1
b86.zt Imidazole	31.8^{j1}	40.0	36.9	42.4	39.7	34.6	42.7
b87.zt N-Methylpyrrole	24.6^{f}	31.1	26.0	35.8	33.5	25.6	33.6
b88.zt N-Methylmethanimine	18.5^{c}	14.8	12.8	15.6	15.6	12.4	14.9
b89.zt N-Benzylideneaniline	60.6^{c}	68.3	54.9	67.6	67.7	47.3	66.1
c01.zt Water	-57.8^{d}	−56.5	−56.7	−58.9	−58.5	−58.8	−58.0
c02.zt Methanol	-48.1^{b}	−49.3	−50.3	−50.1	−49.8	−51.4	−49.7
c03.zt Ethanol	-56.2^{b}	−56.9	−59.1	−56.7	−57.2	−60.8	−56.6
c04.zt 1-Propanol	-61.2^{b}	−61.9	−65.6	−61.9	−62.2	−67.9	−61.6
c05.zt 1-Butanol	-65.8^{b}	−66.4	−71.6	−66.5	−66.9	−74.8	−66.6
c06.zt 1-Pentanol	-70.7^{b}	−71.0	−77.6	−71.3	−71.8	−81.9	−71.7
c07.zt 1-Hexanol	-75.7^{b}	−75.5	−83.7	−76.0	−76.6	−89.0	−76.7
c08.zt 1-Heptanol	-79.1^{b}	−80.1	−89.8	−80.8	−81.5	−96.1	−81.8
c09.zt 1-Octanol	-85.3^{b}	−84.7	−95.9	−85.5	−86.3	−103.1	−86.9
c10.zt 1-Nonanol	-91.1^{b}	−89.2	−101.9	−90.3	−91.1	−110.2	−91.9
c11.zt 2-Propanol	-65.1^{b}	−66.3	−70.1	−67.0	−66.6	−72.5	−66.5
c12.zt Isobutanol	-67.8^{b}	−67.9	−73.5	−69.6	−68.1	−76.7	−68.5
c13.zt 2-Butanol	-70.0^{b}	−71.1	−76.5	−71.9	−71.3	−79.5	−71.3
c14.zt tert-Butanol	-74.7^{b}	−76.8	−82.4	−78.1	−75.9	−84.5	−76.1
c15.zt 2-Pentanol	-75.2^{b}	−75.6	−82.5	−76.5	−76.0	−86.5	−76.2
c16.zt 3-Pentanol	-75.2^{b}	−75.8	−82.8	−76.6	−75.8	−86.4	−75.9
c17.zt 2-Methyl-1-butanol	-72.2^{f}	−72.3	−79.5	−72.8	−72.0	−82.8	−72.2
c18.zt 3-Methyl-1-butanol	-72.0^{b}	−72.2	−79.4	−74.2	−72.8	−83.6	−73.7
c19.zt 2-Methyl-2-butanol	-79.1^{b}	−80.7	−88.2	−82.0	−79.4	−90.7	−79.7
c20.zt 3-Methyl-2-butanol	-75.3^{b}	−77.2	−84.6	−78.3	−76.2	−87.3	−76.7
c21.zt 2-Ethyl-1-hexanol	-87.3^{b}	−84.3	−96.8	−86.8	−85.0	−103.6	−86.6
c22.zt Ethylene glycol	-92.6^{c}	−92.8	−95.5	−93.0	−93.2	−97.5	−92.5
c23.zt 1,2-Propanediol	-104.6^{b}	−103.4	−107.8	−105.3	−104.0	−110.8	−103.9
c24.zt 1,3-Butanediol	-107.5^{b}	−107.3	−113.2	−109.9	−108.3	−117.3	−109.2
c25.zt 2,3-Butanediol	-115.3^{b}	−111.9	−118.0	−113.6	−111.2	−120.4	−111.4
c26.zt Glycerol	-139.3^{b}	−140.9	−145.8	−143.0	−141.7	−149.2	−141.6
c27.zt L-Erythritol	-185.3^{b}	−188.2	−195.4	−190.5	−187.9	−198.8	−187.8
c28.zt Allyl alcohol	-29.6^{b}	−30.6	−33.5	−30.9	−30.6	−35.2	−30.8
c29.zt tert-Pentyl alcohol	-78.7^{d}	−76.1	−83.8	−78.4	−74.6	−86.2	−75.9
c30.zt Cyclopentanol	-58.0^{b}	−61.9	−68.4	−62.7	−62.8	−72.7	−62.4
c31.zt Cyclohexanol	-68.4^{b}	−68.9	−77.5	−70.2	−69.9	−82.9	−70.6
c32.zt cis-2-Methylcyclohexanol	-78.2^{c}	−73.9	−84.7	−75.4	−74.0	−90.3	−75.0
c33.zt trans-2-Methylcyclohexanol	-84.3^{c}	−75.9	−86.5	−77.7	−76.0	−91.9	−77.3
c34.zt cis-3-Methylcyclohexanol	-83.9^{c}	−75.7	−86.1	−77.5	−76.2	−91.9	−77.6
c35.zt trans-3-Methylcyclohexanol	-78.7^{c}	−74.7	−85.3	−76.5	−75.3	−91.2	−76.5
c36.zt cis-4-Methylcyclohexanol	-83.1^{c}	−74.6	−85.2	−76.4	−75.3	−91.1	−76.5

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Table S69: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
c37.zt trans-4-Methylcyclohexanol	−87.8[c]	−75.7	−86.2	−77.6	−76.2	−91.9	−77.6
c38.zt Phenol	−23.0[b]	−21.7	−27.2	−22.4	−23.6	−32.3	−23.2
c39.zt Benzyl alcohol	−22.6[f]	−27.1	−34.3	−27.8	−27.3	−38.5	−27.6
c40.zt o-Cresol	−30.7[b]	−30.5	−37.7	−31.4	−32.0	−43.1	−31.7
c41.zt m-Cresol	−31.6[b]	−31.1	−38.3	−32.6	−32.6	−43.7	−32.4
c42.zt p-Cresol	−30.0[b]	−30.6	−37.7	−31.5	−32.2	−43.3	−32.0
c43.zt 2,3-Xylenol	−37.6[b]	−39.5	−48.7	−40.3	−39.8	−53.8	−39.5
c44.zt 2,4-Xylenol	−38.9[b]	−39.5	−48.4	−40.5	−40.3	−54.0	−40.1
c45.zt 2,5-Xylenol	−38.6[b]	−39.9	−48.8	−41.4	−40.6	−54.3	−40.3
c46.zt 2,6-Xylenol	−38.7[b]	−39.4	−48.4	−40.4	−40.0	−53.8	−39.7
c47.zt 3,4-Xylenol	−37.4[b]	−39.9	−48.9	−41.0	−40.6	−54.5	−40.6
c48.zt 3,5-Xylenol	−38.6[b]	−40.5	−49.3	−42.7	−41.7	−55.1	−41.5
c49.zt Hydroquinone	−63.4[b]	−60.6	−66.7	−63.1	−64.5	−74.0	−64.3
c50.zt Furfuryl alcohol	−50.6[b]	−49.3	−54.2	−50.5	−49.4	−57.0	−49.0
c51.zt Diethylene glycol	−136.5[c]	−132.2	−138.0	−134.6	−130.0	−138.9	−132.2
c52.zt Dimethyl ether	−44.0[b]	−45.6	−47.7	−45.9	−42.8	−46.2	−44.3
c53.zt Diethyl ether	−60.3[b]	−61.1	−65.9	−60.2	−58.4	−65.7	−59.4
c54.zt Dipropyl ether	−69.8[b]	−71.1	−78.9	−70.5	−68.1	−79.9	−69.4
c55.zt Dibutyl ether	−79.8[b]	−80.1	−90.9	−79.8	−77.7	−93.9	−79.4
c56.zt Diisopropyl ether	−76.2[b]	−77.7	−86.2	−78.1	−74.1	−86.8	−76.2
c57.zt di-sec-Butyl ether	−86.3[b]	−84.8	−97.5	−85.8	−80.9	−99.3	−83.5
c58.zt di-tert-Butyl ether	−86.5[c]	−92.3	−105.7	−94.6	−85.1	−104.9	−88.7
c59.zt Methyl ethyl ether	−51.7[b]	−53.4	−56.8	−53.0	−50.6	−56.0	−51.9
c60.zt Methyl propyl ether	−56.8[b]	−58.4	−63.3	−58.1	−55.5	−63.0	−56.9
c61.zt Methyl isopropyl ether	−60.2[b]	−61.7	−66.9	−61.9	−58.6	−66.5	−60.3
c62.zt Methyl tert-butyl ether	−67.7[c]	−70.5	−77.9	−71.4	−66.1	−77.2	−68.3
c63.zt Isopropyl tert-Butyl ether	−85.6[d]	−86.6	−97.5	−88.1	−81.4	−97.6	−84.4
c64.zt Dimethoxymethane	−83.3[b]	−79.9	−83.7	−78.9	−71.4	−77.3	−75.1
c65.zt 1,1-Dimethoxyethane	−93.3[b]	−91.6	−97.7	−93.4	−83.3	−92.5	−88.0
c66.zt 2,2-Diethoxypropane	−121.1[c]	−120.7	−131.4	−120.8	−111.0	−126.9	−109.4
c67.zt Divinyl ether	−3.3[b]	4.5	1.2	3.9	4.6	−0.6	2.9
c68.zt Ethyl vinyl ether	−33.6[b]	−28.2	−32.3	−28.1	−26.8	−33.1	−28.1
c69.zt Ethylene oxide	−12.6[b]	−13.3	−14.8	−10.1	−8.8	−11.2	−5.1
c70.zt Propylene oxide	−22.6[b]	−21.2	−24.0	−18.4	−17.1	−21.5	−13.7
c71.zt Oxetane	−19.2[c]	−17.7	−20.6	−18.8	−15.8	−20.5	−17.2
c72.zt Tetrahydrofuran	−44.0[c]	−47.9	−52.5	−48.9	−46.3	−53.5	−47.3
c73.zt Tetrahydropyran	−53.4[c]	−53.1	−59.6	−54.5	−51.7	−61.8	−53.8
c74.zt 1,3-Dioxolan	−71.2[c]	−78.5	−82.0	−79.9	−70.8	−76.2	−74.0
c75.zt 1,4-Dioxane	−75.5[b]	−76.5	−81.8	−79.3	−72.4	−80.5	−76.3
c76.zt 1,3-Dioxane	−83.7[b]	−82.9	−88.3	−84.7	−75.9	−84.1	−80.7
c77.zt 2-Methyl-1,3-dioxan	−95.4[b]	−95.0	−101.8	−96.0	−87.6	−98.0	−92.2
c78.zt 4-Methyl-1,3-dioxan	−90.5[b]	−92.6	−99.6	−94.1	−85.0	−95.6	−90.0
c79.zt cis-2,4-Dimethyl-1,3-dioxan	−102.3[b]	−104.6	−113.0	−105.4	−96.5	−109.4	−101.5
c80.zt 4,5-Dimethyl-1,3-dioxan	−98.2[b]	−99.7	−108.6	−101.7	−90.8	−104.3	−96.5
c81.zt 5,5-Dimethyl-1,3-dioxan	−100.7[b]	−98.2	−107.5	−101.0	−88.6	−102.6	−94.7
c82.zt 2-cis-4-trans-6-Trimethyl- 1,3-dioxan	−106.8[b]	−112.2	−122.7	−113.6	−103.6	−119.3	−108.8
c83.zt 2-Methoxytetrahydropyran	−95.5[c]	−97.2	−106.1	−99.2	−90.3	−103.6	−95.2
c84.zt 1,3-Dioxacycloheptane	−82.8[c]	−84.1	−91.3	−86.1	−77.6	−88.6	−82.9
c85.zt a-Trioxan	−113.3[c]	−116.3	−120.4	−117.4	−100.5	−107.0	−109.0
c86.zt Anisole	−17.3[b]	−16.0	−23.0	−16.3	−14.1	−25.0	−15.4
c87.zt Furan	−8.3[b]	−2.9	−5.9	−3.4	−2.7	−7.4	−2.2
c88.zt Dihydropyran	−27.0[f]	−24.5	−30.1	−26.2	−24.3	−33.0	−26.0
c89.zt Formaldehyde	−25.9[c]	−30.3	−30.9	−30.0	−31.9	−32.8	−32.3
c90.zt Acetaldehyde	−39.7[b]	−44.2	−45.8	−44.1	−46.5	−49.1	−46.7
c91.zt Propanal	−45.5[b]	−48.2	−51.3	−48.7	−50.5	−55.3	−50.5
c92.zt Butanal	−48.9[b]	−53.0	−57.5	−53.6	−55.4	−62.4	−55.6
c93.zt Pentanal	−54.5[d]	−57.5	−63.5	−58.3	−60.2	−69.4	−60.6
c94.zt Hexanal	−59.4[d]	−62.1	−69.6	−63.1	−65.1	−76.5	−65.7
c95.zt Heptanal	−63.1[d]	−66.7	−75.7	−67.8	−69.9	−83.6	−70.8
c96.zt Octanal	−69.2[d]	−71.2	−81.8	−72.6	−74.7	−90.6	−75.8
c97.zt 2-Methylpropanal	−52.2[b]	−55.2	−60.0	−55.4	−57.1	−64.3	−57.5
c98.zt 2-Butanone	−57.0[b]	−62.4	−66.9	−62.2	−63.4	−70.3	−63.0
c99.zt 2-Butenal	−24.0[b]	−28.5	−32.1	−28.4	−30.1	−35.8	−30.3

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Table S69: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
c100.zt Glyoxal	−50.7[c]	−59.1	−60.6	−58.5	−62.6	−65.0	−63.1
c101.zt Benzaldehyde	−8.8[c]	−14.5	−20.9	−13.6	−15.6	−25.6	−15.7
c102.zt Acetic anhydride	−137.1[b]	−139.5	−143.9	−139.7	−138.8	−145.7	−143.4
c103.zt Maleic anhydride	−95.2[c]	−87.1	−90.4	−87.4	−87.2	−92.5	−90.4
c104.zt Acetone	−51.9[b]	−57.4	−60.4	−57.8	−59.3	−63.9	−59.3
c105.zt 3-Pentanone	−61.6[b]	−67.1	−73.4	−67.0	−67.9	−77.3	−67.1
c106.zt 2-Pentanone	−61.9[b]	−67.0	−73.0	−66.9	−68.3	−77.5	−68.5
c107.zt 3-Methyl-2-butanone	−62.8[k1]	−69.2	−75.5	−69.4	−69.8	−79.3	−69.5
c108.zt 2-Hexanone	−66.9[b]	−71.6	−79.1	−71.7	−73.1	−84.5	−73.5
c109.zt 3,3-Dimethyl-2-butanone	−69.5[k1]	−76.9	−85.5	−77.5	−74.9	−88.2	−75.7
c110.zt 3-Hexanone	−66.5[b]	−71.7	−79.4	−71.7	−72.8	−84.4	−72.2
c111.zt 2-Methyl-3-pentanone	−68.4[l1]	−73.9	−82.0	−74.3	−73.9	−85.7	−73.5
c112.zt 2,2-Dimethyl-3-pentaone	−75.0[l1]	−81.3	−91.6	−82.0	−78.9	−94.1	−79.8
c113.zt 2,4-Dimethyl-3-pentanone	−74.4[l1]	−80.7	−90.5	−81.5	−79.8	−94.5	−80.0
c114.zt Isopropyl tert-butyl ketone	−80.8[b]	−88.0	−100.4	−89.4	−85.1	−103.5	−86.3
c115.zt Diacetyl	−78.2[b]	−88.8	−93.0	−89.0	−90.7	−97.3	−90.5
c116.zt Acetylacetone	−90.5[b]	−99.2	−105.2	−99.3	−101.8	−111.0	−101.6
c117.zt p-Benzoquinone	−29.3[b]	−32.5	−37.9	−31.6	−32.9	−41.3	−32.0
c118.zt Cyclopentanone	−46.0[b]	−55.0	−60.6	−54.7	−57.5	−66.1	−56.9
c119.zt Cyclohexanone	−54.0[b]	−59.9	−67.6	−60.0	−62.1	−73.7	−61.8
c120.zt Cycloheptanone	−59.1[c]	−59.3	−69.1	−59.8	−61.7	−76.5	−61.7
c121.zt Acetophenone	−20.7[c]	−27.4	−35.5	−26.5	−27.6	−40.0	−26.9
c122.zt Furfural	−36.1[c]	−50.7	−56.4	−50.9	−50.8	−59.6	−49.6
c123.zt Tropolone	−37.1[c]	−32.0	−39.1	−32.9	−34.4	−45.4	−32.2
c124.zt Formic acid	−90.6[b]	−86.9	−87.8	−88.0	−88.2	−89.7	−89.6
c125.zt Acetic acid	−103.3[b]	−101.0	−103.0	−102.2	−102.7	−106.0	−103.8
c126.zt Propionic acid	−108.4[c]	−106.3	−109.8	−107.6	−107.5	−112.9	−108.4
c127.zt n-Butyric acid	−113.7[c]	−111.2	−116.2	−112.0	−112.3	−120.0	−113.4
c128.zt n-Valeric acid	−117.1[c]	−115.6	−122.1	−117.2	−117.1	−127.0	−118.4
c129.zt Hexanoic acid	−122.5[c]	−120.3	−128.3	−121.5	−121.9	−134.1	−123.5
c130.zt Heptanoic acid	−127.7[c]	−124.8	−134.3	−126.3	−126.8	−141.2	−128.5
c131.zt Oxalic acid	−173.0[c]	−162.5	−165.0	−163.1	−164.2	−168.1	−164.3
c132.zt Maleic acid	−162.4[c]	−149.1	−153.9	−150.6	−150.5	−157.9	−152.0
c133.zt Succinic acid	−196.7[c]	−184.8	−190.2	−186.5	−187.2	−195.5	−189.0
c134.zt Acrylic acid	−80.4[d]	−68.9	−71.7	−69.6	−69.2	−73.6	−70.1
c135.zt Benzoic acid	−70.7[c]	−71.1	−78.0	−71.2	−71.0	−81.8	−71.3
c136.zt Methyl formate	−85.0[c]	−81.4	−83.5	−82.1	−79.4	−82.6	−82.1
c137.zt Ethyl acetate	−106.3[b]	−103.9	−108.5	−105.0	−102.1	−109.2	−104.7
c138.zt Ethyl propionate	−111.1[c]	−109.1	−115.2	−109.8	−106.8	−116.1	−109.2
c139.zt Isopropyl acrylate	−89.7[m1]	−86.9	−95.2	−88.1	−83.8	−96.5	−86.4
c140.zt Methyl valerate	−112.7[c]	−110.4	−118.1	−111.7	−108.2	−120.0	−111.3
c141.zt n-Butyl acetate	−116.1[c]	−113.4	−121.0	−114.8	−111.6	−123.2	−114.6
c142.zt Methyl caproate	−118.0[c]	−114.9	−124.2	−116.5	−113.0	−127.1	−116.4
c143.zt Ethyl pentanoate	−121.2[c]	−118.4	−127.6	−119.8	−116.4	−130.2	−119.3
c144.zt Vinyl acetate	−75.3[c]	−71.3	−75.2	−72.3	−70.4	−76.5	−73.2
c145.zt Methyl crotonate	−81.7[c]	−79.3	−84.6	−80.1	−76.6	−84.9	−79.0
c146.zt Ethyl crotonate	−89.8[c]	−87.6	−94.2	−88.4	−84.9	−95.1	−86.9
c147.zt Ethyl pent-4-ynotate	−55.7[c]	−48.5	−55.9	−50.3	−46.5	−57.7	−48.9
c148.zt Ethyl pent-3-ynoate	−56.8[c]	−50.6	−57.6	−52.3	−50.0	−60.7	−52.3
c149.zt Ethyl pent-2-ynoate	−59.8[c]	−47.1	−54.0	−47.4	−45.5	−56.1	−46.7
c150.zt Ethyl b-vinylacrylate	−69.2[b]	−62.5	−69.8	−63.6	−59.1	−70.4	−61.8
c151.zt Ethyl 4-pentenoate	−92.2[c]	−88.1	−96.5	−89.6	−85.6	−98.3	−88.4
c152.zt Ethyl cis-3-pentenoate	−92.7[c]	−90.8	−99.2	−91.8	−88.6	−101.4	−91.2
c153.zt Ethyl trans-3-pentenoate	−93.2[c]	−92.1	−100.2	−92.9	−89.8	−102.2	−92.3
c154.zt Ethyl cis-2-pentenoate	−94.3[c]	−90.9	−99.4	−92.0	−88.3	−101.1	−90.5
c155.zt Ethyl trans-2-pentenoate	−94.2[c]	−92.1	−100.3	−93.0	−89.4	−101.8	−91.6
c156.zt n-Propyl crotonate	−94.5[c]	−92.5	−100.7	−93.5	−89.7	−102.1	−91.8
c157.zt Isopropyl crotonate	−98.2[c]	−97.3	−105.8	−98.1	−94.1	−107.0	−96.6
c158.zt Propiolactone	−67.6[c]	−54.2	−56.8	−55.3	−54.0	−58.3	−56.4
c159.zt Ethylene carbonate	−121.5[c]	−120.4	−123.7	−120.7	−113.3	−118.5	−117.6
c160.zt 4-Hydroxy-3-pentene-2-one	−92.1[n1]	−94.1	−99.8	−96.2	−97.2	−106.0	−97.3
c161.zt Hydrogen peroxide	−32.5[o1]	−35.3	−35.8	−34.8	−36.9	−37.6	−36.0
c162.zt Dimethyl peroxide	−30.1[c]	−37.3	−39.9	−36.1	−30.7	−34.6	−31.7
c163.zt Diethyl peroxide	−46.1[c]	−52.6	−57.8	−49.5	−46.0	−53.8	−46.1

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Table S69: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
c164.zt Ozone	34.1^{f}	37.9	37.5	39.7	48.7	48.1	52.8
c165.zt Carbon monoxide	−26.4^{f}	−20.3	−20.5	−19.3	−21.5	−21.8	−17.5
c166.zt Carbon dioxide	−94.0^{f}	−80.5	−80.9	−81.8	−87.7	−88.4	−89.4
c167.zt Ketene	−11.4^{f}	−5.1	−6.1	−6.5	−11.0	−12.6	−10.9
c168.zt Carbon suboxide	−22.4^{f}	−3.2	−4.4	−6.5	−16.9	−18.9	−16.2
c169.zt Pentamethylene formal	−80.5^{c}	−86.3	−95.5	−88.9	−80.6	−94.3	−86.5
c170.zt 1,3-Dioxaindane	−71.5^{f}	−70.0	−77.8	−73.1	−73.3	−85.4	−72.6
c171.zt Furoic acid	−93.2^{c}	−87.4	−92.2	−88.3	−86.9	−94.4	−86.7
c172.zt Fumeric Acid	−161.5^{c}	−154.0	−158.5	−155.7	−155.5	−162.4	−157.2
c173.zt 1-Ethyoxypropane	−65.1^{c}	−66.1	−72.4	−65.3	−63.2	−72.8	−64.4
c174.zt 3,3-Dimethyl oxetane	−35.4^{c}	−34.5	−40.9	−35.9	−31.5	−41.2	−33.4
c175.zt 3-Oxabicyclo[3.2.2]nonan	−53.2^{p1}	−50.1	−62.4	−52.2	−48.9	−67.3	−51.6
c176.zt 1,2-Diethyoxyethane	−97.6^{c}	−101.2	−109.1	−99.8	−95.1	−107.1	−97.8
c177.zt 2,2-Dimethoxypropane	−102.7^{c}	−107.8	−115.6	−109.0	−99.0	−110.7	−103.5
c178.zt 2-Ethylhexanal	−71.6^{b}	−72.4	−83.9	−73.2	−74.1	−91.2	−75.4
c179.zt 4-Heptanone	−71.3^{q1}	−76.3	−85.7	−76.6	−77.3	−91.0	−78.3
c180.zt 5-Nonanone	−82.4^{k1}	−85.5	−97.8	−86.2	−87.2	−105.6	−87.4
c181.zt 6-Undecanone	−92.6^{q1}	−94.6	−110.1	−95.6	−96.9	−119.7	−97.5
c182.zt 3-Methyl-2-pentanone	−67.9^{q1}	−73.3	−81.3	−73.7	−73.8	−85.9	−73.9
c183.zt 3,3-Dimethyl-2-pentanone	−72.6^{q1}	−80.2	−90.7	−80.8	−78.3	−94.1	−78.9
c184.zt 4-Methyl-2-pentanone	−69.6^{q1}	−73.4	−81.6	−74.0	−74.3	−86.5	−74.6
c185.zt 4,4-Dimethyl-2-pentanone	−76.6^{q1}	−80.9	−91.4	−82.1	−80.0	−95.6	−81.2
c186.zt 3,3,4-Trimethyl-2-pentanone	−78.5^{q1}	−86.2	−99.2	−87.6	−83.2	−102.4	−84.6
c187.zt 3,3,4,4-Tetramethyl-2-pentanone	−83.1^{q1}	−92.4	−108.1	−94.4	−86.9	−110.0	−89.3
c188.zt di-tert-Butyl ketone	−82.7^{l1}	−92.3	−107.2	−93.8	−86.7	−108.7	−88.4
c189.zt tert-Butyl neopentyl ketone	−94.1^{l1}	−99.1	−116.0	−101.8	−95.0	−119.5	−97.8
c190.zt Dineopentyl ketone	−100.7^{r1}	−102.1	−121.9	−106.5	−100.3	−126.8	−103.3
c191.zt Cyclooctanone	−64.9^{c}	−62.8	−74.7	−64.1	−65.7	−83.5	−66.8
c192.zt Norbornan-2-one	−40.8^{s1}	−45.8	−54.6	−46.6	−46.7	−60.3	−47.7
c193.zt Norbornan-7-one	−32.0^{s1}	−41.2	−49.9	−41.8	−42.4	−55.9	−43.1
c194.zt Bicyclo[3.2.1]octan-2-one	−51.8^{t1}	−57.0	−68.1	−57.5	−57.9	−74.7	−58.3
c195.zt Bicyclo[3.2.1]octan-3-one	−52.9^{t1}	−58.1	−69.2	−58.7	−59.4	−76.1	−60.0
c196.zt Bicyclo[3.2.1]octan-8-one	−46.2^{t1}	−54.6	−65.7	−55.3	−55.9	−72.7	−56.5
c197.zt Bicyclo[3.3.1]nonane-3-one	−63.8^{t1}	−64.6	−78.1	−65.4	−66.2	−86.6	−67.3
c198.zt Bicyclo[3.3.1]nonane-9-one	−57.3^{t1}	−59.8	−73.2	−60.4	−61.9	−82.0	−62.4
c199.zt Adamantanone	−55.1^{t1}	−64.0	−78.9	−65.1	−63.9	−86.4	−65.5
c200.zt Diadamantanone	−56.6^{t1}	−68.8	−91.5	−71.5	−67.1	−100.8	−71.1
c201.zt Camphor	−63.9^{t1}	−67.2	−83.0	−69.4	−64.5	−87.9	−67.4
c202.zt 2-Methyl-2-propenal	−25.4^{f}	−27.1	−30.9	−26.7	−27.9	−33.9	−28.1
c203.zt 2-Ethylacrolein	−31.4^{f}	−31.1	−36.5	−31.3	−31.7	−40.1	−32.5
c204.zt Xanthone	−23.5^{f}	−26.8	−40.2	−27.7	−24.8	−45.4	−25.7
c205.zt Methyl acetate	−98.8^{c}	−95.6	−98.8	−96.7	−93.8	−99.0	−96.7
c206.zt Isovaleric acid	−123.0^{c}	−111.9	−119.1	−113.0	−112.3	−123.1	−113.6
c207.zt Pivalic acid	−117.4^{c}	−116.5	−123.9	−117.3	−114.3	−125.7	−115.5
c208.zt Octanoic acid	−132.8^{c}	−123.2	−134.3	−125.1	−125.3	−142.1	−127.5
c209.zt 2-Ethylhexanoic acid	−133.7^{c}	−124.1	−136.2	−125.7	−126.3	−142.5	−126.4
c210.zt Methyl heptanoate	−123.5^{c}	−119.4	−130.2	−121.2	−117.9	−134.2	−121.4
c211.zt n-Propyl pentanoate	−127.5^{c}	−123.5	−134.1	−124.6	−121.2	−137.3	−124.2
c212.zt n-Butyl pentanoate	−133.9^{c}	−128.0	−140.1	−129.3	−126.0	−144.3	−129.2
c213.zt Methyl pivalate	−118.2^{c}	−116.9	−125.6	−118.7	−111.6	−124.7	−114.5
c214.zt Ethyl pivalate	−128.1^{c}	−125.1	−135.3	−126.4	−119.8	−134.9	−122.5
c215.zt Methyl isovalerate	−119.0^{c}	−112.3	−120.7	−113.6	−109.3	−121.8	−112.3
c216.zt Ethyl isovalerate	−126.0^{c}	−120.5	−130.6	−122.3	−117.5	−132.0	−120.2
c217.zt Methyl a-methylbutrate	−117.7^{c}	−112.8	−121.0	−114.3	−109.1	−121.6	−111.7
c218.zt Ethyl a-methylbutyrate	−124.9^{c}	−120.9	−130.5	−122.0	−117.3	−131.8	−119.6
c219.zt sec-Butyl butyrate	−130.3^{c}	−128.5	−139.7	−129.4	−125.3	−142.1	−128.6
c220.zt sec-Butyl pentanoate	−137.0^{c}	−133.0	−145.8	−134.1	−130.1	−149.1	−133.6
c221.zt Isopropyl pentanoate	−130.2^{c}	−128.3	−139.3	−129.2	−125.6	−142.1	−128.9
c222.zt Isobutyl pentanoate	−135.9^{c}	−129.8	−142.6	−131.8	−127.0	−146.2	−130.6
c223.zt Butyrolactione	−87.6^{u1}	−88.9	−93.3	−89.7	−87.9	−94.7	−89.8
c224.zt Valerolactone	−90.7^{u1}	−91.0	−97.3	−91.4	−89.2	−98.9	−91.5
c225.zt Caprolactone	−94.7^{v1}	−90.7	−99.1	−91.2	−89.0	−101.7	−91.5
c226.zt Hepanlactone	−98.3^{v1}	−95.9	−106.5	−96.9	−94.2	−110.1	−97.5
c227.zt tert-Butyl hydroperoxide	−58.8^{c}	−62.8	−69.1	−62.4	−59.1	−68.5	−59.3
c228.zt di-tert-Butyl peroxide	−83.4^{c}	−86.9	−100.2	−88.0	−78.8	−98.3	−81.7

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Table S69: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
c229.zt eq-Cyclohexyl hydroperoxide	-55.0^{o1}	−55.7	−64.8	−55.0	−53.5	−67.3	−54.0
c230.zt 1-Methyl cyclohexyl hydroperoxide	-63.0^{o1}	−64.7	−76.2	−64.9	−61.4	−78.5	−62.5
c231.zt 1-Hydroperoxylhexane	-62.0^{o1}	−63.1	−71.7	−61.8	−60.9	−73.9	−61.1
c232.zt 2-Hydroperoxylhexane	-64.0^{o1}	−66.1	−75.3	−65.3	−63.5	−77.2	−63.7
c233.zt 3-Hydroperoxylhexane	-63.0^{o1}	−66.1	−75.5	−67.2	−63.6	−77.6	−64.5
c234.zt Tropone	10.5^{c}	15.2	8.7	15.5	13.5	3.4	14.2
c235.zt Ethyl phenyl ketone	-26.0^{c}	−32.0	−41.3	−30.8	−31.6	−46.4	−30.9
c236.zt Methyl hydroperoxide	-31.3^{w1}	−36.7	−38.1	−35.7	−33.9	−36.1	−33.8
c237.zt Ethyl hydroperoxide	-47.5^{c}	−43.8	−46.6	−43.3	−41.5	−45.8	−41.3
c238.zt Isopropyl hydroperoxide	-47.1^{w1}	−53.2	−57.5	−52.0	−50.3	−57.0	−50.1
d01.zt Formamide	-44.5^{x1}	−39.8	−41.1	−43.2	−46.3	−48.4	−48.5
d02.zt Dimethylformamide	-45.8^{b}	−43.5	−47.6	−39.4	−41.4	−47.7	−45.5
d03.zt Acetamide	-57.0^{f}	−50.7	−53.2	−55.6	−57.4	−61.4	−59.1
d04.zt Butanamide	-66.7^{f}	−60.3	−65.9	−65.9	−66.7	−75.2	−68.7
d05.zt Pentanamide	-69.4^{c}	−64.8	−72.0	−70.1	−71.6	−82.4	−73.6
d06.zt Hexanamide	-78.4^{c}	−69.4	−78.1	−74.9	−76.4	−89.5	−78.7
d07.zt Urea	-58.7^{c}	−39.9	−42.1	−50.6	−49.3	−52.8	−54.2
d08.zt Oxamide	-96.2^{c}	−80.4	−83.9	−88.7	−92.8	−98.1	−94.8
d09.zt n-Propylcarbamate	-112.7^{c}	−99.1	−104.9	−105.1	−101.8	−110.6	−106.2
d10.zt e-Caprolactam	-58.8^{c}	−50.7	−59.9	−53.0	−55.7	−69.5	−59.2
d11.zt N,N-Dimethylbutryamide	-64.7^{f}	−62.7	−71.5	−60.3	−60.0	−73.3	−64.0
d12.zt Nitromethane	-17.9^{b}	−17.3	−19.1	−17.0	−15.7	−18.5	−12.9
d13.zt Nitroethane	-24.4^{b}	−23.4	−26.6	−23.8	−22.0	−27.0	−20.4
d14.zt 1-Nitropropane	-30.0^{b}	−28.2	−32.9	−28.8	−26.8	−34.0	−25.3
d15.zt 2-Nitropropane	-33.2^{b}	−31.2	−36.1	−32.7	−29.9	−37.4	−28.6
d16.zt 1-Nitrobutane	-34.4^{b}	−32.8	−39.0	−33.5	−31.5	−40.9	−30.2
d17.zt 2-Nitrobutane	-39.1^{b}	−36.2	−42.9	−38.0	−34.8	−44.9	−33.7
d18.zt Nitric acid	-32.1^{y}	−33.6	−34.6	−35.9	−33.4	−35.1	−33.4
d19.zt Methyl nitrate	-29.1^{b}	−32.7	−34.9	−34.9	−28.4	−31.8	−29.8
d20.zt Ethyl nitrate	-36.8^{b}	−41.6	−45.1	−43.0	−36.6	−42.0	−37.8
d21.zt n-Propylnitrate	-41.6^{b}	−46.7	−51.7	−48.3	−41.5	−49.1	−42.7
d22.zt Isopropylnitrate	-45.6^{b}	−51.7	−57.0	−53.6	−46.1	−54.0	−47.4
d23.zt Nitrous acid	-18.3^{f}	−19.7	−20.3	−19.9	−26.8	−27.8	−25.8
d24.zt Methyl nitrite	-15.6^{f}	−16.8	−18.4	−17.4	−20.0	−22.6	−20.3
d25.zt Methacrylamide	-37.7^{f}	−33.5	−38.4	−38.2	−38.7	−46.3	−40.3
d26.zt N-Methylacetamide	-59.3^{f}	−51.4	−55.3	−52.4	−54.1	−60.2	−56.4
d27.zt 5-Methylisoxazole	3.6^{b}	12.6	8.7	14.3	13.0	6.8	13.1
d28.zt 3-Methylisoxazole	4.8^{b}	16.4	12.4	15.8	16.1	9.9	15.6
d29.zt 3,5-Dimethylisoxazole	-4.3^{b}	5.2	−0.2	5.0	5.0	−3.3	4.6
d30.zt 3,4,5-Trimethylisoxazole	-4.8^{b}	−3.4	−10.6	−3.1	−3.1	−14.1	−3.6
d31.zt Isocyanic acid	-24.3^{f}	−7.2	−7.9	−13.8	−19.5	−20.7	−25.0
d32.zt Propanamide	-61.9^{f}	−55.7	−59.8	−60.6	−62.0	−68.4	−63.5
d33.zt Dimethylaminomethane	-48.6^{f}	−47.2	−52.2	−46.3	−41.1	−48.5	−45.6
d34.zt N-Butyl acetamide	-72.8^{b}	−65.8	−74.3	−68.0	−69.1	−81.8	−73.1
d35.zt Isophthalamide	-91.4^{f}	−57.4	−67.7	−66.8	−67.9	−83.5	−71.6
d36.zt Glycine	-93.7^{b}	−88.2	−91.3	−92.6	−91.3	−96.1	−92.5
d37.zt L-Alanine	-99.1^{y1}	−95.1	−99.8	−100.7	−98.0	−105.3	−99.3
d38.zt L-Valine	-108.8^{b}	−109.5	−118.1	−112.1	−111.4	−124.2	−109.8
d39.zt L-Leucine	-116.3^{b}	−113.6	−123.8	−116.5	−115.7	−130.9	−114.8
d40.zt Benzamide	-24.1^{f}	−20.1	−27.7	−24.3	−25.2	−36.9	−26.7
d41.zt 2-Methyl propanamide	-67.5^{f}	−62.8	−68.7	−68.1	−68.3	−77.2	−70.3

a M.W.Chase, C.A.Davies, J.R.Downey, D.R.Frurip, R.A.McDonald, and A.N.Syverud, "JANAF Thermochemical Tables", 3rd edition, J.Phys.Chem.Ref.Data 14, Suppl.1 (1985). b J.D.Cox, G.Pilcher, "Thermochemistry of Organic and Organometallic Compounds", Academic Press Inc., New York (1970). c J.B.Pedley, R.D.Naylor, S.P.Kirby, "Thermochemical Data of Organic Compounds", 2 ed., Chapman and Hall, New York (1986). d R.D.Stull, E.F.J.Westrum, G.C.Sinke, "The Chemical Thermodynamics of Organic Compounds", John Wiley & Sons, Inc., New York (1969). e S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, W.G.Mallard, J.Phys.Chem.Ref.Data, Suppl. 17 (1998). f H.Y.Afeefy, J.F.Liebman, and S.E.Stein, "Neutral Thermochemical Data", 20899 (http://webbook.nist.gov) ed.; P.J.Linstrom, and W.G.Mallard, Ed., National Institute of Standards and Technology, Gaithersburg, MD (2001). g W.V.Steele, R.D.Chirico, A.Nguyen, I.A.Hossenlopp, and N.K.Smith, Am.Inst.Chem.Eng.Symp.Ser. (AIChE Symp.Ser.) 138 (1990). h W.R.Roth, O.Adamczak, R.Breuckmann, H.W.Lennartz, and R.Boese, Chem.Ber. 124, 2499-2521 (1991). i W.Fang and D.W.Rogers, J.Org.Chem. 57, 2294 (1992). j S.W.Benson and H.E.O'Neal, "Kinetic Data on Gas Phase Unimolecular Reactions" (1970). k R.B.Turner, P.Goebel, B.J.Mallon, W.v.E.Doering, J.F.J.Coburn, and M.Pomerantz, J.Am.Chem.Soc. 90, 4315 (1968). l T.V.Siretskaya, V.V.Takhistov, S.M.Pimenova, V.M.Orlov, and V.N.Pustobaev, React.Kinet.Catal.Lett. 31, 15 (1986). m D.w.Rogers, O.A.Dagdagan, and N.L.Allinger, J.Am.Chem.Soc.

101, 671 (1979). n R.Shaw, "The Chemistry of the Carbon-Carbon Triple Bond", John Wiley & Sons, New York, Vol. 1 (1978). o N.D.Lebedeva, V.L.Ryadnenko, N.N.Kiseleva, and L.F.Nazarova, Vses.Konf.Kalorim.Rasshir.Tezisy.Dokl.7th. 1, 91 (1977). p value, S.F.N.M. q P.v.R.Schleyer, J.E.Williams, and K.R.Blanchard, J.Am.Chem.Soc. 92, 2377 (1970). r T.Bally, H.Baumgaertel, U.Buechler, E.Haselbach, W.Lohr, J.P.Maier, and J.Vogt, Helv.Chim.Acta. 61, 741 (1978). s W.D.Good, R.T.Moore, A.g.Osborn, and D.R.Douslin, J.Chem.Thermodyn. 6, 303 (1974). t M.P.Kozina, L.P.Timofeeva, S.M.Skuratov, N.A.Belikova, E.M.Milvitskaya, and A.F.Plate, J.Chem.Thermodyn. 3, 563 (1971). u K.B.Wiberg, and J.J.Wendoloski, J.Am.Chem.Soc. 104, 5679 (1982). v T.Clark, T.M.O.Knox, M.A.McKervey, H.Mackle, and J.J.Rooney, J.Am.Chem.Soc. 101, 2404 (1979). w S.P.Verevkin, M.Nolke, H.D.Beckhaus, and C.Ruchardt, J.Org.Chem. 62, 4683 (1997). x J.D.Cox, D.D.Wagman, V.A.Medvedev, "CODATA Key Values for Thermodynamics", Hemisphere Publishing Corp., New York (1984). y M.W.J.Chase, J.Phys.Chem.Ref.Data Monograph 9, 1 (1998). z X.W.An, and M.Mansson, J.Chem.Thermodyn. 15, 287 (1983). a1 H.D.Beckhaus, B.Dogan, J.Pakusch, S.Verevkin, and C.Ruchardt, Chem.Ber. 123, 2153 (1990). b1 R.A.L.Peerboom, S.Ingemann, N.M.M.Nibbering, and J.F.Liebman, J.Chem.Soc,.Perkin.Trans.2. 1, 1825 (1990). c1 A.H.LauFer, and H.Okabe, J.Phys.Chem. 76, 3504 (1972). d1 W.V.Steele, D.G.Archer, R.D.Chirico, W.B.Collier, I.A.Hossenlopp, A.Nguyen, N.K.Smith, and B.E.Gammon, J.Chem.Thermodyn. 20, 1233 (1988). e1 M.A.V.Silva, M.A.R.Matos, and V.M.F.Morais, J.Chem.Soc,.Faraday.Trans. 91, 1907 (1995). f1 W.V.Steele, R.D.Chirico, I.A.Hossenlopp, A.Nguyen, N.K.Smith, and B.E.Gammon, J.Chem.Thermodyn. 21, 81 (1989). g1 R.Sabbah, and L.Elwatik, Thermochim.Acta. 176, 163 (1991). h1 D.M.McEachern, J.C.Iniguez, and H.C.Ornelas, J.Chem.Eng.Data. 20, 226 (1975). i1 R.Sabbah and I.Antipine, Bull.Soc.Chim.France. 3, 392 (1987). j1 P.Jimenez, M.V.Roux, C.Turrion, and F.Gomis, J.Chem.Thermodyn. 19, 985 (1987). k1 A.Harrop, A.J.Head, and G.B.Lewis, J.Chem.Thermodyn. 2, 203 (1970). l1 P.Sellers, J.Chem.Thermodyn. 2, 211 (1970). m1 W.V.Steele, R.D.Chirico, S.E.Knipmeyer, A.Nguyen, and N.K.Smith, J.Chem.Eng.Data. 41, 1285 (1996). n1 T.P.Melia and R.Merrifield, J.Appl.Chem. 19, 79 (1969). o1 K.S.Chen and N.L.Allinger, J.Comput.Chem. 14, 755 (1993). p1 S.W.S.Wong and E.F.Westrum, J.Am.Chem.Soc. 93, 5317 (1971). q1 J.E.Dubois and H.Herzog, J.Chem.Soc.Chem.Commun. 16, 932 (1972). r1 P.Seller, Acta.Chemica.Scandinava. 25, 2099 (1971). s1 W.V.Steele, J.Chem.Thermodyn. 10, 585 (1978). t1 N.L.Allinger, K.S.Chen, M.Rahman, and A.Pathiaseril, J.Am.Chem.Soc. 113, 4505 (1991). u1 M.Luisa, G.Pilcher, M.Y.Yang, J.M.Brown, and A.D.Conn, J.Chem.Thermodyn. 22, 885 (1990). v1 K.B.Wiberg and R.F.Waldron, J.Am.Chem.Soc. 113, 7697 (1991). w1 S.L.Khursan and V.S.Martem'yanov, Russ.J.Phys.Chem.(Engl.Transl). 65, 321 (1991). x1 A.Bauder and H.H.Gunthard, Helv.Chim.Acta. 41, 670 (1958). y1 S.N.Ngauv, R.Sabbah, and M.Laffitte, Thermochim.Acta. 20, 371 (1977).

Table S70: Benchmark Results for the PDDG Set. Ionization Potentials (eV)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
01.zt Hydrogen	15.98[a]	15.68	15.68	15.64	15.65	15.65	15.67
02.zt Methane	14.00[a]	13.64	13.64	13.66	14.17	14.17	14.30
03.zt Ethane	12.10[b]	11.92	11.92	11.93	12.30	12.30	12.43
04.zt n-Propane	11.50[a]	11.39	11.39	11.36	11.69	11.69	11.82
05.zt n-Butane	11.20[c]	10.95	10.94	10.82	11.47	11.47	11.53
06.zt n-Pentane	10.90[c]	10.66	10.66	10.49	11.35	11.34	11.31
12.zt 2-Methylpropane	11.40[a]	11.06	11.07	10.96	11.41	11.41	11.53
13.zt 2,2-Dimethylpropane	11.30[a]	10.82	10.82	10.70	11.31	11.31	11.31
14.zt 2-Methylbutane	11.00[c]	10.65	10.65	10.53	11.13	11.13	11.17
49.zt Ethylene	10.51[a]	10.74	10.74	10.53	11.05	11.05	10.87
50.zt Propene	9.88[b]	9.97	9.97	9.80	10.27	10.27	10.15
51.zt 1-Butene	9.63[c]	9.93	9.93	9.74	10.26	10.26	10.13
52.zt 1-Pentene	9.52[c]	9.86	9.85	9.67	10.21	10.21	10.09
67.zt 2-Methyl-2-butene	8.68[c]	8.94	8.94	8.80	9.19	9.19	9.11
68.zt 2-Methyl-1-butene	9.15[c]	9.47	9.47	9.29	9.78	9.78	9.67
69.zt 3-Methyl-1-butene	9.53[c]	9.88	9.88	9.67	10.25	10.25	10.09
97.zt Allene	11.40[a]	10.16	10.16	9.97	10.44	10.45	10.31
98.zt 1,2-Butadiene	9.33[c]	9.49	9.49	9.33	9.75	9.75	9.66
106.zt 1,4-Pentadiene	9.62[c]	9.89	9.90	9.71	10.16	10.17	10.04
112.zt Acetylene	11.40[a]	11.55	11.55	11.35	11.79	11.79	11.64
113.zt Propyne	10.37[a]	10.64	10.64	10.47	10.88	10.88	10.78
114.zt 1-Butyne	10.20[c]	10.51	10.51	10.32	10.76	10.76	10.67
121.zt 2-Butyne	9.59[c]	9.91	9.91	9.76	10.14	10.15	10.07
128.zt 1,3-Butadiyne	10.17[a]	10.30	10.30	10.06	10.47	10.47	10.29
137.zt Benzene	9.24[a]	9.59	9.59	9.41	9.91	9.91	9.76
138.zt Naphthalene	8.15[a]	8.51	8.51	8.31	8.79	8.79	8.63
139.zt Anthracene	7.44[d]	7.81	7.81	7.59	8.07	8.07	7.91
144.zt Toluene	8.82[b]	9.17	9.17	9.00	9.46	9.46	9.35
145.zt Ethylbenzene	8.80[e]	9.14	9.14	8.96	9.47	9.47	9.35
163.zt Cyclopropane	11.00[b]	10.88	10.88	10.71	11.47	11.47	11.38
164.zt Cyclobutane	11.00[f]	10.38	10.38	10.24	10.98	10.98	10.97
164.zt Cyclobutane	10.70[c]	10.38	10.38	10.24	10.98	10.98	10.97
165.zt Cyclopentane	10.70[c]	10.91	10.91	10.87	11.28	11.29	11.38
166.zt Cyclohexane	10.30[c]	10.15	10.15	10.04	10.70	10.69	10.70
205.zt Cyclopropene	9.86[a]	9.84	9.84	9.70	10.13	10.13	10.06
206.zt Cyclobutene	9.43[a]	9.65	9.64	9.49	9.93	9.93	9.82
207.zt Cyclopentene	9.18[a]	9.22	9.22	9.09	9.51	9.51	9.44
208.zt Cyclohexene	8.94[c]	9.29	9.29	9.14	9.59	9.59	9.51
219.zt 1,3,5-Cycloheptatriene	8.50[d]	8.57	8.58	8.39	8.82	8.84	8.72
220.zt 1,3-Cyclopentadiene	8.57[a]	8.82	8.82	8.63	9.10	9.10	8.97
230.zt Bicyclo[2.2.2]octane	9.47[d]	9.77	9.77	9.66	10.25	10.25	10.25
242.zt Adamantane	9.75[d]	9.59	9.59	9.49	10.06	10.06	10.07
b01.zt Nitrogen	15.60[b]	15.46	15.46	15.55	14.51	14.51	14.73
b02.zt Ammonia	10.85[b]	10.67	10.67	10.84	11.23	11.23	11.30
b03.zt Methylamine	9.45[f]	9.75	9.75	9.91	10.00	10.01	10.13
b04.zt Ethylamine	9.50[d]	9.60	9.60	9.75	9.84	9.84	9.95
b07.zt Dimethylamine	8.93[f]	9.23	9.23	9.41	9.24	9.25	9.38
b08.zt Trimethylamine	8.54[f]	8.84	8.85	9.07	8.67	8.69	8.87
b15.zt Hydrocyanic acid	13.60[b]	13.91	13.91	13.89	13.94	13.94	13.86
b16.zt Acetonitrile	12.21[g]	12.50	12.50	12.52	12.63	12.63	12.67
b17.zt Propionitrile	11.85[d]	12.06	12.06	12.11	12.25	12.25	12.36
b20.zt Cyanogen	13.36[g]	13.27	13.27	13.36	13.22	13.22	13.33
b22.zt Acrylonitrile	10.91[g]	10.88	10.88	10.80	11.09	11.09	11.06
b27.zt Methylhydrazine	9.30[e]	9.57	9.57	9.80	9.75	9.75	10.00
b34.zt Isocyanomethane	11.30[d]	12.14	12.14	12.12	12.20	12.20	12.31
b40.zt Aziridine	9.80[b]	10.13	10.13	10.19	10.39	10.39	10.41
b46.zt Pyrrole	8.21[g]	8.46	8.47	8.27	8.65	8.65	8.49
b50.zt Pyridine	9.67[h]	9.96	9.96	9.78	10.13	10.13	10.08
b51.zt Pyridazine	9.31[d]	9.91	9.91	9.75	9.96	9.96	10.14
b52.zt Pyrimidine	9.73[d]	10.03	10.03	9.89	10.04	10.04	10.10
b53.zt Pyrazine	9.63[d]	9.68	9.68	9.51	9.76	9.76	9.82
b65.zt Aniline	8.05[d]	8.24	8.24	8.15	8.42	8.43	8.47
b66.zt Phenyl cyanide	9.73[d]	9.91	9.91	9.81	10.16	10.16	10.12

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Table S70: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
c01.zt Water	12.62[b]	12.91	12.91	12.88	13.12	13.12	13.05
c02.zt Methanol	10.96[a]	11.22	11.22	11.17	11.60	11.60	11.66
c03.zt Ethanol	10.63[d]	10.88	10.88	10.85	11.21	11.21	11.28
c16.zt 3-Pentanol	10.25[d]	10.32	10.32	10.27	10.80	10.80	10.87
c52.zt Dimethyl ether	10.04[a]	10.51	10.51	10.43	10.94	10.94	11.03
c53.zt Diethyl ether	9.64[d]	10.23	10.23	10.16	10.60	10.60	10.68
c69.zt Ethylene oxide	10.57[a]	11.31	11.31	11.21	11.79	11.79	11.84
c86.zt Anisole	8.40[d]	8.74	8.74	8.59	9.15	9.15	9.07
c87.zt Furan	8.88[a]	9.03	9.03	8.83	9.45	9.45	9.30
c89.zt Formaldehyde	10.88[b]	11.03	11.03	10.91	11.26	11.26	11.25
c90.zt Acetaldehyde	10.21[a]	10.62	10.62	10.51	10.94	10.94	10.91
c92.zt Butanal	9.84[d]	10.27	10.27	10.14	10.65	10.65	10.62
c99.zt 2-Butenal	9.86[d]	10.30	10.30	10.19	10.63	10.63	10.55
c100.zt Glyoxal	10.59[a]	10.57	10.57	10.50	10.75	10.75	10.72
c101.zt Benzaldehyde	9.72[d]	9.93	9.94	9.79	10.26	10.27	10.15
c103.zt Maleic anhydride	11.11[d]	11.72	11.72	11.68	12.07	12.07	11.99
c104.zt Acetone	9.72[a]	10.31	10.31	10.19	10.67	10.67	10.58
c116.zt Acetylacetone	9.63[d]	10.30	10.30	10.18	10.68	10.69	10.59
c124.zt Formic acid	11.51[a]	11.72	11.72	11.65	12.12	12.12	12.09
c125.zt Acetic acid	10.85[d]	11.33	11.33	11.26	11.76	11.76	11.70
c126.zt Propionic acid	10.60[d]	11.07	11.07	11.00	11.49	11.49	11.44
c131.zt Oxalic acid	11.20[d]	11.41	11.41	11.36	11.62	11.62	11.53
c135.zt Benzoic acid	9.80[e]	10.08	10.08	9.92	10.34	10.34	10.19
c136.zt Methyl formate	11.02[a]	11.24	11.24	11.18	11.70	11.70	11.72
c158.zt Propiolactone	10.60[e]	10.96	10.96	10.89	11.39	11.39	11.36
c162.zt Dimethyl peroxide	9.71[d]	10.71	10.72	10.66	11.16	11.19	11.23
c164.zt Ozone	12.75[f]	12.85	12.85	12.80	13.27	13.27	13.10
c165.zt Carbon monoxide	14.01[a]	13.60	13.60	13.36	13.68	13.68	13.42
c166.zt Carbon dioxide	13.78[a]	13.27	13.27	13.21	13.57	13.57	13.47
c167.zt Ketene	9.64[a]	9.75	9.75	9.59	9.97	9.97	9.82
c205.zt Methyl acetate	10.60[e]	10.90	10.90	10.84	11.39	11.39	11.37
d12.zt Nitromethane	11.30[e]	11.84	11.84	11.84	11.74	11.74	11.55
d24.zt Methyl nitrite	11.00[e]	10.97	10.98	10.94	11.06	11.06	11.07
d31.zt Isocyanic acid	11.60[e]	11.34	11.34	11.44	11.43	11.43	11.54
d37.zt L-Alanine	9.60[i]	9.92	9.92	10.09	10.07	10.07	10.23

a J.W.Robinson (ed.), "Handbook of Spectroscopy", Vol.1, CRC Press, Baton Rouge, 1980. b D.W.Turner, C.Baker, A.D.Baker, and C.R.Brundle, "Molecular Photoelectron Spectroscopy", Wiley-Interscience, London, 1970. c G.Bieri, F.Burger, E.Heilbronner, and J.P.Maier, Helv.Chim.Acta 60, 2213 (1977). d W.G.Mallard and P.J.Linstrom (eds.), "NIST Chemistry WebBook", NIST Standard Reference Data Base 69, National Institute of Standards and Technology, Gaithersburg MD, 20899; http://webbook.nist.gov/chemistry e Taken from the experimental data quoted in: J.J.P.Stewart, J.Comput.Chem. 10, 221 (1989). f Taken from the experimental data quoted in: M.J.S. Dewar, W.Thiel, J.Am.Chem.Soc. 99, 4907 (1977). g S.G.Lias, J.E.Bartmess, J.F.Liebman, J.L.Holmes, R.D.Levin, and W.G.Mallard, "Gas Phase Ion and Neutral Thermochemistry", J.Phys.Chem.Ref.Data 17, Suppl. 1 (1988). h From experimental data of dubious accuracy quoted in: J.J.P.Stewart, J.Comput.Chem. 10, 221 (1991). Original source: G.Dittmer and U.Niemann, Philips J.Res. 37, 1 (1982). i Reference not defined

Table S71: Benchmark Results for the PM7-CHNOF Set. Heats of Formation (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 3 Hydrogen (Geo)	0.0[a]	−3.4	−3.5	−0.1	−0.0	−0.1	0.0
# 588 Nitrogen (Geo)	0.0[a]	2.8	2.6	1.5	2.6	2.2	4.6
# 1029 Oxygen, triplet state (Geo)	0.0[a]	2.0	1.9	3.9	−2.6	−2.8	0.4
# 1030 Oxygen (Singlet)	22.0[a]	29.4	29.3	31.4	25.9	25.7	29.0
# 1532 Fluorine (Geo)	0.0[a]	0.6	0.5	−0.9	−1.7	−1.8	−1.3
# 49 Methylene, singlet (Geo)	99.8[a]	103.9	103.7	98.4	101.3	100.8	96.9
# 50 Methylene, triplet (Geo)	99.8[a]	91.9	91.6	89.6	90.3	89.8	88.7
# 54 Methane (Geo)	−17.9[a]	−19.3	−19.9	−19.3	−18.0	−19.1	−17.8
# 60 Acetylene (Geo)	54.3[a]	54.2	53.6	53.9	54.7	53.7	54.2
# 64 Ethylene (Geo)	12.4[a]	12.9	11.7	12.9	13.9	12.0	13.7
# 69 Ethane (Geo)	−20.0[a]	−21.2	−23.0	−20.8	−20.8	−23.6	−20.0
# 84 Allene (Geo)	45.6[a]	45.9	44.3	45.7	45.5	42.9	45.7
# 85 Cyclopropene (Geo)	66.2[a]	67.4	65.7	66.9	65.5	62.8	65.6
# 88 Propyne (Geo)	44.4[a]	44.5	42.9	44.3	44.1	41.5	44.3
# 93 Cyclopropane (Geo)	12.7[a]	9.9	7.6	10.7	10.1	6.3	11.9
# 96 Propene (Geo)	4.9[a]	4.7	2.3	4.8	5.0	1.1	5.0
# 99 Propane (Geo)	−24.8[a]	−25.5	−28.7	−25.2	−25.4	−30.4	−24.8
# 105 Diacetylene (Geo)	113.0[a]	118.0	116.6	116.8	116.1	113.7	115.9
# 109 Vinylacetylene (Geo)	72.8[a]	71.2	69.0	70.7	71.2	67.6	70.9
# 115 Bicyclobutane (Geo)	51.9[a]	62.0	59.0	61.7	59.9	55.2	61.4
# 117 2-Butyne (Geo)	34.7[a]	35.1	32.4	34.5	33.8	29.6	34.1
# 121 1,3-Butadiene (Geo)	26.0[a]	29.4	26.3	29.3	30.3	25.5	29.8
# 125 1-Butene (Geo)	−0.2[a]	0.1	−3.8	0.1	0.3	−5.7	0.3
# 127 Cyclobutane (Geo)	6.8[a]	3.0	−1.0	2.4	2.9	−3.3	3.3
# 129 Isobutene (Geo)	−4.3[a]	−4.3	−8.2	−4.0	−3.9	−10.0	−3.6
# 131 trans-2-Butene (Geo)	−3.0[a]	−3.8	−7.5	−3.7	−4.0	−9.8	−3.9
# 135 n-Butane (Geo)	−30.4[a]	−30.1	−34.8	−29.9	−30.3	−37.5	−29.8
# 136 Isobutane (Geo)	−32.4[a]	−31.8	−36.7	−31.9	−31.3	−38.8	−31.1
# 146 Cyclopentadiene (Geo)	32.1[a]	33.3	29.3	33.5	32.6	26.2	32.2
# 156 Spiropentane (Geo)	44.3[a]	42.8	38.4	43.6	41.0	34.3	42.7
# 167 Neopentane (Geo)	−40.3[a]	−39.6	−46.4	−40.2	−37.6	−48.1	−38.2
# 173 Benzene (Geo)	19.8[a]	18.8	13.8	19.7	18.5	10.6	18.9
# 175 Fulvene (Geo)	47.5[a]	56.9	52.1	57.3	57.4	49.9	56.9
# 186 Cyclohexene (Geo)	−1.1[a]	0.4	−6.4	0.6	−1.1	−11.6	−0.9
# 194 Cyclohexane (Geo)	−29.5[a]	−27.1	−35.0	−27.2	−28.5	−40.5	−28.5
# 279 Naphthalene (Geo)	36.0[a]	34.8	25.3	35.8	35.7	21.0	35.7
# 324 Biphenyl, for torsion (Torsion angle) (Geo)	43.5[a]	39.0	27.0	40.1	40.1	21.8	40.0
# 48 Methylidyne	142.4[a]	140.0	139.9	136.0	138.1	137.9	134.7
# 53 Methyl, cation	261.0[a]	255.7	255.3	248.1	262.4	261.6	255.0
# 61 Vinyl, cation	266.0[a]	258.5	257.6	252.3	262.9	261.5	258.1
# 62 Vinyl	59.6[a]	67.4	66.6	66.5	66.4	64.9	66.1
# 63 Ethylene, cation	257.0[a]	244.8	243.6	238.9	251.5	249.6	246.3
# 66 Methylmethylene	90.3[a]	74.1	72.9	71.3	72.0	70.1	72.1
# 67 Ethyl, cation	216.0[a]	213.4	211.9	208.1	219.2	216.8	215.3
# 68 Ethyl radical	25.0[a]	24.8	23.3	23.9	24.6	22.3	23.7
# 81 Cyclopropenyl, cation	257.0[a]	259.4	258.0	253.8	262.2	260.0	258.3
# 82 Propynyl, cation	281.0[a]	276.4	275.1	269.6	280.9	278.7	275.2
# 89 Allyl, cation	226.0[a]	223.7	221.5	217.8	230.7	227.3	225.5
# 90 Cyclopropyl, cation	235.0[a]	223.7	221.5	217.8	230.7	227.3	225.5
# 91 Propenyl, cation	237.0[a]	225.7	223.8	220.7	230.2	227.2	227.3
# 92 Allyl	40.0[a]	42.9	40.8	41.9	43.6	40.2	42.1
# 97 i-Propyl radical	16.8[a]	14.3	11.6	14.1	13.4	9.0	13.2
# 111 1,2-Butadiene	38.8[a]	38.1	35.2	38.1	37.6	33.0	38.0
# 113 1-Butyne	39.5[a]	39.5	36.5	39.3	39.2	34.6	39.5
# 118 Cyclobutene	37.5[a]	41.3	38.2	40.2	40.8	35.8	40.0
# 119 Methyl cyclopropene	58.2[a]	59.7	56.7	59.7	57.3	52.7	57.3
# 120 Methylenecyclopropane	47.9[a]	45.0	42.0	45.4	43.7	39.1	44.7
# 122 2-Butenyl, cation	200.0[a]	199.8	196.4	194.2	206.2	200.8	201.7
# 123 Cyclobutyl, cation	213.0[a]	214.4	210.9	209.0	224.9	219.3	220.5
# 126 cis-2-Butene	−1.9[a]	−2.1	−6.1	−2.1	−2.3	−8.5	−2.2
# 133 Isobutyl, cation	176.0[a]	158.2	153.9	155.0	163.5	156.8	162.3
# 134 Isobutyl	4.5[a]	3.2	−1.1	3.6	2.4	−4.2	2.9
# 145 Cyclopentadienyl, anion	21.3[a]	28.2	24.6	32.2	20.9	15.2	23.0
# 148 1,2-Dimethyl cyclopropene	46.4[a]	52.2	48.0	51.6	49.2	42.7	49.0

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 149 1,4-Pentadiene	25.3[a]	25.8	21.2	25.5	26.2	19.2	25.4
# 150 1,cis-3-Pentadiene	19.1[a]	22.4	17.8	22.1	22.8	15.6	22.1
# 151 1,trans-3-Pentadiene	18.1[a]	21.4	16.9	21.5	21.8	14.7	21.4
# 152 Bicyclo(2.1.0)-pentane	37.3[a]	40.1	35.4	39.5	39.0	31.6	39.3
# 153 Cyclopentene	8.3[a]	6.8	1.9	7.0	5.7	−1.9	5.5
# 154 Isoprene	18.0[a]	21.0	16.3	21.3	22.1	14.8	21.9
# 155 Methylene cyclobutane	29.1[a]	25.4	20.8	24.9	25.6	18.3	25.5
# 158 Cyclopentyl, cation	188.0[a]	183.8	178.5	179.4	189.3	181.0	186.8
# 159 2-Methyl-2-butene	−9.9[a]	−11.6	−17.2	−11.5	−11.4	−19.9	−11.3
# 160 cis-2-Pentene	−6.1[a]	−6.9	−11.8	−7.1	−7.2	−15.6	−7.3
# 161 cis-Dimethylcyclopropane	1.3[a]	0.6	−5.0	1.1	0.1	−8.4	1.1
# 162 Cyclopentane	−18.3[a]	−19.7	−25.5	−19.9	−20.8	−29.8	−20.3
# 163 trans-2-Pentene	−7.9[a]	−8.3	−13.5	−8.3	−8.6	−16.6	−8.6
# 164 Neopentyl, anion	3.2[a]	5.3	−0.8	6.3	2.9	−6.3	5.1
# 165 Isopentane	−36.8[a]	−35.9	−42.4	−36.1	−35.5	−45.4	−35.5
# 166 n-Pentane	−35.1[a]	−34.7	−40.8	−34.7	−35.2	−44.6	−34.9
# 171 C6H5 radical	74.3[a]	71.5	67.0	72.9	70.4	63.2	72.4
# 176 (E)-1,3,5-Hexatriene	40.1[a]	44.8	39.7	44.5	45.8	37.9	44.7
# 177 (Z)-1,3,5-Hexatriene	41.1[a]	46.7	41.5	46.8	47.7	39.5	47.0
# 178 1,3-Cyclohexadiene	25.4[a]	25.9	20.0	26.5	24.8	15.6	24.9
# 179 1,4-Cyclohexadiene	25.0[a]	26.8	21.0	26.8	24.8	15.8	24.6
# 180 1,2-Dimethylcyclobutene	19.8[a]	21.4	15.3	21.3	20.9	11.7	21.2
# 181 1,5-Hexadiene	20.1[a]	21.0	14.9	20.6	21.2	11.9	20.2
# 182 1-Methyl cyclopentene	−1.0[a]	−2.8	−9.2	−3.0	−3.7	−13.7	−3.7
# 183 3-Methyl cyclopentene	2.3[a]	−0.2	−6.8	−0.3	−0.7	−10.9	−0.9
# 184 4-Methyl cyclopentene	3.5[a]	−0.4	−7.1	−0.6	−1.1	−11.3	−1.3
# 185 Bicyclopropyl	30.9[a]	30.7	24.7	30.9	30.2	21.0	31.9
# 188 Cyclohexyl, cation	177.0[a]	171.1	163.7	166.2	179.5	168.0	176.9
# 189 1-Hexene	−10.1[a]	−9.1	−16.0	−9.4	−9.4	−19.9	−9.9
# 190 2,3-Dimethyl-1-butene	−15.7[a]	−14.8	−22.3	−14.9	−13.5	−25.0	−13.9
# 191 2,3-Dimethyl-2-butene	−16.8[a]	−19.8	−27.2	−19.7	−18.9	−30.2	−18.9
# 192 (Z)-3-Methyl-2-pentene	−14.8[a]	−15.0	−22.4	−15.0	−14.6	−25.8	−14.6
# 193 4-Methyl-1-pentene	−11.8[a]	−10.8	−18.2	−11.5	−10.3	−21.4	−11.3
# 196 2,2-Dimethyl butane	−44.3[a]	−42.8	−51.6	−43.4	−40.7	−54.0	−41.5
# 197 2,3-Dimethyl butane	−42.5[a]	−41.1	−49.7	−41.7	−39.8	−52.8	−40.4
# 198 2-Methyl pentane	−41.7[a]	−40.4	−48.5	−40.9	−40.3	−52.5	−40.6
# 199 3-Methyl pentane	−41.1[a]	−39.9	−48.2	−40.2	−39.5	−52.0	−39.9
# 200 n-Hexane	−39.9[a]	−39.2	−46.9	−39.4	−40.0	−51.6	−39.9
# 203 Benzyl, cation	212.0[a]	214.6	208.4	210.2	221.7	212.0	217.8
# 204 Tropylium, cation	209.0[a]	206.2	200.0	202.4	211.2	201.4	208.9
# 205 Cycloheptatriene	43.2[a]	46.7	39.8	46.7	46.1	35.4	45.8
# 206 Norbornadiene	59.7[a]	51.8	44.8	51.4	52.0	41.1	50.6
# 207 Toluene	12.0[a]	9.5	2.9	9.7	9.6	−0.6	9.9
# 208 1,2-Dimethyl cyclopentene	−9.9[a]	−12.1	−20.3	−11.7	−12.5	−25.0	−12.1
# 209 1-Ethyl cyclopentene	−6.0[a]	−6.9	−15.1	−6.7	−7.8	−20.2	−7.3
# 210 1-Methyl cyclohexene	−19.4[a]	−9.2	−17.8	−9.2	−10.3	−23.3	−10.3
# 211 Norbornane	−12.4[a]	−12.5	−21.5	−13.3	−12.4	−26.3	−13.2
# 212 1,1-Dimethyl cyclopentane	−33.0[a]	−34.4	−44.3	−35.8	−34.4	−49.1	−34.8
# 213 1,2-cis-Dimethyl cyclopentane	−31.0[a]	−31.7	−41.6	−32.1	−31.9	−46.6	−31.8
# 214 1,2-trans-Dimethyl cyclopentane	−32.7[a]	−33.9	−43.4	−34.5	−34.1	−48.5	−34.4
# 215 1,3-cis-Dimethyl cyclopentane	−31.9[a]	−33.7	−43.1	−34.8	−34.1	−48.2	−34.8
# 216 1-Heptene	−14.9[a]	−13.7	−22.1	−14.2	−14.2	−27.0	−14.9
# 217 Ethyl cyclopentane	−30.4[a]	−31.1	−40.5	−31.4	−32.0	−46.1	−31.8
# 218 Methyl-cyclohexane	−37.0[a]	−33.9	−43.7	−34.7	−34.8	−49.5	−35.6
# 219 2,2,3-Trimethyl butane	−48.7[a]	−47.5	−58.6	−48.5	−44.4	−60.9	−45.8
# 220 2,2-Dimethyl pentane	−49.3[a]	−47.3	−57.7	−48.2	−45.5	−61.1	−46.6
# 221 2,3-Dimethyl pentane	−47.6[a]	−44.8	−55.4	−45.6	−43.8	−59.5	−44.7
# 222 2,4-Dimethyl pentane	−48.3[a]	−44.7	−54.9	−46.3	−44.2	−59.4	−45.9
# 223 2-Methyl hexane	−46.6[a]	−45.0	−54.6	−45.6	−45.1	−59.6	−45.7
# 224 3,3-Dimethyl pentane	−48.2[a]	−45.7	−56.5	−46.3	−43.5	−59.6	−44.4
# 225 3-Ethyl pentane	−45.3[a]	−42.5	−52.8	−43.2	−42.5	−57.8	−43.3
# 226 3-Methyl hexane	−46.0[a]	−44.4	−54.3	−45.0	−44.4	−59.1	−45.0
# 227 n-Heptane	−44.8[a]	−43.8	−53.0	−44.2	−44.8	−58.7	−45.0
# 228 Cubane	148.7[a]	144.6	137.2	141.2	146.4	134.8	144.1
# 229 Cyclooctatetraene	70.7[a]	75.2	67.2	74.3	73.9	61.6	72.1

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 230 Styrene	35.3[a]	34.7	27.3	35.4	35.6	24.1	35.4
# 231 Ethylbenzene	7.2[a]	4.8	−3.5	5.4	5.0	−7.7	5.1
# 232 m-Xylene	4.1[a]	0.2	−7.9	0.3	0.7	−11.9	0.9
# 233 o-Xylene	4.6[a]	0.3	−8.1	0.9	1.3	−11.7	1.4
# 234 p-Xylene	4.3[a]	0.3	−7.8	0.4	0.8	−11.8	1.0
# 235 1,5-Cyclooctadiene	13.7[a]	24.8	14.7	23.8	23.2	7.9	21.6
# 236 4-Vinyl cyclohexene	16.6[a]	18.7	9.2	18.1	18.3	3.9	17.0
# 237 1-Octyne	19.3[a]	20.9	11.9	20.0	19.8	6.2	19.2
# 238 2,5-Dimethyl 2,4-hexadiene	−4.6[a]	−3.9	−13.4	−3.7	−3.4	−17.7	−3.6
# 239 2-Octyne	15.2[a]	16.0	7.5	15.6	14.2	1.2	14.6
# 240 3,4-Dimethyl-(E,E)-2,4-hexadiene	−0.5[a]	−2.6	−12.5	−2.8	−1.5	−16.4	−2.1
# 241 3,4-Dimethyl-(E,Z)-2,4-hexadiene	0.7[a]	−2.7	−12.8	−3.1	−1.8	−16.8	−2.5
# 242 3,4-Dimethyl-(Z,Z)-2,4-hexadiene	−0.9[a]	−3.1	−13.5	−3.8	−2.1	−17.4	−3.1
# 243 3-Octyne	14.9[a]	15.5	7.1	15.3	14.2	1.3	14.8
# 244 4-Octyne	14.4[a]	15.2	6.8	14.4	14.0	1.1	14.1
# 245 Bicyclo(2.2.2)-octane	−24.1[a]	−22.2	−33.6	−22.8	−23.4	−40.5	−23.9
# 246 Bicyclo-2,2,2-octane	−23.7[a]	−22.2	−33.6	−22.3	−23.4	−40.5	−23.3
# 247 1-Octene	−19.8[a]	−18.3	−28.2	−18.9	−19.1	−34.0	−20.0
# 248 Ethylcyclohexane	−41.0[a]	−38.0	−49.5	−38.9	−38.9	−56.2	−40.0
# 249 2,2,3,3-Tetramethyl butane	−54.0[a]	−53.4	−67.1	−54.9	−48.1	−68.3	−50.3
# 250 2,2,3,3-Tetramethylbutane	−53.8[a]	−53.4	−67.0	−55.4	−48.1	−68.3	−50.9
# 251 2,2,3-Trimethyl pentane	−52.6[a]	−51.3	−64.3	−52.6	−48.3	−67.5	−50.1
# 252 2,2,4-Trimethyl pentane	−53.6[a]	−51.6	−64.2	−53.2	−49.4	−68.1	−51.4
# 253 2,2-Dimethyl hexane	−53.7[a]	−51.8	−63.8	−53.0	−50.3	−68.2	−51.7
# 254 2,3,3-Trimethyl pentane	−51.7[a]	−50.2	−63.3	−51.2	−46.9	−66.4	−48.5
# 255 2,3,4-Trimethyl pentane	−52.0[a]	−48.3	−61.1	−49.4	−46.7	−65.6	−48.1
# 256 2,3-Dimethyl hexane	−51.1[a]	−49.4	−61.5	−50.4	−48.6	−66.6	−49.8
# 257 2,4-Dimethyl hexane	−52.4[a]	−50.1	−62.1	−51.3	−49.4	−67.2	−50.9
# 258 2,5-Dimethyl hexane	−53.2[a]	−50.7	−62.4	−51.8	−50.2	−67.6	−51.5
# 259 2-Methyl heptane	−51.5[a]	−49.5	−60.7	−50.4	−50.0	−66.7	−50.8
# 260 3,3-Dimethyl hexane	−52.6[a]	−50.2	−62.6	−51.1	−48.3	−66.7	−49.6
# 261 3,4-Dimethyl hexane	−50.9[a]	−48.1	−60.3	−48.9	−47.0	−65.2	−48.2
# 262 3-Ethyl hexane	−50.4[a]	−47.0	−58.9	−48.1	−47.3	−64.9	−48.4
# 263 3-Ethyl-2-methyl pentane	−50.5[a]	−47.3	−59.7	−48.4	−46.4	−64.8	−47.8
# 264 3-Ethyl-3-methyl pentane	−51.4[a]	−46.7	−59.7	−47.4	−44.5	−63.7	−45.6
# 265 3-Methyl heptane	−50.8[a]	−49.0	−60.4	−49.8	−49.2	−66.3	−50.1
# 266 4-Methyl heptane	−50.7[a]	−48.9	−60.4	−49.8	−49.2	−66.3	−50.1
# 267 n-Octane	−49.9[a]	−48.3	−59.0	−48.9	−49.7	−65.8	−50.1
# 270 alpha-Methyl styrene	28.3[a]	25.8	16.5	26.5	27.1	13.0	27.0
# 271 Cyclopropyl benzene	36.0[a]	34.8	25.8	35.8	35.1	21.3	36.1
# 272 1,3,5-Trimethyl cyclohexane	−51.5[a]	−47.5	−61.0	−49.6	−47.3	−67.4	−49.7
# 273 cis-cis-trans-1,3,5-Trimethyl cyclohexane	−49.4[a]	−45.8	−59.6	−47.5	−45.4	−66.0	−47.5
# 274 3,3-Diethylpentane	−55.4[a]	−51.5	−66.7	−52.6	−48.8	−71.2	−50.5
# 275 n-Nonane	−54.7[a]	−52.9	−65.1	−53.7	−54.5	−72.9	−55.1
# 278 Azulene	73.5[a]	83.4	74.0	82.7	82.5	68.1	81.6
# 281 1,4-Dicyclopropylbuta-1,3-diyne	134.3[a]	148.8	141.1	148.4	145.3	133.4	148.5
# 282 1-Butynl benzene	59.4[a]	60.3	51.4	60.8	59.8	46.1	60.8
# 283 2a,4a,6a,6b-Tetrahydrocyclopentapentalene	53.1[a]	52.0	40.9	51.2	52.7	35.7	50.8
# 284 Bulvalene	79.8[a]	84.5	73.3	85.5	83.5	66.5	84.3
# 285 Diisopropenyldiacetylene	118.1[a]	129.8	121.9	128.9	127.5	115.4	128.6
# 286 Tricyclo[6.2.0.0]deca-1(8),2,6-triene	74.0[a]	73.7	64.2	73.2	74.2	59.6	74.0
# 287 1,2,6,7-Cyclodecatetraene	85.1[a]	87.9	76.4	85.4	85.1	67.8	82.8
# 288 Dispiro[2.2.2.2]deca-4,9-diene	72.3[a]	71.3	60.5	71.4	72.0	55.6	72.5
# 289 Tetralin	6.2[a]	3.2	−8.3	3.5	2.9	−14.7	2.6
# 290 (1-Methylpropyl) benzene	−4.2[a]	−5.7	−17.8	−5.7	−4.7	−22.9	−5.5
# 291 (2-Methylpropyl) benzene	−5.2[a]	−6.1	−18.3	−6.5	−5.4	−23.7	−6.6
# 292 1,2,3,4-Tetramethyl benzene	−8.6[a]	−15.3	−27.6	−14.7	−12.7	−31.3	−12.6
# 293 1,2,3,4-Tetramethylfulvene	19.9[a]	18.9	7.0	19.5	20.9	3.0	21.0
# 294 1,2,3,5-Tetramethyl benzene	−10.3[a]	−16.7	−28.7	−16.9	−14.6	−32.8	−14.6
# 295 1,2,4,5-Tetramethyl benzene	−11.3[a]	−17.8	−29.9	−17.6	−15.7	−33.9	−16.0
# 296 tert-Butyl benzene	−5.4[a]	−7.8	−20.5	−7.9	−4.8	−23.8	−5.8
# 297 Tetrahydrotriquinacene	3.0[a]	−2.0	−15.3	−3.0	−2.2	−22.1	−3.2
# 298 1,2,3,4,5-Pentamethyl-1,3-cyclopentadiene	−5.9[a]	−10.3	−23.4	−10.3	−8.7	−28.2	−9.2
# 299 Adamantane	−31.9[a]	−30.4	−45.6	−31.5	−30.2	−53.1	−32.0
# 300 Camphene	−6.8[a]	−6.1	−20.7	−7.8	−2.4	−24.2	−5.0

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 301 Perhydrotriquinacene	-24.5^{a}	−28.5	−43.0	−29.6	−29.1	−50.6	−29.7
# 302 1-Methyl-4-(1-methylethyl)-cyclohexene	-26.5^{a}	−20.9	−36.0	−22.1	−21.2	−43.6	−22.9
# 303 4-Methyl-1-(1-methylethyl)-cyclohexene	-26.6^{a}	−26.5	−40.7	−27.6	−26.1	−47.3	−27.7
# 304 cis-Decalin	-40.5^{a}	−29.4	−44.6	−30.5	−31.2	−53.8	−32.2
# 305 Spiro(4-5)decane	-34.7^{a}	−36.5	−51.7	−37.9	−36.7	−59.4	−38.2
# 306 trans-Decalin	-43.5^{a}	−38.5	−53.6	−40.5	−39.8	−62.3	−42.3
# 307 (E)-2,2,5,5-Tetramethyl-3-hexene	-39.9^{a}	−39.7	−54.8	−41.8	−35.3	−57.6	−38.1
# 308 (Z)-2,2,5,5-Tetramethyl-3-hexene	-30.3^{a}	−29.6	−45.6	−31.5	−25.4	−49.0	−28.0
# 309 1-Decene	-29.8^{a}	−27.4	−40.3	−28.4	−28.7	−48.2	−30.2
# 310 Butyl cyclohexane	-51.0^{a}	−47.1	−61.7	−48.5	−48.6	−70.4	−50.2
# 311 Pentyl cyclopentane	-45.2^{a}	−44.8	−58.8	−45.7	−46.5	−67.4	−47.6
# 312 2,2,5,5-Tetramethylhexane	-68.0^{a}	−64.3	−80.8	−66.6	−60.5	−84.7	−63.5
# 313 3,3,4,4-Tetramethylhexane	-63.5^{a}	−58.3	−76.2	−59.9	−52.6	−78.9	−55.3
# 314 n-Decane	-59.7^{a}	−57.5	−71.2	−58.4	−59.3	−79.9	−60.2
# 315 Pentamethylbenzene	-16.1^{a}	−23.2	−37.4	−22.6	−19.9	−41.3	−20.0
# 316 1,1,4-Trimethylcycloheptane	-50.3^{a}	−42.5	−61.0	−45.4	−43.0	−70.2	−46.6
# 317 Hexyl cyclopentane	-50.1^{a}	−49.3	−64.8	−50.4	−51.3	−74.4	−52.1
# 318 Pentyl cyclohexane	-55.9^{a}	−51.6	−67.8	−53.3	−53.4	−77.5	−55.3
# 319 Undecane	-64.6^{a}	−62.0	−77.3	−63.2	−64.2	−87.0	−65.3
# 320 Acenaphthylene	61.6^{a}	67.0	55.6	68.0	67.9	50.3	67.5
# 321 Biphenylene	100.5^{a}	103.7	93.3	105.4	103.2	87.1	104.4
# 322 Acenaphthene	37.4^{a}	33.9	21.6	34.7	34.3	15.3	34.2
# 325 Hexamethylbenzene	-18.5^{a}	−28.0	−44.5	−27.0	−23.7	−48.4	−23.7
# 326 Hexylcyclohexane	-60.8^{a}	−56.2	−73.9	−58.0	−58.2	−84.6	−60.4
# 327 n-Duodecane	-69.2^{a}	−66.6	−83.4	−67.9	−69.0	−94.1	−70.4
# 331 Fluorene	41.8^{a}	40.7	27.6	41.6	41.3	21.3	41.2
# 333 Tri-t-butylmethane	-56.2^{a}	−49.7	−75.9	−52.6	−41.3	−79.2	−46.1
# 334 Tridecane	-74.4^{a}	−71.1	−89.4	−72.7	−73.8	−101.2	−75.4
# 335 Anthracene	55.2^{a}	55.5	41.4	56.4	57.5	35.8	57.0
# 336 Diphenylethyne	92.0^{a}	95.6	83.2	96.4	95.7	76.6	96.5
# 337 Phenanthrene	49.5^{a}	46.8	32.4	48.0	49.1	27.0	48.8
# 338 9,10-Dihydro-phenanthrene	37.1^{a}	31.6	16.1	32.4	33.2	9.6	32.5
# 339 9-Methyl-9H-fluorene	35.4^{a}	33.8	18.5	34.3	35.4	12.4	34.7
# 340 Octalene	131.8^{a}	134.3	117.9	131.6	133.3	108.9	129.0
# 341 Stilbene	53.4^{a}	55.8	41.8	56.8	56.9	35.4	56.2
# 342 1,2,3,4-Tetrahydrophenanthrene	22.1^{a}	20.2	3.7	20.7	21.4	−3.5	20.9
# 343 4,4'-Dimethylbiphenyl	26.6^{a}	20.5	5.2	20.1	22.4	−0.7	21.9
# 344 Bibenzyl	32.4^{a}	30.3	15.1	30.8	30.6	7.5	29.6
# 346 1,4,5,8-Tetramethynaphthalene	19.5^{a}	11.2	−6.5	12.1	15.5	−11.1	15.3
# 347 1,2,3,4,5,6,7,8-Octahydro-anthracene	-8.9^{a}	−12.0	−30.3	−12.5	−12.5	−39.9	−13.7
# 348 Diadamantane	-34.9^{a}	−35.4	−58.3	−38.1	−33.6	−67.7	−37.9
# 349 1,3,5,7-Tetramethyladamantane	-68.0^{a}	−64.8	−89.0	−69.6	−58.6	−94.2	−65.3
# 350 (E)-3,4-Di-tert-butyl-3-hexene	-40.2^{a}	−43.6	−69.8	−46.0	−35.2	−73.2	−39.5
# 351 Cyclotetradecane	-57.2^{a}	−50.8	−74.5	−54.9	−55.0	−89.1	−59.9
# 352 n-Nonylcyclopentane	-64.8^{a}	−63.0	−83.1	−64.7	−65.8	−95.7	−67.3
# 353 Octylcyclohexane	-70.7^{a}	−65.3	−86.1	−67.5	−67.9	−98.8	−70.5
# 354 3,3,4,4-Tetraethylhexane	-63.5^{a}	−54.0	−82.1	−56.6	−48.4	−88.7	−52.7
# 355 Octamethylhexane	-59.3^{a}	−58.8	−87.9	−62.0	−46.4	−88.6	−51.8
# 356 Tetradecane	-79.4^{a}	−75.7	−95.5	−77.4	−78.7	−108.3	−80.5
# 357 4-Methylphenanthrene	46.8^{a}	43.3	26.7	44.4	46.5	21.3	46.2
# 358 1-Methyldiadamantane	-39.8^{a}	−42.3	−67.9	−45.8	−38.4	−76.3	−43.9
# 359 3-Methyladamantane	-37.6^{a}	−40.9	−66.2	−44.2	−38.2	−75.6	−43.4
# 360 4-Methyldiadamantane	-43.5^{a}	−44.0	−69.2	−47.7	−40.7	−78.0	−46.2
# 361 6-(1,1-dimethylethyl)-2,3-dihydro-1,1-dimethyl-1H-Indene	-24.9^{a}	−32.1	−53.8	−33.8	−27.0	−59.0	−29.8
# 362 n-Nonylcyclohexane	-75.6^{a}	−69.9	−92.1	−72.3	−72.8	−105.8	−75.6
# 363 Pentadecane	-84.8^{a}	−80.3	−101.6	−82.1	−83.5	−115.3	−85.6
# 364 Fluoranthene	69.8^{a}	68.7	52.5	69.9	70.4	45.7	70.2
# 365 Pyrene	53.9^{a}	54.4	37.6	55.4	57.7	32.1	57.1
# 366 2,7-Dimethylphenanthrene	34.2^{a}	28.2	10.5	29.0	31.2	4.3	30.6
# 367 4,5,9,10-Tetrahydropyrene	21.6^{a}	23.8	4.8	24.1	25.4	−3.1	24.2
# 368 9,10-Dimethylphenanthrene	40.0^{a}	32.9	14.3	34.5	36.8	8.7	36.8
# 369 (2.2)Metaparacyclophane	52.2^{a}	43.9	20.7	39.1	45.5	11.3	38.0
# 370 [2.2]Metacyclophane	40.7^{a}	45.1	22.4	41.0	45.8	12.5	38.7
# 371 [2.2]Paracyclophane	58.5^{a}	49.6	25.9	43.7	50.6	15.8	41.7
# 372 1,2,3,6,7,8-Hexahydropyrene	9.7^{a}	11.6	−9.8	10.0	12.3	−19.7	9.1

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Table S71: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 373 Tricyclo[8.2.2.2]-hexadecane	−36.4[a]	−9.7	−39.7	−12.8	−14.7	−57.9	−18.8
# 374 1-Hexadecene	−59.4[a]	−54.7	−76.8	−56.9	−57.8	−90.7	−60.6
# 375 Decylcyclohexane	−80.5[a]	−74.4	−98.2	−77.0	−77.6	−112.9	−80.7
# 376 n-Undecylcyclopentane	−74.7[a]	−72.1	−95.2	−74.2	−75.5	−109.8	−77.5
# 377 n-Dodecylcyclopentane	−79.6[a]	−76.7	−101.3	−78.9	−80.3	−116.9	−82.6
# 378 Undecylcyclohexane	−85.4[a]	−79.0	−104.3	−81.8	−82.4	−120.0	−85.8
# 379 Heptadecane	−94.2[a]	−89.4	−113.7	−91.6	−93.2	−129.5	−95.7
# 380 p-Terphenyl	66.6[a]	59.2	40.1	60.4	61.8	32.8	61.0
# 381 2,5-Diphenyl-1,5-hexadiene	68.0[a]	62.7	40.4	61.6	65.7	33.1	62.4
# 382 3,4,5,6-Tetramethylphenanthrene	38.3[a]	22.9	−0.4	22.4	28.8	−5.9	26.5
# 383 [3.3]Paracyclophane	30.9[a]	24.0	−3.9	17.2	24.0	−16.5	14.6
# 384 1,1'-(1,1,2,2-Tetramethyl-1,2-ethanediyl)bis-benzene	13.7[a]	9.4	−17.7	7.0	17.3	−22.4	12.0
# 385 Dodecylcyclohexane	−90.4[a]	−83.6	−110.4	−86.5	−87.3	−127.1	−90.8
# 386 n-Tridecylcyclopentane	−84.6[a]	−81.3	−107.4	−83.7	−85.1	−124.0	−87.6
# 387 1,1,2,2-Tetra-t-butylethane	−59.9[a]	−50.3	−89.9	−56.6	−40.0	−96.5	−49.2
# 388 Octadecane	−99.1[a]	−93.9	−119.8	−96.4	−98.0	−136.6	−100.8
# 392 2,6-Diphenyl-1,6-heptadiene	61.9[a]	58.7	35.6	58.0	61.3	27.3	58.2
# 393 n-Tetradecylcyclopentane	−89.5[a]	−85.8	−113.5	−88.4	−90.0	−131.1	−92.7
# 394 n-Tridecylcyclohexane	−95.3[a]	−88.1	−116.5	−91.3	−92.1	−134.2	−95.9
# 395 Nonadecane	−104.0[a]	−98.5	−125.9	−101.1	−102.9	−143.7	−105.9
# 396 9,10-Dihydro-9,10[1',2']benzanthracene	76.9[a]	65.3	42.3	65.7	68.6	34.1	65.7
# 397 3,9-Dimethylbenz[a]anthracene	45.1[a]	46.7	24.3	47.4	50.9	17.0	49.6
# 398 5,6-Dimethyl chrysene	62.7[a]	52.2	28.3	53.4	57.8	21.8	56.7
# 399 9,10-Dimethyl-1,2-benzanthracene	66.3[a]	57.8	33.8	59.0	63.4	27.4	62.5
# 400 1,3,5-Tri-tert-butyl pentalene	3.4[a]	9.2	−21.0	5.7	18.1	−26.0	12.8
# 401 Hexacyclopropylethane	111.5[a]	121.5	86.6	117.3	128.3	78.6	126.2
# 402 Tetra-tert-butyltetrahedrane	6.2[a]	45.7	9.3	39.0	47.2	−4.1	39.8
# 403 Meso-3,4-dicyclohexyl-2,5-dimethylhexane	−71.6[a]	−70.4	−108.8	−77.7	−69.2	−124.1	−78.7
# 404 Tetradecylcyclohexane	−100.2[a]	−92.7	−122.5	−96.0	−96.9	−141.2	−101.0
# 405 Eicosane	−108.9[a]	−103.1	−132.0	−105.9	−107.7	−150.7	−110.9
# 406 1,8-Paracyclophane	6.9[a]	11.0	−20.5	5.6	11.0	−34.4	3.3
# 407 Hexadecylcyclopentane	−99.3[a]	−93.5	−124.7	−96.4	−98.1	−144.3	−101.3
# 408 Pentadecylcyclohexane	−105.1[a]	−96.1	−127.8	−99.5	−100.6	−147.4	−104.7
# 410 1,1'-Diphenyl-1,1'-bicyclopentyl	26.6[a]	20.3	−14.8	15.5	26.3	−24.5	19.0
# 411 DL-3,4-di-1-cyclohexen-1-yl-2,2,5,5-tetramethyl hexane	−50.4[a]	−42.0	−84.8	−51.6	−34.5	−95.6	−47.4
# 412 Meso-3,4-di-1-cyclohexen-1-yl-2,2,5,5-tetramethyl hexane	−58.4[a]	−41.0	−83.8	−50.5	−33.6	−94.7	−46.4
# 413 n-Hexadecylcyclohexane	−110.1[a]	−101.8	−134.7	−105.5	−106.6	−155.4	−111.1
# 414 p-Quaterphenyl	91.4[a]	79.4	53.2	80.7	83.4	43.9	81.9
# 415 1,1'-Diphenyl-1,1'-bicyclohexyl	10.4[a]	7.7	−32.5	1.6	14.5	−43.6	4.6
# 416 6,6'-Paracyclophane	−18.5[a]	−5.2	−40.7	−10.0	−6.2	−57.9	−13.4
# 418 Tetraphenylmethane	93.9[a]	82.9	49.4	79.9	90.6	42.5	83.3
# 419 9,9'-Bi-9H-fluorene	95.4[a]	89.3	56.7	86.2	92.9	45.3	86.8
# 420 1,1,1,2-Tetraphenylethane	87.3[a]	80.6	44.6	76.3	87.4	35.0	78.5
# 421 1,1,2,2-Tetraphenylethane	85.4[a]	80.7	45.7	76.2	84.5	33.9	76.0
# 422 Pentacyclo hexacosa nonane	78.0[a]	74.6	30.7	62.1	78.0	15.0	60.3
# 423 2,3-Dimethyl-2,3-bis(4-t-butylphenyl)butane	−33.3[a]	−43.5	−86.4	−48.5	−29.2	−91.6	−37.8
# 424 11-n-butyl docosane	−141.8[a]	−129.1	−168.8	−134.0	−134.4	−192.8	−140.1
# 425 5-n-butyl docosane	−140.4[a]	−129.1	−168.8	−134.0	−134.3	−192.8	−140.1
# 426 9,9'-Dimethyl-9,9'-bifluorene	94.3[a]	75.6	36.4	70.9	84.8	27.9	75.9
# 427 1,1-Diphenyl-1,1-bicyclooctyl	16.6[a]	27.4	−23.8	18.3	30.4	−42.6	17.0
# 428 11-Decyl heneicosane	−167.3[a]	−153.2	−200.3	−158.8	−159.6	−229.0	−166.4
# 429 2,4,5,7-Tetramethyl-4,5-bis(4-t-butylphenyl) octane	−60.6[a]	−63.5	−121.4	−73.7	−47.6	−130.7	−63.4
# 430 Dotriacontane	−166.5[a]	−157.8	−204.9	−162.9	−165.7	−235.7	−171.8
# 431 4,5-Dipropyl-4,5-bis(4-t-butylphenyl) octane	−50.8[a]	−65.5	−127.9	−76.4	−50.8	−139.9	−66.4
# 432 5,6-Dibutyl-5,6-bis(4-t-butylphenyl) decane	−58.6[a]	−77.5	−147.6	−90.1	−63.8	−163.1	−81.1
# 433 5,6-Dibutyl-5,6-bis(4-tert-butylphenyl)decane	−58.6[a]	−70.2	−142.5	−84.4	−70.0	−159.3	−76.2
# 447 Hydrogen cyanide (Geo)	32.3[a]	26.1	25.7	25.5	25.3	24.7	25.4
# 454 Methylamine (Geo)	−5.5[a]	−4.1	−5.6	−6.3	−5.8	−8.1	−5.6
# 459 Acetonitrile (Geo)	17.7[a]	17.5	16.2	17.3	15.3	13.2	15.3
# 460 Methyl isocyanide (Geo)	39.1[a]	38.3	36.9	37.6	26.7	24.4	21.8
# 462 Ethyleneimine (Azirane) (Geo)	30.2[a]	36.3	34.3	36.0	35.4	32.3	38.0
# 467 Dimethylamine (Geo)	−4.4[a]	−5.1	−7.9	−4.2	−2.2	−6.5	−3.2
# 472 Acrylonitrile (Geo)	44.1[a]	45.6	43.6	45.3	43.7	40.5	43.6
# 476 Trimethylamine (Geo)	−5.7[a]	−8.0	−12.4	−4.5	−0.1	−6.7	−2.9
# 484 Pyrrole (Geo)	25.9[a]	33.7	30.2	35.6	32.0	26.3	33.9

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 493 Pyridine (Geo)	34.6[a]	30.8	26.3	33.5	29.4	22.3	31.8
# 689 s-Triazine (Geo)	54.0[a]	59.7	56.1	62.7	55.6	49.8	54.6
# 449 Hydrogen isocyanide	43.5[a]	42.9	42.5	37.1	26.8	26.1	22.0
# 450 CH2-NH2, cation	178.0[a]	174.9	173.7	172.9	173.4	171.6	175.4
# 451 CH2-NH2, radical	0.0[a]	29.3	28.2	28.0	25.2	23.3	27.3
# 452 CH3-NH.	37.0[a]	41.9	40.8	40.0	39.0	37.1	36.5
# 453 CH3NH, anion	30.5[a]	31.9	30.8	27.1	25.6	23.8	24.5
# 464 Dimethyl nitrogen, anion	24.7[a]	17.4	15.1	15.7	17.1	13.4	14.6
# 466 Ethylamine	−11.4[a]	−8.9	−11.7	−10.9	−12.1	−16.5	−11.9
# 473 Ethyl cyanide	12.1[a]	12.3	9.6	12.1	10.2	6.0	10.5
# 474 Cyclopropylamine	18.4[a]	22.1	18.6	19.8	19.5	14.1	20.8
# 475 Isopropylamine	−20.0[a]	−15.0	−19.5	−18.5	−18.3	−25.1	−18.6
# 477 n-Propylamine	−16.8[a]	−13.5	−17.8	−15.6	−16.9	−23.5	−16.8
# 481 (E)-2-Butenenitrile	33.6[a]	35.7	32.5	35.4	33.6	28.5	33.6
# 482 (Z)-2-Butenenitrile	32.0[a]	36.4	33.0	36.2	34.2	28.8	34.3
# 483 3-Butenenitrile	37.7[a]	39.0	35.6	38.5	37.0	31.8	36.5
# 486 Butanenitrile	7.4[a]	7.5	3.3	7.1	5.3	−1.1	5.4
# 487 Isobutane nitrile	5.6[a]	5.1	0.8	4.6	3.5	−3.1	3.6
# 488 Pyrrolidine	−0.8[a]	0.0	−5.3	0.6	0.4	−7.8	−0.0
# 489 2-Butylamine	−25.4[a]	−19.4	−25.5	−23.1	−22.7	−32.0	−23.3
# 490 2-Methyl-1-propylamine	−23.6[a]	−19.5	−25.7	−23.4	−21.7	−31.0	−22.6
# 491 N-Butylamine	−22.7[a]	−18.0	−23.7	−21.6	−20.9	−29.7	−21.5
# 492 t-Butylamine	−28.9[a]	−22.3	−28.7	−27.4	−24.6	−34.3	−25.6
# 495 N-Methyl pyrrole	24.6[a]	31.1	26.0	35.8	33.5	25.6	33.6
# 496 1,2,3,6-Tetrahydropyridine	7.1[a]	20.8	14.4	22.0	20.6	10.8	19.8
# 497 2-Cyanobutane	0.6[a]	0.6	−5.4	−0.0	−0.8	−9.9	−1.0
# 498 Butyl cyanide	2.7[a]	2.9	−2.8	2.3	0.5	−8.1	0.4
# 499 t-Butylnitrile	−0.8[a]	−3.7	−10.0	−4.6	−3.9	−13.3	−4.3
# 500 Cyclopentylamine	−13.1[a]	−9.9	−17.0	−14.6	−13.8	−24.6	−14.2
# 501 Piperidine	−11.3[a]	−6.7	−14.1	−5.7	−7.2	−18.5	−8.2
# 502 N-Methyl-n-butylamine	−25.9[a]	−19.2	−26.4	−19.7	−17.7	−28.6	−19.5
# 503 1-Cyclopentenecarbonitrile	37.4[a]	37.3	31.3	37.1	34.7	25.6	35.3
# 504 2-Cyclopentenecarbonitrile	33.9[a]	37.4	31.3	36.8	35.0	25.6	34.8
# 505 2-Methyl pyridine	23.6[a]	22.8	16.8	23.5	20.9	11.5	22.5
# 506 3-Methyl pyridine	24.8[a]	21.2	15.2	23.4	20.3	10.8	22.1
# 507 4-Methyl pyridine	24.8[a]	21.2	15.1	23.2	20.4	10.9	21.9
# 508 Aniline	20.8[a]	25.2	19.0	22.0	22.3	12.7	22.0
# 509 2,5-Dimethyl-1H-pyrrole	9.5[a]	18.3	11.8	18.1	14.8	4.7	16.5
# 510 Cyclopentanecarbonitrile	11.7[a]	9.8	3.3	9.2	8.0	−2.7	7.7
# 511 2-Methylpiperidine	−20.2[a]	−13.3	−22.4	−16.5	−13.3	−27.0	−16.1
# 512 Cyclohexamethylenimine	−10.8[a]	−5.0	−14.5	−4.8	−7.0	−21.3	−8.6
# 513 Cyclohexanamine	−25.1[a]	−17.3	−26.5	−22.8	−21.2	−35.1	−22.9
# 514 Di-n-propylamine	−27.8[a]	−24.3	−32.9	−25.8	−23.6	−36.6	−25.8
# 515 Diiospropylamine	−32.6[a]	−25.1	−34.7	−27.3	−25.6	−39.7	−27.8
# 516 Triethylamine	−22.1[a]	−17.3	−27.2	−17.8	−14.9	−29.4	−18.9
# 518 Phenyl cyanide	51.5[a]	49.7	43.7	50.1	48.0	38.6	48.3
# 519 1-Cyclohexenecarbonitrile	24.3[a]	29.5	21.5	29.0	26.8	14.6	26.8
# 520 2,6-Dimethylpyridine	13.4[a]	14.5	6.9	14.3	12.5	0.8	13.2
# 521 2-Cyclohexenecarbonitrile	26.2[a]	31.1	22.9	30.5	28.6	16.1	28.0
# 522 Benzylamine	21.0[a]	21.7	13.8	20.1	18.7	6.7	18.6
# 523 m-Toluidine	14.6[a]	15.8	8.0	12.5	13.3	1.4	13.0
# 524 N-Methylaniline	20.1[a]	25.5	17.7	26.1	26.5	14.6	25.5
# 525 o-Toluidine	12.7[a]	16.6	8.6	13.3	14.3	2.1	14.1
# 526 p-Toluidine	10.0[a]	16.3	8.6	13.0	13.8	1.9	13.4
# 527 Cyanocyclohexane	−0.9[a]	2.5	−6.7	1.3	0.1	−13.8	−0.8
# 528 Cyclohexanecarbonitrile	−0.9[a]	2.5	−6.7	1.3	0.1	−13.8	−0.8
# 529 Hexahydro-1H-pyrrolizine	−0.9[a]	−2.6	−12.9	−0.3	1.5	−13.8	−0.6
# 530 n-Heptanenitrile	−7.4[a]	−6.2	−14.9	−7.2	−9.1	−22.3	−9.7
# 531 Isopropylbutylamine	−39.4[a]	−29.5	−40.1	−31.4	−29.6	−45.3	−31.9
# 532 1-Norbornylcyanide	18.0[a]	15.6	5.1	14.0	15.5	−0.3	14.4
# 533 1-Norbornylisocyanide	39.6[a]	36.1	25.5	32.0	24.8	8.8	18.4
# 534 5-Ethyl-2-methyl-pyridine	8.3[a]	8.5	−0.8	9.6	7.3	−6.9	9.2
# 535 N,N-Dimethyl aniline	24.0[a]	24.9	15.2	27.6	30.5	15.8	27.6
# 536 N-Ethyl aniline	13.4[a]	20.7	11.1	21.1	20.4	6.0	19.2
# 537 3-Azabicyclo[3.2.2]nonane	−10.4[a]	−2.3	−15.5	−1.8	−3.7	−23.4	−5.1

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 538 n-Heptyl cyanide	-12.1^a	−10.8	−21.0	−11.9	−14.0	−29.4	−14.8
# 539 N-(2-Methylpropylidene)-butylamine	-21.8^a	−16.7	−29.8	−21.4	−18.3	−35.1	−20.7
# 540 2-Methyl-N-(2-methylpropyl)-1-propanamine	-43.2^a	−36.5	−49.1	−39.1	−34.8	−53.5	−38.2
# 541 Di-sec-butylamine	-43.9^a	−34.0	−47.1	−36.6	−34.4	−53.5	−37.2
# 542 Dibutylamine	-40.9^a	−33.4	−45.0	−35.3	−33.2	−50.7	−35.9
# 543 N-(2-Methylpropyl)-1-butanamine	-41.8^a	−34.9	−47.0	−37.2	−34.1	−52.2	−37.1
# 544 n-Octylamine	-41.5^a	−36.2	−48.0	−40.5	−40.2	−58.0	−41.7
# 545 Isoquinoline	48.9^a	46.9	37.9	49.8	46.7	32.7	48.4
# 546 Quinoline	47.9^a	48.7	39.7	50.4	48.0	34.1	49.7
# 547 2,6-Dimethylbenzonitrile	34.9^a	30.1	20.4	29.9	29.8	15.0	29.4
# 548 (1a,2a,4a)-Bicyclo[2.2.2]oct-5-ene-2-carbonitrile	36.2^a	32.6	20.8	31.7	31.1	13.3	29.7
# 549 (1a,2b,4a)-Bicyclo[2.2.2]oct-5-ene-2-carbonitrile	36.6^a	32.4	20.5	31.5	31.2	13.3	29.7
# 550 1,2,3,4-Tetrahydroquinoline	19.6^a	22.4	11.5	21.6	22.5	5.9	20.6
# 551 5,6,7,8-Tetrahydroquinoline	17.0^a	15.7	4.7	16.6	13.6	−3.0	15.2
# 552 N,N-Dimethyl m-toluidine	17.4^a	15.6	4.2	17.6	21.6	4.4	18.5
# 553 N,N-Dimethyl p-toluidine	16.5^a	16.0	4.7	18.8	22.1	5.0	19.0
# 554 N-Ethyl m-toluidine	7.3^a	11.4	0.1	11.6	11.4	−5.4	10.1
# 555 cis-3,7a-H-cis-5,8-H-3,5-Dimethylpyrrolizidine	-15.9^a	−16.3	−30.4	−19.1	−12.8	−33.5	−17.7
# 556 Decahydro trans-quinoline	-27.0^a	−18.1	−32.7	−19.9	−18.9	−40.5	−22.4
# 557 2,2,6,6-Tetramethyl piperidine	-38.2^a	−30.1	−46.0	−35.3	−30.7	−52.3	−32.7
# 558 2-Methyl-quinoline	38.0^a	40.5	30.0	40.1	39.4	23.2	40.8
# 559 4-Methyl-quinoline	38.7^a	39.5	28.7	41.2	39.7	23.1	41.3
# 560 6-Methyl-quinoline	38.5^a	39.1	28.5	40.7	38.8	22.6	40.5
# 561 8-Methyl-quinoline	40.1^a	39.3	28.6	40.8	39.1	22.6	40.7
# 562 2,4,6-Trimethyl-benzonitrile	25.4^a	20.6	9.2	19.5	20.7	3.1	20.0
# 563 2,4,6-Trimethylphenyl isocyanide	56.6^a	42.1	30.6	38.6	31.5	14.1	25.9
# 564 N,N-Diethyl aniline	14.8^a	16.6	2.7	16.9	19.8	−0.7	15.8
# 565 n-Nonyl cyanide	-21.9^a	−19.9	−33.2	−21.4	−23.6	−43.5	−24.9
# 566 2,6-Dimethyl quinoline	28.9^a	31.0	18.8	30.4	30.3	11.8	31.6
# 567 2,7-Dimethyl quinoline	29.1^a	30.9	18.8	30.4	30.4	11.8	31.6
# 568 1-Adamantyl cyanide	-1.8^a	−3.7	−20.5	−6.0	−3.3	−28.4	−6.1
# 569 1-Adamantyl isocyanide	17.5^a	16.7	−0.2	12.0	6.1	−19.2	−1.9
# 570 2-Methyl-6-t-butylaniline	-10.7^a	−5.0	−21.4	−9.3	−3.5	−27.8	−5.5
# 571 n-Undecanenitrile	-27.1^a	−24.5	−39.3	−26.2	−28.5	−50.6	−30.0
# 572 Carbazole	50.1^a	58.7	46.3	58.0	57.6	38.6	57.1
# 573 2-Biphenylamine	44.1^a	45.1	31.4	41.9	44.1	23.4	43.1
# 574 Biphenylamine	48.2^a	56.0	42.8	55.0	55.7	35.6	53.9
# 575 2-n-Butyl-2-methylhexanenitrile	-31.8^a	−30.7	−49.8	−34.1	−31.5	−59.4	−35.0
# 576 6,7-Benzoquinoline	58.2^a	60.3	46.5	62.2	61.0	39.9	61.9
# 577 a-Benzoquinoline	59.8^a	59.3	45.6	61.0	59.8	38.8	61.3
# 578 Acridine	65.5^a	71.7	58.2	72.0	71.5	50.8	72.7
# 579 Benzo[f]quinoline	55.9^a	60.6	46.8	62.4	61.2	40.0	62.7
# 580 Phenanthridine	57.5^a	60.3	46.5	62.2	61.0	39.9	61.9
# 581 N-Methylcarbazole	47.6^a	55.8	41.4	59.1	59.3	37.5	57.8
# 582 1,2,3,4-Tetrahydro-N-methylcarbazole	22.3^a	31.9	15.5	34.8	34.0	9.3	32.7
# 583 9-Ethyl-9H-carbazole	40.6^a	50.7	34.2	53.1	53.3	28.6	51.1
# 584 Tetradecanenitrile	-41.8^a	−38.2	−57.5	−40.4	−43.0	−71.8	−45.2
# 585 Dioctylamine	-76.5^a	−69.9	−93.6	−73.3	−71.9	−107.3	−76.4
# 586 Triphenylamine	78.1^a	83.6	61.6	83.8	88.3	55.9	83.4
# 587 Trioctylamine	-114.0^a	−101.1	−138.5	−104.8	−102.6	−158.1	−111.5
# 593 Diazomethane	71.0^a	60.5	59.4	64.2	57.2	55.5	63.1
# 594 N=N-CH2-	79.0^a	87.4	86.4	89.3	80.2	78.5	91.8
# 595 Methylhydrazine	22.6^a	17.0	14.6	18.9	18.6	14.9	18.6
# 599 1,1-Dimethylhydrazine	20.0^a	14.8	10.8	17.8	21.4	15.4	22.2
# 600 1,2-Dimethylhydrazine	22.0^a	17.1	13.2	26.3	28.4	22.8	24.4
# 601 Ethylenediamine	-4.1^a	4.1	0.0	−0.6	−2.7	−8.9	−3.0
# 602 1H-Pyrazole	42.9^a	47.8	44.6	52.0	49.3	44.3	52.1
# 603 Imidazole	31.8^a	40.0	36.9	42.4	39.7	34.6	42.7
# 604 1,2-Propanediamine	-12.8^a	−4.1	−9.8	−10.0	−10.5	−19.2	−11.4
# 606 Fumaronitrile	81.3^a	79.7	76.9	79.7	75.2	70.8	75.8
# 607 1,3-Diazine	47.0^a	44.5	40.4	48.0	41.9	35.4	43.8
# 608 Pyrazine	46.9^a	44.9	40.9	50.0	42.0	35.5	47.8
# 609 Pyridazine	66.5^a	48.4	44.3	55.3	51.1	44.6	56.0
# 610 Succinonitrile	50.1^a	47.7	44.0	47.3	43.4	37.7	43.4
# 611 2-Methyl-1H-imidazole	21.5^a	33.5	28.9	33.9	31.4	24.3	34.3

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 612 (Dimethylamino) acetonitrile	27.3[a]	27.5	22.0	29.6	29.6	21.3	28.6
# 613 1,4,5,6-Tetrahydropyrimidine	13.2[a]	26.3	20.4	26.2	26.1	17.2	20.8
# 614 Piperazine	6.0[a]	13.5	6.7	13.2	15.3	4.9	12.3
# 615 2-Aminopyridine	28.2[a]	36.6	31.0	32.8	32.6	23.9	32.5
# 616 3-Aminopyridine	34.5[a]	36.5	30.8	35.6	32.8	23.9	35.2
# 617 4-Aminopyridine	31.0[a]	36.0	30.4	34.3	32.6	23.8	33.5
# 618 Dimethyl propanedinitrile	47.1[a]	38.0	32.4	37.7	35.5	27.0	35.9
# 619 2-Ethyl-1H-imidazole	16.3[a]	28.4	22.3	28.8	26.5	17.1	29.4
# 620 Diethylcyanamide	15.2[a]	23.7	16.5	25.9	27.6	16.9	23.5
# 621 Butylmethyldiazene	18.9[a]	13.1	5.9	12.0	14.1	3.2	15.9
# 622 Butylmethyldiazine	18.9[a]	13.1	5.9	12.0	14.1	3.2	15.9
# 623 N,N-Dimethyl-1,3-propanediamine	−8.3[a]	−4.1	−12.7	−5.5	0.2	−12.7	−4.3
# 624 2-Cyanopyridine	67.1[a]	67.0	61.5	68.2	62.3	53.7	65.4
# 625 3-Cyanopyridine	66.4[a]	63.2	57.7	65.6	60.3	51.5	62.7
# 626 4-Cyanopyridine	67.8[a]	63.6	58.1	66.1	60.7	52.0	63.2
# 627 2,3-Dimethyl pyrazine	30.1[a]	28.6	21.2	30.9	24.8	13.6	30.0
# 628 Hexanedinitrile	35.7[a]	36.9	30.2	35.8	32.3	22.1	31.7
# 629 Phenylhydrazine	48.5[a]	47.9	40.5	49.5	48.9	37.5	49.0
# 630 3(Dimethylamino) propanenitrile	21.6[a]	16.9	8.3	18.5	21.6	8.8	17.6
# 631 Tetramethyldiazetine	35.9[a]	38.6	29.0	41.0	47.3	32.8	49.5
# 632 Triethylenediamine	11.5[a]	28.3	18.1	36.0	38.9	23.4	35.4
# 633 1,2-Diisopropyldiazene	8.6[a]	4.7	−4.8	3.6	6.2	−8.0	8.4
# 634 Dipropyldiazene	12.4[a]	8.0	−0.6	6.0	8.7	−4.2	10.2
# 635 1H-Benzimidazole	43.4[a]	57.5	50.2	57.6	56.6	45.1	57.2
# 636 1H-Indazole	58.1[a]	64.4	57.0	68.0	65.5	54.0	68.0
# 637 1-Methyl-1-phenylhydrazine	50.4[a]	47.2	38.0	49.7	52.8	39.0	51.4
# 638 t-Butylmalononitrile	30.3[a]	27.4	17.4	25.6	26.0	11.3	24.5
# 639 Trimethyl pyrazine	17.8[a]	20.4	11.5	21.4	16.2	2.7	21.2
# 640 1-Piperidineacetonitrile	19.8[a]	25.3	15.0	24.5	24.9	8.6	21.1
# 641 3,3,5,5-Tetramethyl-1-pyrazoline	9.4[a]	−5.8	−17.4	−4.3	1.0	−16.2	1.7
# 642 m-Dicyanobenzene	86.7[a]	82.6	75.5	82.7	79.2	68.2	79.8
# 643 o-Dicyanobenzene	87.8[a]	83.8	76.5	84.1	80.2	69.0	81.1
# 644 p-Dicyanobenzene	85.6[a]	82.3	75.1	82.3	78.9	67.8	79.5
# 645 Phthalazine	78.8[a]	65.0	56.5	71.7	68.2	54.9	71.7
# 646 Quinazoline	58.1[a]	62.3	53.9	64.8	60.4	47.3	61.3
# 647 Quinoxaline	57.4[a]	64.7	56.3	67.8	61.9	48.8	66.8
# 648 n-Pentylmalonodinitrile	32.5[a]	29.1	19.0	28.1	24.7	9.6	24.3
# 649 Tetramethylbutanedinitrile	24.0[a]	15.2	2.9	12.7	16.3	−1.8	14.1
# 650 Tetramethylpyrazine	13.1[a]	12.7	2.0	12.2	8.1	−8.0	12.6
# 651 1,4-Dimethyl-2,3-diaza-bicyclo[2.2.2]oct-2-ene	22.1[a]	7.0	−6.2	9.0	13.6	−6.2	15.3
# 652 3,4,5,6-Tetrahydro-3,3,6,6-tetramethylpyridazine	10.0[a]	−3.6	−17.5	−2.3	3.4	−17.1	1.3
# 653 Di-n-butyldiazene	2.2[a]	−1.1	−12.8	−3.4	−0.9	−18.2	0.2
# 654 Di-tert-butyldiazene	−8.7[a]	−10.7	−24.3	−14.9	−7.2	−27.2	−7.7
# 655 1,2-Dibutylhydrazine	−14.2[a]	−10.3	−23.3	−8.7	−7.5	−25.2	−5.5
# 656 3-Quinolinamine	49.8[a]	54.6	44.4	52.5	51.4	35.8	52.9
# 657 5-Quinolinamine	50.3[a]	55.5	45.2	53.1	52.3	36.4	53.6
# 658 6-Quinolinamine	49.3[a]	54.5	44.4	52.2	51.2	35.6	52.6
# 659 8-Quinolinamine	44.8[a]	52.8	42.5	50.4	49.2	33.4	50.8
# 660 2-(Diethylamino)-pentanenitrile	−1.1[a]	4.4	−10.2	3.4	3.5	−18.6	−1.3
# 661 2,2-Bipyridyl	69.1[a]	65.1	54.4	67.2	62.4	45.9	66.1
# 662 2,4-Bipyridyl	67.9[a]	65.3	54.5	68.9	63.4	46.7	67.2
# 663 4,4'-Bipyridine	70.1[a]	63.6	52.7	68.5	62.7	45.9	66.4
# 664 2,3-Dimethyl quinoxaline	41.3[a]	48.2	36.4	48.3	44.8	26.8	48.6
# 665 alpha N,N-dimethylamino phenylacetonitrile	52.7[a]	49.6	36.6	51.7	53.2	34.4	50.1
# 666 Ethyl(1,1-dimethylpropyl)malonodinitrile	14.6[a]	10.5	−6.0	7.4	12.0	−12.1	9.1
# 667 Meso-2,3-diethyl-2,3-dimethylsuccinodinitrile	15.3[a]	8.4	−8.1	5.2	10.0	−14.1	7.1
# 668 Methyl(1,1,2-trimethylpropyl)malonodinitrile	19.0[a]	11.4	−5.8	7.9	13.7	−11.3	10.3
# 669 Phenazine	80.9[a]	90.1	77.3	90.9	87.1	67.4	91.7
# 670 Phenazone	89.9[a]	77.4	64.2	83.3	83.3	63.1	86.5
# 671 cis-Azobenzene	107.7[a]	86.4	72.2	91.0	91.8	70.6	91.5
# 672 Diphenyl diazene	96.9[a]	91.0	78.3	90.6	91.7	72.3	94.6
# 673 4,4'-Dimethyl-2,2'-bipyridine	50.0[a]	46.1	32.1	46.6	44.5	23.2	46.4
# 674 1,(1-Piperidinyl) cyclohexanecarbonitrile	0.8[a]	8.2	−12.0	5.5	10.4	−19.2	4.4
# 677 a-Phenyl-1-piperidineacetonitrile	45.4[a]	47.2	28.7	45.9	49.9	22.8	44.2
# 680 2,2'-Biquinoline	101.8[a]	101.2	81.3	100.9	99.8	69.6	102.0

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 681 Tetraisobutylsuccinonitrile	−26.7[a]	−33.3	−72.8	−44.5	−28.9	−84.8	−40.9
# 690 Ethylenetricarbonitrile	124.4[a]	119.1	115.1	120.1	111.4	105.4	113.5
# 691 1,1,1-Ethanetricarbonitrile	101.0[a]	85.6	80.6	86.5	80.1	72.5	82.0
# 693 1,3,5-Tricyanobenzene	121.8[a]	117.3	109.0	117.4	111.9	99.2	113.0
# 694 1,1,1-Tricyano-2-phenyl ethane	129.2[a]	111.3	98.5	110.9	106.4	87.3	106.1
# 695 2,2',6',2'-Terpyridine	94.3[a]	99.9	82.7	101.1	95.8	69.7	100.6
# 698 1-H Tetrazole	76.6[a]	70.7	68.3	75.2	73.5	69.6	74.0
# 699 2-H-Tetrazole	79.9[a]	72.0	69.6	77.3	74.1	70.3	77.2
# 701 1,3,5,7-Tetraazaadamantane	47.6[a]	63.9	50.9	72.3	84.4	64.8	70.1
# 705 Melamine	12.4[a]	68.5	61.8	45.9	60.1	49.7	46.4
# 729 Formaldehyde (Geo)	−26.0[a]	−30.3	−30.9	−30.0	−31.9	−32.8	−32.3
# 735 Methanol (Geo)	−48.1[a]	−49.3	−50.3	−50.1	−49.8	−51.4	−49.7
# 741 Ketene (Geo)	−11.4[a]	−5.1	−6.1	−6.5	−11.0	−12.6	−10.9
# 744 Acetaldehyde (Geo)	−39.7[a]	−44.2	−45.8	−44.1	−46.5	−49.1	−46.7
# 747 Dimethyl ether (Geo)	−44.0[a]	−45.6	−47.7	−45.9	−42.8	−46.2	−44.3
# 754 Acetone (Geo)	−52.0[a]	−57.6	−60.5	−57.3	−59.4	−64.0	−58.9
# 762 Furan (Geo)	−8.3[a]	−2.9	−5.9	−3.4	−2.7	−7.4	−2.2
# 1053 Formic acid (Geo)	−90.5[a]	−86.9	−87.8	−88.0	−88.2	−89.7	−89.6
# 1054 trans Glyoxal (Geo)	−50.7[a]	−59.1	−60.6	−58.5	−61.8	−64.2	−62.6
# 1059 Methyl formate (Geo)	−83.6[a]	−81.4	−83.5	−82.1	−79.4	−82.6	−82.1
# 1096 p-Benzoquinone (Geo)	−29.3[a]	−32.5	−37.9	−31.6	−32.9	−41.3	−32.0
# 1376 Formic acid, dimer (Geo)	−194.9[a]	−188.3	−191.4	−191.5	−193.2	−198.0	−197.8
# 727 HCO, cation	199.0[a]	194.8	194.5	190.8	192.6	192.0	190.3
# 728 HCO	10.4[a]	0.1	−0.3	−0.2	−4.4	−4.9	−3.1
# 731 CH2OH, cation	168.0[a]	166.4	165.7	162.3	172.4	171.2	171.0
# 733 Methoxy, radical	−0.5[a]	0.4	−0.4	1.3	1.3	−0.0	1.7
# 734 Methoxy, anion	−36.0[a]	−46.1	−46.9	−42.4	−51.1	−52.4	−48.6
# 745 Ethylene oxide	−12.6[a]	−13.3	−14.8	−10.1	−8.8	−11.2	−5.1
# 746 Ethoxy, anion	−47.5[a]	−52.7	−54.6	−49.9	−58.1	−61.2	−56.3
# 749 Ethanol	−56.2[a]	−56.9	−59.1	−56.7	−57.2	−60.8	−56.6
# 755 Propanal	−45.5[a]	−49.1	−52.1	−49.0	−51.2	−55.9	−51.4
# 756 Trimethylene oxide	−19.2[a]	−17.7	−20.6	−18.8	−15.8	−20.5	−17.2
# 757 Isopropanol	−65.1[a]	−66.7	−70.5	−68.7	−67.2	−73.1	−67.5
# 758 Methyl ethyl ether	−51.7[a]	−53.4	−56.8	−53.0	−50.6	−56.0	−51.9
# 759 Propanol	−61.2[a]	−61.5	−65.3	−62.9	−62.5	−68.4	−62.6
# 760 Acetyl acetylene	15.6[a]	11.2	8.5	10.9	9.8	5.5	10.2
# 763 2,3-Dihydrofuran	−17.3[a]	−19.1	−22.9	−20.6	−19.0	−25.0	−20.1
# 764 Crotonaldehyde	−24.0[a]	−27.9	−31.5	−27.9	−29.5	−35.1	−30.0
# 765 Divinyl ether	−3.3[a]	4.0	0.4	2.5	4.8	−0.7	2.9
# 766 Butanal	−48.9[a]	−53.7	−58.1	−53.6	−56.0	−62.9	−56.4
# 767 Isobutanal	−51.6[a]	−56.0	−60.7	−56.2	−57.1	−64.3	−57.5
# 768 Methyl ethyl ketone	−57.1[a]	−62.4	−66.9	−62.2	−63.7	−70.7	−63.0
# 769 Tetrahydrofuran	−44.0[a]	−47.9	−52.5	−48.9	−46.1	−53.5	−47.3
# 770 Diethyl ether	−60.3[a]	−61.1	−65.9	−60.2	−58.4	−65.7	−59.4
# 771 t-Butanol	−74.7[a]	−76.8	−82.4	−78.1	−75.9	−84.5	−76.1
# 773 2,3-Dihydro-5-methyl-furan	−31.1[a]	−30.2	−35.4	−31.1	−30.2	−38.2	−30.8
# 774 2-Ethylacrolein	−31.4[a]	−32.1	−37.5	−31.9	−32.9	−41.2	−33.2
# 775 3,4-Dihydro-2H-pyran	−27.0[a]	−24.5	−30.1	−26.2	−24.3	−33.0	−26.0
# 776 3-Penten-2-one	−32.6[a]	−42.0	−47.0	−41.9	−43.1	−50.8	−42.7
# 777 Cyclopentanone	−46.0[a]	−55.0	−60.6	−54.7	−57.5	−66.1	−56.9
# 778 Diethyl ketone	−61.6[a]	−67.1	−73.4	−66.9	−67.9	−76.7	−67.9
# 779 Tetrahydropyran	−53.4[a]	−53.1	−59.6	−54.5	−51.7	−61.8	−53.8
# 780 t-Butyl methyl ether	−67.8[a]	−70.5	−77.9	−71.4	−66.1	−77.2	−68.3
# 781 Phenoxy, anion	−40.5[a]	−39.2	−44.3	−36.1	−46.2	−54.4	−43.3
# 782 Phenol	−23.0[a]	−21.7	−27.2	−22.4	−23.6	−32.3	−23.2
# 783 4-Methyl-3-penten-2-one	−42.6[a]	−51.2	−58.0	−51.1	−51.7	−62.2	−51.2
# 784 Cyclohexanone	−54.0[a]	−59.9	−67.6	−60.0	−62.1	−73.7	−61.8
# 785 Methyl neopentyl ketone	−76.6[a]	−76.9	−85.5	−77.5	−75.4	−88.2	−75.7
# 786 Di-isopropyl ether	−76.3[a]	−76.1	−85.1	−77.9	−72.6	−85.9	−75.2
# 787 Benzaldehyde	−8.8[a]	−14.5	−20.9	−13.6	−15.6	−25.6	−15.7
# 788 Anisole	−17.3[a]	−16.0	−23.0	−16.3	−14.1	−25.0	−15.4
# 789 m-Cresol	−31.9[a]	−31.1	−38.3	−32.6	−32.6	−43.7	−32.4
# 790 o-Cresol	−30.7[a]	−30.5	−37.7	−31.4	−32.0	−43.1	−31.7
# 791 p-Cresol	−29.9[a]	−30.6	−37.7	−31.5	−32.2	−43.3	−32.0
# 792 2-Methyl-5-hexen-3-yn-2-ol	11.0[a]	6.8	−0.4	5.1	7.6	−3.3	7.5

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 793 2-Norbornanone	-40.8^{a}	−45.8	−54.6	−46.6	−46.7	−60.3	−47.7
# 794 cis-2,3-Epoxybicyclo[2.2.1]heptane	-12.9^{a}	−6.8	−15.4	−5.2	−1.8	−15.1	0.1
# 795 Norbornan-7-one	-32.0^{a}	−41.2	−49.9	−41.8	−42.4	−55.9	−43.1
# 796 1-Methoxy cyclohexene	-38.5^{a}	−37.0	−45.9	−37.7	−35.9	−49.5	−37.3
# 797 Bicyclo[2.2.1]heptan-7-ol	-52.0^{a}	−52.9	−62.8	−56.0	−52.6	−67.7	−54.1
# 798 cis-1,2-Epoxycycloheptane	-36.4^{a}	−27.6	−37.0	−26.0	−25.1	−39.4	−22.9
# 799 Cycloheptanone	-59.3^{a}	−59.3	−69.1	−59.8	−61.7	−76.5	−61.7
# 800 2,4-Dimethyl 3-pentanone	-74.4^{a}	−80.7	−90.5	−81.5	−79.8	−94.5	−80.6
# 801 2-Methyl cis-cyclohexanol	-71.9^{a}	−73.9	−84.8	−76.6	−74.1	−90.5	−75.5
# 802 3,3-Dimethyl-2-pentanone	-72.6^{a}	−80.2	−90.7	−80.8	−78.4	−94.1	−78.9
# 803 4-Heptanone	-71.3^{a}	−76.3	−85.7	−76.6	−77.6	−91.2	−77.3
# 804 Heptanal	-63.1^{a}	−67.4	−76.4	−67.9	−70.5	−84.1	−71.5
# 805 t-Butyl ethyl ketone	-75.0^{a}	−81.3	−91.6	−82.0	−79.3	−94.7	−79.7
# 806 n-Heptanol	-81.2^{a}	−80.1	−89.8	−80.8	−81.5	−96.1	−81.8
# 807 t-Butyl isopropyl ether	-85.5^{a}	−86.6	−97.5	−88.1	−81.4	−97.6	−84.4
# 808 Benzofuran	3.3^{a}	9.2	2.1	8.5	9.3	−1.8	9.4
# 809 1,3-Dihydro isobenzofuran	-7.2^{a}	−16.2	−24.3	−16.9	−13.8	−26.3	−15.4
# 810 1-Phenylethenol	-11.0^{a}	−7.3	−15.4	−8.2	−7.9	−20.4	−8.0
# 811 2,3-Dihydro-benzofuran	-11.1^{a}	−14.8	−22.8	−15.9	−14.2	−26.6	−15.2
# 812 Acetophenone	-20.7^{a}	−27.4	−35.5	−26.5	−27.6	−40.0	−26.9
# 813 2,3-Dimethyl phenol	-37.6^{a}	−39.5	−48.7	−40.3	−39.8	−53.8	−39.5
# 814 2,4-Dimethyl phenol	-39.0^{a}	−39.5	−48.4	−40.5	−40.3	−54.0	−40.1
# 815 2,5-Dimethyl phenol	-38.7^{a}	−39.9	−48.8	−40.8	−40.6	−54.3	−40.3
# 816 2,6-Dimethyl phenol	-38.7^{a}	−39.0	−48.0	−40.4	−40.0	−53.8	−39.9
# 817 2-Ethyl phenol	-34.7^{a}	−35.1	−44.2	−36.3	−36.4	−50.2	−36.3
# 818 3,4-Dimethyl phenol	-37.4^{a}	−39.9	−48.9	−41.0	−40.6	−54.5	−40.6
# 819 3,5-Dimethyl phenol	-38.6^{a}	−40.5	−49.3	−42.2	−41.6	−55.1	−42.0
# 820 3-Ethyl phenol	-34.9^{a}	−35.8	−44.7	−36.9	−37.2	−50.8	−37.1
# 821 4-Ethyl phenol	-34.5^{a}	−35.3	−44.2	−36.4	−36.8	−50.4	−36.8
# 822 Benzyl alcohol	-22.6^{a}	−31.5	−40.4	−32.6	−32.1	−45.7	−32.8
# 823 Ethoxybenzene	-24.3^{a}	−24.0	−32.4	−23.7	−22.1	−35.0	−23.1
# 824 Phenetole	-26.3^{a}	−23.5	−32.4	−24.8	−21.7	−35.1	−23.6
# 825 1-Methylnorcamphor	-48.9^{a}	−54.8	−65.7	−56.0	−54.8	−71.2	−56.2
# 826 Bicyclo[2.2.2]octanone	-52.2^{a}	−57.3	−68.4	−57.4	−58.8	−75.6	−59.0
# 827 Bicyclo[3.2.1]octan-2-one	-52.0^{a}	−57.0	−68.1	−57.5	−57.9	−74.7	−58.3
# 828 Bicyclo[3.2.1]octan-3-one	-52.9^{a}	−58.1	−69.2	−58.7	−59.4	−76.1	−60.0
# 829 Bicyclo[3.2.1]octan-8-one	-46.2^{a}	−54.6	−65.7	−55.3	−55.9	−72.7	−56.5
# 830 cis-Bicyclo[3.3.0]-octan-2-one	-55.0^{a}	−60.3	−70.9	−60.6	−62.4	−78.3	−62.2
# 831 trans-Bicyclo[3.3.0]-octan-2-one	-49.4^{a}	−46.3	−56.7	−47.3	−49.3	−65.0	−50.0
# 832 3-Oxabicyclo[3,2,2]nonane	-53.2^{a}	−50.1	−62.4	−52.2	−48.9	−67.3	−51.6
# 833 6-Methyl-5-hepten-2-one	-60.1^{a}	−57.8	−67.8	−58.2	−59.4	−74.4	−59.8
# 834 8-Oxatricyclo[3,2,1,0(1,5)]octane	6.4^{a}	28.7	17.2	30.8	34.1	16.7	33.5
# 835 Bicyclo(2.2.2)octan-2-ol	-68.0^{a}	−64.5	−76.8	−67.0	−65.2	−83.7	−66.3
# 836 cis-1,2-Epoxycyclooctane	-39.5^{a}	−24.6	−36.2	−23.3	−23.0	−40.3	−21.0
# 837 Cyclooctanone	-65.1^{a}	−62.8	−74.7	−64.1	−65.7	−83.6	−66.8
# 838 2,2,4-Trimethyl-3-pentanone	-80.9^{a}	−88.0	−100.4	−89.4	−85.1	−103.5	−86.3
# 839 2-Octanone	-82.5^{a}	−80.7	−91.3	−81.2	−83.0	−98.9	−83.2
# 840 3,3,4-Trimethyl pentan-2-one	-78.5^{a}	−86.2	−99.2	−87.6	−83.2	−102.4	−84.6
# 841 3-Octanone	-80.9^{a}	−80.9	−91.6	−81.3	−82.4	−98.5	−82.4
# 842 4-Octanone	-83.5^{a}	−80.9	−91.8	−81.3	−82.4	−98.3	−82.3
# 843 Octanal	-69.8^{a}	−72.0	−82.5	−72.7	−75.3	−91.2	−76.6
# 844 1-Octanol	-85.3^{a}	−84.7	−95.9	−85.5	−86.3	−103.1	−86.9
# 845 1-Tert-butoxybutane	-86.3^{a}	−87.8	−99.6	−88.6	−83.4	−101.1	−86.4
# 846 2-(1,1-Dimethylethoxy)-butane	-90.8^{a}	−90.9	−103.9	−92.9	−85.4	−104.5	−88.9
# 847 Di-n-butyl ether	-79.8^{a}	−80.1	−90.9	−79.8	−77.7	−93.9	−79.4
# 848 Di-sec-butyl ether	-86.3^{a}	−85.2	−97.8	−87.5	−81.2	−99.6	−84.3
# 849 sec-Butyl-tert-butyl ether	-88.0^{a}	−89.6	−102.1	−91.1	−84.3	−102.7	−87.4
# 850 tert-Butyl ether	-86.3^{a}	−92.3	−105.7	−94.6	−85.1	−104.9	−88.7
# 851 tert-Butyl isobutyl ether	-88.0^{a}	−89.6	−102.1	−91.1	−84.3	−102.7	−87.4
# 852 3,4-Dihydro-1H-2-benzopyran	-15.1^{a}	−22.2	−32.3	−23.2	−19.5	−35.0	−21.9
# 853 3,4-Dihydro-2H-1-benzopyran	-19.7^{a}	−21.8	−31.8	−23.1	−20.6	−36.0	−22.4
# 854 Benzyl methyl ketone	-22.6^{a}	−32.3	−42.2	−32.0	−33.3	−48.4	−33.7
# 855 2(-1-Methylethyl)-phenol	-41.9^{a}	−41.4	−52.4	−42.8	−41.7	−58.3	−42.0
# 856 2,4,6-Trimethyl phenol	-42.3^{a}	−48.4	−59.0	−49.7	−48.6	−64.8	−48.7
# 857 3(-1-Methylethyl)-phenol	-41.9^{a}	−42.1	−53.1	−43.6	−42.8	−59.3	−43.2

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 858 4-(-1-Methylethyl)-phenol	−41.9[a]	−41.6	−52.5	−43.1	−42.3	−58.8	−42.8
# 859 2,6,6-Trimethyl-2-cyclohexen-1-one	−55.6[a]	−57.7	−70.2	−58.4	−55.7	−74.4	−56.4
# 860 Bicycle[3.3.1]nonan-9-one -check -3-one	−57.3[a]	−60.4	−73.8	−61.3	−61.4	−81.6	−62.4
# 861 cis Octahydro-2H-inden-2-one	−59.7[a]	−62.3	−75.1	−62.9	−65.3	−84.4	−66.0
# 862 trans Octahydro-2H-inden-2-one	−59.6[a]	−64.1	−76.8	−65.6	−66.8	−85.7	−68.7
# 863 Cyclononanone	−66.9[a]	−64.1	−78.4	−66.1	−67.3	−88.4	−69.2
# 864 2,6-Dimethyl-4-heptanone	−85.5[a]	−89.1	−102.5	−90.6	−89.0	−108.7	−90.2
# 865 2-Nonanone	−81.4[a]	−85.3	−97.4	−86.0	−87.8	−106.0	−88.3
# 866 3,3,4,4-Tetramethyl-2-pentanone	−83.1[a]	−92.4	−108.1	−94.4	−86.9	−110.0	−89.3
# 867 5-Nonanone	−82.4[a]	−84.5	−96.5	−86.2	−86.9	−105.0	−88.3
# 868 Di-tert-butyl ketone	−82.7[a]	−92.3	−107.2	−93.8	−86.7	−108.7	−88.4
# 869 1-Nonanol	−89.8[a]	−89.2	−101.9	−90.3	−91.1	−110.2	−91.9
# 870 Amyl-t-butyl ether	−91.0[a]	−92.4	−105.7	−93.1	−88.3	−108.2	−91.0
# 871 Butyl 1,1-dimethylpropyl ether	−91.3[a]	−91.7	−105.6	−92.4	−87.0	−107.5	−89.7
# 872 4-Phenyl-3-buten-2-one	−11.5[a]	−11.7	−21.8	−11.2	−12.1	−27.7	−12.1
# 873 2-Adamantone	−55.1[a]	−64.0	−78.9	−65.1	−63.9	−86.4	−65.5
# 874 2-Isopropyl-4-methylphenol	−47.4[a]	−49.5	−62.4	−52.2	−49.1	−68.5	−49.8
# 875 2-Isopropyl-5-methylphenol	−44.1[a]	−50.7	−63.4	−52.3	−50.6	−69.6	−51.1
# 876 2-Isopropyl-6-methylphenol	−45.4[a]	−49.4	−62.4	−52.0	−48.7	−68.2	−49.3
# 877 2-Methyl-5-isopropylphenol	−46.4[a]	−50.9	−63.6	−52.4	−50.7	−69.9	−51.2
# 878 3-Isopropyl-2-methylphenol	−43.6[a]	−48.9	−62.0	−50.2	−48.3	−68.0	−48.7
# 879 3-Methyl-2-isopropylphenol	−41.0[a]	−48.0	−61.4	−51.0	−47.0	−67.0	−47.5
# 880 3-Methyl-5-isopropylphenol	−50.2[a]	−51.5	−64.1	−53.7	−51.7	−70.7	−52.3
# 881 4-Isopropyl-2-methylphenol	−49.4[a]	−50.5	−63.2	−52.1	−50.3	−69.5	−50.9
# 882 4-Isopropyl-3-methylphenol	−44.0[a]	−47.2	−60.4	−48.8	−47.2	−66.9	−47.9
# 883 4-Methyl-3-isopropylphenol	−44.2[a]	−47.2	−60.4	−48.8	−47.2	−66.9	−47.9
# 884 m-tert-Butylphenol	−44.3[a]	−48.5	−61.8	−50.3	−47.1	−67.1	−48.2
# 885 o-sec-Butylphenol	−45.8[a]	−45.0	−58.0	−46.6	−45.0	−64.6	−45.8
# 886 o-tert-Butylphenol	−47.6[a]	−47.8	−61.3	−50.0	−45.9	−66.1	−47.2
# 887 p-sec-Butylphenol	−45.6[a]	−45.8	−58.5	−47.6	−46.6	−65.7	−47.5
# 888 p-tert-Butyl phenol	−44.5[a]	−47.9	−61.2	−49.7	−46.6	−66.5	−47.8
# 889 1-Adamantol	−74.3[a]	−76.5	−92.5	−79.2	−75.1	−99.1	−77.5
# 890 2-Adamantol	−71.5[a]	−71.9	−88.2	−75.5	−71.1	−95.4	−73.8
# 891 Camphor	−63.9[a]	−67.2	−83.0	−69.4	−64.5	−87.9	−67.4
# 892 Octahydro-3a-methyl-cis-2H-inden-2-one	−68.6[a]	−72.7	−88.1	−74.4	−73.6	−96.5	−76.0
# 893 Octahydro-3a-methyl-trans-2H-inden-2-one	−65.8[a]	−69.2	−84.6	−71.0	−69.8	−92.8	−72.5
# 894 Beta-caran-3-ol	−61.9[a]	−57.3	−72.8	−59.2	−56.7	−79.5	−58.0
# 895 Cyclodecanone	−72.9[a]	−66.5	−82.8	−69.1	−70.1	−93.9	−72.6
# 896 2,2,5,5-Tetramethyl-3-hexanone	−94.1[a]	−99.3	−116.0	−101.8	−95.0	−119.5	−97.8
# 897 Decanol	−94.5[a]	−93.8	−108.0	−95.0	−96.0	−117.3	−97.0
# 898 Dipentyl ether	−93.1[a]	−87.5	−101.6	−88.7	−86.0	−107.2	−88.7
# 899 2,4,5-Trimethyl-acetophenone	−45.2[a]	−54.3	−68.0	−54.1	−52.6	−73.2	−52.9
# 900 2,4,6-Trimethyl-acetophenone	−49.0[a]	−53.3	−67.2	−53.6	−52.3	−73.0	−53.0
# 901 2-tert-Butyl-p-cresol	−49.5[a]	−56.7	−71.9	−59.7	−54.4	−75.5	−56.5
# 902 3-Methyl-2-phenylbutane-2-ol	−50.5[a]	−57.6	−73.2	−59.4	−53.4	−76.6	−55.2
# 903 Cycloundecanone	−77.0[a]	−69.7	−88.0	−72.4	−73.2	−100.0	−76.5
# 904 2,2,6,6-Tetramethyl-4-heptanone	−100.7[a]	−104.0	−122.4	−107.0	−100.3	−127.2	−103.7
# 905 Dipentyl ketone	−92.6[a]	−94.6	−110.0	−95.6	−96.9	−119.5	−98.1
# 906 Decyl methyl ether	−91.1[a]	−90.3	−105.8	−91.3	−89.3	−112.5	−92.3
# 907 Dibenzofuran	11.3[a]	17.2	5.7	16.5	17.5	−0.2	17.3
# 908 m-Hydroxybiphenyl	5.1[a]	−1.5	−14.1	−2.1	−2.0	−21.2	−2.2
# 909 o-Hydroxybiphenyl	4.0[a]	−0.2	−12.9	−1.0	−0.4	−19.9	−0.8
# 910 p-Hydroxybiphenyl	0.0[a]	−1.3	−13.8	−1.9	−1.8	−21.0	−2.0
# 911 Isobutyl phenyl ketone	−38.4[a]	−51.6	−67.4	−52.4	−50.0	−73.4	−51.3
# 912 2,6-Diisopropylphenol	−60.7[a]	−60.3	−77.2	−62.8	−58.3	−83.4	−59.8
# 913 Benzophenone	11.9[a]	3.0	−10.6	4.0	4.4	−16.4	4.3
# 914 Anthone	5.6[a]	−1.2	−16.1	−0.9	0.0	−22.8	−0.5
# 915 1,1'-Diadamantylketone	−87.9[a]	−89.9	−126.5	−94.6	−84.1	−137.8	−91.2
# 1051 Formate, anion	−106.6[a]	−111.8	−112.4	−109.0	−118.7	−119.8	−118.1
# 1056 Acetate, anion	−122.5[a]	−121.9	−123.6	−120.5	−127.6	−130.5	−127.0
# 1057 Acetic acid	−103.3[a]	−101.0	−103.0	−102.2	−102.7	−106.0	−103.8
# 1058 Acetic acid	−103.3[a]	−101.0	−103.0	−102.2	−102.7	−106.0	−103.8
# 1061 Dimethyl peroxide	−30.1[a]	−37.3	−39.9	−36.1	−30.7	−34.6	−31.7
# 1062 Ethylene glycol	−93.9[a]	−91.7	−94.6	−94.8	−93.6	−98.1	−94.5
# 1067 2-Oxo-propanal	−64.8[a]	−74.0	−76.8	−73.2	−77.0	−81.4	−76.6

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Table S71: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 1068 2-Propenoic acid	−79.0[a]	−74.4	−77.2	−75.4	−74.8	−79.2	−75.6
# 1069 beta-Propiolactone	−67.6[a]	−54.2	−56.8	−55.3	−54.0	−58.3	−56.4
# 1070 1,3-Dioxalane	−72.1[a]	−78.5	−82.0	−79.9	−70.8	−76.2	−74.0
# 1071 Ethyl formate	−95.2[a]	−89.8	−93.3	−90.6	−87.7	−93.2	−90.4
# 1072 Methyl acetate	−97.9[a]	−95.7	−99.0	−96.2	−93.8	−99.0	−96.7
# 1073 Propionic acid	−108.4[a]	−106.3	−109.8	−107.6	−107.5	−113.0	−108.4
# 1074 1,3-Propanediol	−97.6[a]	−97.5	−101.7	−97.7	−98.1	−104.5	−97.8
# 1075 2-Methoxyethanol	−90.1[a]	−89.2	−93.1	−89.1	−86.3	−92.4	−87.6
# 1076 Dimethoxymethane	−83.2[a]	−85.6	−89.7	−86.7	−78.3	−84.5	−82.6
# 1077 Propylene glycol	−102.7[a]	−101.4	−105.9	−103.8	−102.1	−108.9	−102.5
# 1078 2-Butenoic acid	−88.1[a]	−84.7	−88.8	−85.7	−85.6	−91.9	−86.1
# 1079 2-Methyl-2-propenic acid	−87.8[a]	−83.7	−88.0	−84.3	−83.5	−90.2	−83.9
# 1080 Diacetyl	−78.2[a]	−89.2	−93.4	−88.5	−91.6	−98.2	−90.5
# 1081 gamma Butyrolactone	−87.0[a]	−88.9	−93.3	−89.7	−87.9	−94.7	−89.4
# 1082 Methyl 2-propenoate	−79.6[a]	−69.2	−73.1	−69.9	−66.0	−72.2	−68.5
# 1083 1,1 Dimethoxy ethene	−67.1[a]	−59.4	−64.3	−58.5	−51.3	−58.7	−54.6
# 1084 1,3 Dioxan	−80.9[a]	−82.9	−88.3	−84.7	−75.9	−84.1	−80.7
# 1085 1,4-Dioxane	−75.5[a]	−76.5	−81.8	−79.3	−72.4	−80.5	−76.3
# 1086 Ethyl acetate	−106.5[a]	−103.9	−108.5	−104.7	−102.1	−109.2	−104.7
# 1087 1,2-Dimethoxyethane	−81.9[a]	−85.5	−90.7	−85.3	−79.5	−87.4	−82.6
# 1088 1,4 Butandiol	−101.8[a]	−102.7	−108.4	−103.1	−103.6	−112.2	−103.4
# 1089 Diethyl peroxide	−46.1[a]	−48.9	−54.7	−49.4	−44.4	−53.0	−45.9
# 1090 Dimethyl acetal	−93.1[a]	−95.1	−100.7	−94.8	−86.5	−95.1	−90.9
# 1091 Acetylacetone	−91.9[a]	−99.2	−105.2	−99.3	−101.8	−111.0	−101.6
# 1092 Ethyl propionate	−111.5[a]	−109.1	−115.2	−110.2	−106.8	−116.1	−109.2
# 1093 Isopropyl acetate	−115.1[a]	−113.7	−120.2	−114.2	−111.3	−121.1	−113.8
# 1094 1,5 Pentandiol	−105.6[a]	−107.2	−114.3	−107.7	−108.3	−119.1	−108.3
# 1097 1,2-Benzenediol	−65.7[a]	−56.6	−62.7	−59.1	−60.3	−69.9	−60.1
# 1098 Hydroquinone	−66.2[a]	−60.6	−66.7	−63.1	−64.5	−74.0	−64.3
# 1099 Resorcinol	−68.0[a]	−62.6	−68.8	−65.0	−66.1	−75.7	−65.6
# 1100 1,3-Cyclohexanedione	−80.2[a]	−90.8	−98.1	−90.3	−94.4	−105.6	−94.2
# 1101 1,4-Cyclohexanedione	−79.5[a]	−90.4	−97.8	−90.2	−93.5	−104.8	−93.1
# 1102 2,4-Hexanedione	−105.1[a]	−104.4	−112.3	−104.7	−106.1	−118.1	−106.1
# 1103 2-Oxepanone	−94.7[a]	−91.6	−100.1	−93.2	−89.5	−102.3	−92.9
# 1104 3-Methyl-2,4-pentandione	−102.5[a]	−106.1	−114.1	−106.4	−107.2	−119.2	−107.1
# 1105 Ethyl-(E)-2-butenoate	−89.8[a]	−87.6	−94.2	−88.6	−84.9	−95.1	−86.9
# 1106 1,1-Dimethoxy-2-butene	−72.4[a]	−76.2	−84.1	−77.3	−67.9	−79.1	−72.2
# 1107 4-Hydroxy-4-methylpentan-2-one	−116.2[a]	−120.3	−129.3	−122.1	−119.9	−133.4	−120.4
# 1108 5,5-Dimethyl-1,3-dioxane	−100.7[a]	−98.2	−107.5	−101.0	−88.6	−102.6	−94.7
# 1109 cis-2,4-Dimethyl-1,3-dioxane	−102.3[a]	−104.6	−113.0	−105.4	−96.5	−109.4	−101.5
# 1110 Ethyl butanoate	−115.9[a]	−113.8	−121.4	−114.8	−111.6	−123.2	−114.3
# 1111 Hexanoic acid	−122.5[a]	−120.3	−128.3	−121.5	−121.9	−134.1	−123.5
# 1112 Methyl 2-methylbutanoate	−117.7[a]	−112.7	−121.0	−114.3	−109.1	−121.6	−111.7
# 1113 Methyl 2,2-dimethyl-propanoate	−118.2[a]	−117.1	−125.7	−118.7	−111.6	−124.7	−114.5
# 1114 Methyl 3-methylbutanoate	−119.0[a]	−112.3	−120.7	−113.5	−109.3	−121.8	−112.3
# 1115 Methyl pentanoate	−112.7[a]	−110.4	−118.1	−111.7	−108.2	−120.0	−111.3
# 1116 t-Butyl acetate	−123.4[a]	−123.9	−132.5	−125.6	−119.9	−132.9	−123.6
# 1117 trans 4,5-Dimethyl-1,3-dioxane	−98.2[a]	−99.7	−108.6	−101.7	−90.8	−104.3	−96.5
# 1118 1,1-Diethoxy ethane	−108.4[a]	−110.4	−119.5	−112.4	−103.0	−116.5	−107.8
# 1119 1,1-Dimethoxy-butane	−101.7[a]	−104.8	−113.7	−105.0	−96.1	−109.3	−100.9
# 1120 1,2-Diethoxy ethane	−97.6[a]	−101.2	−109.1	−99.8	−95.1	−107.1	−97.8
# 1121 1,6-Hexanediol	−109.8[a]	−111.9	−120.5	−112.6	−113.3	−126.4	−113.5
# 1122 2,3-Dimethyl-2,3-butanediol	−129.2[a]	−133.4	−143.9	−136.8	−129.8	−145.4	−131.0
# 1124 3-(2-Furanyl)-2-propenal	−25.3[a]	−21.1	−27.4	−21.5	−22.0	−31.7	−22.3
# 1125 Benzoic acid	−70.1[a]	−71.1	−78.0	−71.2	−71.0	−81.8	−71.3
# 1126 Phenyl formate	−51.5[a]	−49.3	−56.1	−48.3	−47.4	−58.0	−49.7
# 1127 Tropolone	−37.2[a]	−24.9	−32.0	−25.6	−27.3	−38.3	−26.2
# 1128 3-Methyl-1,2-benzenediol	−71.5[a]	−70.0	−77.9	−72.5	−73.3	−80.3	−72.6
# 1129 4-Methyl 1,2-Benzenediol	−71.3[a]	−65.7	−73.4	−68.4	−69.1	−81.0	−69.0
# 1130 Ethyl 2-methylene-3-butenoate	−69.2[a]	−61.6	−69.4	−62.4	−56.8	−68.8	−59.2
# 1131 Ethyl 2-pentynoate	−59.8[a]	−47.1	−54.0	−48.0	−45.5	−56.1	−46.7
# 1132 Ethyl 3-pentynoate	−56.8[a]	−50.5	−58.2	−52.6	−50.0	−60.6	−52.9
# 1133 Ethyl 4-pentynoate	−55.7[a]	−48.5	−55.9	−50.3	−46.5	−57.7	−48.9
# 1134 3,5-Heptanedione	−104.9[a]	−108.7	−118.8	−109.7	−110.4	−125.0	−110.5
# 1135 3-Ethyl-2,4-pentanedione	−105.1[a]	−110.8	−120.7	−111.6	−111.8	−126.6	−112.3

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 1136 5-Methyl-2,4-hexanedione	-108.2^{a}	-111.2	-120.9	-112.0	-112.2	-126.7	-112.6
# 1137 Butyl 2-propenoate	-89.7^{a}	-86.9	-95.2	-88.1	-83.8	-96.5	-86.4
# 1138 Ethyl (Z)-2-pentenoate	-94.3^{a}	-92.1	-100.3	-93.2	-89.4	-101.8	-91.6
# 1139 Ethyl (Z)-3-pentenoate	-92.6^{a}	-92.1	-100.2	-93.2	-89.8	-102.2	-92.3
# 1140 Ethyl 4-pentenoate	-92.1^{a}	-88.1	-96.5	-89.3	-85.6	-98.3	-88.4
# 1141 Ethyl trans-2-pentenoate	-94.2^{a}	-92.1	-100.3	-93.2	-89.4	-101.8	-91.6
# 1142 Heptanolactone	-98.3^{a}	-90.5	-101.2	-91.5	-88.8	-104.7	-91.6
# 1143 Isopropyl 2-butenoate	-98.2^{a}	-97.3	-105.8	-98.1	-94.1	-107.0	-96.6
# 1144 Propyl (E)-2-butenoate	-94.4^{a}	-92.5	-100.7	-93.5	-89.7	-102.1	-91.8
# 1145 (2a,4a,6b)-2,4,6-Trimethyl-1,3-dioxane	-106.8^{a}	-114.1	-124.3	-114.8	-105.5	-120.7	-110.7
# 1146 1,1-Dimethoxycyclopentane	-95.0^{a}	-101.8	-112.5	-102.9	-92.5	-108.5	-96.9
# 1147 1,1-Dimethylpropyl acetate	-128.8^{a}	-128.1	-138.7	-129.3	-123.6	-139.3	-126.7
# 1148 Ethyl 2-methylbutanoate	-123.3^{a}	-120.8	-130.8	-122.2	-117.3	-132.1	-120.0
# 1149 Ethyl 3-methylbutanoate	-126.0^{a}	-120.4	-130.6	-122.3	-117.5	-132.5	-120.7
# 1150 Ethyl pentanoate	-121.2^{a}	-118.4	-127.5	-119.8	-116.4	-130.2	-119.3
# 1151 Methyl 3,3-dimethylbutanoate	-122.3^{a}	-120.1	-130.8	-122.0	-115.4	-131.4	-119.3
# 1152 Methyl hexanoate	-118.0^{a}	-114.9	-124.2	-116.3	-113.0	-127.1	-116.4
# 1153 1,3-Diethoxypropane	-104.3^{a}	-106.2	-115.6	-104.9	-100.4	-114.6	-103.5
# 1154 1,7-Heptanediol	-114.1^{a}	-116.4	-126.6	-117.3	-118.0	-133.4	-118.5
# 1155 m-Methylbenzoic acid	-78.4^{a}	-80.4	-89.0	-81.3	-79.9	-93.1	-80.3
# 1156 Methyl benzoate	-66.8^{a}	-65.7	-74.0	-65.7	-62.1	-74.9	-64.2
# 1157 o-Methylbenzoic acid	-76.6^{a}	-79.6	-88.5	-80.1	-78.6	-92.3	-79.1
# 1158 p-Methylbenzoic acid	-79.0^{a}	-80.8	-89.4	-81.7	-80.4	-93.6	-81.4
# 1159 1,3-Dioxolane-2-phenyl	-49.1^{a}	-60.2	-70.7	-62.1	-51.0	-66.9	-54.9
# 1160 2,3-Dimethylbenzoic acid	-82.7^{a}	-88.9	-99.7	-89.3	-86.4	-102.8	-86.8
# 1161 2,4-Dimethylbenzoic acid	-84.8^{a}	-90.1	-100.6	-91.2	-88.8	-104.8	-89.9
# 1162 2,5-Dimethylbenzoic acid	-83.9^{a}	-89.5	-100.0	-90.0	-88.1	-104.2	-88.7
# 1163 2,6-Dimethylbenzoic acid	-81.6^{a}	-88.1	-98.9	-88.7	-86.4	-102.9	-87.3
# 1164 2-Ethylbenzoic acid	-81.4^{a}	-83.8	-94.7	-84.8	-82.3	-98.8	-83.2
# 1165 3,4-Dimethylbenzoic acid	-86.6^{a}	-90.0	-100.5	-90.5	-88.7	-104.7	-89.3
# 1166 3,5-Dimethylbenzoic acid	-87.1^{a}	-89.7	-99.9	-91.4	-88.8	-104.4	-89.4
# 1167 3-Ethylbenzoic acid	-82.9^{a}	-85.1	-95.5	-85.6	-84.5	-100.3	-85.1
# 1168 4-Ethylbenzoic acid	-85.0^{a}	-85.6	-95.9	-86.1	-85.0	-100.7	-85.5
# 1169 Methyl 4-methylbenzoate	-74.7^{a}	-75.3	-85.2	-76.1	-71.4	-86.6	-73.6
# 1170 1,2-Naphthalenediol	-47.9^{a}	-44.9	-55.7	-47.1	-47.0	-63.7	-46.3
# 1171 1,3-Naphthalenediol	-50.5^{a}	-47.4	-58.2	-49.5	-49.3	-65.8	-48.9
# 1172 1,4-Naphthalenediol	-47.1^{a}	-45.7	-56.5	-47.7	-47.7	-64.3	-47.3
# 1173 2,3-Naphthalenediol	-46.1^{a}	-41.4	-52.2	-43.8	-43.7	-60.2	-43.8
# 1174 1-Phenyl-1,3-butanedione	-58.3^{a}	-69.4	-80.9	-69.2	-69.0	-86.1	-68.9
# 1175 2,3,4-Trimethylbenzoic acid	-90.2^{a}	-95.8	-108.6	-96.4	-93.2	-112.5	-93.8
# 1176 2,3,5-Trimethylbenzoic acid	-91.3^{a}	-98.0	-110.5	-98.6	-95.1	-114.0	-95.8
# 1177 2,3,6-Trimethylbenzoic acid	-88.7^{a}	-96.3	-109.1	-97.2	-93.8	-113.1	-95.0
# 1178 2,4,5-Trimethylbenzoic acid	-92.3^{a}	-99.0	-111.5	-99.8	-96.9	-115.8	-97.7
# 1179 2,4,6-Trimethylbenzoic acid	-89.4^{a}	-97.8	-110.3	-99.2	-95.6	-114.5	-96.6
# 1180 2-Isopropyl benzoic acid	-85.8^{a}	-90.5	-103.3	-91.5	-87.7	-107.0	-89.0
# 1181 2-Methyl-2-phenyl-1,3-dioxolane	-62.6^{a}	-73.3	-85.8	-74.9	-63.2	-81.9	-67.1
# 1182 3,4,5-Trimethylbenzoic acid	-93.2^{a}	-97.8	-110.3	-98.4	-95.8	-114.6	-96.4
# 1183 3-Isopropyl benzoic acid	-89.8^{a}	-91.6	-104.0	-92.5	-90.2	-108.8	-91.3
# 1184 4-Isopropyl benzoic acid	-91.5^{a}	-91.8	-104.2	-92.7	-90.5	-109.1	-91.6
# 1185 2-Isopropyl-6-methyl-pyrocatechol	-90.6^{a}	-89.9	-103.4	-93.1	-91.4	-111.7	-91.5
# 1186 Cyclohexyl butanoate	-130.4^{a}	-126.3	-140.7	-127.8	-124.1	-145.6	-128.0
# 1187 Ethyl octanoate	-136.2^{a}	-132.2	-146.0	-133.9	-130.9	-151.5	-134.5
# 1188 1,10-Decanediol	-125.0^{a}	-130.1	-144.9	-131.6	-132.6	-154.7	-133.8
# 1189 1-Naphthoic acid	-53.3^{a}	-55.2	-67.0	-55.3	-52.8	-71.0	-53.3
# 1190 Isonaphthoic acid	-55.6^{a}	-55.1	-66.7	-55.2	-53.9	-71.7	-54.6
# 1191 2,3,4,5-Tetramethylbenzoic acid	-95.3^{a}	-105.0	-119.7	-105.4	-101.1	-123.2	-101.6
# 1192 2,3,4,6-Tetramethylbenzoic acid	-95.2^{a}	-104.3	-119.1	-105.2	-101.2	-123.3	-102.4
# 1193 2,3,5,6-Tetramethylbenzoic acid	-95.6^{a}	-104.5	-119.3	-105.7	-101.3	-123.3	-102.8
# 1194 p-tert-Butyl benzoic acid	-95.2^{a}	-98.2	-112.9	-99.4	-94.8	-116.9	-96.5
# 1195 Oxacyclododecan-2-one	-123.6^{a}	-115.8	-134.7	-120.3	-115.5	-142.9	-122.0
# 1196 Ethyl nonanoate	-141.1^{a}	-136.8	-152.1	-138.6	-135.7	-158.5	-138.9
# 1197 1,1-Dibutoxypropane	-132.1^{a}	-135.1	-151.5	-135.3	-126.4	-150.6	-131.6
# 1198 5,5-Dimethyl-2-phenyl-1,3-dioxane	-74.4^{a}	-78.1	-94.5	-80.2	-66.8	-91.2	-73.6
# 1199 Pentamethylbenzoic acid	-101.1^{a}	-109.8	-126.8	-110.6	-105.6	-130.9	-106.9
# 1200 2,2,6,6-Tetramethyl-3,5-heptanedione	-126.3^{a}	-141.6	-162.4	-146.0	-137.8	-167.6	-141.3

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 1201 Ethyl decanoate	−146.3[a]	−141.3	−158.2	−143.4	−140.6	−165.6	−144.6
# 1202 Xanthone	−23.5[a]	−26.8	−40.2	−27.7	−24.8	−45.4	−25.7
# 1203 Phenyl benzoate	−34.0[a]	−35.9	−49.3	−36.1	−32.8	−53.3	−35.3
# 1204 9,10-Anthroquinone	−18.1[a]	−32.7	−47.5	−31.4	−30.4	−53.0	−29.5
# 1205 9,10-Phenanthroquinone	−11.1[a]	−23.6	−38.5	−21.6	−21.6	−44.4	−20.7
# 1318 1,3,5-Trioxane	−111.3[a]	−114.5	−118.6	−116.3	−99.1	−105.5	−107.2
# 1319 Methyl hydroxyacetate	−133.1[a]	−130.5	−134.3	−132.3	−128.2	−134.1	−130.6
# 1320 Glycerol	−138.1[a]	−139.3	−144.4	−143.4	−140.1	−147.9	−140.8
# 1323 Maleic anhydride	−95.2[a]	−87.1	−90.4	−87.4	−87.2	−92.5	−90.4
# 1324 Acetic anhydride	−137.1[a]	−139.5	−143.9	−139.7	−138.8	−145.7	−142.3
# 1325 Trimethoxymethane	−127.1[a]	−129.8	−136.2	−131.1	−115.0	−124.5	−122.5
# 1326 2,5,8-Trioxanonane	−124.6[a]	−125.5	−133.8	−124.8	−116.1	−128.7	−120.9
# 1328 m-Salicylic acid	−112.1[a]	−110.8	−118.4	−112.7	−112.5	−124.2	−112.9
# 1329 o-Salicylic acid	−118.5[a]	−114.7	−122.5	−116.8	−116.0	−128.0	−115.9
# 1330 p-Salicylic acid	−117.7[a]	−112.3	−119.8	−114.1	−113.8	−125.5	−114.0
# 1331 2,3-Butanediol, 2,3-dimethyl-, monoformate	−161.7[a]	−162.7	−174.8	−164.4	−155.8	−173.8	−159.8
# 1332 Trimethoxymethyl benzene	−103.6[a]	−112.5	−125.9	−113.9	−94.9	−115.5	−103.0
# 1333 1-tert-Butoxy-3-propoxy-2-propanol	−169.2[a]	−169.9	−186.1	−172.4	−162.1	−185.8	−166.8
# 1334 1-Butoxy-3-tert-butyl-2-propanol	−172.8[a]	−175.6	−193.1	−177.3	−167.7	−193.5	−172.9
# 1335 Benzoic acid, anhydride	−76.3[a]	−79.4	−93.2	−79.0	−75.2	−97.7	−78.7
# 1375 Oxalic acid	−175.0[a]	−162.5	−165.0	−163.1	−164.2	−168.1	−164.3
# 1378 Dioxybismethanol	−124.5[a]	−123.2	−127.0	−125.6	−115.4	−121.2	−119.0
# 1380 1,4-Dioxan-2,5-dione	−146.3[a]	−146.1	−151.0	−147.0	−141.1	−148.6	−146.1
# 1381 Dimethyl oxalate	−169.5[a]	−158.8	−163.6	−159.9	−152.9	−160.4	−157.1
# 1382 1,3,5,7-Tetroxane	−148.2[a]	−151.3	−157.9	−152.5	−130.9	−140.7	−142.9
# 1383 Dimethyl malonate	−176.4[a]	−171.4	−177.8	−173.1	−167.4	−177.1	−172.7
# 1384 Ethylmalonic acid	−203.1[a]	−195.3	−202.8	−197.7	−196.6	−207.9	−199.0
# 1385 Methylene diacetate	−186.6[a]	−185.7	−191.9	−186.0	−178.8	−188.4	−184.3
# 1386 Tetramethoxymethane	−173.8[a]	−180.0	−188.5	−180.6	−157.6	−170.2	−167.9
# 1387 1,1-Diacetoxyethane	−194.2[a]	−198.5	−207.0	−199.6	−191.0	−203.6	−197.2
# 1388 Dimethyl methylmalonate	−183.7[a]	−180.2	−188.5	−182.1	−174.3	−187.0	−179.9
# 1389 2,2-Diacetoxypropane	−199.3[a]	−207.5	−217.9	−208.8	−198.2	−213.7	−205.5
# 1390 Diethyl malonate	−190.1[a]	−188.4	−198.2	−191.1	−184.2	−197.9	−189.0
# 1391 Dimethyl dimethylmalonate	−191.9[a]	−190.2	−200.8	−191.6	−180.7	−197.3	−187.0
# 1392 3,5,7,9-Tetraoxyundecane	−177.1[a]	−175.7	−187.0	−176.5	−158.9	−173.5	−167.0
# 1393 12-Crown-4	−150.8[a]	−149.4	−163.7	−155.5	−140.4	−161.4	−151.8
# 1394 5,8-Dihydroxy-1,4-naphthalenedione	−119.3[a]	−120.7	−132.3	−123.7	−121.2	−139.0	−120.1
# 1395 Dimethyl isophthalate	−150.4[a]	−149.0	−160.6	−150.2	−141.7	−159.5	−146.4
# 1396 Dimethyl phthalate	−144.9[a]	−144.8	−157.3	−146.8	−137.9	−156.5	−143.5
# 1397 1-(tert-Butyldioxy)-3-propoxy-2-propanol	−157.0[a]	−157.7	−175.1	−162.0	−149.9	−173.9	−154.2
# 1400 Benzal diacetate	−167.3[a]	−166.6	−180.5	−168.0	−157.9	−178.5	−164.7
# 1401 1-Butoxy-1-tert-butyldioxy-2-propanol	−161.3[a]	−175.3	−194.8	−178.2	−163.7	−190.6	−168.9
# 1402 1,1-Ethanediol, 2-phenyl-, diacetate	−167.3[a]	−173.0	−188.7	−174.5	−164.8	−188.0	−172.3
# 1403 Benzyl diacetate	−161.8[a]	−173.0	−188.7	−174.5	−164.8	−188.0	−172.3
# 1406 1,4,9,10-Anthracenetetrone	−50.0[a]	−70.8	−86.1	−69.0	−70.5	−93.8	−69.9
# 1407 1,4-Dihydroxy-9,10-anthracenedione	−112.6[a]	−121.0	−137.4	−123.9	−120.0	−145.0	−119.0
# 1408 Diphenyl oxalate	−104.5[a]	−99.4	−114.2	−100.4	−94.5	−117.2	−99.3
# 1409 Dimethyl naphthalene-2,6-dicarboxylate	−132.7[a]	−133.6	−149.9	−134.6	−125.0	−149.7	−130.1
# 1412 p-Diacetylbenzene diethyl ketal	−189.7[a]	−205.0	−233.6	−209.1	−182.7	−225.7	−190.1
# 1431 Tartronic acid	−227.5[a]	−220.1	−224.6	−223.1	−221.0	−228.1	−222.7
# 1432 1,3,5,7,9-pentaoxecane	−186.4[a]	−194.2	−203.5	−195.8	−167.6	−181.3	−182.0
# 1433 3,5,7,9,11-Pentaoxa-tridecane	−216.5[a]	−219.1	−231.6	−220.6	−195.5	−215.2	−208.2
# 1434 15-Crown-5	−191.1[a]	−192.2	−210.9	−198.7	−179.8	−206.7	−193.9
# 1447 Trimethyl methanetricarboxylate	−252.1[a]	−247.1	−257.2	−250.6	−239.7	−254.8	−248.7
# 1448 Triethyl methanetricarboxylate	−280.4[a]	−273.4	−289.0	−278.7	−265.2	−286.6	−273.7
# 1449 Triethyl 1,1,1-ethanetricarboxylate	−286.2[a]	−283.9	−302.1	−289.9	−273.1	−299.3	−282.7
# 1466 Tetraethylpyromellitate	−353.0[a]	−338.3	−365.2	−346.5	−324.5	−364.7	−338.4
# 1467 Tetrapropyl 1,2,4,5-benzene tetracarboxylate	−370.0[a]	−360.6	−395.9	−367.5	−344.5	−394.9	−360.0
# 1496 Fluoromethane (Geo)	−56.8[a]	−60.4	−61.1	−58.6	−57.3	−58.5	−57.8
# 1498 Fluoroacetylene (Geo)	30.0[a]	26.9	26.2	26.8	23.9	22.9	24.1
# 1500 Fluoroethylene (Geo)	−32.5[a]	−32.3	−33.5	−31.7	−32.2	−34.1	−32.6
# 1586 Trifluoromethane (Geo)	−166.3[a]	−166.8	−167.6	−168.0	−162.0	−163.3	−162.4
# 1494 Fluoromethyl, cation	200.3[a]	193.7	193.2	191.7	199.2	198.4	198.8
# 1502 CH3CHF, cation	166.0[a]	158.1	156.6	155.6	161.7	159.2	161.4
# 1503 Fluoroethane	−62.9[a]	−67.5	−69.4	−66.1	−65.8	−68.8	−65.9

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 1505 2-Fluoropropane	−69.4[a]	−76.2	−79.4	−75.4	−75.1	−80.2	−75.3
# 1506 Fluorobenzene	−27.8[a]	−27.3	−32.3	−26.7	−28.0	−35.9	−27.9
# 1507 Fluorocyclohexane	−80.4[a]	−78.4	−86.3	−78.1	−78.0	−90.2	−79.0
# 1508 1-Fluorononane	−101.2[a]	−99.6	−111.8	−99.3	−99.3	−117.8	−100.9
# 1544 Difluoromethyl, cation	142.4[a]	136.8	136.3	135.6	141.5	140.6	144.8
# 1545 Difluoromethane, cation	185.2[a]	173.7	172.9	173.1	180.1	178.9	182.5
# 1546 Difluoromethane	−108.1[a]	−110.9	−111.6	−109.4	−106.6	−107.8	−107.1
# 1550 gem-Difluoroethylene	−80.5[a]	−72.2	−73.5	−70.8	−71.7	−73.7	−72.2
# 1551 CH3CF2, cation	107.0[a]	106.6	105.1	103.1	108.4	105.9	111.2
# 1552 1,1-Difluoroethane	−118.8[a]	−121.8	−123.6	−121.5	−119.4	−122.4	−119.8
# 1554 1,2-Difluorobenzene	−67.7[a]	−69.1	−74.1	−68.7	−69.9	−77.9	−70.0
# 1555 1,3-Difluorobenzene	−73.9[a]	−72.9	−78.0	−72.5	−74.0	−82.0	−74.0
# 1556 1,4-Difluorobenzene	−73.3[a]	−72.6	−77.6	−72.2	−73.5	−81.5	−73.8
# 1585 Trifluoromethane, cation	151.9[a]	137.2	136.4	134.4	143.8	142.2	147.4
# 1588 Trifluoroethylene	−117.3[a]	−116.4	−117.7	−116.3	−115.9	−118.0	−116.3
# 1589 CF3CH2, cation	114.0[a]	111.1	109.5	101.3	118.7	116.1	112.4
# 1590 CH2F.CF2, cation	81.0[a]	75.0	73.4	73.1	80.4	77.8	82.9
# 1591 CF3CH2.	−123.6[a]	−127.3	−129.0	−132.1	−124.3	−126.9	−126.7
# 1592 1,1,1-Trifluoroethane	−178.9[a]	−178.4	−180.4	−181.8	−176.3	−179.4	−176.9
# 1593 (Trifluoromethyl)-benzene	−138.9[a]	−145.5	−152.3	−147.9	−141.6	−152.1	−142.8
# 1594 Trifluoromethylbenzene	−143.2[a]	−145.5	−152.3	−147.9	−141.6	−152.2	−142.2
# 1617 1,2,4,5-Tetrafluorobenzene	−154.6[a]	−154.5	−159.7	−154.6	−155.9	−164.1	−156.2
# 1618 1-Fluoro-3-(trifluoro-methyl)benzene	−189.4[a]	−190.3	−197.1	−193.7	−186.9	−197.5	−188.3
# 1625 Pentafluorobenzene	−192.5[a]	−191.8	−197.1	−191.8	−192.7	−201.0	−192.7
# 1626 2,3,4,5,6-Pentafluorotoluene	−201.6[a]	−200.9	−207.7	−201.3	−200.6	−211.3	−201.1
# 921 Hydrogen isocyanate (Geo)	−24.3[a]	−7.2	−7.9	−13.8	−19.5	−20.7	−25.0
# 924 Formamide (Geo)	−44.5[a]	−39.8	−41.1	−43.2	−46.3	−48.4	−48.5
# 1358 Pro-pro (Geo)	−131.4[a]	−126.2	−143.7	−129.1	−124.4	−149.8	−132.0
# 1360 Val-val (Geo)	−160.6[a]	−163.6	−182.6	−173.1	−167.4	−195.0	−173.8
# 1362 Ile-ile (Geo)	−176.5[a]	−171.8	−194.8	−181.7	−175.4	−208.6	−182.4
# 1456 Trinitromethane (Geo)	−3.2[a]	6.1	1.1	0.9	9.0	1.6	13.4
# 1473 Pentaerythritol tetranitrate (Geo)	−92.5[a]	−117.4	−134.2	−127.3	−96.9	−121.6	−105.5
# 925 Acetaldoxime	−5.4[a]	−2.7	−5.1	−5.5	−8.4	−12.2	−10.2
# 926 Acetamide	−57.0[a]	−50.7	−53.2	−55.6	−57.4	−61.4	−59.1
# 927 Isoxazole	19.6[a]	23.9	21.3	25.1	24.2	20.0	24.2
# 928 Oxalone	−3.7[a]	2.8	0.3	3.8	5.2	1.1	7.7
# 929 Acrylamine	−31.1[a]	−24.4	−27.6	−29.4	−29.9	−35.0	−31.8
# 930 Methoxyacetonitrile	−8.5[a]	−10.7	−13.7	−10.8	−10.0	−14.7	−11.3
# 931 Dimethylformamide	−45.8[a]	−43.5	−47.6	−39.4	−41.4	−47.7	−45.5
# 932 N-Methyl acetamide	−59.3[a]	−50.6	−54.7	−51.6	−53.2	−59.6	−55.9
# 933 Propanamide	−61.9[a]	−55.3	−59.3	−60.9	−61.7	−68.0	−64.1
# 934 Dimethylaminomethanol	−48.6[a]	−47.0	−52.1	−45.0	−41.3	−48.8	−45.4
# 935 3-Methyl isoxazole	8.5[a]	16.4	12.4	15.8	16.1	9.9	15.6
# 936 5-Methyl isoxazole	8.1[a]	12.6	8.7	14.3	13.0	6.8	13.1
# 937 2-Pyrrolidinone	−47.2[a]	−42.5	−47.6	−44.9	−46.9	−54.7	−49.9
# 938 4,5-Dihydro-2-methyl oxazole	−31.2[a]	−25.6	−30.2	−27.4	−23.9	−31.1	−25.7
# 939 Methacrylamide	−37.7[a]	−33.5	−38.4	−38.2	−38.7	−46.3	−40.3
# 940 2-Methyl propanamide	−67.5[a]	−62.8	−68.7	−68.1	−68.3	−77.2	−70.3
# 941 Butanamide	−66.7[a]	−60.1	−65.7	−65.9	−66.7	−75.2	−68.7
# 942 Isobutylamide	−67.5[a]	−62.8	−68.7	−68.1	−68.3	−77.2	−70.3
# 944 N,N-Diethyl-hydroxylamine	−29.1[a]	−24.5	−30.9	−25.0	−23.1	−32.8	−28.3
# 945 2-Pyridinol	−19.0[a]	−11.5	−16.5	−11.9	−14.9	−22.8	−14.2
# 946 3-Pyridinol	−10.4[a]	−9.0	−14.1	−7.5	−11.8	−19.8	−8.9
# 947 4-Pyridinol	−7.2[a]	−9.9	−15.0	−9.0	−12.5	−20.5	−10.7
# 948 Pyridine 1 oxide	21.0[a]	25.6	20.5	28.0	26.8	18.7	33.7
# 949 3,5-Dimethyl isoxazole	−4.3[a]	5.2	−0.2	5.0	5.0	−3.3	4.6
# 950 1-Methyl-2-pyrrolidinone	−50.4[a]	−46.2	−52.8	−44.7	−45.8	−56.0	−49.8
# 951 2-Ethyl-4,5-dihydro-oxazole	−35.6[a]	−30.6	−36.8	−32.5	−28.6	−38.1	−30.9
# 952 N,N-Dimethylamino-2-propen-3-al	−24.9[a]	−20.0	−26.3	−15.5	−17.2	−26.8	−19.8
# 953 1-(Dimethylamino)-2-propanone	−43.0[a]	−48.7	−56.3	−46.5	−42.6	−53.9	−46.1
# 954 2,2-Dimethyl-propanamide	−74.8[a]	−70.8	−78.9	−77.0	−74.5	−86.6	−76.9
# 955 N,N-Dimethyl propanamide	−59.8[a]	−57.8	−65.2	−55.2	−55.0	−66.1	−58.7
# 956 2-Hydroxy-6-methylpyridine	−28.8[a]	−19.6	−26.2	−22.1	−23.5	−33.7	−23.7
# 957 2-Methyl-3-pyridinol	−20.2[a]	−16.9	−23.6	−16.8	−20.0	−30.5	−17.2
# 958 3-Hydroxy-2-methylpyridine	−20.2[a]	−16.6	−23.3	−17.3	−19.9	−30.3	−17.4

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 959 3-Hydroxy-6-methylpyridine	−16.7[a]	−16.7	−23.3	−17.4	−20.2	−30.4	−17.6
# 960 4-Hydroxy-2-methylpyridine	−17.1[a]	−18.1	−24.7	−18.8	−21.2	−31.4	−20.2
# 961 6-Methyl-2(1H)-pyridinone	−28.8[a]	−19.8	−26.5	−21.4	−25.3	−35.7	−26.2
# 962 m-Amino phenol	−23.6[a]	−16.0	−22.7	−20.8	−20.6	−31.0	−20.6
# 963 o-Amino phenol	−25.0[a]	−14.6	−21.5	−18.8	−19.6	−30.2	−19.1
# 964 p-Amino phenol	−21.6[a]	−13.9	−20.6	−18.8	−18.6	−29.0	−19.0
# 965 Trimethyl isoxazole	−4.8[a]	−3.4	−10.6	−3.1	−3.1	−14.1	−3.6
# 966 Caprolactam	−57.3[a]	−47.5	−56.8	−49.5	−52.1	−66.1	−55.0
# 967 Cyclohexanone oxime	−17.9[a]	−13.3	−22.1	−15.6	−19.8	−33.0	−22.0
# 968 N,N-Diethyl acetamide	−68.6[a]	−61.8	−71.4	−60.8	−61.2	−75.5	−65.9
# 969 N,N-Dimethylbutyramine	−64.7[a]	−62.7	−71.5	−60.3	−60.0	−73.3	−64.0
# 970 Benzoxazole	10.8[a]	17.1	10.5	17.1	18.4	8.1	19.8
# 971 Isocyanatobenzene	−3.5[a]	17.1	10.5	14.5	7.8	−2.3	2.9
# 972 Benzamide	−24.1[a]	−20.1	−27.7	−24.3	−25.2	−36.9	−26.7
# 973 N,N-Dimethylamino-2,4-pentadiene-5-al	−6.9[a]	−3.1	−11.5	1.1	0.1	−12.7	−3.1
# 974 2-Methoxy-3,3-dimethylbutanenitrile	−39.4[a]	−43.6	−54.3	−45.9	−38.7	−54.5	−42.0
# 975 N,N-Diethylaminoacetone	−55.8[a]	−55.7	−67.3	−56.3	−52.5	−69.7	−57.3
# 976 N,N-Dimethyl-tert-butylcarboxamide	−68.4[a]	−70.0	−81.8	−68.0	−64.0	−81.5	−68.6
# 977 alpha-oxo Benzeneacetonitrile	28.1[a]	17.4	9.8	17.8	15.0	3.3	16.1
# 978 1,3-dimethyl-2-nitroso-benzene	33.4[a]	19.7	10.1	19.9	17.3	2.7	19.0
# 979 N-methyl-N-phenyl formamide	−18.1[a]	−11.6	−21.0	−8.4	−9.8	−24.2	−14.0
# 980 Octanone-1-oxime	−35.7[a]	−30.5	−41.9	−34.3	−37.4	−54.6	−40.4
# 981 Octanone-2-oxime	−43.2[a]	−33.6	−45.3	−36.5	−40.1	−57.7	−42.8
# 982 Octanone-3-oxime	−41.3[a]	−34.0	−46.1	−37.0	−39.9	−57.9	−42.4
# 983 Octanone-4-oxime	−43.3[a]	−34.1	−46.3	−37.1	−39.9	−57.9	−42.4
# 984 2(1H)-Quinolinone	−6.1[a]	0.1	−9.6	−1.5	−3.5	−18.4	−5.5
# 985 3-Phenyl isoxazole	33.3[a]	47.0	37.9	46.9	48.0	33.8	46.6
# 986 4-Quinolinol	5.0[a]	7.1	−2.5	7.2	5.7	−9.2	7.0
# 987 5-Phenyl isoxazole	38.3[a]	42.5	33.5	44.4	44.1	30.1	44.1
# 988 8-Quinolinol	1.6[a]	5.8	−3.8	6.1	3.3	−11.5	5.4
# 989 a-Cyanoacetophenone	16.8[a]	10.5	1.3	10.9	7.7	−6.3	7.9
# 990 2,4,6-Trimethylnitrosobenzene	25.7[a]	9.7	−1.6	9.2	7.7	−9.3	9.4
# 991 N,N-Dimethyl benzamide	−20.6[a]	−21.9	−33.1	−18.9	−18.2	−35.1	−22.4
# 992 N,N-Dimethyamino-2,4,6-heptatriene-7-al	5.2[a]	12.7	2.3	16.6	16.2	0.4	12.4
# 993 2,2,6,6-Tetramethyl-4-piperidinone	−65.4[a]	−64.7	−80.5	−70.0	−64.2	−87.4	−67.9
# 994 2-Methyl-4-hydroxyquinoline	−5.6[a]	−1.2	−12.4	−3.3	−3.0	−20.1	−2.0
# 995 2-Methyl-8-quinolinol	−9.4[a]	−2.5	−13.7	−3.8	−5.3	−22.5	−3.6
# 996 3-Methyl-5-phenyl isoxazole	24.5[a]	35.0	24.6	35.1	36.1	19.9	35.5
# 997 4-Methyl-2-hydroxyquinoline	−14.6[a]	−3.6	−15.0	−5.3	−5.0	−22.4	−5.5
# 998 5-Methyl-3-phenyl isoxazole	23.6[a]	35.7	25.2	36.6	36.7	20.5	36.1
# 999 beta-Cyanopropiophenone	7.2[a]	1.6	−9.1	1.6	−0.5	−16.8	−0.6
# 1000 2,4,6-Trimethylbenzonitrile, N-oxide	32.7[a]	35.9	24.0	31.1	30.2	12.3	30.3
# 1001 2-(Dimethylamino)-acetophenone	−11.1[a]	−18.4	−31.7	−16.0	−10.4	−30.1	−14.5
# 1002 N,N,4-Trimethyl benzamide	−26.9[a]	−31.4	−44.2	−28.6	−27.3	−46.6	−31.6
# 1003 (E)-3-(Methylamino)-1-phenyl-but-2-enone	−12.8[a]	−9.6	−23.0	−9.4	−9.2	−29.4	−9.8
# 1004 1-Propanone, 2-(dimethylamino)-1-phenyl-	−16.7[a]	−23.9	−39.4	−21.3	−16.0	−38.8	−20.2
# 1005 2-Propanamine, 2-methyl-N-(phenylmethyle	7.4[a]	8.8	−6.2	9.1	12.8	−9.6	14.8
# 1006 1-Adamantanecarboxamide	−76.2[a]	−67.6	−86.5	−74.9	−72.1	−100.1	−77.2
# 1007 N,N-Dimethylnonamide	−89.4[a]	−85.4	−101.9	−84.1	−84.1	−108.7	−89.3
# 1008 Phenoxazine	22.5[a]	32.0	18.9	29.6	33.7	13.8	30.4
# 1009 2-(Diethylamino)-1-phenylethanone	−23.0[a]	−25.1	−42.9	−25.9	−19.0	−44.7	−24.8
# 1010 9,10-Dihydro-9-oxoacridine	8.3[a]	11.6	−2.8	10.9	11.4	−10.5	11.0
# 1011 Benzenamine, N-(phenylmethylene)-, N-oxide	62.9[a]	63.4	47.8	64.2	65.8	42.6	69.1
# 1012 1-Propanone, 2-(diethylamino)-1-phenyl-	−29.7[a]	−30.3	−50.3	−31.3	−25.1	−54.1	−31.1
# 1013 N,N-Dimethyl-1-adamantylcarboxamide	−68.4[a]	−69.3	−91.9	−69.4	−64.5	−97.7	−72.0
# 1014 4-Isopropylbenzylidene t-butylamine N-oxide	−12.2[a]	−11.5	−31.9	−12.0	−6.2	−36.4	−5.1
# 1017 Urea	−58.7[a]	−39.9	−42.1	−50.6	−49.3	−52.8	−54.2
# 1018 N-Methyl urea	−56.3[a]	−40.9	−44.5	−47.5	−46.3	−51.8	−51.7
# 1019 Dimethyl furazan	25.6[a]	33.2	27.9	33.4	31.5	23.4	30.6
# 1020 Isopropylurea	−69.3[a]	−52.8	−59.6	−61.2	−59.5	−69.7	−65.5
# 1021 5-Amino-3,4-dimethylisoxazole	1.2[a]	13.7	6.9	9.5	10.9	0.6	8.8
# 1022 (1-Methylpropyl) urea	−73.4[a]	−57.3	−66.1	−66.2	−64.1	−77.1	−70.6
# 1023 N,N-diethylurea	−65.1[a]	−51.6	−60.8	−56.1	−54.0	−67.5	−61.3
# 1024 Tetramethylurea	−49.1[a]	−42.5	−51.4	−37.9	−33.5	−46.7	−42.1
# 1027 4-Amino-2(1H)-pyrimidinone	−14.2[a]	9.5	3.8	2.3	2.9	−5.9	−0.7

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 1213 Methyl nitrite	-15.8^{a}	−16.8	−18.4	−17.4	−20.0	−22.6	−20.3
# 1214 Nitromethane	-17.9^{a}	−17.3	−19.1	−17.0	−15.7	−18.5	−12.9
# 1215 Ethyl nitrite	-25.9^{a}	−24.9	−27.9	−25.8	−28.1	−32.8	−28.3
# 1216 Glycine	-93.7^{a}	−90.8	−93.9	−93.3	−94.1	−99.0	−94.2
# 1217 Methyl carbamate	-101.6^{a}	−85.9	−88.9	−92.0	−88.7	−93.3	−93.3
# 1218 Nitroethane	-23.5^{a}	−23.4	−26.6	−23.8	−22.1	−26.8	−19.8
# 1219 Alanine	-99.1^{a}	−98.4	−103.2	−102.2	−101.2	−108.5	−101.4
# 1220 beta-Alanine	-101.0^{a}	−94.1	−98.6	−98.6	−97.7	−104.7	−99.1
# 1221 Isopropylnitrite	-31.9^{a}	−35.0	−39.5	−35.5	−37.4	−44.3	−37.6
# 1222 N-Methylglycine	-87.8^{a}	−89.6	−94.1	−90.8	−88.4	−95.3	−90.7
# 1223 Propyl nitrite	-28.4^{a}	−30.3	−34.7	−30.4	−33.1	−39.7	−33.1
# 1224 Urethane	-106.7^{a}	−94.2	−98.4	−99.8	−97.0	−103.6	−101.3
# 1225 Methyl cyanoacetate	-58.2^{a}	−57.7	−62.0	−58.5	−57.8	−64.4	−60.4
# 1226 Succinimide	-89.8^{a}	−79.7	−84.6	−83.5	−88.3	−95.9	−93.3
# 1227 2-Nitrobutane	-39.1^{a}	−36.2	−42.9	−38.0	−34.8	−44.9	−33.7
# 1228 2-Nitroisobutane	-42.2^{a}	−39.8	−46.7	−42.2	−37.8	−48.2	−37.3
# 1229 4-Aminobutanoic acid	-105.0^{a}	−98.8	−104.9	−103.4	−102.6	−111.9	−104.1
# 1230 Isobutyl nitrite	-36.1^{a}	−36.8	−43.0	−37.3	−38.9	−48.2	−39.4
# 1231 n-Butyl nitrite	-34.8^{a}	−34.2	−40.1	−35.4	−37.6	−46.6	−38.0
# 1232 Sec-butyl nitrite	-36.5^{a}	−39.8	−46.0	−40.4	−41.9	−51.3	−42.2
# 1233 t-Butyl nitrite	-41.0^{a}	−45.6	−52.1	−46.6	−46.6	−56.5	−47.1
# 1234 Diethanolamine	-94.9^{a}	−86.5	−93.2	−91.2	−86.7	−96.8	−89.8
# 1235 N-Methylmaleimide	-61.2^{a}	−44.4	−50.0	−44.7	−46.5	−55.2	−53.8
# 1236 Glutarimide	-94.1^{a}	−87.4	−94.2	−90.6	−94.8	−105.2	−99.6
# 1237 N-Methylsuccinimide	-93.1^{a}	−82.8	−89.3	−83.1	−86.3	−96.2	−92.7
# 1238 Proline	-87.5^{a}	−87.9	−95.3	−90.6	−88.9	−100.8	−90.7
# 1239 5-Aminovaleric acid	-110.0^{a}	−103.5	−111.1	−108.3	−107.6	−119.1	−109.4
# 1240 N,N-Dimethylglycine methyl ester	-88.5^{a}	−86.7	−94.4	−84.8	−77.2	−88.6	−82.5
# 1241 tert-Pentyl nitrite	-45.8^{a}	−49.6	−58.1	−50.7	−50.1	−62.8	−50.7
# 1242 Valine	-108.2^{a}	−109.5	−118.1	−114.1	−111.4	−124.2	−112.6
# 1243 1,1-Dimethoxy-trimethylamine	-85.0^{a}	−85.9	−94.6	−83.9	−71.6	−84.4	−80.0
# 1244 Niacin	-52.9^{a}	−57.7	−64.2	−56.1	−58.9	−69.0	−57.6
# 1245 Nitrobenzene	15.4^{a}	13.0	6.4	12.1	14.3	4.1	18.0
# 1247 Ethyl 2-cyanopropionate	-74.6^{a}	−74.7	−82.3	−76.0	−73.6	−85.0	−76.1
# 1248 Ethyl N,N-dimethylglycinate	-97.3^{a}	−94.9	−104.1	−93.4	−85.3	−99.0	−90.8
# 1249 Hexanoic acid, 6-amino-	-115.3^{a}	−108.1	−117.3	−111.8	−113.2	−127.0	−115.3
# 1250 Isoleucine	-110.0^{a}	−110.7	−121.3	−116.3	−113.1	−128.8	−115.6
# 1251 Leucine	-113.1^{a}	−113.5	−123.6	−118.1	−115.8	−130.8	−117.2
# 1252 Methyl N,N-dimethylalaninate	-94.3^{a}	−93.7	−103.5	−91.6	−84.3	−98.4	−89.1
# 1253 N,N-Dimethylacetamide dimethyl acetal	-92.5^{a}	−94.3	−105.5	−94.3	−79.3	−95.6	−88.0
# 1254 m-Aminobenzoic acid	-69.2^{a}	−64.6	−72.8	−68.9	−67.1	−79.6	−68.0
# 1255 o-Aminobenzoic acid	-70.8^{a}	−67.3	−75.7	−72.0	−70.0	−82.8	−70.4
# 1256 p-Aminobenzoic acid	-70.2^{a}	−66.5	−74.6	−70.9	−69.3	−81.9	−70.1
# 1257 p-Nitrotoluene	7.4^{a}	2.9	−5.2	1.4	4.6	−8.0	7.8
# 1258 Phenylnitromethane	7.3^{a}	8.2	−0.2	7.9	9.7	−3.0	11.3
# 1260 Methyl N,N-,a,a-tetramethylglycinate	-108.1^{a}	−99.8	−112.2	−98.8	−89.4	−107.4	−95.0
# 1261 2,6-Dimethylnitrobenzene	2.1^{a}	−4.3	−14.7	−5.4	−1.0	−16.8	2.1
# 1262 2-Amino-2-phenylacetic acid	-67.0^{a}	−65.8	−76.0	−69.9	−68.1	−83.6	−69.6
# 1263 2-Nitro-m-xylene	2.1^{a}	−4.3	−14.7	−5.4	−1.0	−16.8	2.1
# 1264 N-Phenylglycine	-64.2^{a}	−60.0	−69.9	−60.5	−60.7	−75.5	−62.2
# 1265 8-Aminocaprylic acid	-125.0^{a}	−117.3	−129.5	−122.7	−122.1	−140.4	−124.6
# 1266 2-Methyl-1H-isoindole-1,3(2H)-dione	-55.9^{a}	−43.4	−53.4	−43.2	−44.9	−60.3	−51.6
# 1267 Nitromesitylene	-6.4^{a}	−14.2	−26.3	−16.0	−10.5	−28.8	−8.0
# 1268 Phenylalanine	-69.3^{a}	−71.0	−83.1	−75.7	−73.7	−91.7	−75.8
# 1269 2,2,6,6-Tetramethyl-4-oxo-1-piperidinyloxy	-51.5^{a}	−64.7	−80.8	−67.6	−60.5	−84.1	−65.5
# 1270 1-Hydroxy-2,2,6,6-tetramethyl-4-piperidinone	-71.2^{a}	−75.1	−92.1	−80.6	−70.8	−95.6	−79.8
# 1271 4-Hydroxy-2,2,6,6-tetramethyl-1-piperidinyloxy	-69.6^{a}	−74.3	−91.3	−78.2	−69.0	−93.8	−74.6
# 1272 1-Hydroxy-2,2,6,6-tetramethyl-4-piperidinol	-82.5^{a}	−83.7	−101.5	−90.0	−78.3	−104.3	−87.9
# 1273 1-Nitroso-2-naphthalenol	8.6^{a}	6.8	−4.6	6.0	5.2	−12.4	8.2
# 1274 1-Nitroso-4-naphthalenol	17.8^{a}	11.0	−0.3	10.4	7.5	−9.8	9.8
# 1275 2-Nitroso-1-naphthalenol	8.9^{a}	6.6	−4.8	6.0	4.8	−12.6	8.1
# 1276 N,N-Dimethyl 4-methoxybenzamide	-53.7^{a}	−57.0	−70.3	−55.3	−51.0	−70.9	−56.8
# 1277 1-Nitroadamantane	-45.7^{a}	−40.0	−57.5	−44.3	−37.1	−63.2	−39.1
# 1278 2-Nitroadamantane	-43.0^{a}	−36.6	−54.3	−39.6	−34.3	−60.5	−35.7
# 1279 Phenol, 2-[(phenylimino)methyl]-, N-oxide	12.9^{a}	14.5	−0.8	13.4	13.7	−9.4	13.4

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Table S71: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 1280 Benzenamine, N-[(4-methoxyphenyl)methyle]-, N-oxide	26.2[a]	25.1	8.7	25.7	30.9	6.0	33.4
# 1281 N-(3-Phenoxy-2-hydroxypropyl)aniline	−44.1[a]	−28.7	−47.1	−33.1	−26.1	−54.3	−30.2
# 1283 Oxalamide	−92.5[a]	−80.4	−83.9	−88.7	−92.8	−98.1	−94.8
# 1285 N-Nitrodimethylamine	−3.2[a]	−7.1	−11.4	−4.4	1.5	−5.1	1.7
# 1286 Acetyl-urea	−105.6[a]	−84.7	−89.7	−93.7	−94.6	−102.3	−102.0
# 1287 Propanediamide	−99.5[a]	−87.6	−92.7	−97.2	−99.9	−107.7	−103.2
# 1288 Pyrazine-1,4-dioxide	36.3[a]	37.4	32.1	41.0	40.9	32.7	53.7
# 1289 Uracil	−72.4[a]	−52.5	−57.8	−57.1	−61.2	−69.4	−68.2
# 1290 Thymine	−78.6[a]	−62.1	−69.0	−67.3	−69.8	−80.4	−76.9
# 1291 m-Nitroaniline	14.9[a]	19.3	11.5	14.3	17.9	5.9	20.8
# 1292 p-Nitroaniline	13.2[a]	16.5	8.7	11.5	14.8	2.9	18.7
# 1293 Lysine	−102.5[a]	−100.1	−111.0	−107.2	−106.4	−122.5	−108.2
# 1294 Isophthalamide	−70.3[a]	−59.2	−69.5	−68.3	−69.2	−84.9	−72.5
# 1295 Teraphthalamide	−69.7[a]	−58.6	−68.9	−67.8	−68.7	−84.4	−72.1
# 1296 N,N-Dimethyl-m-nitroaniline	17.4[a]	18.5	7.1	19.9	25.4	8.2	26.3
# 1297 N,N-Dimethyl-p-nitroaniline	16.1[a]	16.1	4.8	18.9	22.7	5.5	24.6
# 1298 Tryptophan	−51.6[a]	−41.1	−56.8	−46.9	−44.8	−68.0	−47.6
# 1300 Imidodicarbonic diamide	−104.4[a]	−78.0	−82.6	−92.0	−90.9	−97.9	−100.4
# 1301 Histidine	−63.5[a]	−48.6	−58.5	−52.3	−52.5	−67.3	−51.8
# 1302 Argenine	−84.3[a]	−59.2	−71.5	−75.9	−70.1	−88.3	−79.5
# 1340 Methyl nitrate	−29.1[a]	−32.7	−34.9	−34.9	−28.4	−31.8	−29.8
# 1341 Oxamic acid	−132.0[a]	−122.2	−125.1	−127.0	−129.6	−133.5	−131.1
# 1342 Ethyl nitrate	−36.8[a]	−41.6	−45.1	−43.0	−36.6	−42.0	−37.8
# 1343 Serine	−133.5[a]	−131.3	−136.8	−137.4	−135.2	−143.4	−136.8
# 1344 2-Nitrofuran	−6.9[a]	−3.0	−7.2	−4.4	−0.8	−7.5	3.9
# 1345 Threonine	−140.5[a]	−140.6	−147.9	−146.0	−143.5	−154.5	−145.1
# 1346 m-Nitrophenol	−25.2[a]	−25.9	−33.1	−28.5	−26.4	−37.5	−22.9
# 1347 o-Nitrophenol	−30.8[a]	−30.4	−37.7	−32.8	−29.6	−41.0	−25.5
# 1348 p-Nitrophenol	−27.4[a]	−28.4	−35.5	−30.8	−28.4	−39.5	−24.4
# 1349 Tyrosine	−111.6[a]	−111.0	−123.6	−117.5	−115.4	−134.3	−117.6
# 1352 Barbituric acid	−121.8[a]	−107.7	−113.7	−114.3	−119.8	−128.9	−130.2
# 1353 Asparagine	−137.8[a]	−132.0	−139.4	−141.7	−141.1	−152.4	−144.2
# 1354 GLY-GLY	−136.4[a]	−125.8	−132.8	−130.3	−132.6	−143.1	−135.6
# 1355 Glutamine	−142.4[a]	−135.9	−145.0	−146.1	−145.4	−159.0	−149.3
# 1356 ALA-ALA	−152.4[a]	−141.2	−151.8	−149.8	−147.2	−163.1	−151.2
# 1357 8-Hydroxy-5-nitroquinoline	−0.4[a]	−0.7	−12.3	−2.0	−0.4	−18.1	5.5
# 1364 LEU-LEU	−177.1[a]	−171.4	−193.1	−182.2	−176.3	−208.0	−183.1
# 1366 1,3,5-Triazine-2,4,6(1H,3H,5H)-trione	−134.8[a]	−99.4	−104.9	−110.2	−113.0	−121.4	−129.3
# 1367 1,3,5-Trimethyl-s-triazine-2,4,6-trione	−141.1[a]	−108.9	−119.5	−110.0	−105.2	−121.2	−126.6
# 1368 2,4,6-Trimethoxy-s-triazine	−70.1[a]	−43.6	−52.9	−53.3	−41.2	−55.3	−55.1
# 1413 Aspartic acid	−185.9[a]	−181.3	−188.2	−187.0	−185.3	−195.7	−187.4
# 1414 Glutamic acid	−189.7[a]	−188.2	−196.8	−193.7	−191.9	−204.7	−193.8
# 1415 4-Nitrocatechol	−69.3[a]	−66.9	−74.7	−70.9	−68.9	−80.9	−64.6
# 1416 p-Nitrobenzoic acid	−68.7[a]	−74.4	−83.0	−76.4	−73.0	−86.2	−70.2
# 1419 Dinitromethane	−13.3[a]	−7.9	−11.1	−9.7	−5.4	−10.3	−1.5
# 1420 m-Dinitrobenzene	11.3[a]	11.4	3.2	8.7	14.2	1.6	21.0
# 1421 o-Dinitrobenzene	20.2[a]	11.4	3.2	8.7	14.2	1.6	21.0
# 1422 p-Dinitrobenzene	13.3[a]	11.4	3.2	8.6	14.2	1.5	20.8
# 1423 2,4-Dinitrotoluene	7.9[a]	1.6	−8.5	−1.2	5.4	−10.0	12.3
# 1424 Dinitrophenylmethane	8.3[a]	14.5	4.1	11.6	18.0	2.3	19.5
# 1425 N,N'-Bis(m-methoxyphenyl) terephthalamide	−81.3[a]	−68.5	−96.4	−74.8	−67.4	−109.3	−76.2
# 1426 N,N'-Bis(o-methoxyphenyl) terephthalamide	−74.2[a]	−70.3	−99.0	−77.2	−68.1	−110.7	−77.2
# 1427 N,N'-Bis(p-methoxyphenyl) terephthalamide	−76.6[a]	−66.8	−94.8	−73.2	−65.7	−107.6	−74.7
# 1428 Methyldinitramine	10.3[a]	13.5	9.2	12.6	21.6	15.0	21.2
# 1438 SER-SER	−211.6[a]	−214.2	−226.3	−226.7	−220.9	−238.9	−226.1
# 1439 THR-THR	−230.2[a]	−232.7	−249.4	−246.1	−236.7	−260.9	−243.0
# 1458 1,1,1-Trinitroethane	−12.4[a]	−6.9	−13.9	−13.9	−4.2	−14.6	−1.0
# 1459 2,4,6-Trinitrotoluene	12.9[a]	4.9	−7.1	0.2	10.9	−7.4	20.8
# 1460 2-(Diacetoxymethyl)-5-nitrofuran	−184.4[a]	−186.4	−199.1	−188.6	−175.3	−194.2	−177.1
# 1461 ASP-ASP	−269.0[a]	−256.5	−272.4	−266.5	−265.3	−288.4	−275.5
# 1462 2,4,6-Trinitroanisole	−5.8[a]	−16.3	−28.9	−22.3	−6.8	−25.7	1.7
# 1463 2,4,6-Trinitrophenetole	−20.1[a]	−25.7	−40.5	−33.3	−16.7	−38.7	−9.4
# 1471 Glycerol trinitrate	−64.7[a]	−84.9	−94.8	−92.6	−72.0	−86.5	−77.3
# 1475 Bis(2,2,2-trinitroethyl)-amine	11.3[a]	15.2	−4.6	−3.1	22.9	−5.7	24.8

a Taken from the experimental and high-level ab initio data quoted in: http://openmopac.net/PM7_accuracy/molecules.html

; J.J.P.Stewart, J.Mol.Model. 19, 1 (2013).

Table S72: Benchmark Results for the PM7-CHNOF Set. Ionization Potentials (eV)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 3 Hydrogen (Geo)	15.40[a]	15.68	15.68	15.64	15.65	15.65	15.67
# 588 Nitrogen (Geo)	15.60[a]	15.46	15.46	15.55	14.51	14.51	14.73
# 54 Methane (Geo)	13.60[a]	13.64	13.64	13.66	14.17	14.17	14.30
# 60 Acetylene (Geo)	11.40[a]	11.55	11.55	11.35	11.79	11.79	11.64
# 64 Ethylene (Geo)	10.50[a]	10.74	10.74	10.53	11.05	11.05	10.87
# 69 Ethane (Geo)	12.00[a]	11.92	11.92	11.93	12.30	12.30	12.43
# 84 Allene (Geo)	10.10[a]	10.16	10.16	9.97	10.44	10.45	10.31
# 85 Cyclopropene (Geo)	9.90[a]	9.84	9.84	9.70	10.13	10.13	10.06
# 88 Propyne (Geo)	10.40[a]	10.64	10.64	10.47	10.88	10.88	10.78
# 93 Cyclopropane (Geo)	11.00[a]	10.88	10.88	10.71	11.47	11.47	11.38
# 96 Propene (Geo)	9.90[a]	9.99	9.99	9.81	10.28	10.29	10.16
# 99 Propane (Geo)	11.50[a]	11.39	11.39	11.36	11.69	11.69	11.82
# 105 Diacetylene (Geo)	10.20[a]	10.30	10.30	10.06	10.47	10.47	10.29
# 107 CH2=C=C=CH2 (Geo)	9.10[a]	9.35	9.35	9.11	9.60	9.60	9.39
# 117 2-Butyne (Geo)	9.60[a]	9.91	9.91	9.76	10.14	10.14	10.07
# 121 1,3-Butadiene (Geo)	9.10[a]	9.32	9.32	9.10	9.61	9.61	9.43
# 125 1-Butene (Geo)	9.70[a]	9.93	9.93	9.74	10.26	10.26	10.13
# 127 Cyclobutane (Geo)	10.70[a]	10.38	10.38	10.24	10.98	10.98	10.97
# 135 n-Butane (Geo)	11.20[a]	10.95	10.94	10.82	11.47	11.47	11.53
# 136 Isobutane (Geo)	11.40[a]	11.06	11.07	10.96	11.41	11.41	11.53
# 146 Cyclopentadiene (Geo)	8.60[a]	8.82	8.82	8.63	9.10	9.10	8.97
# 167 Neopentane (Geo)	11.30[a]	10.82	10.82	10.70	11.31	11.31	11.31
# 173 Benzene (Geo)	9.20[a]	9.59	9.59	9.41	9.91	9.91	9.76
# 186 Cyclohexene (Geo)	10.30[a]	9.29	9.29	9.14	9.59	9.59	9.51
# 194 Cyclohexane (Geo)	10.30[a]	10.16	10.16	10.05	10.72	10.71	10.73
# 279 Naphthalene (Geo)	8.10[a]	8.51	8.51	8.31	8.79	8.79	8.63
# 111 1,2-Butadiene	9.10[a]	9.49	9.49	9.33	9.75	9.75	9.66
# 113 1-Butyne	10.20[a]	10.51	10.51	10.32	10.76	10.76	10.67
# 118 Cyclobutene	9.40[a]	9.65	9.64	9.49	9.93	9.93	9.82
# 153 Cyclopentene	9.20[a]	9.22	9.22	9.09	9.51	9.51	9.44
# 162 Cyclopentane	10.50[a]	10.91	10.91	10.87	11.28	11.29	11.38
# 166 n-Pentane	10.30[a]	10.66	10.66	10.49	11.35	11.34	11.31
# 205 Cycloheptatriene	8.50[a]	8.57	8.58	8.39	8.82	8.84	8.72
# 207 Toluene	8.80[a]	9.16	9.16	9.00	9.46	9.46	9.35
# 231 Ethylbenzene	8.80[a]	9.14	9.14	8.96	9.47	9.47	9.35
# 245 Bicyclo(2.2.2)-octane	9.40[a]	9.76	9.75	9.64	10.23	10.23	10.23
# 299 Adamantane	9.60[a]	9.59	9.59	9.49	10.06	10.06	10.07
# 335 Anthracene	8.20[a]	7.81	7.81	7.59	8.07	8.07	7.91
# 447 Hydrogen cyanide (Geo)	13.60[a]	13.91	13.91	13.89	13.94	13.94	13.86
# 454 Methylamine (Geo)	9.60[a]	9.75	9.75	9.91	10.00	10.01	10.13
# 459 Acetonitrile (Geo)	12.20[a]	12.50	12.50	12.52	12.63	12.63	12.67
# 460 Methyl isocyanide (Geo)	11.30[a]	12.14	12.14	12.12	12.20	12.20	12.31
# 462 Ethyleneimine (Azirane) (Geo)	9.90[a]	10.13	10.13	10.19	10.39	10.39	10.41
# 467 Dimethylamine (Geo)	8.90[a]	9.23	9.23	9.41	9.24	9.25	9.38
# 470 CH.C.CN (Geo)	11.80[a]	11.58	11.58	11.49	11.67	11.67	11.65
# 472 Acrylonitrile (Geo)	10.90[a]	10.88	10.88	10.80	11.09	11.09	11.06
# 476 Trimethylamine (Geo)	8.50[a]	8.84	8.85	9.07	8.67	8.69	8.87
# 484 Pyrrole (Geo)	8.20[a]	8.46	8.47	8.27	8.65	8.65	8.49
# 493 Pyridine (Geo)	9.70[a]	9.96	9.96	9.78	10.13	10.13	10.08
# 466 Ethylamine	9.50[a]	9.60	9.60	9.63	9.95	9.95	10.01
# 473 Ethyl cyanide	11.90[a]	12.06	12.06	12.11	12.25	12.25	12.36
# 508 Aniline	7.70[a]	8.24	8.24	8.15	8.42	8.43	8.47
# 518 Phenyl cyanide	9.70[a]	9.91	9.91	9.81	10.16	10.16	10.12
# 593 Diazomethane	9.00[a]	8.84	8.84	8.74	8.75	8.75	8.63
# 595 Methylhydrazine	9.30[a]	9.73	9.73	9.98	9.90	9.91	10.11
# 687 Methyl Azide	9.80[a]	9.63	9.64	9.77	9.25	9.25	9.44
# 729 Formaldehyde (Geo)	10.10[a]	11.03	11.03	10.91	11.26	11.26	11.25
# 735 Methanol (Geo)	11.00[a]	11.22	11.22	11.17	11.60	11.60	11.66
# 741 Ketene (Geo)	9.60[a]	9.75	9.75	9.59	9.97	9.97	9.82
# 744 Acetaldehyde (Geo)	10.20[a]	10.62	10.62	10.51	10.94	10.94	10.91
# 747 Dimethyl ether (Geo)	10.00[a]	10.51	10.51	10.43	10.94	10.94	11.03
# 752 Acrolein (Geo)	10.10[a]	10.55	10.55	10.44	10.86	10.86	10.82
# 754 Acetone (Geo)	9.70[a]	10.29	10.29	10.17	10.65	10.65	10.56
# 762 Furan (Geo)	8.90[a]	9.03	9.03	8.83	9.45	9.45	9.30

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Table S72: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 1053 Formic acid (Geo)	11.50[a]	11.72	11.72	11.65	12.12	12.12	12.09
# 1054 trans Glyoxal (Geo)	10.60[a]	10.57	10.57	10.50	10.77	10.77	10.74
# 1059 Methyl formate (Geo)	11.00[a]	11.24	11.24	11.18	11.70	11.70	11.72
# 745 Ethylene oxide	10.60[a]	11.31	11.31	11.21	11.79	11.79	11.84
# 749 Ethanol	10.60[a]	10.88	10.88	10.85	11.21	11.21	11.28
# 755 Propanal	10.00[a]	10.38	10.38	10.28	10.71	10.71	10.69
# 766 Butanal	9.80[a]	10.33	10.32	10.20	10.71	10.70	10.69
# 770 Diethyl ether	9.60[a]	10.23	10.23	10.16	10.60	10.60	10.68
# 787 Benzaldehyde	9.70[a]	9.93	9.94	9.79	10.26	10.27	10.15
# 788 Anisole	8.40[a]	8.74	8.74	8.59	9.15	9.15	9.07
# 1057 Acetic acid	10.80[a]	11.33	11.33	11.26	11.76	11.76	11.70
# 1058 Acetic acid	10.80[a]	11.33	11.33	11.26	11.76	11.76	11.70
# 1061 Dimethyl peroxide	10.60[a]	10.71	10.72	10.66	11.16	11.19	11.23
# 1069 beta-Propiolactone	10.60[a]	10.96	10.96	10.89	11.39	11.39	11.36
# 1072 Methyl acetate	10.60[a]	11.04	11.04	10.82	11.39	11.39	11.37
# 1073 Propionic acid	10.50[a]	11.07	11.07	11.00	11.48	11.48	11.44
# 1091 Acetylacetone	9.10[a]	10.30	10.30	10.18	10.68	10.69	10.59
# 1125 Benzoic acid	9.80[a]	10.08	10.08	9.92	10.34	10.34	10.19
# 1323 Maleic anhydride	10.80[a]	11.72	11.72	11.68	12.07	12.07	12.00
# 1329 o-Salicylic acid	9.80[a]	9.23	9.23	9.13	9.51	9.51	9.44
# 1375 Oxalic acid	11.20[a]	11.41	11.41	11.36	11.62	11.62	11.53
# 1496 Fluoromethane (Geo)	13.30[a]	13.07	13.07	13.11	13.41	13.41	13.67
# 1498 Fluoroacetylene (Geo)	11.30[a]	11.33	11.33	11.21	11.52	11.52	11.51
# 1500 Fluoroethylene (Geo)	10.60[a]	10.59	10.59	10.44	10.85	10.85	10.81
# 1586 Trifluoromethane (Geo)	14.80[a]	14.17	14.17	14.19	14.45	14.45	14.78
# 1503 Fluoroethane	12.40[a]	12.01	12.01	12.02	12.28	12.28	12.47
# 1505 2-Fluoropropane	11.10[a]	11.59	11.59	11.51	11.92	11.92	12.09
# 1506 Fluorobenzene	9.20[a]	9.58	9.58	9.43	9.85	9.85	9.79
# 1546 Difluoromethane	13.20[a]	12.98	12.98	13.02	13.23	13.23	13.54
# 1550 gem-Difluoroethylene	10.70[a]	10.38	10.38	10.27	10.56	10.56	10.63
# 1552 1,1-Difluoroethane	12.80[a]	12.30	12.30	12.28	12.69	12.69	12.91
# 1588 Trifluoroethylene	10.50[a]	10.40	10.40	10.30	10.53	10.53	10.66
# 1592 1,1,1-Trifluoroethane	13.80[a]	13.23	13.23	13.21	13.78	13.78	13.98
# 1594 Trifluoromethylbenze	9.70[a]	10.20	10.20	10.01	10.47	10.48	10.35
# 1625 Pentafluorobenzene	9.80[a]	10.19	10.19	10.08	10.30	10.30	10.39
# 921 Hydrogen isocyanate	11.60[a]	11.34	11.34	11.44	11.43	11.43	11.54
# 1213 Methyl nitrite	11.00[a]	10.97	10.98	10.94	11.06	11.06	11.07
# 1214 Nitromethane	11.30[a]	11.84	11.84	11.84	11.74	11.74	11.55
# 1219 Alanine	8.90[a]	9.84	9.84	9.86	10.06	10.07	10.11
# 1245 Nitrobenzene	9.90[a]	10.50	10.50	10.32	10.81	10.81	10.66

a Taken from the experimental and high-level ab initio data quoted in: http://openmopac.net/PM7_accuracy/molecules.html ; J.J.P.Stewart, J.Mol.Model. 19, 1 (2013).

Table S73: Benchmark Results for the C7H10O2 Set. Atomization Enthalpies at 298 K (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1	1909.1[a]	1905.9	1905.9	1907.7	1903.6	1903.6	1903.5
gdb 2	1908.3[a]	1904.9	1904.9	1907.0	1902.3	1902.2	1902.4
gdb 3	1904.5[a]	1896.8	1896.8	1898.9	1897.4	1897.4	1896.9
gdb 4	1906.2[a]	1904.5	1904.5	1906.8	1903.3	1903.2	1903.1
gdb 5	1907.7[a]	1905.2	1905.2	1907.6	1904.2	1904.2	1904.3
gdb 6	1904.3[a]	1896.8	1896.8	1898.9	1897.3	1897.3	1896.8
gdb 7	1907.7[a]	1904.4	1904.4	1906.4	1903.4	1903.4	1903.0
gdb 8	1910.1[a]	1906.7	1906.7	1908.2	1906.2	1906.2	1905.7
gdb 9	1907.9[a]	1904.8	1904.8	1906.0	1904.1	1904.1	1903.2
gdb 10	1906.5[a]	1902.4	1902.4	1903.9	1900.9	1900.8	1900.6
gdb 11	1899.8[a]	1891.4	1891.4	1892.5	1887.9	1887.9	1890.1
gdb 12	1908.0[a]	1901.6	1901.6	1903.0	1901.4	1901.4	1901.5
gdb 13	1895.5[a]	1886.7	1886.6	1888.7	1884.1	1884.1	1885.8
gdb 14	1905.8[a]	1899.2	1899.2	1900.9	1898.5	1898.4	1898.7
gdb 15	1911.0[a]	1904.2	1904.2	1905.5	1905.9	1905.9	1904.6
gdb 16	1903.9[a]	1896.8	1896.8	1899.1	1896.6	1896.6	1897.3
gdb 17	1905.0[a]	1900.8	1900.8	1903.0	1899.8	1899.8	1899.8
gdb 18	1894.1[a]	1890.0	1890.0	1890.8	1885.7	1885.7	1887.1
gdb 19	1903.7[a]	1896.7	1896.7	1899.4	1895.6	1895.6	1896.4
gdb 20	1902.6[a]	1897.4	1897.4	1899.0	1896.3	1896.3	1896.4
gdb 21	1892.5[a]	1887.8	1887.8	1889.0	1883.6	1883.6	1885.4
gdb 22	1906.0[a]	1903.0	1903.0	1904.6	1902.4	1902.4	1902.0
gdb 23	1906.0[a]	1898.4	1898.4	1900.4	1899.7	1899.7	1898.5
gdb 24	1898.1[a]	1890.5	1890.5	1891.5	1886.7	1886.6	1888.1
gdb 25	1908.9[a]	1904.3	1904.3	1905.3	1904.3	1904.2	1903.8
gdb 26	1907.8[a]	1900.6	1900.5	1901.9	1902.3	1902.3	1901.1
gdb 27	1899.8[a]	1892.5	1892.5	1892.9	1889.4	1889.4	1890.6
gdb 28	1909.0[a]	1906.1	1906.1	1907.2	1906.4	1906.3	1905.9
gdb 29	1897.9[a]	1891.1	1891.1	1891.9	1889.4	1889.4	1890.0
gdb 30	1908.1[a]	1903.4	1903.4	1905.1	1903.0	1903.0	1902.8
gdb 31	1895.5[a]	1888.9	1888.9	1890.3	1886.6	1886.6	1887.4
gdb 32	1903.8[a]	1900.4	1900.4	1902.1	1900.1	1900.0	1899.9
gdb 33	1902.8[a]	1899.0	1899.0	1900.7	1898.7	1898.7	1898.5
gdb 34	1892.7[a]	1885.3	1885.3	1886.9	1883.0	1883.0	1883.9
gdb 35	1894.8[a]	1886.5	1886.6	1887.6	1883.0	1882.9	1884.7
gdb 36	1908.9[a]	1904.8	1904.8	1905.6	1904.8	1904.8	1904.7
gdb 37	1907.8[a]	1900.6	1900.5	1901.8	1902.4	1902.3	1901.1
gdb 38	1899.4[a]	1892.4	1892.4	1892.8	1889.1	1889.1	1891.1
gdb 39	1904.7[a]	1899.8	1899.8	1901.2	1899.7	1899.7	1899.2
gdb 40	1892.5[a]	1885.5	1885.4	1886.6	1883.0	1882.9	1883.7
gdb 41	1903.7[a]	1898.7	1898.7	1900.0	1898.6	1898.6	1898.1
gdb 42	1894.7[a]	1886.5	1886.5	1887.4	1882.9	1882.9	1884.5
gdb 43	1906.1[a]	1901.3	1901.3	1902.1	1901.5	1901.5	1900.8
gdb 44	1896.6[a]	1889.0	1889.0	1889.4	1885.8	1885.7	1887.1
gdb 45	1908.0[a]	1903.2	1903.2	1904.9	1902.9	1902.9	1902.6
gdb 46	1905.9[a]	1898.3	1898.3	1900.1	1899.7	1899.7	1898.7
gdb 47	1897.7[a]	1888.0	1888.0	1889.5	1885.9	1885.9	1887.1
gdb 48	1901.8[a]	1897.5	1897.4	1899.7	1896.7	1896.7	1896.7
gdb 49	1892.4[a]	1882.7	1882.7	1884.1	1879.6	1879.6	1880.6
gdb 50	1905.4[a]	1899.5	1899.5	1900.0	1899.3	1899.3	1898.8
gdb 51	1902.9[a]	1894.6	1894.6	1896.8	1896.2	1896.2	1895.5
gdb 52	1898.2[a]	1890.2	1890.2	1890.3	1886.8	1886.7	1888.0
gdb 53	1893.9[a]	1888.8	1888.8	1889.2	1885.2	1885.2	1886.3
gdb 54	1905.8[a]	1899.6	1899.6	1900.1	1899.5	1899.5	1899.1
gdb 55	1896.1[a]	1888.5	1888.5	1889.2	1886.6	1886.5	1887.2
gdb 56	1894.2[a]	1890.3	1890.3	1890.6	1886.7	1886.7	1888.0
gdb 57	1905.4[a]	1899.5	1899.5	1899.8	1899.4	1899.4	1898.6
gdb 58	1902.8[a]	1894.6	1894.6	1896.5	1896.2	1896.2	1895.4
gdb 59	1898.1[a]	1890.2	1890.2	1890.8	1886.7	1886.7	1887.9
gdb 60	1893.6[a]	1889.1	1889.1	1889.2	1885.3	1885.3	1886.1
gdb 61	1907.6[a]	1901.5	1901.5	1902.9	1902.5	1902.5	1902.3
gdb 62	1900.2[a]	1892.3	1892.3	1892.0	1889.4	1889.4	1890.5

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 63	1896.2[a]	1891.3	1891.3	1890.9	1888.0	1888.0	1888.7
gdb 64	1905.7[a]	1899.5	1899.5	1899.8	1899.5	1899.5	1898.8
gdb 65	1895.9[a]	1888.4	1888.4	1888.9	1886.4	1886.4	1886.9
gdb 66	1894.9[a]	1889.5	1889.5	1889.5	1886.2	1886.2	1887.2
gdb 67	1903.3[a]	1897.0	1897.0	1899.6	1896.9	1896.8	1897.2
gdb 68	1895.7[a]	1885.3	1885.3	1886.6	1883.1	1883.1	1883.7
gdb 69	1893.1[a]	1887.1	1887.0	1887.8	1883.2	1883.2	1884.6
gdb 70	1894.8[a]	1886.7	1886.7	1887.3	1882.6	1883.2	1884.9
gdb 71	1893.7[a]	1888.6	1888.6	1888.1	1885.0	1885.0	1885.8
gdb 72	1893.7[a]	1887.5	1887.5	1887.7	1884.4	1884.4	1885.8
gdb 73	1902.3[a]	1895.5	1895.5	1897.5	1896.4	1896.4	1896.7
gdb 74	1890.4[a]	1882.6	1882.6	1883.9	1879.6	1879.6	1881.0
gdb 75	1892.8[a]	1887.6	1887.6	1887.6	1883.8	1883.8	1884.9
gdb 76	1891.5[a]	1885.3	1885.3	1885.9	1881.8	1881.8	1883.3
gdb 77	1900.1[a]	1893.1	1893.1	1895.7	1893.8	1893.8	1894.3
gdb 78	1863.7[a]	1865.6	1865.6	1868.1	1857.9	1857.8	1863.5
gdb 79	1856.9[a]	1859.9	1859.9	1864.0	1854.6	1854.6	1859.8
gdb 80	1865.3[a]	1865.1	1865.1	1868.3	1857.5	1857.5	1863.6
gdb 81	1855.6[a]	1858.6	1858.6	1861.9	1853.1	1853.1	1858.0
gdb 82	1855.7[a]	1856.0	1856.0	1860.1	1851.5	1851.5	1857.1
gdb 83	1859.4[a]	1862.7	1862.7	1865.8	1854.7	1854.7	1860.0
gdb 84	1868.4[a]	1867.7	1867.7	1869.9	1860.2	1860.2	1865.8
gdb 85	1862.5[a]	1861.0	1861.0	1864.3	1856.4	1856.4	1861.0
gdb 86	1866.5[a]	1865.8	1865.8	1868.8	1858.0	1857.9	1864.1
gdb 87	1869.8[a]	1870.5	1870.5	1872.2	1862.9	1862.8	1868.0
gdb 88	1864.3[a]	1869.3	1869.3	1871.9	1861.5	1861.4	1865.7
gdb 89	1866.1[a]	1871.7	1871.7	1874.2	1863.9	1863.9	1867.8
gdb 90	1865.3[a]	1871.5	1871.5	1873.1	1863.6	1863.6	1867.3
gdb 91	1855.1[a]	1860.0	1860.0	1861.5	1854.8	1854.8	1858.3
gdb 92	1840.0[a]	1837.5	1837.5	1839.4	1832.2	1832.2	1836.0
gdb 93	1837.5[a]	1835.1	1835.0	1836.5	1829.8	1829.8	1833.3
gdb 94	1835.6[a]	1832.7	1832.7	1834.0	1827.8	1827.8	1831.7
gdb 95	1838.9[a]	1836.6	1836.6	1833.9	1829.0	1829.0	1827.7
gdb 96	1836.4[a]	1834.3	1834.3	1831.7	1827.4	1827.4	1826.2
gdb 97	1831.6[a]	1813.5	1813.5	1812.0	1807.5	1807.5	1804.0
gdb 98	1842.0[a]	1827.0	1827.0	1826.2	1823.0	1823.0	1821.4
gdb 99	1840.1[a]	1824.9	1824.9	1824.0	1820.7	1820.7	1819.3
gdb 100	1847.8[a]	1837.7	1837.7	1834.0	1829.4	1829.4	1824.2
gdb 101	1832.3[a]	1820.8	1820.8	1823.1	1819.6	1819.6	1822.0
gdb 102	1870.0[a]	1870.9	1870.9	1869.9	1864.5	1864.5	1863.6
gdb 103	1826.4[a]	1810.3	1810.2	1808.9	1804.4	1804.4	1801.2
gdb 104	1820.2[a]	1806.5	1806.4	1809.8	1802.5	1802.4	1804.2
gdb 105	1838.1[a]	1823.7	1823.7	1823.3	1819.4	1819.4	1818.1
gdb 106	1831.0[a]	1819.0	1819.0	1821.1	1817.9	1817.9	1820.2
gdb 107	1844.5[a]	1836.1	1836.1	1832.6	1827.6	1827.5	1822.6
gdb 108	1841.9[a]	1828.0	1828.0	1827.5	1823.6	1823.6	1822.1
gdb 109	1839.2[a]	1835.0	1835.0	1834.0	1828.8	1828.8	1827.2
gdb 110	1870.4[a]	1871.6	1871.6	1870.8	1864.9	1864.9	1864.2
gdb 111	1871.1[a]	1874.9	1874.9	1875.9	1868.3	1868.2	1871.8
gdb 112	1841.0[a]	1829.1	1829.1	1832.3	1827.4	1827.4	1830.3
gdb 113	1841.7[a]	1833.2	1833.2	1835.7	1830.3	1830.3	1833.1
gdb 114	1839.0[a]	1834.9	1834.9	1836.6	1830.4	1830.4	1833.2
gdb 115	1850.3[a]	1844.8	1844.8	1844.6	1837.1	1837.1	1835.8
gdb 116	1856.3[a]	1846.8	1846.8	1850.7	1845.3	1845.3	1850.3
gdb 117	1864.4[a]	1857.5	1857.5	1860.0	1851.8	1851.8	1857.2
gdb 118	1858.5[a]	1843.1	1843.1	1846.1	1842.4	1842.4	1846.3
gdb 119	1860.0[a]	1846.4	1846.4	1849.1	1844.8	1844.8	1848.7
gdb 120	1859.1[a]	1845.8	1845.8	1848.5	1844.0	1844.0	1847.7
gdb 121	1866.1[a]	1857.3	1857.3	1856.9	1851.0	1851.0	1850.9
gdb 122	1881.1[a]	1879.7	1879.7	1881.4	1874.9	1874.6	1877.9
gdb 123	1877.0[a]	1876.3	1876.3	1879.3	1874.3	1874.3	1877.8
gdb 124	1879.9[a]	1879.4	1879.4	1882.0	1876.0	1876.0	1879.5
gdb 125	1882.7[a]	1882.5	1882.5	1884.8	1878.1	1878.1	1881.8
gdb 126	1888.6[a]	1882.9	1882.9	1881.6	1876.4	1876.4	1874.9
gdb 127	1886.4[a]	1888.2	1888.2	1890.9	1879.6	1879.6	1884.3

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 128	1886.2[a]	1885.8	1885.8	1889.3	1880.3	1880.3	1883.6
gdb 129	1892.7[a]	1894.0	1894.0	1896.7	1885.6	1885.5	1889.4
gdb 130	1886.3[a]	1883.1	1883.1	1883.1	1875.1	1875.1	1875.0
gdb 131	1886.2[a]	1882.2	1882.2	1882.2	1874.4	1874.4	1875.0
gdb 132	1889.5[a]	1885.4	1885.4	1884.9	1877.2	1877.2	1876.2
gdb 133	1880.8[a]	1885.2	1885.2	1888.0	1879.1	1879.1	1882.3
gdb 134	1885.7[a]	1891.2	1891.2	1893.4	1882.7	1882.7	1886.8
gdb 135	1885.7[a]	1886.0	1886.0	1885.3	1878.3	1878.3	1877.4
gdb 136	1859.0[a]	1859.6	1859.6	1864.0	1854.7	1854.7	1859.1
gdb 137	1863.1[a]	1863.3	1863.3	1866.6	1856.0	1856.0	1861.2
gdb 138	1861.8[a]	1856.9	1856.9	1856.9	1850.8	1850.8	1850.5
gdb 139	1862.4[a]	1859.7	1859.7	1859.9	1852.8	1852.8	1852.6
gdb 140	1886.7[a]	1885.5	1885.5	1887.8	1879.3	1879.3	1884.3
gdb 141	1888.4[a]	1888.8	1888.8	1891.7	1883.4	1883.4	1887.7
gdb 142	1882.8[a]	1881.9	1881.9	1885.1	1878.6	1878.6	1882.3
gdb 143	1880.3[a]	1879.9	1879.9	1883.1	1876.6	1876.6	1880.6
gdb 144	1884.8[a]	1884.3	1884.3	1887.1	1879.2	1879.1	1882.8
gdb 145	1865.6[a]	1860.6	1860.6	1863.5	1853.9	1853.9	1859.1
gdb 146	1862.4[a]	1855.3	1855.3	1859.6	1851.8	1851.8	1856.9
gdb 147	1866.6[a]	1859.1	1859.1	1861.5	1853.0	1853.0	1858.5
gdb 148	1856.9[a]	1844.4	1844.4	1847.7	1842.3	1842.3	1846.1
gdb 149	1860.2[a]	1845.7	1845.7	1848.5	1844.3	1844.3	1847.8
gdb 150	1859.8[a]	1843.8	1843.8	1847.1	1842.3	1842.3	1846.4
gdb 151	1852.1[a]	1836.9	1836.9	1842.1	1831.2	1831.2	1838.3
gdb 152	1846.5[a]	1830.1	1830.1	1836.3	1826.1	1826.1	1832.7
gdb 153	1838.6[a]	1827.2	1827.2	1829.6	1823.8	1823.8	1825.6
gdb 154	1841.8[a]	1829.5	1829.5	1832.3	1825.2	1825.1	1826.8
gdb 155	1842.9[a]	1828.0	1827.9	1831.5	1825.1	1825.0	1828.1
gdb 156	1840.6[a]	1826.1	1826.1	1829.4	1823.5	1823.4	1826.9
gdb 157	1846.1[a]	1836.9	1836.9	1837.2	1830.1	1830.1	1829.8
gdb 158	1842.8[a]	1834.3	1834.3	1834.6	1827.8	1827.8	1827.8
gdb 159	1875.5[a]	1868.1	1868.1	1872.1	1861.9	1861.9	1866.6
gdb 160	1869.7[a]	1864.5	1864.5	1868.9	1859.9	1859.8	1864.3
gdb 161	1872.3[a]	1865.1	1865.1	1870.0	1860.7	1860.7	1864.9
gdb 162	1877.2[a]	1870.1	1870.1	1874.2	1862.9	1862.9	1868.1
gdb 163	1876.9[a]	1872.2	1872.2	1874.4	1866.1	1866.0	1868.2
gdb 164	1877.6[a]	1872.9	1872.9	1874.9	1866.9	1866.9	1868.8
gdb 165	1854.0[a]	1834.4	1834.4	1838.7	1828.4	1828.4	1834.9
gdb 166	1852.3[a]	1828.1	1828.1	1833.9	1825.6	1825.5	1831.4
gdb 167	1853.3[a]	1831.9	1831.9	1836.6	1826.1	1826.1	1832.7
gdb 168	1847.2[a]	1828.6	1828.6	1831.4	1825.2	1825.1	1826.9
gdb 169	1843.5[a]	1827.6	1827.6	1830.0	1823.7	1823.7	1825.7
gdb 170	1842.4[a]	1826.6	1826.6	1829.0	1822.7	1822.7	1824.4
gdb 171	1870.7[a]	1865.6	1865.6	1868.9	1859.6	1859.6	1862.6
gdb 172	1879.7[a]	1885.0	1885.0	1888.0	1874.7	1874.7	1878.7
gdb 173	1873.4[a]	1873.0	1873.0	1875.6	1865.4	1865.4	1868.2
gdb 174	1882.2[a]	1882.2	1882.2	1885.0	1874.8	1874.8	1876.9
gdb 175	1886.5[a]	1883.8	1883.8	1887.7	1874.7	1874.7	1880.3
gdb 176	1879.5[a]	1876.4	1876.4	1879.1	1870.5	1870.4	1873.0
gdb 177	1881.7[a]	1878.4	1878.4	1881.5	1872.3	1872.3	1874.7
gdb 178	1856.1[a]	1845.4	1845.4	1849.7	1838.6	1838.5	1843.6
gdb 179	1845.7[a]	1838.1	1838.1	1839.8	1832.8	1832.8	1833.2
gdb 180	1844.2[a]	1836.5	1836.5	1838.5	1832.0	1832.0	1833.1
gdb 181	1865.2[a]	1862.4	1862.3	1865.3	1857.5	1857.5	1862.2
gdb 182	1865.0[a]	1866.0	1866.0	1868.7	1861.5	1861.5	1864.5
gdb 183	1872.8[a]	1869.6	1869.6	1868.8	1862.8	1862.8	1861.6
gdb 184	1870.7[a]	1865.5	1865.5	1864.6	1858.8	1858.8	1858.1
gdb 185	1868.1[a]	1871.2	1871.2	1873.7	1863.2	1863.0	1866.5
gdb 186	1865.5[a]	1864.8	1864.8	1864.3	1857.4	1857.4	1856.3
gdb 187	1863.3[a]	1862.7	1862.7	1862.7	1855.7	1855.7	1855.1
gdb 188	1861.4[a]	1856.2	1856.2	1859.2	1853.1	1853.1	1855.7
gdb 189	1875.3[a]	1864.8	1864.8	1864.5	1859.5	1859.4	1858.4
gdb 190	1855.0[a]	1860.2	1860.2	1865.4	1856.3	1856.3	1861.7
gdb 191	1911.8[a]	1917.1	1917.1	1920.4	1910.2	1910.2	1913.6
gdb 192	1915.6[a]	1921.4	1921.4	1923.7	1911.7	1911.7	1915.6

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 193	1914.3[a]	1922.1	1922.1	1924.5	1912.0	1912.0	1915.9
gdb 194	1911.3[a]	1917.5	1917.5	1920.6	1908.2	1908.2	1912.8
gdb 195	1868.2[a]	1868.1	1868.1	1871.2	1862.5	1862.5	1867.6
gdb 196	1872.6[a]	1872.7	1872.7	1875.2	1868.0	1867.9	1871.1
gdb 197	1878.8[a]	1880.4	1880.4	1882.7	1873.2	1873.2	1877.4
gdb 198	1864.5[a]	1862.4	1862.4	1862.8	1856.9	1856.9	1857.6
gdb 199	1866.6[a]	1864.3	1864.3	1865.3	1859.1	1859.0	1859.9
gdb 200	1871.2[a]	1870.2	1870.2	1873.4	1864.7	1864.7	1869.4
gdb 201	1865.3[a]	1864.4	1864.4	1867.9	1860.9	1860.9	1865.3
gdb 202	1864.4[a]	1861.4	1861.4	1865.0	1859.7	1859.7	1863.6
gdb 203	1877.3[a]	1876.6	1876.6	1878.3	1870.1	1870.1	1873.2
gdb 204	1887.3[a]	1893.7	1893.7	1898.6	1887.5	1887.5	1891.7
gdb 205	1895.1[a]	1902.2	1902.2	1906.2	1893.8	1893.8	1899.0
gdb 206	1896.2[a]	1904.2	1904.2	1907.9	1895.5	1895.4	1899.5
gdb 207	1895.8[a]	1901.2	1901.2	1904.9	1892.8	1892.7	1898.1
gdb 208	1890.0[a]	1895.8	1895.8	1900.9	1890.0	1890.0	1894.8
gdb 209	1896.6[a]	1894.1	1894.1	1897.7	1888.9	1888.9	1892.1
gdb 210	1891.9[a]	1890.4	1890.4	1894.2	1885.4	1885.4	1889.6
gdb 211	1891.5[a]	1897.4	1897.4	1899.4	1889.0	1889.0	1891.8
gdb 212	1892.0[a]	1897.1	1897.1	1899.3	1889.1	1889.1	1892.1
gdb 213	1886.4[a]	1888.4	1888.4	1891.0	1881.7	1881.7	1886.0
gdb 214	1890.2[a]	1894.4	1894.4	1897.4	1887.2	1887.2	1891.1
gdb 215	1882.7[a]	1884.9	1884.9	1888.4	1880.4	1880.4	1884.2
gdb 216	1890.9[a]	1889.9	1889.9	1889.2	1882.3	1882.3	1880.9
gdb 217	1892.1[a]	1889.9	1889.9	1889.6	1882.8	1882.8	1882.3
gdb 218	1890.5[a]	1889.4	1889.4	1889.0	1881.9	1881.9	1881.1
gdb 219	1887.7[a]	1889.9	1889.9	1894.8	1883.7	1883.7	1888.5
gdb 220	1891.9[a]	1897.2	1897.2	1901.0	1888.6	1888.6	1894.1
gdb 221	1891.3[a]	1896.4	1896.4	1900.2	1888.1	1888.1	1892.9
gdb 222	1891.9[a]	1889.2	1889.2	1892.6	1883.1	1883.1	1886.5
gdb 223	1891.2[a]	1890.5	1890.5	1893.4	1884.9	1884.9	1888.3
gdb 224	1900.2[a]	1904.5	1904.5	1907.2	1894.5	1894.5	1899.1
gdb 225	1892.6[a]	1895.9	1895.9	1899.1	1888.3	1888.3	1891.8
gdb 226	1902.4[a]	1909.0	1909.0	1910.1	1897.8	1897.8	1900.3
gdb 227	1894.9[a]	1899.0	1899.0	1902.0	1891.7	1891.7	1894.8
gdb 228	1900.3[a]	1902.6	1902.6	1905.5	1895.2	1895.2	1898.1
gdb 229	1865.8[a]	1863.3	1863.3	1865.6	1859.6	1859.5	1863.0
gdb 230	1859.9[a]	1865.0	1865.0	1869.5	1861.3	1861.3	1865.5
gdb 231	1864.9[a]	1854.0	1854.0	1853.5	1848.4	1848.3	1847.7
gdb 232	1870.5[a]	1876.8	1876.8	1881.6	1868.1	1868.1	1874.4
gdb 233	1871.3[a]	1867.0	1867.0	1871.1	1862.3	1862.2	1867.0
gdb 234	1872.8[a]	1869.9	1869.9	1874.4	1864.9	1864.9	1869.7
gdb 235	1885.5[a]	1881.5	1881.5	1885.8	1873.0	1873.0	1879.6
gdb 236	1878.8[a]	1875.0	1875.0	1877.9	1869.4	1869.4	1872.2
gdb 237	1880.4[a]	1874.2	1874.2	1876.9	1868.6	1868.6	1871.6
gdb 238	1881.0[a]	1873.5	1873.5	1876.6	1867.5	1867.5	1870.0
gdb 239	1881.2[a]	1875.3	1875.2	1879.6	1870.0	1870.0	1874.5
gdb 240	1878.3[a]	1872.4	1872.4	1876.6	1867.4	1867.4	1872.1
gdb 241	1886.5[a]	1880.8	1880.8	1884.7	1873.8	1873.7	1878.6
gdb 242	1889.0[a]	1898.4	1898.4	1900.4	1890.5	1890.5	1893.6
gdb 243	1885.1[a]	1890.7	1890.7	1894.1	1886.7	1886.7	1889.7
gdb 244	1881.3[a]	1887.3	1887.3	1890.6	1883.3	1883.3	1886.6
gdb 245	1888.9[a]	1893.9	1893.9	1896.5	1887.6	1887.6	1891.3
gdb 246	1889.6[a]	1892.3	1892.3	1891.7	1885.5	1885.5	1884.4
gdb 247	1890.0[a]	1891.3	1891.3	1890.5	1884.3	1884.3	1882.8
gdb 248	1888.8[a]	1889.1	1889.1	1888.2	1882.6	1882.5	1881.4
gdb 249	1867.5[a]	1860.5	1860.5	1863.4	1854.3	1854.3	1859.8
gdb 250	1864.0[a]	1857.3	1857.3	1861.1	1853.9	1853.9	1858.4
gdb 251	1868.3[a]	1864.9	1864.9	1867.1	1857.6	1857.6	1862.8
gdb 252	1869.5[a]	1862.3	1862.3	1862.6	1855.9	1855.9	1856.0
gdb 253	1863.7[a]	1858.7	1858.7	1859.0	1852.5	1852.5	1852.5
gdb 254	1862.7[a]	1857.6	1857.6	1857.9	1851.2	1851.2	1851.2
gdb 255	1862.4[a]	1849.7	1849.7	1853.2	1848.0	1848.0	1851.6
gdb 256	1862.6[a]	1851.2	1851.2	1854.2	1848.7	1848.7	1852.4
gdb 257	1862.7[a]	1850.6	1850.6	1853.8	1848.0	1848.0	1851.7

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 258	1876.2[a]	1871.6	1871.6	1875.6	1863.7	1863.7	1868.8
gdb 259	1869.2[a]	1865.2	1865.2	1869.6	1860.7	1860.7	1864.8
gdb 260	1867.4[a]	1864.1	1864.1	1868.1	1859.4	1859.4	1863.8
gdb 261	1870.1[a]	1866.6	1866.6	1870.5	1861.3	1861.3	1865.2
gdb 262	1869.0[a]	1865.5	1865.5	1869.2	1860.9	1860.9	1865.1
gdb 263	1869.4[a]	1865.6	1865.6	1869.7	1860.5	1860.5	1864.5
gdb 264	1877.6[a]	1872.5	1872.5	1874.7	1865.9	1865.8	1867.8
gdb 265	1876.3[a]	1872.4	1872.4	1874.3	1866.0	1865.9	1868.0
gdb 266	1843.2[a]	1827.9	1827.9	1831.0	1825.1	1825.1	1828.0
gdb 267	1841.3[a]	1825.0	1825.0	1828.0	1822.6	1822.6	1825.7
gdb 268	1841.4[a]	1826.8	1826.8	1829.6	1824.0	1824.0	1827.0
gdb 269	1838.5[a]	1823.8	1823.8	1826.5	1821.1	1821.1	1824.6
gdb 270	1848.6[a]	1839.1	1839.1	1839.0	1832.1	1832.1	1831.0
gdb 271	1846.8[a]	1836.3	1836.3	1836.3	1829.5	1829.5	1829.1
gdb 272	1868.2[a]	1869.0	1869.0	1871.5	1863.5	1863.5	1866.1
gdb 273	1865.3[a]	1865.0	1865.0	1868.1	1860.6	1860.6	1863.6
gdb 274	1861.3[a]	1861.6	1861.5	1864.5	1857.1	1857.1	1860.6
gdb 275	1871.5[a]	1873.2	1873.2	1872.9	1864.9	1864.9	1863.8
gdb 276	1874.6[a]	1868.9	1868.9	1867.9	1861.5	1861.5	1859.7
gdb 277	1870.0[a]	1864.6	1864.6	1863.6	1857.5	1857.4	1856.4
gdb 278	1863.1[a]	1862.7	1862.7	1863.6	1855.6	1855.6	1856.0
gdb 279	1868.8[a]	1860.8	1860.8	1859.9	1854.3	1854.3	1852.9
gdb 280	1862.4[a]	1859.7	1859.7	1862.6	1855.3	1855.3	1858.8
gdb 281	1859.6[a]	1856.3	1856.3	1855.3	1850.8	1850.8	1849.6
gdb 282	1855.0[a]	1852.3	1852.3	1854.0	1850.8	1850.8	1854.1
gdb 283	1870.0[a]	1859.9	1859.9	1855.9	1852.9	1852.9	1847.7
gdb 284	1880.8[a]	1882.4	1882.4	1883.9	1875.5	1875.5	1878.5
gdb 285	1877.0[a]	1876.9	1876.9	1878.9	1870.0	1870.0	1874.3
gdb 286	1881.2[a]	1883.7	1883.7	1885.7	1877.0	1876.9	1880.7
gdb 287	1869.2[a]	1868.6	1868.6	1871.9	1865.4	1865.4	1869.4
gdb 288	1871.0[a]	1868.6	1868.6	1871.5	1865.3	1865.3	1869.4
gdb 289	1872.4[a]	1871.4	1871.4	1873.4	1867.5	1867.5	1870.2
gdb 290	1867.4[a]	1863.8	1863.8	1867.0	1861.9	1861.9	1866.0
gdb 291	1871.0[a]	1867.6	1867.6	1868.1	1861.8	1861.8	1862.2
gdb 292	1871.3[a]	1866.6	1866.6	1866.5	1860.9	1860.9	1860.7
gdb 293	1886.9[a]	1899.9	1899.9	1904.1	1894.3	1894.3	1898.4
gdb 294	1892.0[a]	1903.9	1903.9	1907.0	1896.0	1896.0	1900.5
gdb 295	1888.8[a]	1899.6	1899.6	1903.8	1893.7	1893.6	1897.9
gdb 296	1893.2[a]	1895.0	1894.9	1898.3	1890.4	1890.4	1893.7
gdb 297	1887.1[a]	1889.5	1889.5	1894.4	1883.4	1883.4	1888.4
gdb 298	1891.7[a]	1894.9	1894.9	1898.4	1886.3	1886.3	1891.6
gdb 299	1883.5[a]	1885.7	1885.7	1890.5	1879.6	1879.6	1884.6
gdb 300	1884.7[a]	1888.3	1888.3	1892.9	1882.4	1882.4	1887.1
gdb 301	1883.9[a]	1883.6	1883.6	1886.8	1877.8	1877.8	1880.8
gdb 302	1888.9[a]	1887.6	1887.6	1891.2	1881.5	1881.5	1884.8
gdb 303	1887.8[a]	1887.3	1887.3	1890.3	1881.6	1881.6	1884.6
gdb 304	1868.0[a]	1865.3	1865.3	1868.7	1860.6	1860.6	1864.1
gdb 305	1866.0[a]	1862.4	1862.4	1864.9	1858.6	1858.6	1862.1
gdb 306	1864.3[a]	1861.9	1861.9	1864.6	1858.2	1858.2	1861.7
gdb 307	1870.5[a]	1868.4	1868.4	1869.1	1861.1	1861.1	1861.2
gdb 308	1872.1[a]	1866.0	1866.0	1865.3	1859.5	1859.5	1858.5
gdb 309	1872.1[a]	1866.7	1866.7	1866.1	1860.6	1860.5	1859.8
gdb 310	1884.7[a]	1889.6	1889.6	1891.8	1883.9	1883.9	1887.2
gdb 311	1882.2[a]	1886.7	1886.7	1889.5	1883.7	1883.7	1886.7
gdb 312	1881.8[a]	1888.4	1888.4	1891.1	1883.9	1883.9	1887.1
gdb 313	1890.3[a]	1893.0	1893.0	1895.0	1886.4	1886.4	1890.1
gdb 314	1879.3[a]	1881.2	1881.2	1884.2	1878.9	1878.9	1882.0
gdb 315	1878.5[a]	1883.8	1883.8	1886.7	1879.8	1879.8	1883.4
gdb 316	1880.4[a]	1885.8	1885.6	1888.8	1881.9	1881.9	1885.3
gdb 317	1887.6[a]	1889.0	1889.0	1888.3	1882.7	1882.6	1881.3
gdb 318	1885.0[a]	1886.8	1886.8	1886.2	1880.3	1880.3	1879.4
gdb 319	1886.7[a]	1888.1	1888.1	1887.6	1881.7	1881.7	1880.6
gdb 320	1857.6[a]	1857.7	1857.7	1860.9	1854.9	1854.9	1859.7
gdb 321	1848.2[a]	1839.0	1839.0	1841.2	1834.2	1834.1	1835.7
gdb 322	1848.4[a]	1838.5	1838.5	1839.6	1833.0	1833.0	1834.0

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 323	1847.8[a]	1841.1	1841.1	1844.4	1838.4	1838.4	1841.9
gdb 324	1846.6[a]	1836.1	1836.1	1839.2	1835.1	1835.1	1838.4
gdb 325	1851.3[a]	1847.5	1847.5	1851.1	1842.1	1842.1	1848.0
gdb 326	1865.0[a]	1862.3	1862.3	1866.6	1857.1	1857.0	1861.7
gdb 327	1861.4[a]	1858.7	1858.7	1863.1	1853.8	1853.8	1858.1
gdb 328	1861.7[a]	1868.4	1868.4	1873.8	1859.6	1859.6	1866.2
gdb 329	1870.1[a]	1861.5	1861.5	1865.1	1856.6	1856.6	1859.7
gdb 330	1859.9[a]	1857.1	1857.1	1856.6	1850.6	1850.6	1849.7
gdb 331	1860.6[a]	1856.1	1856.0	1855.2	1850.7	1850.7	1850.3
gdb 332	1859.1[a]	1857.7	1857.7	1859.6	1852.3	1852.3	1856.6
gdb 333	1870.1[a]	1862.5	1862.5	1858.6	1854.0	1854.0	1848.7
gdb 334	1864.1[a]	1858.1	1858.1	1862.0	1855.5	1855.5	1859.3
gdb 335	1864.1[a]	1857.1	1857.1	1860.3	1854.4	1854.4	1858.1
gdb 336	1864.1[a]	1861.2	1861.2	1863.6	1856.7	1856.7	1859.9
gdb 337	1862.9[a]	1854.2	1854.2	1857.1	1852.7	1852.7	1856.2
gdb 338	1847.1[a]	1841.9	1841.9	1844.7	1838.5	1838.5	1841.7
gdb 339	1865.7[a]	1867.2	1867.2	1870.3	1860.7	1860.7	1866.0
gdb 340	1861.1[a]	1857.0	1857.0	1857.3	1849.8	1849.8	1849.7
gdb 341	1870.1[a]	1865.9	1865.9	1866.3	1859.0	1859.0	1859.1
gdb 342	1871.5[a]	1862.2	1862.2	1861.3	1856.0	1856.0	1854.5
gdb 343	1865.8[a]	1860.9	1860.9	1860.5	1854.9	1854.9	1854.6
gdb 344	1891.7[a]	1893.0	1893.0	1896.0	1885.2	1885.2	1891.6
gdb 345	1886.8[a]	1889.2	1889.2	1893.8	1884.1	1884.1	1889.8
gdb 346	1887.9[a]	1891.5	1891.5	1895.1	1885.9	1885.9	1890.9
gdb 347	1896.2[a]	1899.7	1899.7	1903.3	1892.4	1892.4	1897.9
gdb 348	1869.6[a]	1865.5	1865.5	1868.1	1860.6	1860.6	1866.1
gdb 349	1869.8[a]	1864.7	1864.7	1864.9	1858.7	1858.7	1859.5
gdb 350	1866.3[a]	1863.5	1863.5	1863.2	1856.9	1856.9	1857.3
gdb 351	1896.0[a]	1897.3	1897.3	1899.2	1889.7	1889.7	1895.4
gdb 352	1890.6[a]	1892.5	1892.5	1895.7	1887.3	1887.2	1891.9
gdb 353	1895.8[a]	1896.7	1896.7	1898.5	1888.7	1888.7	1894.4
gdb 354	1866.6[a]	1871.1	1871.1	1873.2	1866.6	1866.6	1869.6
gdb 355	1831.3[a]	1813.0	1813.5	1815.8	1808.8	1808.8	1809.7
gdb 356	1829.9[a]	1811.3	1811.3	1813.5	1807.0	1806.9	1808.2
gdb 357	1870.4[a]	1872.1	1872.1	1875.1	1867.3	1867.3	1871.0
gdb 358	1868.1[a]	1869.3	1869.3	1872.0	1864.4	1864.4	1868.4
gdb 359	1827.4[a]	1811.2	1811.2	1813.7	1806.9	1806.9	1808.4
gdb 360	1824.9[a]	1809.0	1809.0	1811.5	1804.9	1804.9	1806.6
gdb 361	1839.8[a]	1825.7	1824.5	1827.8	1823.5	1821.9	1825.3
gdb 362	1837.1[a]	1822.5	1822.5	1825.8	1820.2	1820.2	1823.8
gdb 363	1872.5[a]	1872.7	1872.7	1875.9	1867.6	1867.5	1871.4
gdb 364	1869.7[a]	1870.0	1870.0	1873.1	1865.2	1865.2	1869.5
gdb 365	1861.1[a]	1866.5	1866.5	1870.1	1858.3	1858.3	1863.0
gdb 366	1860.8[a]	1858.9	1858.9	1861.3	1853.6	1853.6	1856.0
gdb 367	1863.2[a]	1860.8	1860.8	1861.2	1853.6	1853.5	1853.7
gdb 368	1861.5[a]	1861.4	1861.4	1861.7	1853.9	1853.8	1853.2
gdb 369	1865.3[a]	1860.8	1860.8	1859.3	1852.7	1852.7	1850.1
gdb 370	1876.1[a]	1878.5	1878.5	1881.4	1872.8	1872.8	1875.5
gdb 371	1882.0[a]	1884.7	1884.7	1886.6	1876.3	1876.3	1879.8
gdb 372	1880.4[a]	1878.1	1878.1	1877.7	1870.3	1870.2	1869.2
gdb 373	1848.3[a]	1840.7	1840.7	1843.6	1837.5	1837.4	1839.9
gdb 374	1852.5[a]	1850.8	1850.8	1850.9	1843.7	1843.7	1842.7
gdb 375	1848.0[a]	1846.5	1846.5	1846.1	1839.3	1839.3	1838.7
gdb 376	1872.3[a]	1866.4	1866.4	1865.5	1858.6	1858.6	1857.2
gdb 377	1885.0[a]	1891.5	1891.5	1892.9	1882.0	1882.0	1884.2
gdb 378	1885.2[a]	1891.6	1891.6	1893.2	1882.4	1882.3	1884.7
gdb 379	1885.1[a]	1884.9	1884.8	1887.3	1878.1	1878.0	1881.7
gdb 380	1885.8[a]	1889.4	1889.4	1891.1	1881.8	1881.8	1883.7
gdb 381	1879.0[a]	1879.1	1879.1	1882.2	1874.6	1874.6	1877.3
gdb 382	1884.1[a]	1882.4	1882.4	1882.3	1874.5	1874.5	1874.1
gdb 383	1886.3[a]	1887.0	1887.0	1885.9	1878.2	1878.2	1876.0
gdb 384	1882.3[a]	1880.5	1880.5	1880.1	1872.3	1872.3	1871.6
gdb 385	1869.0[a]	1867.4	1867.3	1870.8	1864.1	1864.0	1867.0
gdb 386	1871.8[a]	1868.9	1868.9	1868.0	1862.3	1862.2	1861.1
gdb 387	1869.6[a]	1878.7	1878.7	1881.8	1870.2	1870.2	1873.9

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 388	1869.9[a]	1866.7	1866.7	1870.1	1863.4	1863.3	1865.7
gdb 389	1863.7[a]	1862.6	1862.6	1865.6	1859.8	1859.8	1862.6
gdb 390	1868.6[a]	1871.8	1871.8	1871.8	1864.0	1864.0	1862.8
gdb 391	1869.0[a]	1870.1	1870.1	1869.9	1862.9	1862.9	1862.1
gdb 392	1869.8[a]	1873.2	1873.2	1873.4	1865.9	1865.8	1865.0
gdb 393	1847.1[a]	1843.4	1843.4	1845.6	1837.9	1837.9	1840.0
gdb 394	1849.3[a]	1841.7	1841.7	1844.6	1837.8	1837.8	1839.9
gdb 395	1844.4[a]	1837.3	1837.3	1839.8	1834.0	1834.0	1836.7
gdb 396	1854.8[a]	1851.4	1851.4	1851.4	1843.4	1843.4	1841.8
gdb 397	1848.4[a]	1846.5	1846.5	1846.1	1838.8	1838.8	1837.7
gdb 398	1852.6[a]	1850.0	1850.0	1849.5	1841.5	1841.4	1839.5
gdb 399	1864.2[a]	1865.3	1865.3	1864.0	1859.6	1859.6	1857.6
gdb 400	1869.4[a]	1868.8	1868.8	1863.9	1860.0	1860.0	1853.9
gdb 401	1865.5[a]	1860.2	1860.2	1862.8	1855.7	1855.7	1858.1
gdb 402	1870.7[a]	1864.6	1864.6	1863.7	1856.5	1856.5	1854.6
gdb 403	1865.2[a]	1864.5	1864.5	1865.3	1856.4	1856.3	1856.5
gdb 404	1868.0[a]	1862.2	1862.2	1861.0	1856.8	1856.8	1855.6
gdb 405	1856.0[a]	1854.0	1854.0	1856.9	1851.8	1851.8	1855.1
gdb 406	1876.2[a]	1867.3	1867.3	1862.9	1859.2	1859.2	1853.6
gdb 407	1864.1[a]	1860.4	1860.4	1859.1	1854.7	1854.6	1853.4
gdb 408	1867.6[a]	1868.1	1868.1	1871.5	1862.9	1862.9	1865.9
gdb 409	1867.4[a]	1863.7	1863.7	1866.5	1860.4	1860.4	1863.2
gdb 410	1867.7[a]	1863.9	1863.9	1866.9	1860.7	1860.7	1863.7
gdb 411	1871.7[a]	1867.5	1867.5	1866.7	1860.5	1860.5	1859.0
gdb 412	1872.9[a]	1868.1	1868.1	1867.3	1861.4	1861.4	1860.2
gdb 413	1867.5[a]	1873.5	1873.4	1873.7	1865.5	1865.5	1864.8
gdb 414	1863.2[a]	1865.8	1865.8	1864.6	1858.1	1858.1	1856.2
gdb 415	1864.6[a]	1864.3	1864.3	1863.2	1858.4	1858.4	1856.2
gdb 416	1862.2[a]	1865.2	1865.2	1866.8	1859.7	1859.7	1861.9
gdb 417	1869.9[a]	1868.1	1868.1	1863.5	1858.8	1858.7	1852.5
gdb 418	1867.0[a]	1862.5	1862.5	1861.3	1855.4	1855.4	1854.3
gdb 419	1868.1[a]	1861.7	1861.7	1860.4	1856.2	1856.2	1854.7
gdb 420	1865.1[a]	1863.9	1863.9	1865.3	1858.3	1858.3	1861.9
gdb 421	1874.7[a]	1866.3	1866.3	1861.6	1857.5	1857.5	1851.5
gdb 422	1865.9[a]	1862.9	1862.9	1861.7	1856.9	1856.9	1855.6
gdb 423	1866.7[a]	1863.6	1863.6	1862.2	1856.5	1856.5	1855.0
gdb 424	1869.8[a]	1868.0	1868.0	1867.2	1860.7	1860.7	1860.6
gdb 425	1872.4[a]	1871.4	1871.4	1873.4	1864.8	1864.8	1869.6
gdb 426	1871.3[a]	1868.1	1868.1	1867.6	1861.1	1861.0	1861.1
gdb 427	1870.3[a]	1867.7	1867.7	1867.3	1860.4	1860.4	1860.2
gdb 428	1846.2[a]	1840.3	1840.3	1835.0	1830.4	1830.4	1823.7
gdb 429	1847.2[a]	1842.2	1842.2	1837.2	1832.1	1832.1	1824.9
gdb 430	1860.6[a]	1851.9	1851.9	1851.7	1844.2	1844.1	1843.1
gdb 431	1859.5[a]	1850.5	1850.5	1850.6	1843.0	1842.9	1842.3
gdb 432	1863.2[a]	1854.6	1854.6	1852.9	1845.9	1845.9	1842.8
gdb 433	1859.5[a]	1862.4	1862.3	1864.0	1855.8	1855.7	1858.3
gdb 434	1867.4[a]	1864.7	1864.7	1863.4	1857.4	1857.4	1855.3
gdb 435	1864.1[a]	1861.0	1861.0	1859.6	1854.8	1854.8	1852.7
gdb 436	1865.6[a]	1863.3	1863.3	1862.0	1856.4	1856.3	1854.8
gdb 437	1862.9[a]	1860.2	1860.2	1859.1	1853.9	1853.9	1852.4
gdb 438	1872.1[a]	1864.8	1864.8	1860.0	1855.7	1855.6	1849.3
gdb 439	1849.1[a]	1841.9	1841.8	1844.8	1836.3	1836.3	1838.5
gdb 440	1849.8[a]	1845.4	1845.4	1845.2	1837.4	1837.4	1836.2
gdb 441	1848.1[a]	1843.7	1843.7	1843.6	1835.9	1835.9	1835.1
gdb 442	1873.1[a]	1871.3	1871.3	1870.1	1864.2	1864.2	1863.5
gdb 443	1874.0[a]	1871.7	1871.7	1870.5	1864.7	1864.7	1864.1
gdb 444	1857.5[a]	1848.8	1848.8	1849.2	1841.8	1841.8	1841.4
gdb 445	1859.5[a]	1850.4	1850.3	1848.8	1842.4	1842.3	1839.9
gdb 446	1855.9[a]	1859.8	1859.8	1861.5	1852.9	1852.9	1856.0
gdb 447	1860.4[a]	1858.3	1858.3	1857.2	1852.7	1852.7	1851.0
gdb 448	1864.1[a]	1861.2	1861.2	1860.0	1855.1	1855.1	1853.6
gdb 449	1845.8[a]	1839.0	1839.0	1837.8	1831.8	1831.7	1829.5
gdb 450	1843.6[a]	1834.5	1834.5	1833.6	1829.7	1829.7	1828.1
gdb 451	1841.2[a]	1836.5	1836.4	1834.9	1829.9	1829.8	1828.0
gdb 452	1849.3[a]	1845.4	1845.3	1841.7	1835.8	1835.7	1830.1

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 453	1845.8[a]	1840.6	1840.6	1835.6	1831.3	1831.3	1824.1
gdb 454	1845.3[a]	1839.5	1839.5	1834.9	1831.0	1830.9	1824.5
gdb 455	1846.0[a]	1838.5	1838.5	1837.7	1833.0	1833.0	1830.7
gdb 456	1848.5[a]	1845.5	1845.5	1841.5	1836.2	1836.1	1830.5
gdb 457	1860.9[a]	1852.4	1852.4	1851.3	1844.3	1844.3	1842.0
gdb 458	1858.6[a]	1850.7	1850.7	1851.4	1843.6	1843.6	1843.0
gdb 459	1860.8[a]	1865.1	1865.1	1867.9	1858.5	1858.5	1860.9
gdb 460	1862.3[a]	1862.3	1862.3	1861.5	1855.8	1855.8	1853.8
gdb 461	1869.8[a]	1863.3	1863.3	1858.7	1854.8	1854.8	1849.1
gdb 462	1847.2[a]	1839.5	1839.4	1842.8	1834.3	1834.3	1837.0
gdb 463	1845.6[a]	1841.5	1841.5	1841.8	1834.1	1834.0	1833.6
gdb 464	1846.1[a]	1841.5	1841.5	1841.8	1834.6	1834.6	1834.3
gdb 465	1847.8[a]	1843.6	1843.9	1844.3	1836.5	1836.5	1835.7
gdb 466	1844.5[a]	1841.2	1841.1	1839.6	1833.6	1833.5	1831.0
gdb 467	1844.5[a]	1836.9	1836.9	1835.9	1831.5	1831.5	1829.5
gdb 468	1846.3[a]	1841.3	1841.2	1839.8	1833.3	1833.4	1830.5
gdb 469	1847.8[a]	1845.4	1845.4	1841.5	1835.7	1835.6	1830.2
gdb 470	1865.5[a]	1865.1	1865.1	1863.7	1857.5	1857.4	1855.4
gdb 471	1869.2[a]	1863.2	1863.2	1858.5	1854.3	1854.3	1848.4
gdb 472	1861.2[a]	1859.8	1859.8	1859.0	1853.8	1853.8	1852.3
gdb 473	1865.1[a]	1865.7	1865.7	1864.8	1858.4	1858.4	1856.4
gdb 474	1873.0[a]	1871.5	1871.5	1870.1	1864.2	1864.2	1863.4
gdb 475	1872.0[a]	1869.5	1869.5	1868.7	1862.4	1862.4	1862.0
gdb 476	1872.9[a]	1871.5	1871.5	1870.0	1864.0	1864.0	1863.2
gdb 477	1861.7[a]	1852.6	1852.5	1856.9	1847.4	1847.4	1851.2
gdb 478	1862.7[a]	1853.1	1853.1	1855.6	1846.8	1846.7	1848.5
gdb 479	1857.9[a]	1849.2	1849.2	1853.2	1844.3	1844.3	1848.7
gdb 480	1860.2[a]	1851.4	1851.4	1853.4	1845.5	1845.5	1847.7
gdb 481	1858.8[a]	1863.7	1863.6	1866.3	1856.7	1856.7	1860.6
gdb 482	1860.0[a]	1853.7	1853.7	1856.9	1851.4	1851.4	1854.5
gdb 483	1862.4[a]	1857.6	1857.6	1860.5	1854.9	1854.9	1858.1
gdb 484	1858.7[a]	1856.7	1856.7	1858.9	1853.1	1853.0	1856.1
gdb 485	1862.3[a]	1859.8	1859.8	1862.1	1855.7	1855.7	1858.9
gdb 486	1865.4[a]	1856.5	1856.5	1859.3	1850.4	1850.4	1852.5
gdb 487	1860.9[a]	1852.6	1852.6	1855.1	1846.6	1846.6	1849.2
gdb 488	1862.4[a]	1854.3	1854.3	1858.7	1849.0	1849.0	1853.1
gdb 489	1853.5[a]	1847.3	1847.3	1851.8	1841.7	1841.7	1845.3
gdb 490	1849.1[a]	1843.9	1843.9	1847.9	1838.4	1838.4	1842.3
gdb 491	1851.3[a]	1846.7	1846.7	1850.8	1841.4	1841.4	1845.4
gdb 492	1850.4[a]	1845.8	1845.8	1849.8	1840.4	1840.4	1844.3
gdb 493	1846.2[a]	1842.4	1842.4	1846.2	1837.2	1837.2	1841.6
gdb 494	1845.8[a]	1842.5	1842.5	1846.2	1837.4	1837.3	1841.8
gdb 495	1875.3[a]	1874.0	1874.0	1876.8	1868.7	1868.7	1872.9
gdb 496	1875.4[a]	1872.5	1872.5	1875.5	1866.7	1866.7	1870.8
gdb 497	1872.9[a]	1870.4	1870.4	1873.3	1864.9	1864.9	1869.5
gdb 498	1875.3[a]	1874.5	1874.5	1877.1	1868.7	1868.7	1872.6
gdb 499	1864.5[a]	1855.6	1855.6	1859.7	1850.8	1850.8	1854.4
gdb 500	1863.2[a]	1852.1	1852.1	1856.7	1847.0	1847.0	1851.7
gdb 501	1860.4[a]	1851.9	1851.9	1856.6	1846.8	1846.8	1851.5
gdb 502	1866.1[a]	1857.0	1857.0	1859.3	1851.0	1851.0	1853.3
gdb 503	1857.3[a]	1851.0	1851.0	1855.0	1845.7	1845.7	1850.1
gdb 504	1855.5[a]	1857.9	1857.9	1862.4	1849.5	1849.5	1855.3
gdb 505	1861.3[a]	1856.6	1856.6	1860.0	1850.4	1850.4	1853.9
gdb 506	1853.3[a]	1846.6	1846.6	1851.1	1841.7	1841.7	1846.6
gdb 507	1853.4[a]	1849.1	1849.1	1853.6	1844.1	1844.1	1848.8
gdb 508	1853.7[a]	1847.9	1847.9	1851.9	1842.6	1842.6	1846.9
gdb 509	1854.0[a]	1846.8	1846.8	1850.8	1841.8	1841.8	1846.7
gdb 510	1854.2[a]	1846.7	1846.7	1850.8	1842.1	1842.1	1846.3
gdb 511	1861.8[a]	1850.5	1850.5	1852.9	1844.7	1844.7	1847.1
gdb 512	1876.0[a]	1873.5	1873.5	1878.1	1868.3	1868.3	1872.5
gdb 513	1887.4[a]	1891.0	1891.0	1893.2	1881.2	1881.2	1884.2
gdb 514	1881.2[a]	1879.4	1879.4	1883.1	1871.3	1871.2	1876.1
gdb 515	1864.8[a]	1866.3	1866.3	1868.9	1857.5	1857.5	1860.8
gdb 516	1853.0[a]	1844.4	1844.4	1848.1	1839.9	1839.9	1843.1
gdb 517	1872.9[a]	1866.6	1866.6	1870.3	1861.2	1861.2	1865.0

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 518	1874.2[a]	1867.9	1867.9	1871.0	1862.6	1862.6	1866.5
gdb 519	1881.0[a]	1877.7	1877.7	1879.6	1870.9	1870.9	1873.1
gdb 520	1873.3[a]	1867.2	1867.2	1870.6	1862.1	1862.1	1865.7
gdb 521	1860.7[a]	1858.2	1858.2	1862.6	1853.2	1853.2	1857.3
gdb 522	1867.9[a]	1866.4	1866.4	1869.3	1858.1	1858.1	1862.6
gdb 523	1859.6[a]	1853.2	1853.2	1857.0	1848.6	1848.6	1852.3
gdb 524	1860.6[a]	1852.3	1852.3	1855.6	1847.2	1847.2	1851.0
gdb 525	1863.5[a]	1856.5	1856.5	1858.9	1850.2	1850.2	1853.5
gdb 526	1866.0[a]	1873.6	1873.6	1877.5	1865.4	1865.4	1870.0
gdb 527	1865.0[a]	1862.9	1862.9	1867.0	1858.5	1858.5	1862.3
gdb 528	1861.8[a]	1861.6	1861.6	1865.1	1856.8	1856.8	1860.9
gdb 529	1865.0[a]	1855.6	1855.6	1858.9	1852.0	1852.0	1855.2
gdb 530	1845.6[a]	1838.9	1838.9	1843.1	1834.6	1834.6	1838.8
gdb 531	1873.4[a]	1873.5	1873.5	1877.6	1867.9	1867.9	1871.8
gdb 532	1873.7[a]	1873.7	1873.7	1878.0	1868.1	1868.1	1872.0
gdb 533	1870.4[a]	1867.0	1867.0	1870.2	1862.1	1862.1	1865.1
gdb 534	1843.4[a]	1833.5	1833.5	1836.3	1829.3	1829.3	1832.5
gdb 535	1868.9[a]	1868.6	1868.6	1872.6	1863.8	1863.7	1867.9
gdb 536	1873.4[a]	1872.4	1872.4	1876.5	1867.3	1867.3	1870.8
gdb 537	1872.7[a]	1881.0	1881.0	1885.0	1872.1	1872.1	1876.8
gdb 538	1869.9[a]	1865.4	1865.4	1869.0	1861.0	1861.0	1863.9
gdb 539	1869.1[a]	1870.4	1870.4	1874.3	1865.3	1865.3	1869.0
gdb 540	1867.3[a]	1868.0	1868.0	1871.8	1862.9	1862.9	1866.9
gdb 541	1869.9[a]	1870.4	1870.4	1874.3	1864.9	1864.8	1868.5
gdb 542	1866.8[a]	1867.4	1867.4	1871.1	1862.4	1862.3	1866.7
gdb 543	1868.6[a]	1869.9	1869.7	1873.7	1864.7	1864.6	1868.9
gdb 544	1891.2[a]	1896.2	1896.2	1898.7	1891.7	1891.7	1895.6
gdb 545	1874.4[a]	1877.8	1877.8	1880.6	1869.9	1869.9	1875.6
gdb 546	1868.1[a]	1867.0	1867.0	1869.7	1862.3	1862.3	1866.4
gdb 547	1866.5[a]	1864.7	1864.7	1867.3	1860.1	1860.1	1864.0
gdb 548	1889.5[a]	1895.1	1895.1	1897.9	1885.2	1885.2	1888.9
gdb 549	1885.5[a]	1880.1	1880.1	1883.8	1874.1	1874.1	1878.6
gdb 550	1888.9[a]	1884.1	1884.1	1887.3	1877.8	1877.8	1880.9
gdb 551	1885.2[a]	1879.4	1879.3	1883.0	1873.2	1873.2	1877.6
gdb 552	1869.7[a]	1880.3	1880.3	1884.8	1871.2	1871.2	1876.3
gdb 553	1868.4[a]	1869.0	1869.0	1873.4	1863.7	1863.7	1868.0
gdb 554	1867.8[a]	1867.6	1867.6	1871.7	1862.8	1862.8	1867.3
gdb 555	1868.7[a]	1869.9	1869.9	1874.3	1864.8	1864.8	1869.1
gdb 556	1863.1[a]	1861.3	1861.3	1863.9	1855.1	1855.0	1859.1
gdb 557	1856.9[a]	1846.0	1846.0	1849.0	1844.2	1844.2	1847.2
gdb 558	1856.2[a]	1848.6	1848.6	1851.5	1845.8	1845.8	1849.1
gdb 559	1870.3[a]	1874.9	1874.9	1879.7	1868.9	1868.8	1873.1
gdb 560	1865.0[a]	1862.8	1862.8	1865.9	1857.8	1857.8	1861.5
gdb 561	1871.5[a]	1868.3	1868.3	1871.5	1863.8	1863.8	1867.5
gdb 562	1870.1[a]	1868.7	1868.7	1871.9	1864.3	1864.3	1868.1
gdb 563	1872.7[a]	1864.1	1864.1	1867.3	1858.5	1858.5	1861.8
gdb 564	1868.4[a]	1866.9	1866.9	1872.1	1860.9	1860.9	1866.1
gdb 565	1872.8[a]	1865.7	1865.6	1868.7	1860.1	1860.1	1863.5
gdb 566	1899.5[a]	1900.2	1900.2	1903.8	1893.5	1893.5	1897.2
gdb 567	1906.6[a]	1907.9	1907.9	1910.4	1898.6	1898.5	1903.0
gdb 568	1898.2[a]	1898.9	1898.9	1902.9	1892.6	1892.6	1897.0
gdb 569	1897.1[a]	1897.4	1897.3	1901.6	1891.0	1891.0	1895.7
gdb 570	1899.2[a]	1901.2	1901.2	1905.0	1895.0	1895.0	1899.4
gdb 571	1877.5[a]	1880.2	1880.2	1882.9	1876.8	1876.7	1879.8
gdb 572	1881.0[a]	1883.0	1883.0	1885.6	1879.4	1879.4	1882.7
gdb 573	1881.4[a]	1882.3	1882.3	1885.1	1879.0	1879.0	1882.4
gdb 574	1878.6[a]	1880.3	1880.3	1883.2	1877.7	1877.6	1880.7
gdb 575	1881.8[a]	1883.0	1883.0	1884.9	1877.3	1877.3	1880.6
gdb 576	1883.7[a]	1885.3	1885.3	1887.9	1881.3	1881.3	1884.9
gdb 577	1881.0[a]	1879.6	1879.6	1884.4	1871.4	1871.4	1877.8
gdb 578	1875.7[a]	1873.4	1873.4	1878.2	1868.6	1868.5	1873.2
gdb 579	1876.6[a]	1873.6	1873.6	1878.2	1869.1	1869.1	1874.2
gdb 580	1867.5[a]	1862.2	1862.2	1865.6	1858.0	1858.0	1862.6
gdb 581	1864.9[a]	1861.6	1861.6	1865.0	1857.1	1857.1	1861.9
gdb 582	1864.2[a]	1860.7	1860.7	1864.1	1855.9	1855.9	1860.8

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 583	1897.5[a]	1902.2	1902.2	1905.3	1895.0	1895.0	1899.4
gdb 584	1896.8[a]	1902.8	1902.8	1905.4	1895.3	1895.3	1899.8
gdb 585	1891.8[a]	1896.2	1896.2	1898.6	1888.6	1888.6	1893.6
gdb 586	1886.0[a]	1892.1	1892.1	1895.7	1887.3	1887.3	1891.9
gdb 587	1894.9[a]	1902.6	1902.6	1905.6	1894.5	1894.5	1898.7
gdb 588	1894.0[a]	1901.7	1901.7	1904.4	1893.3	1893.2	1897.2
gdb 589	1910.5[a]	1918.0	1918.0	1920.0	1908.8	1908.8	1911.8
gdb 590	1912.2[a]	1916.4	1916.4	1918.9	1907.8	1907.8	1911.8
gdb 591	1906.1[a]	1912.2	1912.2	1915.5	1905.7	1905.7	1908.9
gdb 592	1905.7[a]	1909.9	1909.9	1914.0	1903.9	1903.9	1908.2
gdb 593	1911.3[a]	1913.6	1913.6	1916.7	1905.2	1905.2	1910.0
gdb 594	1899.2[a]	1902.3	1902.3	1905.4	1894.4	1894.4	1899.5
gdb 595	1899.8[a]	1903.3	1903.3	1906.6	1895.6	1895.6	1900.9
gdb 596	1898.7[a]	1900.7	1900.7	1903.5	1892.7	1892.7	1898.1
gdb 597	1893.9[a]	1894.3	1894.3	1898.1	1889.5	1889.5	1894.0
gdb 598	1896.9[a]	1897.9	1897.9	1900.1	1890.9	1890.9	1895.4
gdb 599	1868.1[a]	1860.3	1860.3	1863.3	1856.7	1856.7	1860.6
gdb 600	1893.7[a]	1897.5	1897.5	1900.7	1890.5	1890.4	1895.9
gdb 601	1888.5[a]	1891.1	1891.1	1894.5	1886.2	1886.2	1890.6
gdb 602	1892.5[a]	1896.6	1896.6	1899.6	1889.2	1889.2	1894.4
gdb 603	1879.1[a]	1877.1	1877.1	1880.4	1874.4	1874.4	1878.0
gdb 604	1885.6[a]	1886.6	1886.6	1889.5	1881.1	1881.1	1885.5
gdb 605	1876.1[a]	1874.8	1874.8	1878.1	1871.8	1871.8	1876.2
gdb 606	1888.5[a]	1891.6	1891.6	1893.8	1885.0	1885.0	1889.3
gdb 607	1880.4[a]	1880.7	1880.7	1884.0	1877.5	1877.5	1881.5
gdb 608	1897.7[a]	1901.0	1901.0	1902.6	1893.2	1893.2	1897.4
gdb 609	1886.4[a]	1888.7	1888.7	1891.8	1884.3	1884.3	1888.7
gdb 610	1892.1[a]	1893.7	1893.7	1896.0	1887.2	1887.1	1891.6
gdb 611	1891.8[a]	1896.1	1896.1	1898.6	1890.9	1890.9	1895.0
gdb 612	1891.7[a]	1896.0	1896.0	1898.8	1887.6	1887.6	1892.9
gdb 613	1885.1[a]	1890.1	1890.1	1893.8	1884.7	1884.6	1889.5
gdb 614	1884.3[a]	1889.4	1889.4	1892.9	1883.7	1883.7	1888.7
gdb 615	1890.6[a]	1895.9	1895.9	1898.9	1888.1	1888.1	1893.6
gdb 616	1885.4[a]	1888.5	1888.5	1890.1	1882.3	1882.3	1886.6
gdb 617	1879.6[a]	1883.5	1883.5	1886.6	1880.0	1880.0	1883.7
gdb 618	1878.9[a]	1880.2	1880.2	1883.0	1876.6	1876.6	1880.5
gdb 619	1875.6[a]	1876.9	1876.8	1879.4	1874.0	1874.0	1877.6
gdb 620	1881.4[a]	1884.6	1884.6	1886.8	1881.1	1881.1	1884.4
gdb 621	1882.4[a]	1885.2	1885.2	1887.7	1880.9	1880.8	1884.3
gdb 622	1887.8[a]	1891.9	1891.9	1893.6	1885.3	1885.2	1889.1
gdb 623	1893.1[a]	1899.3	1899.3	1901.4	1892.3	1892.3	1896.8
gdb 624	1886.9[a]	1896.2	1896.2	1898.9	1891.1	1891.1	1895.1
gdb 625	1889.7[a]	1895.0	1895.0	1897.4	1890.3	1890.3	1894.2
gdb 626	1889.1[a]	1895.6	1895.6	1898.6	1890.7	1890.7	1895.2
gdb 627	1895.6[a]	1899.0	1899.0	1900.6	1891.3	1891.3	1896.5
gdb 628	1891.9[a]	1896.3	1896.3	1899.3	1891.3	1891.3	1895.8
gdb 629	1893.0[a]	1897.0	1897.0	1900.2	1891.8	1891.7	1896.1
gdb 630	1897.1[a]	1898.7	1898.7	1900.7	1891.7	1891.7	1896.3
gdb 631	1896.9[a]	1909.0	1909.0	1911.0	1900.9	1900.9	1904.7
gdb 632	1894.9[a]	1905.4	1905.4	1907.2	1896.8	1896.8	1900.9
gdb 633	1891.1[a]	1900.2	1900.2	1902.9	1894.6	1894.6	1898.0
gdb 634	1895.2[a]	1904.1	1904.1	1905.7	1895.3	1895.3	1899.1
gdb 635	1899.4[a]	1907.4	1907.4	1908.8	1899.6	1899.5	1902.7
gdb 636	1897.0[a]	1906.8	1906.8	1908.4	1898.5	1898.5	1901.8
gdb 637	1873.3[a]	1873.2	1873.2	1875.5	1865.6	1865.6	1872.1
gdb 638	1860.4[a]	1857.7	1857.7	1860.0	1852.0	1852.0	1857.9
gdb 639	1848.7[a]	1848.1	1848.1	1851.0	1843.9	1843.9	1849.1
gdb 640	1846.7[a]	1851.8	1851.7	1855.4	1847.1	1847.1	1852.3
gdb 641	1856.2[a]	1858.3	1858.3	1860.0	1851.2	1851.2	1856.9
gdb 642	1871.5[a]	1876.8	1876.8	1878.2	1874.5	1874.5	1871.2
gdb 643	1871.8[a]	1874.2	1874.2	1875.4	1872.3	1872.3	1872.7
gdb 644	1871.4[a]	1877.0	1876.5	1875.4	1871.8	1871.7	1868.5
gdb 645	1867.8[a]	1872.5	1872.5	1869.8	1868.3	1868.1	1864.1
gdb 646	1873.1[a]	1876.5	1876.5	1874.1	1872.6	1872.6	1868.4
gdb 647	1885.2[a]	1883.4	1883.4	1883.6	1881.9	1881.9	1882.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 648	1892.2[a]	1894.8	1894.8	1897.7	1894.3	1894.2	1897.9
gdb 649	1888.9[a]	1894.6	1894.6	1898.0	1893.6	1893.6	1896.7
gdb 650	1897.5[a]	1895.3	1895.3	1897.5	1894.8	1894.8	1896.6
gdb 651	1910.0[a]	1916.8	1916.8	1919.2	1914.7	1914.7	1917.8
gdb 652	1907.1[a]	1914.5	1914.5	1916.6	1912.8	1912.8	1915.0
gdb 653	1910.5[a]	1917.7	1917.7	1919.8	1916.1	1916.1	1918.4
gdb 654	1876.8[a]	1876.7	1876.7	1879.7	1876.6	1876.6	1879.5
gdb 655	1873.4[a]	1874.1	1874.1	1877.0	1874.2	1874.2	1877.4
gdb 656	1897.6[a]	1884.5	1884.5	1887.0	1883.6	1883.6	1886.8
gdb 657	1870.8[a]	1875.7	1875.7	1877.2	1876.2	1876.2	1878.2
gdb 658	1895.8[a]	1880.5	1880.4	1881.9	1880.4	1880.4	1882.4
gdb 659	1874.9[a]	1875.5	1875.5	1874.7	1873.6	1873.6	1872.0
gdb 660	1897.1[a]	1907.3	1907.3	1909.7	1906.8	1906.8	1909.1
gdb 661	1893.1[a]	1902.0	1902.0	1904.6	1901.5	1901.5	1904.4
gdb 662	1919.7[a]	1909.2	1909.2	1910.6	1908.7	1908.7	1910.9
gdb 663	1913.5[a]	1921.1	1921.1	1923.5	1919.7	1919.7	1922.6
gdb 664	1913.2[a]	1919.8	1919.8	1922.2	1918.2	1918.2	1921.6
gdb 665	1910.0[a]	1917.5	1917.5	1919.6	1915.8	1915.8	1918.3
gdb 666	1916.7[a]	1924.7	1924.7	1926.6	1922.9	1922.9	1924.7
gdb 667	1933.5[a]	1930.7	1930.7	1931.9	1928.2	1928.1	1930.8
gdb 668	1918.0[a]	1927.4	1927.4	1929.2	1925.4	1925.3	1926.9
gdb 669	1929.0[a]	1929.9	1929.9	1931.0	1927.3	1927.3	1930.1
gdb 670	1915.7[a]	1923.4	1923.4	1925.1	1922.1	1922.1	1924.3
gdb 671	1913.4[a]	1922.0	1922.0	1923.8	1920.5	1920.5	1922.8
gdb 672	1912.1[a]	1920.1	1920.1	1921.9	1918.3	1918.3	1920.4
gdb 673	1931.9[a]	1930.6	1930.6	1931.1	1928.0	1928.0	1930.1
gdb 674	1932.8[a]	1935.3	1935.3	1936.1	1933.9	1933.9	1936.0
gdb 675	1914.3[a]	1927.0	1927.0	1928.4	1926.9	1926.9	1928.5
gdb 676	1911.3[a]	1924.1	1924.1	1925.9	1923.9	1923.9	1926.1
gdb 677	1892.2[a]	1897.5	1897.5	1899.8	1897.0	1896.9	1899.7
gdb 678	1893.5[a]	1896.6	1896.6	1899.1	1896.4	1896.4	1899.4
gdb 679	1894.2[a]	1897.0	1897.0	1899.5	1897.1	1897.1	1900.1
gdb 680	1897.4[a]	1900.6	1900.6	1903.2	1900.4	1900.4	1903.4
gdb 681	1918.3[a]	1904.2	1904.2	1905.3	1904.2	1904.2	1906.4
gdb 682	1908.0[a]	1907.6	1907.6	1908.2	1906.2	1906.2	1907.6
gdb 683	1894.0[a]	1898.8	1898.8	1896.6	1896.4	1896.4	1893.6
gdb 684	1909.9[a]	1910.2	1910.2	1910.6	1908.4	1908.4	1909.4
gdb 685	1889.8[a]	1900.4	1900.3	1901.7	1899.8	1899.7	1900.7
gdb 686	1895.5[a]	1906.3	1906.3	1908.2	1904.6	1904.6	1905.9
gdb 687	1893.3[a]	1902.4	1902.4	1904.7	1901.1	1901.1	1903.5
gdb 688	1896.3[a]	1899.5	1899.5	1901.2	1898.8	1898.8	1899.9
gdb 689	1915.1[a]	1905.3	1905.3	1906.2	1904.0	1904.0	1905.9
gdb 690	1874.2[a]	1875.1	1875.1	1877.8	1874.6	1874.6	1877.3
gdb 691	1873.4[a]	1874.2	1874.2	1877.0	1873.8	1873.8	1876.8
gdb 692	1873.0[a]	1874.4	1874.4	1877.2	1873.5	1873.5	1875.9
gdb 693	1894.5[a]	1882.5	1882.5	1884.7	1881.3	1881.3	1884.3
gdb 694	1874.9[a]	1875.8	1875.7	1874.7	1873.5	1873.4	1871.5
gdb 695	1868.6[a]	1874.6	1874.6	1876.0	1874.1	1874.1	1875.5
gdb 696	1871.0[a]	1869.7	1869.7	1871.4	1869.9	1869.8	1871.1
gdb 697	1892.7[a]	1878.3	1878.2	1879.2	1877.8	1877.8	1879.5
gdb 698	1906.9[a]	1904.3	1904.3	1904.7	1901.8	1901.7	1903.9
gdb 699	1892.0[a]	1896.2	1896.2	1897.3	1896.1	1896.1	1897.6
gdb 700	1900.3[a]	1901.1	1901.1	1898.9	1898.1	1898.1	1895.2
gdb 701	1910.9[a]	1914.5	1914.5	1916.1	1912.1	1912.1	1915.0
gdb 702	1915.7[a]	1919.5	1919.5	1920.7	1917.0	1917.0	1919.1
gdb 703	1899.4[a]	1905.4	1905.4	1906.9	1904.9	1904.9	1906.5
gdb 704	1893.9[a]	1900.4	1900.4	1901.8	1899.9	1899.9	1902.0
gdb 705	1896.0[a]	1909.6	1909.6	1911.7	1908.3	1908.3	1910.3
gdb 706	1901.1[a]	1904.1	1904.1	1906.6	1900.4	1900.4	1904.8
gdb 707	1899.6[a]	1901.4	1901.4	1903.5	1899.8	1899.8	1901.8
gdb 708	1904.1[a]	1906.0	1906.0	1908.2	1903.1	1903.1	1906.6
gdb 709	1887.8[a]	1897.4	1897.4	1900.5	1895.5	1895.5	1898.5
gdb 710	1901.4[a]	1899.4	1899.4	1899.5	1897.1	1897.1	1899.2
gdb 711	1887.5[a]	1891.4	1891.4	1892.4	1891.7	1891.7	1893.3
gdb 712	1895.2[a]	1897.2	1897.2	1895.5	1894.8	1894.7	1892.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 713	1915.4[a]	1922.3	1922.3	1924.2	1920.4	1920.4	1922.5
gdb 714	1915.0[a]	1923.6	1923.6	1925.1	1921.2	1921.2	1922.2
gdb 715	1913.8[a]	1920.9	1920.9	1922.8	1918.7	1918.7	1920.6
gdb 716	1910.6[a]	1919.5	1919.5	1921.8	1917.7	1917.7	1920.2
gdb 717	1926.3[a]	1926.2	1926.2	1927.2	1923.0	1922.9	1925.8
gdb 718	1899.5[a]	1897.0	1897.0	1898.6	1894.2	1894.2	1897.7
gdb 719	1910.1[a]	1912.0	1912.0	1914.0	1909.1	1909.1	1912.3
gdb 720	1899.2[a]	1899.6	1899.6	1900.8	1899.3	1899.3	1901.1
gdb 721	1897.0[a]	1899.9	1899.9	1901.4	1899.2	1899.2	1901.2
gdb 722	1894.2[a]	1903.8	1903.8	1905.9	1902.1	1902.1	1904.7
gdb 723	1909.4[a]	1922.2	1922.2	1923.6	1921.4	1921.4	1922.5
gdb 724	1912.6[a]	1924.0	1924.0	1925.6	1923.2	1923.2	1924.9
gdb 725	1915.2[a]	1927.2	1927.1	1928.7	1926.4	1926.4	1927.9
gdb 726	1913.3[a]	1925.4	1925.4	1927.3	1924.7	1924.7	1926.5
gdb 727	1930.2[a]	1932.4	1932.4	1933.3	1930.5	1930.4	1932.5
gdb 728	1919.2[a]	1929.8	1929.8	1930.2	1932.6	1932.6	1932.6
gdb 729	1896.4[a]	1901.0	1901.0	1902.3	1899.6	1899.6	1900.5
gdb 730	1893.7[a]	1898.6	1898.6	1900.0	1897.2	1897.1	1899.0
gdb 731	1896.4[a]	1908.6	1908.6	1910.6	1906.5	1906.5	1908.1
gdb 732	1891.7[a]	1903.9	1903.9	1906.4	1902.0	1902.0	1904.3
gdb 733	1911.3[a]	1914.1	1914.1	1915.6	1910.9	1910.9	1913.1
gdb 734	1892.4[a]	1898.6	1898.5	1896.2	1895.5	1895.5	1892.5
gdb 735	1889.0[a]	1900.3	1900.3	1901.7	1899.0	1899.0	1899.7
gdb 736	1887.4[a]	1897.1	1897.3	1898.5	1896.7	1896.6	1897.6
gdb 737	1906.9[a]	1907.2	1907.2	1907.8	1905.3	1905.3	1906.5
gdb 738	1907.0[a]	1904.5	1904.5	1904.9	1902.3	1902.3	1904.6
gdb 739	1907.4[a]	1904.5	1904.5	1904.7	1903.5	1903.4	1905.4
gdb 740	1899.8[a]	1900.4	1900.3	1898.1	1897.7	1897.6	1894.9
gdb 741	1894.5[a]	1898.4	1898.4	1899.6	1898.3	1898.3	1899.9
gdb 742	1890.7[a]	1896.1	1896.1	1897.2	1894.7	1894.7	1896.3
gdb 743	1895.3[a]	1897.0	1897.0	1898.8	1895.3	1895.3	1896.7
gdb 744	1891.0[a]	1899.2	1899.2	1902.5	1897.4	1897.3	1900.7
gdb 745	1889.8[a]	1897.6	1897.6	1900.3	1895.3	1895.3	1898.4
gdb 746	1903.0[a]	1903.0	1903.0	1904.7	1899.8	1899.8	1903.3
gdb 747	1899.6[a]	1898.8	1898.7	1900.0	1896.7	1896.7	1899.7
gdb 748	1899.3[a]	1897.6	1897.6	1898.7	1896.4	1896.4	1899.4
gdb 749	1895.1[a]	1894.4	1894.4	1892.8	1892.7	1892.6	1890.3
gdb 750	1890.4[a]	1894.1	1894.1	1895.5	1894.3	1894.3	1896.3
gdb 751	1888.0[a]	1893.5	1893.4	1894.9	1892.8	1892.8	1894.4
gdb 752	1894.5[a]	1895.8	1895.8	1896.7	1894.5	1894.5	1895.8
gdb 753	1896.1[a]	1899.2	1899.2	1900.6	1898.2	1898.2	1900.0
gdb 754	1895.4[a]	1904.3	1904.3	1906.1	1902.3	1902.3	1904.7
gdb 755	1892.2[a]	1900.8	1900.8	1903.1	1898.9	1898.9	1901.4
gdb 756	1908.2[a]	1909.6	1909.6	1910.9	1906.4	1906.4	1909.3
gdb 757	1910.6[a]	1909.1	1909.1	1911.0	1906.4	1906.4	1910.6
gdb 758	1889.2[a]	1896.4	1896.4	1897.9	1895.3	1895.3	1898.3
gdb 759	1906.2[a]	1904.6	1904.6	1906.1	1902.2	1902.2	1905.8
gdb 760	1920.3[a]	1930.8	1930.8	1931.4	1933.8	1933.8	1934.3
gdb 761	1896.7[a]	1899.1	1899.1	1896.5	1895.3	1895.3	1891.8
gdb 762	1893.7[a]	1898.1	1898.1	1899.4	1897.7	1897.7	1898.6
gdb 763	1894.4[a]	1900.1	1900.1	1901.2	1897.9	1897.9	1899.0
gdb 764	1893.2[a]	1898.7	1898.7	1900.1	1896.7	1896.7	1898.0
gdb 765	1909.0[a]	1907.0	1907.0	1907.5	1903.6	1903.6	1905.2
gdb 766	1896.4[a]	1896.4	1896.4	1894.8	1893.7	1893.6	1890.8
gdb 767	1890.0[a]	1892.9	1892.9	1894.3	1893.3	1893.3	1895.2
gdb 768	1887.7[a]	1893.8	1893.8	1895.2	1893.0	1892.9	1894.6
gdb 769	1887.8[a]	1892.4	1892.4	1894.1	1891.6	1891.5	1893.5
gdb 770	1899.4[a]	1897.8	1897.8	1899.2	1895.6	1895.6	1898.5
gdb 771	1907.5[a]	1905.9	1905.9	1907.0	1904.1	1904.1	1907.8
gdb 772	1888.3[a]	1896.6	1896.6	1898.0	1895.4	1895.4	1898.5
gdb 773	1894.4[a]	1900.4	1900.4	1902.1	1899.2	1899.2	1902.3
gdb 774	1909.4[a]	1920.5	1920.5	1920.6	1923.6	1923.6	1923.1
gdb 775	1892.7[a]	1898.6	1898.6	1900.2	1897.5	1897.4	1900.5
gdb 776	1891.6[a]	1898.7	1898.7	1900.7	1897.5	1897.5	1900.8
gdb 777	1892.7[a]	1896.1	1896.1	1898.2	1895.7	1895.6	1898.5

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 778	1905.8[a]	1903.2	1903.2	1904.9	1900.2	1900.2	1904.0
gdb 779	1908.7[a]	1917.4	1917.4	1917.1	1919.9	1919.9	1919.5
gdb 780	1889.9[a]	1899.0	1899.0	1899.8	1901.3	1901.2	1901.9
gdb 781	1887.7[a]	1894.4	1894.4	1894.2	1897.4	1897.4	1896.7
gdb 782	1865.1[a]	1866.7	1866.6	1864.4	1863.9	1863.8	1860.9
gdb 783	1887.2[a]	1898.0	1898.0	1899.8	1900.5	1900.5	1902.9
gdb 784	1885.9[a]	1893.7	1893.7	1893.7	1896.6	1896.6	1897.1
gdb 785	1873.3[a]	1871.5	1871.4	1873.2	1869.7	1869.7	1871.4
gdb 786	1868.1[a]	1868.1	1868.1	1869.3	1866.2	1866.2	1867.7
gdb 787	1871.2[a]	1872.1	1872.1	1870.8	1867.6	1867.6	1865.3
gdb 788	1863.0[a]	1866.2	1866.2	1866.9	1866.4	1866.4	1867.1
gdb 789	1868.4[a]	1867.9	1867.9	1865.5	1864.2	1864.1	1860.7
gdb 790	1871.4[a]	1869.6	1869.6	1867.3	1866.2	1866.2	1863.2
gdb 791	1869.6[a]	1873.4	1873.4	1872.0	1868.5	1868.5	1866.6
gdb 792	1870.7[a]	1872.5	1872.5	1874.2	1870.2	1870.1	1871.3
gdb 793	1864.4[a]	1867.4	1867.4	1868.7	1865.0	1865.0	1866.8
gdb 794	1909.0[a]	1919.5	1919.5	1920.6	1921.1	1921.1	1922.4
gdb 795	1886.9[a]	1893.0	1893.0	1895.3	1890.4	1890.4	1893.2
gdb 796	1886.8[a]	1890.5	1890.5	1893.4	1888.0	1888.0	1891.8
gdb 797	1886.9[a]	1891.2	1891.2	1894.2	1889.0	1889.0	1892.6
gdb 798	1890.9[a]	1892.0	1892.0	1893.3	1889.6	1889.6	1890.8
gdb 799	1889.4[a]	1891.8	1891.8	1893.1	1891.9	1891.9	1893.7
gdb 800	1890.1[a]	1891.2	1891.1	1892.4	1890.4	1890.4	1892.7
gdb 801	1891.2[a]	1891.7	1891.7	1893.0	1891.2	1891.2	1893.4
gdb 802	1888.4[a]	1889.4	1889.4	1890.8	1889.3	1889.3	1891.8
gdb 803	1896.8[a]	1893.9	1893.9	1891.8	1891.0	1891.0	1888.5
gdb 804	1904.8[a]	1908.6	1908.6	1910.8	1905.9	1905.9	1908.9
gdb 805	1905.4[a]	1915.2	1915.2	1916.2	1908.3	1908.3	1909.4
gdb 806	1905.5[a]	1910.8	1910.8	1912.5	1907.9	1907.9	1910.3
gdb 807	1892.6[a]	1903.0	1903.0	1905.2	1900.2	1900.2	1902.4
gdb 808	1889.5[a]	1898.7	1898.7	1901.2	1896.4	1896.3	1899.4
gdb 809	1890.5[a]	1901.4	1901.4	1904.2	1898.9	1898.8	1901.8
gdb 810	1894.8[a]	1896.3	1896.3	1898.1	1894.5	1894.5	1896.5
gdb 811	1892.8[a]	1894.7	1894.7	1896.4	1893.1	1893.1	1895.6
gdb 812	1895.2[a]	1896.4	1896.4	1898.2	1895.5	1895.4	1898.6
gdb 813	1895.3[a]	1895.7	1895.7	1897.7	1895.5	1895.5	1898.7
gdb 814	1895.3[a]	1896.0	1896.0	1897.8	1895.4	1895.4	1898.5
gdb 815	1885.3[a]	1888.6	1888.6	1891.7	1887.0	1887.0	1891.1
gdb 816	1883.7[a]	1889.6	1889.6	1892.7	1888.0	1888.0	1891.5
gdb 817	1889.3[a]	1889.6	1889.6	1891.1	1888.0	1888.0	1889.9
gdb 818	1903.0[a]	1907.4	1907.4	1909.7	1905.5	1905.5	1908.7
gdb 819	1886.6[a]	1888.3	1888.3	1889.8	1889.2	1889.2	1891.7
gdb 820	1888.7[a]	1889.9	1889.9	1891.3	1890.4	1890.3	1892.7
gdb 821	1868.8[a]	1871.9	1871.9	1870.8	1868.6	1868.5	1866.6
gdb 822	1869.1[a]	1870.4	1870.4	1872.1	1869.2	1869.2	1870.5
gdb 823	1887.5[a]	1892.9	1892.8	1894.3	1893.6	1893.6	1895.0
gdb 824	1886.0[a]	1893.5	1893.5	1895.1	1892.8	1892.8	1894.4
gdb 825	1890.9[a]	1894.4	1894.4	1892.5	1891.3	1891.3	1888.6
gdb 826	1871.0[a]	1869.5	1869.5	1871.1	1868.9	1868.9	1870.5
gdb 827	1867.8[a]	1866.8	1866.8	1868.3	1866.5	1866.5	1868.4
gdb 828	1869.5[a]	1871.9	1871.9	1870.7	1868.2	1868.2	1866.0
gdb 829	1869.2[a]	1868.1	1868.1	1865.8	1865.9	1865.9	1862.9
gdb 830	1862.6[a]	1864.5	1864.5	1864.8	1865.6	1865.6	1866.4
gdb 831	1867.5[a]	1867.6	1867.6	1865.3	1864.7	1864.7	1861.4
gdb 832	1874.7[a]	1878.8	1878.8	1881.6	1877.2	1877.2	1879.4
gdb 833	1874.9[a]	1877.6	1877.5	1880.1	1876.4	1876.3	1878.9
gdb 834	1868.4[a]	1873.1	1873.1	1875.3	1872.0	1871.9	1875.0
gdb 835	1888.9[a]	1890.3	1890.3	1892.1	1888.5	1888.5	1890.7
gdb 836	1885.2[a]	1892.4	1892.4	1896.0	1890.5	1890.4	1894.0
gdb 837	1904.5[a]	1908.5	1908.5	1911.0	1906.8	1906.8	1910.2
gdb 838	1907.2[a]	1913.7	1913.7	1915.3	1911.1	1911.1	1912.9
gdb 839	1903.8[a]	1908.5	1908.5	1911.0	1906.4	1906.4	1909.8
gdb 840	1904.9[a]	1910.5	1910.5	1912.9	1908.3	1908.3	1911.1
gdb 841	1889.9[a]	1901.7	1901.7	1904.3	1899.8	1899.8	1902.4
gdb 842	1892.6[a]	1893.4	1893.4	1895.4	1892.7	1892.7	1895.5

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 843	1890.8[a]	1900.0	1900.0	1902.7	1898.7	1898.7	1901.5
gdb 844	1889.5[a]	1897.5	1897.5	1899.9	1896.5	1896.5	1899.5
gdb 845	1890.5[a]	1899.7	1899.7	1902.5	1898.6	1898.5	1901.5
gdb 846	1893.6[a]	1894.9	1894.9	1896.9	1894.2	1894.2	1896.3
gdb 847	1917.8[a]	1926.1	1926.1	1926.7	1929.2	1929.2	1930.3
gdb 848	1908.7[a]	1917.6	1917.9	1918.6	1921.3	1921.2	1922.7
gdb 849	1873.5[a]	1877.9	1877.9	1880.6	1876.1	1876.1	1878.9
gdb 850	1868.4[a]	1872.5	1872.5	1874.7	1870.8	1870.7	1873.2
gdb 851	1872.3[a]	1876.9	1876.9	1879.5	1875.1	1875.0	1877.8
gdb 852	1869.1[a]	1875.0	1875.0	1877.6	1873.0	1873.0	1875.6
gdb 853	1869.2[a]	1872.1	1872.1	1870.7	1868.7	1868.7	1866.7
gdb 854	1867.7[a]	1868.9	1868.9	1870.5	1867.8	1867.7	1869.6
gdb 855	1866.4[a]	1868.5	1868.5	1870.3	1867.4	1867.4	1869.0
gdb 856	1884.7[a]	1895.0	1895.0	1896.6	1893.7	1893.6	1895.1
gdb 857	1885.7[a]	1893.4	1893.4	1895.1	1893.7	1893.7	1894.9
gdb 858	1889.6[a]	1894.0	1894.0	1891.9	1891.0	1891.0	1888.8
gdb 859	1884.7[a]	1890.9	1890.9	1892.4	1891.4	1891.3	1892.9
gdb 860	1889.0[a]	1890.1	1890.1	1891.9	1888.4	1888.4	1890.5
gdb 861	1883.3[a]	1889.5	1889.5	1893.0	1887.9	1887.9	1892.1
gdb 862	1885.8[a]	1891.7	1891.7	1894.6	1889.6	1889.5	1893.4
gdb 863	1885.9[a]	1891.4	1891.4	1892.2	1890.6	1890.6	1892.5
gdb 864	1884.7[a]	1889.8	1889.8	1890.7	1889.7	1889.6	1891.8
gdb 865	1893.7[a]	1892.4	1892.4	1890.6	1890.2	1890.2	1888.5
gdb 866	1882.8[a]	1887.2	1887.2	1888.7	1887.2	1887.2	1890.0
gdb 867	1892.4[a]	1893.5	1893.4	1895.4	1892.6	1892.5	1895.1
gdb 868	1891.2[a]	1893.4	1893.3	1894.8	1892.4	1892.4	1895.2
gdb 869	1888.8[a]	1899.2	1899.2	1902.4	1897.8	1897.7	1900.9
gdb 870	1888.3[a]	1899.5	1899.5	1902.3	1897.8	1897.8	1900.5
gdb 871	1890.4[a]	1894.8	1894.8	1896.3	1893.9	1893.8	1897.0
gdb 872	1918.4[a]	1925.9	1925.9	1926.5	1929.1	1929.1	1930.3
gdb 873	1889.4[a]	1894.4	1894.4	1892.3	1890.8	1890.8	1888.1
gdb 874	1885.6[a]	1891.4	1891.4	1892.9	1891.5	1891.4	1893.2
gdb 875	1883.7[a]	1893.2	1893.2	1894.7	1891.5	1891.5	1893.5
gdb 876	1884.6[a]	1895.5	1895.5	1896.9	1893.5	1893.3	1894.7
gdb 877	1908.2[a]	1918.1	1918.1	1918.6	1921.0	1921.4	1922.8
gdb 878	1892.6[a]	1891.6	1891.6	1889.5	1889.3	1889.3	1887.3
gdb 879	1884.1[a]	1887.9	1887.9	1889.4	1887.9	1887.9	1890.5
gdb 880	1884.9[a]	1889.6	1889.6	1891.1	1889.1	1889.1	1891.6
gdb 881	1885.9[a]	1891.2	1891.2	1892.0	1890.5	1890.4	1892.2
gdb 882	1891.8[a]	1897.4	1897.4	1899.1	1896.4	1896.3	1899.9
gdb 883	1888.4[a]	1893.5	1893.5	1895.7	1892.8	1892.8	1896.9
gdb 884	1917.5[a]	1926.2	1926.2	1926.6	1928.7	1928.7	1929.4
gdb 885	1888.6[a]	1893.5	1893.5	1895.5	1892.2	1892.2	1895.8
gdb 886	1887.6[a]	1891.5	1891.5	1893.7	1890.8	1890.8	1894.6
gdb 887	1890.0[a]	1895.3	1895.3	1896.9	1894.1	1894.1	1897.2
gdb 888	1893.6[a]	1905.4	1905.3	1906.5	1907.5	1907.4	1908.1
gdb 889	1891.2[a]	1901.3	1901.2	1901.7	1904.0	1903.6	1904.0
gdb 890	1886.9[a]	1894.7	1894.7	1895.3	1898.0	1897.7	1898.9
gdb 891	1867.9[a]	1867.5	1867.4	1865.2	1864.4	1864.3	1861.7
gdb 892	1869.6[a]	1869.7	1869.7	1867.6	1866.4	1866.3	1863.5
gdb 893	1880.2[a]	1876.1	1876.1	1877.1	1875.2	1874.2	1876.4
gdb 894	1887.9[a]	1894.2	1894.2	1894.6	1897.7	1897.7	1898.9
gdb 895	1892.6[a]	1901.1	1901.1	1902.8	1903.1	1903.0	1905.2
gdb 896	1883.5[a]	1881.3	1881.3	1883.8	1880.5	1880.5	1883.4
gdb 897	1880.9[a]	1878.1	1878.1	1881.1	1877.4	1877.4	1880.7
gdb 898	1886.1[a]	1883.5	1883.5	1884.6	1881.6	1881.5	1882.5
gdb 899	1903.7[a]	1890.8	1890.8	1893.8	1887.8	1887.7	1892.5
gdb 900	1886.1[a]	1889.5	1889.5	1891.0	1890.3	1890.2	1892.3
gdb 901	1886.9[a]	1890.3	1890.2	1891.6	1890.1	1890.1	1892.6
gdb 902	1883.9[a]	1887.2	1887.2	1888.8	1887.8	1887.8	1890.3
gdb 903	1894.6[a]	1892.8	1892.8	1890.8	1890.5	1890.5	1888.2
gdb 904	1901.6[a]	1895.0	1895.0	1894.4	1894.2	1894.2	1896.5
gdb 905	1871.7[a]	1874.1	1874.1	1876.7	1873.0	1872.9	1875.8
gdb 906	1869.0[a]	1871.3	1871.3	1874.0	1870.3	1870.3	1873.5
gdb 907	1887.9[a]	1888.5	1888.5	1891.5	1885.0	1885.0	1889.3

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Table S73: . . . *continued from previous page* . . .

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 908	1895.0[a]	1899.1	1899.0	1900.6	1898.8	1898.8	1902.0
gdb 909	1895.3[a]	1899.3	1899.3	1900.9	1899.0	1898.8	1902.2
gdb 910	1879.7[a]	1875.7	1875.7	1878.7	1875.5	1875.5	1879.0
gdb 911	1881.8[a]	1877.9	1877.8	1879.0	1876.7	1876.6	1877.9
gdb 912	1903.5[a]	1889.2	1889.0	1891.9	1886.4	1886.3	1891.2
gdb 913	1882.6[a]	1886.5	1886.5	1888.0	1887.6	1887.6	1889.8
gdb 914	1885.8[a]	1889.2	1889.1	1890.9	1890.0	1890.0	1892.4
gdb 915	1902.5[a]	1895.6	1895.6	1896.2	1895.5	1895.4	1898.0
gdb 916	1890.0[a]	1899.2	1899.1	1900.8	1902.5	1902.4	1904.6
gdb 917	1866.5[a]	1863.2	1863.1	1865.2	1864.8	1864.7	1867.0
gdb 918	1863.1[a]	1864.2	1864.2	1865.1	1864.4	1864.4	1866.4
gdb 919	1872.0[a]	1874.2	1874.2	1873.1	1871.3	1871.3	1869.5
gdb 920	1880.5[a]	1877.7	1877.7	1879.1	1876.7	1876.6	1879.7
gdb 921	1865.9[a]	1865.6	1865.6	1863.1	1863.8	1863.7	1860.9
gdb 922	1867.7[a]	1868.5	1868.5	1866.2	1866.0	1866.0	1863.0
gdb 923	1879.0[a]	1873.7	1873.7	1874.1	1872.9	1872.9	1874.5
gdb 924	1887.3[a]	1893.5	1893.5	1893.8	1898.3	1898.3	1899.4
gdb 925	1868.2[a]	1867.1	1867.1	1869.0	1868.4	1868.4	1870.2
gdb 926	1869.8[a]	1872.7	1872.7	1871.4	1870.2	1870.1	1868.6
gdb 927	1885.3[a]	1884.4	1884.4	1885.6	1881.9	1881.8	1884.8
gdb 928	1881.5[a]	1879.4	1879.4	1881.2	1877.8	1877.8	1879.5
gdb 929	1880.9[a]	1879.3	1879.3	1882.5	1878.7	1878.7	1882.2
gdb 930	1902.3[a]	1890.4	1890.4	1893.2	1887.7	1887.7	1892.6
gdb 931	1884.8[a]	1890.5	1890.5	1892.3	1890.9	1890.9	1893.0
gdb 932	1891.4[a]	1890.6	1890.6	1888.9	1888.7	1888.6	1887.0
gdb 933	1905.7[a]	1902.4	1902.4	1902.8	1900.7	1900.7	1903.0
gdb 934	1868.1[a]	1869.5	1869.5	1872.5	1868.7	1868.6	1872.2
gdb 935	1868.0[a]	1869.1	1869.1	1872.2	1868.9	1868.8	1872.5
gdb 936	1870.1[a]	1872.5	1872.5	1875.5	1871.9	1871.9	1875.1
gdb 937	1884.9[a]	1886.2	1886.2	1888.7	1883.1	1883.0	1887.3
gdb 938	1915.3[a]	1925.8	1925.8	1926.3	1930.1	1930.1	1931.4
gdb 939	1870.3[a]	1873.2	1873.2	1872.1	1870.4	1870.4	1868.7
gdb 940	1865.3[a]	1864.0	1864.0	1865.7	1865.5	1865.5	1867.5
gdb 941	1866.3[a]	1869.6	1869.6	1870.7	1869.0	1868.9	1870.5
gdb 942	1886.3[a]	1885.0	1884.9	1886.5	1882.1	1882.0	1885.0
gdb 943	1891.4[a]	1900.2	1900.1	1901.8	1903.3	1903.3	1905.6
gdb 944	1890.9[a]	1891.0	1891.0	1889.3	1888.2	1888.2	1886.4
gdb 945	1883.5[a]	1887.2	1887.2	1889.2	1886.8	1886.8	1889.1
gdb 946	1887.7[a]	1894.0	1894.0	1895.6	1893.6	1893.6	1895.7
gdb 947	1907.1[a]	1902.1	1901.9	1902.3	1900.1	1900.0	1902.3
gdb 948	1895.9[a]	1900.0	1900.0	1901.3	1899.6	1899.6	1902.9
gdb 949	1917.1[a]	1911.1	1911.1	1911.9	1909.1	1909.1	1912.6
gdb 950	1915.8[a]	1926.1	1926.1	1926.6	1930.0	1930.0	1930.9
gdb 951	1892.9[a]	1896.4	1896.4	1898.5	1896.1	1896.1	1899.9
gdb 952	1895.2[a]	1900.0	1900.0	1901.2	1899.4	1899.4	1902.6
gdb 953	1915.8[a]	1910.2	1910.2	1910.9	1908.1	1908.1	1911.5
gdb 954	1895.4[a]	1903.5	1903.5	1903.5	1906.5	1906.5	1905.8
gdb 955	1892.5[a]	1896.5	1896.5	1896.8	1899.6	1899.5	1900.3
gdb 956	1853.1[a]	1841.0	1841.0	1842.1	1841.4	1841.4	1841.7
gdb 957	1855.7[a]	1839.8	1839.8	1843.0	1840.0	1840.0	1843.9
gdb 958	1873.8[a]	1849.6	1849.4	1853.2	1848.8	1848.7	1853.5
gdb 959	1864.0[a]	1854.3	1854.3	1856.1	1856.8	1856.7	1858.8
gdb 960	1860.9[a]	1852.2	1852.2	1853.8	1854.5	1854.5	1856.8
gdb 961	1869.4[a]	1865.2	1865.2	1864.0	1863.3	1863.3	1861.7
gdb 962	1861.3[a]	1860.2	1860.2	1861.5	1860.8	1860.8	1863.3
gdb 963	1883.8[a]	1873.0	1873.0	1874.7	1871.3	1871.3	1874.6
gdb 964	1890.6[a]	1898.0	1898.0	1899.5	1898.2	1898.2	1901.0
gdb 965	1910.9[a]	1907.0	1906.9	1907.9	1905.2	1905.2	1908.3
gdb 966	1847.5[a]	1837.5	1837.5	1838.8	1838.0	1838.0	1838.6
gdb 967	1851.8[a]	1839.0	1839.0	1842.2	1839.5	1839.5	1843.7
gdb 968	1870.1[a]	1846.9	1846.5	1850.9	1846.7	1846.6	1851.9
gdb 969	1859.4[a]	1850.7	1850.7	1852.8	1853.1	1853.1	1855.7
gdb 970	1858.1[a]	1858.3	1858.3	1859.4	1858.8	1858.7	1861.3
gdb 971	1881.9[a]	1871.7	1871.7	1874.0	1870.3	1870.3	1873.9
gdb 972	1896.0[a]	1902.5	1902.4	1904.1	1907.2	1907.2	1909.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 973	1890.3[a]	1895.1	1895.1	1895.4	1899.5	1899.5	1900.4
gdb 974	1865.2[a]	1862.7	1862.7	1861.8	1860.9	1860.9	1859.7
gdb 975	1863.7[a]	1855.4	1855.4	1857.6	1857.5	1857.5	1859.8
gdb 976	1861.3[a]	1863.2	1863.2	1864.1	1862.5	1862.5	1864.9
gdb 977	1882.4[a]	1872.7	1872.7	1875.1	1871.1	1871.1	1874.6
gdb 978	1889.5[a]	1897.6	1897.6	1897.9	1896.7	1896.7	1899.4
gdb 979	1910.1[a]	1905.9	1905.8	1907.5	1904.0	1903.9	1907.8
gdb 980	1895.9[a]	1902.8	1902.8	1904.3	1907.0	1907.0	1908.8
gdb 981	1892.6[a]	1899.2	1899.2	1901.2	1899.1	1899.1	1902.2
gdb 982	1889.3[a]	1896.2	1896.2	1896.4	1895.2	1895.2	1897.9
gdb 983	1910.1[a]	1905.8	1905.7	1907.0	1903.8	1903.7	1907.5
gdb 984	1857.6[a]	1861.6	1861.6	1861.6	1861.2	1861.2	1863.9
gdb 985	1860.9[a]	1864.9	1864.9	1864.8	1864.2	1864.2	1866.8
gdb 986	1859.6[a]	1864.2	1864.2	1864.3	1863.2	1863.2	1865.8
gdb 987	1882.0[a]	1875.3	1875.3	1876.9	1873.6	1873.6	1877.0
gdb 988	1883.6[a]	1893.2	1893.2	1894.8	1892.4	1892.4	1891.8
gdb 989	1883.0[a]	1888.5	1888.5	1889.8	1889.9	1889.8	1889.1
gdb 990	1886.8[a]	1886.1	1886.1	1886.8	1883.1	1883.1	1885.2
gdb 991	1883.4[a]	1894.7	1894.7	1896.0	1894.0	1894.0	1893.3
gdb 992	1857.4[a]	1859.9	1859.9	1858.5	1853.7	1853.7	1849.7
gdb 993	1888.9[a]	1889.5	1889.5	1890.7	1886.0	1886.0	1888.9
gdb 994	1880.0[a]	1888.1	1888.0	1889.7	1888.0	1888.0	1888.3
gdb 995	1874.2[a]	1879.3	1879.3	1882.5	1881.3	1881.3	1882.8
gdb 996	1874.8[a]	1882.4	1882.4	1885.1	1883.6	1883.6	1884.7
gdb 997	1856.3[a]	1856.3	1856.2	1856.4	1850.9	1850.9	1848.1
gdb 998	1860.3[a]	1862.3	1862.3	1865.2	1863.7	1863.7	1862.8
gdb 999	1853.6[a]	1858.4	1858.4	1862.0	1860.4	1860.4	1860.6
gdb 1000	1855.1[a]	1855.3	1855.3	1855.1	1850.7	1850.6	1847.6
gdb 1001	1853.5[a]	1853.1	1853.1	1857.3	1850.7	1850.7	1852.8
gdb 1002	1851.9[a]	1851.3	1851.3	1855.0	1849.2	1849.2	1851.4
gdb 1003	1893.0[a]	1893.3	1893.3	1893.7	1891.3	1890.8	1892.7
gdb 1004	1880.6[a]	1888.6	1888.6	1890.8	1890.4	1890.4	1890.5
gdb 1005	1851.9[a]	1853.1	1853.0	1852.7	1849.1	1849.1	1846.2
gdb 1006	1886.6[a]	1881.9	1881.7	1883.5	1879.9	1879.7	1883.0
gdb 1007	1865.9[a]	1873.7	1873.7	1873.8	1872.2	1872.2	1874.0
gdb 1008	1874.0[a]	1880.5	1880.5	1882.9	1883.2	1883.1	1884.0
gdb 1009	1875.3[a]	1881.2	1881.2	1884.2	1883.0	1883.0	1884.5
gdb 1010	1859.3[a]	1855.3	1855.3	1858.1	1858.0	1858.0	1857.8
gdb 1011	1857.8[a]	1854.7	1854.7	1856.6	1857.7	1857.7	1857.2
gdb 1012	1864.3[a]	1873.0	1873.0	1877.3	1872.6	1872.5	1873.1
gdb 1013	1860.9[a]	1858.1	1858.1	1860.8	1861.0	1861.0	1860.7
gdb 1014	1858.8[a]	1859.5	1859.5	1861.9	1856.0	1856.0	1857.0
gdb 1015	1866.1[a]	1873.6	1873.6	1877.8	1872.6	1872.6	1872.5
gdb 1016	1858.4[a]	1860.6	1860.6	1863.4	1856.9	1856.9	1858.0
gdb 1017	1869.9[a]	1880.1	1880.1	1881.6	1870.7	1870.7	1873.6
gdb 1018	1871.6[a]	1882.8	1882.8	1884.2	1873.7	1873.7	1876.0
gdb 1019	1871.1[a]	1881.3	1881.3	1883.8	1877.8	1877.8	1878.9
gdb 1020	1857.4[a]	1855.0	1855.0	1855.0	1850.2	1850.2	1847.1
gdb 1021	1861.8[a]	1857.2	1857.2	1859.8	1860.4	1860.4	1860.3
gdb 1022	1863.9[a]	1868.5	1868.5	1872.1	1868.5	1868.5	1869.7
gdb 1023	1865.8[a]	1869.1	1869.1	1872.7	1869.4	1869.4	1870.3
gdb 1024	1859.5[a]	1858.6	1858.6	1862.7	1856.0	1855.9	1857.8
gdb 1025	1855.3[a]	1853.5	1853.5	1853.5	1849.7	1849.7	1846.7
gdb 1026	1870.3[a]	1877.9	1877.9	1880.4	1875.6	1875.6	1877.0
gdb 1027	1870.9[a]	1880.2	1880.1	1883.0	1872.1	1872.0	1875.6
gdb 1028	1868.6[a]	1879.7	1879.6	1882.1	1871.0	1870.9	1874.1
gdb 1029	1860.7[a]	1861.3	1861.3	1864.2	1858.1	1858.0	1859.3
gdb 1030	1871.2[a]	1877.1	1877.1	1879.7	1875.1	1875.1	1876.6
gdb 1031	1871.6[a]	1878.8	1878.2	1881.2	1876.1	1876.1	1877.2
gdb 1032	1869.9[a]	1878.7	1878.7	1880.5	1870.1	1870.1	1873.2
gdb 1033	1869.1[a]	1871.0	1871.0	1872.7	1863.8	1863.8	1868.4
gdb 1034	1864.0[a]	1864.8	1864.8	1867.5	1860.3	1860.3	1863.8
gdb 1035	1868.5[a]	1868.3	1868.3	1870.7	1861.7	1861.7	1866.7
gdb 1036	1867.4[a]	1870.2	1870.2	1871.4	1863.4	1863.4	1867.5
gdb 1037	1881.5[a]	1888.3	1888.2	1889.4	1889.2	1889.2	1888.8

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1038	1881.7[a]	1884.9	1884.9	1886.9	1886.3	1886.3	1886.8
gdb 1039	1883.0[a]	1886.5	1886.5	1888.8	1888.9	1888.8	1888.7
gdb 1040	1855.4[a]	1853.5	1853.5	1852.3	1849.4	1849.4	1846.1
gdb 1041	1889.6[a]	1884.6	1884.5	1885.9	1883.1	1883.1	1885.9
gdb 1042	1874.5[a]	1881.7	1881.7	1881.8	1882.6	1884.6	1884.0
gdb 1043	1859.4[a]	1855.0	1855.0	1858.6	1859.1	1859.1	1859.0
gdb 1044	1856.2[a]	1854.4	1854.4	1858.1	1853.0	1852.9	1855.4
gdb 1045	1856.2[a]	1854.0	1854.0	1856.6	1858.0	1857.9	1857.9
gdb 1046	1854.4[a]	1852.0	1852.0	1856.2	1851.6	1851.6	1854.3
gdb 1047	1866.8[a]	1872.4	1872.4	1874.7	1865.6	1865.6	1869.2
gdb 1048	1868.9[a]	1875.4	1875.4	1877.6	1868.5	1868.5	1871.5
gdb 1049	1874.4[a]	1878.3	1878.3	1879.7	1881.0	1881.0	1881.5
gdb 1050	1864.3[a]	1869.9	1869.9	1870.1	1869.1	1869.1	1870.6
gdb 1051	1843.8[a]	1843.3	1843.3	1846.8	1844.3	1844.2	1845.2
gdb 1052	1840.3[a]	1839.0	1839.0	1840.5	1834.8	1834.8	1837.9
gdb 1053	1892.6[a]	1889.2	1889.2	1890.3	1888.3	1888.3	1890.8
gdb 1054	1869.0[a]	1875.8	1875.5	1878.4	1874.9	1874.6	1877.5
gdb 1055	1839.1[a]	1838.2	1838.2	1835.1	1831.6	1831.6	1829.6
gdb 1056	1885.5[a]	1880.0	1879.6	1881.0	1878.8	1878.7	1881.5
gdb 1057	1864.0[a]	1869.2	1869.2	1868.9	1868.9	1868.9	1870.5
gdb 1058	1861.4[a]	1866.4	1866.4	1866.0	1866.9	1866.9	1868.7
gdb 1059	1882.1[a]	1893.3	1893.3	1894.4	1892.9	1892.9	1892.0
gdb 1060	1898.2[a]	1909.4	1909.4	1909.1	1910.1	1910.1	1908.6
gdb 1061	1897.6[a]	1909.3	1909.3	1909.8	1910.5	1910.5	1909.9
gdb 1062	1895.4[a]	1905.6	1905.5	1904.6	1907.6	1907.5	1906.2
gdb 1063	1884.1[a]	1891.2	1891.2	1893.4	1890.3	1890.3	1891.1
gdb 1064	1893.2[a]	1903.8	1903.8	1904.2	1905.7	1905.6	1905.6
gdb 1065	1855.3[a]	1849.4	1849.4	1850.2	1847.1	1847.1	1846.6
gdb 1066	1867.5[a]	1858.4	1858.4	1862.2	1859.8	1859.8	1861.0
gdb 1067	1871.2[a]	1862.7	1862.7	1864.4	1861.9	1861.9	1863.2
gdb 1068	1876.4[a]	1878.3	1878.3	1880.6	1879.9	1879.9	1879.9
gdb 1069	1906.0[a]	1915.5	1915.5	1916.9	1917.4	1917.4	1918.5
gdb 1070	1899.5[a]	1906.7	1906.7	1906.7	1908.3	1908.3	1907.9
gdb 1071	1874.5[a]	1876.0	1876.0	1874.6	1871.1	1871.1	1868.8
gdb 1072	1873.7[a]	1869.2	1869.2	1871.0	1868.4	1868.4	1869.3
gdb 1073	1882.3[a]	1885.7	1885.7	1887.6	1885.8	1885.7	1885.6
gdb 1074	1909.8[a]	1920.1	1920.1	1921.8	1920.1	1920.1	1921.1
gdb 1075	1906.8[a]	1916.6	1916.6	1917.9	1917.7	1917.7	1918.5
gdb 1076	1903.3[a]	1914.1	1914.1	1915.7	1910.6	1910.5	1912.5
gdb 1077	1908.7[a]	1918.8	1918.8	1920.2	1918.5	1918.5	1918.7
gdb 1078	1902.8[a]	1913.9	1913.9	1913.7	1914.7	1914.7	1913.6
gdb 1079	1875.8[a]	1877.2	1877.2	1874.6	1872.5	1872.5	1868.5
gdb 1080	1875.4[a]	1877.8	1877.8	1875.2	1873.2	1873.2	1868.9
gdb 1081	1896.2[a]	1905.4	1905.4	1905.6	1907.1	1907.1	1907.1
gdb 1082	1897.3[a]	1910.0	1910.0	1911.1	1910.4	1910.4	1911.5
gdb 1083	1864.3[a]	1853.4	1853.4	1854.4	1852.0	1852.0	1850.4
gdb 1084	1874.6[a]	1857.9	1857.9	1861.5	1860.6	1860.6	1861.8
gdb 1085	1888.3[a]	1888.2	1888.2	1890.6	1886.1	1886.1	1887.8
gdb 1086	1886.9[a]	1886.1	1886.1	1888.8	1884.1	1884.1	1886.2
gdb 1087	1891.2[a]	1890.2	1890.2	1891.1	1887.2	1887.1	1887.0
gdb 1088	1875.9[a]	1867.9	1867.9	1869.3	1868.4	1868.4	1869.0
gdb 1089	1876.9[a]	1867.2	1867.2	1868.6	1867.4	1867.4	1868.5
gdb 1090	1885.1[a]	1881.7	1881.7	1883.9	1884.1	1884.1	1884.3
gdb 1091	1882.0[a]	1878.7	1878.7	1877.2	1874.8	1874.7	1871.7
gdb 1092	1894.6[a]	1900.0	1900.0	1901.4	1899.3	1899.3	1900.0
gdb 1093	1895.7[a]	1901.1	1901.1	1902.4	1899.4	1899.4	1900.5
gdb 1094	1893.3[a]	1898.1	1898.1	1899.6	1896.9	1896.9	1897.9
gdb 1095	1901.4[a]	1901.4	1901.3	1899.0	1897.6	1897.6	1894.0
gdb 1096	1877.6[a]	1880.9	1880.9	1883.2	1878.4	1878.4	1880.1
gdb 1097	1875.3[a]	1878.6	1878.6	1880.9	1876.4	1876.4	1878.7
gdb 1098	1902.0[a]	1913.3	1913.3	1915.2	1911.2	1911.2	1912.6
gdb 1099	1901.4[a]	1908.6	1908.6	1909.8	1906.8	1906.8	1908.7
gdb 1100	1901.9[a]	1908.4	1908.4	1909.6	1906.9	1906.8	1908.8
gdb 1101	1861.6[a]	1852.3	1852.3	1853.1	1851.2	1851.1	1850.5
gdb 1102	1872.6[a]	1857.2	1857.2	1861.4	1860.3	1860.3	1862.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1103	1886.6[a]	1885.2	1885.1	1888.2	1883.8	1883.8	1886.5
gdb 1104	1887.7[a]	1886.9	1886.9	1888.0	1884.5	1884.4	1885.0
gdb 1105	1884.5[a]	1881.0	1881.0	1884.2	1882.7	1882.7	1883.3
gdb 1106	1875.6[a]	1866.9	1866.9	1869.0	1867.5	1867.5	1868.9
gdb 1107	1869.5[a]	1862.1	1862.1	1863.3	1862.7	1862.7	1864.1
gdb 1108	1893.2[a]	1898.3	1898.3	1900.0	1898.1	1898.0	1899.0
gdb 1109	1896.0[a]	1900.6	1900.6	1902.3	1900.1	1900.1	1901.2
gdb 1110	1897.4[a]	1908.4	1908.4	1909.7	1910.3	1910.2	1911.1
gdb 1111	1901.8[a]	1909.1	1909.1	1909.3	1910.8	1910.8	1910.3
gdb 1112	1873.9[a]	1873.2	1873.2	1875.0	1873.3	1873.3	1874.3
gdb 1113	1873.7[a]	1875.5	1875.5	1876.8	1874.4	1874.4	1875.2
gdb 1114	1876.7[a]	1880.7	1880.7	1879.4	1876.7	1876.7	1873.6
gdb 1115	1907.5[a]	1916.2	1916.2	1916.4	1918.4	1918.4	1916.8
gdb 1116	1876.1[a]	1878.0	1878.0	1875.8	1874.8	1874.8	1870.7
gdb 1117	1874.5[a]	1876.6	1876.6	1874.0	1872.7	1872.7	1868.4
gdb 1118	1897.8[a]	1905.2	1905.2	1905.7	1908.6	1908.6	1908.3
gdb 1119	1878.6[a]	1876.4	1876.4	1875.0	1873.1	1873.1	1870.6
gdb 1120	1880.9[a]	1878.6	1878.6	1881.0	1881.7	1881.7	1882.3
gdb 1121	1874.1[a]	1866.7	1866.6	1868.5	1867.5	1867.4	1868.5
gdb 1122	1873.8[a]	1874.3	1874.3	1876.0	1874.6	1874.5	1875.2
gdb 1123	1877.2[a]	1880.7	1880.7	1879.0	1877.1	1877.0	1874.3
gdb 1124	1880.2[a]	1878.0	1878.0	1880.1	1881.5	1881.5	1881.9
gdb 1125	1878.8[a]	1876.3	1876.2	1875.1	1872.7	1872.7	1870.5
gdb 1126	1871.2[a]	1864.9	1864.9	1866.4	1865.3	1865.3	1866.4
gdb 1127	1887.4[a]	1888.1	1888.1	1889.4	1885.1	1885.1	1885.7
gdb 1128	1885.0[a]	1884.8	1884.8	1887.6	1882.9	1882.9	1885.0
gdb 1129	1890.0[a]	1898.5	1898.5	1900.1	1897.6	1897.6	1898.6
gdb 1130	1898.6[a]	1899.7	1899.7	1897.7	1896.4	1896.4	1893.6
gdb 1131	1873.1[a]	1876.4	1876.4	1879.1	1874.4	1874.3	1877.0
gdb 1132	1875.2[a]	1877.6	1877.6	1880.3	1876.1	1876.1	1878.6
gdb 1133	1875.7[a]	1879.7	1879.7	1882.4	1878.0	1878.0	1880.0
gdb 1134	1922.3[a]	1935.0	1935.0	1935.3	1937.9	1937.9	1937.9
gdb 1135	1900.1[a]	1909.4	1909.4	1910.6	1907.5	1907.5	1908.9
gdb 1136	1877.9[a]	1881.9	1881.9	1880.7	1877.7	1877.7	1875.1
gdb 1137	1872.2[a]	1871.4	1871.4	1873.1	1871.6	1871.6	1872.7
gdb 1138	1872.9[a]	1877.2	1877.1	1878.1	1875.3	1875.2	1875.8
gdb 1139	1898.5[a]	1908.6	1908.6	1909.8	1910.7	1910.7	1911.8
gdb 1140	1897.7[a]	1899.5	1899.5	1897.4	1895.7	1895.7	1893.2
gdb 1141	1888.5[a]	1895.4	1895.4	1896.9	1894.8	1894.8	1896.2
gdb 1142	1892.5[a]	1901.9	1898.9	1900.4	1897.4	1897.3	1898.3
gdb 1143	1903.0[a]	1912.8	1912.8	1914.5	1910.5	1910.4	1912.2
gdb 1144	1901.1[a]	1907.8	1907.8	1908.9	1906.2	1906.1	1908.4
gdb 1145	1922.8[a]	1935.6	1935.6	1935.9	1938.0	1938.0	1937.9
gdb 1146	1899.5[a]	1905.8	1905.8	1907.8	1904.1	1904.0	1907.0
gdb 1147	1901.2[a]	1908.1	1908.0	1909.2	1906.3	1906.2	1908.4
gdb 1148	1901.9[a]	1912.7	1912.7	1912.7	1914.5	1914.5	1913.2
gdb 1149	1879.8[a]	1889.8	1889.8	1892.0	1889.1	1889.1	1889.9
gdb 1150	1890.1[a]	1893.6	1893.6	1895.6	1889.2	1889.1	1892.9
gdb 1151	1898.5[a]	1906.1	1906.0	1906.1	1907.8	1907.7	1907.5
gdb 1152	1860.2[a]	1850.1	1850.0	1851.3	1849.5	1849.4	1849.1
gdb 1153	1882.8[a]	1859.9	1859.9	1864.2	1859.3	1859.3	1864.2
gdb 1154	1870.8[a]	1863.3	1863.3	1865.0	1864.8	1864.8	1866.2
gdb 1155	1868.6[a]	1861.1	1861.0	1862.7	1862.2	1862.1	1863.8
gdb 1156	1876.4[a]	1874.2	1874.2	1873.1	1871.3	1871.3	1869.1
gdb 1157	1888.5[a]	1879.1	1879.1	1880.9	1879.0	1879.0	1882.0
gdb 1158	1897.2[a]	1907.0	1907.0	1908.5	1906.3	1905.9	1908.1
gdb 1159	1856.2[a]	1846.7	1846.7	1847.9	1846.4	1846.3	1846.1
gdb 1160	1874.0[a]	1854.5	1854.5	1857.8	1853.5	1853.4	1858.0
gdb 1161	1866.2[a]	1859.9	1859.8	1861.8	1860.9	1860.9	1862.5
gdb 1162	1885.6[a]	1877.5	1877.5	1879.1	1877.5	1877.4	1880.2
gdb 1163	1902.6[a]	1911.5	1911.5	1913.0	1915.1	1915.0	1916.3
gdb 1164	1897.5[a]	1905.2	1905.2	1905.5	1908.1	1908.1	1907.8
gdb 1165	1872.3[a]	1871.9	1871.8	1870.9	1868.9	1868.9	1866.8
gdb 1166	1870.2[a]	1864.4	1864.4	1866.6	1865.4	1865.4	1866.9
gdb 1167	1889.8[a]	1883.8	1883.8	1885.2	1882.3	1882.2	1884.8

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1168	1919.0[a]	1918.6	1918.6	1919.4	1917.0	1916.9	1919.8
gdb 1169	1902.9[a]	1911.8	1911.8	1913.2	1915.0	1915.0	1915.8
gdb 1170	1898.9[a]	1908.3	1908.2	1910.3	1907.0	1907.0	1909.4
gdb 1171	1911.0[a]	1911.5	1911.5	1911.7	1908.9	1908.9	1911.8
gdb 1172	1865.6[a]	1870.5	1870.5	1870.4	1869.5	1869.5	1871.2
gdb 1173	1867.4[a]	1872.9	1872.9	1872.9	1871.2	1871.2	1873.0
gdb 1174	1888.4[a]	1884.5	1884.2	1885.9	1882.7	1882.7	1885.8
gdb 1175	1878.1[a]	1880.9	1880.9	1883.4	1880.0	1880.0	1881.6
gdb 1176	1873.2[a]	1880.7	1880.6	1883.9	1878.8	1878.8	1881.0
gdb 1177	1878.6[a]	1884.3	1884.3	1886.1	1883.9	1883.9	1884.7
gdb 1178	1876.7[a]	1885.2	1885.2	1888.3	1884.7	1884.6	1886.1
gdb 1179	1850.3[a]	1849.0	1849.0	1848.3	1843.0	1843.0	1840.9
gdb 1180	1848.4[a]	1848.5	1848.5	1849.2	1843.0	1843.0	1841.6
gdb 1181	1855.5[a]	1859.8	1859.8	1862.6	1858.8	1858.7	1858.5
gdb 1182	1857.0[a]	1852.8	1852.8	1856.9	1854.8	1854.8	1855.7
gdb 1183	1855.6[a]	1855.9	1855.9	1859.5	1856.1	1856.1	1857.1
gdb 1184	1857.5[a]	1857.9	1857.9	1861.2	1858.5	1858.5	1858.7
gdb 1185	1855.0[a]	1853.3	1853.3	1853.8	1847.2	1847.2	1845.4
gdb 1186	1853.7[a]	1851.8	1851.8	1855.4	1848.3	1848.3	1851.2
gdb 1187	1854.9[a]	1854.0	1854.0	1858.3	1849.6	1849.6	1852.2
gdb 1188	1851.2[a]	1850.6	1850.6	1854.7	1846.2	1846.1	1849.4
gdb 1189	1860.9[a]	1867.0	1867.0	1871.4	1865.3	1865.3	1866.5
gdb 1190	1853.5[a]	1851.5	1851.5	1854.5	1853.4	1853.4	1854.3
gdb 1191	1853.3[a]	1854.7	1854.7	1858.3	1855.4	1855.3	1856.2
gdb 1192	1854.3[a]	1853.1	1853.1	1857.3	1849.6	1849.5	1852.0
gdb 1193	1857.9[a]	1862.8	1862.8	1866.1	1861.6	1861.5	1863.0
gdb 1194	1854.7[a]	1853.8	1853.8	1854.2	1847.9	1847.9	1846.0
gdb 1195	1855.5[a]	1857.2	1857.2	1860.8	1857.8	1857.8	1858.4
gdb 1196	1852.7[a]	1850.2	1850.2	1855.1	1847.2	1847.2	1850.5
gdb 1197	1851.4[a]	1850.8	1850.8	1855.0	1847.2	1847.2	1849.8
gdb 1198	1852.7[a]	1851.4	1851.4	1855.6	1848.2	1848.2	1851.3
gdb 1199	1858.8[a]	1862.9	1862.8	1867.4	1862.0	1862.0	1863.6
gdb 1200	1866.1[a]	1872.0	1871.9	1874.8	1862.6	1862.6	1867.2
gdb 1201	1866.3[a]	1873.3	1873.3	1875.5	1864.0	1864.0	1868.1
gdb 1202	1867.3[a]	1873.7	1873.7	1877.6	1870.4	1870.3	1872.5
gdb 1203	1865.7[a]	1872.0	1872.0	1876.0	1868.5	1868.8	1871.2
gdb 1204	1855.6[a]	1856.1	1856.1	1855.6	1848.8	1848.7	1846.2
gdb 1205	1859.6[a]	1863.6	1863.6	1866.5	1862.1	1862.0	1861.9
gdb 1206	1856.2[a]	1854.4	1854.4	1857.9	1850.0	1850.0	1852.2
gdb 1207	1851.9[a]	1852.7	1852.7	1855.8	1847.9	1847.9	1850.5
gdb 1208	1853.4[a]	1856.2	1856.2	1854.7	1850.3	1850.3	1846.7
gdb 1209	1875.6[a]	1883.9	1883.9	1885.5	1885.3	1885.3	1885.7
gdb 1210	1881.9[a]	1889.9	1889.8	1892.1	1888.6	1888.5	1889.4
gdb 1211	1876.4[a]	1883.0	1883.0	1885.7	1882.2	1882.2	1884.3
gdb 1212	1858.9[a]	1857.2	1857.2	1856.9	1849.8	1849.8	1847.3
gdb 1213	1858.2[a]	1855.3	1855.3	1855.0	1849.2	1849.2	1846.7
gdb 1214	1879.1[a]	1884.7	1884.7	1886.4	1885.7	1885.7	1886.3
gdb 1215	1887.6[a]	1887.6	1887.6	1889.4	1883.3	1883.3	1886.4
gdb 1216	1878.1[a]	1885.3	1885.3	1887.9	1884.9	1884.9	1886.1
gdb 1217	1856.6[a]	1854.2	1854.2	1853.9	1848.4	1848.3	1846.1
gdb 1218	1854.1[a]	1855.5	1855.5	1854.9	1848.4	1848.4	1846.0
gdb 1219	1888.5[a]	1885.3	1885.3	1887.4	1881.2	1881.1	1885.5
gdb 1220	1876.3[a]	1880.8	1880.8	1883.4	1881.5	1881.5	1883.5
gdb 1221	1862.7[a]	1871.9	1871.9	1873.9	1868.1	1868.0	1871.3
gdb 1222	1874.7[a]	1879.4	1879.4	1881.7	1879.8	1879.8	1881.1
gdb 1223	1885.1[a]	1880.7	1880.6	1882.7	1876.1	1876.0	1880.3
gdb 1224	1864.8[a]	1874.1	1874.1	1875.1	1870.2	1870.2	1872.9
gdb 1225	1874.6[a]	1881.9	1881.9	1883.9	1882.0	1882.0	1883.4
gdb 1226	1871.8[a]	1880.0	1880.0	1882.3	1881.1	1881.1	1881.6
gdb 1227	1874.1[a]	1882.6	1882.6	1883.3	1883.3	1883.3	1883.2
gdb 1228	1853.8[a]	1854.2	1854.2	1853.8	1849.5	1849.5	1846.3
gdb 1229	1856.2[a]	1858.9	1858.9	1861.8	1860.3	1860.2	1859.5
gdb 1230	1855.8[a]	1857.6	1857.5	1860.5	1859.5	1859.5	1858.9
gdb 1231	1853.6[a]	1853.7	1853.7	1853.4	1849.6	1849.6	1846.5
gdb 1232	1850.0[a]	1853.3	1853.3	1856.5	1850.8	1850.7	1852.1

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1233	1850.2[a]	1852.0	1852.0	1855.4	1849.7	1849.7	1851.3
gdb 1234	1879.4[a]	1889.1	1888.7	1890.9	1890.5	1890.5	1890.6
gdb 1235	1850.6[a]	1852.2	1852.2	1851.7	1848.5	1848.5	1845.3
gdb 1236	1883.4[a]	1879.8	1880.5	1881.5	1877.7	1877.7	1880.1
gdb 1237	1872.4[a]	1880.2	1880.2	1882.3	1882.9	1882.9	1883.5
gdb 1238	1874.2[a]	1883.8	1883.7	1885.5	1882.3	1882.2	1882.6
gdb 1239	1878.8[a]	1885.4	1885.4	1886.8	1884.3	1884.3	1884.6
gdb 1240	1885.8[a]	1885.7	1885.6	1886.9	1882.0	1881.9	1884.5
gdb 1241	1878.0[a]	1883.6	1883.6	1885.2	1884.7	1884.7	1885.1
gdb 1242	1878.4[a]	1884.4	1884.4	1886.4	1884.7	1884.7	1885.9
gdb 1243	1851.3[a]	1850.1	1850.1	1849.8	1844.5	1844.5	1842.8
gdb 1244	1875.4[a]	1881.3	1881.2	1883.3	1879.1	1879.1	1880.2
gdb 1245	1874.8[a]	1882.7	1882.7	1886.1	1879.4	1879.4	1881.8
gdb 1246	1871.4[a]	1879.9	1879.9	1882.4	1880.5	1880.5	1881.3
gdb 1247	1874.3[a]	1880.8	1880.8	1883.5	1882.2	1882.2	1883.1
gdb 1248	1873.9[a]	1881.5	1881.5	1883.4	1879.7	1879.7	1880.4
gdb 1249	1876.2[a]	1883.5	1883.5	1885.7	1882.9	1882.9	1883.7
gdb 1250	1872.8[a]	1877.6	1877.6	1881.1	1878.9	1878.8	1881.4
gdb 1251	1883.4[a]	1881.0	1881.0	1882.6	1876.6	1876.6	1880.4
gdb 1252	1874.1[a]	1878.4	1878.4	1880.5	1879.7	1879.7	1881.8
gdb 1253	1858.0[a]	1852.6	1852.5	1851.9	1847.0	1847.0	1844.7
gdb 1254	1861.4[a]	1857.4	1857.4	1861.2	1858.0	1858.0	1858.6
gdb 1255	1856.3[a]	1852.2	1852.1	1851.4	1846.7	1846.7	1844.2
gdb 1256	1858.4[a]	1855.8	1855.8	1859.4	1856.3	1856.3	1857.2
gdb 1257	1856.9[a]	1852.1	1852.1	1852.8	1846.3	1846.2	1844.7
gdb 1258	1856.1[a]	1855.0	1855.0	1859.3	1850.4	1850.4	1852.9
gdb 1259	1854.1[a]	1851.8	1851.8	1856.0	1847.6	1847.6	1850.9
gdb 1260	1846.8[a]	1831.0	1831.0	1833.2	1831.1	1831.0	1832.3
gdb 1261	1858.2[a]	1847.0	1846.9	1847.7	1845.4	1845.4	1844.1
gdb 1262	1871.5[a]	1854.3	1854.3	1858.9	1858.4	1858.3	1860.3
gdb 1263	1864.2[a]	1863.3	1863.3	1865.7	1859.4	1859.3	1860.2
gdb 1264	1876.1[a]	1871.0	1871.0	1870.0	1868.0	1868.0	1865.7
gdb 1265	1891.8[a]	1869.5	1869.4	1871.2	1870.1	1870.0	1872.1
gdb 1266	1884.4[a]	1878.9	1878.9	1880.8	1881.7	1881.7	1882.3
gdb 1267	1829.6[a]	1820.3	1820.3	1816.0	1810.8	1810.8	1805.0
gdb 1268	1838.2[a]	1830.5	1830.5	1829.3	1826.9	1826.9	1823.9
gdb 1269	1839.4[a]	1833.3	1833.3	1833.1	1829.2	1829.2	1825.8
gdb 1270	1883.7[a]	1881.0	1881.0	1880.8	1875.8	1875.8	1873.9
gdb 1271	1889.3[a]	1867.9	1867.9	1869.3	1868.2	1868.2	1870.2
gdb 1272	1876.5[a]	1871.9	1871.9	1870.8	1868.6	1868.5	1866.1
gdb 1273	1885.3[a]	1881.1	1881.1	1884.0	1883.7	1883.6	1884.3
gdb 1274	1883.6[a]	1881.2	1881.1	1880.9	1875.9	1875.9	1874.0
gdb 1275	1850.5[a]	1834.7	1834.7	1838.3	1834.6	1834.5	1835.8
gdb 1276	1822.3[a]	1802.7	1802.7	1805.5	1798.2	1798.2	1798.1
gdb 1277	1833.4[a]	1810.1	1810.1	1813.4	1810.4	1810.4	1811.5
gdb 1278	1835.3[a]	1812.0	1812.0	1816.8	1812.4	1812.4	1813.7
gdb 1279	1845.9[a]	1830.6	1830.6	1834.4	1830.9	1830.8	1832.7
gdb 1280	1849.0[a]	1833.4	1833.4	1837.1	1833.7	1833.7	1835.1
gdb 1281	1913.4[a]	1918.6	1918.6	1919.6	1920.3	1920.3	1920.6
gdb 1282	1860.5[a]	1861.5	1861.5	1863.7	1858.1	1858.1	1858.9
gdb 1283	1882.9[a]	1881.1	1881.1	1879.3	1876.2	1876.2	1873.9
gdb 1284	1910.2[a]	1918.2	1918.2	1919.0	1919.9	1919.9	1920.6
gdb 1285	1882.9[a]	1881.8	1881.8	1880.1	1877.0	1876.9	1874.5
gdb 1286	1922.7[a]	1916.6	1916.6	1917.7	1914.0	1914.0	1916.4
gdb 1287	1914.3[a]	1918.6	1918.6	1919.2	1919.8	1919.8	1919.8
gdb 1288	1854.4[a]	1852.7	1852.7	1856.4	1854.6	1854.5	1855.3
gdb 1289	1845.0[a]	1830.3	1830.3	1834.7	1830.5	1830.5	1832.9
gdb 1290	1829.9[a]	1806.8	1806.8	1812.2	1807.8	1807.7	1810.1
gdb 1291	1836.7[a]	1829.6	1829.6	1828.7	1826.2	1826.2	1823.5
gdb 1292	1887.7[a]	1865.3	1865.3	1867.4	1866.0	1866.0	1868.6
gdb 1293	1882.9[a]	1877.9	1877.9	1880.1	1881.0	1881.0	1881.8
gdb 1294	1853.0[a]	1841.0	1841.0	1842.2	1840.1	1840.0	1839.5
gdb 1295	1870.0[a]	1851.7	1851.7	1855.6	1855.8	1855.8	1858.0
gdb 1296	1860.0[a]	1859.2	1859.2	1860.9	1855.6	1855.5	1856.8
gdb 1297	1871.6[a]	1868.5	1868.5	1867.7	1865.0	1865.0	1863.0

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1298	1884.8[a]	1880.0	1880.0	1882.0	1881.9	1881.9	1882.3
gdb 1299	1880.1[a]	1878.5	1878.5	1878.7	1873.6	1873.6	1872.4
gdb 1300	1910.1[a]	1917.6	1917.6	1920.5	1918.7	1918.7	1920.5
gdb 1301	1922.3[a]	1916.1	1916.1	1917.8	1913.4	1913.3	1916.6
gdb 1302	1911.6[a]	1915.6	1915.6	1918.3	1917.0	1917.0	1918.5
gdb 1303	1854.4[a]	1852.2	1852.2	1856.9	1849.1	1849.1	1851.8
gdb 1304	1856.6[a]	1854.9	1854.9	1858.8	1856.1	1856.1	1857.0
gdb 1305	1854.6[a]	1851.8	1851.8	1852.9	1846.7	1846.6	1845.1
gdb 1306	1853.7[a]	1850.5	1850.5	1848.8	1845.3	1845.2	1842.8
gdb 1307	1914.1[a]	1916.0	1916.0	1917.4	1916.8	1916.8	1917.6
gdb 1308	1852.0[a]	1849.9	1849.9	1853.1	1846.9	1846.8	1849.6
gdb 1309	1854.7[a]	1851.6	1851.6	1856.1	1848.6	1848.6	1851.5
gdb 1310	1881.5[a]	1888.0	1887.9	1889.0	1889.4	1889.3	1888.8
gdb 1311	1851.5[a]	1849.9	1849.8	1849.9	1846.5	1846.5	1843.8
gdb 1312	1876.6[a]	1880.7	1880.7	1881.9	1883.7	1883.7	1884.2
gdb 1313	1889.7[a]	1887.3	1887.3	1888.5	1885.0	1884.9	1887.9
gdb 1314	1878.0[a]	1881.9	1881.9	1883.8	1882.7	1882.7	1884.0
gdb 1315	1861.6[a]	1870.4	1870.4	1871.4	1867.2	1867.2	1870.1
gdb 1316	1873.5[a]	1877.4	1877.4	1879.4	1878.6	1878.5	1880.1
gdb 1317	1854.1[a]	1850.0	1850.0	1849.3	1844.6	1844.6	1842.4
gdb 1318	1853.3[a]	1849.0	1849.0	1848.5	1844.5	1844.5	1842.4
gdb 1319	1861.7[a]	1868.5	1868.5	1870.6	1867.6	1867.6	1869.2
gdb 1320	1873.8[a]	1878.5	1878.5	1879.7	1881.2	1881.2	1881.5
gdb 1321	1883.1[a]	1878.2	1878.2	1880.3	1875.1	1875.1	1878.0
gdb 1322	1864.5[a]	1871.3	1871.3	1873.3	1868.9	1868.8	1871.7
gdb 1323	1874.6[a]	1881.0	1881.0	1884.1	1882.6	1882.0	1883.0
gdb 1324	1889.9[a]	1897.7	1897.7	1897.7	1899.3	1899.3	1899.0
gdb 1325	1887.3[a]	1897.8	1897.8	1898.2	1897.8	1897.8	1898.4
gdb 1326	1896.1[a]	1905.7	1905.7	1906.0	1906.9	1906.9	1906.4
gdb 1327	1876.1[a]	1879.7	1879.6	1882.8	1878.6	1878.6	1880.6
gdb 1328	1875.0[a]	1884.6	1884.6	1886.9	1882.6	1882.6	1884.3
gdb 1329	1893.3[a]	1899.1	1899.1	1899.5	1900.3	1900.3	1901.2
gdb 1330	1854.0[a]	1843.5	1843.5	1844.8	1842.1	1842.1	1842.4
gdb 1331	1861.8[a]	1849.2	1849.2	1854.1	1852.0	1852.0	1854.6
gdb 1332	1865.3[a]	1857.0	1857.0	1859.0	1857.7	1857.7	1859.9
gdb 1333	1861.5[a]	1854.6	1854.6	1856.5	1855.3	1855.3	1857.7
gdb 1334	1870.2[a]	1867.5	1867.5	1866.5	1863.8	1863.8	1862.3
gdb 1335	1872.2[a]	1872.4	1872.4	1874.0	1873.9	1873.8	1874.6
gdb 1336	1891.4[a]	1900.2	1900.2	1901.9	1898.6	1898.6	1901.4
gdb 1337	1900.6[a]	1907.8	1907.8	1908.7	1909.2	1909.1	1909.7
gdb 1338	1850.4[a]	1840.1	1840.1	1841.8	1839.3	1839.3	1840.1
gdb 1339	1858.7[a]	1846.6	1846.6	1850.7	1849.9	1849.9	1852.6
gdb 1340	1861.4[a]	1853.6	1853.6	1856.0	1854.5	1854.5	1857.1
gdb 1341	1870.6[a]	1871.4	1871.4	1873.6	1873.4	1873.4	1874.6
gdb 1342	1897.9[a]	1905.1	1905.1	1907.2	1908.2	1908.2	1910.5
gdb 1343	1891.9[a]	1897.7	1897.7	1898.2	1900.6	1900.6	1901.5
gdb 1344	1867.2[a]	1865.5	1865.5	1864.9	1862.0	1861.9	1861.0
gdb 1345	1864.8[a]	1857.5	1857.5	1859.7	1857.9	1857.9	1860.1
gdb 1346	1871.2[a]	1872.4	1872.4	1874.6	1874.0	1873.9	1875.1
gdb 1347	1899.3[a]	1904.8	1904.7	1906.3	1906.0	1906.0	1907.6
gdb 1348	1897.8[a]	1904.8	1904.8	1906.3	1907.5	1907.5	1909.4
gdb 1349	1893.7[a]	1901.7	1901.6	1904.0	1899.9	1899.8	1903.3
gdb 1350	1899.0[a]	1904.7	1904.7	1906.3	1905.8	1905.8	1907.3
gdb 1351	1875.3[a]	1878.7	1878.7	1880.8	1879.0	1879.0	1880.7
gdb 1352	1873.3[a]	1876.6	1876.5	1878.7	1876.9	1876.9	1878.7
gdb 1353	1855.4[a]	1851.4	1851.4	1850.4	1845.8	1845.8	1843.6
gdb 1354	1858.5[a]	1857.6	1857.6	1861.6	1858.7	1858.6	1859.4
gdb 1355	1856.1[a]	1852.0	1852.0	1851.5	1847.2	1847.2	1845.0
gdb 1356	1852.4[a]	1853.1	1853.0	1856.3	1855.2	1855.1	1856.3
gdb 1357	1850.0[a]	1847.7	1847.6	1850.1	1844.4	1844.4	1847.1
gdb 1358	1849.6[a]	1845.3	1845.3	1848.3	1843.0	1843.0	1845.8
gdb 1359	1879.7[a]	1883.8	1883.8	1887.0	1885.6	1885.6	1887.0
gdb 1360	1885.4[a]	1883.5	1883.5	1884.1	1880.3	1880.3	1883.4
gdb 1361	1853.3[a]	1850.2	1850.2	1849.6	1845.6	1845.5	1843.4
gdb 1362	1871.6[a]	1878.1	1878.1	1880.1	1878.4	1878.4	1880.1

... *continued on next page* ...

Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1363	1872.8[a]	1876.9	1876.8	1878.7	1877.5	1877.4	1879.1
gdb 1364	1865.0[a]	1872.2	1872.2	1873.2	1869.1	1869.1	1871.6
gdb 1365	1851.0[a]	1848.6	1848.6	1847.7	1843.4	1843.3	1841.3
gdb 1366	1854.5[a]	1856.3	1856.3	1860.1	1857.1	1857.1	1857.7
gdb 1367	1844.4[a]	1845.2	1845.2	1847.1	1844.0	1843.9	1845.7
gdb 1368	1852.0[a]	1851.0	1851.0	1851.4	1846.4	1846.4	1844.6
gdb 1369	1851.9[a]	1851.9	1851.9	1854.5	1853.6	1853.6	1854.2
gdb 1370	1841.1[a]	1841.5	1841.5	1843.7	1835.0	1835.0	1838.9
gdb 1371	1850.8[a]	1850.0	1850.0	1852.8	1847.0	1847.0	1849.2
gdb 1372	1847.3[a]	1846.7	1846.7	1849.4	1844.0	1844.0	1846.5
gdb 1373	1873.8[a]	1877.7	1877.7	1881.2	1879.1	1879.1	1881.5
gdb 1374	1872.6[a]	1877.0	1877.0	1880.3	1877.4	1877.4	1879.4
gdb 1375	1886.9[a]	1881.7	1881.7	1883.2	1877.9	1877.9	1881.8
gdb 1376	1881.1[a]	1883.5	1883.5	1886.0	1884.8	1884.7	1885.3
gdb 1377	1866.3[a]	1874.1	1874.1	1874.7	1871.6	1871.6	1873.5
gdb 1378	1839.1[a]	1838.1	1838.1	1836.1	1830.0	1830.0	1829.0
gdb 1379	1851.7[a]	1848.7	1848.7	1847.6	1844.1	1844.1	1841.5
gdb 1380	1860.9[a]	1866.3	1868.2	1870.5	1865.0	1864.9	1868.0
gdb 1381	1885.3[a]	1880.1	1879.8	1881.1	1877.3	1877.3	1880.9
gdb 1382	1872.4[a]	1874.8	1874.8	1878.0	1877.3	1877.3	1879.3
gdb 1383	1877.3[a]	1884.0	1884.0	1886.6	1885.2	1885.2	1886.0
gdb 1384	1889.6[a]	1886.4	1886.2	1888.1	1883.9	1883.6	1887.1
gdb 1385	1868.7[a]	1876.9	1876.9	1877.3	1874.1	1874.1	1876.0
gdb 1386	1840.2[a]	1840.5	1840.5	1838.3	1831.9	1831.9	1830.8
gdb 1387	1848.2[a]	1847.7	1847.7	1847.9	1843.3	1843.3	1841.3
gdb 1388	1843.1[a]	1844.2	1844.2	1845.4	1842.0	1842.0	1843.2
gdb 1389	1862.9[a]	1867.6	1867.6	1868.4	1866.3	1866.2	1869.3
gdb 1390	1884.5[a]	1877.5	1877.5	1879.3	1874.7	1874.7	1878.5
gdb 1391	1873.0[a]	1875.3	1875.3	1877.2	1877.7	1877.7	1879.4
gdb 1392	1859.4[a]	1864.2	1864.2	1864.3	1862.3	1862.2	1864.9
gdb 1393	1863.8[a]	1868.3	1868.3	1868.9	1866.4	1866.4	1868.7
gdb 1394	1870.5[a]	1874.5	1874.5	1876.3	1876.3	1876.3	1877.7
gdb 1395	1883.2[a]	1877.6	1877.6	1879.1	1874.9	1874.4	1878.4
gdb 1396	1860.8[a]	1865.9	1865.9	1866.2	1864.0	1863.9	1866.7
gdb 1397	1862.3[a]	1868.9	1868.9	1869.3	1867.0	1867.0	1869.7
gdb 1398	1869.3[a]	1875.0	1875.0	1877.9	1877.1	1877.1	1878.9
gdb 1399	1880.1[a]	1883.0	1883.0	1881.8	1879.2	1879.2	1877.0
gdb 1400	1897.7[a]	1884.6	1884.6	1885.5	1884.0	1884.0	1885.2
gdb 1401	1883.3[a]	1890.9	1890.9	1892.7	1892.0	1891.9	1891.7
gdb 1402	1924.1[a]	1939.1	1939.1	1939.5	1940.6	1940.6	1940.9
gdb 1403	1863.1[a]	1856.1	1856.1	1859.1	1857.4	1857.3	1858.0
gdb 1404	1894.8[a]	1899.4	1899.4	1899.6	1901.9	1901.9	1902.8
gdb 1405	1900.7[a]	1909.7	1909.7	1911.3	1911.6	1911.6	1913.5
gdb 1406	1884.3[a]	1876.6	1876.6	1879.1	1879.7	1879.7	1881.0
gdb 1407	1895.3[a]	1871.3	1871.3	1872.5	1871.3	1871.3	1873.5
gdb 1408	1885.7[a]	1878.7	1878.7	1880.7	1882.0	1882.0	1882.8
gdb 1409	1857.3[a]	1851.1	1851.1	1853.3	1848.9	1848.9	1849.3
gdb 1410	1842.5[a]	1834.4	1834.4	1837.6	1833.2	1833.2	1835.1
gdb 1411	1865.5[a]	1853.8	1853.8	1857.4	1854.5	1854.5	1854.9
gdb 1412	1854.5[a]	1839.7	1839.7	1842.5	1838.9	1838.9	1839.7
gdb 1413	1886.8[a]	1880.4	1880.4	1882.8	1872.5	1872.5	1875.5
gdb 1414	1895.7[a]	1888.3	1888.3	1891.1	1885.8	1885.7	1887.1
gdb 1415	1852.9[a]	1827.0	1827.0	1832.9	1829.8	1829.8	1832.0
gdb 1416	1841.1[a]	1816.7	1816.7	1820.5	1816.7	1816.7	1817.9
gdb 1417	1838.0[a]	1814.3	1814.3	1818.1	1813.3	1813.3	1814.1
gdb 1418	1851.4[a]	1826.6	1826.6	1832.4	1829.2	1829.2	1831.1
gdb 1419	1839.1[a]	1815.6	1815.6	1819.1	1815.3	1815.2	1816.2
gdb 1420	1834.1[a]	1826.9	1826.9	1829.2	1830.9	1830.9	1830.5
gdb 1421	1838.2[a]	1830.5	1830.5	1829.8	1827.4	1827.4	1824.5
gdb 1422	1832.2[a]	1825.9	1825.9	1825.2	1822.7	1822.7	1819.9
gdb 1423	1835.7[a]	1828.7	1828.7	1830.9	1831.7	1831.7	1830.9
gdb 1424	1835.1[a]	1828.9	1828.9	1828.0	1825.2	1825.2	1822.4
gdb 1425	1875.6[a]	1873.4	1873.4	1876.8	1870.1	1870.1	1872.1
gdb 1426	1877.7[a]	1871.7	1871.7	1875.0	1869.5	1869.5	1871.7
gdb 1427	1865.8[a]	1849.8	1849.8	1855.0	1848.6	1848.6	1852.0

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1428	1886.1[a]	1882.2	1882.2	1885.0	1885.1	1885.1	1886.5
gdb 1429	1882.7[a]	1876.1	1876.1	1878.2	1879.6	1879.6	1880.1
gdb 1430	1892.4[a]	1869.8	1869.8	1870.6	1869.3	1869.3	1871.2
gdb 1431	1885.2[a]	1878.1	1878.1	1879.9	1881.3	1881.3	1881.9
gdb 1432	1910.8[a]	1906.0	1906.0	1906.7	1904.2	1904.2	1906.6
gdb 1433	1900.8[a]	1907.1	1907.1	1908.1	1910.4	1910.4	1910.7
gdb 1434	1888.0[a]	1887.2	1887.2	1888.7	1883.3	1883.3	1884.2
gdb 1435	1898.7[a]	1897.0	1897.0	1899.9	1896.9	1896.9	1898.3
gdb 1436	1865.7[a]	1856.1	1856.1	1858.0	1856.1	1856.1	1858.1
gdb 1437	1873.6[a]	1870.3	1870.3	1872.4	1873.5	1873.5	1874.7
gdb 1438	1849.8[a]	1844.2	1844.2	1844.4	1839.1	1839.1	1838.2
gdb 1439	1866.5[a]	1854.8	1854.8	1857.8	1856.6	1856.5	1858.0
gdb 1440	1781.5[a]	1762.3	1762.3	1764.3	1758.6	1758.6	1758.7
gdb 1441	1805.4[a]	1785.4	1785.4	1789.3	1785.3	1785.3	1787.2
gdb 1442	1805.4[a]	1786.6	1786.6	1790.7	1786.0	1786.0	1787.9
gdb 1443	1817.5[a]	1809.1	1809.1	1810.2	1804.9	1804.8	1802.5
gdb 1444	1888.4[a]	1887.7	1887.7	1888.8	1884.3	1884.3	1885.0
gdb 1445	1903.3[a]	1894.4	1894.4	1896.6	1891.0	1890.9	1894.0
gdb 1446	1898.1[a]	1897.2	1897.2	1900.1	1897.7	1897.7	1899.6
gdb 1447	1850.9[a]	1844.5	1844.5	1842.8	1834.8	1834.8	1832.3
gdb 1448	1864.3[a]	1855.9	1855.9	1857.3	1850.0	1850.0	1848.9
gdb 1449	1854.6[a]	1854.4	1854.4	1855.0	1849.5	1849.5	1847.7
gdb 1450	1824.6[a]	1811.8	1811.8	1809.3	1803.5	1803.5	1799.0
gdb 1451	1841.2[a]	1821.9	1821.9	1823.1	1819.2	1819.2	1817.9
gdb 1452	1830.6[a]	1822.5	1822.5	1823.6	1820.1	1820.1	1818.2
gdb 1453	1845.1[a]	1840.9	1840.9	1841.7	1839.2	1839.1	1839.1
gdb 1454	1863.8[a]	1853.6	1853.6	1857.5	1856.1	1856.1	1858.6
gdb 1455	1885.3[a]	1885.2	1885.2	1887.5	1880.7	1880.7	1882.0
gdb 1456	1849.3[a]	1841.6	1841.5	1837.7	1831.1	1831.1	1825.3
gdb 1457	1853.1[a]	1848.5	1848.5	1847.7	1843.5	1843.5	1840.1
gdb 1458	1853.1[a]	1850.4	1850.4	1849.8	1845.3	1845.3	1841.9
gdb 1459	1868.9[a]	1869.5	1869.5	1868.5	1865.0	1865.0	1863.7
gdb 1460	1877.0[a]	1880.5	1880.5	1882.8	1881.2	1881.2	1882.2
gdb 1461	1868.8[a]	1865.3	1865.3	1861.1	1854.2	1854.2	1849.2
gdb 1462	1875.8[a]	1877.4	1877.3	1876.3	1871.3	1871.3	1868.0
gdb 1463	1910.9[a]	1909.6	1909.5	1910.5	1906.3	1906.3	1908.3
gdb 1464	1902.0[a]	1905.6	1905.6	1903.9	1900.9	1900.9	1898.6
gdb 1465	1902.8[a]	1911.2	1911.2	1911.9	1911.5	1911.5	1910.7
gdb 1466	1854.6[a]	1843.7	1843.7	1843.3	1840.7	1840.7	1838.1
gdb 1467	1846.5[a]	1829.9	1829.9	1832.9	1832.0	1831.9	1832.7
gdb 1468	1859.1[a]	1848.8	1848.8	1852.1	1841.3	1841.3	1843.4
gdb 1469	1869.3[a]	1858.5	1858.5	1862.2	1854.5	1854.5	1856.2
gdb 1470	1861.4[a]	1856.1	1856.1	1861.0	1851.9	1851.9	1855.2
gdb 1471	1869.3[a]	1857.9	1857.9	1861.8	1854.7	1854.7	1856.9
gdb 1472	1866.1[a]	1859.5	1859.5	1864.0	1856.2	1856.2	1858.7
gdb 1473	1876.7[a]	1869.6	1869.6	1868.3	1866.6	1866.6	1864.1
gdb 1474	1860.0[a]	1859.9	1859.9	1862.0	1859.6	1859.6	1860.4
gdb 1475	1887.4[a]	1881.0	1881.0	1883.9	1883.3	1883.3	1884.2
gdb 1476	1912.7[a]	1907.4	1907.4	1908.1	1905.4	1905.3	1907.5
gdb 1477	1891.4[a]	1895.6	1895.6	1897.4	1895.0	1895.0	1897.0
gdb 1478	1902.0[a]	1906.3	1906.3	1907.4	1909.5	1909.4	1909.4
gdb 1479	1867.8[a]	1858.5	1858.5	1860.1	1858.3	1858.3	1859.9
gdb 1480	1868.4[a]	1856.8	1856.8	1858.0	1856.2	1856.2	1858.1
gdb 1481	1877.8[a]	1873.3	1873.3	1874.9	1875.8	1875.8	1876.4
gdb 1482	1882.1[a]	1880.3	1880.3	1883.0	1877.9	1877.9	1880.5
gdb 1483	1896.4[a]	1893.2	1893.2	1896.0	1894.0	1893.9	1895.8
gdb 1484	1889.8[a]	1894.5	1894.5	1897.7	1889.8	1889.7	1892.7
gdb 1485	1874.7[a]	1875.3	1875.3	1877.7	1872.9	1872.9	1875.2
gdb 1486	1879.0[a]	1878.7	1878.7	1881.6	1876.5	1876.5	1879.3
gdb 1487	1882.6[a]	1891.9	1891.9	1894.5	1891.8	1891.7	1892.4
gdb 1488	1877.8[a]	1876.1	1876.1	1878.6	1875.7	1875.7	1878.3
gdb 1489	1883.6[a]	1884.0	1884.0	1886.8	1878.4	1878.4	1880.4
gdb 1490	1886.1[a]	1886.1	1886.1	1889.3	1881.9	1881.9	1884.6
gdb 1491	1884.1[a]	1883.6	1883.6	1886.5	1879.7	1879.7	1882.3
gdb 1492	1887.3[a]	1888.0	1888.0	1887.1	1881.6	1881.6	1878.9

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1493	1904.6[a]	1912.7	1912.7	1914.6	1912.8	1912.7	1914.5
gdb 1494	1889.0[a]	1885.8	1885.8	1884.8	1880.4	1880.4	1877.9
gdb 1495	1915.2[a]	1916.0	1916.0	1918.0	1911.9	1911.8	1915.0
gdb 1496	1910.6[a]	1917.2	1917.2	1918.2	1916.4	1916.4	1916.4
gdb 1497	1917.2[a]	1928.2	1928.2	1928.1	1930.2	1930.2	1930.4
gdb 1498	1879.2[a]	1882.3	1882.3	1880.8	1877.7	1877.7	1874.9
gdb 1499	1903.8[a]	1891.7	1891.7	1892.3	1889.7	1889.6	1890.4
gdb 1500	1887.8[a]	1894.0	1894.0	1896.2	1895.3	1895.3	1895.3
gdb 1501	1900.0[a]	1908.5	1908.5	1910.1	1910.6	1910.5	1912.5
gdb 1502	1899.4[a]	1901.5	1901.5	1899.5	1896.5	1896.5	1893.8
gdb 1503	1917.6[a]	1915.7	1915.7	1916.3	1912.5	1912.5	1914.1
gdb 1504	1906.6[a]	1913.4	1913.4	1914.7	1914.2	1914.2	1914.0
gdb 1505	1924.1[a]	1939.2	1939.2	1939.6	1941.3	1941.3	1942.0
gdb 1506	1920.2[a]	1921.9	1921.9	1922.4	1917.8	1917.7	1920.7
gdb 1507	1912.9[a]	1919.6	1919.6	1921.0	1920.1	1920.1	1921.1
gdb 1508	1864.4[a]	1871.7	1871.7	1875.6	1870.1	1870.1	1871.4
gdb 1509	1900.0[a]	1909.4	1909.3	1911.1	1906.2	1906.2	1908.8
gdb 1510	1905.2[a]	1912.9	1912.8	1914.6	1913.0	1913.0	1914.5
gdb 1511	1858.8[a]	1855.7	1855.7	1858.9	1857.7	1857.6	1858.6
gdb 1512	1895.2[a]	1902.0	1902.0	1902.0	1902.8	1902.8	1903.5
gdb 1513	1833.7[a]	1814.9	1814.9	1813.5	1808.1	1808.1	1804.2
gdb 1514	1829.9[a]	1816.3	1816.3	1817.6	1816.7	1816.7	1815.8
gdb 1515	1896.9[a]	1877.8	1877.8	1879.3	1878.6	1878.6	1881.2
gdb 1516	1884.6[a]	1882.8	1882.8	1882.3	1880.5	1880.5	1878.9
gdb 1517	1882.5[a]	1884.0	1884.0	1886.5	1888.0	1888.0	1889.2
gdb 1518	1853.3[a]	1840.0	1840.0	1836.5	1831.1	1831.1	1826.0
gdb 1519	1851.2[a]	1842.6	1842.6	1842.3	1840.2	1840.2	1837.9
gdb 1520	1847.6[a]	1830.1	1830.1	1833.1	1832.5	1832.5	1833.4
gdb 1521	1898.2[a]	1882.2	1882.1	1882.8	1880.8	1880.8	1882.5
gdb 1522	1876.6[a]	1870.7	1870.7	1872.7	1871.4	1871.4	1872.7
gdb 1523	1884.2[a]	1883.6	1883.6	1882.6	1880.0	1880.0	1877.5
gdb 1524	1885.6[a]	1886.6	1886.6	1889.0	1889.9	1889.9	1890.5
gdb 1525	1878.9[a]	1876.2	1876.2	1878.9	1876.1	1876.1	1877.9
gdb 1526	1895.3[a]	1900.4	1900.4	1900.2	1902.0	1901.9	1901.5
gdb 1527	1844.0[a]	1842.9	1842.8	1845.6	1841.8	1841.7	1844.2
gdb 1528	1874.6[a]	1871.3	1871.3	1869.8	1866.6	1866.5	1864.3
gdb 1529	1874.6[a]	1866.4	1866.4	1868.1	1866.2	1866.2	1867.4
gdb 1530	1881.3[a]	1882.5	1882.4	1884.1	1883.5	1883.5	1883.8
gdb 1531	1878.3[a]	1882.4	1882.4	1880.7	1877.7	1877.7	1874.6
gdb 1532	1881.3[a]	1880.1	1880.1	1881.8	1879.8	1879.8	1879.8
gdb 1533	1885.5[a]	1893.0	1893.0	1894.7	1893.8	1893.8	1893.0
gdb 1534	1885.4[a]	1886.1	1886.1	1885.2	1880.4	1880.4	1878.1
gdb 1535	1872.1[a]	1875.8	1875.8	1879.4	1872.9	1872.8	1875.5
gdb 1536	1871.7[a]	1863.1	1863.1	1865.1	1863.3	1863.3	1865.3
gdb 1537	1879.0[a]	1879.3	1879.3	1881.6	1880.9	1880.9	1881.9
gdb 1538	1900.2[a]	1887.5	1887.5	1890.0	1884.8	1884.8	1888.1
gdb 1539	1880.6[a]	1880.2	1880.2	1882.8	1878.4	1878.4	1880.7
gdb 1540	1885.5[a]	1893.1	1893.1	1896.3	1893.9	1893.9	1895.5
gdb 1541	1863.6[a]	1854.0	1854.0	1857.2	1849.7	1849.7	1852.9
gdb 1542	1870.4[a]	1861.1	1861.1	1864.1	1859.4	1859.3	1861.3
gdb 1543	1854.8[a]	1842.1	1842.1	1845.3	1836.9	1836.8	1838.5
gdb 1544	1859.6[a]	1847.5	1847.5	1850.5	1845.9	1845.9	1846.7
gdb 1545	1846.4[a]	1839.0	1839.0	1839.2	1830.6	1830.6	1829.9
gdb 1546	1851.2[a]	1852.2	1852.2	1853.0	1846.4	1846.4	1844.8
gdb 1547	1900.1[a]	1887.7	1887.7	1890.1	1885.1	1885.0	1888.6
gdb 1548	1884.4[a]	1883.3	1883.3	1886.5	1881.7	1881.7	1884.8
gdb 1549	1887.1[a]	1894.3	1894.3	1897.7	1895.1	1895.1	1897.0
gdb 1550	1874.2[a]	1871.7	1871.7	1870.3	1866.5	1866.5	1864.4
gdb 1551	1874.4[a]	1866.0	1866.0	1867.6	1865.2	1865.2	1866.9
gdb 1552	1883.5[a]	1883.8	1883.8	1885.6	1884.4	1884.4	1884.9
gdb 1553	1886.8[a]	1885.3	1885.3	1886.7	1881.6	1881.6	1882.3
gdb 1554	1887.1[a]	1886.6	1886.6	1889.3	1884.4	1884.3	1886.8
gdb 1555	1897.8[a]	1895.8	1895.8	1898.9	1896.6	1896.6	1898.8
gdb 1556	1890.8[a]	1901.0	1901.0	1902.2	1889.2	1889.2	1892.3
gdb 1557	1895.8[a]	1902.1	1902.1	1904.5	1896.8	1896.8	1898.5

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1558	1897.8[a]	1901.5	1901.5	1899.5	1896.3	1896.3	1893.5
gdb 1559	1895.9[a]	1904.0	1904.0	1905.8	1902.1	1902.1	1903.5
gdb 1560	1904.5[a]	1912.5	1912.5	1913.7	1912.8	1912.8	1912.0
gdb 1561	1891.5[a]	1888.8	1888.8	1887.8	1882.6	1882.6	1880.3
gdb 1562	1870.1[a]	1862.5	1862.5	1865.3	1861.1	1861.1	1863.0
gdb 1563	1869.1[a]	1869.1	1869.1	1871.4	1865.9	1865.9	1867.6
gdb 1564	1869.4[a]	1873.9	1873.9	1877.4	1871.3	1871.3	1873.7
gdb 1565	1910.1[a]	1915.9	1915.9	1917.1	1916.8	1916.8	1917.7
gdb 1566	1869.0[a]	1868.9	1868.9	1871.6	1865.8	1865.8	1867.7
gdb 1567	1923.2[a]	1921.1	1921.1	1921.9	1916.7	1916.7	1919.8
gdb 1568	1916.9[a]	1921.4	1921.4	1923.1	1921.4	1921.4	1922.3
gdb 1569	1887.9[a]	1887.6	1887.6	1886.8	1881.1	1881.1	1878.3
gdb 1570	1905.7[a]	1914.9	1914.9	1916.9	1914.7	1914.7	1916.3
gdb 1571	1887.8[a]	1886.8	1886.8	1885.7	1880.8	1880.8	1877.9
gdb 1572	1912.8[a]	1919.2	1919.2	1920.4	1918.9	1918.8	1919.1
gdb 1573	1916.5[a]	1928.3	1928.3	1928.2	1929.6	1929.6	1929.4
gdb 1574	1919.7[a]	1915.7	1915.7	1917.2	1910.8	1910.8	1914.5
gdb 1575	1905.9[a]	1911.7	1911.7	1913.1	1907.9	1907.9	1910.3
gdb 1576	1915.0[a]	1919.3	1919.3	1920.8	1919.1	1919.0	1919.6
gdb 1577	1869.0[a]	1880.7	1880.7	1883.2	1869.8	1869.7	1873.7
gdb 1578	1872.1[a]	1882.9	1882.8	1885.4	1873.1	1873.0	1877.0
gdb 1579	1872.6[a]	1881.2	1881.2	1884.7	1876.9	1876.8	1879.2
gdb 1580	1902.0[a]	1908.1	1908.1	1909.3	1905.2	1905.2	1907.5
gdb 1581	1908.6[a]	1913.7	1913.7	1915.0	1914.1	1914.1	1914.9
gdb 1582	1859.4[a]	1862.0	1862.0	1865.3	1856.0	1855.9	1858.0
gdb 1583	1867.5[a]	1875.1	1875.1	1878.9	1872.0	1872.0	1872.4
gdb 1584	1861.4[a]	1862.8	1862.8	1866.0	1857.1	1857.1	1858.9
gdb 1585	1859.1[a]	1856.9	1856.9	1860.6	1853.4	1853.3	1855.9
gdb 1586	1899.8[a]	1909.3	1909.3	1910.6	1906.4	1906.4	1908.8
gdb 1587	1907.2[a]	1916.1	1916.1	1917.1	1916.4	1916.3	1916.9
gdb 1588	1906.5[a]	1912.5	1912.5	1913.9	1908.3	1908.3	1910.5
gdb 1589	1914.0[a]	1917.9	1917.9	1918.9	1916.9	1916.9	1916.9
gdb 1590	1869.3[a]	1878.9	1878.9	1881.3	1867.9	1867.9	1872.1
gdb 1591	1871.5[a]	1879.9	1879.9	1883.3	1875.2	1875.2	1877.4
gdb 1592	1872.4[a]	1878.8	1878.8	1882.4	1874.5	1874.5	1876.4
gdb 1593	1825.9[a]	1813.5	1813.5	1812.0	1805.6	1805.6	1802.3
gdb 1594	1835.3[a]	1826.0	1826.0	1826.9	1822.7	1822.3	1820.2
gdb 1595	1842.1[a]	1823.8	1823.8	1825.0	1819.7	1819.7	1817.7
gdb 1596	1837.7[a]	1824.1	1824.1	1823.5	1817.9	1817.8	1816.6
gdb 1597	1843.4[a]	1831.5	1831.5	1834.2	1831.7	1831.7	1832.4
gdb 1598	1849.8[a]	1840.7	1840.7	1840.0	1837.5	1837.5	1834.3
gdb 1599	1878.6[a]	1879.5	1879.5	1882.4	1876.9	1876.9	1880.3
gdb 1600	1883.2[a]	1883.1	1883.1	1884.3	1879.6	1879.5	1880.7
gdb 1601	1896.1[a]	1889.0	1889.0	1891.9	1888.7	1888.7	1890.5
gdb 1602	1887.2[a]	1890.9	1890.9	1892.5	1889.9	1889.9	1891.8
gdb 1603	1890.0[a]	1892.7	1892.7	1894.1	1891.6	1891.5	1893.5
gdb 1604	1894.4[a]	1894.7	1894.7	1895.5	1898.1	1898.1	1897.6
gdb 1605	1868.5[a]	1873.9	1873.9	1876.4	1864.8	1864.8	1869.3
gdb 1606	1871.4[a]	1878.0	1877.9	1880.5	1869.4	1869.4	1873.4
gdb 1607	1871.8[a]	1877.0	1877.0	1880.4	1873.9	1873.8	1876.2
gdb 1608	1878.9[a]	1879.7	1879.7	1878.8	1876.1	1876.1	1874.5
gdb 1609	1901.6[a]	1888.1	1888.0	1889.4	1886.5	1886.5	1888.3
gdb 1610	1882.7[a]	1890.4	1890.4	1892.6	1891.8	1891.8	1892.0
gdb 1611	1890.8[a]	1897.1	1897.1	1897.1	1899.3	1899.2	1899.4
gdb 1612	1893.6[a]	1903.9	1903.9	1905.9	1905.3	1905.2	1907.2
gdb 1613	1895.4[a]	1901.9	1901.9	1902.0	1902.8	1902.8	1903.5
gdb 1614	1871.3[a]	1875.1	1875.1	1872.1	1869.7	1869.7	1865.3
gdb 1615	1873.9[a]	1877.7	1877.7	1877.6	1874.9	1874.9	1870.1
gdb 1616	1882.6[a]	1883.8	1883.8	1884.7	1885.1	1884.9	1882.6
gdb 1617	1896.0[a]	1905.0	1905.0	1904.9	1906.6	1906.6	1906.1
gdb 1618	1886.4[a]	1894.4	1894.4	1894.8	1896.7	1896.7	1898.2
gdb 1619	1871.4[a]	1870.4	1870.4	1868.0	1865.6	1865.6	1862.4
gdb 1620	1876.2[a]	1873.7	1873.6	1871.5	1869.3	1869.3	1866.4
gdb 1621	1873.9[a]	1876.7	1876.7	1877.5	1880.1	1880.1	1879.2
gdb 1622	1834.9[a]	1815.8	1815.8	1814.3	1808.2	1808.7	1804.9

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1623	1838.1[a]	1821.0	1821.0	1823.0	1820.0	1820.0	1818.7
gdb 1624	1846.8[a]	1830.2	1830.2	1829.5	1824.8	1824.8	1822.9
gdb 1625	1844.9[a]	1829.2	1829.2	1828.2	1823.7	1823.7	1822.1
gdb 1626	1850.9[a]	1840.7	1840.6	1836.7	1830.8	1830.8	1825.2
gdb 1627	1849.8[a]	1835.0	1835.0	1837.6	1836.1	1836.1	1836.7
gdb 1628	1845.6[a]	1833.5	1833.5	1836.0	1834.5	1834.5	1835.3
gdb 1629	1853.7[a]	1845.4	1845.4	1845.0	1841.8	1841.8	1838.6
gdb 1630	1874.3[a]	1874.3	1874.3	1873.4	1866.8	1866.8	1865.8
gdb 1631	1876.3[a]	1878.9	1878.9	1881.4	1877.5	1877.5	1878.9
gdb 1632	1829.1[a]	1813.2	1813.2	1812.0	1806.3	1806.2	1803.2
gdb 1633	1830.8[a]	1817.2	1817.2	1819.4	1816.4	1816.4	1815.8
gdb 1634	1843.1[a]	1828.1	1828.1	1827.7	1823.0	1823.0	1821.9
gdb 1635	1842.0[a]	1831.3	1831.3	1834.3	1833.3	1833.3	1834.6
gdb 1636	1899.2[a]	1883.0	1883.0	1884.6	1881.7	1881.7	1884.1
gdb 1637	1880.8[a]	1879.0	1879.0	1878.1	1876.2	1876.2	1874.5
gdb 1638	1880.5[a]	1883.7	1883.7	1886.2	1887.1	1887.1	1887.8
gdb 1639	1871.3[a]	1870.0	1870.0	1867.7	1866.2	1866.1	1863.1
gdb 1640	1874.7[a]	1872.2	1872.2	1870.0	1869.1	1869.1	1866.1
gdb 1641	1875.7[a]	1877.5	1877.5	1878.7	1880.4	1880.4	1879.6
gdb 1642	1848.8[a]	1839.1	1839.1	1835.6	1829.7	1829.7	1824.7
gdb 1643	1845.8[a]	1831.1	1831.0	1830.6	1825.5	1825.5	1823.8
gdb 1644	1850.5[a]	1844.0	1844.0	1843.9	1840.9	1840.9	1838.4
gdb 1645	1849.3[a]	1835.9	1835.9	1838.8	1837.0	1837.0	1837.7
gdb 1646	1896.3[a]	1880.4	1880.4	1881.6	1878.8	1878.7	1881.1
gdb 1647	1875.1[a]	1872.9	1872.9	1874.8	1871.7	1871.7	1873.3
gdb 1648	1879.9[a]	1879.6	1879.6	1878.6	1876.2	1876.2	1874.2
gdb 1649	1882.5[a]	1884.0	1884.0	1886.4	1887.0	1886.9	1887.4
gdb 1650	1874.8[a]	1874.4	1874.4	1873.7	1866.4	1866.3	1865.8
gdb 1651	1878.4[a]	1879.7	1879.7	1882.4	1878.5	1878.5	1880.2
gdb 1652	1872.0[a]	1867.0	1867.0	1868.7	1867.1	1867.0	1868.9
gdb 1653	1869.4[a]	1868.9	1868.9	1870.1	1867.4	1867.4	1869.3
gdb 1654	1877.4[a]	1877.8	1877.8	1876.7	1873.4	1873.4	1871.1
gdb 1655	1876.9[a]	1877.9	1877.9	1879.9	1880.6	1880.6	1881.1
gdb 1656	1870.6[a]	1870.4	1870.4	1868.0	1866.4	1866.3	1863.4
gdb 1657	1872.0[a]	1872.2	1872.2	1870.2	1868.1	1868.1	1865.0
gdb 1658	1875.2[a]	1873.0	1872.8	1873.8	1876.4	1876.3	1875.5
gdb 1659	1867.3[a]	1870.1	1870.1	1867.7	1865.7	1865.7	1863.1
gdb 1660	1872.4[a]	1872.4	1872.4	1870.3	1868.6	1868.6	1865.3
gdb 1661	1873.9[a]	1877.2	1876.2	1877.1	1879.9	1879.9	1878.0
gdb 1662	1892.2[a]	1898.2	1898.2	1898.6	1900.9	1900.9	1901.8
gdb 1663	1872.6[a]	1872.0	1872.0	1873.8	1871.6	1871.6	1872.8
gdb 1664	1874.3[a]	1876.8	1876.8	1875.5	1872.4	1872.4	1870.7
gdb 1665	1879.0[a]	1884.8	1884.8	1887.2	1885.4	1885.4	1885.6
gdb 1666	1844.6[a]	1839.9	1839.9	1836.3	1829.3	1829.3	1824.1
gdb 1667	1845.4[a]	1832.2	1832.2	1831.6	1825.8	1825.8	1823.8
gdb 1668	1853.1[a]	1849.7	1849.7	1849.2	1844.5	1844.5	1841.4
gdb 1669	1852.0[a]	1850.2	1850.2	1849.5	1844.7	1844.7	1841.1
gdb 1670	1884.7[a]	1883.5	1883.5	1884.5	1879.3	1879.8	1881.5
gdb 1671	1884.1[a]	1884.3	1884.3	1887.5	1881.6	1881.5	1884.5
gdb 1672	1894.6[a]	1890.7	1890.7	1893.9	1890.6	1890.6	1892.7
gdb 1673	1887.9[a]	1896.5	1896.5	1898.1	1894.7	1894.7	1896.3
gdb 1674	1893.9[a]	1895.5	1895.5	1893.6	1891.4	1891.4	1889.5
gdb 1675	1896.3[a]	1903.4	1903.4	1904.7	1904.1	1904.1	1904.1
gdb 1676	1871.9[a]	1874.0	1874.0	1877.0	1871.4	1871.4	1874.8
gdb 1677	1871.2[a]	1872.7	1872.7	1875.5	1870.4	1870.4	1873.8
gdb 1678	1874.0[a]	1876.5	1876.5	1879.4	1873.9	1873.9	1876.6
gdb 1679	1876.7[a]	1885.9	1885.9	1888.9	1885.5	1885.5	1886.9
gdb 1680	1847.4[a]	1840.1	1840.1	1841.1	1838.8	1838.7	1839.1
gdb 1681	1875.2[a]	1855.2	1855.2	1858.8	1853.5	1853.5	1858.5
gdb 1682	1862.3[a]	1850.3	1850.3	1854.3	1853.5	1853.5	1856.1
gdb 1683	1863.6[a]	1853.2	1853.1	1855.0	1853.9	1853.9	1856.5
gdb 1684	1882.9[a]	1871.2	1871.2	1873.0	1870.1	1870.1	1873.6
gdb 1685	1870.2[a]	1868.6	1868.5	1870.9	1871.7	1871.6	1873.3
gdb 1686	1898.9[a]	1906.5	1906.5	1908.3	1909.6	1909.6	1912.0
gdb 1687	1893.7[a]	1898.5	1898.5	1899.0	1900.1	1900.1	1901.0

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1688	1889.6[a]	1882.5	1882.5	1884.4	1879.6	1879.6	1883.1
gdb 1689	1869.4[a]	1868.1	1868.1	1867.2	1864.4	1864.3	1863.1
gdb 1690	1868.9[a]	1860.9	1860.9	1863.0	1861.1	1861.0	1863.4
gdb 1691	1877.2[a]	1878.9	1878.8	1881.0	1880.4	1880.3	1881.2
gdb 1692	1915.5[a]	1915.9	1915.9	1917.3	1912.6	1912.5	1916.5
gdb 1693	1902.2[a]	1911.2	1911.2	1913.1	1912.4	1912.4	1914.1
gdb 1694	1898.6[a]	1906.8	1906.8	1908.3	1909.4	1909.4	1911.2
gdb 1695	1897.3[a]	1905.4	1905.4	1907.5	1903.3	1903.2	1906.5
gdb 1696	1915.2[a]	1913.5	1913.5	1915.0	1910.3	1910.3	1915.1
gdb 1697	1903.3[a]	1911.3	1911.3	1912.8	1912.4	1912.3	1913.5
gdb 1698	1880.7[a]	1883.6	1883.6	1882.5	1878.2	1878.2	1875.6
gdb 1699	1841.8[a]	1841.8	1841.8	1845.3	1835.2	1835.1	1839.8
gdb 1700	1851.3[a]	1849.4	1849.4	1852.7	1846.8	1846.7	1849.4
gdb 1701	1917.7[a]	1929.9	1929.9	1930.5	1931.7	1931.9	1932.8
gdb 1702	1892.5[a]	1903.7	1903.7	1904.5	1904.2	1904.2	1904.8
gdb 1703	1873.8[a]	1877.9	1877.8	1876.5	1872.8	1872.8	1870.6
gdb 1704	1868.8[a]	1868.3	1868.3	1869.9	1867.7	1867.7	1869.3
gdb 1705	1871.5[a]	1875.1	1875.1	1876.3	1872.6	1872.5	1873.5
gdb 1706	1880.2[a]	1885.5	1885.5	1887.2	1885.5	1885.4	1885.4
gdb 1707	1876.3[a]	1879.9	1879.9	1878.6	1875.6	1875.5	1873.3
gdb 1708	1896.6[a]	1884.7	1884.7	1885.5	1882.0	1882.0	1883.5
gdb 1709	1877.7[a]	1878.2	1878.2	1879.9	1876.4	1876.4	1877.2
gdb 1710	1882.1[a]	1889.2	1889.2	1890.9	1889.6	1889.6	1888.8
gdb 1711	1893.6[a]	1903.5	1903.5	1905.0	1904.5	1904.5	1906.7
gdb 1712	1894.9[a]	1895.0	1895.0	1893.0	1890.4	1890.3	1888.5
gdb 1713	1885.0[a]	1890.4	1890.4	1892.5	1888.8	1888.8	1891.2
gdb 1714	1891.8[a]	1899.2	1899.2	1900.6	1896.5	1896.5	1897.9
gdb 1715	1900.0[a]	1902.8	1902.8	1903.9	1903.4	1903.4	1903.0
gdb 1716	1874.2[a]	1877.0	1876.9	1875.9	1868.1	1868.1	1866.9
gdb 1717	1879.7[a]	1882.7	1882.7	1881.5	1876.9	1876.9	1874.0
gdb 1718	1897.9[a]	1904.3	1904.3	1906.1	1901.6	1901.6	1904.6
gdb 1719	1909.0[a]	1909.7	1909.7	1911.2	1910.7	1910.7	1911.7
gdb 1720	1840.6[a]	1837.3	1837.3	1834.7	1829.5	1829.5	1828.4
gdb 1721	1843.9[a]	1842.4	1842.4	1843.1	1841.1	1841.1	1842.4
gdb 1722	1918.8[a]	1930.1	1930.1	1930.6	1931.4	1931.4	1932.2
gdb 1723	1896.5[a]	1901.1	1901.1	1903.1	1898.2	1898.1	1901.7
gdb 1724	1898.2[a]	1905.1	1905.1	1906.6	1902.0	1902.0	1904.8
gdb 1725	1908.2[a]	1910.1	1910.1	1911.3	1910.5	1910.5	1910.7
gdb 1726	1866.7[a]	1871.0	1871.0	1873.4	1861.2	1861.2	1866.6
gdb 1727	1862.5[a]	1865.1	1865.1	1868.6	1858.1	1858.1	1862.5
gdb 1728	1867.9[a]	1868.0	1868.0	1871.1	1858.5	1858.5	1864.7
gdb 1729	1864.6[a]	1871.1	1871.1	1873.8	1862.2	1862.2	1867.2
gdb 1730	1872.5[a]	1875.7	1875.7	1879.1	1871.1	1871.1	1874.0
gdb 1731	1873.7[a]	1877.0	1877.0	1880.3	1872.5	1872.5	1875.6
gdb 1732	1848.3[a]	1830.9	1830.9	1834.2	1831.1	1831.0	1832.7
gdb 1733	1859.9[a]	1846.6	1846.6	1850.3	1848.6	1848.6	1849.3
gdb 1734	1857.2[a]	1839.4	1839.4	1842.3	1838.6	1838.6	1839.5
gdb 1735	1872.4[a]	1865.9	1865.9	1869.4	1864.5	1864.5	1866.8
gdb 1736	1864.5[a]	1852.8	1852.8	1855.4	1849.4	1849.4	1852.2
gdb 1737	1874.3[a]	1870.6	1870.6	1873.3	1869.5	1869.5	1871.1
gdb 1738	1870.9[a]	1863.4	1863.4	1867.1	1862.8	1862.7	1865.3
gdb 1739	1873.3[a]	1861.6	1861.6	1863.9	1862.0	1862.0	1862.7
gdb 1740	1881.0[a]	1874.8	1874.7	1877.9	1877.2	1877.2	1877.5
gdb 1741	1847.2[a]	1831.6	1831.6	1834.5	1831.2	1831.2	1832.5
gdb 1742	1858.3[a]	1843.9	1843.9	1847.7	1846.6	1846.6	1847.8
gdb 1743	1851.0[a]	1835.3	1835.2	1837.8	1834.7	1834.7	1835.7
gdb 1744	1873.7[a]	1875.2	1875.2	1879.5	1869.6	1869.6	1873.6
gdb 1745	1876.9[a]	1885.1	1885.1	1890.0	1881.4	1881.3	1884.6
gdb 1746	1878.4[a]	1880.2	1880.2	1884.2	1877.4	1877.4	1879.4
gdb 1747	1869.7[a]	1865.0	1865.0	1867.6	1858.2	1858.2	1863.5
gdb 1748	1860.6[a]	1848.8	1848.8	1851.2	1846.0	1846.0	1849.5
gdb 1749	1861.4[a]	1848.6	1848.6	1851.8	1845.8	1845.8	1849.6
gdb 1750	1870.5[a]	1861.8	1861.8	1865.2	1862.2	1862.2	1865.0
gdb 1751	1868.3[a]	1861.4	1861.4	1864.6	1861.4	1861.4	1864.3
gdb 1752	1871.1[a]	1865.1	1865.1	1868.8	1864.9	1864.9	1867.7

... *continued on next page* ...

Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1753	1869.9[a]	1856.3	1856.3	1858.9	1857.6	1857.6	1858.9
gdb 1754	1884.1[a]	1886.8	1886.8	1889.7	1882.6	1882.6	1886.0
gdb 1755	1891.7[a]	1896.9	1896.8	1898.3	1889.4	1889.3	1892.9
gdb 1756	1879.1[a]	1879.7	1879.7	1882.7	1875.9	1875.9	1879.7
gdb 1757	1887.7[a]	1888.0	1887.9	1891.0	1888.1	1888.1	1890.2
gdb 1758	1890.2[a]	1893.1	1893.1	1895.7	1892.8	1892.8	1894.4
gdb 1759	1901.0[a]	1909.8	1909.8	1912.2	1908.5	1908.4	1910.9
gdb 1760	1898.0[a]	1905.0	1905.0	1907.7	1903.7	1903.6	1906.6
gdb 1761	1895.7[a]	1905.0	1905.0	1907.7	1903.2	1903.2	1905.7
gdb 1762	1925.4[a]	1912.7	1912.7	1913.9	1911.4	1911.4	1913.6
gdb 1763	1905.9[a]	1914.3	1914.3	1917.0	1916.0	1916.0	1917.1
gdb 1764	1912.0[a]	1900.8	1900.8	1902.1	1898.2	1898.2	1900.4
gdb 1765	1898.3[a]	1894.6	1894.6	1895.2	1892.2	1892.2	1892.3
gdb 1766	1905.1[a]	1897.0	1897.0	1900.1	1898.5	1898.5	1900.3
gdb 1767	1903.4[a]	1898.4	1898.4	1901.5	1899.6	1899.6	1901.6
gdb 1768	1862.1[a]	1854.5	1854.5	1852.5	1846.1	1846.1	1842.9
gdb 1769	1866.5[a]	1856.9	1856.9	1857.4	1852.1	1852.1	1850.6
gdb 1770	1870.8[a]	1861.4	1861.4	1865.3	1862.2	1862.2	1863.3
gdb 1771	1837.4[a]	1819.6	1819.6	1816.6	1812.7	1812.7	1807.2
gdb 1772	1847.6[a]	1824.3	1824.3	1825.0	1822.1	1822.1	1818.4
gdb 1773	1848.7[a]	1828.5	1828.5	1833.2	1831.5	1831.5	1832.6
gdb 1774	1861.0[a]	1849.1	1849.1	1849.5	1848.6	1848.6	1848.2
gdb 1775	1869.6[a]	1852.6	1852.6	1856.2	1855.8	1855.1	1857.3
gdb 1776	1894.9[a]	1895.2	1895.2	1899.4	1893.9	1893.9	1896.2
gdb 1777	1889.5[a]	1887.6	1887.6	1889.3	1886.1	1886.1	1887.6
gdb 1778	1900.0[a]	1894.3	1894.3	1897.0	1895.9	1895.9	1897.1
gdb 1779	1895.7[a]	1893.2	1893.2	1893.1	1890.2	1890.2	1889.2
gdb 1780	1836.0[a]	1817.8	1817.8	1815.6	1810.7	1810.6	1806.2
gdb 1781	1846.5[a]	1821.9	1821.9	1822.8	1818.8	1818.8	1817.2
gdb 1782	1886.3[a]	1883.6	1883.6	1885.5	1881.7	1881.7	1884.0
gdb 1783	1884.9[a]	1883.2	1883.2	1885.2	1880.8	1880.8	1883.1
gdb 1784	1889.9[a]	1887.2	1887.1	1887.8	1884.1	1884.1	1884.3
gdb 1785	1895.5[a]	1890.3	1890.3	1893.3	1890.9	1890.9	1892.9
gdb 1786	1896.0[a]	1902.9	1902.9	1905.4	1900.3	1900.3	1903.2
gdb 1787	1912.4[a]	1908.8	1908.8	1910.9	1904.6	1904.5	1908.4
gdb 1788	1900.9[a]	1902.1	1902.1	1903.5	1899.4	1899.4	1900.3
gdb 1789	1906.6[a]	1910.4	1910.4	1913.0	1911.0	1911.0	1912.2
gdb 1790	1884.8[a]	1881.9	1881.9	1884.2	1880.3	1880.3	1883.0
gdb 1791	1889.0[a]	1886.5	1886.5	1887.6	1883.9	1883.9	1885.1
gdb 1792	1892.9[a]	1889.0	1889.0	1892.5	1890.4	1890.4	1893.2
gdb 1793	1866.8[a]	1857.0	1857.0	1855.3	1848.8	1848.7	1846.0
gdb 1794	1874.3[a]	1862.8	1862.8	1863.7	1858.1	1858.1	1857.0
gdb 1795	1875.0[a]	1867.4	1867.4	1866.3	1859.0	1859.0	1857.6
gdb 1796	1881.6[a]	1877.4	1877.4	1877.8	1872.0	1872.0	1870.8
gdb 1797	1856.8[a]	1853.3	1853.3	1855.2	1845.8	1845.8	1846.9
gdb 1798	1859.2[a]	1855.0	1855.0	1858.3	1850.8	1850.8	1852.4
gdb 1799	1868.0[a]	1854.5	1854.5	1857.2	1848.4	1848.4	1850.7
gdb 1800	1866.6[a]	1854.1	1854.1	1856.5	1847.7	1847.7	1849.7
gdb 1801	1873.2[a]	1859.5	1859.5	1864.1	1857.0	1857.0	1860.5
gdb 1802	1873.0[a]	1859.0	1859.0	1863.7	1856.2	1856.2	1860.0
gdb 1803	1867.2[a]	1852.3	1852.3	1856.1	1854.6	1854.5	1856.9
gdb 1804	1869.7[a]	1854.1	1854.1	1856.9	1855.7	1855.7	1856.9
gdb 1805	1856.3[a]	1847.8	1847.8	1848.5	1845.9	1845.9	1845.8
gdb 1806	1837.4[a]	1818.0	1818.0	1819.8	1813.0	1813.0	1813.2
gdb 1807	1833.3[a]	1815.8	1815.8	1817.2	1811.5	1811.5	1812.2
gdb 1808	1850.6[a]	1825.2	1825.2	1830.4	1824.5	1824.5	1827.5
gdb 1809	1845.1[a]	1821.9	1821.9	1826.8	1821.5	1821.5	1824.9
gdb 1810	1831.7[a]	1815.0	1814.9	1813.2	1808.4	1808.3	1804.7
gdb 1811	1843.1[a]	1820.5	1820.5	1822.0	1817.9	1817.8	1816.8
gdb 1812	1878.5[a]	1854.5	1854.4	1857.6	1853.4	1853.4	1858.0
gdb 1813	1853.7[a]	1842.6	1842.5	1843.1	1842.9	1842.9	1842.9
gdb 1814	1868.6[a]	1850.0	1849.9	1854.5	1853.5	1853.5	1856.3
gdb 1815	1915.0[a]	1914.4	1914.4	1915.8	1910.7	1910.7	1914.1
gdb 1816	1913.3[a]	1911.7	1911.7	1913.9	1908.0	1908.0	1912.0
gdb 1817	1904.7[a]	1906.2	1906.2	1907.6	1904.0	1904.0	1905.4

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1818	1907.3[a]	1913.0	1913.0	1915.5	1913.7	1913.7	1915.4
gdb 1819	1875.0[a]	1867.8	1867.7	1866.6	1859.4	1859.4	1857.8
gdb 1820	1881.0[a]	1877.8	1877.8	1878.2	1872.5	1872.5	1870.9
gdb 1821	1871.1[a]	1871.4	1871.4	1875.7	1869.3	1869.2	1872.2
gdb 1822	1867.2[a]	1857.4	1857.4	1855.9	1849.1	1849.1	1846.4
gdb 1823	1875.3[a]	1863.6	1863.6	1864.5	1859.0	1859.0	1857.5
gdb 1824	1866.5[a]	1858.2	1858.2	1862.4	1857.3	1857.2	1859.0
gdb 1825	1884.2[a]	1883.2	1883.2	1886.3	1881.3	1881.2	1884.4
gdb 1826	1889.2[a]	1886.6	1886.6	1888.0	1883.9	1883.9	1885.3
gdb 1827	1895.7[a]	1891.2	1891.2	1895.0	1892.1	1892.1	1894.8
gdb 1828	1912.4[a]	1909.1	1909.1	1911.0	1904.7	1904.7	1908.2
gdb 1829	1894.6[a]	1900.3	1900.3	1903.5	1897.6	1897.6	1900.9
gdb 1830	1901.2[a]	1902.2	1902.2	1903.5	1899.4	1899.4	1900.3
gdb 1831	1908.9[a]	1909.3	1909.3	1911.8	1910.0	1910.0	1910.7
gdb 1832	1877.8[a]	1883.3	1883.3	1887.9	1880.0	1880.0	1883.9
gdb 1833	1877.1[a]	1874.9	1874.8	1879.2	1874.1	1874.1	1875.7
gdb 1834	1872.5[a]	1873.2	1873.2	1874.3	1868.4	1868.3	1868.0
gdb 1835	1861.5[a]	1854.0	1854.0	1853.5	1846.7	1846.7	1845.2
gdb 1836	1861.0[a]	1851.3	1851.3	1851.1	1843.7	1843.7	1842.7
gdb 1837	1866.9[a]	1857.3	1857.3	1855.2	1848.4	1848.4	1844.5
gdb 1838	1868.7[a]	1858.3	1858.3	1858.9	1854.1	1854.1	1852.4
gdb 1839	1864.1[a]	1858.7	1858.7	1862.3	1856.5	1856.5	1858.1
gdb 1840	1885.2[a]	1882.7	1882.7	1885.0	1881.3	1881.3	1884.2
gdb 1841	1883.1[a]	1881.0	1881.0	1883.8	1879.4	1879.3	1882.6
gdb 1842	1889.0[a]	1886.2	1886.2	1887.2	1883.4	1883.3	1884.5
gdb 1843	1893.8[a]	1889.7	1889.7	1893.0	1891.0	1891.0	1893.4
gdb 1844	1880.4[a]	1854.5	1854.5	1857.7	1853.1	1853.1	1857.7
gdb 1845	1859.6[a]	1847.3	1847.3	1847.9	1847.0	1847.0	1846.6
gdb 1846	1868.4[a]	1850.4	1850.3	1854.1	1854.2	1854.1	1856.7
gdb 1847	1891.4[a]	1897.3	1897.3	1899.3	1895.4	1895.4	1897.5
gdb 1848	1893.6[a]	1896.3	1896.3	1899.4	1894.2	1894.2	1897.6
gdb 1849	1889.3[a]	1894.4	1894.4	1897.2	1892.5	1892.5	1895.2
gdb 1850	1897.6[a]	1898.6	1898.6	1899.8	1896.4	1896.4	1896.9
gdb 1851	1903.1[a]	1903.9	1903.9	1906.1	1905.5	1905.5	1906.2
gdb 1852	1894.2[a]	1898.8	1898.8	1901.3	1888.7	1888.7	1894.3
gdb 1853	1898.0[a]	1903.3	1903.3	1905.4	1893.0	1893.0	1897.7
gdb 1854	1891.9[a]	1895.8	1895.8	1898.7	1888.5	1888.5	1892.5
gdb 1855	1899.1[a]	1905.0	1905.0	1906.6	1895.2	1895.2	1899.5
gdb 1856	1896.7[a]	1899.2	1899.2	1902.9	1895.1	1895.1	1899.0
gdb 1857	1898.3[a]	1901.3	1901.3	1905.2	1897.3	1897.3	1901.0
gdb 1858	1896.9[a]	1898.9	1898.9	1900.4	1898.8	1898.8	1900.5
gdb 1859	1915.5[a]	1909.4	1909.4	1910.0	1907.1	1907.0	1909.2
gdb 1860	1906.0[a]	1905.0	1905.0	1906.1	1908.6	1908.6	1908.4
gdb 1861	1905.7[a]	1906.4	1906.4	1907.7	1909.8	1909.8	1909.9
gdb 1862	1906.1[a]	1904.4	1904.3	1902.1	1900.9	1900.9	1897.6
gdb 1863	1877.8[a]	1872.9	1872.9	1871.3	1869.7	1869.7	1867.8
gdb 1864	1869.8[a]	1860.1	1860.1	1861.4	1861.3	1861.2	1862.8
gdb 1865	1877.0[a]	1872.6	1872.6	1874.6	1876.1	1876.1	1877.6
gdb 1866	1876.8[a]	1871.8	1871.7	1874.0	1875.3	1875.2	1876.9
gdb 1867	1850.3[a]	1834.2	1834.2	1836.5	1836.7	1836.7	1836.7
gdb 1868	1856.9[a]	1845.1	1845.1	1844.2	1842.8	1842.7	1839.6
gdb 1869	1856.5[a]	1844.3	1844.3	1843.6	1842.0	1842.0	1839.4
gdb 1870	1856.1[a]	1843.8	1843.8	1839.7	1835.0	1835.0	1829.0
gdb 1871	1856.4[a]	1849.0	1849.0	1852.0	1853.2	1853.1	1853.0
gdb 1872	1866.6[a]	1865.7	1865.7	1868.1	1866.2	1866.2	1867.4
gdb 1873	1875.0[a]	1871.3	1871.2	1870.2	1868.2	1868.2	1865.6
gdb 1874	1876.2[a]	1872.2	1872.2	1871.2	1869.1	1869.1	1866.7
gdb 1875	1880.9[a]	1870.1	1870.1	1865.8	1860.5	1860.5	1855.2
gdb 1876	1874.0[a]	1874.8	1874.8	1877.1	1878.3	1878.3	1878.1
gdb 1877	1859.8[a]	1851.1	1851.1	1852.6	1849.7	1849.7	1850.0
gdb 1878	1858.7[a]	1846.9	1846.9	1845.6	1838.8	1838.8	1836.5
gdb 1879	1864.7[a]	1852.9	1852.9	1857.1	1856.8	1856.7	1858.5
gdb 1880	1850.0[a]	1839.9	1839.9	1843.0	1839.7	1839.7	1841.6
gdb 1881	1859.5[a]	1843.1	1843.1	1846.4	1842.9	1842.9	1845.2
gdb 1882	1850.2[a]	1838.7	1838.7	1838.3	1831.6	1831.6	1830.5

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1883	1851.3[a]	1848.0	1848.0	1852.0	1850.9	1850.8	1852.0
gdb 1884	1878.8[a]	1876.9	1876.9	1879.5	1876.2	1876.2	1878.9
gdb 1885	1887.4[a]	1884.2	1884.2	1886.9	1887.4	1887.4	1888.1
gdb 1886	1907.6[a]	1907.9	1907.9	1905.9	1905.2	1905.2	1903.0
gdb 1887	1914.6[a]	1909.6	1909.6	1910.0	1908.5	1908.5	1910.8
gdb 1888	1904.1[a]	1908.0	1908.0	1909.3	1911.7	1911.6	1912.3
gdb 1889	1890.6[a]	1886.8	1886.8	1889.3	1890.2	1890.2	1890.8
gdb 1890	1846.1[a]	1829.7	1829.7	1828.2	1824.7	1824.7	1822.8
gdb 1891	1844.9[a]	1828.7	1828.6	1827.3	1823.8	1823.7	1821.8
gdb 1892	1852.3[a]	1841.7	1841.7	1837.7	1832.5	1832.4	1826.8
gdb 1893	1852.6[a]	1842.3	1842.3	1841.6	1840.0	1840.0	1837.4
gdb 1894	1847.5[a]	1833.7	1833.7	1836.2	1834.7	1834.6	1835.1
gdb 1895	1885.7[a]	1872.7	1872.7	1874.3	1872.1	1872.1	1875.6
gdb 1896	1867.4[a]	1857.1	1857.1	1858.3	1859.1	1859.0	1861.1
gdb 1897	1866.9[a]	1857.4	1857.4	1858.6	1859.3	1859.3	1861.2
gdb 1898	1875.2[a]	1870.3	1870.3	1868.9	1867.9	1867.9	1866.0
gdb 1899	1874.3[a]	1870.6	1870.3	1872.4	1875.1	1875.0	1876.4
gdb 1900	1892.4[a]	1893.7	1893.7	1895.0	1893.1	1893.1	1895.1
gdb 1901	1892.7[a]	1894.2	1894.2	1895.5	1892.7	1892.7	1894.9
gdb 1902	1890.8[a]	1894.0	1894.0	1895.3	1893.3	1893.3	1894.9
gdb 1903	1899.5[a]	1896.8	1896.8	1894.7	1893.3	1893.3	1890.5
gdb 1904	1901.3[a]	1901.0	1901.0	1902.8	1903.2	1903.1	1903.7
gdb 1905	1885.4[a]	1881.0	1881.0	1883.3	1883.4	1883.4	1883.9
gdb 1906	1888.4[a]	1886.0	1886.0	1887.6	1887.2	1887.2	1886.9
gdb 1907	1880.2[a]	1876.9	1876.9	1875.5	1873.0	1873.0	1870.3
gdb 1908	1895.9[a]	1899.8	1899.8	1901.1	1899.2	1899.2	1901.0
gdb 1909	1896.0[a]	1899.8	1899.8	1901.1	1898.0	1897.9	1899.6
gdb 1910	1911.1[a]	1906.1	1906.0	1906.3	1903.5	1903.4	1905.6
gdb 1911	1902.2[a]	1903.1	1903.1	1900.8	1899.2	1899.2	1896.0
gdb 1912	1903.9[a]	1906.1	1906.1	1907.1	1909.2	1909.2	1909.0
gdb 1913	1883.8[a]	1880.1	1880.1	1882.0	1882.8	1882.7	1882.7
gdb 1914	1887.0[a]	1884.8	1884.8	1886.0	1886.0	1886.0	1885.4
gdb 1915	1880.4[a]	1877.2	1877.2	1875.5	1873.2	1873.2	1870.1
gdb 1916	1887.8[a]	1887.3	1887.3	1889.9	1887.6	1887.6	1888.4
gdb 1917	1887.4[a]	1885.3	1885.3	1884.5	1878.9	1878.9	1876.8
gdb 1918	1876.3[a]	1873.3	1873.3	1875.5	1876.0	1876.0	1877.3
gdb 1919	1874.9[a]	1872.1	1872.1	1870.6	1868.0	1868.0	1866.1
gdb 1920	1872.6[a]	1864.1	1864.1	1865.7	1864.1	1864.1	1865.4
gdb 1921	1879.3[a]	1877.6	1877.6	1879.0	1878.5	1878.5	1878.6
gdb 1922	1850.1[a]	1840.7	1840.6	1836.6	1831.7	1831.6	1826.0
gdb 1923	1846.5[a]	1831.0	1831.0	1830.2	1826.0	1826.0	1824.1
gdb 1924	1851.3[a]	1842.2	1842.2	1842.0	1840.1	1840.1	1837.7
gdb 1925	1887.8[a]	1891.0	1891.0	1892.5	1891.0	1891.0	1893.3
gdb 1926	1889.5[a]	1895.2	1895.2	1896.9	1893.8	1893.8	1895.8
gdb 1927	1896.8[a]	1895.8	1895.8	1893.8	1892.6	1892.5	1890.4
gdb 1928	1894.5[a]	1896.8	1896.8	1898.5	1900.5	1900.5	1901.2
gdb 1929	1871.8[a]	1868.3	1868.3	1867.0	1865.9	1865.8	1864.2
gdb 1930	1887.0[a]	1877.1	1877.0	1878.1	1875.1	1875.0	1878.3
gdb 1931	1869.0[a]	1859.8	1859.8	1861.7	1861.6	1861.6	1863.7
gdb 1932	1872.2[a]	1869.0	1869.0	1871.3	1873.8	1873.8	1875.2
gdb 1933	1866.2[a]	1865.4	1865.4	1867.8	1866.0	1866.0	1867.3
gdb 1934	1877.2[a]	1873.5	1873.5	1872.5	1870.5	1870.5	1867.6
gdb 1935	1881.0[a]	1870.2	1870.2	1865.8	1860.9	1860.8	1855.4
gdb 1936	1881.4[a]	1873.4	1873.4	1872.5	1870.8	1870.8	1868.3
gdb 1937	1873.9[a]	1874.2	1874.2	1876.6	1877.8	1877.8	1877.8
gdb 1938	1843.1[a]	1833.6	1833.6	1832.5	1831.4	1831.4	1828.0
gdb 1939	1842.8[a]	1834.1	1834.1	1836.4	1839.0	1838.9	1838.4
gdb 1940	1841.9[a]	1833.3	1833.3	1835.8	1837.8	1837.8	1837.7
gdb 1941	1842.8[a]	1833.3	1833.3	1832.3	1831.1	1831.1	1827.8
gdb 1942	1841.1[a]	1833.8	1833.8	1836.2	1838.4	1838.4	1838.1
gdb 1943	1846.0[a]	1835.8	1835.8	1834.9	1833.8	1833.7	1830.2
gdb 1944	1840.2[a]	1828.6	1828.6	1823.8	1820.0	1820.0	1813.7
gdb 1945	1863.0[a]	1855.2	1855.2	1856.6	1853.7	1853.6	1853.5
gdb 1946	1859.8[a]	1849.3	1849.2	1847.5	1840.9	1840.9	1838.1
gdb 1947	1868.4[a]	1856.9	1856.9	1857.6	1852.7	1852.7	1851.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 1948	1868.3[a]	1857.5	1857.5	1861.4	1860.0	1860.0	1861.4
gdb 1949	1851.9[a]	1845.4	1845.4	1848.4	1842.9	1842.9	1844.2
gdb 1950	1850.8[a]	1843.0	1843.0	1846.1	1841.9	1841.9	1843.5
gdb 1951	1848.0[a]	1839.5	1839.4	1838.9	1831.7	1831.6	1830.4
gdb 1952	1850.8[a]	1840.8	1840.8	1840.4	1833.2	1833.2	1831.9
gdb 1953	1855.3[a]	1853.0	1853.0	1853.5	1847.6	1847.6	1845.5
gdb 1954	1853.1[a]	1844.1	1844.1	1847.4	1843.6	1843.6	1845.3
gdb 1955	1855.6[a]	1855.4	1855.4	1859.4	1857.0	1857.0	1857.7
gdb 1956	1867.0[a]	1864.2	1864.2	1862.9	1858.0	1858.0	1856.4
gdb 1957	1876.6[a]	1868.6	1868.6	1863.9	1859.5	1859.5	1853.3
gdb 1958	1869.6[a]	1863.9	1863.9	1862.8	1858.2	1858.2	1856.3
gdb 1959	1870.1[a]	1867.6	1867.6	1870.1	1868.4	1868.4	1869.4
gdb 1960	1875.6[a]	1871.4	1871.4	1870.3	1869.1	1869.1	1865.9
gdb 1961	1848.7[a]	1833.0	1833.0	1835.8	1830.1	1830.1	1832.6
gdb 1962	1853.3[a]	1842.6	1842.6	1842.3	1835.6	1835.6	1834.6
gdb 1963	1849.7[a]	1840.5	1840.5	1840.0	1833.7	1833.7	1832.9
gdb 1964	1855.8[a]	1846.6	1846.6	1850.2	1846.4	1846.3	1848.3
gdb 1965	1851.1[a]	1843.1	1843.1	1846.3	1843.1	1843.0	1845.3
gdb 1966	1873.6[a]	1865.4	1865.4	1864.5	1857.3	1857.3	1856.2
gdb 1967	1876.6[a]	1872.3	1872.3	1875.1	1870.7	1870.7	1872.3
gdb 1968	1880.7[a]	1870.1	1870.1	1865.8	1860.8	1860.8	1855.5
gdb 1969	1878.2[a]	1874.1	1874.1	1873.2	1871.4	1871.4	1868.8
gdb 1970	1874.4[a]	1874.1	1874.1	1876.3	1877.7	1877.7	1877.8
gdb 1971	1868.4[a]	1863.0	1863.0	1861.7	1857.1	1857.1	1856.1
gdb 1972	1879.6[a]	1870.0	1870.0	1865.6	1861.0	1861.0	1855.5
gdb 1973	1869.0[a]	1861.4	1861.4	1861.1	1854.9	1854.9	1854.3
gdb 1974	1869.7[a]	1865.5	1865.5	1868.6	1865.4	1865.4	1867.3
gdb 1975	1880.5[a]	1872.4	1872.3	1871.2	1870.0	1870.0	1867.2
gdb 1976	1863.1[a]	1855.2	1855.2	1856.7	1853.6	1853.6	1853.4
gdb 1977	1859.9[a]	1849.3	1849.3	1847.7	1840.9	1840.9	1838.2
gdb 1978	1868.9[a]	1855.8	1855.8	1856.8	1851.5	1851.5	1850.3
gdb 1979	1869.1[a]	1856.9	1856.9	1861.0	1859.5	1859.5	1860.7
gdb 1980	1869.8[a]	1866.6	1866.6	1870.0	1862.4	1862.4	1866.0
gdb 1981	1874.4[a]	1867.7	1867.7	1867.0	1860.6	1860.6	1859.6
gdb 1982	1877.6[a]	1870.3	1870.3	1869.7	1863.4	1863.4	1862.7
gdb 1983	1874.9[a]	1872.3	1872.3	1875.4	1871.9	1871.9	1874.1
gdb 1984	1874.7[a]	1871.9	1871.9	1874.9	1871.3	1871.3	1873.4
gdb 1985	1861.4[a]	1848.9	1848.8	1852.2	1846.6	1846.6	1848.5
gdb 1986	1850.8[a]	1842.6	1842.6	1845.8	1841.8	1841.8	1843.5
gdb 1987	1854.8[a]	1853.4	1853.4	1853.8	1847.9	1847.9	1845.6
gdb 1988	1850.8[a]	1841.5	1841.4	1841.1	1833.6	1833.6	1832.3
gdb 1989	1847.9[a]	1839.0	1839.0	1838.6	1831.2	1831.2	1830.1
gdb 1990	1853.3[a]	1844.1	1844.1	1847.2	1842.8	1842.8	1844.3
gdb 1991	1856.6[a]	1856.2	1856.2	1859.9	1857.6	1857.6	1857.8
gdb 1992	1887.3[a]	1888.7	1888.7	1890.2	1879.2	1879.1	1881.6
gdb 1993	1886.6[a]	1888.3	1888.3	1889.7	1878.6	1878.6	1881.0
gdb 1994	1885.0[a]	1879.6	1879.6	1879.4	1871.3	1871.3	1870.8
gdb 1995	1886.6[a]	1881.2	1881.2	1880.2	1872.2	1872.2	1870.3
gdb 1996	1879.8[a]	1877.6	1877.6	1877.3	1869.3	1869.3	1868.7
gdb 1997	1881.5[a]	1880.7	1880.7	1883.8	1879.3	1879.3	1881.5
gdb 1998	1889.9[a]	1887.4	1887.4	1890.0	1885.4	1885.4	1886.1
gdb 1999	1882.0[a]	1880.8	1880.8	1883.8	1879.2	1879.2	1881.1
gdb 2000	1873.4[a]	1872.2	1872.1	1875.3	1864.0	1864.0	1868.0
gdb 2001	1872.6[a]	1868.0	1868.0	1868.3	1860.9	1860.8	1860.0
gdb 2002	1866.3[a]	1863.1	1863.1	1862.7	1856.4	1856.4	1855.5
gdb 2003	1869.1[a]	1865.9	1865.9	1865.9	1858.8	1858.8	1857.8
gdb 2004	1875.9[a]	1870.6	1870.6	1874.6	1870.3	1870.3	1872.4
gdb 2005	1873.0[a]	1867.2	1867.2	1870.8	1867.3	1867.3	1869.8
gdb 2006	1875.3[a]	1870.4	1870.4	1874.4	1870.2	1870.1	1872.4
gdb 2007	1887.1[a]	1887.4	1887.4	1890.1	1887.3	1887.3	1888.0
gdb 2008	1889.4[a]	1887.1	1887.1	1886.0	1880.3	1880.2	1877.6
gdb 2009	1872.9[a]	1867.5	1867.5	1866.6	1860.4	1860.4	1860.2
gdb 2010	1876.1[a]	1872.7	1872.7	1875.2	1872.2	1872.2	1874.1
gdb 2011	1893.6[a]	1897.2	1897.2	1898.3	1897.4	1897.4	1899.2
gdb 2012	1909.8[a]	1906.4	1906.4	1906.8	1903.7	1903.7	1906.2

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2013	1907.3[a]	1902.6	1902.6	1903.2	1900.9	1900.9	1903.4
gdb 2014	1902.6[a]	1903.4	1903.4	1901.1	1900.8	1900.8	1898.1
gdb 2015	1899.9[a]	1904.7	1904.6	1905.8	1908.3	1908.3	1908.3
gdb 2016	1896.9[a]	1895.1	1895.1	1893.2	1892.8	1892.7	1890.9
gdb 2017	1888.2[a]	1893.7	1893.7	1895.3	1893.4	1893.3	1895.1
gdb 2018	1885.9[a]	1892.0	1892.0	1893.8	1891.5	1891.4	1893.4
gdb 2019	1895.4[a]	1896.9	1896.9	1898.5	1900.6	1900.6	1901.4
gdb 2020	1876.5[a]	1870.7	1870.7	1866.0	1861.8	1861.8	1856.2
gdb 2021	1876.5[a]	1873.6	1873.6	1872.6	1871.1	1871.1	1868.3
gdb 2022	1867.7[a]	1866.7	1866.7	1869.5	1868.2	1868.2	1869.4
gdb 2023	1858.5[a]	1857.0	1857.0	1858.7	1855.3	1855.3	1858.5
gdb 2024	1877.3[a]	1869.1	1869.1	1864.5	1861.0	1861.0	1855.6
gdb 2025	1877.3[a]	1871.6	1871.6	1870.5	1870.1	1870.1	1867.4
gdb 2026	1862.4[a]	1865.6	1865.6	1867.5	1867.3	1867.3	1868.9
gdb 2027	1863.8[a]	1863.9	1863.9	1866.6	1864.0	1864.0	1865.3
gdb 2028	1882.1[a]	1872.9	1872.9	1872.0	1870.4	1870.4	1867.4
gdb 2029	1881.7[a]	1870.2	1870.2	1866.0	1860.8	1860.8	1855.3
gdb 2030	1874.4[a]	1874.5	1874.4	1876.8	1878.3	1878.3	1877.7
gdb 2031	1874.3[a]	1865.7	1865.7	1864.9	1857.6	1857.6	1856.4
gdb 2032	1876.7[a]	1870.9	1870.9	1873.6	1869.2	1869.2	1870.4
gdb 2033	1866.1[a]	1866.1	1866.1	1870.6	1865.3	1865.2	1868.5
gdb 2034	1868.0[a]	1864.8	1864.8	1868.5	1860.3	1860.3	1864.0
gdb 2035	1876.9[a]	1869.3	1869.3	1868.8	1862.0	1862.0	1861.0
gdb 2036	1877.4[a]	1869.9	1869.9	1869.4	1862.9	1862.9	1862.1
gdb 2037	1876.4[a]	1871.3	1871.3	1874.3	1871.0	1871.0	1872.7
gdb 2038	1875.3[a]	1871.3	1871.3	1874.3	1871.0	1871.0	1873.0
gdb 2039	1871.2[a]	1874.1	1874.1	1878.5	1873.4	1873.4	1876.0
gdb 2040	1876.8[a]	1874.3	1874.2	1876.7	1876.9	1876.9	1878.1
gdb 2041	1881.5[a]	1878.8	1878.8	1880.3	1879.5	1879.5	1879.9
gdb 2042	1869.5[a]	1862.5	1862.5	1864.1	1862.1	1862.1	1863.6
gdb 2043	1875.4[a]	1872.3	1872.3	1870.9	1867.8	1867.8	1866.2
gdb 2044	1846.1[a]	1831.6	1831.6	1834.3	1828.3	1828.3	1830.9
gdb 2045	1854.9[a]	1845.1	1845.1	1845.2	1837.9	1837.9	1836.7
gdb 2046	1850.1[a]	1840.7	1840.7	1840.3	1833.7	1833.7	1833.1
gdb 2047	1858.4[a]	1848.3	1848.3	1851.9	1847.8	1847.8	1849.3
gdb 2048	1851.6[a]	1843.4	1843.4	1846.6	1843.2	1843.2	1845.3
gdb 2049	1852.9[a]	1843.0	1843.0	1846.8	1842.9	1842.9	1844.2
gdb 2050	1843.2[a]	1829.1	1829.1	1827.9	1823.8	1823.8	1821.8
gdb 2051	1850.1[a]	1840.6	1840.6	1836.7	1831.6	1831.6	1826.2
gdb 2052	1850.9[a]	1842.2	1842.2	1842.1	1839.9	1839.9	1837.6
gdb 2053	1847.0[a]	1835.4	1835.4	1838.3	1835.8	1835.8	1836.3
gdb 2054	1888.9[a]	1878.5	1878.5	1879.8	1876.5	1876.4	1879.8
gdb 2055	1865.7[a]	1858.1	1858.1	1859.5	1859.5	1859.5	1861.5
gdb 2056	1871.8[a]	1868.6	1868.6	1867.6	1865.8	1865.8	1864.5
gdb 2057	1873.3[a]	1869.9	1869.9	1872.6	1874.5	1874.5	1876.1
gdb 2058	1904.3[a]	1904.0	1904.0	1901.9	1901.3	1901.2	1898.5
gdb 2059	1908.9[a]	1904.7	1904.7	1904.6	1903.3	1903.3	1905.4
gdb 2060	1909.9[a]	1906.1	1906.1	1906.6	1903.7	1903.7	1906.2
gdb 2061	1890.1[a]	1893.1	1893.1	1895.0	1892.6	1892.6	1894.9
gdb 2062	1901.5[a]	1905.1	1905.1	1906.0	1908.7	1908.6	1908.5
gdb 2063	1866.8[a]	1861.7	1861.7	1860.5	1855.4	1855.4	1854.6
gdb 2064	1879.7[a]	1870.1	1870.1	1865.7	1861.0	1861.0	1855.4
gdb 2065	1869.2[a]	1861.3	1861.3	1861.0	1855.1	1855.1	1854.5
gdb 2066	1880.0[a]	1871.8	1871.8	1870.5	1869.5	1869.5	1866.4
gdb 2067	1870.2[a]	1867.8	1867.8	1870.1	1868.2	1868.2	1870.0
gdb 2068	1868.4[a]	1867.7	1867.7	1869.8	1867.7	1867.7	1869.0
gdb 2069	1864.9[a]	1862.4	1862.4	1861.4	1855.7	1855.7	1854.3
gdb 2070	1877.0[a]	1868.7	1868.7	1864.1	1859.4	1859.4	1853.2
gdb 2071	1869.7[a]	1864.0	1864.0	1863.1	1858.2	1858.2	1856.4
gdb 2072	1875.9[a]	1871.0	1871.0	1869.9	1868.5	1868.5	1865.1
gdb 2073	1870.5[a]	1868.2	1868.2	1870.8	1869.0	1869.0	1869.8
gdb 2074	1866.1[a]	1867.1	1867.1	1869.8	1867.0	1867.0	1868.1
gdb 2075	1888.8[a]	1894.9	1894.9	1896.6	1893.1	1893.1	1895.3
gdb 2076	1885.2[a]	1889.2	1889.2	1891.0	1888.5	1888.5	1891.2
gdb 2077	1897.1[a]	1895.9	1895.9	1894.1	1892.6	1892.6	1890.7

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2078	1894.8[a]	1897.1	1897.1	1898.6	1900.2	1900.2	1901.0
gdb 2079	1875.8[a]	1871.8	1871.8	1874.5	1872.7	1872.7	1875.3
gdb 2080	1910.6[a]	1906.1	1906.1	1906.2	1903.0	1903.0	1904.8
gdb 2081	1895.8[a]	1899.2	1899.2	1900.5	1897.3	1897.3	1898.9
gdb 2082	1892.6[a]	1895.1	1895.1	1896.9	1894.2	1894.2	1896.2
gdb 2083	1902.9[a]	1902.8	1902.8	1900.3	1898.7	1898.7	1895.3
gdb 2084	1904.4[a]	1905.0	1905.0	1906.3	1908.2	1908.2	1907.6
gdb 2085	1873.4[a]	1868.8	1868.8	1868.1	1861.9	1861.9	1861.5
gdb 2086	1874.0[a]	1871.3	1871.3	1874.6	1870.2	1870.2	1873.4
gdb 2087	1874.9[a]	1870.8	1870.8	1873.7	1870.9	1870.9	1873.8
gdb 2088	1869.0[a]	1858.3	1858.3	1861.8	1855.0	1855.0	1856.8
gdb 2089	1871.4[a]	1862.6	1862.6	1866.7	1859.6	1859.6	1861.7
gdb 2090	1870.0[a]	1859.4	1859.4	1862.9	1856.5	1856.4	1858.3
gdb 2091	1869.8[a]	1858.5	1858.5	1860.3	1852.3	1852.3	1852.8
gdb 2092	1876.5[a]	1864.9	1864.9	1870.2	1865.1	1865.1	1867.7
gdb 2093	1853.6[a]	1826.0	1826.0	1831.3	1828.9	1828.9	1830.6
gdb 2094	1845.0[a]	1820.6	1820.6	1823.4	1820.3	1820.3	1820.1
gdb 2095	1850.4[a]	1824.3	1824.3	1829.6	1827.3	1827.3	1829.2
gdb 2096	1847.5[a]	1822.4	1822.4	1825.3	1822.3	1822.3	1822.0
gdb 2097	1836.5[a]	1817.6	1817.5	1818.5	1813.0	1813.0	1810.9
gdb 2098	1871.0[a]	1850.2	1850.2	1855.0	1849.4	1849.4	1852.3
gdb 2099	1860.3[a]	1844.9	1844.9	1847.2	1840.6	1840.6	1841.2
gdb 2100	1876.9[a]	1854.1	1854.1	1859.2	1856.5	1856.5	1858.6
gdb 2101	1859.0[a]	1841.0	1841.0	1844.8	1845.3	1845.3	1846.4
gdb 2102	1862.5[a]	1846.0	1846.0	1849.8	1848.6	1848.6	1849.9
gdb 2103	1855.5[a]	1835.9	1835.9	1838.4	1837.3	1837.3	1838.2
gdb 2104	1862.2[a]	1846.1	1846.1	1849.6	1849.3	1849.3	1850.2
gdb 2105	1853.0[a]	1834.7	1834.7	1836.9	1835.8	1835.8	1836.6
gdb 2106	1851.3[a]	1835.5	1835.5	1837.5	1835.5	1835.5	1835.9
gdb 2107	1858.9[a]	1844.2	1844.2	1847.9	1847.3	1847.2	1848.2
gdb 2108	1856.6[a]	1841.8	1841.8	1845.4	1846.1	1846.1	1847.0
gdb 2109	1854.3[a]	1838.2	1838.2	1839.9	1838.8	1838.8	1838.7
gdb 2110	1892.7[a]	1884.9	1884.9	1886.1	1878.5	1878.5	1880.8
gdb 2111	1893.7[a]	1884.2	1884.2	1886.8	1883.7	1883.7	1885.4
gdb 2112	1895.4[a]	1886.6	1886.6	1887.5	1880.5	1880.5	1882.6
gdb 2113	1898.4[a]	1891.4	1891.4	1894.8	1890.0	1890.0	1894.4
gdb 2114	1876.0[a]	1871.9	1871.9	1874.8	1871.2	1871.2	1873.1
gdb 2115	1872.5[a]	1865.4	1865.4	1868.9	1865.0	1865.0	1867.4
gdb 2116	1872.4[a]	1866.4	1866.4	1869.9	1864.8	1864.8	1867.1
gdb 2117	1867.3[a]	1854.9	1854.9	1857.6	1851.7	1851.7	1854.3
gdb 2118	1881.5[a]	1875.8	1875.8	1879.1	1878.4	1878.4	1879.1
gdb 2119	1841.1[a]	1823.8	1823.8	1827.8	1818.2	1818.1	1822.6
gdb 2120	1842.8[a]	1827.9	1827.9	1829.4	1822.7	1822.7	1822.9
gdb 2121	1832.7[a]	1818.5	1818.5	1820.0	1815.2	1815.2	1815.8
gdb 2122	1850.3[a]	1830.2	1830.2	1835.1	1829.8	1829.8	1833.1
gdb 2123	1849.0[a]	1829.6	1829.6	1833.9	1829.8	1829.8	1833.0
gdb 2124	1847.5[a]	1827.6	1827.6	1832.9	1827.7	1827.7	1831.2
gdb 2125	1841.5[a]	1828.8	1828.8	1831.6	1824.1	1824.1	1826.9
gdb 2126	1843.3[a]	1829.8	1829.8	1832.1	1825.0	1825.0	1827.5
gdb 2127	1837.3[a]	1824.8	1824.8	1828.6	1820.3	1820.3	1823.5
gdb 2128	1850.4[a]	1836.5	1836.5	1837.9	1829.6	1829.6	1830.6
gdb 2129	1853.6[a]	1837.6	1837.6	1842.2	1836.2	1836.2	1839.3
gdb 2130	1850.0[a]	1840.0	1840.0	1845.0	1838.3	1838.3	1841.4
gdb 2131	1853.3[a]	1837.1	1837.1	1841.2	1835.3	1835.2	1838.1
gdb 2132	1842.7[a]	1826.4	1826.4	1830.5	1822.6	1822.6	1825.9
gdb 2133	1840.7[a]	1827.1	1827.1	1828.9	1822.5	1822.5	1823.3
gdb 2134	1852.4[a]	1836.5	1836.5	1841.0	1835.0	1835.0	1838.1
gdb 2135	1852.7[a]	1837.5	1837.5	1841.3	1835.9	1835.9	1838.7
gdb 2136	1894.8[a]	1896.8	1896.8	1898.3	1889.7	1889.7	1893.3
gdb 2137	1885.4[a]	1883.5	1883.5	1886.6	1878.9	1878.9	1882.4
gdb 2138	1892.1[a]	1891.6	1891.6	1893.2	1885.5	1885.5	1888.1
gdb 2139	1893.0[a]	1892.0	1892.0	1895.4	1889.7	1889.7	1892.4
gdb 2140	1868.8[a]	1866.2	1866.2	1869.7	1859.6	1859.6	1863.1
gdb 2141	1876.1[a]	1867.7	1867.7	1871.0	1861.3	1861.3	1863.9
gdb 2142	1869.3[a]	1865.9	1865.9	1870.1	1859.4	1859.3	1863.1

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2143	1878.9[a]	1874.4	1874.3	1878.2	1871.0	1871.0	1873.4
gdb 2144	1873.6[a]	1874.9	1874.9	1880.1	1871.1	1871.1	1874.8
gdb 2145	1870.7[a]	1862.7	1862.7	1866.5	1859.7	1859.7	1861.7
gdb 2146	1873.9[a]	1862.5	1862.5	1865.8	1859.8	1859.8	1861.0
gdb 2147	1870.1[a]	1858.6	1858.6	1860.5	1852.3	1852.3	1853.0
gdb 2148	1873.1[a]	1861.3	1861.3	1864.9	1858.5	1858.5	1860.3
gdb 2149	1877.9[a]	1866.0	1866.0	1871.2	1866.5	1866.5	1868.7
gdb 2150	1871.9[a]	1869.2	1869.2	1871.5	1861.7	1861.7	1866.7
gdb 2151	1865.2[a]	1852.8	1852.8	1855.7	1849.8	1849.8	1853.4
gdb 2152	1863.7[a]	1852.7	1852.7	1855.5	1849.1	1849.1	1852.5
gdb 2153	1872.4[a]	1870.0	1870.0	1873.2	1867.9	1867.8	1870.2
gdb 2154	1871.2[a]	1866.3	1866.3	1870.2	1864.9	1864.9	1867.8
gdb 2155	1859.4[a]	1845.5	1845.5	1849.3	1847.9	1847.9	1849.0
gdb 2156	1859.5[a]	1840.7	1840.7	1843.5	1840.2	1840.2	1841.1
gdb 2157	1869.3[a]	1857.8	1857.8	1859.9	1851.7	1851.7	1852.6
gdb 2158	1873.5[a]	1861.5	1861.5	1865.1	1859.0	1859.0	1860.7
gdb 2159	1878.1[a]	1866.2	1866.2	1871.4	1866.4	1866.4	1869.0
gdb 2160	1868.5[a]	1850.0	1850.0	1854.9	1848.6	1848.6	1851.5
gdb 2161	1869.8[a]	1849.5	1849.5	1854.7	1848.2	1848.2	1851.4
gdb 2162	1857.8[a]	1843.3	1843.3	1845.8	1838.5	1838.5	1839.4
gdb 2163	1867.5[a]	1851.5	1851.5	1853.7	1850.5	1850.4	1849.7
gdb 2164	1859.8[a]	1845.9	1845.9	1847.8	1841.3	1841.3	1841.8
gdb 2165	1871.7[a]	1852.1	1852.1	1856.7	1850.6	1850.6	1853.5
gdb 2166	1877.9[a]	1857.3	1857.3	1862.4	1859.3	1859.3	1861.1
gdb 2167	1889.9[a]	1886.1	1886.1	1888.8	1877.4	1877.4	1881.5
gdb 2168	1884.6[a]	1878.9	1878.9	1882.7	1872.7	1872.7	1876.1
gdb 2169	1885.2[a]	1879.1	1879.1	1882.0	1872.5	1872.5	1874.8
gdb 2170	1883.9[a]	1879.2	1879.2	1881.9	1873.1	1873.1	1875.4
gdb 2171	1890.0[a]	1884.5	1884.5	1889.0	1881.5	1881.5	1885.0
gdb 2172	1890.2[a]	1883.0	1883.0	1887.9	1879.6	1879.6	1883.4
gdb 2173	1863.6[a]	1847.1	1847.1	1852.2	1840.2	1840.2	1846.6
gdb 2174	1856.7[a]	1842.5	1842.5	1844.9	1838.0	1838.0	1838.9
gdb 2175	1854.2[a]	1840.4	1840.4	1842.5	1837.0	1837.0	1838.5
gdb 2176	1867.7[a]	1847.4	1847.4	1853.0	1846.7	1846.7	1850.6
gdb 2177	1866.0[a]	1846.1	1846.1	1851.3	1846.4	1846.4	1850.3
gdb 2178	1866.3[a]	1861.9	1861.9	1866.4	1858.7	1858.7	1861.5
gdb 2179	1871.4[a]	1871.3	1871.3	1876.5	1870.3	1870.2	1872.7
gdb 2180	1865.3[a]	1861.0	1861.0	1865.3	1857.8	1857.8	1860.5
gdb 2181	1864.4[a]	1862.7	1862.7	1866.7	1858.8	1858.8	1860.5
gdb 2182	1861.5[a]	1859.6	1859.6	1864.0	1855.5	1855.5	1857.8
gdb 2183	1869.3[a]	1870.5	1870.5	1875.6	1869.5	1869.5	1871.2
gdb 2184	1898.2[a]	1901.1	1901.1	1903.8	1891.9	1891.9	1895.9
gdb 2185	1900.2[a]	1903.8	1903.8	1906.2	1894.2	1894.2	1897.4
gdb 2186	1898.0[a]	1894.5	1894.5	1897.3	1887.6	1887.6	1890.3
gdb 2187	1898.9[a]	1894.7	1894.7	1898.2	1891.0	1891.0	1893.8
gdb 2188	1875.2[a]	1876.7	1876.7	1880.6	1870.8	1870.8	1874.9
gdb 2189	1875.3[a]	1876.7	1876.7	1881.1	1870.7	1870.7	1874.8
gdb 2190	1875.5[a]	1885.6	1885.6	1890.5	1881.8	1881.8	1885.1
gdb 2191	1879.9[a]	1881.8	1881.8	1885.9	1879.2	1879.2	1881.7
gdb 2192	1898.0[a]	1894.9	1894.9	1897.9	1888.1	1888.1	1890.6
gdb 2193	1898.8[a]	1902.8	1902.8	1905.2	1892.8	1892.8	1896.0
gdb 2194	1896.7[a]	1900.6	1900.6	1903.6	1890.5	1890.5	1894.2
gdb 2195	1897.3[a]	1899.9	1899.9	1902.8	1890.4	1890.4	1894.5
gdb 2196	1900.8[a]	1901.4	1901.4	1905.4	1897.5	1897.5	1899.9
gdb 2197	1898.4[a]	1898.4	1898.4	1902.9	1894.7	1894.7	1897.9
gdb 2198	1859.6[a]	1841.0	1841.0	1844.6	1845.3	1845.3	1846.3
gdb 2199	1855.9[a]	1840.1	1840.1	1843.7	1844.6	1844.6	1845.6
gdb 2200	1850.3[a]	1833.3	1833.3	1835.6	1833.4	1833.4	1834.2
gdb 2201	1852.4[a]	1833.0	1833.0	1835.4	1833.9	1833.9	1834.9
gdb 2202	1890.8[a]	1880.8	1880.8	1883.8	1880.5	1880.5	1882.5
gdb 2203	1890.6[a]	1881.7	1881.7	1883.2	1875.3	1875.3	1877.9
gdb 2204	1893.5[a]	1883.6	1883.6	1884.7	1877.5	1877.4	1879.8
gdb 2205	1893.3[a]	1882.6	1882.6	1885.2	1882.6	1882.6	1884.3
gdb 2206	1896.6[a]	1885.6	1885.6	1888.8	1888.7	1888.7	1890.3
gdb 2207	1882.9[a]	1879.7	1879.7	1883.1	1875.7	1875.7	1879.5

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2208	1891.4[a]	1891.2	1891.2	1893.7	1884.4	1884.3	1888.7
gdb 2209	1893.8[a]	1893.1	1893.1	1895.1	1886.5	1886.5	1890.5
gdb 2210	1885.5[a]	1881.6	1881.6	1884.7	1877.9	1877.9	1881.4
gdb 2211	1890.6[a]	1888.1	1888.1	1889.9	1882.5	1882.5	1885.3
gdb 2212	1893.6[a]	1892.8	1892.8	1895.9	1892.2	1892.2	1894.7
gdb 2213	1891.1[a]	1887.0	1887.0	1890.4	1887.0	1887.0	1889.8
gdb 2214	1892.4[a]	1888.3	1888.3	1891.1	1888.8	1888.8	1890.5
gdb 2215	1869.0[a]	1860.9	1860.9	1865.0	1857.7	1857.7	1860.0
gdb 2216	1873.9[a]	1862.5	1862.5	1865.7	1859.9	1859.9	1861.0
gdb 2217	1870.6[a]	1859.5	1859.5	1861.1	1853.2	1853.2	1853.5
gdb 2218	1874.8[a]	1864.4	1864.4	1869.4	1865.0	1865.0	1867.1
gdb 2219	1894.3[a]	1897.7	1897.7	1901.1	1888.1	1888.1	1892.6
gdb 2220	1898.9[a]	1902.9	1902.9	1905.4	1893.0	1893.0	1896.3
gdb 2221	1898.2[a]	1895.5	1895.5	1898.0	1888.7	1888.7	1891.0
gdb 2222	1894.1[a]	1896.2	1896.2	1900.7	1892.4	1892.4	1895.4
gdb 2223	1898.0[a]	1894.8	1894.8	1898.2	1891.6	1891.6	1893.8
gdb 2224	1894.3[a]	1898.6	1898.6	1899.1	1886.9	1886.9	1888.9
gdb 2225	1892.1[a]	1892.9	1892.9	1894.8	1884.9	1884.9	1886.6
gdb 2226	1891.7[a]	1896.5	1896.5	1897.4	1884.7	1884.7	1886.9
gdb 2227	1896.0[a]	1899.9	1899.9	1900.4	1888.6	1888.6	1890.6
gdb 2228	1891.2[a]	1891.2	1891.2	1894.5	1886.6	1886.6	1888.7
gdb 2229	1882.0[a]	1876.5	1876.5	1880.7	1870.0	1870.0	1873.9
gdb 2230	1887.6[a]	1884.0	1884.0	1887.1	1875.1	1875.1	1879.5
gdb 2231	1885.1[a]	1878.8	1878.8	1881.9	1872.2	1872.2	1874.6
gdb 2232	1883.9[a]	1879.2	1879.2	1881.8	1873.1	1873.1	1875.4
gdb 2233	1890.1[a]	1882.7	1882.7	1887.6	1879.7	1879.7	1883.4
gdb 2234	1890.5[a]	1884.2	1884.2	1888.6	1881.5	1881.5	1884.7
gdb 2235	1890.0[a]	1883.1	1883.1	1887.2	1880.0	1880.0	1882.4
gdb 2236	1876.2[a]	1876.9	1876.9	1881.0	1871.2	1871.2	1875.2
gdb 2237	1879.0[a]	1886.8	1886.8	1891.6	1883.4	1883.4	1886.8
gdb 2238	1871.6[a]	1867.4	1867.4	1870.6	1866.3	1866.3	1868.4
gdb 2239	1873.7[a]	1868.3	1868.3	1871.8	1867.0	1867.0	1869.5
gdb 2240	1873.2[a]	1860.4	1860.4	1863.0	1861.0	1861.0	1862.3
gdb 2241	1865.9[a]	1853.1	1853.1	1855.6	1850.1	1850.1	1852.8
gdb 2242	1874.0[a]	1866.0	1866.0	1869.4	1865.2	1865.2	1867.6
gdb 2243	1879.2[a]	1870.7	1870.7	1874.0	1873.8	1873.8	1874.6
gdb 2244	1873.7[a]	1868.1	1868.1	1871.2	1867.8	1867.7	1869.9
gdb 2245	1872.1[a]	1863.7	1863.7	1867.0	1863.2	1863.2	1865.6
gdb 2246	1870.5[a]	1862.0	1862.0	1865.1	1861.9	1861.9	1864.2
gdb 2247	1871.7[a]	1866.5	1866.5	1869.4	1865.9	1865.9	1867.9
gdb 2248	1873.0[a]	1859.7	1859.7	1861.7	1860.7	1860.7	1861.4
gdb 2249	1864.3[a]	1851.2	1851.2	1853.5	1848.4	1848.4	1851.0
gdb 2250	1877.4[a]	1869.2	1869.1	1872.3	1873.2	1873.2	1873.9
gdb 2251	1867.1[a]	1864.2	1864.2	1868.1	1857.8	1857.8	1861.5
gdb 2252	1876.6[a]	1868.4	1868.4	1871.3	1862.3	1862.3	1864.4
gdb 2253	1869.8[a]	1866.3	1866.3	1870.1	1860.0	1860.0	1863.5
gdb 2254	1879.1[a]	1874.7	1874.7	1878.4	1871.5	1871.5	1873.4
gdb 2255	1873.4[a]	1874.6	1874.6	1879.6	1871.0	1871.0	1874.5
gdb 2256	1874.9[a]	1875.1	1875.1	1880.2	1871.6	1871.6	1875.4
gdb 2257	1869.7[a]	1865.4	1865.4	1867.9	1858.6	1858.6	1863.7
gdb 2258	1863.9[a]	1850.3	1850.3	1853.5	1847.8	1847.8	1851.4
gdb 2259	1863.1[a]	1850.5	1850.5	1853.0	1848.0	1848.0	1851.4
gdb 2260	1870.1[a]	1862.7	1862.7	1865.7	1863.5	1863.5	1866.0
gdb 2261	1870.8[a]	1863.7	1863.7	1867.0	1863.6	1863.6	1866.4
gdb 2262	1870.0[a]	1863.1	1863.1	1866.5	1863.8	1863.8	1866.1
gdb 2263	1895.3[a]	1898.8	1898.8	1901.7	1894.2	1894.2	1896.9
gdb 2264	1896.6[a]	1904.6	1904.6	1904.9	1894.0	1894.0	1896.4
gdb 2265	1901.0[a]	1903.3	1903.3	1907.2	1901.9	1901.9	1904.1
gdb 2266	1914.4[a]	1920.3	1920.3	1922.2	1917.9	1917.9	1920.5
gdb 2267	1932.7[a]	1929.2	1929.2	1930.1	1925.7	1925.7	1928.2
gdb 2268	1916.4[a]	1923.9	1923.9	1924.9	1920.7	1920.7	1921.7
gdb 2269	1910.1[a]	1915.3	1915.3	1917.4	1912.5	1912.5	1915.1
gdb 2270	1919.9[a]	1925.1	1925.1	1927.6	1925.6	1925.6	1927.2
gdb 2271	1885.6[a]	1882.0	1882.0	1881.2	1873.1	1873.1	1872.3
gdb 2272	1887.7[a]	1883.5	1883.5	1882.0	1874.1	1874.1	1871.9

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2273	1883.3[a]	1879.7	1879.7	1879.5	1870.8	1870.8	1870.3
gdb 2274	1890.4[a]	1892.8	1892.8	1893.9	1882.9	1882.9	1884.9
gdb 2275	1891.7[a]	1894.2	1894.2	1895.1	1884.7	1884.7	1886.5
gdb 2276	1886.6[a]	1886.0	1886.0	1885.9	1880.3	1880.3	1878.4
gdb 2277	1886.4[a]	1885.6	1885.6	1888.4	1882.2	1882.2	1884.0
gdb 2278	1904.5[a]	1911.3	1911.3	1912.9	1901.8	1901.8	1905.3
gdb 2279	1901.7[a]	1909.0	1909.0	1910.9	1898.9	1898.8	1902.6
gdb 2280	1902.1[a]	1906.6	1906.6	1909.8	1902.8	1902.7	1905.6
gdb 2281	1903.1[a]	1909.9	1909.9	1911.8	1900.1	1900.1	1903.8
gdb 2282	1903.5[a]	1910.5	1910.5	1912.0	1900.9	1900.9	1904.3
gdb 2283	1902.3[a]	1906.5	1906.5	1909.9	1902.9	1902.9	1905.7
gdb 2284	1906.7[a]	1913.3	1913.3	1914.8	1910.9	1910.9	1912.8
gdb 2285	1904.6[a]	1910.7	1910.7	1912.9	1908.3	1908.3	1910.6
gdb 2286	1914.9[a]	1918.8	1918.8	1921.0	1919.9	1919.9	1920.8
gdb 2287	1891.4[a]	1900.0	1900.0	1902.5	1892.3	1892.3	1896.3
gdb 2288	1895.1[a]	1904.1	1904.1	1906.8	1893.8	1893.8	1899.3
gdb 2289	1898.1[a]	1908.0	1908.0	1909.4	1898.4	1898.4	1903.0
gdb 2290	1899.2[a]	1905.4	1905.4	1908.5	1901.5	1901.5	1904.3
gdb 2291	1913.0[a]	1917.8	1917.8	1919.3	1915.1	1915.1	1917.1
gdb 2292	1931.1[a]	1927.1	1927.1	1928.5	1923.4	1923.4	1926.1
gdb 2293	1916.7[a]	1924.0	1924.0	1925.1	1920.9	1920.8	1921.7
gdb 2294	1912.8[a]	1918.1	1918.1	1920.5	1915.5	1915.5	1918.4
gdb 2295	1921.5[a]	1923.9	1923.9	1926.2	1924.6	1924.6	1925.7
gdb 2296	1884.3[a]	1884.3	1884.3	1886.6	1882.9	1882.9	1885.2
gdb 2297	1905.4[a]	1894.5	1894.5	1895.9	1892.0	1892.0	1894.1
gdb 2298	1888.3[a]	1894.1	1894.1	1896.8	1894.4	1894.4	1895.3
gdb 2299	1887.9[a]	1895.1	1895.1	1898.3	1895.8	1895.8	1897.3
gdb 2300	1881.7[a]	1882.5	1882.5	1884.6	1880.7	1880.7	1882.5
gdb 2301	1853.6[a]	1853.3	1853.3	1853.9	1847.2	1847.2	1845.0
gdb 2302	1848.9[a]	1841.8	1841.7	1841.3	1833.3	1833.3	1831.9
gdb 2303	1855.4[a]	1850.9	1850.9	1853.8	1847.6	1847.6	1848.4
gdb 2304	1858.6[a]	1861.2	1861.2	1865.0	1860.8	1860.8	1860.9
gdb 2305	1881.1[a]	1875.3	1875.3	1878.2	1876.7	1876.7	1878.0
gdb 2306	1870.4[a]	1859.4	1859.4	1860.2	1860.4	1860.3	1861.9
gdb 2307	1890.9[a]	1890.3	1890.3	1893.5	1886.7	1886.7	1888.9
gdb 2308	1890.1[a]	1890.2	1890.2	1893.4	1886.6	1886.5	1888.8
gdb 2309	1894.8[a]	1901.5	1901.5	1905.2	1900.1	1900.1	1901.2
gdb 2310	1876.3[a]	1877.8	1877.8	1880.0	1875.2	1875.2	1877.9
gdb 2311	1874.9[a]	1877.3	1877.3	1879.5	1874.7	1874.6	1876.9
gdb 2312	1882.0[a]	1890.7	1890.7	1893.7	1890.4	1890.3	1892.1
gdb 2313	1848.4[a]	1837.6	1837.6	1839.0	1830.3	1830.3	1831.3
gdb 2314	1840.7[a]	1826.0	1826.0	1830.6	1821.5	1821.5	1824.9
gdb 2315	1861.2[a]	1854.8	1854.8	1857.6	1850.8	1850.8	1851.5
gdb 2316	1854.2[a]	1840.1	1840.1	1844.6	1838.1	1838.1	1840.7
gdb 2317	1838.5[a]	1826.4	1826.4	1829.8	1821.2	1821.2	1824.5
gdb 2318	1837.6[a]	1826.0	1826.0	1829.7	1821.3	1821.2	1824.4
gdb 2319	1842.7[a]	1829.5	1829.5	1832.5	1824.5	1824.5	1827.3
gdb 2320	1848.8[a]	1836.4	1836.3	1837.6	1829.0	1829.0	1830.0
gdb 2321	1850.7[a]	1841.8	1841.8	1846.8	1840.2	1840.1	1843.2
gdb 2322	1855.3[a]	1846.5	1846.5	1850.4	1844.2	1844.1	1846.3
gdb 2323	1861.3[a]	1853.0	1853.0	1855.5	1848.8	1848.7	1849.2
gdb 2324	1853.0[a]	1838.3	1838.3	1842.9	1836.7	1836.7	1839.6
gdb 2325	1852.1[a]	1842.5	1842.5	1846.2	1837.0	1837.0	1840.3
gdb 2326	1851.1[a]	1841.7	1841.7	1844.8	1836.7	1836.7	1840.1
gdb 2327	1854.7[a]	1843.6	1843.6	1848.1	1838.7	1838.7	1842.3
gdb 2328	1854.4[a]	1844.1	1844.1	1848.5	1839.3	1839.3	1842.6
gdb 2329	1849.8[a]	1840.7	1840.6	1844.4	1835.1	1835.1	1838.6
gdb 2330	1855.7[a]	1854.2	1854.1	1858.4	1851.3	1851.3	1854.2
gdb 2331	1859.0[a]	1855.4	1855.4	1860.2	1852.7	1852.6	1855.4
gdb 2332	1858.4[a]	1856.0	1856.0	1860.7	1853.0	1853.0	1855.5
gdb 2333	1870.7[a]	1867.5	1867.5	1870.2	1861.7	1861.7	1865.3
gdb 2334	1879.4[a]	1882.0	1882.0	1885.4	1878.9	1878.9	1881.7
gdb 2335	1902.1[a]	1906.0	1906.0	1907.5	1904.8	1904.7	1906.4
gdb 2336	1897.6[a]	1911.1	1911.1	1913.4	1909.0	1909.0	1911.4
gdb 2337	1913.3[a]	1916.4	1916.4	1918.1	1913.1	1913.1	1916.1

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2338	1895.5[a]	1900.4	1900.4	1901.7	1898.8	1898.8	1900.4
gdb 2339	1903.9[a]	1917.3	1917.3	1919.5	1918.3	1918.3	1919.0
gdb 2340	1875.2[a]	1876.1	1876.1	1878.7	1874.8	1874.8	1877.9
gdb 2341	1875.2[a]	1877.8	1877.8	1880.6	1876.1	1876.1	1878.7
gdb 2342	1872.7[a]	1874.7	1874.6	1877.2	1873.0	1873.0	1876.0
gdb 2343	1877.5[a]	1887.0	1887.0	1890.4	1887.6	1887.6	1889.8
gdb 2344	1854.5[a]	1848.9	1848.9	1848.8	1841.4	1841.3	1840.5
gdb 2345	1851.1[a]	1842.0	1842.0	1845.1	1838.2	1838.2	1840.2
gdb 2346	1850.7[a]	1847.4	1847.4	1847.1	1839.3	1839.3	1838.2
gdb 2347	1858.7[a]	1860.6	1860.6	1861.3	1855.3	1855.3	1853.5
gdb 2348	1854.6[a]	1854.6	1854.6	1858.1	1851.8	1851.8	1853.4
gdb 2349	1878.0[a]	1872.6	1872.6	1872.0	1865.2	1865.1	1864.4
gdb 2350	1870.4[a]	1869.9	1869.9	1873.1	1865.0	1865.0	1868.2
gdb 2351	1874.5[a]	1869.7	1869.7	1869.2	1861.8	1861.8	1861.0
gdb 2352	1879.4[a]	1882.7	1882.7	1882.8	1877.3	1877.3	1875.5
gdb 2353	1877.0[a]	1877.9	1877.9	1880.7	1875.3	1875.3	1876.9
gdb 2354	1863.6[a]	1852.7	1852.7	1855.2	1845.8	1845.8	1848.1
gdb 2355	1866.1[a]	1854.7	1854.7	1857.2	1848.0	1848.0	1850.1
gdb 2356	1870.5[a]	1866.9	1866.9	1870.0	1862.6	1862.6	1863.5
gdb 2357	1872.5[a]	1860.8	1860.8	1865.6	1857.6	1857.6	1861.2
gdb 2358	1852.7[a]	1844.4	1844.4	1848.5	1838.9	1838.9	1843.4
gdb 2359	1851.8[a]	1843.2	1843.2	1847.2	1837.4	1837.3	1841.7
gdb 2360	1855.2[a]	1845.8	1845.8	1850.0	1840.3	1840.3	1844.5
gdb 2361	1854.6[a]	1845.7	1845.7	1849.6	1840.2	1840.2	1844.5
gdb 2362	1856.5[a]	1854.6	1854.6	1859.5	1851.3	1851.2	1854.7
gdb 2363	1859.3[a]	1857.4	1857.4	1862.1	1854.0	1853.9	1857.4
gdb 2364	1858.1[a]	1857.0	1857.0	1861.8	1853.7	1853.7	1856.8
gdb 2365	1877.1[a]	1870.4	1870.4	1872.5	1872.8	1872.8	1874.1
gdb 2366	1876.5[a]	1870.8	1870.8	1872.3	1873.5	1873.5	1873.8
gdb 2367	1867.7[a]	1858.1	1858.1	1859.6	1857.5	1857.5	1859.5
gdb 2368	1871.1[a]	1859.8	1859.8	1861.5	1859.7	1859.7	1861.8
gdb 2369	1841.0[a]	1821.9	1821.9	1824.8	1819.7	1819.7	1822.9
gdb 2370	1839.1[a]	1824.2	1824.2	1826.3	1821.1	1821.1	1824.2
gdb 2371	1843.9[a]	1823.7	1823.7	1826.8	1821.8	1821.8	1824.9
gdb 2372	1842.0[a]	1825.8	1825.8	1828.2	1823.1	1823.0	1826.1
gdb 2373	1853.4[a]	1838.9	1838.9	1842.8	1839.4	1839.4	1841.7
gdb 2374	1848.5[a]	1839.0	1839.0	1842.1	1839.0	1839.0	1841.2
gdb 2375	1845.1[a]	1835.0	1835.0	1838.5	1835.5	1835.5	1837.4
gdb 2376	1840.7[a]	1825.4	1825.3	1824.6	1820.5	1820.5	1819.3
gdb 2377	1844.3[a]	1828.1	1828.1	1827.6	1823.7	1823.7	1822.5
gdb 2378	1850.5[a]	1840.7	1840.7	1840.8	1838.5	1838.5	1836.4
gdb 2379	1842.7[a]	1830.9	1830.9	1833.7	1831.8	1831.8	1832.6
gdb 2380	1882.9[a]	1871.0	1871.0	1872.6	1870.3	1870.2	1873.9
gdb 2381	1862.8[a]	1853.8	1853.8	1855.7	1855.4	1855.3	1858.0
gdb 2382	1865.7[a]	1855.5	1855.4	1857.6	1857.4	1857.2	1859.8
gdb 2383	1873.5[a]	1869.2	1869.2	1872.0	1873.4	1873.3	1875.1
gdb 2384	1879.1[a]	1878.4	1878.4	1881.0	1872.3	1872.3	1876.2
gdb 2385	1886.8[a]	1885.8	1885.8	1888.4	1883.2	1883.1	1885.4
gdb 2386	1902.3[a]	1908.6	1908.6	1910.1	1907.6	1907.6	1909.5
gdb 2387	1918.4[a]	1922.8	1922.8	1924.1	1919.8	1919.8	1922.4
gdb 2388	1915.9[a]	1920.2	1920.2	1922.1	1917.2	1917.2	1920.2
gdb 2389	1900.1[a]	1906.7	1906.7	1908.2	1905.6	1905.6	1907.8
gdb 2390	1904.8[a]	1919.1	1919.1	1921.3	1920.4	1920.4	1921.3
gdb 2391	1875.9[a]	1870.7	1870.7	1870.1	1863.1	1863.1	1862.3
gdb 2392	1875.3[a]	1870.4	1870.4	1869.6	1862.5	1862.5	1861.3
gdb 2393	1870.3[a]	1869.2	1869.2	1872.8	1864.3	1864.3	1867.5
gdb 2394	1882.0[a]	1883.9	1883.9	1883.8	1878.6	1878.5	1876.0
gdb 2395	1875.1[a]	1881.2	1881.2	1885.3	1878.7	1878.7	1880.8
gdb 2396	1877.8[a]	1877.3	1877.3	1880.0	1875.0	1874.9	1876.3
gdb 2397	1852.3[a]	1847.7	1847.7	1847.5	1839.8	1839.8	1838.9
gdb 2398	1852.7[a]	1847.9	1847.9	1847.5	1839.8	1839.8	1838.5
gdb 2399	1851.5[a]	1842.6	1842.6	1845.8	1838.7	1838.7	1840.7
gdb 2400	1858.5[a]	1860.9	1860.9	1861.5	1855.1	1855.1	1852.9
gdb 2401	1857.0[a]	1855.0	1854.9	1858.7	1853.4	1853.4	1854.2
gdb 2402	1855.8[a]	1856.0	1855.9	1859.3	1852.9	1852.9	1854.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2403	1870.9[a]	1872.2	1872.2	1874.9	1870.4	1870.4	1873.4
gdb 2404	1871.5[a]	1874.0	1874.0	1876.6	1872.2	1872.2	1875.5
gdb 2405	1875.3[a]	1876.3	1876.3	1879.0	1874.7	1874.7	1877.6
gdb 2406	1880.2[a]	1889.0	1889.0	1892.6	1888.5	1888.4	1890.2
gdb 2407	1888.3[a]	1886.7	1886.7	1889.7	1884.6	1884.5	1887.0
gdb 2408	1913.7[a]	1916.8	1916.8	1918.4	1913.3	1913.3	1916.0
gdb 2409	1895.4[a]	1908.7	1908.7	1911.6	1906.5	1906.5	1909.1
gdb 2410	1900.2[a]	1904.1	1904.1	1905.6	1902.7	1902.7	1904.4
gdb 2411	1898.9[a]	1902.7	1902.7	1904.0	1901.2	1901.2	1902.4
gdb 2412	1904.8[a]	1915.4	1915.4	1917.6	1916.3	1916.3	1916.4
gdb 2413	1879.5[a]	1877.9	1877.8	1881.5	1871.7	1871.6	1875.8
gdb 2414	1882.1[a]	1889.1	1889.1	1892.4	1885.3	1885.3	1888.3
gdb 2415	1885.4[a]	1885.3	1885.3	1888.2	1882.6	1882.6	1884.8
gdb 2416	1863.8[a]	1849.5	1849.5	1851.9	1848.0	1848.0	1847.6
gdb 2417	1856.5[a]	1843.8	1843.8	1845.8	1838.7	1838.7	1839.5
gdb 2418	1868.8[a]	1851.5	1851.5	1856.1	1850.1	1850.1	1853.0
gdb 2419	1874.3[a]	1856.8	1856.8	1862.1	1858.8	1858.8	1861.0
gdb 2420	1873.5[a]	1870.8	1870.8	1873.6	1869.4	1869.4	1871.2
gdb 2421	1873.2[a]	1861.5	1861.5	1864.2	1861.9	1861.9	1863.2
gdb 2422	1866.4[a]	1854.6	1854.6	1857.3	1851.3	1851.3	1854.0
gdb 2423	1874.6[a]	1869.2	1869.2	1872.6	1867.5	1867.5	1869.8
gdb 2424	1878.8[a]	1876.0	1876.0	1879.4	1877.9	1877.9	1878.7
gdb 2425	1885.9[a]	1890.7	1890.7	1893.3	1885.8	1885.8	1888.8
gdb 2426	1878.8[a]	1881.4	1881.4	1884.9	1876.7	1876.7	1880.7
gdb 2427	1894.5[a]	1902.3	1902.3	1903.2	1894.6	1894.5	1897.5
gdb 2428	1889.8[a]	1893.7	1893.7	1896.8	1891.9	1891.9	1893.7
gdb 2429	1882.9[a]	1879.2	1879.2	1881.5	1872.7	1872.7	1875.0
gdb 2430	1882.1[a]	1876.6	1876.6	1880.0	1869.6	1869.6	1872.4
gdb 2431	1883.9[a]	1878.6	1878.6	1882.9	1872.0	1872.0	1875.8
gdb 2432	1890.4[a]	1887.5	1887.5	1890.2	1878.9	1878.9	1883.0
gdb 2433	1887.3[a]	1882.8	1882.8	1885.7	1879.2	1879.2	1880.5
gdb 2434	1888.8[a]	1882.4	1882.4	1887.5	1879.0	1879.0	1882.8
gdb 2435	1878.2[a]	1871.4	1871.4	1876.0	1865.9	1865.9	1870.2
gdb 2436	1880.3[a]	1873.8	1873.8	1877.9	1868.6	1868.6	1872.5
gdb 2437	1890.3[a]	1880.7	1880.7	1885.5	1878.6	1878.6	1881.6
gdb 2438	1888.0[a]	1879.2	1879.2	1883.9	1876.5	1876.5	1879.7
gdb 2439	1871.3[a]	1866.8	1866.7	1869.9	1865.8	1865.8	1867.8
gdb 2440	1870.6[a]	1858.0	1858.0	1860.4	1858.7	1858.7	1860.0
gdb 2441	1870.1[a]	1857.5	1857.5	1860.1	1858.0	1857.9	1859.3
gdb 2442	1871.2[a]	1866.0	1866.0	1869.5	1865.0	1865.0	1867.3
gdb 2443	1872.2[a]	1863.3	1863.3	1866.6	1863.1	1863.1	1865.6
gdb 2444	1863.4[a]	1850.9	1850.9	1853.2	1847.8	1847.8	1850.7
gdb 2445	1876.5[a]	1868.8	1868.8	1872.2	1872.6	1872.6	1873.4
gdb 2446	1889.0[a]	1886.9	1886.9	1889.3	1880.5	1880.5	1883.8
gdb 2447	1891.9[a]	1891.7	1891.7	1894.3	1884.3	1884.3	1888.8
gdb 2448	1885.4[a]	1882.0	1882.0	1885.0	1878.0	1878.0	1881.5
gdb 2449	1894.0[a]	1890.4	1890.4	1893.2	1890.2	1890.2	1891.8
gdb 2450	1894.0[a]	1893.3	1893.3	1896.3	1892.0	1892.0	1894.4
gdb 2451	1880.8[a]	1877.4	1877.4	1880.2	1870.7	1870.7	1873.2
gdb 2452	1886.1[a]	1883.6	1883.6	1886.9	1874.3	1874.3	1878.9
gdb 2453	1884.1[a]	1879.5	1879.5	1882.2	1872.6	1872.6	1874.8
gdb 2454	1882.9[a]	1878.6	1878.6	1882.4	1872.0	1872.0	1875.6
gdb 2455	1888.7[a]	1884.9	1884.9	1887.7	1881.6	1881.6	1882.3
gdb 2456	1887.8[a]	1884.9	1884.9	1889.1	1881.5	1881.5	1884.0
gdb 2457	1887.3[a]	1883.9	1883.9	1888.4	1880.5	1880.5	1883.9
gdb 2458	1884.1[a]	1887.4	1887.4	1890.3	1882.8	1882.8	1886.2
gdb 2459	1891.6[a]	1897.1	1897.1	1898.6	1889.4	1889.4	1893.1
gdb 2460	1881.3[a]	1882.0	1882.0	1884.9	1878.1	1878.1	1881.6
gdb 2461	1886.2[a]	1888.7	1888.7	1891.4	1884.6	1884.6	1887.9
gdb 2462	1888.6[a]	1889.9	1889.9	1892.8	1889.8	1889.8	1891.7
gdb 2463	1891.3[a]	1895.2	1895.2	1897.8	1894.5	1894.5	1896.4
gdb 2464	1890.3[a]	1893.8	1893.8	1896.2	1893.1	1893.1	1894.7
gdb 2465	1836.2[a]	1825.8	1825.8	1826.9	1819.8	1819.8	1820.5
gdb 2466	1831.9[a]	1818.1	1818.1	1820.8	1814.3	1814.3	1815.1
gdb 2467	1840.1[a]	1824.2	1824.2	1828.6	1818.2	1818.2	1822.8

... *continued on next page* ...

Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2468	1849.2[a]	1837.5	1837.5	1839.2	1835.2	1835.2	1834.1
gdb 2469	1847.2[a]	1830.3	1830.3	1835.6	1830.1	1830.1	1833.4
gdb 2470	1845.9[a]	1830.7	1830.7	1835.1	1829.9	1829.9	1833.1
gdb 2471	1886.6[a]	1893.7	1893.7	1896.7	1887.9	1887.9	1891.8
gdb 2472	1893.4[a]	1897.9	1897.9	1900.3	1890.9	1890.9	1894.8
gdb 2473	1895.6[a]	1902.7	1902.7	1905.4	1900.4	1900.4	1902.6
gdb 2474	1869.6[a]	1867.8	1867.8	1868.2	1859.7	1859.7	1859.0
gdb 2475	1864.0[a]	1863.3	1863.3	1863.2	1855.5	1855.5	1855.0
gdb 2476	1872.0[a]	1870.2	1870.2	1869.9	1862.2	1862.2	1861.1
gdb 2477	1874.5[a]	1876.5	1876.5	1879.1	1867.6	1867.6	1871.1
gdb 2478	1879.5[a]	1876.3	1876.2	1876.3	1871.6	1871.6	1869.1
gdb 2479	1877.5[a]	1877.4	1877.4	1881.2	1874.9	1874.8	1876.6
gdb 2480	1876.3[a]	1874.9	1874.9	1878.4	1872.5	1872.5	1874.5
gdb 2481	1888.3[a]	1891.9	1891.9	1893.6	1891.3	1891.2	1893.2
gdb 2482	1891.6[a]	1894.2	1894.1	1895.8	1893.3	1893.3	1895.4
gdb 2483	1891.2[a]	1894.1	1894.1	1895.6	1893.9	1893.9	1895.6
gdb 2484	1897.2[a]	1897.8	1897.8	1899.3	1901.6	1901.6	1902.1
gdb 2485	1901.6[a]	1910.7	1910.7	1912.8	1901.3	1901.3	1905.5
gdb 2486	1901.2[a]	1910.1	1910.1	1913.4	1906.7	1906.6	1909.2
gdb 2487	1899.7[a]	1908.1	1908.1	1911.3	1905.1	1905.1	1907.8
gdb 2488	1923.4[a]	1911.5	1911.5	1912.6	1909.8	1909.8	1911.8
gdb 2489	1899.0[a]	1907.9	1907.9	1910.8	1906.3	1906.3	1909.0
gdb 2490	1898.4[a]	1905.4	1905.4	1908.0	1903.9	1903.9	1906.7
gdb 2491	1899.0[a]	1908.2	1908.2	1910.2	1906.3	1906.3	1908.0
gdb 2492	1905.1[a]	1912.6	1912.6	1915.6	1914.4	1914.4	1914.9
gdb 2493	1901.8[a]	1910.6	1910.6	1912.6	1901.2	1901.2	1905.4
gdb 2494	1902.7[a]	1911.0	1911.0	1914.2	1907.9	1907.9	1910.2
gdb 2495	1901.4[a]	1908.2	1908.2	1911.2	1905.1	1905.1	1907.5
gdb 2496	1852.3[a]	1840.3	1840.3	1843.1	1834.8	1834.8	1836.2
gdb 2497	1849.6[a]	1838.7	1838.7	1840.8	1834.0	1834.0	1835.8
gdb 2498	1853.5[a]	1843.0	1843.0	1844.9	1837.7	1837.7	1838.6
gdb 2499	1863.2[a]	1848.1	1848.1	1852.5	1840.7	1840.7	1847.0
gdb 2500	1863.5[a]	1850.9	1850.9	1852.7	1849.3	1849.3	1848.2
gdb 2501	1866.1[a]	1850.0	1850.0	1855.7	1848.8	1848.8	1852.9
gdb 2502	1862.5[a]	1847.4	1847.4	1852.6	1846.7	1846.7	1850.6
gdb 2503	1860.5[a]	1849.0	1849.0	1852.1	1845.3	1845.3	1849.2
gdb 2504	1863.8[a]	1850.9	1850.9	1853.8	1848.2	1848.2	1851.9
gdb 2505	1871.0[a]	1866.5	1866.5	1869.4	1859.6	1859.6	1865.0
gdb 2506	1870.8[a]	1858.4	1858.4	1861.3	1858.7	1858.6	1860.3
gdb 2507	1869.9[a]	1864.3	1864.3	1867.9	1863.8	1863.8	1866.4
gdb 2508	1867.8[a]	1864.0	1864.0	1867.4	1863.1	1863.1	1865.7
gdb 2509	1905.4[a]	1912.2	1912.2	1913.3	1909.4	1909.4	1911.2
gdb 2510	1921.7[a]	1920.4	1920.4	1920.9	1916.9	1916.9	1919.2
gdb 2511	1899.3[a]	1908.4	1908.4	1909.9	1906.3	1906.3	1908.4
gdb 2512	1890.6[a]	1900.8	1900.8	1901.3	1890.8	1890.8	1892.9
gdb 2513	1918.0[a]	1919.8	1919.8	1920.4	1917.1	1917.1	1920.0
gdb 2514	1894.8[a]	1903.0	1903.0	1904.7	1902.6	1902.5	1905.1
gdb 2515	1872.8[a]	1874.8	1874.8	1873.5	1867.5	1867.4	1866.1
gdb 2516	1900.3[a]	1903.8	1904.1	1905.2	1902.4	1902.4	1904.9
gdb 2517	1900.0[a]	1904.2	1904.2	1905.2	1902.3	1902.3	1904.8
gdb 2518	1868.9[a]	1865.8	1865.8	1868.2	1860.7	1860.7	1864.0
gdb 2519	1891.4[a]	1895.3	1895.3	1897.3	1888.9	1888.9	1892.6
gdb 2520	1885.4[a]	1892.8	1892.8	1895.4	1888.1	1888.0	1891.4
gdb 2521	1919.6[a]	1924.6	1924.6	1925.9	1924.9	1924.9	1924.8
gdb 2522	1918.4[a]	1924.3	1924.3	1925.8	1924.7	1924.7	1925.3
gdb 2523	1930.7[a]	1926.4	1926.4	1927.3	1922.9	1922.9	1925.3
gdb 2524	1899.5[a]	1905.3	1905.3	1906.7	1903.7	1903.7	1906.0
gdb 2525	1899.4[a]	1903.5	1903.5	1904.6	1902.0	1902.0	1903.8
gdb 2526	1913.7[a]	1911.2	1911.2	1911.8	1908.8	1908.8	1911.4
gdb 2527	1914.0[a]	1921.9	1921.9	1922.9	1922.3	1922.2	1922.4
gdb 2528	1887.7[a]	1887.4	1887.4	1885.9	1881.0	1881.0	1877.9
gdb 2529	1930.4[a]	1925.5	1925.5	1926.2	1922.2	1922.2	1924.3
gdb 2530	1917.9[a]	1922.8	1922.8	1924.1	1923.4	1923.4	1923.8
gdb 2531	1900.4[a]	1909.7	1909.7	1911.1	1906.8	1906.8	1908.8
gdb 2532	1909.0[a]	1914.1	1914.1	1915.2	1914.5	1914.5	1914.8

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2533	1874.0[a]	1876.0	1876.0	1874.7	1868.4	1868.4	1866.8
gdb 2534	1916.2[a]	1913.7	1913.3	1913.8	1911.1	1911.0	1914.1
gdb 2535	1896.0[a]	1904.4	1904.4	1906.0	1903.7	1903.7	1906.3
gdb 2536	1897.0[a]	1902.4	1902.4	1904.0	1900.7	1900.6	1903.8
gdb 2537	1897.8[a]	1904.2	1904.2	1905.3	1902.6	1902.6	1905.3
gdb 2538	1876.8[a]	1873.3	1873.3	1877.6	1873.7	1873.7	1875.4
gdb 2539	1888.5[a]	1885.4	1885.4	1888.0	1888.7	1888.7	1889.4
gdb 2540	1878.1[a]	1878.1	1878.1	1880.5	1877.4	1877.4	1879.7
gdb 2541	1893.1[a]	1902.2	1902.2	1902.6	1891.9	1891.8	1894.0
gdb 2542	1894.3[a]	1903.5	1903.5	1903.7	1893.6	1893.6	1895.6
gdb 2543	1892.7[a]	1897.0	1897.0	1900.1	1893.3	1893.3	1895.8
gdb 2544	1889.7[a]	1889.3	1889.3	1892.0	1886.3	1886.2	1888.1
gdb 2545	1877.8[a]	1875.4	1875.4	1874.2	1867.2	1867.2	1866.3
gdb 2546	1877.0[a]	1879.2	1879.2	1881.6	1873.4	1873.4	1876.6
gdb 2547	1869.5[a]	1871.5	1871.5	1872.5	1867.2	1867.2	1866.8
gdb 2548	1892.6[a]	1897.5	1897.5	1900.3	1888.5	1888.5	1893.9
gdb 2549	1896.2[a]	1902.2	1902.2	1904.4	1892.9	1892.9	1897.2
gdb 2550	1890.0[a]	1894.5	1894.5	1897.5	1888.2	1888.2	1892.0
gdb 2551	1896.1[a]	1902.3	1902.3	1904.5	1893.0	1893.0	1897.4
gdb 2552	1888.0[a]	1887.1	1887.0	1885.9	1880.6	1880.6	1878.0
gdb 2553	1870.2[a]	1869.8	1869.8	1869.4	1862.3	1862.3	1862.3
gdb 2554	1901.4[a]	1908.3	1908.3	1910.5	1899.4	1899.4	1903.1
gdb 2555	1900.0[a]	1907.6	1907.6	1909.6	1898.3	1898.3	1901.9
gdb 2556	1893.1[a]	1897.0	1897.0	1900.2	1893.3	1893.3	1895.8
gdb 2557	1894.8[a]	1903.6	1903.6	1904.0	1893.6	1893.6	1895.7
gdb 2558	1893.1[a]	1902.1	1902.1	1902.6	1891.6	1891.6	1894.0
gdb 2559	1889.7[a]	1898.7	1898.7	1901.5	1892.2	1892.1	1895.9
gdb 2560	1895.2[a]	1905.2	1905.2	1907.3	1896.1	1896.1	1900.7
gdb 2561	1895.2[a]	1905.2	1905.2	1907.3	1896.2	1896.1	1901.0
gdb 2562	1887.9[a]	1888.3	1888.3	1891.2	1885.6	1885.6	1887.8
gdb 2563	1877.0[a]	1876.2	1876.2	1879.4	1870.8	1870.8	1874.8
gdb 2564	1900.7[a]	1908.9	1908.9	1911.0	1900.7	1900.6	1904.5
gdb 2565	1914.4[a]	1922.1	1922.1	1923.3	1922.2	1922.2	1922.4
gdb 2566	1899.1[a]	1905.8	1905.8	1907.5	1904.2	1904.1	1906.7
gdb 2567	1908.7[a]	1910.1	1910.1	1911.4	1907.6	1907.6	1911.2
gdb 2568	1918.8[a]	1923.1	1923.1	1924.4	1923.3	1923.3	1923.1
gdb 2569	1908.6[a]	1915.1	1915.1	1916.6	1915.7	1915.7	1916.3
gdb 2570	1897.6[a]	1903.8	1903.8	1905.0	1902.1	1902.1	1904.9
gdb 2571	1916.4[a]	1914.2	1914.1	1914.8	1912.1	1912.1	1915.2
gdb 2572	1889.0[a]	1885.8	1885.8	1888.4	1889.0	1889.0	1889.6
gdb 2573	1887.7[a]	1888.2	1888.2	1891.1	1885.4	1885.4	1887.5
gdb 2574	1889.1[a]	1888.5	1888.5	1891.4	1885.4	1885.4	1887.4
gdb 2575	1899.9[a]	1907.9	1907.9	1909.9	1898.4	1898.4	1901.9
gdb 2576	1901.1[a]	1908.3	1908.3	1910.6	1899.2	1899.2	1903.0
gdb 2577	1900.7[a]	1908.8	1908.8	1911.0	1900.5	1900.4	1904.4
gdb 2578	1908.8[a]	1910.1	1910.1	1910.5	1907.2	1907.1	1910.1
gdb 2579	1913.3[a]	1911.6	1911.6	1912.2	1909.4	1909.4	1912.3
gdb 2580	1897.8[a]	1903.9	1903.9	1905.0	1902.4	1902.4	1905.2
gdb 2581	1909.4[a]	1914.2	1914.1	1915.5	1914.2	1914.2	1914.7
gdb 2582	1900.8[a]	1910.1	1910.1	1911.8	1906.9	1906.8	1909.1
gdb 2583	1877.4[a]	1879.0	1879.0	1881.7	1873.0	1873.0	1877.0
gdb 2584	1874.4[a]	1876.3	1876.3	1875.4	1868.4	1868.4	1867.1
gdb 2585	1915.8[a]	1913.4	1913.4	1914.2	1910.9	1910.9	1914.1
gdb 2586	1896.1[a]	1904.4	1904.4	1906.1	1903.5	1903.5	1906.2
gdb 2587	1878.1[a]	1878.0	1878.0	1880.4	1877.2	1877.2	1879.5
gdb 2588	1877.2[a]	1876.0	1876.0	1879.4	1870.7	1870.6	1874.7
gdb 2589	1908.8[a]	1910.0	1909.9	1911.3	1907.4	1907.4	1911.1
gdb 2590	1899.0[a]	1905.9	1905.9	1907.6	1904.5	1904.5	1907.1
gdb 2591	1877.1[a]	1874.6	1874.6	1873.3	1866.3	1866.2	1865.4
gdb 2592	1896.8[a]	1903.9	1903.9	1905.3	1901.7	1901.7	1904.6
gdb 2593	1897.2[a]	1902.5	1902.5	1904.2	1900.8	1900.7	1904.1
gdb 2594	1870.6[a]	1868.0	1868.0	1866.8	1861.3	1861.3	1860.8
gdb 2595	1912.2[a]	1911.1	1911.1	1911.7	1908.1	1908.1	1910.5
gdb 2596	1897.9[a]	1904.2	1904.2	1905.9	1902.2	1902.2	1904.6
gdb 2597	1898.5[a]	1905.1	1905.0	1906.7	1903.0	1903.0	1905.5

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2598	1878.1[a]	1881.1	1881.1	1879.7	1877.8	1877.8	1875.2
gdb 2599	1881.0[a]	1886.6	1886.6	1889.2	1888.2	1888.2	1888.3
gdb 2600	1887.1[a]	1881.1	1881.1	1882.0	1883.4	1883.4	1883.1
gdb 2601	1885.4[a]	1878.9	1878.9	1881.0	1883.0	1883.0	1883.3
gdb 2602	1883.2[a]	1877.4	1877.4	1875.7	1874.7	1874.7	1871.6
gdb 2603	1885.6[a]	1878.1	1878.1	1879.7	1881.9	1881.9	1881.8
gdb 2604	1899.2[a]	1894.9	1894.9	1897.4	1895.6	1895.6	1897.1
gdb 2605	1892.7[a]	1890.0	1890.0	1891.1	1887.2	1887.2	1887.6
gdb 2606	1900.5[a]	1896.2	1896.2	1899.5	1897.1	1897.1	1899.1
gdb 2607	1882.5[a]	1889.7	1889.7	1892.0	1890.0	1890.0	1891.0
gdb 2608	1884.6[a]	1892.4	1892.4	1895.7	1893.2	1893.2	1894.5
gdb 2609	1882.0[a]	1881.2	1881.1	1883.7	1879.8	1879.8	1882.2
gdb 2610	1875.1[a]	1876.5	1876.5	1878.8	1874.6	1874.6	1876.8
gdb 2611	1913.7[a]	1916.7	1916.6	1918.2	1916.0	1916.0	1916.9
gdb 2612	1913.9[a]	1919.9	1919.9	1921.6	1919.2	1919.2	1920.1
gdb 2613	1912.9[a]	1919.6	1919.6	1920.0	1920.9	1920.9	1920.9
gdb 2614	1900.9[a]	1909.4	1909.4	1911.0	1911.2	1911.2	1913.0
gdb 2615	1880.4[a]	1883.2	1883.2	1886.0	1882.3	1882.3	1884.7
gdb 2616	1875.8[a]	1878.7	1878.7	1881.0	1877.8	1877.7	1880.5
gdb 2617	1902.4[a]	1892.3	1892.3	1894.3	1890.5	1890.5	1892.8
gdb 2618	1882.9[a]	1890.7	1890.7	1893.9	1891.6	1891.6	1892.6
gdb 2619	1900.7[a]	1907.9	1907.9	1908.4	1909.3	1909.3	1908.9
gdb 2620	1901.9[a]	1907.6	1907.6	1909.1	1910.5	1910.5	1910.7
gdb 2621	1904.7[a]	1905.9	1905.9	1904.1	1902.6	1902.6	1900.2
gdb 2622	1910.3[a]	1907.3	1907.3	1908.2	1905.3	1905.3	1907.4
gdb 2623	1897.7[a]	1903.4	1903.4	1901.2	1900.1	1900.1	1897.2
gdb 2624	1891.2[a]	1899.1	1899.1	1900.7	1899.4	1899.4	1900.6
gdb 2625	1908.8[a]	1910.6	1910.6	1911.3	1907.9	1907.9	1909.6
gdb 2626	1900.6[a]	1907.5	1907.5	1908.1	1909.2	1909.2	1908.4
gdb 2627	1908.8[a]	1915.7	1915.7	1917.5	1916.1	1916.1	1916.3
gdb 2628	1916.7[a]	1917.9	1917.9	1918.5	1914.3	1914.3	1917.2
gdb 2629	1924.8[a]	1934.2	1934.2	1933.7	1936.1	1936.1	1935.7
gdb 2630	1857.3[a]	1853.2	1853.2	1856.2	1854.2	1854.1	1855.0
gdb 2631	1860.3[a]	1853.5	1853.5	1857.1	1854.7	1854.6	1855.7
gdb 2632	1859.3[a]	1854.7	1854.7	1857.7	1856.0	1856.0	1856.6
gdb 2633	1887.7[a]	1887.3	1887.3	1890.3	1888.5	1888.5	1889.2
gdb 2634	1888.8[a]	1886.2	1886.1	1885.5	1880.9	1880.9	1878.3
gdb 2635	1886.6[a]	1886.6	1886.6	1886.1	1881.7	1881.7	1879.0
gdb 2636	1900.5[a]	1908.5	1908.5	1910.0	1911.0	1910.9	1912.4
gdb 2637	1916.0[a]	1918.7	1918.7	1919.7	1919.4	1919.4	1919.5
gdb 2638	1915.9[a]	1920.3	1920.3	1921.3	1921.2	1921.2	1921.5
gdb 2639	1923.5[a]	1937.6	1937.6	1938.0	1940.4	1940.4	1940.8
gdb 2640	1862.7[a]	1866.7	1866.7	1870.3	1865.5	1865.5	1867.1
gdb 2641	1864.2[a]	1867.4	1867.4	1872.2	1866.2	1866.1	1867.9
gdb 2642	1854.3[a]	1850.1	1850.1	1852.8	1852.7	1852.7	1853.7
gdb 2643	1857.7[a]	1852.9	1852.9	1856.0	1855.9	1855.8	1856.7
gdb 2644	1895.0[a]	1901.0	1901.0	1901.1	1902.5	1902.5	1903.0
gdb 2645	1826.2[a]	1812.4	1812.4	1813.7	1813.1	1813.1	1812.3
gdb 2646	1836.2[a]	1818.3	1818.3	1822.9	1823.9	1823.8	1825.7
gdb 2647	1895.5[a]	1876.4	1876.4	1878.0	1877.8	1877.8	1880.2
gdb 2648	1879.6[a]	1880.9	1880.9	1883.2	1885.2	1885.2	1886.4
gdb 2649	1848.1[a]	1839.7	1839.7	1839.2	1837.5	1837.5	1835.2
gdb 2650	1843.6[a]	1825.9	1825.9	1829.4	1828.8	1828.7	1829.8
gdb 2651	1850.9[a]	1844.2	1844.2	1846.9	1848.2	1848.2	1848.4
gdb 2652	1880.8[a]	1881.1	1881.1	1883.7	1884.1	1884.0	1885.2
gdb 2653	1896.8[a]	1880.9	1880.9	1881.6	1880.1	1880.1	1881.7
gdb 2654	1875.0[a]	1869.3	1869.3	1871.4	1870.6	1870.6	1871.8
gdb 2655	1883.5[a]	1882.2	1882.2	1885.6	1885.3	1885.3	1886.4
gdb 2656	1875.4[a]	1873.2	1873.1	1876.4	1873.4	1873.4	1875.4
gdb 2657	1881.1[a]	1880.5	1880.5	1882.7	1883.4	1883.4	1883.9
gdb 2658	1894.1[a]	1899.3	1899.3	1899.1	1901.5	1901.5	1900.9
gdb 2659	1840.5[a]	1837.5	1840.3	1843.5	1838.2	1837.3	1842.1
gdb 2660	1851.8[a]	1847.4	1847.4	1850.4	1851.3	1851.2	1852.1
gdb 2661	1876.8[a]	1880.7	1880.7	1879.1	1876.9	1876.9	1873.7
gdb 2662	1882.3[a]	1887.4	1887.4	1888.9	1888.7	1888.7	1888.1

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2663	1884.0[a]	1890.8	1890.8	1893.6	1892.3	1892.3	1892.1
gdb 2664	1801.4[a]	1785.4	1785.4	1789.2	1785.1	1785.1	1785.3
gdb 2665	1798.9[a]	1783.9	1783.9	1787.8	1784.1	1784.1	1784.6
gdb 2666	1818.5[a]	1801.5	1801.5	1806.3	1804.2	1804.2	1806.0
gdb 2667	1869.7[a]	1871.9	1871.9	1876.2	1869.2	1869.2	1872.0
gdb 2668	1869.7[a]	1871.6	1871.5	1875.7	1869.3	1869.3	1871.9
gdb 2669	1878.4[a]	1880.6	1880.6	1884.3	1881.3	1881.3	1882.0
gdb 2670	1898.8[a]	1886.5	1886.5	1889.0	1884.5	1884.5	1887.7
gdb 2671	1881.7[a]	1889.0	1889.0	1892.0	1890.2	1890.2	1892.0
gdb 2672	1883.0[a]	1889.9	1889.9	1894.4	1891.2	1891.2	1893.6
gdb 2673	1848.0[a]	1848.2	1848.2	1848.7	1842.9	1842.9	1841.2
gdb 2674	1861.3[a]	1858.6	1858.6	1863.4	1858.6	1858.6	1860.2
gdb 2675	1890.8[a]	1896.0	1896.0	1899.9	1895.7	1895.7	1897.2
gdb 2676	1892.1[a]	1897.9	1897.9	1901.3	1893.2	1893.2	1895.5
gdb 2677	1899.0[a]	1901.4	1901.4	1905.4	1900.2	1900.2	1902.7
gdb 2678	1901.4[a]	1908.0	1908.0	1910.0	1910.9	1910.9	1912.4
gdb 2679	1894.5[a]	1897.9	1897.9	1897.9	1900.6	1900.5	1901.4
gdb 2680	1870.4[a]	1866.4	1866.4	1868.3	1867.2	1867.1	1869.1
gdb 2681	1867.6[a]	1866.6	1866.6	1867.6	1866.0	1866.0	1867.9
gdb 2682	1871.9[a]	1877.0	1877.0	1879.2	1880.0	1880.0	1881.1
gdb 2683	1899.9[a]	1907.5	1907.5	1907.7	1909.8	1909.8	1909.3
gdb 2684	1868.6[a]	1867.6	1867.6	1865.0	1864.9	1864.8	1862.0
gdb 2685	1872.5[a]	1874.1	1874.1	1875.1	1877.0	1877.0	1876.3
gdb 2686	1877.3[a]	1876.0	1876.0	1877.4	1877.8	1877.8	1878.7
gdb 2687	1875.3[a]	1872.6	1872.6	1874.9	1876.1	1876.1	1877.4
gdb 2688	1873.2[a]	1870.6	1870.6	1869.1	1867.0	1866.9	1865.0
gdb 2689	1855.4[a]	1853.7	1853.7	1856.6	1855.9	1855.8	1854.8
gdb 2690	1860.9[a]	1860.0	1860.0	1864.5	1855.4	1855.3	1857.9
gdb 2691	1864.8[a]	1868.2	1868.2	1875.7	1867.3	1867.2	1869.1
gdb 2692	1873.5[a]	1875.9	1875.9	1874.5	1872.1	1872.1	1870.3
gdb 2693	1869.3[a]	1868.9	1868.9	1870.8	1869.3	1869.2	1870.6
gdb 2694	1876.9[a]	1884.6	1884.6	1887.7	1885.1	1885.1	1885.7
gdb 2695	1906.1[a]	1914.2	1914.1	1915.5	1916.9	1916.9	1917.7
gdb 2696	1876.9[a]	1878.2	1878.2	1877.0	1875.4	1875.3	1873.3
gdb 2697	1897.7[a]	1884.6	1884.5	1885.6	1883.3	1883.2	1884.7
gdb 2698	1879.0[a]	1883.3	1883.3	1886.1	1885.1	1885.1	1885.3
gdb 2699	1893.0[a]	1901.8	1901.8	1903.2	1904.4	1904.4	1906.6
gdb 2700	1892.0[a]	1897.2	1897.2	1897.8	1900.8	1900.7	1901.7
gdb 2701	1897.8[a]	1905.3	1905.3	1907.0	1909.5	1909.5	1911.5
gdb 2702	1904.8[a]	1911.6	1911.6	1913.9	1913.4	1913.4	1914.8
gdb 2703	1917.8[a]	1928.4	1928.4	1929.1	1931.4	1931.3	1932.5
gdb 2704	1865.9[a]	1850.5	1850.5	1854.8	1851.7	1851.7	1852.8
gdb 2705	1859.6[a]	1840.2	1840.2	1843.3	1840.1	1840.1	1840.9
gdb 2706	1859.7[a]	1846.5	1846.4	1850.9	1849.4	1849.4	1850.4
gdb 2707	1861.6[a]	1845.9	1845.9	1850.1	1848.4	1848.4	1849.7
gdb 2708	1851.7[a]	1833.4	1833.4	1836.5	1834.4	1834.4	1835.7
gdb 2709	1839.3[a]	1814.8	1814.8	1817.3	1814.7	1814.7	1815.1
gdb 2710	1849.6[a]	1824.3	1824.3	1830.6	1827.0	1827.0	1829.2
gdb 2711	1837.8[a]	1813.3	1813.3	1816.6	1812.7	1812.7	1813.3
gdb 2712	1847.7[a]	1822.2	1822.2	1828.0	1825.1	1825.1	1827.3
gdb 2713	1838.1[a]	1830.0	1830.0	1828.6	1826.9	1826.9	1823.8
gdb 2714	1840.1[a]	1831.2	1831.2	1833.5	1835.0	1835.0	1834.6
gdb 2715	1837.1[a]	1828.9	1828.9	1827.9	1826.0	1826.0	1823.0
gdb 2716	1838.9[a]	1832.2	1832.2	1835.0	1836.6	1836.6	1836.4
gdb 2717	1885.1[a]	1877.5	1877.5	1879.2	1881.2	1881.2	1881.8
gdb 2718	1885.9[a]	1876.8	1876.8	1878.7	1880.6	1880.6	1881.0
gdb 2719	1895.8[a]	1871.9	1871.9	1872.4	1872.6	1872.6	1874.1
gdb 2720	1884.3[a]	1877.0	1877.0	1879.3	1881.4	1881.4	1882.2
gdb 2721	1879.1[a]	1858.6	1858.6	1862.3	1862.1	1862.1	1863.4
gdb 2722	1877.8[a]	1857.4	1857.4	1860.5	1861.2	1861.2	1862.2
gdb 2723	1866.9[a]	1854.9	1854.9	1854.6	1853.9	1853.8	1851.3
gdb 2724	1876.8[a]	1871.6	1871.6	1876.8	1871.3	1871.3	1873.3
gdb 2725	1875.5[a]	1872.6	1872.6	1874.8	1868.4	1868.4	1868.5
gdb 2726	1873.8[a]	1869.9	1869.9	1874.5	1869.9	1869.9	1872.0
gdb 2727	1867.9[a]	1852.9	1852.9	1856.6	1855.5	1855.5	1857.2

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2728	1858.5[a]	1847.3	1847.3	1847.5	1845.7	1845.7	1844.6
gdb 2729	1868.4[a]	1850.2	1850.1	1853.3	1853.2	1853.1	1854.8
gdb 2730	1856.1[a]	1847.3	1847.3	1845.8	1843.1	1843.1	1839.6
gdb 2731	1857.4[a]	1851.6	1851.6	1851.3	1847.6	1847.6	1844.0
gdb 2732	1851.7[a]	1841.8	1841.8	1837.7	1832.6	1832.6	1826.5
gdb 2733	1854.8[a]	1844.7	1844.7	1844.4	1842.4	1842.4	1839.6
gdb 2734	1857.8[a]	1852.3	1852.3	1855.9	1854.8	1854.8	1854.5
gdb 2735	1887.1[a]	1882.5	1882.5	1885.3	1885.0	1885.0	1886.0
gdb 2736	1886.0[a]	1882.2	1882.2	1885.0	1884.8	1884.7	1885.8
gdb 2737	1886.0[a]	1881.9	1881.9	1884.7	1884.9	1884.9	1885.9
gdb 2738	1877.7[a]	1873.4	1873.4	1874.5	1876.0	1876.0	1876.6
gdb 2739	1868.6[a]	1860.0	1860.0	1861.6	1860.3	1860.3	1861.9
gdb 2740	1872.7[a]	1861.3	1861.3	1862.4	1861.7	1861.7	1863.2
gdb 2741	1877.6[a]	1873.6	1873.6	1875.5	1876.7	1876.7	1877.4
gdb 2742	1851.3[a]	1848.6	1848.6	1844.7	1839.1	1839.1	1833.4
gdb 2743	1855.1[a]	1856.8	1856.8	1856.8	1852.2	1852.1	1848.8
gdb 2744	1851.9[a]	1847.1	1847.1	1850.5	1848.0	1848.0	1847.9
gdb 2745	1851.7[a]	1854.2	1854.2	1849.2	1840.9	1840.9	1843.9
gdb 2746	1848.3[a]	1834.5	1834.5	1836.9	1832.7	1832.7	1835.4
gdb 2747	1851.9[a]	1838.0	1838.0	1840.4	1835.8	1835.8	1838.9
gdb 2748	1863.0[a]	1855.7	1855.6	1857.9	1855.9	1855.9	1857.9
gdb 2749	1859.4[a]	1852.2	1852.1	1854.7	1852.6	1852.6	1854.5
gdb 2750	1859.8[a]	1843.2	1843.2	1845.9	1845.2	1845.0	1846.2
gdb 2751	1884.1[a]	1877.1	1877.1	1879.0	1880.7	1880.7	1881.5
gdb 2752	1882.7[a]	1877.4	1877.4	1880.0	1881.7	1881.7	1882.4
gdb 2753	1883.5[a]	1878.8	1878.8	1881.4	1881.3	1881.3	1881.9
gdb 2754	1870.1[a]	1852.2	1852.2	1856.9	1854.7	1854.7	1857.4
gdb 2755	1871.6[a]	1855.0	1855.0	1858.7	1858.6	1858.6	1860.7
gdb 2756	1902.7[a]	1905.4	1905.4	1906.3	1908.6	1908.6	1908.8
gdb 2757	1903.7[a]	1905.4	1905.4	1906.9	1909.2	1909.2	1909.4
gdb 2758	1894.3[a]	1898.0	1898.0	1899.4	1898.1	1898.1	1899.8
gdb 2759	1912.7[a]	1907.7	1907.7	1908.3	1906.0	1905.9	1908.1
gdb 2760	1887.8[a]	1884.6	1884.6	1887.0	1887.5	1887.5	1888.1
gdb 2761	1884.5[a]	1877.1	1877.1	1879.5	1880.8	1880.8	1881.1
gdb 2762	1883.6[a]	1878.3	1878.3	1879.9	1880.7	1880.6	1880.7
gdb 2763	1885.0[a]	1878.6	1878.6	1880.2	1881.9	1881.9	1882.3
gdb 2764	1875.9[a]	1855.2	1855.2	1858.8	1859.1	1859.1	1860.4
gdb 2765	1876.4[a]	1855.9	1855.9	1860.2	1859.4	1859.4	1861.4
gdb 2766	1834.0[a]	1815.0	1815.0	1816.2	1813.1	1813.1	1811.9
gdb 2767	1844.8[a]	1828.9	1828.9	1834.3	1831.5	1831.5	1832.9
gdb 2768	1861.6[a]	1849.1	1849.1	1852.9	1852.7	1852.7	1855.4
gdb 2769	1887.7[a]	1884.9	1884.9	1888.0	1886.3	1886.2	1887.5
gdb 2770	1886.6[a]	1883.0	1883.0	1885.4	1884.7	1884.7	1885.7
gdb 2771	1885.1[a]	1881.6	1881.5	1884.6	1884.1	1884.1	1885.2
gdb 2772	1870.6[a]	1862.1	1862.1	1864.2	1862.7	1862.6	1864.3
gdb 2773	1877.5[a]	1875.1	1875.1	1876.7	1877.0	1877.0	1877.8
gdb 2774	1877.8[a]	1874.3	1874.3	1875.9	1876.9	1876.8	1877.7
gdb 2775	1883.0[a]	1876.9	1876.9	1878.7	1878.8	1878.8	1879.3
gdb 2776	1883.8[a]	1878.4	1878.4	1880.6	1881.5	1881.5	1882.1
gdb 2777	1875.3[a]	1875.5	1875.5	1879.0	1877.8	1877.7	1879.2
gdb 2778	1873.7[a]	1870.1	1870.1	1872.1	1873.6	1873.6	1875.0
gdb 2779	1874.4[a]	1870.9	1870.9	1873.5	1874.8	1874.8	1876.3
gdb 2780	1868.4[a]	1858.9	1858.9	1860.9	1859.8	1859.8	1861.7
gdb 2781	1903.6[a]	1908.7	1908.7	1909.7	1911.2	1911.1	1911.1
gdb 2782	1915.0[a]	1911.2	1911.2	1912.1	1909.6	1909.6	1911.6
gdb 2783	1901.3[a]	1905.1	1905.1	1906.4	1908.5	1908.5	1908.7
gdb 2784	1883.1[a]	1878.8	1878.7	1881.0	1881.0	1881.0	1881.8
gdb 2785	1885.0[a]	1883.1	1883.1	1884.9	1884.7	1884.7	1884.5
gdb 2786	1888.9[a]	1887.8	1887.8	1890.8	1889.6	1889.6	1890.3
gdb 2787	1870.4[a]	1870.7	1870.7	1872.4	1873.7	1873.7	1874.9
gdb 2788	1875.3[a]	1874.3	1874.3	1876.1	1876.4	1876.4	1877.4
gdb 2789	1835.9[a]	1828.2	1828.2	1829.9	1832.3	1832.3	1832.2
gdb 2790	1831.8[a]	1821.6	1821.6	1824.8	1826.7	1826.7	1826.1
gdb 2791	1836.2[a]	1828.8	1828.8	1831.4	1833.6	1833.6	1833.7
gdb 2792	1838.8[a]	1830.6	1830.6	1832.6	1835.3	1835.2	1835.2

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2793	1842.8[a]	1832.6	1832.6	1832.8	1829.6	1829.6	1826.9
gdb 2794	1839.7[a]	1831.8	1831.8	1834.6	1836.7	1836.6	1836.7
gdb 2795	1859.4[a]	1852.7	1852.6	1853.9	1851.1	1851.1	1851.1
gdb 2796	1864.8[a]	1855.2	1855.2	1858.5	1857.4	1857.4	1858.9
gdb 2797	1847.7[a]	1840.4	1840.4	1843.4	1839.2	1839.2	1841.0
gdb 2798	1850.3[a]	1842.1	1842.1	1845.2	1841.1	1841.1	1842.8
gdb 2799	1850.2[a]	1843.7	1843.7	1847.2	1841.4	1841.4	1843.0
gdb 2800	1851.0[a]	1852.4	1852.4	1855.9	1853.6	1853.6	1854.5
gdb 2801	1849.5[a]	1842.3	1842.3	1841.5	1839.8	1839.8	1837.1
gdb 2802	1853.8[a]	1846.8	1846.8	1847.2	1843.1	1843.1	1840.1
gdb 2803	1852.3[a]	1851.4	1851.4	1854.3	1853.8	1853.8	1852.6
gdb 2804	1854.3[a]	1843.7	1843.6	1847.1	1843.3	1843.3	1846.0
gdb 2805	1846.8[a]	1848.5	1848.5	1852.9	1850.5	1850.5	1852.0
gdb 2806	1830.7[a]	1825.2	1825.2	1827.1	1828.6	1828.6	1828.1
gdb 2807	1858.2[a]	1852.5	1852.5	1855.0	1849.9	1849.9	1849.9
gdb 2808	1853.8[a]	1847.6	1847.6	1850.4	1846.9	1846.9	1846.7
gdb 2809	1864.8[a]	1854.8	1854.8	1858.8	1856.9	1856.9	1858.7
gdb 2810	1885.6[a]	1887.4	1887.4	1889.1	1878.5	1878.5	1881.0
gdb 2811	1879.7[a]	1878.9	1878.9	1881.8	1877.3	1877.3	1879.4
gdb 2812	1887.8[a]	1886.3	1886.3	1888.7	1884.3	1884.3	1885.3
gdb 2813	1870.8[a]	1870.5	1870.5	1874.0	1862.8	1862.8	1867.0
gdb 2814	1868.0[a]	1864.0	1864.0	1868.7	1865.6	1865.6	1867.3
gdb 2815	1869.5[a]	1868.3	1868.2	1871.6	1867.9	1867.8	1870.3
gdb 2816	1859.3[a]	1844.4	1844.4	1848.9	1847.9	1847.8	1849.4
gdb 2817	1857.3[a]	1843.6	1843.5	1847.9	1847.2	1847.2	1848.5
gdb 2818	1851.6[a]	1835.6	1835.6	1838.9	1835.7	1835.6	1836.9
gdb 2819	1849.4[a]	1833.0	1833.0	1835.5	1833.7	1833.7	1834.4
gdb 2820	1855.2[a]	1838.9	1838.9	1843.1	1843.0	1843.0	1844.6
gdb 2821	1851.6[a]	1824.8	1824.8	1831.2	1828.0	1828.0	1830.4
gdb 2822	1843.3[a]	1816.8	1816.8	1820.1	1817.5	1817.4	1818.4
gdb 2823	1847.4[a]	1821.0	1821.0	1827.0	1824.3	1824.3	1826.8
gdb 2824	1839.8[a]	1830.4	1830.4	1832.7	1834.9	1834.9	1834.8
gdb 2825	1840.4[a]	1830.7	1830.7	1833.2	1834.9	1834.8	1834.7
gdb 2826	1843.2[a]	1832.2	1832.2	1832.1	1828.7	1828.7	1826.3
gdb 2827	1840.7[a]	1831.3	1831.3	1830.6	1828.8	1828.8	1825.8
gdb 2828	1840.4[a]	1831.7	1831.7	1834.6	1836.6	1836.6	1836.7
gdb 2829	1853.9[a]	1843.1	1843.1	1842.2	1840.5	1840.4	1837.7
gdb 2830	1847.6[a]	1830.8	1830.8	1833.3	1833.4	1833.4	1833.8
gdb 2831	1853.9[a]	1843.1	1843.1	1842.9	1841.3	1841.3	1838.7
gdb 2832	1854.5[a]	1846.4	1846.4	1849.4	1850.1	1850.1	1850.1
gdb 2833	1858.7[a]	1848.2	1848.2	1853.5	1850.3	1850.3	1852.1
gdb 2834	1856.5[a]	1840.6	1840.6	1844.5	1844.0	1843.9	1845.5
gdb 2835	1847.6[a]	1823.1	1823.1	1830.5	1826.1	1826.1	1829.1
gdb 2836	1848.0[a]	1822.1	1822.1	1828.9	1825.5	1825.5	1827.9
gdb 2837	1849.7[a]	1823.0	1823.0	1829.7	1826.4	1826.4	1828.9
gdb 2838	1859.6[a]	1849.0	1849.0	1854.3	1851.0	1851.0	1852.6
gdb 2839	1858.4[a]	1844.4	1844.4	1849.5	1847.3	1847.3	1849.1
gdb 2840	1858.2[a]	1844.1	1844.1	1849.1	1847.3	1847.3	1848.7
gdb 2841	1848.0[a]	1824.1	1824.1	1830.9	1827.1	1827.1	1829.8
gdb 2842	1876.5[a]	1870.7	1870.7	1874.8	1868.6	1868.5	1870.8
gdb 2843	1872.9[a]	1868.4	1868.4	1872.7	1867.3	1867.3	1870.1
gdb 2844	1869.7[a]	1866.6	1866.6	1870.2	1865.4	1865.4	1867.7
gdb 2845	1877.5[a]	1873.8	1873.8	1878.1	1876.2	1876.2	1877.4
gdb 2846	1860.3[a]	1846.6	1846.6	1851.3	1849.6	1849.6	1851.0
gdb 2847	1861.9[a]	1849.5	1849.5	1853.9	1851.0	1851.0	1852.1
gdb 2848	1862.2[a]	1841.6	1841.6	1844.8	1841.8	1841.8	1842.5
gdb 2849	1860.9[a]	1845.3	1845.3	1849.5	1848.3	1848.3	1849.6
gdb 2850	1859.6[a]	1849.4	1849.4	1854.0	1850.6	1850.6	1851.9
gdb 2851	1861.0[a]	1851.1	1851.1	1856.5	1852.6	1852.6	1854.0
gdb 2852	1863.6[a]	1850.2	1850.2	1855.0	1852.0	1851.9	1852.9
gdb 2853	1871.3[a]	1867.9	1867.9	1872.1	1866.4	1866.4	1869.2
gdb 2854	1878.6[a]	1875.5	1875.5	1879.2	1877.0	1877.0	1878.2
gdb 2855	1866.0[a]	1848.5	1848.5	1853.8	1848.0	1848.0	1851.7
gdb 2856	1870.3[a]	1853.7	1853.7	1861.0	1856.4	1856.4	1859.7
gdb 2857	1870.3[a]	1861.2	1861.2	1865.0	1860.6	1860.6	1862.4

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2858	1871.8[a]	1862.8	1862.8	1866.6	1862.0	1862.0	1864.0
gdb 2859	1878.7[a]	1875.9	1875.8	1879.4	1876.7	1876.7	1877.7
gdb 2860	1856.9[a]	1848.7	1848.7	1850.0	1847.0	1847.0	1847.4
gdb 2861	1857.9[a]	1849.6	1849.6	1851.4	1848.5	1848.5	1848.8
gdb 2862	1862.9[a]	1851.7	1851.7	1855.8	1854.9	1854.9	1856.5
gdb 2863	1864.4[a]	1850.6	1850.6	1854.9	1852.6	1852.6	1853.3
gdb 2864	1859.4[a]	1840.4	1840.4	1843.2	1840.3	1840.3	1840.9
gdb 2865	1858.4[a]	1845.9	1845.9	1850.4	1849.0	1849.0	1850.1
gdb 2866	1859.8[a]	1845.8	1845.8	1849.6	1848.5	1848.5	1849.2
gdb 2867	1850.8[a]	1835.5	1835.5	1837.9	1835.7	1835.7	1836.2
gdb 2868	1897.6[a]	1889.0	1889.0	1892.2	1887.2	1887.2	1888.8
gdb 2869	1891.9[a]	1884.4	1884.4	1886.0	1877.7	1877.7	1880.2
gdb 2870	1902.9[a]	1895.1	1895.1	1899.0	1895.3	1895.3	1896.6
gdb 2871	1893.6[a]	1884.8	1884.8	1888.6	1883.2	1883.2	1885.1
gdb 2872	1900.8[a]	1892.8	1892.8	1896.2	1892.8	1892.8	1894.3
gdb 2873	1891.8[a]	1882.1	1882.1	1884.7	1880.4	1880.4	1882.2
gdb 2874	1896.8[a]	1886.8	1886.7	1890.1	1885.6	1885.6	1887.4
gdb 2875	1889.7[a]	1880.1	1880.1	1883.3	1879.8	1879.7	1881.8
gdb 2876	1889.6[a]	1881.1	1881.1	1882.8	1874.5	1874.5	1877.1
gdb 2877	1898.9[a]	1890.4	1890.4	1894.4	1892.2	1892.2	1894.0
gdb 2878	1890.3[a]	1891.2	1891.2	1893.8	1884.0	1884.0	1888.2
gdb 2879	1881.9[a]	1879.3	1879.3	1883.1	1875.3	1875.3	1879.2
gdb 2880	1891.7[a]	1888.8	1888.8	1891.8	1887.2	1887.2	1890.0
gdb 2881	1895.1[a]	1895.4	1895.4	1898.9	1893.2	1893.2	1895.3
gdb 2882	1894.6[a]	1892.6	1892.6	1896.1	1891.8	1891.8	1893.5
gdb 2883	1852.7[a]	1826.1	1826.1	1832.4	1829.1	1829.1	1831.3
gdb 2884	1850.3[a]	1824.5	1824.5	1829.6	1827.4	1827.4	1829.2
gdb 2885	1841.9[a]	1816.4	1816.4	1819.4	1816.7	1816.6	1817.4
gdb 2886	1850.8[a]	1824.1	1824.1	1830.0	1827.1	1827.1	1829.0
gdb 2887	1842.1[a]	1817.5	1817.5	1820.7	1817.3	1817.3	1817.5
gdb 2888	1867.7[a]	1855.3	1855.3	1860.0	1852.5	1852.5	1854.9
gdb 2889	1864.7[a]	1853.0	1853.0	1856.7	1850.3	1850.3	1852.7
gdb 2890	1869.1[a]	1859.9	1859.9	1865.8	1860.2	1860.2	1863.3
gdb 2891	1867.4[a]	1856.2	1856.2	1859.5	1853.3	1853.3	1855.4
gdb 2892	1867.0[a]	1859.9	1859.9	1864.9	1857.0	1857.0	1859.5
gdb 2893	1868.1[a]	1856.4	1856.4	1860.4	1853.9	1853.9	1856.0
gdb 2894	1873.9[a]	1863.3	1863.3	1868.2	1863.8	1863.8	1866.2
gdb 2895	1855.2[a]	1841.9	1841.9	1844.4	1840.6	1840.6	1841.5
gdb 2896	1870.6[a]	1854.5	1854.5	1860.6	1856.8	1856.8	1859.1
gdb 2897	1892.5[a]	1895.0	1895.0	1898.6	1885.4	1885.4	1890.0
gdb 2898	1896.1[a]	1890.8	1890.8	1893.9	1887.5	1887.5	1890.2
gdb 2899	1894.8[a]	1894.2	1894.2	1899.4	1890.9	1890.9	1894.1
gdb 2900	1839.6[a]	1830.7	1830.7	1833.0	1835.2	1835.2	1835.0
gdb 2901	1840.1[a]	1831.2	1831.2	1833.6	1835.2	1835.2	1834.9
gdb 2902	1843.1[a]	1832.2	1832.2	1832.3	1828.7	1828.7	1826.3
gdb 2903	1840.6[a]	1832.4	1832.4	1835.1	1837.4	1837.4	1837.0
gdb 2904	1841.0[a]	1832.4	1832.4	1831.7	1830.3	1830.3	1827.0
gdb 2905	1878.4[a]	1873.9	1873.9	1873.4	1869.8	1869.8	1866.9
gdb 2906	1874.7[a]	1868.9	1868.9	1867.9	1865.9	1865.9	1863.5
gdb 2907	1871.7[a]	1874.4	1874.4	1875.7	1876.3	1876.2	1875.6
gdb 2908	1863.9[a]	1851.6	1851.6	1853.3	1847.0	1847.0	1846.2
gdb 2909	1863.9[a]	1859.0	1859.0	1863.8	1859.3	1859.3	1860.6
gdb 2910	1873.2[a]	1870.2	1870.2	1868.9	1867.1	1867.1	1864.6
gdb 2911	1864.9[a]	1863.8	1863.8	1865.8	1864.3	1864.3	1865.3
gdb 2912	1876.3[a]	1869.2	1869.2	1868.2	1866.7	1866.7	1864.4
gdb 2913	1872.9[a]	1872.5	1872.5	1874.6	1875.7	1875.6	1875.5
gdb 2914	1870.9[a]	1866.7	1866.7	1870.0	1864.8	1864.8	1867.2
gdb 2915	1879.4[a]	1875.3	1875.3	1878.8	1873.0	1872.9	1874.6
gdb 2916	1871.6[a]	1867.5	1867.5	1871.2	1865.5	1865.5	1867.7
gdb 2917	1882.8[a]	1878.9	1878.9	1882.7	1879.2	1879.2	1879.8
gdb 2918	1872.7[a]	1869.3	1869.3	1872.0	1867.4	1867.4	1869.2
gdb 2919	1870.8[a]	1864.6	1864.6	1867.5	1863.5	1863.5	1866.0
gdb 2920	1870.3[a]	1866.7	1866.7	1870.2	1865.9	1865.9	1868.0
gdb 2921	1868.7[a]	1861.0	1861.0	1864.8	1861.4	1861.4	1864.1
gdb 2922	1877.3[a]	1872.7	1872.7	1876.7	1875.7	1875.7	1876.7

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2923	1865.7[a]	1848.2	1848.2	1853.1	1847.0	1847.0	1850.5
gdb 2924	1867.3[a]	1850.3	1850.3	1854.9	1849.2	1849.2	1852.5
gdb 2925	1861.7[a]	1845.0	1844.9	1851.6	1843.5	1843.5	1848.2
gdb 2926	1875.3[a]	1857.5	1857.5	1863.9	1859.4	1859.4	1861.9
gdb 2927	1868.0[a]	1848.9	1848.9	1853.5	1848.0	1848.0	1851.3
gdb 2928	1867.6[a]	1847.6	1847.6	1852.7	1847.0	1847.0	1850.0
gdb 2929	1876.4[a]	1855.0	1855.0	1859.8	1857.5	1857.5	1859.4
gdb 2930	1846.6[a]	1837.4	1837.4	1840.3	1836.6	1836.5	1838.5
gdb 2931	1854.5[a]	1840.7	1840.7	1844.0	1840.1	1840.0	1842.8
gdb 2932	1847.8[a]	1838.9	1838.9	1842.4	1838.5	1838.4	1840.4
gdb 2933	1847.7[a]	1838.4	1838.4	1841.9	1838.3	1838.3	1840.4
gdb 2934	1850.4[a]	1846.3	1846.3	1850.3	1848.8	1848.8	1849.9
gdb 2935	1859.3[a]	1843.2	1843.2	1848.3	1836.8	1836.8	1843.3
gdb 2936	1863.3[a]	1846.3	1846.3	1851.6	1846.1	1846.1	1850.2
gdb 2937	1861.2[a]	1844.6	1844.6	1849.5	1845.1	1845.1	1849.2
gdb 2938	1888.8[a]	1887.6	1887.6	1890.6	1889.3	1889.3	1890.0
gdb 2939	1876.3[a]	1874.4	1874.4	1879.3	1874.2	1874.2	1875.8
gdb 2940	1887.8[a]	1884.7	1884.7	1887.2	1887.7	1887.6	1888.3
gdb 2941	1888.1[a]	1887.6	1887.6	1889.8	1887.8	1887.8	1888.5
gdb 2942	1886.8[a]	1884.7	1884.7	1888.7	1885.7	1885.7	1887.1
gdb 2943	1886.1[a]	1884.8	1884.8	1888.3	1886.4	1886.4	1887.4
gdb 2944	1885.6[a]	1881.8	1881.8	1884.5	1883.9	1883.9	1885.0
gdb 2945	1877.3[a]	1874.4	1874.4	1879.5	1873.4	1873.3	1875.2
gdb 2946	1870.6[a]	1867.7	1867.7	1872.3	1867.5	1867.5	1869.5
gdb 2947	1875.1[a]	1875.2	1875.2	1879.3	1873.6	1873.6	1875.1
gdb 2948	1886.0[a]	1885.0	1885.0	1887.1	1887.3	1887.2	1888.0
gdb 2949	1878.2[a]	1876.2	1876.2	1878.4	1875.5	1875.5	1878.0
gdb 2950	1886.4[a]	1883.2	1883.2	1885.6	1886.5	1886.5	1887.3
gdb 2951	1897.6[a]	1906.2	1906.2	1906.4	1909.4	1909.4	1909.7
gdb 2952	1898.5[a]	1905.6	1905.6	1907.4	1907.9	1907.9	1908.0
gdb 2953	1909.6[a]	1907.1	1907.1	1908.1	1905.6	1905.6	1907.7
gdb 2954	1892.4[a]	1891.6	1891.6	1894.9	1892.9	1892.9	1895.3
gdb 2955	1896.0[a]	1887.8	1887.8	1889.9	1886.0	1886.0	1888.7
gdb 2956	1901.3[a]	1906.5	1906.5	1907.4	1910.0	1910.0	1910.5
gdb 2957	1901.8[a]	1906.3	1906.3	1907.6	1910.2	1910.2	1910.9
gdb 2958	1912.9[a]	1908.4	1908.4	1908.9	1907.4	1907.4	1909.6
gdb 2959	1910.6[a]	1905.5	1905.5	1906.2	1904.2	1904.2	1906.6
gdb 2960	1899.3[a]	1894.6	1894.6	1896.9	1895.4	1895.3	1896.7
gdb 2961	1893.1[a]	1890.3	1890.3	1891.3	1887.5	1887.5	1887.7
gdb 2962	1902.4[a]	1894.6	1894.6	1897.8	1895.9	1895.9	1897.5
gdb 2963	1872.6[a]	1871.5	1871.5	1873.6	1873.7	1873.7	1875.0
gdb 2964	1877.1[a]	1876.0	1876.0	1877.9	1877.1	1877.1	1877.4
gdb 2965	1868.4[a]	1861.2	1861.2	1863.2	1860.9	1860.8	1862.4
gdb 2966	1887.5[a]	1883.8	1883.8	1886.3	1886.7	1886.7	1887.3
gdb 2967	1903.5[a]	1906.8	1906.8	1907.7	1908.8	1908.8	1908.2
gdb 2968	1893.7[a]	1899.1	1899.0	1901.0	1898.7	1898.7	1900.2
gdb 2969	1901.2[a]	1905.1	1905.1	1906.2	1908.0	1908.0	1907.9
gdb 2970	1876.5[a]	1877.9	1877.9	1880.9	1879.6	1879.6	1880.8
gdb 2971	1871.1[a]	1859.7	1859.7	1861.1	1859.9	1859.9	1861.6
gdb 2972	1877.1[a]	1873.9	1873.9	1875.4	1876.2	1876.2	1877.0
gdb 2973	1894.5[a]	1891.3	1891.3	1895.4	1893.0	1893.0	1895.7
gdb 2974	1881.4[a]	1878.3	1878.3	1880.8	1877.3	1877.3	1879.6
gdb 2975	1891.4[a]	1887.2	1887.2	1891.1	1888.9	1888.9	1891.4
gdb 2976	1877.6[a]	1876.2	1876.2	1878.8	1875.5	1875.5	1878.0
gdb 2977	1885.3[a]	1884.1	1884.1	1886.9	1886.3	1886.3	1887.1
gdb 2978	1874.9[a]	1875.7	1875.7	1877.3	1879.0	1879.0	1879.5
gdb 2979	1870.0[a]	1863.8	1863.7	1865.8	1864.2	1864.2	1865.4
gdb 2980	1894.8[a]	1891.8	1891.8	1896.1	1893.3	1893.3	1896.0
gdb 2981	1885.6[a]	1883.9	1883.9	1885.2	1881.0	1881.0	1881.6
gdb 2982	1862.1[a]	1852.8	1852.8	1851.7	1844.4	1844.4	1842.1
gdb 2983	1871.9[a]	1861.0	1861.0	1862.5	1855.9	1855.9	1854.8
gdb 2984	1865.2[a]	1861.3	1861.3	1864.3	1857.7	1857.6	1858.0
gdb 2985	1883.7[a]	1882.0	1882.0	1883.6	1879.4	1879.4	1881.1
gdb 2986	1890.8[a]	1888.1	1888.1	1891.2	1889.2	1889.1	1891.8
gdb 2987	1882.7[a]	1882.7	1882.7	1886.0	1878.2	1878.1	1880.0

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 2988	1910.1[a]	1909.8	1909.8	1912.1	1905.7	1905.7	1909.3
gdb 2989	1899.6[a]	1902.1	1902.1	1903.8	1899.4	1899.4	1900.9
gdb 2990	1903.7[a]	1908.5	1908.4	1910.4	1908.4	1908.4	1909.4
gdb 2991	1841.6[a]	1827.9	1827.9	1827.3	1822.6	1822.5	1820.9
gdb 2992	1846.0[a]	1840.2	1840.2	1839.2	1837.8	1837.8	1835.5
gdb 2993	1844.7[a]	1832.2	1832.2	1835.0	1833.0	1833.0	1833.7
gdb 2994	1873.6[a]	1870.5	1870.5	1872.3	1873.5	1873.5	1874.6
gdb 2995	1873.9[a]	1871.2	1871.2	1873.7	1874.8	1874.8	1876.1
gdb 2996	1864.7[a]	1856.7	1856.7	1858.3	1857.2	1857.2	1859.1
gdb 2997	1884.4[a]	1890.9	1890.9	1892.8	1890.6	1890.6	1892.5
gdb 2998	1892.7[a]	1895.0	1895.0	1896.4	1898.8	1898.7	1899.6
gdb 2999	1886.9[a]	1877.0	1876.9	1878.4	1875.1	1875.1	1878.4
gdb 3000	1864.6[a]	1856.8	1856.8	1859.0	1858.4	1858.4	1860.7
gdb 3001	1867.9[a]	1867.8	1867.8	1869.7	1872.2	1872.2	1873.9
gdb 3002	1898.3[a]	1895.6	1895.6	1899.6	1896.8	1896.8	1899.1
gdb 3003	1893.6[a]	1890.9	1890.9	1891.9	1888.3	1888.3	1888.7
gdb 3004	1906.0[a]	1895.6	1895.6	1897.5	1892.9	1892.9	1895.5
gdb 3005	1901.7[a]	1894.0	1894.0	1897.2	1895.7	1895.7	1897.5
gdb 3006	1877.1[a]	1873.3	1873.3	1877.1	1873.4	1873.4	1874.8
gdb 3007	1872.8[a]	1871.3	1871.3	1873.4	1867.5	1867.5	1867.6
gdb 3008	1867.5[a]	1855.9	1855.9	1857.6	1850.8	1850.8	1849.9
gdb 3009	1863.2[a]	1858.4	1858.4	1860.4	1854.9	1854.9	1854.3
gdb 3010	1864.0[a]	1853.7	1853.6	1854.2	1849.2	1849.1	1847.7
gdb 3011	1856.4[a]	1847.9	1847.9	1846.1	1839.1	1839.1	1836.3
gdb 3012	1866.3[a]	1859.4	1859.4	1863.0	1860.1	1860.1	1861.0
gdb 3013	1847.6[a]	1824.8	1824.8	1826.6	1821.9	1821.9	1820.3
gdb 3014	1835.1[a]	1822.3	1822.2	1827.4	1820.7	1820.6	1818.7
gdb 3015	1842.7[a]	1819.1	1819.1	1819.8	1817.1	1817.1	1815.1
gdb 3016	1831.0[a]	1814.9	1814.9	1812.2	1807.9	1807.8	1802.8
gdb 3017	1846.9[a]	1828.3	1828.3	1833.6	1831.5	1831.5	1832.6
gdb 3018	1866.5[a]	1851.9	1851.9	1855.1	1855.2	1855.2	1857.4
gdb 3019	1864.6[a]	1848.9	1848.9	1853.0	1852.6	1852.5	1855.0
gdb 3020	1855.4[a]	1845.8	1845.8	1846.4	1845.0	1845.0	1844.8
gdb 3021	1872.5[a]	1871.2	1871.2	1873.3	1867.6	1867.6	1867.5
gdb 3022	1876.8[a]	1873.3	1873.2	1877.1	1873.5	1873.5	1874.9
gdb 3023	1889.6[a]	1886.3	1886.3	1889.7	1881.5	1881.5	1883.3
gdb 3024	1892.0[a]	1891.7	1891.7	1896.6	1891.0	1891.0	1893.2
gdb 3025	1897.6[a]	1895.7	1895.7	1899.7	1896.8	1896.8	1899.4
gdb 3026	1910.0[a]	1898.5	1898.5	1900.2	1896.1	1896.1	1898.6
gdb 3027	1899.3[a]	1895.3	1895.3	1898.7	1896.8	1896.8	1899.0
gdb 3028	1893.1[a]	1890.0	1890.0	1890.8	1887.7	1887.7	1888.0
gdb 3029	1886.9[a]	1885.4	1885.4	1888.8	1881.2	1881.2	1883.1
gdb 3030	1893.4[a]	1892.2	1892.2	1897.1	1891.4	1891.4	1893.7
gdb 3031	1871.9[a]	1858.6	1858.6	1861.9	1861.0	1861.0	1862.1
gdb 3032	1859.3[a]	1850.5	1850.5	1851.2	1848.8	1848.7	1847.5
gdb 3033	1831.0[a]	1814.8	1814.8	1813.1	1807.4	1807.3	1803.4
gdb 3034	1842.6[a]	1821.4	1821.4	1823.3	1818.4	1818.3	1817.1
gdb 3035	1840.5[a]	1826.0	1826.0	1828.3	1823.6	1823.6	1821.7
gdb 3036	1859.7[a]	1847.9	1847.9	1851.1	1850.7	1850.7	1852.4
gdb 3037	1851.7[a]	1842.8	1842.7	1843.0	1841.2	1841.2	1840.1
gdb 3038	1882.8[a]	1878.3	1878.3	1880.8	1876.4	1876.4	1879.2
gdb 3039	1883.1[a]	1880.2	1880.2	1882.2	1878.1	1878.1	1880.3
gdb 3040	1885.6[a]	1882.3	1882.3	1883.0	1879.4	1879.4	1879.6
gdb 3041	1895.0[a]	1888.9	1888.9	1891.4	1889.5	1889.5	1891.5
gdb 3042	1876.6[a]	1851.3	1851.3	1855.1	1850.3	1850.3	1855.2
gdb 3043	1854.6[a]	1844.3	1844.3	1845.5	1843.6	1843.6	1843.8
gdb 3044	1864.9[a]	1850.4	1850.4	1855.2	1854.0	1854.0	1856.8
gdb 3045	1837.4[a]	1819.9	1819.9	1824.6	1816.1	1816.1	1819.6
gdb 3046	1835.5[a]	1822.9	1822.8	1825.1	1818.0	1818.0	1819.0
gdb 3047	1848.2[a]	1838.3	1838.3	1844.5	1836.7	1836.7	1840.1
gdb 3048	1847.8[a]	1834.8	1834.8	1838.4	1833.4	1833.4	1836.1
gdb 3049	1847.9[a]	1834.5	1834.5	1839.8	1833.2	1833.2	1836.3
gdb 3050	1851.0[a]	1840.9	1840.9	1845.1	1838.9	1838.9	1839.7
gdb 3051	1836.9[a]	1820.9	1820.9	1825.0	1815.6	1815.6	1820.0
gdb 3052	1837.1[a]	1824.9	1824.9	1826.5	1819.4	1819.4	1819.8

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3053	1827.1[a]	1814.6	1814.6	1816.4	1810.9	1810.9	1811.8
gdb 3054	1845.5[a]	1830.1	1830.1	1835.8	1830.0	1830.0	1833.6
gdb 3055	1844.4[a]	1829.0	1829.0	1834.3	1829.3	1829.3	1832.9
gdb 3056	1845.4[a]	1828.5	1828.5	1834.4	1828.3	1828.3	1831.8
gdb 3057	1837.3[a]	1822.9	1822.9	1825.1	1822.1	1822.1	1821.1
gdb 3058	1895.3[a]	1893.6	1893.6	1896.5	1894.5	1894.4	1896.5
gdb 3059	1894.6[a]	1891.5	1891.5	1894.0	1892.6	1892.6	1894.2
gdb 3060	1887.3[a]	1886.4	1886.4	1887.7	1883.5	1883.5	1884.1
gdb 3061	1892.3[a]	1897.1	1897.1	1900.4	1894.8	1894.8	1898.0
gdb 3062	1910.5[a]	1905.6	1905.6	1907.6	1901.9	1901.9	1905.5
gdb 3063	1896.7[a]	1898.4	1898.4	1900.0	1896.1	1896.1	1897.2
gdb 3064	1901.8[a]	1906.8	1906.8	1908.9	1907.6	1907.6	1908.9
gdb 3065	1869.1[a]	1869.4	1869.4	1871.4	1866.2	1866.2	1866.1
gdb 3066	1883.9[a]	1883.9	1883.9	1887.3	1880.5	1880.5	1882.3
gdb 3067	1880.5[a]	1880.2	1880.2	1882.6	1875.6	1875.6	1877.5
gdb 3068	1882.2[a]	1881.0	1881.0	1884.8	1877.0	1877.0	1879.3
gdb 3069	1886.5[a]	1888.8	1888.8	1894.6	1887.7	1887.6	1890.6
gdb 3070	1883.1[a]	1881.9	1881.9	1883.3	1879.4	1879.4	1880.9
gdb 3071	1881.3[a]	1879.0	1879.0	1882.2	1877.6	1877.6	1880.7
gdb 3072	1892.8[a]	1886.6	1886.6	1890.9	1887.9	1887.9	1890.9
gdb 3073	1857.8[a]	1850.6	1850.6	1851.7	1846.7	1846.7	1846.2
gdb 3074	1867.3[a]	1855.6	1855.5	1857.2	1851.0	1851.0	1850.3
gdb 3075	1854.8[a]	1845.6	1845.6	1844.1	1837.2	1837.2	1834.7
gdb 3076	1857.5[a]	1851.2	1851.2	1853.0	1849.5	1849.5	1849.7
gdb 3077	1864.9[a]	1855.7	1855.7	1859.3	1858.1	1858.0	1859.5
gdb 3078	1861.8[a]	1852.0	1852.0	1850.4	1843.9	1843.8	1841.2
gdb 3079	1867.7[a]	1857.6	1857.6	1862.7	1857.0	1857.0	1859.1
gdb 3080	1872.3[a]	1860.8	1860.8	1862.5	1856.1	1856.0	1855.3
gdb 3081	1868.1[a]	1861.6	1861.6	1864.6	1857.9	1857.9	1858.0
gdb 3082	1870.5[a]	1863.9	1863.9	1863.0	1855.9	1855.9	1854.7
gdb 3083	1864.3[a]	1866.3	1866.3	1871.6	1864.4	1864.4	1867.7
gdb 3084	1878.7[a]	1874.0	1874.0	1875.1	1868.6	1868.6	1867.5
gdb 3085	1873.4[a]	1870.9	1870.9	1873.9	1868.4	1868.4	1869.2
gdb 3086	1851.4[a]	1849.6	1849.6	1851.7	1842.1	1842.1	1843.5
gdb 3087	1858.2[a]	1853.2	1853.2	1857.2	1849.1	1849.1	1851.1
gdb 3088	1855.7[a]	1853.6	1853.5	1857.5	1849.4	1849.4	1850.9
gdb 3089	1861.0[a]	1850.4	1850.4	1853.0	1843.7	1843.7	1846.0
gdb 3090	1871.5[a]	1856.8	1856.8	1862.2	1853.8	1853.8	1857.8
gdb 3091	1868.6[a]	1864.7	1864.7	1869.1	1861.1	1861.1	1862.6
gdb 3092	1860.9[a]	1849.0	1849.0	1852.6	1851.5	1851.4	1854.1
gdb 3093	1861.8[a]	1848.1	1848.1	1851.6	1849.8	1849.8	1851.4
gdb 3094	1849.6[a]	1843.7	1843.7	1844.3	1841.5	1841.5	1841.3
gdb 3095	1828.8[a]	1811.7	1811.7	1813.3	1806.4	1806.3	1806.4
gdb 3096	1825.6[a]	1810.2	1810.2	1811.6	1805.5	1805.5	1806.1
gdb 3097	1847.3[a]	1824.4	1824.3	1829.7	1824.0	1824.0	1827.6
gdb 3098	1841.5[a]	1820.8	1820.8	1825.7	1820.4	1820.4	1824.3
gdb 3099	1834.4[a]	1824.4	1824.3	1826.9	1821.8	1821.8	1821.6
gdb 3100	1868.1[a]	1857.6	1857.6	1862.1	1858.6	1860.6	1860.7
gdb 3101	1853.6[a]	1847.2	1847.2	1847.9	1846.2	1846.2	1845.5
gdb 3102	1826.3[a]	1811.5	1811.5	1809.6	1804.8	1804.8	1801.0
gdb 3103	1838.0[a]	1818.9	1818.9	1820.7	1816.4	1816.3	1815.8
gdb 3104	1829.7[a]	1818.9	1818.9	1821.9	1816.1	1816.1	1814.9
gdb 3105	1871.1[a]	1848.5	1848.2	1852.3	1847.8	1847.6	1853.0
gdb 3106	1848.1[a]	1839.2	1839.2	1840.1	1839.3	1839.3	1839.4
gdb 3107	1860.4[a]	1847.3	1847.3	1852.5	1850.4	1850.3	1853.5
gdb 3108	1884.3[a]	1884.0	1884.0	1887.4	1880.7	1880.7	1882.4
gdb 3109	1874.5[a]	1879.7	1879.7	1883.7	1876.5	1876.5	1880.0
gdb 3110	1881.5[a]	1880.4	1880.3	1884.5	1878.0	1878.0	1880.4
gdb 3111	1900.3[a]	1902.8	1902.8	1904.3	1900.8	1900.8	1902.4
gdb 3112	1910.9[a]	1908.5	1908.5	1910.6	1905.1	1905.0	1908.7
gdb 3113	1905.3[a]	1909.4	1909.4	1911.6	1910.3	1910.3	1911.8
gdb 3114	1885.5[a]	1878.8	1878.8	1881.5	1877.3	1877.3	1879.5
gdb 3115	1856.2[a]	1848.7	1848.7	1848.6	1844.6	1844.6	1841.3
gdb 3116	1854.8[a]	1849.8	1849.8	1849.9	1845.6	1845.6	1842.4
gdb 3117	1855.4[a]	1845.1	1845.1	1844.8	1842.5	1842.5	1839.4

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3118	1852.1[a]	1841.9	1841.9	1838.0	1832.6	1832.6	1826.7
gdb 3119	1858.1[a]	1853.4	1853.4	1857.2	1855.8	1855.8	1855.6
gdb 3120	1874.7[a]	1876.2	1876.2	1879.0	1877.7	1877.7	1879.2
gdb 3121	1873.4[a]	1872.3	1872.3	1874.8	1875.5	1875.5	1876.8
gdb 3122	1873.8[a]	1871.0	1871.0	1869.6	1867.4	1867.4	1865.6
gdb 3123	1887.3[a]	1883.7	1883.7	1882.1	1878.7	1878.7	1876.2
gdb 3124	1888.0[a]	1887.7	1887.7	1890.7	1889.1	1889.1	1889.7
gdb 3125	1902.1[a]	1908.3	1908.3	1908.9	1910.0	1910.0	1909.7
gdb 3126	1913.1[a]	1910.0	1910.0	1910.6	1908.5	1908.5	1910.5
gdb 3127	1901.8[a]	1907.6	1907.6	1909.2	1910.8	1910.8	1911.3
gdb 3128	1903.9[a]	1906.1	1906.1	1904.1	1902.8	1902.8	1900.4
gdb 3129	1879.4[a]	1878.2	1878.2	1880.9	1879.8	1879.8	1880.7
gdb 3130	1879.9[a]	1879.1	1879.1	1880.9	1879.9	1879.9	1880.4
gdb 3131	1873.4[a]	1870.3	1870.3	1868.8	1866.1	1866.1	1863.8
gdb 3132	1902.9[a]	1909.4	1909.4	1911.5	1910.5	1910.5	1910.3
gdb 3133	1900.6[a]	1908.5	1908.5	1909.5	1909.6	1909.6	1908.9
gdb 3134	1896.6[a]	1900.1	1900.1	1898.2	1895.7	1895.7	1892.8
gdb 3135	1886.1[a]	1885.9	1885.9	1884.9	1880.6	1880.6	1877.6
gdb 3136	1900.1[a]	1908.4	1908.4	1909.3	1909.5	1909.5	1908.9
gdb 3137	1899.3[a]	1904.1	1904.1	1902.3	1900.1	1900.1	1897.5
gdb 3138	1875.2[a]	1879.1	1879.1	1882.4	1878.7	1878.7	1879.8
gdb 3139	1877.3[a]	1877.6	1877.6	1879.4	1877.9	1877.9	1878.0
gdb 3140	1870.5[a]	1869.4	1869.4	1868.2	1864.5	1864.5	1862.8
gdb 3141	1850.0[a]	1840.7	1840.7	1840.7	1833.1	1833.1	1832.1
gdb 3142	1846.2[a]	1838.4	1838.4	1838.0	1831.0	1831.0	1830.3
gdb 3143	1859.9[a]	1851.5	1851.5	1855.6	1849.3	1849.2	1850.7
gdb 3144	1850.5[a]	1846.2	1846.2	1848.9	1843.9	1843.9	1845.8
gdb 3145	1852.1[a]	1852.2	1852.1	1853.5	1846.6	1846.6	1844.7
gdb 3146	1879.9[a]	1884.0	1883.9	1887.3	1884.6	1884.6	1885.0
gdb 3147	1873.5[a]	1874.4	1874.4	1873.2	1870.1	1870.1	1867.7
gdb 3148	1846.1[a]	1838.9	1838.9	1835.2	1829.5	1829.5	1824.1
gdb 3149	1849.6[a]	1845.3	1845.2	1845.9	1841.0	1840.9	1838.8
gdb 3150	1851.8[a]	1848.1	1848.1	1848.6	1843.7	1843.6	1840.7
gdb 3151	1887.5[a]	1879.1	1879.1	1880.5	1876.8	1876.7	1879.8
gdb 3152	1867.8[a]	1866.7	1866.7	1865.7	1863.8	1863.8	1862.4
gdb 3153	1871.9[a]	1873.5	1873.5	1877.0	1876.3	1876.3	1878.0
gdb 3154	1874.3[a]	1874.7	1874.7	1874.3	1869.7	1869.7	1866.9
gdb 3155	1882.3[a]	1877.4	1877.4	1876.9	1872.8	1872.8	1869.6
gdb 3156	1871.0[a]	1866.1	1866.1	1861.7	1856.4	1856.4	1851.1
gdb 3157	1877.8[a]	1870.6	1870.6	1869.8	1867.6	1867.6	1864.9
gdb 3158	1873.5[a]	1878.2	1878.2	1881.3	1880.3	1880.3	1880.1
gdb 3159	1875.1[a]	1874.5	1874.5	1873.9	1869.5	1869.5	1866.6
gdb 3160	1877.8[a]	1876.9	1876.9	1876.2	1871.9	1871.9	1868.6
gdb 3161	1876.2[a]	1870.2	1870.1	1869.4	1866.8	1866.8	1864.4
gdb 3162	1871.3[a]	1865.7	1865.6	1861.2	1855.9	1855.9	1850.7
gdb 3163	1874.1[a]	1877.1	1877.1	1879.7	1878.8	1878.8	1878.3
gdb 3164	1870.6[a]	1863.3	1863.3	1862.6	1854.8	1854.8	1853.6
gdb 3165	1875.2[a]	1873.6	1873.6	1877.0	1869.9	1869.9	1871.1
gdb 3166	1878.0[a]	1874.9	1874.9	1875.8	1869.2	1869.2	1867.7
gdb 3167	1872.9[a]	1867.5	1867.5	1867.1	1860.0	1860.0	1859.4
gdb 3168	1870.5[a]	1865.7	1865.7	1865.2	1858.2	1858.2	1857.4
gdb 3169	1876.4[a]	1875.8	1875.8	1879.3	1873.5	1873.5	1875.0
gdb 3170	1874.8[a]	1873.8	1873.8	1876.0	1871.5	1871.5	1873.1
gdb 3171	1876.6[a]	1879.2	1879.2	1878.9	1873.8	1873.8	1871.5
gdb 3172	1873.0[a]	1868.3	1868.3	1863.9	1858.8	1858.8	1853.3
gdb 3173	1873.9[a]	1876.8	1876.8	1876.2	1872.1	1872.1	1868.6
gdb 3174	1869.4[a]	1871.1	1871.1	1874.6	1871.1	1871.1	1872.1
gdb 3175	1875.3[a]	1876.0	1876.0	1875.6	1871.3	1871.3	1868.1
gdb 3176	1885.6[a]	1891.5	1891.5	1893.4	1890.6	1890.6	1892.6
gdb 3177	1893.7[a]	1893.2	1893.2	1891.6	1890.0	1890.0	1888.5
gdb 3178	1895.6[a]	1900.8	1900.8	1903.1	1902.6	1902.5	1903.1
gdb 3179	1873.2[a]	1867.6	1867.6	1863.2	1858.9	1858.9	1853.4
gdb 3180	1876.8[a]	1874.0	1874.0	1873.0	1870.5	1870.4	1866.7
gdb 3181	1865.2[a]	1867.4	1867.4	1869.7	1866.9	1866.9	1868.1
gdb 3182	1887.0[a]	1885.1	1885.1	1883.6	1880.7	1880.6	1878.1

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3183	1907.4[a]	1906.4	1906.4	1906.9	1903.2	1903.2	1905.2
gdb 3184	1890.7[a]	1895.7	1895.7	1896.8	1895.1	1895.1	1896.8
gdb 3185	1898.1[a]	1901.2	1901.2	1898.8	1897.7	1897.7	1894.6
gdb 3186	1901.2[a]	1906.8	1906.8	1907.6	1908.2	1908.2	1907.5
gdb 3187	1859.7[a]	1845.0	1845.0	1849.7	1848.4	1848.4	1849.7
gdb 3188	1858.7[a]	1844.7	1844.7	1849.1	1848.0	1848.0	1849.2
gdb 3189	1858.4[a]	1837.4	1837.4	1840.8	1837.6	1837.6	1838.8
gdb 3190	1857.3[a]	1838.8	1838.8	1843.0	1843.3	1843.2	1844.6
gdb 3191	1851.4[a]	1831.7	1831.7	1834.6	1833.1	1833.1	1834.3
gdb 3192	1867.2[a]	1855.3	1855.3	1858.5	1852.4	1852.3	1854.0
gdb 3193	1873.4[a]	1860.3	1860.3	1864.7	1857.5	1857.5	1859.4
gdb 3194	1868.4[a]	1857.4	1857.3	1861.2	1854.5	1854.5	1856.2
gdb 3195	1864.3[a]	1853.3	1853.3	1855.7	1846.8	1846.8	1847.9
gdb 3196	1873.8[a]	1862.5	1862.5	1868.5	1862.8	1862.8	1865.8
gdb 3197	1862.7[a]	1858.1	1858.1	1862.3	1854.7	1854.7	1857.3
gdb 3198	1867.2[a]	1867.7	1867.7	1872.7	1866.7	1866.7	1869.2
gdb 3199	1870.0[a]	1858.3	1858.3	1861.6	1855.6	1855.6	1857.6
gdb 3200	1873.4[a]	1862.4	1862.4	1867.1	1859.8	1859.7	1862.0
gdb 3201	1873.0[a]	1862.9	1862.9	1869.1	1863.4	1863.4	1866.4
gdb 3202	1865.1[a]	1863.5	1863.5	1865.6	1864.2	1864.1	1865.3
gdb 3203	1876.3[a]	1872.5	1872.5	1871.3	1869.6	1869.6	1866.8
gdb 3204	1871.0[a]	1872.2	1872.2	1874.2	1876.1	1876.1	1876.1
gdb 3205	1854.0[a]	1843.6	1843.6	1842.7	1840.8	1840.8	1837.9
gdb 3206	1845.1[a]	1830.1	1830.1	1832.4	1832.0	1832.0	1832.3
gdb 3207	1854.8[a]	1844.2	1844.2	1843.9	1841.9	1841.9	1839.0
gdb 3208	1845.1[a]	1831.0	1831.0	1833.8	1833.1	1833.1	1833.4
gdb 3209	1855.0[a]	1847.1	1847.1	1850.1	1850.6	1850.6	1850.4
gdb 3210	1865.6[a]	1865.4	1865.4	1867.9	1867.0	1866.9	1867.9
gdb 3211	1872.8[a]	1871.3	1871.3	1869.9	1869.0	1869.0	1866.0
gdb 3212	1835.9[a]	1823.2	1823.2	1825.5	1818.4	1818.4	1819.5
gdb 3213	1850.9[a]	1835.7	1835.7	1841.3	1834.4	1834.4	1837.9
gdb 3214	1851.1[a]	1841.7	1841.7	1846.2	1840.0	1840.0	1841.4
gdb 3215	1849.7[a]	1835.8	1835.8	1839.5	1834.0	1833.9	1836.7
gdb 3216	1844.5[a]	1830.0	1830.0	1833.2	1826.8	1826.8	1829.6
gdb 3217	1852.2[a]	1846.2	1846.2	1848.9	1845.4	1845.4	1847.3
gdb 3218	1846.2[a]	1841.2	1841.2	1843.8	1840.8	1840.7	1843.0
gdb 3219	1850.3[a]	1840.3	1840.3	1844.1	1840.6	1840.6	1842.1
gdb 3220	1858.1[a]	1854.0	1854.0	1858.7	1850.4	1850.4	1853.7
gdb 3221	1864.0[a]	1864.8	1864.8	1870.4	1863.9	1863.9	1866.5
gdb 3222	1863.3[a]	1854.3	1854.3	1858.5	1851.9	1851.9	1854.3
gdb 3223	1868.1[a]	1859.8	1859.8	1867.0	1860.4	1860.4	1863.9
gdb 3224	1861.6[a]	1860.8	1860.8	1863.2	1861.0	1861.0	1862.3
gdb 3225	1868.7[a]	1869.7	1869.7	1871.6	1873.6	1873.6	1873.7
gdb 3226	1894.7[a]	1885.3	1885.3	1888.9	1883.8	1883.8	1885.7
gdb 3227	1889.9[a]	1880.4	1880.4	1883.7	1879.8	1879.8	1881.8
gdb 3228	1887.2[a]	1879.4	1879.4	1881.5	1872.4	1872.4	1875.3
gdb 3229	1899.3[a]	1889.9	1889.9	1892.5	1891.4	1891.3	1892.4
gdb 3230	1856.4[a]	1842.5	1842.5	1847.1	1845.9	1845.9	1847.4
gdb 3231	1858.3[a]	1844.3	1844.3	1848.6	1847.6	1847.6	1848.8
gdb 3232	1855.6[a]	1835.9	1835.9	1838.8	1835.9	1835.8	1836.9
gdb 3233	1854.7[a]	1838.9	1838.9	1843.1	1843.4	1843.3	1844.7
gdb 3234	1847.4[a]	1831.0	1831.0	1833.7	1831.3	1831.3	1832.4
gdb 3235	1848.1[a]	1830.4	1830.4	1833.2	1831.0	1831.0	1832.3
gdb 3236	1866.6[a]	1856.0	1856.0	1859.4	1852.7	1852.7	1854.7
gdb 3237	1873.5[a]	1860.8	1860.8	1865.1	1857.8	1857.8	1859.7
gdb 3238	1867.9[a]	1855.7	1855.7	1859.7	1852.8	1852.8	1854.9
gdb 3239	1864.0[a]	1852.6	1852.6	1855.4	1846.2	1846.2	1847.6
gdb 3240	1875.4[a]	1864.3	1864.3	1869.0	1863.9	1863.8	1866.4
gdb 3241	1878.2[a]	1874.7	1874.7	1877.8	1868.2	1868.2	1870.8
gdb 3242	1880.0[a]	1874.4	1874.4	1877.9	1867.6	1867.6	1870.5
gdb 3243	1888.0[a]	1882.2	1882.2	1887.3	1879.0	1879.0	1882.4
gdb 3244	1885.4[a]	1878.3	1878.3	1882.9	1874.9	1874.9	1878.9
gdb 3245	1888.1[a]	1882.7	1882.7	1886.3	1879.4	1879.4	1880.7
gdb 3246	1869.7[a]	1866.0	1866.0	1867.4	1865.0	1865.0	1866.1
gdb 3247	1864.7[a]	1863.7	1863.7	1867.8	1863.2	1863.2	1866.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3248	1864.2[a]	1857.8	1857.8	1863.1	1854.2	1854.2	1857.3
gdb 3249	1866.7[a]	1860.0	1860.0	1865.0	1856.6	1856.6	1859.2
gdb 3250	1862.8[a]	1858.1	1858.1	1863.0	1854.5	1854.5	1857.7
gdb 3251	1868.7[a]	1867.9	1867.9	1873.8	1866.4	1866.4	1869.0
gdb 3252	1859.3[a]	1857.0	1857.0	1862.4	1853.7	1853.7	1856.7
gdb 3253	1860.2[a]	1857.9	1857.9	1862.7	1854.1	1854.1	1856.6
gdb 3254	1864.4[a]	1867.1	1867.1	1873.3	1866.4	1866.3	1868.9
gdb 3255	1894.3[a]	1896.8	1896.8	1899.7	1887.1	1887.1	1890.5
gdb 3256	1892.6[a]	1896.0	1896.0	1899.5	1886.5	1886.5	1890.9
gdb 3257	1898.7[a]	1898.3	1898.3	1901.8	1894.2	1894.2	1896.5
gdb 3258	1894.0[a]	1892.0	1892.0	1896.0	1888.2	1888.2	1891.2
gdb 3259	1894.6[a]	1898.5	1898.5	1901.9	1888.4	1888.4	1892.2
gdb 3260	1893.7[a]	1890.5	1890.5	1894.0	1883.6	1883.6	1886.6
gdb 3261	1898.9[a]	1899.3	1899.3	1904.1	1895.5	1895.4	1898.2
gdb 3262	1894.4[a]	1894.6	1894.6	1899.7	1890.9	1890.9	1894.1
gdb 3263	1898.3[a]	1892.8	1892.8	1896.9	1889.1	1889.1	1891.7
gdb 3264	1870.6[a]	1860.1	1860.1	1865.0	1857.5	1857.4	1859.9
gdb 3265	1870.0[a]	1858.4	1858.4	1861.7	1855.8	1855.8	1857.9
gdb 3266	1866.7[a]	1857.7	1857.7	1862.0	1855.0	1855.0	1857.3
gdb 3267	1874.8[a]	1864.4	1864.4	1869.3	1864.8	1864.8	1867.2
gdb 3268	1868.1[a]	1856.7	1856.7	1859.8	1853.8	1853.8	1855.7
gdb 3269	1865.7[a]	1857.3	1857.3	1861.4	1854.6	1854.6	1856.9
gdb 3270	1868.4[a]	1857.4	1857.4	1861.2	1854.7	1854.7	1856.3
gdb 3271	1866.2[a]	1858.3	1858.3	1862.9	1855.2	1855.2	1857.6
gdb 3272	1873.2[a]	1862.6	1862.6	1868.7	1863.2	1863.2	1865.8
gdb 3273	1886.7[a]	1891.3	1891.3	1892.1	1879.8	1879.8	1881.9
gdb 3274	1886.7[a]	1887.7	1887.7	1890.2	1879.6	1879.6	1881.7
gdb 3275	1889.5[a]	1886.9	1886.9	1889.8	1882.4	1882.4	1884.3
gdb 3276	1889.8[a]	1888.2	1888.2	1891.1	1883.7	1883.6	1885.8
gdb 3277	1862.9[a]	1862.0	1862.0	1864.4	1862.3	1862.3	1863.7
gdb 3278	1876.9[a]	1870.8	1870.8	1868.9	1868.3	1868.3	1865.7
gdb 3279	1862.9[a]	1862.6	1862.6	1865.3	1863.1	1863.1	1864.6
gdb 3280	1870.0[a]	1872.0	1872.0	1873.0	1875.8	1875.8	1875.8
gdb 3281	1873.6[a]	1870.1	1870.1	1868.9	1866.9	1866.9	1864.3
gdb 3282	1862.6[a]	1862.0	1862.0	1864.4	1862.1	1862.1	1863.4
gdb 3283	1877.6[a]	1869.3	1869.3	1868.3	1866.9	1866.9	1864.2
gdb 3284	1862.4[a]	1863.0	1863.0	1865.6	1863.2	1863.2	1864.5
gdb 3285	1871.6[a]	1870.9	1870.9	1874.1	1875.6	1875.6	1875.3
gdb 3286	1855.2[a]	1854.8	1854.8	1856.3	1853.0	1853.0	1856.1
gdb 3287	1864.4[a]	1863.6	1863.6	1865.2	1865.3	1865.3	1866.7
gdb 3288	1872.4[a]	1867.2	1867.2	1864.9	1866.1	1866.1	1863.4
gdb 3289	1871.8[a]	1872.9	1872.9	1877.6	1867.1	1867.1	1871.5
gdb 3290	1874.6[a]	1883.5	1883.5	1888.0	1880.0	1880.0	1883.2
gdb 3291	1874.5[a]	1883.7	1883.7	1888.2	1880.3	1880.3	1883.7
gdb 3292	1876.4[a]	1878.0	1878.0	1883.0	1875.6	1875.6	1878.3
gdb 3293	1878.0[a]	1873.6	1873.6	1878.0	1867.4	1867.4	1871.3
gdb 3294	1883.6[a]	1881.0	1881.0	1884.3	1872.4	1872.4	1876.9
gdb 3295	1886.4[a]	1880.4	1880.4	1885.0	1877.5	1877.5	1881.4
gdb 3296	1885.6[a]	1881.6	1881.6	1885.8	1878.8	1878.8	1882.4
gdb 3297	1890.6[a]	1883.1	1883.1	1887.8	1880.5	1880.5	1883.0
gdb 3298	1866.3[a]	1863.7	1863.7	1867.4	1859.6	1859.6	1863.3
gdb 3299	1870.5[a]	1869.7	1869.7	1871.6	1869.5	1869.4	1871.5
gdb 3300	1871.2[a]	1870.2	1870.2	1871.9	1870.1	1870.1	1872.2
gdb 3301	1869.2[a]	1872.9	1872.8	1877.0	1872.4	1872.4	1874.9
gdb 3302	1888.0[a]	1883.9	1883.9	1886.5	1886.8	1886.8	1887.4
gdb 3303	1885.9[a]	1885.0	1884.9	1887.7	1887.5	1887.4	1888.0
gdb 3304	1890.7[a]	1890.4	1890.4	1894.8	1889.2	1889.2	1891.6
gdb 3305	1888.1[a]	1884.2	1884.1	1886.5	1887.7	1887.7	1888.3
gdb 3306	1903.2[a]	1905.1	1905.1	1906.1	1908.2	1908.2	1908.2
gdb 3307	1903.6[a]	1903.8	1903.7	1905.0	1907.8	1907.8	1907.4
gdb 3308	1913.2[a]	1907.4	1907.4	1907.9	1905.3	1905.3	1907.2
gdb 3309	1891.6[a]	1894.9	1894.9	1896.6	1894.6	1894.6	1896.5
gdb 3310	1890.7[a]	1894.9	1894.9	1895.9	1895.3	1895.2	1897.0
gdb 3311	1905.5[a]	1901.2	1901.2	1901.8	1900.1	1900.0	1902.3
gdb 3312	1908.0[a]	1905.1	1905.1	1905.6	1903.2	1903.1	1905.5

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3313	1898.1[a]	1901.9	1901.9	1902.2	1906.0	1906.0	1905.7
gdb 3314	1877.2[a]	1877.3	1877.3	1879.4	1876.9	1876.9	1879.1
gdb 3315	1910.3[a]	1915.8	1915.8	1918.3	1913.1	1913.1	1915.9
gdb 3316	1911.8[a]	1919.7	1919.7	1921.3	1916.5	1916.5	1917.5
gdb 3317	1907.5[a]	1913.0	1913.0	1915.1	1910.3	1910.2	1912.6
gdb 3318	1916.1[a]	1920.9	1920.9	1922.4	1921.2	1921.2	1922.1
gdb 3319	1888.1[a]	1893.9	1893.9	1895.7	1893.1	1893.1	1895.1
gdb 3320	1884.1[a]	1888.2	1888.2	1890.1	1888.2	1888.2	1890.6
gdb 3321	1892.1[a]	1895.0	1894.9	1896.2	1898.8	1898.4	1899.5
gdb 3322	1896.3[a]	1891.5	1891.5	1895.1	1892.9	1892.9	1894.9
gdb 3323	1896.8[a]	1890.0	1890.0	1892.6	1891.8	1891.8	1893.1
gdb 3324	1886.8[a]	1884.0	1884.0	1885.8	1882.5	1882.5	1884.3
gdb 3325	1884.5[a]	1881.3	1881.3	1883.7	1879.8	1879.7	1881.9
gdb 3326	1892.3[a]	1896.1	1896.1	1900.2	1891.3	1891.3	1894.5
gdb 3327	1894.7[a]	1898.4	1898.4	1902.0	1893.7	1893.7	1896.6
gdb 3328	1889.9[a]	1893.6	1893.6	1897.2	1889.3	1889.3	1892.4
gdb 3329	1902.4[a]	1903.4	1903.4	1907.8	1902.3	1902.3	1904.3
gdb 3330	1831.8[a]	1820.3	1820.3	1824.5	1815.8	1815.8	1819.4
gdb 3331	1835.5[a]	1823.2	1823.2	1826.5	1818.2	1818.2	1821.3
gdb 3332	1832.8[a]	1820.6	1820.6	1824.2	1816.0	1816.0	1819.2
gdb 3333	1851.3[a]	1837.3	1837.3	1842.5	1835.3	1835.3	1838.4
gdb 3334	1851.1[a]	1834.8	1834.8	1839.1	1833.5	1833.5	1836.5
gdb 3335	1842.8[a]	1837.2	1837.2	1842.1	1835.0	1835.0	1838.2
gdb 3336	1844.6[a]	1839.3	1839.3	1843.3	1836.9	1836.8	1839.4
gdb 3337	1882.5[a]	1881.3	1881.3	1884.7	1882.3	1882.3	1882.7
gdb 3338	1872.6[a]	1866.0	1866.0	1868.0	1866.2	1866.2	1867.2
gdb 3339	1870.6[a]	1865.0	1865.0	1866.9	1864.8	1864.7	1866.1
gdb 3340	1841.4[a]	1826.4	1826.4	1825.8	1821.4	1820.9	1819.9
gdb 3341	1841.4[a]	1824.1	1824.1	1822.5	1818.9	1818.9	1817.0
gdb 3342	1849.5[a]	1840.8	1840.8	1841.4	1837.1	1837.1	1834.9
gdb 3343	1845.4[a]	1832.1	1832.1	1834.6	1832.5	1832.5	1833.0
gdb 3344	1845.7[a]	1830.9	1830.9	1833.7	1831.4	1831.3	1832.3
gdb 3345	1883.8[a]	1871.4	1871.4	1873.8	1870.9	1870.8	1874.7
gdb 3346	1864.9[a]	1855.7	1855.6	1857.7	1857.4	1857.3	1859.9
gdb 3347	1863.0[a]	1852.5	1852.5	1853.7	1854.1	1854.0	1856.2
gdb 3348	1872.9[a]	1870.5	1870.5	1872.9	1873.6	1873.6	1874.9
gdb 3349	1909.7[a]	1915.3	1915.3	1917.7	1913.0	1913.0	1915.9
gdb 3350	1928.6[a]	1924.8	1924.8	1926.3	1921.4	1921.4	1924.2
gdb 3351	1908.1[a]	1912.4	1912.4	1914.5	1909.9	1909.9	1912.4
gdb 3352	1916.9[a]	1921.6	1921.6	1924.8	1922.3	1922.3	1924.2
gdb 3353	1892.4[a]	1897.0	1897.0	1900.7	1893.1	1893.1	1895.7
gdb 3354	1892.6[a]	1897.0	1896.9	1900.7	1893.1	1893.1	1895.8
gdb 3355	1876.8[a]	1874.0	1874.0	1873.8	1865.2	1865.2	1864.7
gdb 3356	1889.6[a]	1882.8	1882.8	1882.4	1877.2	1877.2	1875.9
gdb 3357	1884.9[a]	1882.6	1882.6	1886.2	1879.3	1879.3	1881.4
gdb 3358	1856.4[a]	1848.0	1848.0	1847.9	1840.7	1840.7	1839.5
gdb 3359	1869.9[a]	1857.3	1857.3	1858.6	1853.0	1853.0	1851.9
gdb 3360	1864.3[a]	1857.4	1857.4	1861.6	1855.6	1855.5	1857.5
gdb 3361	1880.6[a]	1877.0	1877.0	1879.6	1875.8	1875.8	1878.8
gdb 3362	1891.4[a]	1886.1	1886.1	1889.1	1887.2	1887.2	1889.8
gdb 3363	1901.7[a]	1903.8	1903.8	1907.9	1900.1	1900.1	1903.2
gdb 3364	1899.8[a]	1902.4	1902.4	1906.4	1898.6	1898.6	1901.6
gdb 3365	1882.5[a]	1890.4	1890.4	1892.7	1890.7	1890.7	1891.5
gdb 3366	1885.5[a]	1891.8	1891.8	1894.7	1892.2	1892.2	1893.0
gdb 3367	1879.2[a]	1879.9	1879.9	1882.2	1878.2	1878.2	1880.0
gdb 3368	1879.2[a]	1880.1	1880.1	1882.6	1878.5	1878.4	1880.8
gdb 3369	1847.0[a]	1837.7	1837.7	1841.7	1832.4	1832.3	1836.0
gdb 3370	1845.7[a]	1837.2	1837.2	1840.5	1832.1	1832.1	1835.8
gdb 3371	1851.5[a]	1850.7	1850.7	1855.7	1847.7	1847.7	1850.7
gdb 3372	1854.5[a]	1852.1	1852.1	1857.7	1849.3	1849.3	1852.7
gdb 3373	1848.0[a]	1843.1	1843.1	1843.0	1835.2	1835.2	1834.4
gdb 3374	1850.0[a]	1845.2	1845.2	1845.4	1837.5	1837.5	1836.8
gdb 3375	1854.3[a]	1857.9	1857.9	1859.1	1852.4	1852.4	1850.4
gdb 3376	1852.8[a]	1853.1	1853.1	1857.4	1850.7	1850.7	1852.9
gdb 3377	1852.3[a]	1852.5	1852.5	1856.9	1850.0	1850.0	1852.0

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3378	1870.5[a]	1872.0	1872.0	1875.0	1870.6	1870.5	1874.0
gdb 3379	1871.0[a]	1871.4	1871.4	1874.3	1870.2	1870.2	1873.6
gdb 3380	1873.4[a]	1883.1	1883.1	1887.5	1884.2	1884.2	1886.9
gdb 3381	1887.2[a]	1885.8	1885.8	1889.1	1882.8	1882.8	1884.8
gdb 3382	1885.1[a]	1883.5	1883.5	1885.8	1881.0	1880.9	1883.3
gdb 3383	1913.5[a]	1918.3	1918.3	1920.2	1915.2	1915.2	1918.0
gdb 3384	1897.6[a]	1904.0	1904.0	1905.7	1903.0	1903.0	1905.1
gdb 3385	1897.6[a]	1904.2	1904.2	1905.9	1903.0	1903.0	1904.9
gdb 3386	1900.5[a]	1913.3	1913.3	1914.9	1914.5	1914.5	1914.7
gdb 3387	1863.4[a]	1861.6	1861.6	1860.8	1855.4	1855.4	1853.9
gdb 3388	1872.9[a]	1869.9	1869.9	1868.5	1867.5	1867.5	1864.3
gdb 3389	1866.4[a]	1866.7	1864.5	1868.1	1867.7	1867.7	1868.8
gdb 3390	1863.4[a]	1865.9	1865.8	1868.3	1865.7	1865.7	1866.8
gdb 3391	1877.3[a]	1871.6	1871.6	1875.2	1869.6	1869.6	1871.5
gdb 3392	1873.0[a]	1863.8	1863.8	1866.6	1862.3	1862.3	1864.7
gdb 3393	1871.1[a]	1863.6	1863.6	1867.2	1863.7	1863.7	1866.1
gdb 3394	1872.6[a]	1868.0	1868.0	1871.6	1867.4	1867.4	1869.6
gdb 3395	1879.9[a]	1873.7	1873.7	1877.7	1876.3	1876.3	1877.0
gdb 3396	1864.1[a]	1861.2	1861.2	1865.6	1855.0	1855.0	1859.0
gdb 3397	1873.8[a]	1870.5	1870.5	1875.3	1867.7	1867.7	1870.5
gdb 3398	1873.9[a]	1873.3	1873.3	1879.0	1869.9	1869.9	1873.7
gdb 3399	1869.2[a]	1870.8	1870.8	1875.6	1867.5	1867.5	1871.1
gdb 3400	1866.4[a]	1862.8	1862.8	1861.6	1857.2	1857.1	1856.2
gdb 3401	1876.6[a]	1868.6	1868.6	1867.1	1866.9	1866.9	1864.0
gdb 3402	1866.8[a]	1863.4	1863.4	1866.2	1864.1	1864.0	1865.9
gdb 3403	1866.3[a]	1862.8	1862.7	1865.5	1863.3	1863.3	1865.1
gdb 3404	1877.3[a]	1877.1	1877.1	1879.2	1876.9	1876.9	1879.1
gdb 3405	1876.0[a]	1874.4	1874.4	1876.7	1873.7	1873.7	1876.4
gdb 3406	1876.1[a]	1874.1	1874.1	1876.5	1873.7	1873.6	1876.2
gdb 3407	1885.6[a]	1881.8	1881.8	1884.5	1885.1	1885.1	1885.9
gdb 3408	1871.9[a]	1869.0	1869.0	1871.5	1869.7	1869.7	1872.3
gdb 3409	1909.4[a]	1904.8	1904.8	1905.1	1902.8	1902.8	1904.8
gdb 3410	1894.3[a]	1898.4	1898.4	1899.9	1897.4	1897.4	1899.0
gdb 3411	1893.0[a]	1897.2	1897.2	1898.6	1896.8	1896.8	1898.7
gdb 3412	1900.6[a]	1903.6	1903.6	1904.6	1907.1	1907.1	1906.9
gdb 3413	1887.8[a]	1892.5	1892.5	1893.9	1892.0	1892.0	1893.5
gdb 3414	1890.2[a]	1892.2	1892.2	1893.5	1891.2	1891.2	1893.2
gdb 3415	1887.5[a]	1890.3	1890.3	1891.6	1889.6	1889.6	1891.5
gdb 3416	1895.9[a]	1896.9	1896.9	1897.7	1900.1	1900.1	1900.3
gdb 3417	1886.7[a]	1892.2	1892.2	1895.3	1890.7	1890.7	1893.6
gdb 3418	1891.2[a]	1894.0	1894.0	1897.3	1892.6	1892.6	1896.3
gdb 3419	1898.6[a]	1900.9	1900.9	1903.2	1903.1	1903.1	1904.5
gdb 3420	1889.9[a]	1893.5	1893.4	1896.9	1883.6	1883.6	1889.7
gdb 3421	1897.5[a]	1897.9	1897.9	1902.3	1894.1	1894.1	1897.6
gdb 3422	1895.6[a]	1897.1	1897.1	1901.6	1893.8	1893.8	1898.2
gdb 3423	1894.0[a]	1903.2	1903.2	1905.7	1901.9	1901.8	1903.8
gdb 3424	1896.4[a]	1903.4	1903.4	1905.8	1902.4	1902.4	1904.9
gdb 3425	1896.9[a]	1905.9	1905.9	1908.7	1904.7	1904.7	1907.0
gdb 3426	1901.0[a]	1909.1	1909.1	1910.8	1910.7	1910.7	1911.0
gdb 3427	1871.0[a]	1868.5	1868.5	1870.9	1868.9	1868.9	1871.5
gdb 3428	1872.3[a]	1869.2	1869.2	1872.0	1869.5	1869.5	1872.7
gdb 3429	1915.3[a]	1918.8	1918.8	1919.8	1919.7	1919.7	1920.0
gdb 3430	1915.5[a]	1918.7	1918.6	1919.6	1919.5	1919.5	1919.5
gdb 3431	1910.9[a]	1917.0	1917.0	1917.8	1917.8	1917.8	1917.9
gdb 3432	1911.2[a]	1917.2	1917.2	1918.0	1918.1	1918.1	1918.2
gdb 3433	1889.9[a]	1888.6	1888.6	1891.9	1890.4	1890.4	1890.9
gdb 3434	1887.8[a]	1885.4	1885.4	1884.8	1880.1	1880.1	1877.5
gdb 3435	1888.1[a]	1885.9	1885.9	1885.2	1880.7	1880.7	1877.9
gdb 3436	1890.7[a]	1888.6	1888.6	1891.6	1890.5	1890.5	1890.5
gdb 3437	1884.7[a]	1884.0	1884.0	1887.2	1880.0	1880.0	1881.7
gdb 3438	1886.0[a]	1884.8	1884.8	1888.3	1882.4	1882.4	1885.0
gdb 3439	1886.8[a]	1884.9	1884.9	1888.3	1882.1	1882.1	1884.3
gdb 3440	1886.4[a]	1886.5	1886.5	1886.0	1881.7	1881.7	1879.1
gdb 3441	1905.0[a]	1911.0	1911.0	1912.1	1912.6	1912.6	1913.8
gdb 3442	1887.2[a]	1885.5	1885.5	1884.1	1881.3	1881.3	1878.8

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3443	1912.2[a]	1918.9	1918.9	1920.0	1920.1	1920.1	1920.3
gdb 3444	1916.3[a]	1918.3	1918.3	1918.9	1914.9	1914.9	1917.7
gdb 3445	1865.1[a]	1862.9	1862.8	1865.1	1859.9	1859.9	1862.1
gdb 3446	1862.5[a]	1859.9	1859.9	1861.9	1857.2	1857.2	1859.1
gdb 3447	1877.4[a]	1881.1	1881.1	1884.8	1881.1	1881.1	1881.8
gdb 3448	1912.3[a]	1917.1	1917.1	1918.7	1916.1	1916.1	1917.4
gdb 3449	1915.2[a]	1919.6	1919.6	1921.2	1918.9	1918.9	1919.4
gdb 3450	1909.0[a]	1916.0	1916.0	1917.2	1915.5	1915.4	1916.2
gdb 3451	1911.2[a]	1918.9	1918.9	1920.3	1918.5	1918.5	1918.9
gdb 3452	1883.9[a]	1883.4	1883.4	1883.4	1878.0	1878.0	1875.9
gdb 3453	1885.5[a]	1891.8	1891.8	1895.9	1891.5	1891.5	1892.1
gdb 3454	1902.7[a]	1908.4	1908.4	1910.0	1909.6	1909.5	1911.5
gdb 3455	1885.8[a]	1883.4	1883.4	1883.5	1878.6	1878.5	1876.7
gdb 3456	1888.3[a]	1890.4	1890.4	1892.9	1889.7	1889.7	1889.8
gdb 3457	1902.1[a]	1909.2	1909.2	1912.0	1910.5	1910.5	1912.7
gdb 3458	1903.2[a]	1910.0	1910.0	1911.7	1911.0	1911.0	1912.6
gdb 3459	1887.1[a]	1885.1	1885.1	1887.2	1886.5	1886.5	1887.2
gdb 3460	1888.3[a]	1885.5	1885.5	1888.9	1886.7	1886.7	1887.9
gdb 3461	1889.6[a]	1885.2	1885.2	1884.9	1879.7	1879.7	1877.5
gdb 3462	1885.9[a]	1882.7	1882.7	1885.6	1885.3	1885.3	1886.3
gdb 3463	1885.4[a]	1884.0	1884.0	1887.3	1879.1	1879.1	1881.0
gdb 3464	1891.2[a]	1892.3	1892.3	1897.1	1890.8	1890.7	1893.2
gdb 3465	1885.5[a]	1884.2	1884.2	1886.9	1880.8	1880.8	1883.3
gdb 3466	1887.6[a]	1886.2	1886.2	1890.1	1883.0	1883.0	1885.9
gdb 3467	1886.8[a]	1886.2	1886.2	1889.4	1882.5	1882.5	1885.0
gdb 3468	1890.6[a]	1895.5	1895.5	1901.9	1894.5	1894.5	1898.4
gdb 3469	1883.1[a]	1882.4	1882.4	1882.6	1877.3	1877.3	1875.5
gdb 3470	1884.7[a]	1883.4	1883.4	1883.1	1877.8	1877.8	1875.5
gdb 3471	1886.3[a]	1889.7	1889.7	1892.7	1889.8	1889.8	1890.2
gdb 3472	1888.0[a]	1886.1	1886.1	1889.4	1887.3	1887.3	1888.5
gdb 3473	1885.8[a]	1884.1	1884.1	1887.5	1879.1	1879.1	1881.1
gdb 3474	1893.7[a]	1892.8	1892.8	1896.3	1891.3	1891.2	1893.0
gdb 3475	1888.1[a]	1885.0	1885.0	1885.0	1879.3	1879.3	1877.4
gdb 3476	1884.1[a]	1882.2	1882.2	1881.9	1876.8	1876.8	1874.4
gdb 3477	1888.6[a]	1890.1	1890.1	1893.8	1890.2	1890.2	1890.5
gdb 3478	1884.3[a]	1883.4	1883.4	1887.2	1879.8	1879.8	1882.8
gdb 3479	1889.2[a]	1887.5	1887.5	1891.2	1883.9	1883.9	1886.3
gdb 3480	1884.5[a]	1884.5	1884.5	1887.7	1881.1	1881.1	1883.7
gdb 3481	1890.1[a]	1897.4	1897.4	1901.7	1896.4	1896.4	1897.9
gdb 3482	1899.1[a]	1905.7	1905.7	1908.3	1896.0	1896.0	1900.0
gdb 3483	1897.8[a]	1904.7	1904.7	1907.1	1894.8	1894.8	1898.8
gdb 3484	1899.8[a]	1903.5	1903.5	1907.4	1899.9	1899.9	1903.0
gdb 3485	1903.7[a]	1907.4	1907.4	1911.0	1903.7	1903.7	1905.7
gdb 3486	1903.0[a]	1905.3	1905.3	1909.1	1901.9	1901.9	1904.6
gdb 3487	1897.5[a]	1905.0	1905.0	1907.5	1895.9	1895.9	1900.5
gdb 3488	1900.3[a]	1906.9	1906.9	1910.8	1904.2	1904.2	1906.8
gdb 3489	1898.9[a]	1904.8	1904.8	1908.5	1902.5	1902.5	1905.3
gdb 3490	1900.0[a]	1906.5	1906.5	1910.3	1904.0	1904.0	1906.6
gdb 3491	1909.9[a]	1915.8	1915.8	1918.0	1916.4	1916.4	1917.3
gdb 3492	1908.9[a]	1913.6	1913.6	1914.6	1913.9	1913.9	1914.3
gdb 3493	1903.2[a]	1909.4	1909.4	1911.1	1909.2	1909.2	1911.0
gdb 3494	1903.9[a]	1912.7	1912.7	1914.5	1912.2	1912.2	1913.5
gdb 3495	1885.7[a]	1885.6	1885.6	1889.4	1882.8	1882.7	1885.1
gdb 3496	1878.6[a]	1879.2	1879.2	1881.7	1876.4	1876.4	1879.2
gdb 3497	1908.5[a]	1916.1	1916.0	1918.6	1916.9	1916.9	1917.8
gdb 3498	1879.5[a]	1879.0	1879.0	1877.9	1874.6	1874.6	1872.5
gdb 3499	1913.8[a]	1911.9	1911.8	1913.0	1909.1	1909.1	1912.8
gdb 3500	1900.9[a]	1906.7	1906.7	1909.6	1909.2	1909.1	1911.4
gdb 3501	1891.8[a]	1886.2	1886.2	1886.0	1882.1	1882.1	1880.0
gdb 3502	1888.1[a]	1888.2	1888.2	1891.2	1890.3	1890.3	1890.8
gdb 3503	1889.7[a]	1884.7	1884.7	1884.3	1880.1	1880.1	1877.7
gdb 3504	1890.6[a]	1888.0	1887.9	1890.9	1889.9	1889.9	1890.1
gdb 3505	1886.7[a]	1879.9	1879.9	1883.5	1878.3	1878.3	1880.4
gdb 3506	1882.4[a]	1882.4	1882.4	1885.2	1880.2	1880.2	1882.8
gdb 3507	1884.3[a]	1881.1	1881.1	1883.7	1879.0	1879.0	1881.8

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3508	1891.6[a]	1893.1	1893.1	1896.8	1893.5	1893.5	1895.0
gdb 3509	1885.2[a]	1882.4	1882.4	1881.0	1877.5	1877.5	1874.9
gdb 3510	1880.5[a]	1880.2	1880.2	1883.1	1878.6	1878.6	1880.4
gdb 3511	1895.2[a]	1901.4	1901.4	1903.1	1899.1	1899.1	1902.4
gdb 3512	1902.2[a]	1905.5	1905.4	1906.6	1907.1	1907.1	1908.6
gdb 3513	1879.0[a]	1876.9	1876.9	1877.1	1873.1	1873.1	1871.2
gdb 3514	1874.2[a]	1875.0	1875.0	1877.3	1873.9	1873.9	1876.3
gdb 3515	1906.4[a]	1907.8	1907.8	1909.5	1904.4	1904.4	1908.3
gdb 3516	1895.5[a]	1901.4	1901.4	1903.2	1899.4	1899.4	1901.9
gdb 3517	1903.1[a]	1910.6	1910.6	1912.1	1911.3	1911.3	1911.9
gdb 3518	1877.1[a]	1879.1	1879.1	1882.8	1876.7	1876.7	1880.1
gdb 3519	1916.2[a]	1926.9	1926.9	1926.7	1929.4	1929.4	1929.3
gdb 3520	1918.4[a]	1923.1	1923.1	1925.0	1924.7	1924.7	1925.0
gdb 3521	1930.5[a]	1924.9	1924.9	1925.7	1922.5	1922.5	1924.5
gdb 3522	1922.8[a]	1937.3	1937.3	1937.5	1939.7	1939.7	1939.7
gdb 3523	1909.7[a]	1915.7	1915.7	1917.8	1916.3	1916.3	1917.0
gdb 3524	1906.9[a]	1912.5	1912.4	1914.5	1912.5	1912.4	1913.1
gdb 3525	1916.5[a]	1918.6	1918.6	1919.0	1914.8	1914.8	1917.8
gdb 3526	1898.9[a]	1909.0	1909.0	1910.5	1910.5	1910.5	1912.1
gdb 3527	1878.8[a]	1880.9	1880.9	1883.4	1879.3	1879.2	1881.0
gdb 3528	1875.4[a]	1877.3	1877.3	1879.4	1876.0	1876.0	1878.6
gdb 3529	1901.1[a]	1890.6	1890.6	1892.1	1888.5	1888.5	1890.7
gdb 3530	1883.9[a]	1892.2	1892.2	1894.8	1893.2	1893.2	1894.3
gdb 3531	1906.5[a]	1914.8	1914.8	1916.2	1917.3	1917.2	1918.2
gdb 3532	1875.0[a]	1877.1	1877.1	1875.9	1874.2	1874.1	1872.2
gdb 3533	1897.4[a]	1884.4	1884.4	1885.4	1883.4	1883.3	1884.9
gdb 3534	1879.3[a]	1885.0	1885.0	1886.8	1886.7	1886.7	1886.9
gdb 3535	1898.1[a]	1906.0	1906.0	1907.5	1909.5	1909.5	1911.3
gdb 3536	1905.6[a]	1909.9	1909.9	1910.8	1911.7	1911.7	1911.5
gdb 3537	1902.2[a]	1902.2	1902.2	1900.0	1898.5	1898.5	1895.3
gdb 3538	1903.9[a]	1904.8	1904.8	1906.3	1908.4	1908.4	1908.1
gdb 3539	1916.2[a]	1911.8	1911.8	1912.1	1909.4	1909.4	1911.0
gdb 3540	1895.8[a]	1902.3	1902.3	1904.2	1903.0	1902.8	1903.7
gdb 3541	1895.3[a]	1900.1	1900.1	1897.8	1896.7	1896.7	1893.4
gdb 3542	1914.1[a]	1913.9	1913.8	1914.5	1911.5	1911.5	1912.7
gdb 3543	1903.1[a]	1911.4	1911.4	1912.4	1913.1	1913.1	1912.4
gdb 3544	1905.3[a]	1909.0	1909.0	1909.7	1910.5	1910.5	1910.5
gdb 3545	1903.2[a]	1906.2	1906.2	1907.8	1909.4	1909.4	1909.5
gdb 3546	1901.8[a]	1902.1	1902.1	1900.0	1898.4	1898.4	1895.4
gdb 3547	1916.1[a]	1911.8	1911.8	1912.4	1909.6	1909.5	1911.5
gdb 3548	1896.3[a]	1897.7	1897.7	1899.5	1895.1	1895.1	1896.6
gdb 3549	1912.1[a]	1909.2	1909.2	1911.2	1905.3	1905.3	1908.9
gdb 3550	1902.6[a]	1907.5	1907.5	1909.5	1907.9	1907.9	1909.2
gdb 3551	1898.1[a]	1901.6	1901.6	1903.3	1900.5	1900.5	1902.5
gdb 3552	1893.7[a]	1897.5	1897.5	1899.1	1896.5	1896.5	1898.3
gdb 3553	1913.9[a]	1917.2	1917.2	1918.9	1914.4	1914.4	1917.1
gdb 3554	1901.8[a]	1914.1	1914.1	1915.9	1915.3	1915.3	1916.0
gdb 3555	1917.0[a]	1921.2	1921.2	1923.1	1922.4	1922.3	1922.9
gdb 3556	1924.3[a]	1921.2	1921.2	1921.4	1918.0	1918.0	1920.6
gdb 3557	1914.0[a]	1917.6	1917.6	1918.9	1917.8	1917.8	1918.7
gdb 3558	1911.7[a]	1914.6	1914.6	1915.8	1914.9	1914.8	1915.6
gdb 3559	1920.7[a]	1917.3	1917.3	1918.0	1913.2	1913.2	1916.5
gdb 3560	1924.8[a]	1934.1	1934.0	1934.4	1937.0	1937.0	1937.5
gdb 3561	1912.7[a]	1918.6	1918.6	1920.4	1920.2	1920.1	1920.7
gdb 3562	1919.7[a]	1920.4	1920.4	1921.2	1917.5	1917.4	1920.3
gdb 3563	1897.6[a]	1903.4	1903.4	1901.3	1900.5	1900.5	1898.0
gdb 3564	1910.7[a]	1908.8	1908.8	1909.5	1908.3	1908.3	1909.9
gdb 3565	1911.7[a]	1913.2	1913.2	1913.9	1911.1	1911.1	1912.9
gdb 3566	1899.7[a]	1911.5	1911.5	1913.4	1913.7	1913.7	1913.7
gdb 3567	1917.8[a]	1928.5	1928.5	1929.3	1931.8	1931.8	1933.3
gdb 3568	1898.9[a]	1899.6	1899.6	1897.4	1896.7	1896.7	1894.0
gdb 3569	1906.0[a]	1902.2	1902.2	1903.0	1900.5	1900.5	1903.0
gdb 3570	1910.8[a]	1909.3	1909.3	1909.3	1906.7	1906.6	1908.6
gdb 3571	1900.6[a]	1906.8	1906.8	1908.5	1909.2	1909.2	1908.8
gdb 3572	1912.3[a]	1918.9	1918.8	1920.7	1920.3	1920.3	1920.8

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3573	1919.4[a]	1920.6	1920.6	1921.5	1917.4	1917.4	1920.3
gdb 3574	1923.3[a]	1934.4	1934.4	1934.4	1936.9	1936.9	1937.1
gdb 3575	1911.2[a]	1908.5	1908.5	1909.5	1906.0	1906.0	1909.4
gdb 3576	1913.5[a]	1912.0	1912.0	1912.1	1909.5	1909.5	1912.3
gdb 3577	1904.5[a]	1910.9	1910.9	1912.6	1912.2	1912.1	1913.1
gdb 3578	1865.5[a]	1871.7	1871.7	1876.4	1869.8	1869.8	1871.1
gdb 3579	1860.9[a]	1861.1	1861.1	1864.6	1856.4	1856.3	1858.4
gdb 3580	1906.4[a]	1914.9	1914.9	1916.2	1917.1	1917.1	1917.7
gdb 3581	1863.6[a]	1868.6	1868.5	1873.1	1866.3	1866.3	1867.9
gdb 3582	1860.1[a]	1869.9	1869.9	1870.7	1867.7	1867.7	1865.7
gdb 3583	1862.9[a]	1870.2	1870.2	1874.8	1867.8	1867.8	1868.6
gdb 3584	1860.8[a]	1860.5	1860.5	1864.9	1855.7	1855.7	1858.0
gdb 3585	1864.4[a]	1868.4	1868.4	1872.2	1867.2	1867.1	1868.7
gdb 3586	1901.1[a]	1910.2	1910.1	1911.4	1911.5	1911.4	1912.7
gdb 3587	1903.7[a]	1910.1	1910.1	1911.6	1910.0	1910.0	1911.6
gdb 3588	1906.4[a]	1911.1	1911.1	1912.6	1911.0	1911.0	1911.9
gdb 3589	1900.4[a]	1909.6	1909.6	1911.3	1906.2	1906.2	1908.7
gdb 3590	1862.3[a]	1866.5	1866.5	1870.3	1866.5	1866.4	1868.0
gdb 3591	1918.6[a]	1922.0	1922.0	1922.8	1923.5	1923.4	1923.0
gdb 3592	1908.6[a]	1914.1	1914.1	1914.7	1915.6	1915.6	1916.5
gdb 3593	1865.3[a]	1862.6	1862.6	1864.4	1860.9	1860.9	1862.4
gdb 3594	1887.3[a]	1886.3	1886.3	1885.6	1881.4	1881.3	1878.5
gdb 3595	1905.4[a]	1912.6	1912.6	1913.8	1914.2	1914.2	1915.2
gdb 3596	1886.9[a]	1885.5	1885.5	1884.8	1880.9	1880.9	1878.1
gdb 3597	1910.9[a]	1915.9	1915.9	1916.6	1917.1	1917.1	1917.0
gdb 3598	1914.8[a]	1926.6	1926.6	1926.2	1928.6	1928.5	1928.0
gdb 3599	1910.9[a]	1914.3	1914.3	1915.3	1914.4	1914.3	1914.4
gdb 3600	1912.1[a]	1915.6	1915.6	1916.5	1915.4	1915.4	1915.7
gdb 3601	1906.6[a]	1911.8	1911.8	1912.3	1908.5	1908.5	1910.4
gdb 3602	1871.1[a]	1878.8	1878.8	1881.2	1875.0	1875.0	1876.9
gdb 3603	1871.3[a]	1880.5	1880.5	1883.7	1870.9	1870.9	1875.3
gdb 3604	1878.5[a]	1882.6	1882.6	1885.3	1882.4	1882.4	1883.3
gdb 3605	1907.8[a]	1912.1	1912.1	1913.1	1912.8	1912.7	1913.5
gdb 3606	1902.8[a]	1910.4	1910.4	1912.5	1911.7	1911.6	1912.9
gdb 3607	1899.0[a]	1907.8	1907.8	1909.2	1905.8	1905.8	1908.1
gdb 3608	1864.2[a]	1868.4	1868.4	1871.6	1865.9	1865.9	1867.1
gdb 3609	1861.9[a]	1869.9	1869.9	1875.0	1867.0	1866.9	1868.1
gdb 3610	1858.5[a]	1858.5	1858.5	1861.8	1854.0	1853.9	1855.9
gdb 3611	1858.7[a]	1863.0	1863.0	1868.1	1863.6	1863.6	1865.8
gdb 3612	1892.6[a]	1892.3	1892.3	1895.5	1893.3	1893.3	1894.7
gdb 3613	1892.9[a]	1903.2	1903.2	1904.3	1904.2	1904.1	1906.1
gdb 3614	1892.6[a]	1901.7	1901.6	1902.3	1903.4	1903.3	1903.7
gdb 3615	1874.9[a]	1877.1	1877.1	1875.6	1873.8	1873.8	1871.4
gdb 3616	1876.0[a]	1876.4	1876.4	1878.1	1875.2	1875.2	1875.8
gdb 3617	1879.1[a]	1884.0	1884.0	1886.0	1885.6	1885.6	1885.1
gdb 3618	1906.5[a]	1911.6	1911.6	1913.9	1913.1	1913.0	1914.4
gdb 3619	1905.9[a]	1909.8	1909.8	1910.9	1910.8	1910.8	1911.8
gdb 3620	1917.4[a]	1928.0	1928.0	1928.5	1930.9	1930.9	1931.8
gdb 3621	1905.2[a]	1910.4	1910.4	1911.5	1911.8	1911.7	1913.1
gdb 3622	1899.8[a]	1908.5	1908.5	1910.2	1906.4	1906.4	1908.7
gdb 3623	1872.0[a]	1875.6	1875.6	1874.3	1871.7	1871.7	1869.7
gdb 3624	1870.8[a]	1873.7	1873.7	1875.1	1872.2	1872.1	1873.4
gdb 3625	1875.8[a]	1884.3	1884.3	1887.5	1885.3	1885.3	1886.2
gdb 3626	1893.8[a]	1902.1	1902.1	1903.6	1904.7	1904.7	1906.8
gdb 3627	1890.9[a]	1893.2	1893.1	1891.4	1889.8	1889.7	1887.8
gdb 3628	1890.4[a]	1898.2	1898.1	1900.2	1896.6	1896.5	1898.5
gdb 3629	1895.6[a]	1900.6	1900.6	1901.8	1902.5	1902.4	1903.0
gdb 3630	1904.7[a]	1911.7	1911.6	1913.9	1913.3	1913.3	1914.7
gdb 3631	1899.6[a]	1908.3	1908.3	1909.9	1906.3	1906.2	1908.5
gdb 3632	1910.0[a]	1916.6	1916.6	1919.3	1917.2	1917.2	1918.3
gdb 3633	1902.8[a]	1912.3	1912.3	1913.9	1909.9	1909.9	1911.8
gdb 3634	1874.3[a]	1875.9	1875.8	1875.1	1867.8	1867.7	1866.7
gdb 3635	1878.6[a]	1878.8	1878.8	1878.7	1874.6	1874.6	1872.7
gdb 3636	1858.2[a]	1854.2	1854.2	1857.7	1851.0	1850.9	1853.5
gdb 3637	1860.6[a]	1862.5	1862.5	1867.6	1862.9	1862.9	1865.0

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3638	1916.6[a]	1928.1	1928.1	1928.7	1930.9	1930.9	1931.9
gdb 3639	1872.3[a]	1880.2	1880.2	1884.4	1876.5	1876.4	1879.1
gdb 3640	1869.0[a]	1879.8	1879.8	1882.5	1869.6	1869.6	1873.6
gdb 3641	1876.2[a]	1882.0	1882.0	1885.8	1881.9	1881.9	1883.1
gdb 3642	1898.4[a]	1905.7	1905.7	1907.2	1909.2	1909.1	1910.7
gdb 3643	1913.6[a]	1910.7	1910.3	1911.3	1907.6	1907.6	1911.4
gdb 3644	1896.1[a]	1904.3	1904.2	1906.1	1903.1	1903.1	1906.1
gdb 3645	1901.1[a]	1905.7	1905.7	1908.4	1908.0	1908.0	1910.1
gdb 3646	1898.2[a]	1903.8	1903.8	1904.6	1901.9	1901.8	1904.7
gdb 3647	1904.3[a]	1907.2	1907.2	1909.7	1909.2	1909.1	1911.1
gdb 3648	1848.1[a]	1853.6	1853.6	1858.3	1850.9	1850.8	1854.6
gdb 3649	1891.8[a]	1899.7	1899.7	1899.6	1901.0	1901.0	1900.7
gdb 3650	1844.0[a]	1841.9	1841.9	1845.5	1840.8	1840.7	1844.0
gdb 3651	1853.8[a]	1849.9	1849.8	1852.9	1853.3	1853.3	1854.1
gdb 3652	1899.4[a]	1907.8	1907.8	1907.8	1908.8	1908.8	1908.5
gdb 3653	1870.9[a]	1869.6	1869.6	1867.2	1865.8	1865.8	1862.9
gdb 3654	1872.0[a]	1871.8	1871.8	1869.6	1867.9	1867.9	1864.5
gdb 3655	1872.4[a]	1874.7	1874.7	1876.6	1876.9	1876.9	1876.3
gdb 3656	1892.4[a]	1897.2	1897.1	1897.3	1899.7	1899.7	1900.6
gdb 3657	1881.7[a]	1884.4	1884.4	1886.8	1887.7	1887.7	1888.3
gdb 3658	1900.1[a]	1885.4	1885.4	1886.2	1884.5	1884.5	1885.7
gdb 3659	1885.1[a]	1887.7	1887.7	1889.6	1890.0	1890.0	1890.3
gdb 3660	1880.9[a]	1881.9	1881.9	1880.7	1878.5	1878.5	1875.8
gdb 3661	1832.5[a]	1818.5	1818.5	1819.7	1819.1	1819.1	1817.8
gdb 3662	1835.8[a]	1817.5	1817.4	1815.6	1810.7	1810.7	1806.2
gdb 3663	1848.8[a]	1822.9	1822.9	1824.6	1821.3	1821.3	1819.7
gdb 3664	1844.1[a]	1823.7	1823.7	1828.3	1828.4	1828.3	1829.8
gdb 3665	1823.7[a]	1813.7	1813.7	1814.3	1814.1	1814.1	1813.1
gdb 3666	1830.3[a]	1818.7	1818.7	1821.0	1817.0	1817.0	1815.9
gdb 3667	1842.3[a]	1819.5	1819.5	1822.3	1818.2	1818.2	1817.6
gdb 3668	1827.9[a]	1810.5	1810.5	1808.7	1804.1	1804.0	1800.0
gdb 3669	1840.0[a]	1822.0	1822.0	1826.3	1826.7	1826.7	1828.4
gdb 3670	1859.1[a]	1850.1	1850.1	1850.7	1843.5	1843.5	1842.8
gdb 3671	1860.5[a]	1851.4	1851.4	1849.9	1843.5	1843.4	1840.5
gdb 3672	1859.3[a]	1852.9	1852.9	1856.5	1853.0	1853.0	1855.3
gdb 3673	1860.5[a]	1854.6	1854.6	1856.2	1853.5	1853.4	1853.5
gdb 3674	1849.4[a]	1841.4	1841.4	1840.9	1839.0	1839.0	1836.4
gdb 3675	1850.6[a]	1845.4	1845.4	1845.6	1841.4	1841.4	1838.6
gdb 3676	1856.5[a]	1847.7	1847.6	1847.0	1843.7	1843.7	1840.6
gdb 3677	1849.9[a]	1839.0	1839.0	1835.3	1830.0	1830.0	1824.6
gdb 3678	1855.0[a]	1850.4	1850.4	1854.6	1852.9	1852.9	1853.2
gdb 3679	1882.5[a]	1878.8	1878.8	1884.1	1874.3	1874.3	1877.1
gdb 3680	1885.1[a]	1885.3	1885.3	1887.3	1886.8	1886.8	1887.2
gdb 3681	1880.0[a]	1883.0	1883.0	1885.1	1886.7	1886.7	1887.5
gdb 3682	1880.6[a]	1884.5	1884.5	1887.2	1886.9	1886.9	1887.4
gdb 3683	1896.0[a]	1879.6	1879.6	1880.8	1880.3	1880.3	1882.0
gdb 3684	1881.5[a]	1881.6	1881.6	1880.7	1879.1	1879.1	1877.0
gdb 3685	1882.4[a]	1886.0	1886.0	1887.6	1888.0	1888.0	1887.7
gdb 3686	1877.8[a]	1873.7	1873.7	1875.6	1874.6	1874.6	1875.1
gdb 3687	1882.2[a]	1884.6	1884.6	1886.6	1887.8	1887.7	1887.9
gdb 3688	1879.9[a]	1881.8	1881.8	1880.5	1878.3	1878.3	1875.4
gdb 3689	1885.6[a]	1883.3	1883.3	1883.4	1879.1	1879.1	1877.2
gdb 3690	1878.1[a]	1876.6	1876.6	1880.1	1876.8	1876.7	1878.8
gdb 3691	1882.7[a]	1882.8	1882.8	1884.9	1884.7	1884.7	1885.4
gdb 3692	1868.2[a]	1865.7	1865.7	1867.7	1866.6	1866.6	1868.2
gdb 3693	1875.4[a]	1876.0	1876.0	1874.9	1872.8	1872.7	1871.1
gdb 3694	1872.1[a]	1876.9	1876.9	1878.9	1880.3	1880.2	1881.7
gdb 3695	1848.4[a]	1830.0	1830.0	1833.3	1833.2	1833.2	1834.1
gdb 3696	1852.2[a]	1843.3	1843.3	1842.5	1841.2	1841.2	1838.6
gdb 3697	1853.7[a]	1840.3	1840.3	1836.5	1832.0	1832.0	1826.6
gdb 3698	1857.1[a]	1844.7	1844.7	1844.7	1843.2	1843.1	1840.7
gdb 3699	1853.7[a]	1845.2	1845.2	1848.1	1849.8	1849.8	1850.2
gdb 3700	1853.4[a]	1848.7	1848.7	1845.1	1839.9	1839.9	1834.6
gdb 3701	1848.2[a]	1838.1	1838.1	1841.6	1840.9	1840.9	1841.6
gdb 3702	1849.4[a]	1849.7	1849.7	1849.1	1847.1	1847.1	1844.5

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3703	1844.2[a]	1827.1	1827.1	1830.8	1830.0	1830.0	1831.1
gdb 3704	1842.9[a]	1826.9	1826.9	1829.8	1829.3	1829.3	1830.2
gdb 3705	1851.8[a]	1842.7	1842.7	1842.2	1840.6	1840.6	1838.1
gdb 3706	1849.4[a]	1843.8	1843.8	1846.2	1848.0	1848.0	1848.4
gdb 3707	1845.3[a]	1830.1	1830.1	1832.7	1832.6	1832.6	1833.4
gdb 3708	1851.6[a]	1842.8	1842.8	1842.2	1840.6	1840.6	1838.1
gdb 3709	1846.3[a]	1830.2	1830.2	1833.2	1832.7	1832.7	1833.3
gdb 3710	1857.2[a]	1845.6	1845.6	1845.8	1843.5	1843.5	1840.9
gdb 3711	1854.6[a]	1841.0	1841.0	1837.2	1832.5	1832.5	1827.1
gdb 3712	1855.1[a]	1846.2	1846.2	1849.3	1850.8	1850.8	1851.0
gdb 3713	1864.5[a]	1853.4	1853.4	1852.4	1845.8	1845.8	1843.7
gdb 3714	1863.4[a]	1856.0	1856.0	1858.2	1854.8	1854.8	1855.4
gdb 3715	1861.9[a]	1851.6	1851.6	1856.5	1852.6	1852.6	1855.1
gdb 3716	1875.8[a]	1870.1	1870.1	1865.8	1861.6	1861.5	1856.1
gdb 3717	1865.6[a]	1864.3	1864.3	1867.6	1866.0	1866.0	1867.3
gdb 3718	1873.6[a]	1870.3	1870.3	1869.1	1867.9	1867.9	1865.3
gdb 3719	1846.4[a]	1835.2	1835.1	1838.7	1831.9	1831.9	1834.7
gdb 3720	1851.6[a]	1845.4	1845.3	1845.9	1838.2	1838.2	1837.7
gdb 3721	1852.8[a]	1845.2	1845.2	1845.7	1838.3	1838.3	1838.0
gdb 3722	1850.0[a]	1846.7	1846.7	1850.2	1846.1	1846.1	1848.5
gdb 3723	1850.5[a]	1846.7	1846.7	1850.2	1846.3	1846.2	1848.8
gdb 3724	1851.0[a]	1844.0	1843.9	1848.5	1844.7	1844.7	1846.8
gdb 3725	1886.5[a]	1885.1	1885.1	1885.3	1880.5	1880.5	1878.5
gdb 3726	1884.3[a]	1886.7	1886.7	1890.1	1888.5	1888.5	1889.5
gdb 3727	1891.1[a]	1897.4	1897.4	1898.8	1898.7	1898.7	1900.2
gdb 3728	1910.1[a]	1907.4	1907.4	1907.8	1907.5	1907.5	1909.0
gdb 3729	1908.9[a]	1908.6	1908.6	1909.3	1907.2	1907.2	1909.2
gdb 3730	1900.0[a]	1904.6	1904.6	1902.5	1902.5	1902.4	1899.8
gdb 3731	1898.0[a]	1905.4	1905.2	1906.3	1909.3	1909.2	1909.3
gdb 3732	1877.7[a]	1876.6	1876.6	1879.7	1877.1	1877.1	1878.7
gdb 3733	1845.9[a]	1836.2	1836.2	1834.9	1830.3	1830.3	1827.8
gdb 3734	1855.0[a]	1849.2	1849.2	1845.6	1839.6	1839.6	1833.7
gdb 3735	1849.0[a]	1839.2	1839.2	1838.2	1833.4	1833.3	1830.8
gdb 3736	1853.0[a]	1850.9	1850.9	1850.6	1847.7	1847.7	1844.9
gdb 3737	1846.6[a]	1840.3	1840.3	1842.3	1841.3	1841.2	1841.6
gdb 3738	1846.5[a]	1840.1	1840.1	1842.8	1840.9	1840.8	1841.2
gdb 3739	1867.0[a]	1868.5	1868.5	1869.8	1867.4	1867.4	1868.9
gdb 3740	1867.6[a]	1863.9	1863.9	1865.7	1864.9	1864.8	1866.9
gdb 3741	1874.0[a]	1876.1	1876.1	1875.2	1872.6	1872.6	1871.2
gdb 3742	1872.0[a]	1877.7	1877.7	1879.8	1880.6	1880.5	1881.7
gdb 3743	1865.9[a]	1859.8	1859.8	1858.6	1854.4	1854.4	1852.8
gdb 3744	1875.3[a]	1867.2	1867.2	1862.8	1858.4	1858.4	1852.4
gdb 3745	1865.9[a]	1863.2	1863.2	1862.7	1857.2	1857.2	1855.9
gdb 3746	1873.8[a]	1868.7	1868.7	1867.3	1866.3	1866.2	1863.2
gdb 3747	1864.4[a]	1865.1	1865.1	1867.6	1865.3	1865.3	1866.7
gdb 3748	1869.0[a]	1865.9	1865.9	1868.9	1866.8	1866.8	1867.9
gdb 3749	1878.2[a]	1876.8	1876.8	1880.1	1877.2	1877.1	1878.9
gdb 3750	1877.6[a]	1874.3	1874.3	1877.3	1874.7	1874.7	1877.1
gdb 3751	1911.8[a]	1909.2	1909.2	1909.9	1907.3	1907.3	1908.7
gdb 3752	1892.1[a]	1900.3	1900.3	1902.0	1899.4	1899.4	1900.8
gdb 3753	1894.0[a]	1898.2	1898.2	1899.8	1899.2	1899.2	1900.1
gdb 3754	1896.6[a]	1901.6	1901.6	1899.4	1898.5	1898.5	1895.2
gdb 3755	1902.6[a]	1906.8	1906.8	1909.5	1909.2	1909.2	1909.4
gdb 3756	1877.4[a]	1872.4	1872.4	1871.7	1864.9	1864.9	1864.5
gdb 3757	1878.0[a]	1875.6	1875.6	1877.9	1874.6	1874.6	1877.0
gdb 3758	1878.6[a]	1873.6	1873.6	1877.0	1873.9	1873.9	1876.3
gdb 3759	1900.7[a]	1908.8	1908.8	1908.4	1910.4	1910.3	1908.6
gdb 3760	1874.5[a]	1876.4	1876.4	1873.9	1872.0	1872.0	1867.5
gdb 3761	1877.2[a]	1879.0	1879.0	1876.7	1874.6	1874.6	1870.0
gdb 3762	1880.2[a]	1884.3	1884.3	1885.4	1886.2	1886.2	1884.2
gdb 3763	1896.2[a]	1904.8	1904.8	1904.9	1907.6	1907.5	1907.0
gdb 3764	1854.2[a]	1859.4	1859.3	1862.1	1858.9	1858.6	1859.1
gdb 3765	1855.2[a]	1857.1	1857.1	1856.5	1850.1	1850.1	1847.4
gdb 3766	1887.5[a]	1895.1	1895.0	1895.4	1897.7	1897.6	1898.5
gdb 3767	1870.8[a]	1869.0	1869.0	1866.5	1865.4	1865.3	1862.0

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3768	1875.5[a]	1872.6	1872.6	1870.5	1869.1	1869.1	1866.2
gdb 3769	1873.3[a]	1873.5	1873.5	1874.4	1875.8	1875.8	1875.2
gdb 3770	1833.3[a]	1815.4	1815.4	1813.9	1808.7	1808.7	1804.9
gdb 3771	1835.2[a]	1819.2	1819.2	1821.0	1818.8	1818.8	1817.6
gdb 3772	1845.7[a]	1829.2	1829.2	1828.5	1824.5	1824.5	1822.7
gdb 3773	1844.1[a]	1827.5	1827.5	1826.6	1822.8	1822.8	1821.2
gdb 3774	1851.4[a]	1839.6	1839.6	1835.8	1830.5	1830.5	1825.0
gdb 3775	1844.1[a]	1832.3	1832.3	1835.0	1834.0	1834.0	1834.9
gdb 3776	1843.7[a]	1830.3	1830.3	1832.6	1831.9	1831.9	1833.0
gdb 3777	1852.4[a]	1843.7	1843.7	1843.4	1841.1	1841.1	1838.3
gdb 3778	1873.9[a]	1873.7	1873.7	1872.9	1866.9	1866.9	1866.0
gdb 3779	1874.3[a]	1876.9	1876.9	1879.3	1876.2	1876.2	1877.8
gdb 3780	1830.4[a]	1813.2	1813.2	1812.0	1807.0	1807.0	1803.8
gdb 3781	1828.4[a]	1815.3	1815.3	1816.7	1815.4	1815.3	1814.8
gdb 3782	1841.9[a]	1826.0	1826.0	1825.7	1821.6	1821.6	1820.5
gdb 3783	1841.5[a]	1828.8	1828.8	1831.8	1830.6	1830.6	1832.2
gdb 3784	1897.6[a]	1881.2	1881.2	1882.6	1881.0	1881.0	1883.2
gdb 3785	1879.0[a]	1878.6	1878.6	1877.8	1876.5	1876.5	1874.8
gdb 3786	1878.3[a]	1880.6	1880.6	1883.0	1884.9	1884.9	1885.8
gdb 3787	1869.4[a]	1868.3	1868.3	1866.0	1865.3	1865.2	1862.2
gdb 3788	1872.9[a]	1870.7	1870.7	1868.5	1868.3	1868.2	1865.3
gdb 3789	1872.5[a]	1873.2	1873.2	1874.4	1877.0	1877.0	1876.8
gdb 3790	1847.7[a]	1838.6	1838.6	1835.2	1830.0	1829.9	1825.0
gdb 3791	1843.8[a]	1830.3	1830.3	1829.9	1825.4	1825.4	1823.8
gdb 3792	1846.0[a]	1841.4	1841.4	1841.3	1839.0	1839.0	1836.7
gdb 3793	1845.8[a]	1833.1	1833.1	1835.9	1834.7	1834.7	1835.8
gdb 3794	1894.1[a]	1879.3	1879.3	1880.3	1878.7	1878.7	1880.6
gdb 3795	1873.2[a]	1871.3	1871.3	1873.1	1871.0	1871.0	1872.3
gdb 3796	1877.2[a]	1877.7	1877.7	1876.7	1875.2	1875.2	1873.2
gdb 3797	1878.1[a]	1881.1	1881.1	1883.5	1884.8	1884.7	1885.4
gdb 3798	1874.6[a]	1874.5	1874.5	1873.9	1867.3	1867.3	1866.4
gdb 3799	1874.8[a]	1876.9	1876.9	1879.4	1876.3	1876.3	1878.2
gdb 3800	1889.6[a]	1895.8	1895.6	1895.7	1898.9	1898.7	1899.0
gdb 3801	1839.6[a]	1836.4	1836.5	1834.0	1829.4	1829.4	1828.3
gdb 3802	1840.5[a]	1839.3	1839.2	1840.0	1838.5	1838.5	1840.1
gdb 3803	1843.3[a]	1841.4	1841.4	1843.0	1841.4	1841.3	1843.1
gdb 3804	1877.3[a]	1876.7	1876.7	1879.9	1879.0	1879.0	1880.4
gdb 3805	1879.5[a]	1874.7	1874.7	1878.1	1876.5	1876.5	1878.0
gdb 3806	1870.0[a]	1859.4	1859.4	1860.6	1860.5	1860.5	1862.0
gdb 3807	1886.5[a]	1892.2	1892.2	1894.9	1893.0	1893.0	1894.3
gdb 3808	1900.8[a]	1889.9	1889.9	1891.7	1887.5	1887.5	1890.0
gdb 3809	1886.2[a]	1891.8	1891.8	1894.8	1892.5	1892.5	1893.6
gdb 3810	1883.1[a]	1882.8	1882.8	1885.2	1881.4	1881.4	1883.3
gdb 3811	1871.9[a]	1861.7	1861.7	1865.2	1861.1	1861.1	1862.8
gdb 3812	1868.5[a]	1856.8	1856.8	1860.0	1857.3	1857.3	1859.1
gdb 3813	1864.1[a]	1852.8	1852.8	1855.5	1849.5	1849.5	1852.5
gdb 3814	1878.1[a]	1873.8	1873.8	1878.0	1876.3	1876.3	1877.6
gdb 3815	1858.8[a]	1845.8	1845.8	1847.9	1844.3	1844.3	1844.7
gdb 3816	1861.3[a]	1846.8	1846.8	1849.6	1845.7	1845.7	1845.8
gdb 3817	1856.3[a]	1843.7	1843.7	1846.1	1839.1	1839.1	1840.1
gdb 3818	1872.1[a]	1856.1	1856.1	1862.4	1858.4	1858.4	1861.2
gdb 3819	1851.0[a]	1850.9	1850.9	1851.1	1845.4	1845.3	1843.6
gdb 3820	1850.5[a]	1850.8	1850.8	1851.6	1845.2	1845.1	1843.3
gdb 3821	1849.7[a]	1841.5	1841.5	1841.5	1833.6	1833.6	1832.5
gdb 3822	1866.1[a]	1862.6	1862.6	1867.7	1862.8	1862.7	1864.2
gdb 3823	1893.5[a]	1899.3	1899.3	1904.0	1898.9	1898.9	1900.8
gdb 3824	1884.0[a]	1891.7	1891.7	1895.9	1892.9	1892.9	1895.3
gdb 3825	1903.0[a]	1890.8	1890.8	1892.7	1888.8	1888.8	1891.5
gdb 3826	1885.6[a]	1892.4	1892.4	1895.9	1893.6	1893.6	1895.5
gdb 3827	1884.9[a]	1883.8	1883.7	1886.6	1882.7	1882.7	1885.4
gdb 3828	1882.1[a]	1879.1	1879.1	1880.2	1880.8	1880.8	1881.4
gdb 3829	1876.5[a]	1872.3	1872.3	1870.9	1868.4	1868.4	1866.2
gdb 3830	1878.7[a]	1874.6	1874.6	1876.3	1877.8	1877.8	1878.6
gdb 3831	1875.5[a]	1865.5	1865.5	1866.8	1866.1	1866.0	1867.6
gdb 3832	1897.7[a]	1893.7	1893.7	1896.1	1895.2	1895.2	1896.9

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3833	1890.8[a]	1888.4	1888.4	1889.0	1885.6	1885.6	1885.4
gdb 3834	1897.9[a]	1892.4	1892.3	1895.5	1894.1	1894.1	1895.7
gdb 3835	1889.3[a]	1887.5	1887.5	1889.4	1886.2	1886.2	1888.0
gdb 3836	1896.1[a]	1901.6	1901.6	1904.4	1896.3	1896.3	1898.2
gdb 3837	1894.8[a]	1903.2	1903.2	1903.9	1892.7	1892.7	1895.3
gdb 3838	1900.8[a]	1902.7	1902.7	1907.2	1901.6	1901.6	1904.2
gdb 3839	1901.9[a]	1908.2	1908.2	1908.8	1909.7	1909.7	1909.0
gdb 3840	1901.6[a]	1902.1	1902.1	1899.8	1898.2	1898.2	1895.0
gdb 3841	1903.9[a]	1906.4	1906.4	1907.9	1909.4	1909.4	1909.5
gdb 3842	1897.4[a]	1901.7	1901.7	1903.3	1901.3	1901.3	1902.7
gdb 3843	1892.1[a]	1887.3	1887.3	1887.1	1882.3	1882.2	1880.2
gdb 3844	1888.8[a]	1887.1	1887.1	1889.3	1889.2	1889.2	1889.9
gdb 3845	1873.9[a]	1865.3	1865.3	1867.7	1864.6	1864.6	1865.9
gdb 3846	1879.9[a]	1876.4	1876.4	1879.3	1877.1	1877.0	1877.9
gdb 3847	1891.6[a]	1899.5	1899.5	1904.4	1899.2	1899.1	1901.3
gdb 3848	1870.1[a]	1869.1	1869.0	1872.2	1866.2	1866.2	1868.1
gdb 3849	1877.6[a]	1882.1	1882.1	1885.3	1881.9	1881.9	1883.2
gdb 3850	1869.2[a]	1872.7	1872.7	1876.0	1870.1	1870.1	1872.8
gdb 3851	1878.0[a]	1880.8	1880.8	1883.9	1881.2	1881.2	1882.2
gdb 3852	1837.3[a]	1819.0	1819.0	1821.5	1814.3	1814.3	1814.9
gdb 3853	1835.4[a]	1826.4	1826.4	1828.9	1824.5	1824.5	1824.6
gdb 3854	1842.7[a]	1823.8	1823.7	1827.2	1822.0	1822.0	1825.4
gdb 3855	1847.3[a]	1838.3	1838.3	1843.0	1838.3	1838.3	1841.2
gdb 3856	1902.0[a]	1891.3	1891.3	1893.7	1890.2	1890.2	1893.3
gdb 3857	1883.8[a]	1885.9	1885.9	1888.9	1885.6	1885.6	1888.2
gdb 3858	1884.3[a]	1892.9	1892.9	1897.4	1895.1	1895.1	1897.6
gdb 3859	1880.8[a]	1890.4	1890.4	1895.1	1887.6	1887.6	1890.8
gdb 3860	1883.2[a]	1883.8	1883.8	1886.5	1885.3	1885.3	1885.6
gdb 3861	1878.2[a]	1876.4	1876.4	1874.9	1872.2	1872.2	1869.2
gdb 3862	1877.1[a]	1869.9	1869.8	1871.8	1870.3	1870.3	1871.0
gdb 3863	1847.9[a]	1839.5	1839.4	1835.6	1830.0	1830.0	1824.3
gdb 3864	1847.2[a]	1831.1	1831.1	1830.5	1826.1	1826.1	1824.3
gdb 3865	1853.3[a]	1846.1	1846.1	1846.4	1842.5	1842.4	1840.0
gdb 3866	1853.3[a]	1847.4	1847.3	1846.6	1842.9	1842.9	1839.5
gdb 3867	1882.1[a]	1877.9	1877.9	1878.9	1879.7	1879.7	1880.2
gdb 3868	1879.2[a]	1875.3	1875.3	1877.0	1878.4	1878.4	1879.0
gdb 3869	1877.1[a]	1872.4	1872.4	1870.7	1868.7	1868.7	1866.2
gdb 3870	1873.1[a]	1863.9	1863.9	1865.2	1864.6	1864.6	1865.8
gdb 3871	1884.9[a]	1883.0	1883.0	1884.1	1880.0	1880.0	1880.7
gdb 3872	1884.5[a]	1883.0	1883.0	1885.3	1880.9	1880.9	1883.2
gdb 3873	1891.5[a]	1888.6	1888.5	1892.9	1889.5	1889.5	1892.7
gdb 3874	1885.2[a]	1883.9	1883.9	1882.2	1879.3	1879.3	1876.5
gdb 3875	1852.1[a]	1848.4	1848.4	1844.5	1838.5	1838.5	1832.4
gdb 3876	1849.5[a]	1841.5	1841.5	1840.4	1835.3	1835.2	1832.3
gdb 3877	1854.8[a]	1855.9	1855.9	1856.0	1851.2	1851.1	1847.8
gdb 3878	1855.7[a]	1857.0	1857.0	1857.2	1852.5	1852.5	1849.4
gdb 3879	1871.7[a]	1875.7	1875.6	1874.3	1871.9	1871.8	1870.0
gdb 3880	1870.2[a]	1868.6	1868.6	1870.3	1869.2	1869.2	1870.9
gdb 3881	1873.9[a]	1882.8	1882.8	1886.0	1884.5	1884.4	1885.9
gdb 3882	1872.9[a]	1866.6	1866.6	1862.1	1857.1	1857.1	1851.0
gdb 3883	1868.2[a]	1864.7	1864.6	1863.4	1858.6	1858.6	1856.6
gdb 3884	1875.6[a]	1873.7	1873.7	1873.2	1869.4	1869.3	1866.1
gdb 3885	1875.7[a]	1875.2	1875.1	1874.7	1871.3	1871.3	1868.2
gdb 3886	1885.5[a]	1885.4	1885.4	1884.9	1881.0	1881.0	1878.5
gdb 3887	1910.5[a]	1909.2	1909.2	1909.8	1908.5	1908.5	1909.8
gdb 3888	1897.1[a]	1903.7	1903.7	1901.5	1900.6	1900.6	1897.8
gdb 3889	1893.0[a]	1901.9	1901.8	1903.5	1902.4	1902.3	1903.5
gdb 3890	1900.1[a]	1908.2	1908.2	1908.8	1910.1	1910.1	1909.4
gdb 3891	1887.4[a]	1883.0	1883.0	1882.7	1878.8	1878.8	1876.6
gdb 3892	1872.8[a]	1875.9	1875.9	1874.9	1872.1	1872.1	1870.1
gdb 3893	1873.4[a]	1870.5	1870.5	1872.5	1871.3	1871.3	1873.1
gdb 3894	1876.5[a]	1882.9	1882.9	1886.1	1885.1	1885.0	1886.4
gdb 3895	1852.6[a]	1843.1	1843.1	1843.3	1836.0	1836.0	1835.1
gdb 3896	1852.0[a]	1846.3	1846.3	1851.2	1846.0	1845.9	1848.2
gdb 3897	1853.7[a]	1852.2	1852.2	1852.6	1847.5	1847.5	1845.9

... *continued on next page* ...

Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3898	1884.3[a]	1872.5	1872.5	1874.6	1871.9	1871.9	1875.6
gdb 3899	1870.9[a]	1868.1	1868.1	1866.9	1865.5	1865.5	1863.8
gdb 3900	1868.8[a]	1859.7	1859.7	1861.6	1861.6	1861.6	1863.6
gdb 3901	1873.8[a]	1873.4	1873.3	1875.1	1876.2	1876.2	1877.4
gdb 3902	1871.9[a]	1872.5	1872.5	1874.9	1870.2	1870.2	1873.1
gdb 3903	1872.5[a]	1874.3	1874.3	1876.9	1872.1	1872.1	1874.7
gdb 3904	1875.6[a]	1877.1	1877.1	1879.7	1874.9	1874.9	1877.2
gdb 3905	1877.5[a]	1886.2	1886.2	1888.8	1886.3	1886.2	1888.0
gdb 3906	1877.6[a]	1881.3	1881.3	1883.5	1879.5	1879.5	1881.0
gdb 3907	1875.5[a]	1877.8	1877.8	1879.9	1876.5	1876.5	1878.8
gdb 3908	1882.5[a]	1884.4	1884.4	1886.9	1882.7	1882.7	1883.9
gdb 3909	1882.4[a]	1890.6	1890.6	1893.4	1891.4	1891.4	1891.9
gdb 3910	1877.1[a]	1878.9	1878.9	1881.7	1872.8	1872.8	1876.4
gdb 3911	1882.9[a]	1882.7	1882.7	1885.1	1880.0	1880.0	1882.1
gdb 3912	1878.6[a]	1879.2	1879.2	1881.5	1876.4	1876.4	1879.1
gdb 3913	1879.7[a]	1881.2	1881.2	1883.8	1880.0	1879.9	1881.8
gdb 3914	1882.1[a]	1884.2	1884.2	1886.7	1882.7	1882.7	1884.4
gdb 3915	1898.5[a]	1887.8	1887.8	1889.4	1885.9	1885.9	1888.4
gdb 3916	1885.7[a]	1893.0	1893.0	1895.7	1894.2	1894.2	1895.5
gdb 3917	1816.5[a]	1802.8	1802.8	1805.8	1800.3	1800.3	1800.1
gdb 3918	1811.5[a]	1783.4	1783.4	1788.5	1784.7	1784.7	1787.7
gdb 3919	1822.9[a]	1802.3	1802.3	1807.1	1805.3	1805.3	1807.2
gdb 3920	1798.2[a]	1783.1	1783.1	1785.7	1782.5	1782.4	1782.7
gdb 3921	1803.3[a]	1786.0	1786.0	1788.9	1786.0	1786.0	1785.5
gdb 3922	1807.6[a]	1784.1	1784.1	1789.2	1785.1	1785.0	1787.7
gdb 3923	1816.4[a]	1802.4	1802.4	1807.4	1804.6	1804.5	1806.2
gdb 3924	1841.8[a]	1825.9	1825.9	1830.5	1822.2	1822.2	1825.7
gdb 3925	1851.9[a]	1842.2	1842.2	1847.1	1840.7	1840.7	1843.8
gdb 3926	1850.7[a]	1841.7	1841.7	1844.8	1839.8	1839.8	1841.0
gdb 3927	1812.9[a]	1803.0	1803.0	1805.8	1799.9	1799.9	1799.4
gdb 3928	1815.9[a]	1804.2	1804.2	1806.9	1801.0	1801.0	1800.0
gdb 3929	1808.3[a]	1786.0	1786.0	1791.8	1786.5	1786.5	1789.5
gdb 3930	1817.4[a]	1798.5	1798.5	1806.0	1802.1	1802.1	1805.0
gdb 3931	1840.4[a]	1828.0	1828.0	1831.7	1823.6	1823.6	1827.0
gdb 3932	1846.4[a]	1840.8	1840.8	1845.5	1839.1	1839.1	1842.5
gdb 3933	1848.7[a]	1843.3	1843.3	1847.1	1841.3	1841.3	1844.0
gdb 3934	1858.0[a]	1851.8	1851.8	1854.1	1848.0	1848.0	1848.8
gdb 3935	1851.7[a]	1852.3	1852.2	1850.0	1841.9	1841.9	1845.6
gdb 3936	1858.5[a]	1851.3	1851.3	1850.0	1844.4	1844.4	1842.9
gdb 3937	1855.9[a]	1841.9	1841.9	1844.5	1839.9	1839.9	1843.1
gdb 3938	1851.6[a]	1838.0	1838.0	1840.7	1836.6	1836.6	1839.3
gdb 3939	1861.7[a]	1856.6	1856.5	1860.2	1856.6	1856.5	1858.9
gdb 3940	1866.2[a]	1860.9	1860.9	1864.0	1860.2	1860.2	1862.4
gdb 3941	1862.2[a]	1857.7	1857.7	1859.9	1857.3	1857.3	1858.8
gdb 3942	1871.7[a]	1862.5	1862.5	1862.0	1859.2	1859.1	1855.8
gdb 3943	1850.9[a]	1838.0	1838.0	1840.4	1836.5	1836.5	1839.6
gdb 3944	1854.7[a]	1855.4	1855.4	1854.9	1846.7	1846.7	1850.5
gdb 3945	1860.4[a]	1848.3	1848.3	1850.3	1849.6	1849.5	1851.1
gdb 3946	1868.6[a]	1861.6	1861.6	1860.4	1858.2	1858.1	1855.4
gdb 3947	1830.4[a]	1815.0	1815.0	1819.0	1812.5	1812.5	1816.6
gdb 3948	1833.8[a]	1817.9	1817.9	1821.9	1815.4	1815.4	1819.4
gdb 3949	1838.9[a]	1833.4	1833.4	1837.3	1832.3	1832.3	1835.6
gdb 3950	1835.9[a]	1830.7	1830.7	1834.5	1829.4	1829.4	1832.7
gdb 3951	1845.2[a]	1832.4	1832.4	1834.2	1825.4	1825.4	1827.1
gdb 3952	1836.1[a]	1824.7	1824.7	1828.7	1820.4	1820.4	1823.9
gdb 3953	1849.9[a]	1836.4	1836.4	1840.9	1834.9	1834.9	1838.4
gdb 3954	1856.8[a]	1850.5	1850.5	1854.1	1846.5	1846.5	1847.8
gdb 3955	1850.4[a]	1837.4	1837.4	1841.2	1835.6	1835.5	1838.6
gdb 3956	1849.6[a]	1839.3	1839.3	1844.1	1834.6	1834.6	1838.5
gdb 3957	1852.9[a]	1842.3	1842.3	1846.9	1837.7	1837.7	1841.2
gdb 3958	1850.7[a]	1841.1	1841.1	1845.1	1836.1	1836.1	1839.6
gdb 3959	1854.3[a]	1852.6	1852.6	1857.1	1850.1	1850.1	1853.1
gdb 3960	1852.4[a]	1851.9	1851.9	1855.8	1849.3	1849.3	1852.3
gdb 3961	1854.4[a]	1852.4	1852.4	1857.0	1849.8	1849.8	1853.0
gdb 3962	1867.5[a]	1869.8	1869.7	1872.8	1868.0	1868.0	1870.2

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 3963	1893.8[a]	1900.2	1900.2	1902.1	1898.8	1898.8	1900.5
gdb 3964	1868.1[a]	1870.1	1870.1	1873.3	1867.8	1867.8	1870.6
gdb 3965	1876.8[a]	1881.2	1881.2	1886.6	1881.9	1881.9	1884.0
gdb 3966	1876.4[a]	1881.8	1881.7	1885.5	1882.5	1882.4	1883.5
gdb 3967	1872.0[a]	1874.5	1874.5	1877.5	1871.2	1871.2	1873.6
gdb 3968	1878.0[a]	1883.2	1883.2	1886.2	1883.2	1883.2	1884.0
gdb 3969	1877.0[a]	1881.1	1881.1	1885.2	1879.0	1878.9	1882.1
gdb 3970	1875.0[a]	1878.2	1878.2	1881.4	1876.0	1876.0	1879.2
gdb 3971	1886.4[a]	1892.1	1892.1	1895.0	1892.9	1892.9	1894.5
gdb 3972	1886.2[a]	1892.9	1892.9	1896.2	1893.9	1893.8	1895.4
gdb 3973	1903.0[a]	1890.6	1890.6	1892.6	1888.6	1888.6	1891.3
gdb 3974	1878.8[a]	1879.5	1879.4	1881.9	1877.9	1877.9	1880.2
gdb 3975	1881.8[a]	1889.8	1889.8	1894.0	1891.1	1891.1	1893.1
gdb 3976	1881.7[a]	1887.3	1887.2	1889.9	1887.9	1887.9	1889.1
gdb 3977	1880.3[a]	1879.8	1879.8	1882.8	1878.5	1878.5	1881.2
gdb 3978	1866.8[a]	1863.7	1863.7	1865.9	1861.6	1861.6	1863.4
gdb 3979	1877.8[a]	1881.6	1881.6	1886.8	1882.0	1882.0	1883.8
gdb 3980	1889.2[a]	1892.7	1892.7	1894.5	1892.9	1892.8	1894.9
gdb 3981	1896.9[a]	1900.4	1900.4	1901.5	1903.1	1903.1	1903.5
gdb 3982	1842.9[a]	1828.1	1828.1	1827.6	1823.3	1823.3	1821.8
gdb 3983	1850.0[a]	1843.4	1843.4	1842.9	1839.9	1839.9	1837.4
gdb 3984	1878.8[a]	1876.5	1876.4	1878.2	1878.3	1878.3	1879.2
gdb 3985	1879.5[a]	1875.0	1875.0	1878.3	1876.6	1876.6	1878.0
gdb 3986	1869.1[a]	1859.9	1859.9	1861.1	1860.4	1860.4	1862.0
gdb 3987	1870.5[a]	1872.6	1872.6	1875.7	1871.1	1871.0	1874.0
gdb 3988	1873.7[a]	1874.7	1874.7	1877.6	1873.6	1873.6	1876.7
gdb 3989	1875.2[a]	1884.0	1884.0	1887.0	1885.2	1885.2	1887.4
gdb 3990	1881.4[a]	1870.9	1870.8	1872.8	1870.3	1870.2	1873.7
gdb 3991	1865.2[a]	1856.4	1856.3	1858.6	1858.4	1858.4	1860.8
gdb 3992	1871.8[a]	1872.2	1872.1	1875.6	1875.7	1875.7	1877.6
gdb 3993	1882.1[a]	1890.0	1889.9	1894.3	1891.4	1891.4	1893.4
gdb 3994	1880.2[a]	1887.7	1887.7	1890.3	1888.7	1888.6	1889.8
gdb 3995	1877.2[a]	1877.5	1877.5	1880.1	1876.3	1876.3	1878.5
gdb 3996	1852.4[a]	1850.7	1850.7	1852.3	1846.1	1846.1	1844.7
gdb 3997	1851.5[a]	1842.7	1842.6	1846.1	1842.1	1842.1	1843.8
gdb 3998	1849.0[a]	1839.4	1839.4	1839.3	1832.1	1832.1	1831.0
gdb 3999	1851.7[a]	1851.2	1851.2	1856.1	1853.6	1853.5	1855.0
gdb 4000	1875.4[a]	1874.5	1874.5	1877.6	1876.2	1876.2	1877.6
gdb 4001	1874.8[a]	1870.1	1870.1	1872.1	1873.0	1873.0	1873.5
gdb 4002	1870.5[a]	1860.1	1860.1	1862.0	1860.1	1860.0	1862.0
gdb 4003	1842.9[a]	1824.9	1824.9	1828.3	1823.1	1823.1	1826.0
gdb 4004	1841.0[a]	1826.6	1826.6	1829.2	1823.7	1823.6	1826.7
gdb 4005	1851.6[a]	1841.1	1841.1	1844.6	1840.9	1840.9	1843.1
gdb 4006	1847.6[a]	1841.5	1841.5	1844.2	1840.0	1840.0	1842.2
gdb 4007	1881.1[a]	1882.8	1882.8	1886.3	1885.1	1885.1	1885.8
gdb 4008	1874.8[a]	1867.4	1867.4	1869.7	1868.0	1868.0	1869.3
gdb 4009	1887.3[a]	1885.6	1885.6	1889.7	1882.8	1882.8	1885.7
gdb 4010	1889.3[a]	1895.3	1895.2	1899.4	1895.0	1895.0	1896.9
gdb 4011	1851.1[a]	1845.7	1845.7	1845.7	1838.1	1838.1	1837.2
gdb 4012	1849.8[a]	1840.1	1840.1	1843.6	1836.5	1836.5	1838.8
gdb 4013	1854.5[a]	1857.6	1857.6	1859.2	1852.8	1852.8	1851.5
gdb 4014	1853.2[a]	1849.7	1849.7	1853.4	1848.9	1848.9	1850.4
gdb 4015	1912.1[a]	1914.6	1914.6	1916.3	1912.1	1912.0	1914.9
gdb 4016	1893.1[a]	1905.9	1905.9	1908.8	1904.3	1904.2	1906.9
gdb 4017	1897.1[a]	1901.0	1901.0	1902.4	1900.2	1900.2	1901.6
gdb 4018	1901.9[a]	1913.9	1913.8	1917.1	1915.6	1915.6	1916.8
gdb 4019	1874.7[a]	1862.8	1862.8	1866.0	1862.7	1862.7	1864.1
gdb 4020	1873.1[a]	1865.5	1865.5	1869.3	1865.6	1865.6	1868.0
gdb 4021	1865.1[a]	1853.1	1853.1	1855.8	1850.0	1850.0	1852.8
gdb 4022	1880.2[a]	1873.9	1873.9	1877.9	1876.9	1876.9	1878.0
gdb 4023	1862.1[a]	1850.4	1850.4	1853.5	1847.4	1847.4	1851.2
gdb 4024	1869.5[a]	1867.9	1867.9	1872.0	1861.3	1861.2	1866.8
gdb 4025	1871.2[a]	1859.9	1859.9	1863.7	1860.1	1860.1	1862.2
gdb 4026	1864.7[a]	1852.8	1852.8	1855.5	1846.6	1846.6	1848.9
gdb 4027	1865.7[a]	1863.0	1863.0	1867.1	1859.4	1859.4	1861.1

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4028	1875.5[a]	1865.8	1865.8	1869.2	1865.1	1865.1	1866.3
gdb 4029	1873.3[a]	1868.6	1868.6	1872.0	1866.7	1866.7	1868.9
gdb 4030	1865.5[a]	1854.8	1854.8	1857.9	1851.1	1851.1	1854.1
gdb 4031	1883.3[a]	1879.0	1879.0	1881.9	1879.8	1879.8	1880.1
gdb 4032	1841.4[a]	1828.2	1828.2	1831.7	1823.8	1823.8	1826.8
gdb 4033	1837.5[a]	1825.9	1825.9	1830.2	1821.7	1821.7	1825.0
gdb 4034	1848.2[a]	1835.8	1835.8	1837.7	1828.9	1828.9	1830.1
gdb 4035	1847.7[a]	1841.3	1841.3	1845.1	1839.4	1839.4	1842.1
gdb 4036	1845.1[a]	1840.1	1840.1	1845.8	1838.5	1838.5	1841.9
gdb 4037	1855.9[a]	1851.1	1851.1	1854.6	1847.0	1847.0	1847.8
gdb 4038	1871.4[a]	1860.9	1860.9	1864.1	1860.5	1860.5	1862.1
gdb 4039	1868.5[a]	1856.5	1856.5	1859.3	1857.0	1856.9	1858.4
gdb 4040	1870.1[a]	1862.1	1862.1	1865.4	1862.3	1862.3	1864.7
gdb 4041	1862.1[a]	1850.8	1850.8	1853.3	1847.6	1847.6	1850.5
gdb 4042	1876.9[a]	1871.5	1871.5	1875.7	1874.5	1874.5	1875.9
gdb 4043	1887.0[a]	1886.1	1886.1	1888.8	1879.8	1879.8	1883.1
gdb 4044	1883.9[a]	1881.7	1881.7	1885.5	1877.6	1877.6	1881.3
gdb 4045	1895.5[a]	1893.7	1893.7	1897.2	1892.6	1892.6	1894.2
gdb 4046	1862.2[a]	1847.4	1847.4	1849.5	1846.5	1846.4	1846.7
gdb 4047	1870.1[a]	1850.1	1850.1	1855.8	1849.3	1849.3	1852.8
gdb 4048	1856.9[a]	1842.9	1842.9	1845.8	1838.4	1838.4	1839.7
gdb 4049	1875.8[a]	1856.2	1856.2	1862.4	1858.8	1858.8	1861.4
gdb 4050	1839.3[a]	1826.9	1826.9	1828.8	1821.4	1821.4	1822.4
gdb 4051	1843.4[a]	1826.8	1826.8	1831.5	1821.5	1821.4	1826.4
gdb 4052	1849.3[a]	1838.2	1838.2	1840.8	1836.2	1836.2	1836.0
gdb 4053	1859.2[a]	1846.0	1846.0	1848.1	1844.4	1844.4	1844.7
gdb 4054	1861.7[a]	1847.0	1847.0	1849.8	1845.7	1845.7	1845.7
gdb 4055	1868.2[a]	1850.7	1850.7	1856.4	1849.0	1849.0	1852.4
gdb 4056	1854.6[a]	1841.2	1841.1	1844.2	1836.2	1836.2	1837.7
gdb 4057	1871.3[a]	1855.3	1855.3	1861.6	1857.1	1857.1	1859.8
gdb 4058	1882.5[a]	1876.8	1876.8	1880.3	1870.3	1870.3	1873.0
gdb 4059	1882.1[a]	1877.0	1877.0	1881.6	1870.7	1870.7	1874.6
gdb 4060	1887.6[a]	1881.9	1881.9	1884.5	1878.7	1878.7	1880.1
gdb 4061	1888.2[a]	1884.2	1884.2	1889.1	1881.5	1881.5	1884.2
gdb 4062	1851.8[a]	1839.3	1839.3	1842.6	1834.8	1834.8	1836.4
gdb 4063	1862.7[a]	1848.3	1848.3	1855.0	1842.0	1842.0	1849.0
gdb 4064	1857.9[a]	1845.3	1845.3	1847.1	1844.4	1844.4	1844.2
gdb 4065	1855.4[a]	1852.6	1852.6	1854.1	1847.6	1847.6	1846.0
gdb 4066	1859.6[a]	1845.2	1845.2	1849.1	1845.1	1845.1	1847.6
gdb 4067	1848.9[a]	1838.8	1838.8	1838.8	1831.6	1831.6	1830.7
gdb 4068	1861.5[a]	1855.2	1855.2	1859.3	1857.5	1857.5	1859.0
gdb 4069	1853.4[a]	1853.1	1853.1	1854.7	1847.2	1847.2	1845.7
gdb 4070	1850.8[a]	1850.9	1850.9	1851.6	1845.0	1845.0	1842.9
gdb 4071	1863.1[a]	1852.9	1852.9	1856.5	1850.3	1850.3	1851.9
gdb 4072	1846.3[a]	1839.2	1839.2	1839.1	1831.0	1831.0	1829.9
gdb 4073	1865.1[a]	1860.0	1860.0	1863.8	1859.8	1859.8	1861.0
gdb 4074	1870.4[a]	1868.2	1868.2	1868.3	1860.6	1860.6	1859.9
gdb 4075	1829.0[a]	1821.9	1821.9	1824.6	1818.2	1818.2	1821.0
gdb 4076	1874.1[a]	1871.2	1871.2	1872.3	1867.5	1867.5	1866.0
gdb 4077	1869.7[a]	1868.1	1868.1	1871.8	1863.7	1863.7	1867.0
gdb 4078	1874.3[a]	1868.9	1868.9	1868.1	1861.7	1861.7	1860.6
gdb 4079	1868.9[a]	1874.0	1874.0	1877.9	1871.9	1871.9	1874.4
gdb 4080	1878.0[a]	1879.9	1879.9	1880.9	1875.6	1875.6	1874.2
gdb 4081	1885.6[a]	1888.6	1888.6	1891.3	1884.0	1884.0	1887.3
gdb 4082	1880.3[a]	1881.9	1881.9	1885.5	1878.0	1878.0	1881.8
gdb 4083	1889.5[a]	1893.2	1893.2	1895.2	1890.7	1890.7	1892.4
gdb 4084	1889.6[a]	1891.1	1891.1	1893.7	1889.9	1889.9	1892.0
gdb 4085	1877.6[a]	1871.7	1871.7	1876.5	1866.7	1866.7	1871.1
gdb 4086	1885.2[a]	1878.4	1878.4	1882.8	1876.3	1876.3	1879.8
gdb 4087	1853.5[a]	1844.4	1844.4	1848.9	1839.5	1839.5	1844.2
gdb 4088	1853.4[a]	1843.9	1843.9	1848.5	1838.8	1838.8	1843.3
gdb 4089	1854.4[a]	1854.0	1854.0	1858.6	1851.3	1851.3	1855.1
gdb 4090	1854.6[a]	1854.6	1854.6	1860.6	1852.2	1852.2	1856.3
gdb 4091	1885.8[a]	1883.3	1883.3	1886.1	1880.8	1880.8	1883.5
gdb 4092	1888.9[a]	1893.9	1893.9	1896.8	1893.6	1893.6	1895.4

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4093	1894.7[a]	1895.7	1895.7	1899.9	1891.6	1891.6	1894.9
gdb 4094	1899.3[a]	1899.0	1899.0	1901.9	1898.0	1898.0	1900.2
gdb 4095	1887.9[a]	1887.9	1887.9	1891.0	1884.6	1884.6	1887.0
gdb 4096	1892.7[a]	1899.5	1899.5	1903.9	1898.9	1898.9	1900.5
gdb 4097	1878.3[a]	1876.2	1876.2	1879.8	1870.9	1870.9	1874.9
gdb 4098	1881.1[a]	1887.5	1887.5	1890.5	1884.5	1884.5	1887.6
gdb 4099	1886.4[a]	1891.8	1891.8	1895.9	1892.5	1892.5	1894.6
gdb 4100	1885.5[a]	1892.1	1892.1	1895.2	1892.4	1892.4	1893.5
gdb 4101	1901.0[a]	1890.0	1890.0	1891.8	1887.5	1887.5	1890.1
gdb 4102	1883.1[a]	1882.6	1882.6	1885.5	1881.3	1881.3	1884.0
gdb 4103	1900.0[a]	1908.1	1908.1	1910.7	1907.1	1907.1	1909.7
gdb 4104	1897.2[a]	1905.6	1905.6	1907.9	1904.4	1904.4	1906.5
gdb 4105	1921.5[a]	1907.8	1907.8	1909.4	1906.9	1906.8	1909.5
gdb 4106	1903.2[a]	1910.5	1910.5	1914.0	1913.0	1913.0	1914.5
gdb 4107	1914.0[a]	1918.6	1918.5	1920.4	1915.9	1915.9	1918.8
gdb 4108	1914.7[a]	1918.4	1918.4	1920.2	1916.0	1916.0	1918.9
gdb 4109	1901.5[a]	1907.2	1907.2	1908.8	1906.8	1906.8	1908.7
gdb 4110	1902.4[a]	1915.9	1915.9	1917.6	1917.7	1917.6	1918.5
gdb 4111	1870.5[a]	1872.6	1872.6	1875.8	1870.3	1870.3	1872.9
gdb 4112	1869.7[a]	1868.0	1868.0	1870.1	1865.5	1865.5	1867.2
gdb 4113	1877.2[a]	1880.1	1880.1	1884.2	1880.8	1880.8	1882.3
gdb 4114	1888.2[a]	1895.1	1895.1	1898.5	1893.4	1893.3	1896.3
gdb 4115	1892.5[a]	1893.4	1893.4	1895.3	1891.6	1891.6	1892.9
gdb 4116	1898.5[a]	1902.1	1902.1	1904.3	1903.8	1903.8	1905.0
gdb 4117	1896.3[a]	1902.0	1902.0	1904.0	1892.1	1892.1	1896.8
gdb 4118	1894.3[a]	1899.4	1899.4	1901.7	1890.0	1889.9	1895.4
gdb 4119	1898.5[a]	1903.2	1903.2	1905.8	1899.1	1899.1	1901.8
gdb 4120	1895.9[a]	1897.5	1897.5	1899.2	1894.7	1894.7	1896.0
gdb 4121	1893.6[a]	1901.1	1901.1	1904.5	1898.2	1898.2	1901.3
gdb 4122	1903.0[a]	1907.0	1907.0	1909.1	1907.0	1907.0	1907.8
gdb 4123	1880.4[a]	1881.2	1881.2	1885.4	1878.1	1878.1	1880.9
gdb 4124	1870.6[a]	1873.2	1873.2	1876.3	1871.8	1871.8	1874.9
gdb 4125	1873.7[a]	1874.5	1874.5	1877.4	1873.5	1873.5	1876.8
gdb 4126	1875.6[a]	1883.4	1883.4	1887.7	1884.6	1884.6	1887.2
gdb 4127	1897.4[a]	1893.8	1893.8	1897.6	1895.3	1895.3	1897.5
gdb 4128	1897.5[a]	1891.9	1891.9	1894.9	1893.5	1893.5	1895.1
gdb 4129	1890.8[a]	1888.3	1888.2	1888.9	1885.3	1885.3	1885.1
gdb 4130	1887.0[a]	1884.9	1884.9	1887.4	1883.5	1883.5	1885.7
gdb 4131	1895.7[a]	1900.7	1900.7	1902.4	1895.5	1895.5	1897.2
gdb 4132	1893.5[a]	1896.9	1896.9	1900.5	1892.4	1892.4	1895.5
gdb 4133	1892.8[a]	1901.4	1901.4	1902.4	1890.4	1890.4	1893.4
gdb 4134	1900.3[a]	1902.0	1902.0	1905.5	1901.1	1901.1	1903.2
gdb 4135	1885.1[a]	1883.3	1883.2	1884.5	1880.1	1880.1	1880.9
gdb 4136	1884.2[a]	1881.4	1881.4	1884.2	1879.4	1879.3	1882.3
gdb 4137	1894.2[a]	1890.9	1890.9	1893.7	1891.1	1891.1	1893.1
gdb 4138	1845.1[a]	1832.3	1832.3	1834.2	1825.5	1825.5	1827.1
gdb 4139	1840.3[a]	1827.1	1827.1	1830.3	1822.6	1822.6	1825.6
gdb 4140	1838.8[a]	1826.7	1826.7	1830.2	1822.1	1822.1	1825.3
gdb 4141	1850.2[a]	1836.6	1836.6	1841.6	1835.2	1835.2	1838.6
gdb 4142	1850.1[a]	1836.2	1836.2	1840.5	1834.9	1834.9	1838.0
gdb 4143	1859.0[a]	1851.9	1851.9	1855.3	1848.4	1848.4	1849.3
gdb 4144	1884.5[a]	1884.2	1884.2	1885.7	1885.5	1885.5	1885.3
gdb 4145	1877.5[a]	1876.4	1876.3	1875.0	1871.8	1871.8	1869.0
gdb 4146	1875.5[a]	1868.7	1868.7	1870.3	1868.6	1868.6	1869.5
gdb 4147	1847.8[a]	1839.6	1839.5	1835.7	1829.9	1829.9	1824.3
gdb 4148	1844.5[a]	1829.3	1829.3	1828.2	1824.1	1824.0	1822.2
gdb 4149	1854.4[a]	1846.6	1846.6	1846.8	1842.5	1842.5	1840.0
gdb 4150	1853.7[a]	1847.7	1847.7	1847.1	1843.1	1843.1	1839.7
gdb 4151	1884.0[a]	1872.7	1872.7	1874.8	1871.9	1871.9	1875.5
gdb 4152	1871.3[a]	1868.3	1868.2	1867.3	1865.5	1865.4	1864.0
gdb 4153	1866.3[a]	1857.8	1857.7	1859.5	1859.3	1859.3	1861.4
gdb 4154	1875.3[a]	1874.6	1874.6	1877.4	1877.3	1877.3	1878.7
gdb 4155	1911.5[a]	1919.6	1919.6	1921.3	1916.6	1916.6	1918.0
gdb 4156	1928.1[a]	1924.4	1924.4	1926.0	1921.2	1921.2	1924.2
gdb 4157	1912.8[a]	1918.6	1918.6	1921.2	1916.3	1916.3	1919.3

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4158	1918.1[a]	1923.5	1923.5	1925.7	1924.2	1924.2	1926.0
gdb 4159	1894.0[a]	1900.4	1900.4	1903.3	1895.8	1895.8	1897.5
gdb 4160	1891.1[a]	1900.7	1900.7	1901.5	1890.5	1890.5	1893.0
gdb 4161	1883.3[a]	1879.3	1879.3	1878.4	1870.1	1870.1	1868.5
gdb 4162	1875.9[a]	1875.5	1875.5	1875.3	1866.9	1866.9	1866.6
gdb 4163	1888.7[a]	1891.6	1891.6	1893.1	1881.9	1881.9	1884.0
gdb 4164	1886.8[a]	1886.1	1886.1	1887.0	1880.5	1880.5	1879.3
gdb 4165	1891.9[a]	1892.0	1892.0	1895.4	1888.7	1888.7	1889.7
gdb 4166	1861.5[a]	1852.6	1852.6	1850.9	1843.7	1843.6	1840.4
gdb 4167	1860.4[a]	1850.8	1850.8	1850.9	1843.5	1843.5	1842.6
gdb 4168	1871.3[a]	1861.2	1861.2	1862.8	1856.6	1856.6	1855.6
gdb 4169	1862.4[a]	1860.3	1860.3	1862.8	1856.9	1856.8	1856.8
gdb 4170	1883.9[a]	1881.8	1881.8	1883.3	1879.2	1879.1	1880.6
gdb 4171	1881.0[a]	1879.4	1879.4	1882.4	1878.1	1878.1	1881.3
gdb 4172	1889.2[a]	1886.7	1886.7	1890.9	1888.3	1888.2	1891.2
gdb 4173	1893.5[a]	1899.0	1899.0	1900.7	1894.6	1894.5	1895.9
gdb 4174	1891.3[a]	1900.9	1900.9	1901.7	1890.6	1890.6	1893.0
gdb 4175	1901.8[a]	1908.5	1908.5	1910.9	1899.3	1899.3	1903.1
gdb 4176	1903.8[a]	1907.8	1907.8	1911.7	1904.9	1904.9	1907.2
gdb 4177	1928.2[a]	1924.5	1924.5	1926.2	1921.2	1921.2	1924.1
gdb 4178	1912.0[a]	1919.8	1919.8	1921.5	1917.0	1917.0	1918.3
gdb 4179	1909.7[a]	1914.6	1914.6	1916.5	1912.3	1912.3	1914.5
gdb 4180	1917.7[a]	1923.4	1923.4	1925.2	1923.9	1923.9	1925.4
gdb 4181	1900.5[a]	1907.7	1907.7	1909.8	1898.1	1898.1	1901.9
gdb 4182	1901.5[a]	1907.7	1907.7	1911.6	1904.7	1904.7	1907.1
gdb 4183	1902.1[a]	1907.9	1907.9	1908.4	1909.3	1909.3	1908.5
gdb 4184	1903.7[a]	1904.7	1904.7	1906.0	1907.9	1907.9	1907.4
gdb 4185	1902.1[a]	1902.1	1902.1	1899.7	1898.2	1898.2	1894.8
gdb 4186	1895.4[a]	1899.7	1899.7	1901.5	1898.9	1898.9	1900.5
gdb 4187	1891.8[a]	1887.3	1887.3	1887.1	1882.3	1882.3	1880.2
gdb 4188	1878.2[a]	1877.7	1877.7	1879.8	1876.8	1876.8	1879.2
gdb 4189	1886.6[a]	1885.7	1885.7	1888.8	1887.5	1887.5	1888.2
gdb 4190	1891.5[a]	1894.2	1894.2	1895.9	1893.6	1893.6	1895.6
gdb 4191	1891.6[a]	1895.9	1895.9	1897.5	1895.3	1895.3	1896.8
gdb 4192	1896.1[a]	1894.3	1894.3	1892.2	1890.7	1890.7	1888.2
gdb 4193	1898.9[a]	1901.7	1901.7	1902.4	1903.9	1903.9	1904.2
gdb 4194	1895.3[a]	1900.7	1900.7	1901.6	1899.7	1899.7	1901.3
gdb 4195	1909.5[a]	1908.4	1908.3	1908.3	1905.9	1905.9	1907.7
gdb 4196	1899.0[a]	1900.1	1900.1	1898.1	1896.3	1896.2	1893.4
gdb 4197	1902.8[a]	1907.6	1907.6	1909.4	1909.6	1909.5	1909.5
gdb 4198	1885.0[a]	1884.8	1884.8	1884.5	1880.5	1880.5	1878.5
gdb 4199	1870.9[a]	1864.7	1864.6	1860.1	1855.2	1855.1	1849.4
gdb 4200	1866.4[a]	1865.4	1865.3	1864.7	1858.6	1858.6	1857.0
gdb 4201	1872.1[a]	1869.9	1869.9	1868.1	1865.5	1865.5	1862.1
gdb 4202	1875.5[a]	1875.4	1875.4	1874.9	1871.2	1871.2	1868.1
gdb 4203	1891.6[a]	1892.5	1892.5	1890.7	1889.7	1889.4	1887.5
gdb 4204	1885.5[a]	1892.3	1892.3	1894.1	1891.7	1891.7	1894.3
gdb 4205	1895.0[a]	1900.4	1900.4	1903.0	1901.6	1901.6	1902.4
gdb 4206	1875.8[a]	1867.6	1867.6	1863.4	1858.4	1858.3	1853.0
gdb 4207	1867.9[a]	1862.1	1862.1	1861.0	1855.5	1855.5	1854.5
gdb 4208	1879.1[a]	1874.2	1874.2	1873.6	1870.5	1870.4	1867.3
gdb 4209	1875.4[a]	1873.8	1873.8	1872.4	1870.1	1870.1	1867.2
gdb 4210	1884.2[a]	1884.1	1884.1	1882.3	1879.1	1879.1	1876.7
gdb 4211	1905.2[a]	1902.5	1902.5	1903.1	1900.3	1900.2	1902.4
gdb 4212	1898.2[a]	1900.5	1900.5	1898.3	1897.2	1897.2	1894.5
gdb 4213	1892.8[a]	1898.6	1898.6	1899.0	1897.9	1897.9	1899.1
gdb 4214	1902.2[a]	1906.2	1906.2	1907.0	1907.9	1907.9	1907.2
gdb 4215	1880.8[a]	1876.2	1876.2	1876.2	1872.8	1872.8	1870.9
gdb 4216	1876.0[a]	1864.9	1864.9	1868.1	1865.0	1864.9	1866.5
gdb 4217	1873.3[a]	1869.2	1869.2	1872.8	1868.5	1868.5	1870.9
gdb 4218	1878.5[a]	1873.5	1873.5	1877.5	1876.2	1876.2	1877.4
gdb 4219	1853.3[a]	1847.4	1847.4	1847.7	1840.1	1840.1	1839.5
gdb 4220	1854.1[a]	1857.1	1857.1	1857.4	1852.1	1852.0	1850.3
gdb 4221	1852.5[a]	1849.8	1849.8	1854.8	1849.3	1849.3	1851.7
gdb 4222	1887.1[a]	1885.9	1885.9	1888.5	1879.9	1879.8	1883.2

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4223	1892.5[a]	1893.5	1893.5	1896.1	1886.4	1886.4	1890.6
gdb 4224	1894.2[a]	1893.8	1893.8	1897.2	1892.5	1892.4	1894.3
gdb 4225	1873.1[a]	1863.3	1863.3	1866.2	1863.1	1863.1	1864.7
gdb 4226	1868.2[a]	1856.8	1856.8	1859.6	1857.4	1857.4	1858.9
gdb 4227	1870.8[a]	1867.1	1867.0	1870.5	1866.2	1866.2	1868.4
gdb 4228	1876.9[a]	1872.5	1872.5	1876.6	1875.3	1875.3	1876.5
gdb 4229	1873.1[a]	1863.6	1863.6	1867.1	1863.0	1862.9	1864.9
gdb 4230	1868.2[a]	1857.6	1857.6	1860.7	1857.7	1857.7	1859.5
gdb 4231	1871.1[a]	1868.3	1868.3	1872.1	1866.9	1866.9	1869.3
gdb 4232	1877.5[a]	1873.6	1873.6	1876.7	1875.7	1875.7	1876.6
gdb 4233	1870.1[a]	1862.3	1862.3	1866.0	1856.0	1856.0	1859.0
gdb 4234	1867.0[a]	1864.1	1864.1	1868.1	1857.7	1857.6	1861.5
gdb 4235	1874.4[a]	1870.4	1870.4	1874.0	1867.0	1867.0	1869.3
gdb 4236	1877.7[a]	1873.7	1873.7	1878.3	1870.5	1870.4	1873.2
gdb 4237	1848.9[a]	1837.7	1837.7	1839.0	1831.2	1831.2	1832.0
gdb 4238	1860.8[a]	1854.4	1854.4	1857.6	1850.2	1850.2	1850.7
gdb 4239	1848.1[a]	1840.9	1840.9	1847.0	1839.8	1839.8	1843.3
gdb 4240	1873.8[a]	1874.3	1874.3	1878.9	1868.5	1868.5	1873.0
gdb 4241	1877.6[a]	1879.5	1879.5	1884.1	1876.7	1876.7	1879.2
gdb 4242	1877.7[a]	1879.1	1879.1	1882.8	1876.7	1876.7	1879.4
gdb 4243	1881.3[a]	1877.2	1877.2	1880.1	1871.1	1871.0	1873.7
gdb 4244	1887.5[a]	1884.4	1884.4	1887.7	1875.7	1875.7	1880.3
gdb 4245	1885.4[a]	1880.8	1880.8	1883.2	1877.5	1877.5	1878.9
gdb 4246	1887.9[a]	1884.1	1884.1	1889.1	1881.4	1881.4	1884.4
gdb 4247	1876.9[a]	1871.0	1871.0	1870.5	1864.2	1864.2	1863.4
gdb 4248	1877.7[a]	1879.5	1879.5	1879.1	1874.9	1874.9	1873.0
gdb 4249	1871.6[a]	1878.0	1878.0	1881.9	1876.2	1876.2	1878.8
gdb 4250	1849.5[a]	1838.9	1838.9	1843.7	1834.4	1834.4	1838.2
gdb 4251	1850.2[a]	1840.9	1840.9	1844.9	1835.8	1835.7	1839.1
gdb 4252	1849.0[a]	1839.8	1839.8	1843.2	1835.2	1835.2	1838.8
gdb 4253	1854.7[a]	1851.4	1851.4	1855.9	1848.8	1848.8	1851.6
gdb 4254	1851.1[a]	1850.7	1850.7	1855.8	1848.6	1848.6	1851.8
gdb 4255	1853.6[a]	1852.0	1852.0	1857.6	1850.2	1850.2	1853.6
gdb 4256	1890.0[a]	1889.0	1889.0	1892.2	1885.7	1885.7	1887.9
gdb 4257	1893.6[a]	1899.1	1899.1	1903.3	1898.3	1898.3	1899.7
gdb 4258	1902.4[a]	1910.8	1910.8	1914.1	1902.5	1902.4	1907.2
gdb 4259	1911.7[a]	1914.6	1914.6	1916.3	1912.0	1912.0	1914.9
gdb 4260	1893.2[a]	1906.9	1906.9	1909.7	1905.4	1905.4	1908.1
gdb 4261	1901.2[a]	1904.6	1904.6	1906.3	1904.0	1904.0	1905.7
gdb 4262	1900.0[a]	1913.3	1913.3	1916.4	1915.0	1914.9	1916.2
gdb 4263	1870.9[a]	1874.8	1874.8	1878.9	1872.6	1872.6	1875.0
gdb 4264	1872.6[a]	1874.1	1874.1	1876.6	1871.6	1871.6	1874.1
gdb 4265	1871.3[a]	1872.5	1872.5	1874.8	1870.1	1870.1	1873.0
gdb 4266	1874.5[a]	1875.0	1875.0	1877.4	1872.7	1872.7	1875.5
gdb 4267	1877.5[a]	1885.9	1885.8	1888.4	1885.6	1885.6	1887.3
gdb 4268	1902.2[a]	1908.5	1908.5	1910.9	1906.3	1906.3	1908.9
gdb 4269	1902.4[a]	1909.2	1909.1	1911.5	1907.1	1907.0	1909.7
gdb 4270	1905.2[a]	1911.9	1911.9	1914.0	1909.8	1909.8	1912.1
gdb 4271	1911.0[a]	1918.1	1918.1	1921.1	1919.1	1919.1	1920.8
gdb 4272	1889.8[a]	1898.2	1898.2	1901.3	1891.0	1891.0	1895.2
gdb 4273	1895.4[a]	1904.7	1904.7	1907.2	1895.1	1895.1	1900.3
gdb 4274	1898.6[a]	1904.8	1904.8	1908.5	1901.5	1901.5	1904.5
gdb 4275	1898.0[a]	1905.1	1905.1	1908.7	1901.5	1901.5	1904.8
gdb 4276	1868.8[a]	1868.0	1868.0	1870.9	1866.2	1866.2	1867.8
gdb 4277	1891.6[a]	1897.5	1897.5	1899.1	1896.0	1895.9	1897.6
gdb 4278	1896.6[a]	1901.4	1901.4	1903.3	1900.1	1900.0	1902.0
gdb 4279	1894.5[a]	1909.2	1909.1	1912.2	1907.0	1907.0	1909.5
gdb 4280	1901.0[a]	1911.8	1911.8	1913.6	1912.9	1912.8	1913.1
gdb 4281	1877.0[a]	1875.9	1875.9	1878.8	1870.1	1870.1	1874.2
gdb 4282	1882.8[a]	1881.1	1881.1	1883.4	1878.8	1878.8	1881.3
gdb 4283	1883.2[a]	1882.7	1882.7	1886.7	1880.6	1880.6	1883.7
gdb 4284	1885.2[a]	1889.4	1889.4	1892.2	1885.0	1884.9	1888.2
gdb 4285	1892.8[a]	1899.4	1899.4	1901.0	1891.6	1891.6	1895.1
gdb 4286	1890.3[a]	1893.6	1893.6	1897.2	1892.4	1892.4	1894.4
gdb 4287	1890.6[a]	1897.1	1897.1	1899.3	1895.1	1895.1	1896.7

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4288	1891.3[a]	1895.4	1895.4	1897.8	1888.8	1888.7	1893.0
gdb 4289	1893.1[a]	1901.1	1901.1	1903.5	1899.1	1899.1	1901.4
gdb 4290	1883.0[a]	1887.7	1887.7	1890.7	1884.9	1884.8	1888.1
gdb 4291	1885.8[a]	1892.9	1892.9	1895.6	1887.8	1887.8	1891.5
gdb 4292	1891.5[a]	1895.2	1895.2	1897.4	1888.5	1888.5	1892.5
gdb 4293	1893.5[a]	1900.4	1900.4	1904.2	1898.5	1898.5	1901.5
gdb 4294	1895.1[a]	1901.8	1901.8	1905.4	1900.0	1900.0	1902.6
gdb 4295	1870.5[a]	1866.9	1866.9	1869.6	1861.8	1861.8	1865.3
gdb 4296	1876.7[a]	1878.1	1878.1	1881.3	1875.8	1875.8	1878.9
gdb 4297	1877.5[a]	1881.3	1881.3	1885.6	1879.0	1879.0	1882.4
gdb 4298	1916.0[a]	1919.8	1919.8	1922.1	1920.8	1920.8	1921.6
gdb 4299	1923.3[a]	1920.5	1920.5	1920.7	1916.9	1916.9	1919.4
gdb 4300	1887.1[a]	1885.9	1885.9	1885.2	1880.7	1880.7	1877.9
gdb 4301	1904.6[a]	1912.4	1912.4	1915.0	1914.1	1914.1	1915.9
gdb 4302	1886.1[a]	1885.0	1885.0	1884.3	1880.4	1880.4	1877.5
gdb 4303	1911.0[a]	1915.9	1915.8	1916.5	1917.0	1917.0	1917.0
gdb 4304	1909.0[a]	1918.2	1918.2	1919.1	1919.4	1919.4	1919.4
gdb 4305	1880.8[a]	1881.0	1881.0	1879.4	1876.8	1876.8	1874.1
gdb 4306	1903.9[a]	1912.2	1912.2	1913.3	1913.2	1913.2	1914.1
gdb 4307	1908.2[a]	1912.6	1912.6	1913.8	1913.3	1913.2	1914.0
gdb 4308	1902.8[a]	1909.1	1909.0	1910.2	1911.6	1911.6	1912.8
gdb 4309	1870.2[a]	1867.8	1867.8	1869.9	1864.8	1864.8	1866.2
gdb 4310	1877.3[a]	1884.1	1884.0	1888.3	1883.6	1883.6	1884.7
gdb 4311	1877.9[a]	1874.4	1874.4	1876.4	1872.4	1872.4	1874.4
gdb 4312	1892.4[a]	1896.6	1896.6	1899.4	1894.7	1894.7	1897.2
gdb 4313	1892.5[a]	1900.4	1900.4	1904.1	1898.6	1898.6	1901.4
gdb 4314	1913.4[a]	1917.4	1917.4	1919.7	1917.4	1917.4	1918.2
gdb 4315	1916.7[a]	1917.4	1917.4	1918.9	1917.4	1917.4	1917.9
gdb 4316	1908.8[a]	1913.0	1913.0	1913.8	1913.5	1913.5	1913.7
gdb 4317	1910.0[a]	1916.2	1916.2	1917.8	1916.7	1916.6	1917.2
gdb 4318	1888.7[a]	1889.3	1889.3	1892.2	1889.9	1889.9	1890.3
gdb 4319	1898.4[a]	1904.2	1904.2	1905.0	1902.3	1902.3	1905.1
gdb 4320	1906.4[a]	1908.6	1908.6	1909.8	1910.0	1910.0	1911.4
gdb 4321	1903.9[a]	1910.9	1910.9	1912.4	1910.4	1910.4	1911.9
gdb 4322	1906.2[a]	1910.1	1910.1	1911.6	1909.7	1909.7	1910.6
gdb 4323	1886.1[a]	1885.4	1885.4	1888.9	1882.3	1882.3	1884.2
gdb 4324	1879.8[a]	1880.5	1880.5	1882.9	1877.4	1877.4	1879.9
gdb 4325	1907.5[a]	1915.7	1915.7	1917.1	1916.8	1916.8	1917.5
gdb 4326	1878.9[a]	1879.7	1879.7	1879.7	1875.1	1875.1	1873.4
gdb 4327	1913.2[a]	1910.9	1910.9	1912.2	1908.2	1908.1	1912.0
gdb 4328	1900.4[a]	1907.1	1907.1	1910.0	1909.8	1909.7	1912.0
gdb 4329	1890.4[a]	1886.5	1886.5	1886.3	1882.0	1882.0	1880.0
gdb 4330	1887.3[a]	1886.5	1886.5	1888.7	1888.2	1888.2	1888.8
gdb 4331	1887.8[a]	1882.7	1882.7	1882.4	1878.6	1878.6	1876.5
gdb 4332	1890.5[a]	1886.6	1886.6	1886.4	1881.9	1881.9	1879.9
gdb 4333	1886.9[a]	1887.2	1887.2	1890.5	1888.5	1888.4	1889.2
gdb 4334	1881.7[a]	1881.2	1881.1	1885.3	1878.5	1878.5	1881.1
gdb 4335	1879.5[a]	1877.4	1877.4	1877.9	1873.7	1873.7	1872.5
gdb 4336	1885.5[a]	1883.4	1883.4	1886.0	1881.2	1881.2	1883.6
gdb 4337	1884.0[a]	1880.7	1880.7	1882.9	1878.4	1878.4	1880.8
gdb 4338	1895.8[a]	1894.4	1894.4	1896.3	1894.7	1894.6	1895.1
gdb 4339	1909.0[a]	1910.6	1910.6	1911.4	1907.5	1907.5	1911.1
gdb 4340	1905.8[a]	1912.7	1912.7	1915.6	1914.1	1914.1	1915.8
gdb 4341	1886.7[a]	1883.6	1883.6	1882.6	1878.4	1878.4	1876.0
gdb 4342	1904.8[a]	1906.5	1906.5	1907.8	1908.3	1908.3	1909.8
gdb 4343	1881.1[a]	1876.3	1876.3	1875.5	1872.5	1872.5	1869.9
gdb 4344	1911.5[a]	1909.1	1909.0	1909.9	1906.2	1906.2	1909.3
gdb 4345	1908.3[a]	1912.9	1912.9	1915.3	1913.8	1913.8	1914.7
gdb 4346	1916.6[a]	1927.7	1927.7	1928.1	1929.8	1929.8	1929.9
gdb 4347	1914.4[a]	1918.4	1918.4	1920.1	1918.9	1918.9	1919.1
gdb 4348	1920.4[a]	1917.0	1917.0	1917.8	1913.1	1913.1	1915.8
gdb 4349	1906.6[a]	1911.6	1911.6	1912.3	1908.8	1908.8	1910.7
gdb 4350	1894.9[a]	1899.8	1899.8	1897.5	1896.1	1896.1	1892.7
gdb 4351	1912.0[a]	1910.5	1910.5	1911.3	1907.8	1907.8	1909.2
gdb 4352	1894.5[a]	1904.2	1904.2	1905.9	1902.6	1902.6	1903.7

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4353	1903.3[a]	1912.4	1912.4	1914.5	1914.1	1914.1	1913.6
gdb 4354	1917.8[a]	1928.2	1928.2	1928.8	1930.9	1930.9	1931.9
gdb 4355	1898.4[a]	1900.6	1900.6	1898.6	1896.5	1896.5	1893.4
gdb 4356	1909.2[a]	1905.7	1905.7	1906.3	1902.8	1902.7	1904.8
gdb 4357	1896.9[a]	1902.2	1902.2	1903.0	1900.3	1900.3	1901.4
gdb 4358	1903.5[a]	1907.5	1907.5	1908.0	1909.2	1909.2	1908.5
gdb 4359	1915.1[a]	1919.8	1919.8	1921.5	1920.4	1920.4	1920.7
gdb 4360	1921.3[a]	1917.9	1917.9	1918.8	1914.4	1914.4	1917.3
gdb 4361	1906.5[a]	1912.2	1912.2	1913.0	1909.2	1909.2	1911.1
gdb 4362	1899.9[a]	1902.9	1902.9	1903.9	1901.2	1901.1	1903.1
gdb 4363	1911.8[a]	1907.9	1907.9	1909.0	1905.2	1905.1	1908.2
gdb 4364	1906.4[a]	1911.5	1911.5	1913.0	1913.0	1912.9	1913.9
gdb 4365	1924.7[a]	1934.0	1934.0	1934.2	1936.5	1936.5	1936.7
gdb 4366	1906.4[a]	1907.4	1907.4	1909.2	1904.2	1904.2	1908.3
gdb 4367	1899.7[a]	1905.7	1905.7	1906.9	1903.9	1903.9	1906.3
gdb 4368	1905.6[a]	1910.3	1910.3	1912.7	1912.4	1912.3	1913.4
gdb 4369	1908.2[a]	1916.9	1916.9	1918.9	1918.2	1918.2	1918.4
gdb 4370	1901.9[a]	1911.8	1911.8	1913.1	1909.8	1909.7	1911.3
gdb 4371	1873.4[a]	1874.8	1874.8	1873.6	1867.2	1867.2	1866.0
gdb 4372	1880.1[a]	1879.3	1879.3	1877.6	1875.0	1875.0	1872.2
gdb 4373	1869.2[a]	1875.8	1875.8	1880.0	1872.4	1872.4	1874.9
gdb 4374	1868.8[a]	1876.2	1876.2	1879.4	1872.2	1872.2	1874.5
gdb 4375	1871.5[a]	1877.4	1877.4	1882.2	1874.5	1874.4	1877.5
gdb 4376	1879.1[a]	1883.5	1883.5	1886.2	1883.2	1883.2	1883.8
gdb 4377	1871.0[a]	1879.6	1879.6	1882.2	1875.3	1875.3	1879.9
gdb 4378	1872.1[a]	1878.6	1878.6	1881.4	1874.9	1874.9	1876.9
gdb 4379	1871.4[a]	1882.7	1882.7	1885.0	1872.3	1872.2	1875.8
gdb 4380	1870.7[a]	1882.0	1882.0	1884.8	1871.5	1871.5	1875.7
gdb 4381	1879.6[a]	1887.9	1887.9	1891.7	1886.8	1886.8	1887.4
gdb 4382	1910.3[a]	1916.0	1915.9	1916.5	1916.8	1916.8	1916.8
gdb 4383	1899.6[a]	1909.6	1909.6	1910.9	1907.7	1907.7	1909.8
gdb 4384	1915.6[a]	1919.5	1919.5	1919.8	1920.0	1920.0	1919.2
gdb 4385	1907.3[a]	1913.1	1913.1	1913.7	1910.1	1910.1	1911.8
gdb 4386	1871.2[a]	1877.2	1877.1	1880.5	1873.8	1873.7	1876.2
gdb 4387	1879.6[a]	1884.1	1884.1	1888.0	1884.0	1883.9	1885.1
gdb 4388	1908.2[a]	1913.8	1913.8	1915.5	1915.3	1915.3	1915.8
gdb 4389	1901.6[a]	1908.1	1908.1	1909.3	1906.0	1906.0	1908.0
gdb 4390	1903.2[a]	1904.7	1904.7	1905.6	1902.9	1902.9	1905.7
gdb 4391	1910.8[a]	1910.8	1910.8	1912.8	1913.0	1913.0	1914.1
gdb 4392	1916.4[a]	1928.0	1928.0	1928.6	1930.3	1930.2	1930.8
gdb 4393	1895.5[a]	1901.5	1901.5	1903.0	1899.3	1899.3	1902.4
gdb 4394	1897.2[a]	1902.2	1902.1	1903.5	1900.1	1900.1	1903.3
gdb 4395	1903.1[a]	1906.7	1906.7	1909.1	1908.3	1908.3	1909.7
gdb 4396	1870.0[a]	1875.8	1875.7	1878.6	1867.5	1867.5	1871.5
gdb 4397	1870.1[a]	1875.0	1875.0	1878.0	1867.3	1867.2	1871.5
gdb 4398	1869.6[a]	1873.0	1872.9	1876.4	1871.2	1871.1	1873.9
gdb 4399	1864.2[a]	1864.7	1864.7	1867.3	1858.4	1858.4	1862.8
gdb 4400	1864.3[a]	1866.3	1866.3	1868.4	1857.8	1857.8	1863.1
gdb 4401	1871.0[a]	1870.7	1870.7	1872.6	1862.8	1862.8	1868.4
gdb 4402	1870.9[a]	1871.8	1871.8	1874.5	1868.8	1868.8	1871.7
gdb 4403	1895.4[a]	1902.9	1902.9	1904.3	1902.3	1902.3	1904.9
gdb 4404	1902.3[a]	1908.6	1908.6	1910.9	1911.3	1911.3	1912.6
gdb 4405	1859.0[a]	1855.6	1855.6	1859.0	1852.0	1852.0	1854.5
gdb 4406	1857.1[a]	1854.7	1854.7	1858.1	1851.8	1851.8	1854.3
gdb 4407	1865.1[a]	1868.9	1868.8	1872.6	1867.6	1867.5	1868.8
gdb 4408	1892.5[a]	1903.4	1903.4	1904.6	1903.9	1903.8	1905.6
gdb 4409	1834.6[a]	1816.8	1816.8	1819.2	1811.7	1811.7	1812.3
gdb 4410	1830.8[a]	1814.6	1814.6	1816.5	1810.2	1810.2	1811.3
gdb 4411	1837.6[a]	1827.2	1827.1	1829.5	1825.0	1825.0	1824.8
gdb 4412	1846.2[a]	1825.4	1825.3	1831.9	1824.9	1824.9	1828.5
gdb 4413	1839.5[a]	1821.8	1821.8	1825.1	1819.8	1819.8	1823.1
gdb 4414	1840.9[a]	1826.7	1826.7	1829.4	1823.7	1823.7	1826.8
gdb 4415	1847.6[a]	1839.3	1839.3	1843.9	1839.1	1839.1	1841.5
gdb 4416	1852.0[a]	1841.7	1841.7	1846.3	1841.7	1841.6	1844.0
gdb 4417	1902.4[a]	1891.2	1891.2	1893.6	1889.8	1889.8	1892.8

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4418	1880.8[a]	1883.3	1883.3	1886.2	1882.7	1882.7	1885.3
gdb 4419	1879.1[a]	1881.2	1881.2	1883.8	1880.7	1880.7	1883.6
gdb 4420	1885.4[a]	1893.0	1893.0	1897.4	1894.7	1894.7	1896.9
gdb 4421	1873.5[a]	1876.2	1876.2	1875.3	1872.1	1872.1	1870.0
gdb 4422	1870.8[a]	1868.6	1868.5	1870.4	1869.2	1869.1	1870.8
gdb 4423	1872.4[a]	1872.6	1872.5	1874.0	1871.5	1871.5	1873.1
gdb 4424	1881.0[a]	1885.4	1885.4	1887.5	1886.6	1886.6	1887.0
gdb 4425	1849.1[a]	1840.6	1840.6	1840.6	1833.1	1833.1	1832.2
gdb 4426	1848.7[a]	1840.8	1840.8	1840.7	1833.6	1833.5	1832.9
gdb 4427	1847.7[a]	1834.0	1834.0	1837.2	1830.5	1830.5	1833.1
gdb 4428	1854.1[a]	1851.8	1851.8	1852.0	1846.6	1846.6	1844.8
gdb 4429	1854.7[a]	1846.7	1846.7	1851.3	1845.8	1845.7	1847.3
gdb 4430	1856.5[a]	1850.4	1850.4	1854.8	1848.4	1848.3	1850.2
gdb 4431	1883.5[a]	1884.9	1884.9	1887.6	1882.2	1882.1	1884.5
gdb 4432	1897.8[a]	1887.5	1887.4	1888.9	1885.2	1885.2	1887.6
gdb 4433	1879.7[a]	1880.9	1880.9	1883.6	1879.3	1879.3	1881.1
gdb 4434	1879.0[a]	1881.8	1881.8	1884.3	1880.0	1880.0	1881.8
gdb 4435	1878.9[a]	1880.1	1880.1	1882.3	1878.8	1878.8	1881.2
gdb 4436	1885.1[a]	1892.7	1892.7	1896.7	1893.7	1893.7	1895.2
gdb 4437	1877.8[a]	1879.3	1879.3	1882.3	1873.3	1873.3	1876.8
gdb 4438	1884.7[a]	1891.6	1891.6	1895.8	1888.2	1888.1	1890.5
gdb 4439	1883.4[a]	1882.8	1882.8	1885.3	1879.9	1879.9	1881.9
gdb 4440	1893.1[a]	1901.9	1901.9	1902.8	1903.6	1903.6	1904.3
gdb 4441	1840.6[a]	1838.6	1838.5	1840.5	1833.1	1833.1	1837.0
gdb 4442	1847.5[a]	1853.6	1853.5	1858.0	1850.4	1850.4	1853.2
gdb 4443	1852.5[a]	1849.0	1849.0	1852.1	1846.9	1846.9	1849.5
gdb 4444	1896.3[a]	1894.2	1894.2	1892.1	1890.5	1890.5	1887.8
gdb 4445	1889.1[a]	1893.4	1893.4	1895.0	1892.7	1892.7	1894.4
gdb 4446	1894.0[a]	1896.7	1896.5	1898.2	1895.2	1895.1	1897.1
gdb 4447	1900.2[a]	1902.6	1902.6	1904.5	1904.7	1904.7	1905.1
gdb 4448	1895.3[a]	1900.1	1900.1	1897.7	1896.3	1896.3	1892.7
gdb 4449	1893.9[a]	1899.7	1899.7	1901.3	1899.8	1899.8	1900.5
gdb 4450	1894.2[a]	1904.4	1904.4	1906.0	1902.7	1902.7	1903.5
gdb 4451	1903.3[a]	1909.3	1909.3	1910.3	1910.7	1910.7	1909.6
gdb 4452	1877.8[a]	1874.7	1874.7	1873.1	1866.4	1866.4	1865.6
gdb 4453	1886.0[a]	1881.3	1881.3	1880.8	1876.6	1876.6	1874.3
gdb 4454	1881.4[a]	1879.1	1879.1	1882.1	1877.7	1877.7	1879.6
gdb 4455	1829.4[a]	1817.0	1817.0	1818.9	1813.5	1813.5	1814.6
gdb 4456	1837.1[a]	1825.4	1825.4	1828.9	1825.5	1825.5	1825.7
gdb 4457	1844.1[a]	1828.3	1828.3	1833.6	1827.9	1827.9	1831.6
gdb 4458	1847.6[a]	1834.8	1834.8	1837.9	1833.1	1833.1	1836.4
gdb 4459	1854.4[a]	1841.3	1841.3	1843.6	1839.0	1839.0	1842.0
gdb 4460	1855.2[a]	1841.7	1841.7	1844.2	1839.4	1839.4	1842.5
gdb 4461	1860.4[a]	1853.5	1853.5	1852.5	1846.4	1846.4	1844.9
gdb 4462	1860.9[a]	1846.0	1846.0	1848.0	1847.2	1847.2	1848.4
gdb 4463	1862.7[a]	1847.6	1847.6	1850.2	1848.6	1848.6	1849.9
gdb 4464	1869.0[a]	1861.9	1861.9	1861.3	1858.2	1858.2	1855.0
gdb 4465	1859.5[a]	1855.6	1855.6	1858.2	1855.0	1854.9	1856.7
gdb 4466	1885.4[a]	1892.2	1892.2	1894.5	1887.6	1887.6	1890.8
gdb 4467	1893.7[a]	1899.6	1899.6	1902.5	1898.4	1898.4	1900.2
gdb 4468	1885.8[a]	1892.3	1892.3	1895.5	1887.2	1887.1	1891.1
gdb 4469	1892.3[a]	1896.2	1896.2	1898.7	1894.4	1894.3	1896.7
gdb 4470	1886.7[a]	1890.0	1890.0	1892.0	1890.1	1890.1	1892.4
gdb 4471	1892.3[a]	1895.4	1895.4	1897.3	1894.9	1894.9	1897.1
gdb 4472	1898.3[a]	1900.0	1900.0	1901.0	1902.6	1902.6	1902.9
gdb 4473	1921.0[a]	1907.7	1907.7	1909.3	1906.4	1906.4	1909.0
gdb 4474	1894.4[a]	1902.5	1902.5	1905.4	1901.3	1901.2	1903.8
gdb 4475	1898.2[a]	1905.1	1905.1	1908.0	1904.2	1904.2	1907.1
gdb 4476	1903.9[a]	1911.0	1911.0	1914.5	1913.4	1913.3	1914.8
gdb 4477	1828.9[a]	1814.2	1814.2	1817.3	1811.0	1811.0	1812.2
gdb 4478	1838.9[a]	1827.9	1827.9	1829.4	1822.2	1822.1	1822.9
gdb 4479	1845.9[a]	1834.5	1834.5	1835.9	1831.9	1831.9	1830.9
gdb 4480	1845.4[a]	1829.7	1829.7	1835.9	1829.8	1829.8	1833.6
gdb 4481	1859.8[a]	1847.7	1847.7	1851.7	1844.4	1844.4	1848.7
gdb 4482	1861.5[a]	1851.0	1851.0	1853.3	1847.7	1847.7	1851.1

... *continued on next page* ...

Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4483	1871.7[a]	1859.8	1859.8	1863.4	1860.1	1860.1	1861.9
gdb 4484	1868.6[a]	1861.6	1861.6	1866.2	1860.8	1860.8	1863.9
gdb 4485	1850.8[a]	1837.8	1837.8	1841.0	1832.9	1832.9	1834.8
gdb 4486	1850.8[a]	1838.6	1838.6	1840.4	1834.7	1834.7	1836.6
gdb 4487	1857.6[a]	1844.0	1844.0	1845.7	1843.2	1843.2	1842.9
gdb 4488	1863.3[a]	1846.8	1846.8	1852.4	1846.0	1846.0	1850.2
gdb 4489	1829.6[a]	1818.8	1818.8	1819.1	1814.5	1814.5	1814.1
gdb 4490	1868.4[a]	1865.6	1865.6	1866.2	1858.8	1858.7	1858.6
gdb 4491	1874.0[a]	1870.4	1870.4	1870.2	1866.1	1866.1	1864.1
gdb 4492	1837.6[a]	1827.3	1827.3	1830.6	1828.4	1828.4	1830.4
gdb 4493	1901.8[a]	1907.1	1907.1	1911.2	1905.1	1905.1	1907.9
gdb 4494	1921.0[a]	1907.4	1907.3	1908.9	1906.3	1906.3	1909.0
gdb 4495	1897.3[a]	1904.9	1904.9	1908.1	1904.0	1904.0	1906.9
gdb 4496	1898.1[a]	1905.1	1905.1	1908.0	1904.2	1904.2	1907.1
gdb 4497	1904.6[a]	1910.2	1910.2	1912.3	1912.2	1912.2	1913.3
gdb 4498	1896.7[a]	1894.4	1894.4	1892.4	1890.6	1890.6	1888.0
gdb 4499	1887.6[a]	1891.6	1891.6	1893.3	1890.1	1890.1	1892.0
gdb 4500	1892.9[a]	1896.0	1896.0	1897.7	1894.3	1894.3	1896.4
gdb 4501	1899.0[a]	1903.9	1903.9	1905.7	1905.4	1905.4	1905.6
gdb 4502	1892.9[a]	1893.4	1893.4	1895.3	1891.5	1891.5	1892.7
gdb 4503	1886.8[a]	1892.0	1892.0	1895.2	1890.3	1890.3	1893.4
gdb 4504	1892.9[a]	1896.3	1896.3	1900.0	1894.5	1894.4	1898.2
gdb 4505	1900.7[a]	1903.3	1903.2	1906.9	1904.9	1904.9	1906.8
gdb 4506	1893.3[a]	1899.0	1899.0	1901.8	1889.0	1889.0	1894.0
gdb 4507	1890.5[a]	1894.4	1894.4	1897.1	1887.3	1887.3	1891.4
gdb 4508	1900.2[a]	1903.7	1903.7	1907.4	1899.8	1899.8	1902.3
gdb 4509	1894.5[a]	1897.7	1897.7	1902.2	1894.2	1894.2	1898.2
gdb 4510	1897.7[a]	1899.9	1899.9	1897.5	1895.2	1895.2	1891.7
gdb 4511	1892.6[a]	1897.8	1897.8	1899.3	1896.4	1896.4	1898.1
gdb 4512	1896.3[a]	1902.4	1902.3	1903.2	1900.1	1900.0	1901.0
gdb 4513	1903.2[a]	1906.8	1906.8	1907.1	1907.8	1907.8	1906.3
gdb 4514	1870.6[a]	1869.7	1869.7	1869.0	1861.8	1861.8	1861.9
gdb 4515	1877.8[a]	1876.3	1876.3	1876.6	1871.7	1871.7	1870.2
gdb 4516	1871.9[a]	1870.6	1870.6	1873.2	1869.8	1869.8	1872.9
gdb 4517	1861.5[a]	1850.9	1850.9	1853.2	1847.6	1847.6	1851.1
gdb 4518	1871.0[a]	1860.5	1860.5	1862.8	1860.7	1860.7	1862.2
gdb 4519	1871.0[a]	1867.5	1867.5	1871.7	1866.3	1866.3	1868.7
gdb 4520	1901.9[a]	1908.3	1908.3	1912.5	1906.5	1906.5	1909.5
gdb 4521	1868.2[a]	1865.9	1865.9	1868.8	1860.3	1860.3	1864.1
gdb 4522	1878.6[a]	1874.8	1874.8	1877.9	1872.9	1872.8	1874.9
gdb 4523	1879.3[a]	1880.2	1880.2	1884.1	1877.7	1877.7	1880.5
gdb 4524	1889.3[a]	1892.5	1892.5	1895.0	1885.7	1885.7	1890.0
gdb 4525	1885.6[a]	1892.8	1892.8	1895.8	1887.6	1887.6	1891.5
gdb 4526	1892.8[a]	1900.8	1900.8	1904.4	1898.9	1898.9	1901.4
gdb 4527	1891.8[a]	1898.4	1898.4	1900.8	1896.5	1896.5	1898.8
gdb 4528	1918.0[a]	1919.6	1919.6	1920.6	1920.1	1920.1	1919.9
gdb 4529	1906.6[a]	1911.8	1911.8	1912.4	1908.7	1908.7	1910.4
gdb 4530	1903.5[a]	1904.4	1904.4	1905.4	1903.0	1903.0	1905.9
gdb 4531	1910.8[a]	1910.6	1910.6	1912.6	1912.8	1912.7	1913.9
gdb 4532	1912.5[a]	1918.6	1918.6	1919.4	1919.1	1919.1	1918.7
gdb 4533	1903.6[a]	1911.2	1911.2	1912.6	1908.9	1908.9	1910.6
gdb 4534	1873.3[a]	1875.1	1875.0	1874.2	1867.4	1867.4	1866.4
gdb 4535	1880.9[a]	1882.2	1882.1	1880.7	1877.4	1877.3	1874.3
gdb 4536	1895.6[a]	1903.3	1903.2	1905.2	1902.4	1902.3	1905.4
gdb 4537	1901.8[a]	1908.9	1908.9	1911.2	1911.6	1911.6	1912.9
gdb 4538	1868.5[a]	1865.0	1864.9	1868.3	1859.6	1859.6	1863.6
gdb 4539	1880.2[a]	1873.2	1873.1	1875.3	1871.8	1871.8	1873.4
gdb 4540	1898.6[a]	1904.3	1904.3	1906.4	1902.3	1902.2	1905.1
gdb 4541	1914.1[a]	1911.0	1911.0	1911.2	1908.4	1908.4	1911.0
gdb 4542	1905.1[a]	1910.9	1910.9	1913.7	1912.6	1912.6	1914.1
gdb 4543	1877.7[a]	1874.7	1874.7	1873.1	1866.1	1866.1	1865.4
gdb 4544	1886.5[a]	1883.2	1883.2	1882.7	1878.0	1878.0	1875.5
gdb 4545	1896.1[a]	1901.0	1900.9	1903.4	1899.2	1899.2	1902.8
gdb 4546	1904.7[a]	1906.8	1906.8	1907.8	1908.4	1908.4	1909.9
gdb 4547	1866.9[a]	1867.1	1867.1	1867.2	1859.2	1859.2	1859.7

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4548	1880.0[a]	1878.2	1878.2	1877.3	1873.7	1873.6	1871.7
gdb 4549	1899.6[a]	1906.2	1906.2	1907.5	1904.1	1904.0	1906.3
gdb 4550	1908.1[a]	1912.2	1912.2	1914.7	1913.4	1913.4	1914.4
gdb 4551	1916.7[a]	1927.7	1927.7	1927.9	1929.6	1929.6	1929.5
gdb 4552	1911.6[a]	1907.7	1907.7	1908.7	1904.9	1904.9	1908.0
gdb 4553	1895.9[a]	1901.4	1901.4	1903.5	1899.1	1899.1	1902.1
gdb 4554	1898.7[a]	1904.9	1904.9	1906.2	1902.5	1902.5	1905.1
gdb 4555	1903.0[a]	1908.2	1908.2	1910.5	1909.3	1909.3	1910.0
gdb 4556	1869.5[a]	1870.6	1870.6	1872.3	1861.9	1861.9	1867.4
gdb 4557	1867.6[a]	1869.7	1869.7	1870.9	1861.3	1861.2	1866.3
gdb 4558	1864.2[a]	1864.7	1864.7	1867.4	1858.4	1858.4	1862.8
gdb 4559	1871.1[a]	1873.1	1873.1	1874.4	1864.6	1864.6	1869.7
gdb 4560	1871.3[a]	1872.5	1872.5	1876.5	1869.9	1869.9	1873.5
gdb 4561	1872.2[a]	1871.9	1871.9	1876.7	1869.0	1869.0	1872.8
gdb 4562	1900.2[a]	1902.0	1902.0	1903.7	1900.0	1900.0	1903.2
gdb 4563	1903.0[a]	1904.3	1904.3	1905.2	1902.7	1902.7	1905.5
gdb 4564	1909.4[a]	1910.1	1910.1	1911.9	1911.7	1911.7	1912.7
gdb 4565	1869.9[a]	1876.0	1876.0	1879.0	1871.2	1871.2	1873.6
gdb 4566	1873.1[a]	1880.7	1880.7	1884.3	1876.0	1875.9	1878.0
gdb 4567	1870.2[a]	1877.5	1877.5	1880.8	1872.5	1872.5	1874.8
gdb 4568	1872.4[a]	1878.3	1878.3	1881.0	1874.2	1874.1	1876.0
gdb 4569	1870.3[a]	1879.4	1879.4	1881.6	1868.3	1868.3	1872.4
gdb 4570	1878.1[a]	1887.1	1887.1	1889.8	1884.5	1884.4	1884.7
gdb 4571	1867.1[a]	1873.0	1873.0	1875.6	1864.8	1864.8	1869.3
gdb 4572	1871.5[a]	1875.6	1875.6	1878.4	1873.1	1873.1	1875.3
gdb 4573	1868.5[a]	1871.5	1871.5	1875.8	1869.7	1869.7	1872.7
gdb 4574	1896.3[a]	1901.7	1901.6	1903.2	1899.7	1899.7	1902.7
gdb 4575	1898.6[a]	1904.9	1904.9	1905.7	1902.9	1902.8	1905.5
gdb 4576	1911.5[a]	1911.8	1911.8	1912.5	1912.9	1912.9	1913.5
gdb 4577	1896.8[a]	1901.5	1901.5	1903.1	1899.2	1899.1	1901.7
gdb 4578	1899.4[a]	1903.3	1903.3	1904.2	1901.1	1901.1	1902.8
gdb 4579	1908.2[a]	1910.7	1910.7	1913.1	1912.1	1912.1	1912.8
gdb 4580	1878.4[a]	1878.1	1878.1	1880.9	1875.5	1875.5	1878.8
gdb 4581	1867.2[a]	1868.5	1868.5	1871.0	1859.2	1859.2	1865.2
gdb 4582	1864.3[a]	1864.9	1864.9	1867.9	1858.6	1858.6	1863.1
gdb 4583	1871.6[a]	1871.5	1871.5	1873.9	1862.2	1862.1	1868.0
gdb 4584	1869.9[a]	1871.5	1871.5	1874.2	1868.2	1868.2	1871.1
gdb 4585	1872.4[a]	1872.0	1872.0	1876.9	1869.2	1869.2	1873.3
gdb 4586	1873.7[a]	1873.7	1873.7	1877.1	1870.3	1870.2	1873.6
gdb 4587	1874.6[a]	1883.7	1883.7	1885.4	1884.2	1884.2	1884.0
gdb 4588	1878.0[a]	1886.7	1886.7	1889.3	1887.3	1887.3	1886.5
gdb 4589	1873.2[a]	1881.4	1881.4	1883.0	1881.3	1881.3	1881.9
gdb 4590	1877.5[a]	1884.9	1884.9	1886.4	1885.0	1885.0	1884.4
gdb 4591	1877.3[a]	1885.9	1885.9	1887.9	1887.4	1887.1	1886.4
gdb 4592	1880.4[a]	1887.6	1887.6	1889.3	1888.9	1888.9	1888.1
gdb 4593	1849.4[a]	1850.1	1850.1	1849.1	1845.7	1845.8	1842.5
gdb 4594	1849.7[a]	1852.1	1852.1	1851.3	1847.1	1847.1	1844.1
gdb 4595	1851.4[a]	1858.5	1858.5	1861.3	1858.6	1858.6	1857.6
gdb 4596	1870.6[a]	1877.5	1877.5	1879.3	1879.8	1879.8	1880.7
gdb 4597	1885.5[a]	1884.1	1884.1	1885.1	1881.8	1881.3	1883.6
gdb 4598	1872.2[a]	1880.6	1880.6	1882.6	1882.8	1882.8	1883.4
gdb 4599	1872.3[a]	1877.1	1877.0	1879.1	1879.4	1879.4	1880.8
gdb 4600	1859.8[a]	1866.6	1866.7	1867.2	1865.3	1865.3	1866.8
gdb 4601	1870.1[a]	1877.3	1877.2	1879.0	1878.9	1878.8	1879.5
gdb 4602	1854.6[a]	1854.2	1854.2	1856.5	1856.2	1856.2	1855.9
gdb 4603	1854.3[a]	1854.6	1854.6	1857.0	1856.7	1856.7	1856.1
gdb 4604	1855.3[a]	1852.2	1852.2	1851.7	1848.2	1848.2	1845.5
gdb 4605	1855.9[a]	1852.8	1852.8	1856.1	1857.0	1857.0	1856.3
gdb 4606	1852.5[a]	1854.8	1854.8	1857.6	1851.9	1851.9	1853.0
gdb 4607	1850.0[a]	1851.5	1851.5	1854.3	1848.7	1848.7	1850.4
gdb 4608	1851.1[a]	1853.0	1853.0	1855.8	1850.6	1850.6	1851.8
gdb 4609	1857.6[a]	1867.0	1867.0	1870.1	1865.8	1865.8	1865.7
gdb 4610	1852.1[a]	1849.2	1849.2	1848.7	1845.4	1845.3	1841.8
gdb 4611	1850.2[a]	1848.7	1848.7	1847.7	1844.4	1844.4	1841.2
gdb 4612	1843.4[a]	1844.1	1844.1	1846.2	1842.7	1842.6	1843.7

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4613	1854.0[a]	1854.6	1854.6	1857.1	1855.8	1855.8	1855.3
gdb 4614	1853.8[a]	1853.3	1853.3	1855.7	1856.0	1856.0	1855.6
gdb 4615	1856.1[a]	1852.9	1852.9	1855.8	1856.2	1856.2	1855.8
gdb 4616	1852.3[a]	1853.2	1853.1	1856.2	1851.2	1851.1	1852.6
gdb 4617	1857.5[a]	1863.5	1863.4	1868.0	1864.3	1864.2	1865.3
gdb 4618	1855.3[a]	1852.4	1852.4	1851.8	1848.5	1848.5	1845.8
gdb 4619	1857.6[a]	1855.6	1855.6	1858.3	1858.4	1858.4	1858.2
gdb 4620	1850.7[a]	1847.7	1847.7	1847.6	1844.5	1844.5	1841.8
gdb 4621	1849.7[a]	1848.1	1848.1	1847.2	1844.7	1844.7	1841.5
gdb 4622	1842.9[a]	1843.3	1843.3	1845.1	1842.5	1842.5	1843.5
gdb 4623	1852.6[a]	1853.4	1853.4	1856.1	1855.3	1855.3	1854.8
gdb 4624	1849.4[a]	1851.2	1851.2	1854.0	1849.1	1849.1	1850.5
gdb 4625	1852.5[a]	1852.2	1852.2	1855.1	1850.4	1850.4	1852.0
gdb 4626	1852.1[a]	1852.5	1852.5	1855.4	1850.2	1850.2	1851.3
gdb 4627	1857.8[a]	1863.2	1863.2	1867.8	1863.9	1863.9	1864.7
gdb 4628	1864.0[a]	1873.3	1873.3	1875.0	1865.2	1865.2	1868.0
gdb 4629	1863.6[a]	1874.6	1874.6	1876.4	1866.2	1866.2	1868.7
gdb 4630	1865.3[a]	1874.0	1874.0	1876.6	1872.0	1872.0	1873.0
gdb 4631	1865.2[a]	1872.0	1872.0	1874.6	1870.6	1870.5	1871.6
gdb 4632	1879.4[a]	1883.1	1883.1	1885.0	1885.8	1885.7	1885.5
gdb 4633	1886.7[a]	1884.3	1884.3	1885.1	1883.2	1883.2	1885.6
gdb 4634	1875.9[a]	1883.2	1883.1	1885.0	1885.4	1885.4	1885.1
gdb 4635	1871.3[a]	1877.3	1876.9	1879.4	1879.6	1879.3	1880.6
gdb 4636	1875.2[a]	1880.9	1880.8	1882.1	1882.9	1882.9	1883.0
gdb 4637	1852.5[a]	1850.8	1850.8	1849.9	1847.4	1847.3	1844.5
gdb 4638	1853.8[a]	1855.5	1855.5	1858.1	1857.5	1857.5	1857.2
gdb 4639	1851.8[a]	1850.0	1850.0	1849.3	1847.4	1847.3	1844.5
gdb 4640	1851.8[a]	1852.8	1852.8	1855.2	1856.1	1856.1	1855.7
gdb 4641	1849.3[a]	1848.2	1848.2	1851.2	1847.5	1847.4	1849.1
gdb 4642	1847.1[a]	1846.4	1846.4	1849.8	1845.5	1845.5	1847.4
gdb 4643	1877.3[a]	1884.0	1884.0	1885.3	1886.5	1886.5	1886.2
gdb 4644	1888.8[a]	1887.7	1887.7	1888.9	1886.6	1886.6	1887.6
gdb 4645	1848.1[a]	1847.8	1847.8	1846.8	1844.7	1844.7	1841.6
gdb 4646	1839.8[a]	1843.1	1843.1	1844.0	1842.5	1842.5	1843.1
gdb 4647	1885.2[a]	1880.2	1879.9	1881.1	1878.6	1878.6	1881.7
gdb 4648	1859.8[a]	1866.3	1866.3	1866.3	1866.0	1866.0	1867.4
gdb 4649	1869.3[a]	1875.0	1875.0	1876.6	1878.6	1878.6	1879.2
gdb 4650	1875.5[a]	1883.6	1883.6	1885.6	1884.7	1884.6	1884.5
gdb 4651	1876.9[a]	1886.9	1886.9	1887.6	1887.3	1887.3	1886.2
gdb 4652	1885.5[a]	1882.1	1882.1	1883.4	1879.9	1879.9	1882.3
gdb 4653	1897.3[a]	1907.8	1907.7	1907.3	1908.5	1908.3	1906.4
gdb 4654	1879.5[a]	1884.8	1884.8	1887.4	1883.5	1883.5	1884.4
gdb 4655	1878.5[a]	1889.0	1889.0	1890.6	1887.3	1887.3	1887.2
gdb 4656	1887.2[a]	1886.8	1886.8	1888.1	1881.4	1881.4	1884.4
gdb 4657	1881.3[a]	1885.5	1885.5	1887.6	1887.0	1887.0	1886.9
gdb 4658	1878.3[a]	1886.5	1886.5	1888.7	1887.3	1887.2	1886.7
gdb 4659	1889.3[a]	1887.6	1887.6	1888.5	1885.2	1885.2	1887.1
gdb 4660	1876.4[a]	1882.2	1882.2	1885.0	1882.1	1882.0	1883.5
gdb 4661	1876.9[a]	1881.3	1881.2	1882.8	1881.8	1881.7	1881.9
gdb 4662	1887.6[a]	1883.8	1883.8	1885.5	1880.7	1880.7	1883.8
gdb 4663	1899.0[a]	1906.7	1906.7	1906.7	1907.5	1907.4	1906.9
gdb 4664	1855.8[a]	1847.2	1847.1	1848.1	1845.4	1845.3	1844.1
gdb 4665	1876.2[a]	1855.0	1855.0	1857.8	1853.3	1853.3	1856.5
gdb 4666	1863.3[a]	1851.5	1851.5	1855.4	1853.8	1853.8	1855.2
gdb 4667	1871.3[a]	1864.4	1864.3	1866.1	1864.6	1864.6	1865.1
gdb 4668	1869.4[a]	1863.5	1863.5	1865.1	1863.2	1863.2	1864.1
gdb 4669	1874.1[a]	1873.5	1873.5	1871.9	1869.2	1869.0	1865.7
gdb 4670	1889.3[a]	1880.2	1880.2	1881.5	1877.8	1877.8	1879.9
gdb 4671	1881.2[a]	1879.1	1879.1	1881.3	1880.5	1880.5	1880.2
gdb 4672	1897.7[a]	1906.7	1906.7	1907.9	1905.0	1905.0	1906.3
gdb 4673	1916.4[a]	1913.8	1913.8	1914.9	1911.4	1911.4	1913.4
gdb 4674	1907.2[a]	1912.3	1912.3	1913.7	1913.9	1913.9	1913.5
gdb 4675	1851.4[a]	1845.2	1845.1	1846.2	1843.7	1843.7	1843.3
gdb 4676	1873.6[a]	1854.3	1854.3	1858.2	1853.0	1853.0	1857.3
gdb 4677	1860.7[a]	1849.8	1849.8	1854.5	1853.3	1853.2	1855.5

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4678	1869.3[a]	1862.0	1862.0	1864.0	1862.2	1862.2	1863.2
gdb 4679	1886.7[a]	1878.0	1878.0	1880.0	1876.5	1876.5	1879.1
gdb 4680	1875.0[a]	1875.9	1875.9	1878.6	1878.1	1878.1	1878.3
gdb 4681	1902.3[a]	1911.0	1911.0	1912.3	1913.9	1913.8	1914.4
gdb 4682	1899.1[a]	1907.2	1907.2	1907.3	1909.2	1909.2	1908.1
gdb 4683	1872.1[a]	1871.1	1871.1	1869.8	1867.5	1867.4	1864.9
gdb 4684	1866.6[a]	1862.2	1862.1	1864.2	1862.5	1862.0	1863.1
gdb 4685	1885.8[a]	1878.8	1878.8	1880.3	1876.5	1876.5	1879.0
gdb 4686	1873.4[a]	1874.2	1874.2	1876.7	1876.4	1876.3	1876.9
gdb 4687	1914.3[a]	1913.0	1913.0	1913.7	1910.4	1910.3	1913.0
gdb 4688	1904.4[a]	1909.1	1909.0	1911.0	1910.4	1910.3	1911.1
gdb 4689	1902.3[a]	1911.9	1911.9	1913.2	1914.0	1913.9	1914.6
gdb 4690	1898.4[a]	1907.3	1907.2	1909.0	1905.2	1905.1	1906.9
gdb 4691	1914.1[a]	1913.1	1913.1	1913.7	1910.3	1910.3	1912.8
gdb 4692	1900.8[a]	1907.1	1907.1	1909.0	1908.9	1908.9	1909.8
gdb 4693	1873.3[a]	1879.0	1879.0	1881.4	1879.5	1879.4	1880.4
gdb 4694	1875.8[a]	1882.9	1882.9	1885.4	1883.6	1883.6	1884.2
gdb 4695	1888.3[a]	1888.7	1888.7	1889.3	1885.2	1885.2	1887.0
gdb 4696	1887.3[a]	1883.2	1883.2	1884.9	1880.5	1880.5	1883.7
gdb 4697	1877.4[a]	1882.2	1882.2	1883.8	1885.2	1885.2	1885.0
gdb 4698	1889.4[a]	1888.1	1888.1	1888.4	1886.5	1886.4	1888.0
gdb 4699	1890.3[a]	1886.2	1886.2	1887.8	1885.1	1885.1	1887.2
gdb 4700	1863.4[a]	1869.2	1869.2	1869.1	1867.5	1867.5	1869.0
gdb 4701	1888.4[a]	1884.8	1884.8	1886.5	1882.5	1882.5	1885.4
gdb 4702	1886.1[a]	1881.2	1881.1	1883.0	1879.4	1879.3	1882.9
gdb 4703	1873.2[a]	1877.1	1877.1	1879.1	1879.4	1879.3	1880.0
gdb 4704	1874.5[a]	1879.7	1879.6	1882.4	1880.4	1880.3	1881.4
gdb 4705	1864.3[a]	1872.6	1872.6	1873.5	1869.0	1869.0	1870.8
gdb 4706	1872.7[a]	1877.9	1877.9	1880.1	1878.7	1878.6	1879.4
gdb 4707	1885.1[a]	1882.2	1882.2	1883.7	1878.9	1878.9	1881.9
gdb 4708	1871.9[a]	1875.5	1875.5	1878.5	1876.1	1876.1	1878.5
gdb 4709	1872.3[a]	1878.0	1878.0	1880.1	1877.7	1877.7	1879.3
gdb 4710	1861.9[a]	1868.6	1868.6	1870.0	1864.9	1864.9	1868.1
gdb 4711	1853.1[a]	1849.2	1849.2	1849.2	1844.0	1844.0	1842.4
gdb 4712	1842.4[a]	1841.3	1841.3	1839.9	1831.6	1831.6	1831.0
gdb 4713	1845.2[a]	1845.7	1845.6	1847.7	1842.9	1842.9	1844.6
gdb 4714	1856.6[a]	1855.2	1855.2	1858.7	1856.4	1856.4	1857.2
gdb 4715	1852.5[a]	1848.6	1848.6	1848.8	1844.3	1844.3	1842.6
gdb 4716	1842.4[a]	1843.4	1843.4	1845.4	1841.2	1841.2	1843.2
gdb 4717	1841.0[a]	1840.9	1840.9	1839.6	1832.1	1832.1	1831.3
gdb 4718	1853.2[a]	1851.4	1851.4	1854.8	1853.2	1853.2	1854.2
gdb 4719	1839.4[a]	1838.8	1838.7	1841.4	1831.9	1831.9	1835.9
gdb 4720	1838.4[a]	1837.2	1837.2	1839.8	1830.7	1830.7	1835.1
gdb 4721	1849.9[a]	1846.1	1846.1	1850.2	1843.9	1843.9	1847.1
gdb 4722	1846.4[a]	1842.5	1842.5	1846.7	1840.6	1840.6	1844.3
gdb 4723	1882.7[a]	1888.5	1888.5	1890.6	1889.7	1889.7	1889.7
gdb 4724	1866.7[a]	1878.2	1878.2	1878.9	1875.8	1875.8	1873.8
gdb 4725	1853.2[a]	1852.1	1852.0	1851.7	1847.8	1847.7	1844.8
gdb 4726	1841.4[a]	1842.7	1842.7	1840.8	1834.4	1834.4	1832.6
gdb 4727	1879.4[a]	1886.0	1886.0	1888.6	1884.4	1884.4	1885.6
gdb 4728	1881.2[a]	1888.5	1888.5	1890.1	1886.6	1886.5	1886.4
gdb 4729	1867.2[a]	1877.4	1877.4	1879.1	1872.6	1872.5	1874.9
gdb 4730	1851.2[a]	1850.3	1850.2	1850.2	1843.3	1843.3	1841.5
gdb 4731	1850.5[a]	1853.5	1853.5	1852.6	1845.9	1845.8	1842.9
gdb 4732	1838.0[a]	1841.0	1841.0	1840.2	1830.9	1830.9	1830.0
gdb 4733	1855.7[a]	1860.3	1860.3	1863.1	1858.3	1858.3	1858.0
gdb 4734	1874.5[a]	1880.5	1880.5	1882.6	1880.8	1880.8	1881.6
gdb 4735	1873.3[a]	1884.3	1884.3	1883.1	1882.0	1882.0	1882.2
gdb 4736	1861.3[a]	1871.3	1871.3	1872.9	1868.5	1868.5	1870.4
gdb 4737	1874.6[a]	1881.6	1881.6	1884.4	1879.8	1879.8	1881.2
gdb 4738	1877.1[a]	1886.7	1886.7	1888.9	1884.7	1884.6	1885.2
gdb 4739	1864.3[a]	1874.2	1874.2	1876.1	1869.6	1869.5	1871.9
gdb 4740	1876.7[a]	1882.6	1882.6	1884.6	1882.6	1882.6	1883.5
gdb 4741	1878.3[a]	1884.9	1884.9	1886.1	1884.6	1884.6	1884.3
gdb 4742	1865.6[a]	1873.9	1873.9	1875.8	1870.8	1870.7	1873.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4743	1873.8[a]	1876.6	1876.6	1878.2	1876.1	1876.0	1877.9
gdb 4744	1877.4[a]	1879.8	1879.8	1882.2	1879.8	1879.8	1881.1
gdb 4745	1862.5[a]	1868.3	1868.3	1870.3	1865.0	1864.9	1868.3
gdb 4746	1873.7[a]	1878.0	1878.0	1880.8	1877.8	1877.8	1880.1
gdb 4747	1883.5[a]	1883.7	1883.7	1885.6	1878.8	1878.8	1882.8
gdb 4748	1873.9[a]	1881.9	1881.9	1883.8	1881.3	1881.3	1882.6
gdb 4749	1861.1[a]	1868.6	1868.6	1870.5	1865.3	1865.2	1868.7
gdb 4750	1879.1[a]	1885.7	1885.7	1887.6	1887.3	1887.3	1887.0
gdb 4751	1877.3[a]	1886.9	1886.9	1889.0	1887.9	1887.9	1887.4
gdb 4752	1866.3[a]	1875.5	1875.4	1876.0	1873.7	1873.7	1874.6
gdb 4753	1850.2[a]	1848.4	1848.3	1847.7	1844.4	1844.4	1841.5
gdb 4754	1848.6[a]	1849.9	1849.9	1849.4	1845.4	1845.4	1842.2
gdb 4755	1837.2[a]	1837.9	1837.9	1835.8	1830.6	1830.6	1828.9
gdb 4756	1856.1[a]	1857.9	1857.9	1861.1	1858.8	1858.8	1857.9
gdb 4757	1873.7[a]	1878.5	1878.5	1880.5	1881.2	1881.2	1882.1
gdb 4758	1872.3[a]	1880.2	1880.2	1882.4	1882.4	1882.4	1882.9
gdb 4759	1861.1[a]	1868.5	1868.5	1869.1	1867.8	1867.8	1869.8
gdb 4760	1880.2[a]	1886.3	1886.3	1888.4	1887.0	1887.0	1886.7
gdb 4761	1881.9[a]	1886.3	1886.2	1888.6	1887.2	1887.2	1886.6
gdb 4762	1868.7[a]	1875.9	1875.9	1876.6	1873.2	1873.2	1874.2
gdb 4763	1877.5[a]	1881.9	1881.9	1884.5	1882.3	1882.3	1883.4
gdb 4764	1879.0[a]	1882.5	1882.5	1885.4	1883.1	1883.0	1883.9
gdb 4765	1865.7[a]	1871.5	1871.5	1872.7	1868.6	1868.5	1870.9
gdb 4766	1868.4[a]	1873.0	1873.0	1876.3	1873.6	1873.6	1876.4
gdb 4767	1870.4[a]	1875.7	1875.7	1879.2	1876.4	1876.4	1878.7
gdb 4768	1861.0[a]	1866.7	1866.7	1868.2	1863.8	1863.8	1867.4
gdb 4769	1851.6[a]	1847.9	1847.9	1848.3	1842.1	1842.1	1840.4
gdb 4770	1852.3[a]	1849.5	1849.5	1849.9	1843.5	1843.5	1841.3
gdb 4771	1842.1[a]	1838.7	1838.7	1837.7	1829.5	1829.4	1829.0
gdb 4772	1858.5[a]	1856.1	1856.1	1860.2	1856.1	1856.0	1856.7
gdb 4773	1850.7[a]	1847.0	1847.0	1847.5	1842.1	1842.1	1840.4
gdb 4774	1850.4[a]	1847.9	1847.9	1848.3	1843.1	1843.1	1840.9
gdb 4775	1841.7[a]	1838.2	1838.1	1837.2	1829.9	1829.8	1829.4
gdb 4776	1857.2[a]	1854.1	1854.1	1855.5	1854.3	1854.3	1854.0
gdb 4777	1871.7[a]	1875.6	1875.6	1877.9	1878.3	1878.3	1879.2
gdb 4778	1871.9[a]	1876.7	1876.7	1879.4	1879.7	1879.7	1880.5
gdb 4779	1863.1[a]	1868.6	1868.6	1869.3	1867.5	1867.5	1869.5
gdb 4780	1873.3[a]	1878.3	1878.3	1879.8	1878.5	1878.5	1879.3
gdb 4781	1885.4[a]	1881.7	1881.7	1883.2	1878.8	1878.7	1881.6
gdb 4782	1876.9[a]	1881.8	1881.8	1883.6	1882.3	1882.2	1882.5
gdb 4783	1863.8[a]	1870.9	1870.9	1872.6	1868.3	1868.2	1871.1
gdb 4784	1870.5[a]	1874.5	1874.5	1877.7	1875.5	1875.5	1878.1
gdb 4785	1869.7[a]	1876.6	1876.6	1879.9	1877.0	1877.0	1879.2
gdb 4786	1861.5[a]	1866.5	1866.5	1868.2	1863.4	1863.4	1866.7
gdb 4787	1877.9[a]	1882.3	1882.3	1885.0	1883.0	1882.9	1884.3
gdb 4788	1867.5[a]	1872.9	1872.9	1874.3	1870.3	1870.2	1872.7
gdb 4789	1839.7[a]	1837.8	1837.7	1836.6	1829.6	1829.6	1829.0
gdb 4790	1849.2[a]	1846.4	1846.4	1846.7	1841.8	1841.7	1840.2
gdb 4791	1875.3[a]	1879.2	1879.2	1881.4	1881.5	1881.4	1882.4
gdb 4792	1864.3[a]	1868.9	1868.9	1870.0	1868.0	1867.9	1870.1
gdb 4793	1877.3[a]	1881.2	1881.2	1883.7	1882.7	1882.6	1884.0
gdb 4794	1888.6[a]	1888.3	1888.3	1889.3	1885.2	1885.2	1887.9
gdb 4795	1862.1[a]	1875.2	1871.0	1876.5	1872.5	1872.4	1871.4
gdb 4796	1873.5[a]	1877.6	1877.6	1880.4	1876.1	1876.1	1877.9
gdb 4797	1858.9[a]	1869.3	1869.3	1871.1	1861.7	1861.7	1864.6
gdb 4798	1869.8[a]	1874.3	1874.3	1876.6	1876.9	1876.9	1877.8
gdb 4799	1860.8[a]	1868.8	1868.8	1869.4	1866.7	1866.6	1868.3
gdb 4800	1871.8[a]	1878.5	1878.5	1881.4	1878.3	1878.2	1879.4
gdb 4801	1863.0[a]	1869.6	1869.6	1870.8	1865.7	1865.7	1867.7
gdb 4802	1835.0[a]	1835.7	1835.7	1834.7	1828.0	1827.9	1827.7
gdb 4803	1849.7[a]	1846.3	1846.2	1846.2	1841.9	1841.9	1840.2
gdb 4804	1844.0[a]	1845.8	1845.8	1848.1	1843.4	1843.4	1845.2
gdb 4805	1874.4[a]	1878.2	1878.2	1879.1	1880.8	1880.8	1881.5
gdb 4806	1886.3[a]	1884.1	1884.1	1884.8	1881.7	1881.7	1884.7
gdb 4807	1864.1[a]	1871.5	1871.5	1872.3	1870.2	1870.2	1872.4

... *continued on next page* ...

Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4808	1885.2[a]	1879.5	1879.5	1881.3	1877.0	1877.0	1880.8
gdb 4809	1860.9[a]	1866.2	1866.2	1868.0	1865.0	1865.0	1868.7
gdb 4810	1871.3[a]	1873.2	1873.1	1874.7	1874.8	1874.8	1876.6
gdb 4811	1859.7[a]	1864.6	1864.6	1865.3	1862.6	1862.6	1865.2
gdb 4812	1861.1[a]	1865.0	1865.0	1866.4	1863.3	1863.2	1866.2
gdb 4813	1869.8[a]	1872.7	1872.7	1874.1	1874.1	1874.0	1875.6
gdb 4814	1882.9[a]	1876.8	1876.8	1878.7	1874.0	1873.8	1877.9
gdb 4815	1861.3[a]	1868.6	1868.6	1869.1	1866.0	1865.9	1868.6
gdb 4816	1860.2[a]	1866.3	1866.3	1867.6	1864.5	1864.5	1867.6
gdb 4817	1871.0[a]	1873.5	1873.5	1876.2	1875.8	1875.8	1877.9
gdb 4818	1856.8[a]	1852.0	1852.0	1854.0	1852.7	1852.7	1853.2
gdb 4819	1853.9[a]	1848.7	1848.6	1851.5	1850.8	1850.8	1851.7
gdb 4820	1843.7[a]	1839.8	1839.8	1842.3	1838.1	1838.1	1840.4
gdb 4821	1856.4[a]	1851.5	1851.5	1854.6	1852.8	1852.8	1854.0
gdb 4822	1857.6[a]	1852.2	1852.2	1855.4	1853.9	1853.9	1854.7
gdb 4823	1858.5[a]	1850.9	1850.9	1854.6	1853.1	1853.0	1853.9
gdb 4824	1845.9[a]	1839.5	1839.5	1843.1	1838.2	1838.2	1841.2
gdb 4825	1845.2[a]	1830.2	1830.2	1833.8	1829.4	1829.4	1831.1
gdb 4826	1846.2[a]	1831.8	1831.8	1834.9	1831.1	1831.1	1832.3
gdb 4827	1836.2[a]	1822.7	1822.7	1825.4	1818.5	1818.5	1821.6
gdb 4828	1856.8[a]	1846.9	1846.9	1848.3	1848.3	1848.3	1846.8
gdb 4829	1828.8[a]	1805.3	1805.3	1809.8	1805.3	1805.3	1807.3
gdb 4830	1833.0[a]	1809.8	1809.8	1813.8	1809.7	1809.7	1811.3
gdb 4831	1822.8[a]	1799.8	1799.8	1803.5	1796.5	1796.5	1800.0
gdb 4832	1843.6[a]	1820.2	1820.2	1825.0	1822.9	1822.9	1824.6
gdb 4833	1832.1[a]	1825.3	1825.3	1825.0	1821.4	1821.4	1818.9
gdb 4834	1831.1[a]	1825.7	1825.6	1825.2	1822.2	1822.2	1819.5
gdb 4835	1820.8[a]	1815.3	1815.3	1814.2	1808.7	1808.7	1807.8
gdb 4836	1830.6[a]	1826.6	1826.6	1828.9	1829.0	1828.9	1827.7
gdb 4837	1881.1[a]	1875.0	1874.9	1877.4	1877.7	1877.7	1878.7
gdb 4838	1889.1[a]	1866.2	1866.2	1867.8	1866.3	1866.2	1868.7
gdb 4839	1880.5[a]	1874.7	1874.7	1876.5	1878.4	1878.3	1879.2
gdb 4840	1871.3[a]	1865.5	1865.5	1867.3	1865.5	1865.5	1868.0
gdb 4841	1864.8[a]	1848.6	1848.6	1852.7	1852.3	1852.3	1854.6
gdb 4842	1852.7[a]	1843.4	1843.4	1844.0	1841.2	1841.2	1840.2
gdb 4843	1869.5[a]	1852.9	1852.8	1856.8	1856.6	1856.6	1858.7
gdb 4844	1859.4[a]	1843.3	1843.3	1846.9	1843.6	1843.6	1847.6
gdb 4845	1856.8[a]	1857.8	1857.8	1859.8	1853.5	1853.5	1854.8
gdb 4846	1864.8[a]	1865.8	1865.8	1867.2	1861.2	1861.1	1861.2
gdb 4847	1848.5[a]	1851.4	1851.3	1852.4	1845.1	1845.1	1847.5
gdb 4848	1870.0[a]	1867.4	1867.4	1871.8	1867.0	1867.0	1868.8
gdb 4849	1881.3[a]	1878.0	1878.0	1879.0	1879.2	1879.2	1879.1
gdb 4850	1872.9[a]	1871.3	1871.3	1870.1	1867.1	1867.1	1864.6
gdb 4851	1882.9[a]	1883.3	1883.3	1885.4	1884.4	1884.4	1884.2
gdb 4852	1873.0[a]	1873.0	1873.0	1874.8	1871.0	1871.0	1872.7
gdb 4853	1885.1[a]	1881.1	1881.1	1882.4	1882.6	1882.6	1882.8
gdb 4854	1879.8[a]	1877.0	1877.0	1876.6	1870.6	1870.6	1869.3
gdb 4855	1881.5[a]	1880.2	1880.2	1879.3	1873.9	1873.9	1871.7
gdb 4856	1869.9[a]	1869.6	1869.6	1868.2	1860.2	1860.1	1859.7
gdb 4857	1888.4[a]	1889.4	1889.4	1891.7	1888.5	1888.5	1888.7
gdb 4858	1908.5[a]	1914.9	1914.9	1917.2	1915.0	1915.0	1916.7
gdb 4859	1909.2[a]	1916.4	1916.3	1917.7	1916.5	1916.5	1916.9
gdb 4860	1898.0[a]	1906.6	1906.6	1907.8	1903.3	1903.2	1905.8
gdb 4861	1911.1[a]	1914.4	1914.4	1916.5	1914.7	1914.7	1916.3
gdb 4862	1925.5[a]	1920.4	1920.4	1921.7	1917.0	1916.9	1919.9
gdb 4863	1912.2[a]	1917.3	1917.3	1919.0	1917.7	1917.7	1918.6
gdb 4864	1902.0[a]	1907.6	1907.6	1908.7	1904.7	1904.7	1907.4
gdb 4865	1857.2[a]	1854.7	1854.7	1858.3	1851.3	1851.3	1853.5
gdb 4866	1862.4[a]	1864.5	1864.5	1868.8	1864.1	1864.1	1865.5
gdb 4867	1857.3[a]	1854.4	1854.4	1857.5	1855.0	1854.9	1855.6
gdb 4868	1857.6[a]	1853.4	1853.4	1856.7	1854.0	1854.0	1855.1
gdb 4869	1855.7[a]	1851.1	1851.1	1851.4	1845.6	1845.6	1843.9
gdb 4870	1856.7[a]	1853.1	1853.0	1856.0	1854.8	1854.8	1855.3
gdb 4871	1845.7[a]	1843.5	1843.5	1846.4	1841.3	1841.3	1843.8
gdb 4872	1858.9[a]	1854.0	1854.0	1857.0	1857.5	1857.4	1857.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4873	1858.4[a]	1853.5	1853.5	1853.9	1849.3	1849.3	1846.7
gdb 4874	1853.0[a]	1848.5	1848.5	1848.5	1844.4	1844.3	1842.4
gdb 4875	1856.2[a]	1852.0	1852.0	1853.7	1854.2	1854.2	1854.2
gdb 4876	1913.5[a]	1916.7	1916.7	1919.2	1916.3	1916.3	1917.7
gdb 4877	1913.3[a]	1918.3	1918.3	1919.8	1918.1	1918.0	1918.3
gdb 4878	1899.2[a]	1905.9	1905.8	1906.9	1902.5	1902.5	1904.8
gdb 4879	1851.1[a]	1849.3	1849.3	1853.1	1845.3	1845.3	1848.3
gdb 4880	1857.5[a]	1853.9	1853.9	1857.8	1850.5	1850.5	1853.1
gdb 4881	1852.1[a]	1855.4	1855.4	1855.1	1849.0	1849.0	1850.2
gdb 4882	1842.9[a]	1843.1	1843.1	1846.3	1835.6	1835.6	1839.9
gdb 4883	1860.8[a]	1866.9	1866.9	1867.0	1865.7	1865.6	1863.7
gdb 4884	1846.8[a]	1839.5	1839.4	1840.4	1837.8	1837.7	1838.0
gdb 4885	1851.0[a]	1839.8	1839.8	1843.4	1838.2	1838.2	1841.9
gdb 4886	1855.4[a]	1845.1	1845.1	1849.2	1847.8	1847.8	1850.5
gdb 4887	1864.6[a]	1854.1	1854.1	1855.9	1854.1	1854.1	1856.4
gdb 4888	1859.2[a]	1857.2	1857.2	1858.6	1856.3	1856.3	1858.5
gdb 4889	1874.8[a]	1869.8	1869.8	1871.9	1871.2	1871.2	1872.3
gdb 4890	1852.9[a]	1848.8	1848.8	1849.0	1844.2	1844.2	1842.6
gdb 4891	1843.2[a]	1841.0	1841.0	1843.6	1839.9	1839.9	1842.7
gdb 4892	1853.7[a]	1850.4	1850.4	1853.6	1851.8	1851.7	1852.8
gdb 4893	1841.6[a]	1838.5	1838.5	1841.7	1832.4	1832.4	1837.0
gdb 4894	1854.2[a]	1849.8	1849.8	1853.7	1846.7	1846.7	1849.3
gdb 4895	1850.9[a]	1846.2	1846.2	1848.6	1843.1	1843.1	1845.9
gdb 4896	1853.9[a]	1851.8	1851.8	1851.0	1847.6	1847.5	1844.6
gdb 4897	1898.2[a]	1906.2	1906.2	1907.9	1908.7	1908.7	1910.7
gdb 4898	1856.7[a]	1854.2	1854.2	1857.9	1850.7	1850.6	1852.9
gdb 4899	1850.2[a]	1857.8	1857.8	1862.3	1852.9	1852.9	1856.3
gdb 4900	1858.0[a]	1861.0	1861.0	1865.2	1860.1	1860.1	1862.2
gdb 4901	1851.4[a]	1847.5	1847.5	1847.5	1840.3	1842.5	1838.5
gdb 4902	1845.8[a]	1841.3	1841.2	1844.2	1839.7	1839.7	1842.2
gdb 4903	1856.2[a]	1852.7	1852.7	1856.2	1853.2	1853.1	1854.0
gdb 4904	1855.6[a]	1850.5	1850.5	1850.8	1844.7	1844.7	1843.1
gdb 4905	1857.3[a]	1852.8	1852.7	1856.2	1854.1	1854.1	1855.4
gdb 4906	1848.2[a]	1842.9	1842.9	1845.7	1841.1	1841.1	1843.5
gdb 4907	1890.5[a]	1898.9	1898.9	1898.7	1899.9	1899.8	1899.2
gdb 4908	1853.1[a]	1849.9	1849.9	1849.8	1844.3	1844.3	1842.1
gdb 4909	1850.2[a]	1849.9	1849.9	1848.8	1843.2	1843.1	1840.6
gdb 4910	1843.7[a]	1846.9	1846.9	1850.0	1843.6	1843.5	1845.5
gdb 4911	1854.8[a]	1858.0	1858.0	1861.8	1855.6	1855.5	1856.0
gdb 4912	1858.5[a]	1856.3	1856.3	1858.8	1858.7	1858.7	1858.4
gdb 4913	1856.7[a]	1851.4	1851.4	1851.1	1847.6	1847.6	1844.9
gdb 4914	1846.9[a]	1843.1	1843.1	1846.5	1842.9	1842.9	1844.6
gdb 4915	1894.3[a]	1899.7	1899.7	1900.0	1901.5	1901.4	1901.6
gdb 4916	1867.2[a]	1866.4	1866.4	1865.3	1862.2	1862.2	1860.6
gdb 4917	1866.3[a]	1859.8	1859.8	1861.7	1859.3	1859.3	1860.7
gdb 4918	1863.5[a]	1865.2	1865.2	1866.8	1862.3	1862.3	1864.4
gdb 4919	1874.0[a]	1872.2	1872.2	1874.7	1872.9	1872.9	1874.2
gdb 4920	1891.2[a]	1899.2	1899.2	1900.4	1896.2	1896.2	1899.1
gdb 4921	1903.2[a]	1908.0	1908.0	1910.4	1908.3	1908.3	1910.2
gdb 4922	1842.9[a]	1842.1	1843.5	1846.3	1841.9	1841.8	1844.1
gdb 4923	1851.7[a]	1847.4	1847.4	1846.9	1843.1	1843.1	1840.8
gdb 4924	1855.8[a]	1854.3	1854.3	1857.3	1851.9	1851.9	1853.2
gdb 4925	1854.5[a]	1852.2	1852.1	1855.2	1849.6	1849.6	1851.6
gdb 4926	1843.4[a]	1845.4	1845.3	1847.8	1838.6	1838.6	1841.7
gdb 4927	1898.2[a]	1905.2	1905.2	1906.5	1907.2	1907.2	1908.9
gdb 4928	1853.6[a]	1851.6	1851.6	1855.2	1847.8	1847.8	1850.2
gdb 4929	1855.4[a]	1852.0	1852.0	1855.7	1848.1	1848.1	1851.2
gdb 4930	1854.5[a]	1854.0	1854.0	1856.9	1849.2	1849.2	1851.1
gdb 4931	1851.7[a]	1857.9	1857.9	1862.1	1852.1	1852.1	1854.9
gdb 4932	1843.6[a]	1845.2	1845.2	1848.3	1836.8	1836.8	1840.9
gdb 4933	1860.9[a]	1864.0	1864.0	1867.8	1862.2	1862.1	1863.6
gdb 4934	1896.1[a]	1904.5	1904.5	1906.4	1901.4	1901.3	1904.0
gdb 4935	1891.3[a]	1897.9	1897.9	1899.1	1894.7	1894.7	1897.4
gdb 4936	1900.6[a]	1906.5	1906.5	1908.6	1906.9	1906.9	1908.8
gdb 4937	1865.7[a]	1874.7	1874.7	1876.7	1864.0	1864.0	1867.8

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 4938	1867.0[a]	1877.8	1877.8	1879.8	1867.2	1867.2	1870.4
gdb 4939	1865.0[a]	1874.2	1874.2	1875.9	1864.6	1864.6	1868.1
gdb 4940	1857.0[a]	1866.1	1866.1	1868.8	1858.1	1858.1	1862.0
gdb 4941	1869.3[a]	1875.8	1875.8	1878.6	1871.8	1871.8	1873.5
gdb 4942	1868.9[a]	1872.9	1872.9	1876.5	1869.1	1869.0	1871.8
gdb 4943	1835.7[a]	1827.8	1827.8	1827.0	1824.6	1824.5	1821.8
gdb 4944	1832.9[a]	1825.1	1825.1	1825.2	1823.8	1823.8	1819.3
gdb 4945	1824.7[a]	1816.8	1816.8	1816.0	1811.2	1811.1	1810.0
gdb 4946	1826.3[a]	1817.5	1817.5	1820.7	1818.2	1818.2	1819.8
gdb 4947	1837.2[a]	1830.0	1830.0	1832.3	1833.5	1833.5	1833.2
gdb 4948	1882.2[a]	1876.2	1876.2	1878.6	1879.5	1879.4	1880.3
gdb 4949	1889.2[a]	1867.1	1867.1	1868.2	1867.6	1867.5	1869.4
gdb 4950	1881.1[a]	1874.2	1874.2	1876.3	1878.0	1878.0	1878.7
gdb 4951	1870.8[a]	1864.9	1864.9	1867.1	1865.6	1865.6	1867.9
gdb 4952	1831.0[a]	1807.5	1807.5	1811.3	1808.4	1808.4	1809.7
gdb 4953	1833.1[a]	1808.5	1808.5	1811.8	1808.9	1808.9	1810.2
gdb 4954	1824.5[a]	1800.9	1800.9	1804.5	1797.4	1797.4	1800.0
gdb 4955	1835.7[a]	1810.6	1810.6	1817.2	1810.7	1810.7	1814.9
gdb 4956	1843.3[a]	1818.6	1818.6	1824.2	1822.6	1822.6	1825.0
gdb 4957	1844.1[a]	1828.3	1828.3	1830.3	1828.2	1828.2	1829.5
gdb 4958	1851.7[a]	1832.5	1832.5	1836.3	1832.8	1832.8	1834.2
gdb 4959	1845.0[a]	1831.9	1831.9	1836.3	1831.8	1831.8	1834.7
gdb 4960	1834.4[a]	1817.0	1817.0	1820.0	1814.8	1814.7	1818.0
gdb 4961	1859.2[a]	1843.8	1843.8	1848.3	1846.4	1846.4	1847.8
gdb 4962	1850.1[a]	1833.8	1833.8	1836.2	1834.4	1834.4	1835.4
gdb 4963	1838.4[a]	1823.3	1823.3	1825.3	1820.4	1820.4	1822.5
gdb 4964	1845.6[a]	1833.3	1831.6	1835.4	1832.9	1831.3	1834.1
gdb 4965	1859.4[a]	1844.4	1844.4	1846.8	1846.4	1846.4	1846.9
gdb 4966	1843.8[a]	1829.2	1829.2	1832.1	1829.8	1829.8	1831.4
gdb 4967	1845.4[a]	1830.8	1830.8	1834.5	1830.7	1830.6	1832.3
gdb 4968	1843.7[a]	1830.3	1830.3	1834.9	1830.0	1829.9	1833.5
gdb 4969	1832.8[a]	1817.5	1817.5	1820.3	1813.8	1813.8	1817.1
gdb 4970	1856.4[a]	1843.8	1843.8	1848.4	1846.4	1846.3	1847.9
gdb 4971	1846.2[a]	1829.6	1829.6	1832.0	1830.3	1830.3	1831.6
gdb 4972	1848.9[a]	1831.4	1831.4	1833.9	1832.2	1832.2	1833.5
gdb 4973	1845.4[a]	1827.1	1827.0	1829.8	1828.2	1828.2	1829.6
gdb 4974	1842.9[a]	1827.1	1827.1	1830.7	1827.9	1827.9	1830.9
gdb 4975	1837.4[a]	1820.9	1820.9	1823.0	1818.4	1818.3	1820.7
gdb 4976	1834.3[a]	1818.3	1818.2	1820.5	1815.0	1815.0	1817.9
gdb 4977	1854.7[a]	1837.6	1837.6	1840.1	1841.5	1841.5	1842.3
gdb 4978	1847.6[a]	1845.0	1844.9	1849.2	1837.9	1837.9	1842.1
gdb 4979	1856.5[a]	1851.3	1851.3	1854.5	1848.5	1848.4	1850.8
gdb 4980	1857.5[a]	1845.6	1845.6	1848.5	1843.1	1843.1	1846.1
gdb 4981	1856.2[a]	1849.0	1849.0	1852.3	1846.0	1846.0	1850.2
gdb 4982	1858.0[a]	1854.5	1854.5	1857.5	1850.5	1850.5	1854.3
gdb 4983	1856.0[a]	1845.0	1844.9	1847.1	1842.1	1842.1	1845.1
gdb 4984	1867.8[a]	1860.9	1860.9	1864.3	1860.5	1860.5	1863.1
gdb 4985	1869.0[a]	1866.5	1866.5	1869.6	1865.4	1865.4	1867.4
gdb 4986	1868.2[a]	1856.5	1856.5	1858.9	1857.0	1857.0	1858.5
gdb 4987	1872.4[a]	1867.8	1867.8	1871.1	1867.3	1867.2	1870.2
gdb 4988	1884.9[a]	1882.0	1882.0	1884.4	1884.1	1884.1	1885.1
gdb 4989	1881.6[a]	1875.3	1875.3	1877.7	1878.7	1878.7	1879.7
gdb 4990	1881.7[a]	1874.6	1874.6	1876.8	1878.6	1878.6	1879.4
gdb 4991	1892.1[a]	1868.2	1868.2	1869.3	1869.2	1869.2	1870.9
gdb 4992	1871.3[a]	1864.6	1864.6	1867.1	1865.9	1865.8	1868.6
gdb 4993	1872.7[a]	1854.2	1854.2	1857.1	1858.6	1858.5	1859.6
gdb 4994	1863.5[a]	1852.1	1852.1	1851.9	1851.1	1851.1	1848.7
gdb 4995	1874.5[a]	1854.5	1854.5	1857.8	1858.7	1858.7	1859.8
gdb 4996	1864.5[a]	1845.4	1845.4	1848.3	1846.1	1846.1	1848.8
gdb 4997	1867.1[a]	1864.7	1864.7	1866.2	1861.2	1861.2	1861.5
gdb 4998	1862.9[a]	1857.8	1857.8	1862.2	1854.8	1854.8	1858.7
gdb 4999	1871.4[a]	1864.8	1864.8	1868.1	1865.0	1865.0	1866.7
gdb 5000	1855.8[a]	1843.7	1843.7	1844.0	1842.5	1842.5	1841.3
gdb 5001	1857.8[a]	1839.5	1839.5	1842.5	1839.1	1839.0	1842.4
gdb 5002	1863.5[a]	1847.2	1847.2	1848.9	1849.8	1849.8	1851.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5003	1906.7[a]	1895.8	1895.8	1897.7	1893.8	1893.8	1896.2
gdb 5004	1890.3[a]	1887.5	1887.5	1888.4	1885.3	1885.3	1885.7
gdb 5005	1888.8[a]	1884.2	1884.2	1887.2	1882.4	1882.4	1886.2
gdb 5006	1896.6[a]	1891.9	1891.9	1893.9	1893.2	1893.2	1894.8
gdb 5007	1864.5[a]	1863.5	1863.5	1864.8	1860.5	1860.4	1860.5
gdb 5008	1855.2[a]	1847.8	1847.8	1846.1	1839.6	1839.5	1836.7
gdb 5009	1853.1[a]	1842.7	1842.6	1843.1	1835.0	1835.0	1835.4
gdb 5010	1860.0[a]	1849.8	1849.8	1850.6	1845.8	1845.8	1844.7
gdb 5011	1858.9[a]	1852.6	1852.6	1853.8	1849.9	1849.9	1849.4
gdb 5012	1829.3[a]	1812.4	1812.4	1809.8	1805.6	1805.5	1800.6
gdb 5013	1833.7[a]	1810.2	1810.2	1811.2	1804.8	1804.7	1804.7
gdb 5014	1840.7[a]	1817.6	1817.6	1818.8	1816.1	1816.1	1814.5
gdb 5015	1830.8[a]	1818.8	1818.8	1820.0	1817.8	1817.8	1815.9
gdb 5016	1853.3[a]	1842.6	1842.6	1843.4	1842.2	1842.1	1842.1
gdb 5017	1855.3[a]	1838.9	1838.9	1842.5	1839.1	1839.1	1843.1
gdb 5018	1861.0[a]	1846.7	1846.7	1850.4	1850.5	1850.5	1852.8
gdb 5019	1865.0[a]	1863.7	1863.7	1865.2	1860.5	1860.5	1860.8
gdb 5020	1881.7[a]	1879.4	1879.4	1880.9	1875.1	1875.1	1876.3
gdb 5021	1904.7[a]	1893.6	1893.6	1895.6	1891.2	1891.2	1893.9
gdb 5022	1890.8[a]	1887.8	1887.8	1888.7	1885.5	1885.5	1885.7
gdb 5023	1886.4[a]	1881.1	1881.1	1884.0	1879.3	1879.3	1882.9
gdb 5024	1896.1[a]	1891.8	1891.8	1895.1	1893.4	1893.4	1895.5
gdb 5025	1883.1[a]	1880.5	1880.5	1883.1	1877.0	1877.0	1878.7
gdb 5026	1869.8[a]	1851.2	1851.2	1855.0	1855.6	1855.5	1857.3
gdb 5027	1873.1[a]	1853.0	1853.0	1856.4	1857.4	1857.3	1859.1
gdb 5028	1857.9[a]	1847.4	1847.4	1847.7	1846.1	1846.0	1844.2
gdb 5029	1863.0[a]	1843.7	1843.7	1847.1	1844.2	1844.2	1847.4
gdb 5030	1862.5[a]	1861.5	1861.5	1863.4	1857.6	1857.6	1858.4
gdb 5031	1868.2[a]	1865.7	1865.7	1868.2	1861.8	1861.8	1862.2
gdb 5032	1861.9[a]	1857.9	1857.9	1862.1	1854.3	1854.3	1858.0
gdb 5033	1870.5[a]	1866.9	1866.9	1872.3	1867.3	1867.2	1869.6
gdb 5034	1884.4[a]	1883.2	1883.2	1885.2	1882.0	1881.9	1883.7
gdb 5035	1881.7[a]	1880.0	1880.0	1882.5	1878.9	1878.8	1881.0
gdb 5036	1888.4[a]	1886.1	1886.1	1886.6	1883.4	1883.4	1882.8
gdb 5037	1882.6[a]	1878.7	1878.7	1881.3	1877.3	1877.3	1880.6
gdb 5038	1893.0[a]	1888.1	1888.1	1889.8	1889.9	1889.8	1891.1
gdb 5039	1884.1[a]	1877.5	1877.5	1879.3	1880.9	1880.9	1881.4
gdb 5040	1881.1[a]	1874.4	1874.4	1872.8	1872.1	1872.0	1869.2
gdb 5041	1893.7[a]	1870.8	1870.8	1871.5	1871.8	1871.8	1873.1
gdb 5042	1884.5[a]	1875.7	1875.7	1877.6	1880.0	1880.0	1880.2
gdb 5043	1873.5[a]	1866.6	1866.6	1868.3	1867.6	1867.6	1869.8
gdb 5044	1838.0[a]	1829.7	1829.7	1828.5	1826.5	1826.5	1823.5
gdb 5045	1843.1[a]	1833.5	1833.5	1832.5	1830.3	1830.3	1826.8
gdb 5046	1836.0[a]	1827.3	1827.3	1826.2	1825.0	1825.0	1821.9
gdb 5047	1834.3[a]	1823.3	1823.3	1818.6	1814.6	1814.6	1808.4
gdb 5048	1826.8[a]	1818.6	1818.6	1817.2	1812.9	1812.9	1811.4
gdb 5049	1828.0[a]	1821.3	1821.3	1823.4	1822.4	1822.4	1823.8
gdb 5050	1838.2[a]	1831.3	1831.3	1833.7	1835.3	1835.2	1835.1
gdb 5051	1886.4[a]	1881.3	1881.3	1880.6	1876.8	1876.8	1874.9
gdb 5052	1873.8[a]	1871.0	1871.0	1873.8	1870.5	1870.5	1873.4
gdb 5053	1886.7[a]	1881.8	1881.8	1883.5	1883.6	1883.5	1884.3
gdb 5054	1884.1[a]	1878.7	1878.7	1880.5	1881.9	1881.9	1882.4
gdb 5055	1893.7[a]	1870.5	1870.5	1871.3	1871.7	1871.6	1873.1
gdb 5056	1882.5[a]	1875.8	1875.8	1877.9	1880.4	1880.4	1881.0
gdb 5057	1881.1[a]	1874.4	1874.4	1872.9	1872.0	1872.0	1869.2
gdb 5058	1873.4[a]	1866.9	1866.9	1868.5	1867.6	1867.5	1869.5
gdb 5059	1886.5[a]	1881.5	1881.5	1880.7	1877.0	1877.0	1875.0
gdb 5060	1874.5[a]	1871.0	1871.0	1873.3	1870.7	1870.7	1873.4
gdb 5061	1884.9[a]	1882.4	1882.4	1885.1	1884.4	1884.4	1885.5
gdb 5062	1870.3[a]	1860.7	1860.7	1862.1	1861.3	1861.3	1862.7
gdb 5063	1867.7[a]	1858.6	1858.5	1859.9	1859.5	1859.5	1860.7
gdb 5064	1874.5[a]	1869.5	1869.5	1867.8	1865.9	1865.9	1863.3
gdb 5065	1867.3[a]	1863.0	1863.0	1864.4	1863.0	1863.0	1865.2
gdb 5066	1876.8[a]	1874.4	1874.4	1876.0	1876.6	1876.6	1877.2
gdb 5067	1881.9[a]	1877.1	1877.1	1879.0	1880.1	1880.0	1880.4

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5068	1881.7[a]	1878.1	1878.1	1879.7	1880.5	1880.5	1880.6
gdb 5069	1876.2[a]	1871.8	1871.8	1870.5	1869.0	1868.9	1866.2
gdb 5070	1871.5[a]	1866.6	1866.6	1868.7	1867.2	1867.2	1869.4
gdb 5071	1893.0[a]	1897.0	1897.0	1898.6	1897.2	1897.2	1898.7
gdb 5072	1911.4[a]	1906.8	1906.8	1907.5	1905.1	1905.1	1907.0
gdb 5073	1899.4[a]	1899.6	1899.6	1897.2	1896.4	1896.3	1892.9
gdb 5074	1891.7[a]	1894.9	1894.9	1895.8	1895.0	1894.9	1896.6
gdb 5075	1902.4[a]	1905.7	1905.7	1907.0	1908.2	1908.2	1908.2
gdb 5076	1883.0[a]	1881.0	1881.0	1879.8	1876.6	1876.6	1874.1
gdb 5077	1882.4[a]	1878.8	1878.8	1880.9	1881.6	1881.6	1881.7
gdb 5078	1882.4[a]	1877.7	1877.7	1879.1	1880.0	1880.0	1879.7
gdb 5079	1876.5[a]	1872.4	1872.4	1870.6	1869.4	1869.3	1866.1
gdb 5080	1871.2[a]	1867.0	1867.0	1868.8	1867.2	1867.2	1868.9
gdb 5081	1881.7[a]	1878.0	1878.0	1877.4	1872.9	1872.9	1871.0
gdb 5082	1883.5[a]	1880.1	1880.1	1880.0	1875.0	1875.0	1873.0
gdb 5083	1875.3[a]	1873.9	1873.9	1876.8	1872.2	1872.1	1874.7
gdb 5084	1885.8[a]	1883.7	1883.7	1885.7	1883.8	1883.8	1884.3
gdb 5085	1871.1[a]	1867.3	1867.3	1866.0	1864.5	1864.5	1862.5
gdb 5086	1866.6[a]	1857.9	1857.9	1859.7	1859.0	1859.0	1860.5
gdb 5087	1862.9[a]	1860.1	1860.1	1862.0	1860.5	1860.5	1863.8
gdb 5088	1871.7[a]	1870.9	1870.9	1872.8	1873.6	1873.9	1874.8
gdb 5089	1840.0[a]	1831.0	1831.0	1829.7	1827.7	1827.7	1824.3
gdb 5090	1841.2[a]	1831.8	1831.8	1830.7	1828.8	1828.8	1825.6
gdb 5091	1834.0[a]	1823.2	1823.2	1818.4	1814.6	1814.6	1808.3
gdb 5092	1839.0[a]	1829.6	1829.6	1828.9	1827.3	1827.3	1824.0
gdb 5093	1829.7[a]	1820.6	1820.6	1819.4	1815.1	1815.1	1813.5
gdb 5094	1828.7[a]	1820.1	1820.1	1822.4	1821.9	1821.9	1823.4
gdb 5095	1839.6[a]	1830.8	1830.8	1833.3	1835.2	1835.2	1835.0
gdb 5096	1848.9[a]	1838.3	1838.3	1834.3	1829.5	1829.5	1823.5
gdb 5097	1842.5[a]	1832.1	1832.0	1831.2	1826.7	1826.7	1825.6
gdb 5098	1846.3[a]	1831.6	1831.6	1834.4	1833.9	1833.9	1834.2
gdb 5099	1850.8[a]	1842.8	1842.7	1842.0	1839.8	1839.8	1836.8
gdb 5100	1848.5[a]	1843.0	1843.0	1840.8	1838.0	1838.0	1835.0
gdb 5101	1838.3[a]	1829.7	1829.7	1828.9	1826.5	1826.5	1823.4
gdb 5102	1837.3[a]	1828.8	1828.7	1827.9	1826.4	1826.4	1823.2
gdb 5103	1825.1[a]	1818.0	1818.0	1819.9	1819.3	1819.3	1820.8
gdb 5104	1834.8[a]	1829.1	1829.1	1830.8	1832.9	1832.9	1832.7
gdb 5105	1874.9[a]	1865.4	1865.4	1861.0	1856.2	1856.1	1850.6
gdb 5106	1863.0[a]	1860.1	1860.1	1858.7	1854.1	1854.0	1853.0
gdb 5107	1865.1[a]	1864.1	1864.1	1866.3	1864.1	1864.0	1865.1
gdb 5108	1873.1[a]	1870.2	1870.2	1869.1	1866.5	1866.5	1863.9
gdb 5109	1874.6[a]	1872.0	1872.0	1870.8	1868.0	1868.0	1864.8
gdb 5110	1840.2[a]	1831.2	1831.2	1830.1	1827.8	1827.8	1824.6
gdb 5111	1841.3[a]	1831.9	1831.9	1831.0	1828.9	1828.9	1825.8
gdb 5112	1839.5[a]	1830.4	1830.3	1829.7	1828.3	1828.3	1824.9
gdb 5113	1834.0[a]	1823.3	1823.3	1818.8	1814.5	1814.5	1808.4
gdb 5114	1829.4[a]	1821.4	1821.4	1823.6	1822.9	1822.9	1824.1
gdb 5115	1829.9[a]	1821.0	1821.0	1819.9	1815.4	1815.4	1813.8
gdb 5116	1839.1[a]	1831.5	1831.5	1833.9	1835.4	1835.3	1835.3
gdb 5117	1852.6[a]	1842.3	1842.3	1840.8	1834.2	1834.2	1831.7
gdb 5118	1844.5[a]	1837.0	1837.0	1838.1	1832.4	1832.4	1834.2
gdb 5119	1856.6[a]	1849.3	1849.3	1850.7	1847.0	1847.0	1847.1
gdb 5120	1862.2[a]	1850.5	1850.5	1851.3	1846.7	1846.7	1845.5
gdb 5121	1843.8[a]	1833.8	1833.8	1833.6	1826.6	1826.6	1825.4
gdb 5122	1843.8[a]	1833.3	1833.3	1833.2	1826.2	1826.2	1825.3
gdb 5123	1836.5[a]	1827.9	1827.9	1830.7	1824.0	1823.9	1827.3
gdb 5124	1844.4[a]	1830.4	1830.4	1833.7	1826.9	1826.9	1831.1
gdb 5125	1846.5[a]	1837.9	1837.9	1840.9	1836.5	1836.5	1838.3
gdb 5126	1854.3[a]	1841.4	1841.4	1844.9	1840.2	1840.2	1842.7
gdb 5127	1848.8[a]	1845.2	1845.2	1845.6	1840.5	1840.5	1838.4
gdb 5128	1884.6[a]	1881.1	1881.1	1880.1	1876.8	1876.8	1874.6
gdb 5129	1882.7[a]	1878.9	1878.8	1878.4	1873.8	1873.8	1872.0
gdb 5130	1883.5[a]	1880.8	1880.8	1880.4	1875.4	1875.4	1873.1
gdb 5131	1873.1[a]	1872.5	1872.5	1875.5	1870.1	1870.1	1872.7
gdb 5132	1885.8[a]	1883.9	1883.9	1884.9	1883.5	1883.5	1883.5

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Table S73: . . . *continued from previous page* . . .

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5133	1877.3[a]	1876.0	1876.0	1878.6	1874.9	1874.9	1877.7
gdb 5134	1887.3[a]	1881.6	1881.6	1880.6	1877.7	1877.7	1875.3
gdb 5135	1902.2[a]	1903.5	1903.5	1901.4	1901.1	1901.1	1898.6
gdb 5136	1911.6[a]	1907.7	1907.7	1908.2	1906.9	1906.8	1908.8
gdb 5137	1909.3[a]	1905.2	1905.2	1906.0	1904.4	1904.4	1906.6
gdb 5138	1890.3[a]	1896.0	1896.0	1896.8	1896.3	1896.3	1898.5
gdb 5139	1901.3[a]	1905.7	1905.7	1905.6	1907.9	1907.9	1907.8
gdb 5140	1884.1[a]	1880.8	1880.8	1879.7	1876.4	1876.4	1874.0
gdb 5141	1875.1[a]	1865.5	1865.5	1861.0	1856.2	1856.2	1850.4
gdb 5142	1861.8[a]	1859.3	1859.3	1857.8	1853.0	1853.0	1851.7
gdb 5143	1851.4[a]	1851.9	1851.9	1854.1	1848.9	1848.9	1851.8
gdb 5144	1873.1[a]	1870.6	1870.6	1869.5	1866.7	1866.7	1863.9
gdb 5145	1862.3[a]	1862.3	1862.3	1864.9	1861.9	1861.9	1863.4
gdb 5146	1878.6[a]	1872.1	1872.1	1871.1	1868.2	1868.2	1864.9
gdb 5147	1849.4[a]	1837.8	1837.7	1833.7	1828.9	1828.9	1823.2
gdb 5148	1840.3[a]	1830.8	1830.8	1830.0	1825.0	1825.0	1823.8
gdb 5149	1833.4[a]	1819.8	1819.7	1822.2	1818.5	1818.5	1820.5
gdb 5150	1852.8[a]	1843.7	1843.7	1843.0	1840.5	1840.5	1837.6
gdb 5151	1843.7[a]	1830.3	1830.3	1833.0	1832.3	1832.3	1832.9
gdb 5152	1848.4[a]	1841.6	1841.6	1841.0	1840.4	1837.9	1835.1
gdb 5153	1863.4[a]	1855.8	1855.8	1857.6	1856.7	1856.7	1858.6
gdb 5154	1871.5[a]	1868.3	1868.3	1867.1	1864.9	1864.9	1863.2
gdb 5155	1863.4[a]	1860.4	1860.4	1862.6	1860.6	1860.5	1863.8
gdb 5156	1873.7[a]	1871.2	1871.1	1873.1	1873.6	1873.6	1874.6
gdb 5157	1884.1[a]	1880.7	1880.7	1879.9	1876.1	1876.1	1873.8
gdb 5158	1888.3[a]	1881.0	1881.0	1880.0	1878.0	1878.0	1875.5
gdb 5159	1912.1[a]	1907.4	1907.4	1908.2	1905.3	1905.3	1907.2
gdb 5160	1890.9[a]	1894.9	1894.8	1896.8	1894.8	1894.8	1896.6
gdb 5161	1900.0[a]	1900.1	1900.1	1897.7	1896.7	1896.6	1893.1
gdb 5162	1890.1[a]	1892.0	1892.0	1892.9	1892.2	1892.2	1893.5
gdb 5163	1903.5[a]	1906.3	1906.3	1907.6	1908.1	1908.1	1907.7
gdb 5164	1864.0[a]	1863.2	1863.2	1865.2	1859.4	1859.3	1863.5
gdb 5165	1874.3[a]	1872.8	1872.8	1873.9	1871.1	1871.1	1873.4
gdb 5166	1888.0[a]	1882.4	1882.4	1881.5	1878.3	1878.3	1875.8
gdb 5167	1834.0[a]	1810.8	1810.8	1813.9	1811.5	1811.4	1812.1
gdb 5168	1838.9[a]	1813.4	1813.4	1817.0	1814.2	1814.2	1814.9
gdb 5169	1837.0[a]	1812.8	1812.8	1816.2	1812.9	1812.9	1813.2
gdb 5170	1828.1[a]	1808.8	1808.8	1810.5	1804.6	1804.6	1803.2
gdb 5171	1827.1[a]	1803.7	1803.6	1806.7	1800.0	1800.0	1802.2
gdb 5172	1836.4[a]	1809.5	1809.5	1815.2	1809.7	1809.6	1813.7
gdb 5173	1844.3[a]	1817.7	1817.7	1822.1	1820.9	1820.9	1822.7
gdb 5174	1849.5[a]	1832.7	1832.7	1835.3	1833.3	1833.3	1834.4
gdb 5175	1851.9[a]	1835.1	1835.1	1837.8	1835.8	1835.8	1836.7
gdb 5176	1839.1[a]	1821.3	1821.3	1823.7	1819.2	1819.2	1821.9
gdb 5177	1848.6[a]	1833.2	1833.2	1836.9	1833.0	1833.0	1835.8
gdb 5178	1859.0[a]	1843.5	1843.5	1846.0	1845.4	1845.4	1846.1
gdb 5179	1849.2[a]	1832.8	1832.8	1834.9	1833.0	1833.0	1833.7
gdb 5180	1847.9[a]	1832.6	1832.6	1834.8	1833.1	1833.1	1833.3
gdb 5181	1845.4[a]	1831.4	1831.4	1835.0	1831.2	1831.2	1833.9
gdb 5182	1853.8[a]	1838.6	1838.6	1842.5	1842.2	1842.2	1843.4
gdb 5183	1889.3[a]	1882.2	1882.2	1883.6	1875.9	1875.9	1878.0
gdb 5184	1885.1[a]	1877.0	1877.0	1878.9	1870.4	1870.4	1874.1
gdb 5185	1891.0[a]	1882.4	1882.4	1883.9	1880.3	1880.3	1881.4
gdb 5186	1848.1[a]	1832.0	1832.0	1835.0	1832.0	1832.0	1833.3
gdb 5187	1855.3[a]	1837.0	1836.9	1840.5	1836.9	1836.9	1837.9
gdb 5188	1848.4[a]	1836.8	1836.8	1841.3	1835.4	1835.4	1838.2
gdb 5189	1856.6[a]	1845.1	1845.1	1849.8	1847.1	1847.1	1848.3
gdb 5190	1860.5[a]	1849.3	1849.3	1852.5	1846.0	1846.0	1848.9
gdb 5191	1858.2[a]	1853.6	1853.6	1857.0	1848.8	1848.8	1852.8
gdb 5192	1872.7[a]	1870.2	1870.2	1872.9	1868.2	1868.2	1869.7
gdb 5193	1867.0[a]	1861.6	1861.6	1865.4	1860.3	1860.3	1863.1
gdb 5194	1871.0[a]	1859.9	1859.9	1862.5	1859.8	1859.8	1860.9
gdb 5195	1862.4[a]	1850.4	1850.4	1852.9	1844.6	1844.5	1845.7
gdb 5196	1855.8[a]	1843.9	1843.9	1847.3	1838.2	1838.2	1841.9
gdb 5197	1864.8[a]	1852.4	1852.4	1854.9	1849.8	1849.8	1851.5

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5198	1866.3[a]	1857.0	1857.0	1861.2	1854.8	1854.8	1857.1
gdb 5199	1867.1[a]	1854.6	1854.6	1858.2	1852.5	1852.5	1854.3
gdb 5200	1833.2[a]	1808.5	1808.5	1812.3	1809.4	1809.4	1810.4
gdb 5201	1836.1[a]	1810.4	1810.4	1814.2	1811.1	1811.1	1812.5
gdb 5202	1837.9[a]	1811.2	1811.2	1817.9	1811.4	1811.4	1815.8
gdb 5203	1841.8[a]	1817.3	1817.3	1822.9	1821.0	1820.9	1823.4
gdb 5204	1846.7[a]	1830.5	1830.5	1833.7	1831.2	1831.2	1832.6
gdb 5205	1854.7[a]	1834.3	1834.3	1838.1	1834.8	1834.8	1836.0
gdb 5206	1845.8[a]	1832.0	1832.0	1836.6	1832.1	1832.1	1835.3
gdb 5207	1855.0[a]	1843.3	1843.3	1848.0	1846.0	1846.0	1847.5
gdb 5208	1849.3[a]	1832.4	1832.4	1834.8	1832.6	1832.6	1833.5
gdb 5209	1852.0[a]	1834.0	1834.0	1836.6	1834.6	1834.5	1835.3
gdb 5210	1848.9[a]	1830.5	1830.5	1833.4	1831.9	1831.9	1833.0
gdb 5211	1847.6[a]	1832.2	1832.2	1836.0	1832.2	1832.2	1835.2
gdb 5212	1855.1[a]	1839.6	1839.6	1843.6	1843.2	1843.2	1844.5
gdb 5213	1836.8[a]	1812.3	1812.3	1815.7	1812.8	1812.8	1813.5
gdb 5214	1836.3[a]	1811.8	1811.8	1815.3	1812.5	1812.5	1813.4
gdb 5215	1839.8[a]	1815.3	1815.3	1818.9	1815.4	1815.3	1815.6
gdb 5216	1828.4[a]	1809.1	1809.1	1810.9	1804.8	1804.8	1803.6
gdb 5217	1839.0[a]	1812.0	1812.0	1817.7	1811.7	1811.7	1815.6
gdb 5218	1829.7[a]	1805.8	1805.8	1809.1	1802.3	1802.3	1804.5
gdb 5219	1846.1[a]	1819.9	1819.9	1825.6	1823.7	1823.6	1825.8
gdb 5220	1852.6[a]	1838.1	1838.1	1840.9	1833.9	1833.9	1834.9
gdb 5221	1856.3[a]	1835.8	1836.3	1841.5	1832.3	1832.2	1837.4
gdb 5222	1862.2[a]	1844.2	1844.2	1849.4	1843.7	1843.7	1846.9
gdb 5223	1858.4[a]	1842.9	1842.9	1845.3	1842.3	1842.3	1842.3
gdb 5224	1850.0[a]	1845.4	1845.4	1849.9	1839.2	1839.2	1844.1
gdb 5225	1859.3[a]	1854.0	1854.0	1858.3	1851.3	1851.3	1854.0
gdb 5226	1856.5[a]	1851.3	1851.3	1856.1	1848.7	1848.7	1852.1
gdb 5227	1848.8[a]	1831.1	1831.1	1833.9	1831.9	1831.9	1833.2
gdb 5228	1848.6[a]	1830.9	1830.8	1833.7	1831.5	1831.5	1833.0
gdb 5229	1848.1[a]	1828.9	1828.8	1832.0	1830.5	1830.5	1831.8
gdb 5230	1844.7[a]	1826.7	1826.7	1830.4	1827.8	1827.7	1830.8
gdb 5231	1838.5[a]	1819.2	1819.2	1822.0	1817.3	1817.3	1820.4
gdb 5232	1856.8[a]	1840.2	1840.2	1844.2	1843.7	1843.7	1845.1
gdb 5233	1848.2[a]	1831.6	1831.6	1834.0	1832.3	1832.3	1833.4
gdb 5234	1845.8[a]	1829.0	1829.0	1831.5	1829.6	1829.6	1830.9
gdb 5235	1843.8[a]	1827.3	1827.3	1829.9	1827.8	1827.8	1828.9
gdb 5236	1846.9[a]	1830.5	1830.5	1832.8	1831.5	1831.4	1831.9
gdb 5237	1842.1[a]	1826.7	1826.7	1830.3	1827.9	1827.9	1830.8
gdb 5238	1835.7[a]	1817.9	1817.9	1820.1	1815.8	1815.8	1818.6
gdb 5239	1852.1[a]	1837.5	1837.5	1840.1	1841.1	1841.1	1842.1
gdb 5240	1884.9[a]	1876.9	1876.9	1878.8	1870.8	1870.8	1873.5
gdb 5241	1887.6[a]	1879.2	1879.2	1880.7	1873.1	1873.1	1875.5
gdb 5242	1877.5[a]	1868.5	1868.5	1871.2	1865.0	1865.0	1868.6
gdb 5243	1889.8[a]	1880.2	1880.2	1883.2	1879.4	1879.4	1881.5
gdb 5244	1892.3[a]	1882.4	1882.4	1885.0	1881.8	1881.7	1883.4
gdb 5245	1863.0[a]	1851.2	1851.2	1853.4	1845.2	1845.2	1846.1
gdb 5246	1855.9[a]	1844.2	1844.2	1847.5	1838.0	1838.0	1843.1
gdb 5247	1855.1[a]	1846.4	1846.3	1850.5	1840.2	1840.2	1844.4
gdb 5248	1864.8[a]	1852.0	1852.0	1854.3	1849.6	1849.6	1851.1
gdb 5249	1862.9[a]	1854.1	1854.1	1858.6	1852.0	1851.9	1854.7
gdb 5250	1867.1[a]	1854.3	1854.3	1857.8	1852.3	1852.3	1854.1
gdb 5251	1860.6[a]	1848.2	1848.2	1851.0	1845.6	1845.6	1848.2
gdb 5252	1858.7[a]	1851.4	1851.4	1854.5	1847.3	1847.3	1851.5
gdb 5253	1860.6[a]	1855.8	1855.8	1858.9	1851.6	1851.6	1855.6
gdb 5254	1867.9[a]	1861.2	1861.2	1864.5	1860.6	1860.6	1863.1
gdb 5255	1869.7[a]	1865.9	1865.9	1869.0	1864.6	1864.6	1866.7
gdb 5256	1868.8[a]	1858.3	1858.3	1860.8	1859.0	1859.0	1860.1
gdb 5257	1873.2[a]	1868.9	1868.9	1872.1	1868.3	1868.2	1871.2
gdb 5258	1885.2[a]	1882.2	1882.2	1884.6	1884.2	1884.2	1885.3
gdb 5259	1888.6[a]	1896.7	1896.7	1897.5	1886.1	1886.1	1888.8
gdb 5260	1889.9[a]	1898.2	1898.2	1898.8	1887.9	1887.9	1890.3
gdb 5261	1884.5[a]	1887.2	1887.2	1889.4	1878.6	1878.6	1883.4
gdb 5262	1887.4[a]	1891.3	1891.3	1892.7	1881.9	1881.9	1885.4

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5263	1879.0[a]	1882.5	1882.5	1885.5	1875.1	1875.1	1879.7
gdb 5264	1889.4[a]	1892.6	1892.6	1895.6	1888.6	1888.5	1891.3
gdb 5265	1893.6[a]	1897.1	1897.0	1899.0	1892.7	1892.7	1894.0
gdb 5266	1887.6[a]	1890.4	1890.4	1893.8	1886.7	1886.7	1890.0
gdb 5267	1869.3[a]	1870.5	1870.5	1874.1	1868.3	1868.3	1870.6
gdb 5268	1868.1[a]	1864.0	1864.0	1866.6	1862.2	1862.2	1863.7
gdb 5269	1879.7[a]	1878.3	1878.3	1881.0	1877.5	1877.5	1880.0
gdb 5270	1900.7[a]	1887.9	1887.9	1889.8	1886.2	1886.2	1888.7
gdb 5271	1873.9[a]	1873.9	1873.9	1876.4	1872.8	1872.8	1875.2
gdb 5272	1873.7[a]	1880.2	1880.2	1883.2	1878.2	1878.2	1881.5
gdb 5273	1881.0[a]	1885.9	1885.9	1889.3	1887.6	1887.6	1889.5
gdb 5274	1841.7[a]	1833.6	1833.6	1833.4	1825.8	1825.8	1824.8
gdb 5275	1843.8[a]	1835.8	1835.8	1835.7	1827.8	1827.8	1826.7
gdb 5276	1838.6[a]	1838.2	1838.2	1838.4	1829.4	1829.3	1828.9
gdb 5277	1837.6[a]	1832.6	1832.6	1835.4	1826.5	1826.5	1829.5
gdb 5278	1847.4[a]	1844.9	1844.9	1845.6	1840.0	1840.0	1838.3
gdb 5279	1846.5[a]	1838.8	1838.8	1842.0	1837.0	1837.0	1838.8
gdb 5280	1849.7[a]	1841.2	1841.2	1844.3	1839.6	1839.6	1840.9
gdb 5281	1865.3[a]	1856.2	1856.2	1858.2	1856.8	1856.8	1858.9
gdb 5282	1868.4[a]	1858.3	1858.2	1860.4	1859.1	1859.1	1861.1
gdb 5283	1864.8[a]	1861.3	1861.3	1863.7	1861.3	1861.2	1864.4
gdb 5284	1871.8[a]	1871.9	1871.8	1874.4	1873.8	1873.8	1874.9
gdb 5285	1872.3[a]	1872.6	1872.6	1875.2	1866.1	1866.1	1870.4
gdb 5286	1886.0[a]	1883.1	1883.1	1886.3	1880.7	1880.7	1883.3
gdb 5287	1881.6[a]	1878.9	1878.9	1882.3	1876.2	1876.2	1879.4
gdb 5288	1898.5[a]	1886.9	1886.9	1888.7	1884.8	1884.8	1887.2
gdb 5289	1877.5[a]	1876.9	1876.9	1879.5	1875.9	1875.9	1878.5
gdb 5290	1877.3[a]	1877.2	1877.2	1879.4	1875.7	1875.7	1877.6
gdb 5291	1871.8[a]	1880.0	1880.0	1882.7	1877.4	1877.4	1880.1
gdb 5292	1882.2[a]	1886.9	1886.9	1890.1	1888.4	1888.4	1890.0
gdb 5293	1874.8[a]	1874.0	1874.0	1876.7	1867.5	1867.5	1871.7
gdb 5294	1883.3[a]	1880.7	1880.7	1884.1	1878.1	1878.0	1881.1
gdb 5295	1883.1[a]	1880.4	1880.3	1883.7	1877.4	1877.4	1880.1
gdb 5296	1849.1[a]	1835.9	1835.9	1838.8	1831.2	1831.2	1832.6
gdb 5297	1851.4[a]	1838.9	1838.9	1841.2	1834.3	1834.3	1835.2
gdb 5298	1844.9[a]	1834.1	1834.1	1836.4	1829.4	1829.4	1831.1
gdb 5299	1852.7[a]	1835.6	1835.6	1840.8	1831.2	1831.2	1836.3
gdb 5300	1854.5[a]	1840.7	1840.7	1843.3	1839.6	1839.6	1840.1
gdb 5301	1860.2[a]	1843.4	1843.4	1848.9	1842.6	1842.6	1846.3
gdb 5302	1864.0[a]	1847.1	1847.0	1851.9	1846.4	1846.4	1849.4
gdb 5303	1859.5[a]	1847.9	1847.9	1850.7	1845.1	1845.0	1848.0
gdb 5304	1856.3[a]	1845.5	1845.5	1847.9	1842.5	1842.5	1845.8
gdb 5305	1857.0[a]	1854.3	1854.3	1857.4	1850.0	1849.9	1853.8
gdb 5306	1867.7[a]	1856.1	1856.0	1859.0	1856.2	1856.2	1858.0
gdb 5307	1869.3[a]	1866.0	1866.0	1869.6	1864.3	1864.3	1866.8
gdb 5308	1869.5[a]	1863.3	1863.3	1866.6	1862.7	1862.7	1865.1
gdb 5309	1914.1[a]	1918.4	1918.4	1919.8	1920.5	1920.5	1920.6
gdb 5310	1925.3[a]	1919.8	1919.8	1920.6	1917.9	1917.9	1919.8
gdb 5311	1860.5[a]	1861.1	1861.1	1861.3	1858.2	1858.2	1857.9
gdb 5312	1882.0[a]	1881.2	1881.2	1879.9	1877.0	1876.9	1874.5
gdb 5313	1909.4[a]	1918.1	1918.1	1919.4	1920.5	1920.4	1921.2
gdb 5314	1882.5[a]	1882.1	1882.1	1880.9	1877.9	1877.9	1875.4
gdb 5315	1914.0[a]	1919.6	1919.6	1921.5	1921.6	1921.6	1921.7
gdb 5316	1925.8[a]	1920.2	1920.1	1920.8	1918.1	1918.0	1920.0
gdb 5317	1896.2[a]	1903.0	1903.0	1904.2	1901.4	1901.4	1903.4
gdb 5318	1902.9[a]	1907.8	1907.8	1908.9	1909.8	1909.8	1910.1
gdb 5319	1864.9[a]	1866.9	1866.9	1869.2	1865.2	1865.2	1867.0
gdb 5320	1864.3[a]	1860.8	1860.8	1861.9	1859.6	1859.6	1860.5
gdb 5321	1911.5[a]	1915.8	1915.8	1917.4	1917.4	1917.4	1917.9
gdb 5322	1913.7[a]	1917.5	1917.5	1918.4	1919.0	1919.0	1918.8
gdb 5323	1910.2[a]	1914.9	1914.9	1916.4	1916.4	1916.4	1917.1
gdb 5324	1912.6[a]	1917.2	1917.2	1918.3	1918.6	1918.6	1919.0
gdb 5325	1925.0[a]	1920.0	1920.0	1920.9	1917.7	1917.7	1920.0
gdb 5326	1902.1[a]	1907.5	1907.5	1908.8	1905.4	1905.4	1907.4
gdb 5327	1918.8[a]	1915.6	1915.6	1916.2	1912.9	1912.9	1915.5

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5328	1912.0[a]	1915.7	1915.7	1917.0	1917.3	1917.3	1917.5
gdb 5329	1907.8[a]	1915.5	1915.5	1917.1	1917.3	1917.3	1918.2
gdb 5330	1908.1[a]	1914.7	1914.7	1915.3	1916.3	1916.3	1916.4
gdb 5331	1880.6[a]	1879.3	1879.3	1878.4	1874.7	1874.6	1872.5
gdb 5332	1881.1[a]	1880.5	1880.5	1879.7	1875.5	1875.5	1872.7
gdb 5333	1885.9[a]	1886.7	1886.7	1889.8	1887.3	1887.3	1887.7
gdb 5334	1911.4[a]	1915.7	1915.7	1917.1	1917.4	1917.4	1917.9
gdb 5335	1925.2[a]	1919.6	1919.6	1920.4	1917.2	1917.2	1919.3
gdb 5336	1912.9[a]	1917.2	1917.2	1919.2	1918.8	1918.8	1919.3
gdb 5337	1894.2[a]	1903.1	1903.1	1904.6	1901.6	1901.6	1903.7
gdb 5338	1900.2[a]	1906.2	1906.2	1907.7	1908.4	1908.4	1909.5
gdb 5339	1863.1[a]	1862.4	1862.4	1862.5	1859.0	1859.0	1858.8
gdb 5340	1870.8[a]	1866.8	1866.8	1871.3	1867.9	1867.9	1869.8
gdb 5341	1884.3[a]	1880.8	1880.8	1879.8	1876.8	1876.8	1874.6
gdb 5342	1884.2[a]	1882.9	1882.9	1885.5	1885.3	1885.3	1885.9
gdb 5343	1874.9[a]	1876.4	1876.4	1879.0	1875.9	1875.9	1877.3
gdb 5344	1881.2[a]	1879.9	1879.9	1878.7	1876.0	1876.0	1873.3
gdb 5345	1883.4[a]	1882.3	1882.3	1884.6	1884.7	1884.7	1885.3
gdb 5346	1879.5[a]	1878.2	1878.2	1880.8	1875.1	1875.1	1877.0
gdb 5347	1863.9[a]	1862.9	1862.9	1864.6	1859.6	1859.6	1860.2
gdb 5348	1871.4[a]	1867.3	1867.3	1871.9	1868.2	1868.2	1870.1
gdb 5349	1859.5[a]	1860.4	1860.4	1862.0	1857.1	1857.1	1857.7
gdb 5350	1864.8[a]	1864.1	1864.1	1866.3	1860.9	1860.8	1861.1
gdb 5351	1869.4[a]	1865.8	1865.8	1869.7	1866.5	1866.5	1868.4
gdb 5352	1884.4[a]	1880.9	1880.9	1879.9	1876.9	1876.9	1874.8
gdb 5353	1884.8[a]	1883.4	1883.4	1886.0	1885.9	1885.9	1886.6
gdb 5354	1879.6[a]	1877.9	1877.9	1877.1	1873.1	1873.1	1871.2
gdb 5355	1881.2[a]	1880.2	1880.2	1879.7	1875.1	1875.1	1872.8
gdb 5356	1885.1[a]	1887.3	1887.3	1890.3	1887.5	1887.4	1887.8
gdb 5357	1875.0[a]	1876.4	1876.4	1878.7	1875.2	1875.2	1877.4
gdb 5358	1881.9[a]	1879.6	1879.6	1878.5	1876.2	1876.2	1873.8
gdb 5359	1886.0[a]	1895.5	1895.5	1896.1	1885.6	1885.6	1887.9
gdb 5360	1885.8[a]	1895.4	1895.4	1896.0	1885.6	1885.5	1887.9
gdb 5361	1888.2[a]	1891.4	1891.4	1894.5	1888.6	1888.6	1891.3
gdb 5362	1890.3[a]	1895.4	1895.4	1897.4	1891.6	1891.6	1892.8
gdb 5363	1888.0[a]	1892.2	1892.2	1895.2	1889.3	1889.3	1891.8
gdb 5364	1882.2[a]	1880.4	1880.4	1883.4	1878.6	1878.6	1881.1
gdb 5365	1881.3[a]	1879.4	1879.4	1882.3	1877.6	1877.5	1880.0
gdb 5366	1882.5[a]	1882.7	1882.7	1885.3	1881.1	1881.1	1883.9
gdb 5367	1907.3[a]	1915.3	1915.3	1917.1	1916.9	1916.9	1918.0
gdb 5368	1908.0[a]	1914.7	1914.7	1915.6	1916.2	1916.2	1916.4
gdb 5369	1914.5[a]	1915.5	1915.5	1916.0	1913.1	1913.1	1915.9
gdb 5370	1909.0[a]	1915.0	1915.0	1916.3	1917.4	1917.3	1918.0
gdb 5371	1911.5[a]	1916.0	1915.9	1917.4	1917.4	1917.4	1917.7
gdb 5372	1913.2[a]	1916.2	1916.2	1917.0	1917.5	1917.5	1917.3
gdb 5373	1900.1[a]	1906.1	1906.1	1907.7	1908.5	1908.5	1909.6
gdb 5374	1883.6[a]	1880.9	1880.9	1879.9	1876.9	1876.8	1874.7
gdb 5375	1884.8[a]	1883.3	1883.3	1885.9	1885.8	1885.7	1886.4
gdb 5376	1880.7[a]	1881.6	1881.6	1880.6	1877.8	1877.8	1875.5
gdb 5377	1882.9[a]	1882.0	1882.0	1884.4	1884.5	1884.4	1885.2
gdb 5378	1884.0[a]	1880.6	1880.5	1879.8	1876.3	1876.2	1874.3
gdb 5379	1885.2[a]	1884.5	1884.5	1887.3	1886.7	1886.7	1887.0
gdb 5380	1879.6[a]	1879.0	1879.0	1881.6	1875.8	1875.8	1877.6
gdb 5381	1885.9[a]	1880.4	1880.4	1879.5	1877.7	1877.7	1875.5
gdb 5382	1881.8[a]	1880.7	1880.7	1883.7	1878.8	1878.8	1881.2
gdb 5383	1882.3[a]	1880.3	1880.3	1883.4	1878.6	1878.5	1881.1
gdb 5384	1915.0[a]	1915.5	1915.5	1916.1	1913.3	1913.2	1916.1
gdb 5385	1908.9[a]	1914.6	1914.6	1915.5	1917.0	1917.0	1917.7
gdb 5386	1881.0[a]	1879.2	1879.2	1877.1	1874.8	1874.8	1871.7
gdb 5387	1875.2[a]	1876.6	1876.6	1879.4	1875.8	1875.8	1877.4
gdb 5388	1893.8[a]	1903.1	1903.1	1905.0	1901.4	1901.3	1903.9
gdb 5389	1900.4[a]	1906.1	1906.4	1908.4	1908.0	1908.0	1909.2
gdb 5390	1881.4[a]	1880.2	1880.1	1879.1	1876.6	1876.6	1874.2
gdb 5391	1874.5[a]	1876.1	1876.1	1878.4	1875.1	1875.1	1877.3
gdb 5392	1918.4[a]	1915.2	1915.1	1915.8	1912.0	1911.9	1914.4

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5393	1901.7[a]	1906.3	1906.3	1907.6	1904.0	1904.0	1906.1
gdb 5394	1913.0[a]	1916.7	1916.7	1918.0	1917.5	1917.5	1917.6
gdb 5395	1881.7[a]	1881.8	1881.8	1884.4	1880.1	1880.1	1883.0
gdb 5396	1882.1[a]	1876.9	1876.9	1879.0	1880.0	1880.0	1880.6
gdb 5397	1880.2[a]	1875.8	1875.8	1878.4	1880.0	1880.0	1880.6
gdb 5398	1876.1[a]	1871.6	1871.5	1870.3	1868.9	1868.9	1866.4
gdb 5399	1872.4[a]	1869.5	1869.4	1870.6	1868.5	1868.4	1870.3
gdb 5400	1875.9[a]	1877.9	1877.9	1876.8	1875.4	1875.4	1873.3
gdb 5401	1893.6[a]	1878.6	1878.6	1879.8	1879.3	1879.3	1880.8
gdb 5402	1866.0[a]	1873.3	1873.3	1874.5	1872.0	1871.9	1873.8
gdb 5403	1878.7[a]	1883.2	1883.2	1885.7	1885.8	1885.8	1886.5
gdb 5404	1910.6[a]	1917.7	1917.7	1919.5	1919.0	1919.0	1920.1
gdb 5405	1897.1[a]	1904.6	1904.6	1906.2	1902.7	1902.6	1905.2
gdb 5406	1920.9[a]	1934.8	1934.8	1935.2	1937.8	1937.8	1938.1
gdb 5407	1857.5[a]	1852.4	1852.3	1855.9	1854.3	1854.3	1855.5
gdb 5408	1848.1[a]	1842.9	1842.9	1845.5	1841.8	1841.7	1844.1
gdb 5409	1855.2[a]	1851.4	1851.4	1854.4	1852.9	1852.8	1853.7
gdb 5410	1856.4[a]	1851.6	1851.6	1855.0	1853.0	1852.9	1854.0
gdb 5411	1854.2[a]	1850.4	1850.4	1853.5	1852.5	1852.4	1853.1
gdb 5412	1844.6[a]	1840.1	1840.0	1842.6	1838.9	1838.8	1841.3
gdb 5413	1845.5[a]	1840.9	1840.9	1843.4	1839.4	1839.4	1841.8
gdb 5414	1858.2[a]	1855.0	1855.0	1857.5	1858.4	1858.4	1858.1
gdb 5415	1847.2[a]	1843.3	1843.3	1845.7	1843.7	1843.6	1845.1
gdb 5416	1842.9[a]	1840.0	1840.0	1842.3	1839.8	1839.7	1842.0
gdb 5417	1852.9[a]	1850.0	1849.9	1853.3	1852.6	1852.5	1853.6
gdb 5418	1912.1[a]	1914.9	1914.9	1917.2	1915.8	1915.8	1917.1
gdb 5419	1910.2[a]	1913.8	1913.8	1915.3	1914.8	1914.8	1915.9
gdb 5420	1897.2[a]	1902.0	1902.0	1904.0	1899.4	1899.3	1902.1
gdb 5421	1852.6[a]	1850.3	1850.3	1854.3	1848.0	1847.9	1850.9
gdb 5422	1845.1[a]	1844.4	1844.3	1847.1	1837.5	1837.5	1841.4
gdb 5423	1851.7[a]	1855.3	1855.3	1859.6	1851.2	1851.2	1854.6
gdb 5424	1859.1[a]	1860.7	1860.7	1865.0	1860.8	1860.8	1862.8
gdb 5425	1892.4[a]	1896.3	1896.3	1896.5	1899.9	1899.9	1900.6
gdb 5426	1843.7[a]	1840.1	1840.1	1842.8	1839.1	1839.1	1841.4
gdb 5427	1831.7[a]	1828.4	1828.4	1830.3	1824.1	1824.1	1828.0
gdb 5428	1855.4[a]	1850.7	1850.7	1854.3	1852.3	1852.2	1853.3
gdb 5429	1898.6[a]	1905.1	1905.1	1906.6	1908.4	1908.4	1910.1
gdb 5430	1881.8[a]	1875.5	1875.5	1878.0	1879.0	1879.0	1880.1
gdb 5431	1880.4[a]	1874.2	1874.2	1877.0	1879.0	1879.0	1880.1
gdb 5432	1892.1[a]	1868.2	1868.1	1869.8	1869.4	1869.4	1871.5
gdb 5433	1871.4[a]	1864.9	1864.8	1866.6	1865.7	1865.6	1868.1
gdb 5434	1868.0[a]	1849.3	1849.3	1853.6	1854.0	1854.0	1856.2
gdb 5435	1870.2[a]	1850.0	1849.9	1854.0	1854.7	1854.6	1857.1
gdb 5436	1861.1[a]	1841.5	1841.5	1845.0	1842.6	1842.6	1846.6
gdb 5437	1880.5[a]	1875.4	1875.4	1878.3	1878.7	1878.7	1879.8
gdb 5438	1880.1[a]	1873.7	1873.6	1876.0	1877.7	1877.7	1878.6
gdb 5439	1870.7[a]	1867.8	1867.8	1869.4	1867.1	1867.1	1869.1
gdb 5440	1880.7[a]	1876.4	1876.4	1879.2	1879.8	1879.8	1880.6
gdb 5441	1879.9[a]	1876.5	1876.5	1878.4	1879.3	1879.2	1879.5
gdb 5442	1870.1[a]	1865.9	1865.9	1867.7	1866.2	1866.2	1868.4
gdb 5443	1846.9[a]	1840.0	1840.0	1841.6	1835.2	1835.2	1837.1
gdb 5444	1857.2[a]	1850.1	1850.1	1852.7	1848.3	1848.3	1848.8
gdb 5445	1833.5[a]	1825.6	1825.6	1828.2	1821.7	1821.7	1825.3
gdb 5446	1844.6[a]	1836.1	1836.1	1839.8	1835.2	1835.1	1837.5
gdb 5447	1833.6[a]	1808.9	1808.9	1815.2	1809.5	1809.4	1814.1
gdb 5448	1839.8[a]	1815.9	1815.9	1823.3	1820.4	1820.4	1823.5
gdb 5449	1847.3[a]	1829.9	1829.9	1833.1	1831.0	1830.9	1832.5
gdb 5450	1845.1[a]	1829.7	1829.7	1833.1	1829.7	1829.6	1832.8
gdb 5451	1837.6[a]	1820.7	1820.7	1823.0	1818.0	1817.9	1820.9
gdb 5452	1854.4[a]	1837.8	1837.8	1841.0	1841.0	1841.0	1842.4
gdb 5453	1848.7[a]	1836.4	1836.4	1840.3	1834.9	1834.8	1837.8
gdb 5454	1854.2[a]	1842.4	1842.4	1847.7	1845.1	1845.1	1847.1
gdb 5455	1848.9[a]	1832.7	1832.7	1835.8	1833.1	1833.1	1834.5
gdb 5456	1850.6[a]	1837.9	1837.9	1841.0	1836.2	1836.2	1838.6
gdb 5457	1839.2[a]	1824.5	1824.5	1826.6	1820.9	1820.9	1823.6

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5458	1856.3[a]	1843.1	1843.1	1847.7	1845.6	1845.6	1847.2
gdb 5459	1844.3[a]	1828.2	1828.2	1831.3	1828.8	1828.8	1830.7
gdb 5460	1843.0[a]	1827.1	1827.1	1830.1	1828.0	1828.0	1829.3
gdb 5461	1843.8[a]	1829.6	1829.5	1832.8	1829.7	1829.7	1832.7
gdb 5462	1835.2[a]	1819.4	1819.4	1821.4	1816.3	1816.3	1819.1
gdb 5463	1852.2[a]	1836.6	1836.6	1841.0	1840.6	1840.6	1842.5
gdb 5464	1883.5[a]	1876.2	1876.2	1878.4	1869.9	1869.9	1872.7
gdb 5465	1878.5[a]	1869.5	1869.5	1871.6	1864.8	1864.8	1868.3
gdb 5466	1888.0[a]	1879.2	1879.2	1882.7	1878.3	1878.3	1880.6
gdb 5467	1833.5[a]	1808.9	1808.9	1813.1	1810.2	1810.2	1811.7
gdb 5468	1838.2[a]	1811.6	1811.6	1817.0	1812.0	1811.9	1816.1
gdb 5469	1826.7[a]	1801.5	1801.5	1804.8	1799.1	1799.1	1802.2
gdb 5470	1842.5[a]	1817.2	1817.1	1823.7	1821.2	1821.2	1824.0
gdb 5471	1831.2[a]	1807.8	1807.8	1811.7	1808.7	1808.7	1810.1
gdb 5472	1832.5[a]	1807.8	1807.8	1811.8	1807.9	1807.8	1809.0
gdb 5473	1835.6[a]	1809.7	1809.7	1815.1	1809.9	1809.8	1813.9
gdb 5474	1824.1[a]	1800.2	1800.2	1803.0	1797.3	1797.2	1800.1
gdb 5475	1843.9[a]	1817.8	1817.8	1824.2	1822.0	1822.0	1824.6
gdb 5476	1838.9[a]	1830.0	1829.9	1829.5	1827.4	1827.4	1824.7
gdb 5477	1826.8[a]	1818.5	1818.5	1820.5	1819.7	1819.7	1821.3
gdb 5478	1827.9[a]	1819.5	1819.5	1818.1	1813.9	1813.9	1812.5
gdb 5479	1836.9[a]	1827.7	1827.7	1829.5	1831.5	1831.5	1831.4
gdb 5480	1834.2[a]	1825.8	1825.8	1823.9	1822.3	1822.3	1819.3
gdb 5481	1834.3[a]	1826.5	1826.5	1826.1	1824.5	1824.5	1821.7
gdb 5482	1825.8[a]	1816.7	1818.6	1820.8	1817.4	1817.4	1820.6
gdb 5483	1824.8[a]	1817.3	1817.3	1815.9	1811.4	1811.3	1810.1
gdb 5484	1838.3[a]	1829.8	1829.8	1831.6	1833.4	1833.4	1833.0
gdb 5485	1861.1[a]	1857.3	1857.3	1859.8	1851.8	1851.8	1855.5
gdb 5486	1859.8[a]	1853.1	1853.0	1856.1	1848.5	1848.4	1852.7
gdb 5487	1868.5[a]	1865.0	1865.0	1868.4	1863.4	1863.4	1865.5
gdb 5488	1866.9[a]	1860.5	1860.5	1863.1	1859.5	1859.5	1861.8
gdb 5489	1853.0[a]	1835.3	1835.3	1840.1	1831.7	1831.7	1837.0
gdb 5490	1858.7[a]	1841.6	1841.6	1847.2	1841.9	1841.9	1845.6
gdb 5491	1875.1[a]	1873.7	1873.7	1876.3	1872.1	1872.1	1874.7
gdb 5492	1882.4[a]	1882.4	1882.4	1885.9	1883.4	1883.4	1884.5
gdb 5493	1863.1[a]	1860.1	1860.1	1865.0	1856.4	1856.4	1860.4
gdb 5494	1864.3[a]	1861.8	1861.8	1866.6	1862.5	1862.5	1865.3
gdb 5495	1873.0[a]	1869.1	1869.1	1871.3	1868.9	1868.8	1871.7
gdb 5496	1884.8[a]	1881.3	1881.3	1884.4	1883.9	1883.9	1885.2
gdb 5497	1881.5[a]	1875.1	1875.1	1877.6	1878.7	1878.7	1879.7
gdb 5498	1882.4[a]	1874.0	1874.0	1876.5	1878.2	1878.2	1878.8
gdb 5499	1889.1[a]	1866.7	1866.7	1867.9	1867.4	1867.4	1869.3
gdb 5500	1872.0[a]	1865.4	1865.4	1867.0	1865.9	1865.9	1868.2
gdb 5501	1907.9[a]	1904.3	1904.3	1905.2	1903.7	1903.7	1905.8
gdb 5502	1888.7[a]	1894.9	1894.9	1895.3	1895.5	1895.4	1897.2
gdb 5503	1899.1[a]	1904.1	1904.0	1904.2	1907.0	1907.0	1906.8
gdb 5504	1885.0[a]	1883.1	1883.1	1884.4	1880.8	1880.8	1881.4
gdb 5505	1882.1[a]	1880.0	1880.0	1882.3	1877.9	1877.9	1881.3
gdb 5506	1894.5[a]	1890.7	1890.7	1894.3	1892.3	1892.3	1894.6
gdb 5507	1862.2[a]	1854.5	1854.4	1856.7	1855.5	1855.5	1857.5
gdb 5508	1859.9[a]	1858.3	1858.3	1860.0	1858.5	1858.5	1861.5
gdb 5509	1870.6[a]	1868.1	1868.1	1869.4	1870.8	1870.8	1871.8
gdb 5510	1870.6[a]	1852.0	1852.0	1855.8	1856.6	1856.6	1858.4
gdb 5511	1873.0[a]	1852.5	1852.5	1856.3	1856.7	1856.7	1858.2
gdb 5512	1858.9[a]	1847.0	1847.0	1847.2	1846.4	1846.3	1844.5
gdb 5513	1863.5[a]	1844.4	1844.4	1847.4	1845.3	1845.3	1848.8
gdb 5514	1862.2[a]	1860.8	1860.8	1862.9	1857.4	1857.4	1858.5
gdb 5515	1864.3[a]	1859.1	1859.1	1862.9	1856.0	1856.0	1859.5
gdb 5516	1854.2[a]	1852.7	1852.6	1853.5	1844.8	1844.7	1847.0
gdb 5517	1869.6[a]	1865.2	1865.2	1869.9	1866.2	1866.1	1868.5
gdb 5518	1850.4[a]	1840.4	1840.4	1841.0	1839.2	1839.1	1838.5
gdb 5519	1854.3[a]	1840.6	1840.6	1843.7	1839.7	1839.7	1843.3
gdb 5520	1862.2[a]	1847.4	1847.4	1851.0	1850.4	1850.4	1852.4
gdb 5521	1885.3[a]	1883.8	1883.8	1885.0	1881.8	1881.8	1882.6
gdb 5522	1900.2[a]	1890.2	1890.2	1892.5	1888.5	1888.5	1891.6

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5523	1884.7[a]	1882.9	1882.8	1885.4	1881.1	1881.1	1885.0
gdb 5524	1891.9[a]	1888.8	1888.8	1892.4	1891.2	1891.2	1893.8
gdb 5525	1859.5[a]	1859.6	1859.6	1861.4	1856.7	1856.7	1857.6
gdb 5526	1851.4[a]	1851.3	1851.3	1851.8	1844.0	1844.0	1846.0
gdb 5527	1848.9[a]	1840.7	1840.7	1839.1	1832.5	1832.4	1830.1
gdb 5528	1845.9[a]	1835.6	1835.5	1835.7	1827.7	1827.6	1829.1
gdb 5529	1841.9[a]	1838.3	1838.3	1838.9	1831.6	1831.6	1833.1
gdb 5530	1856.7[a]	1846.1	1846.1	1846.9	1842.7	1842.7	1841.8
gdb 5531	1853.3[a]	1848.0	1848.0	1849.8	1845.8	1845.7	1846.0
gdb 5532	1822.5[a]	1806.9	1806.9	1804.7	1800.3	1800.3	1796.0
gdb 5533	1828.5[a]	1807.2	1807.1	1807.9	1802.1	1802.1	1802.5
gdb 5534	1817.0[a]	1806.1	1806.1	1806.9	1801.4	1801.4	1801.6
gdb 5535	1834.9[a]	1813.3	1813.2	1814.8	1812.4	1812.4	1811.3
gdb 5536	1822.8[a]	1813.4	1813.3	1814.9	1812.9	1812.8	1811.7
gdb 5537	1846.6[a]	1838.4	1838.4	1839.3	1837.9	1837.9	1838.0
gdb 5538	1851.6[a]	1837.7	1837.7	1841.4	1838.3	1838.2	1843.0
gdb 5539	1853.7[a]	1842.3	1842.3	1846.9	1846.8	1846.7	1849.7
gdb 5540	1868.7[a]	1867.8	1867.8	1869.6	1860.6	1860.6	1864.1
gdb 5541	1878.3[a]	1876.1	1876.1	1879.1	1873.1	1873.1	1875.5
gdb 5542	1882.6[a]	1877.1	1877.1	1878.0	1879.6	1879.6	1879.6
gdb 5543	1882.3[a]	1875.6	1875.6	1877.9	1879.4	1879.4	1879.6
gdb 5544	1876.5[a]	1872.2	1872.1	1870.6	1869.4	1869.4	1866.5
gdb 5545	1872.7[a]	1869.4	1869.3	1870.3	1868.4	1868.3	1869.9
gdb 5546	1844.9[a]	1836.3	1836.3	1832.5	1827.1	1827.1	1821.4
gdb 5547	1839.7[a]	1834.3	1834.3	1833.1	1826.9	1826.8	1825.3
gdb 5548	1837.9[a]	1833.7	1833.7	1832.2	1826.3	1826.3	1824.6
gdb 5549	1852.6[a]	1844.2	1844.2	1844.1	1840.6	1840.6	1837.7
gdb 5550	1846.4[a]	1841.0	1840.9	1840.7	1837.4	1837.4	1834.8
gdb 5551	1867.2[a]	1864.9	1864.9	1863.8	1861.9	1861.9	1860.3
gdb 5552	1861.9[a]	1864.0	1864.0	1865.8	1862.4	1862.4	1865.4
gdb 5553	1868.9[a]	1869.8	1869.8	1871.2	1871.7	1871.7	1872.7
gdb 5554	1864.6[a]	1861.0	1861.0	1856.4	1851.6	1851.5	1846.3
gdb 5555	1860.8[a]	1861.6	1861.6	1859.6	1853.7	1853.7	1852.0
gdb 5556	1869.7[a]	1868.9	1868.9	1868.3	1864.9	1864.9	1862.4
gdb 5557	1881.4[a]	1879.1	1879.1	1878.4	1874.6	1874.6	1872.9
gdb 5558	1870.0[a]	1868.1	1868.1	1866.0	1859.9	1859.9	1859.1
gdb 5559	1907.3[a]	1905.5	1905.5	1906.4	1904.0	1904.0	1905.9
gdb 5560	1897.6[a]	1901.3	1901.2	1899.2	1898.2	1898.2	1895.7
gdb 5561	1885.6[a]	1894.9	1894.9	1896.2	1893.3	1893.3	1894.9
gdb 5562	1898.7[a]	1906.1	1906.1	1907.8	1908.3	1908.3	1908.7
gdb 5563	1840.4[a]	1831.1	1831.1	1830.0	1825.3	1825.2	1824.1
gdb 5564	1831.6[a]	1816.9	1816.9	1819.2	1816.1	1816.1	1818.2
gdb 5565	1851.3[a]	1841.6	1841.6	1841.5	1838.8	1838.8	1836.4
gdb 5566	1842.1[a]	1826.7	1828.2	1828.6	1828.3	1828.3	1828.8
gdb 5567	1844.5[a]	1828.4	1828.4	1831.6	1829.0	1829.0	1830.8
gdb 5568	1844.4[a]	1826.1	1826.1	1829.3	1827.6	1827.6	1829.1
gdb 5569	1843.8[a]	1830.7	1830.7	1834.1	1830.4	1830.4	1833.3
gdb 5570	1838.4[a]	1819.2	1819.2	1823.4	1816.0	1815.9	1819.1
gdb 5571	1855.4[a]	1839.7	1839.7	1844.2	1843.6	1843.6	1845.2
gdb 5572	1856.8[a]	1845.0	1845.0	1848.2	1839.2	1839.2	1841.0
gdb 5573	1851.5[a]	1839.2	1839.2	1842.3	1833.4	1833.4	1837.4
gdb 5574	1862.4[a]	1850.1	1850.1	1854.4	1848.2	1848.1	1850.7
gdb 5575	1847.4[a]	1841.0	1841.0	1845.1	1834.7	1834.7	1839.5
gdb 5576	1854.8[a]	1849.4	1849.4	1853.2	1846.4	1846.4	1849.5
gdb 5577	1855.3[a]	1842.6	1842.6	1845.6	1837.1	1837.1	1840.9
gdb 5578	1850.9[a]	1843.4	1843.4	1847.4	1838.0	1838.0	1842.3
gdb 5579	1862.1[a]	1849.3	1849.3	1852.2	1847.2	1847.2	1849.3
gdb 5580	1859.8[a]	1851.8	1851.8	1856.9	1850.2	1850.2	1853.4
gdb 5581	1863.5[a]	1857.5	1857.5	1855.6	1851.7	1851.7	1850.6
gdb 5582	1850.1[a]	1850.4	1850.3	1852.1	1847.2	1847.2	1849.9
gdb 5583	1874.4[a]	1868.0	1868.0	1867.1	1865.1	1865.1	1862.7
gdb 5584	1860.3[a]	1859.3	1859.3	1860.8	1859.1	1859.0	1860.1
gdb 5585	1873.0[a]	1869.7	1869.7	1871.9	1869.1	1869.1	1871.7
gdb 5586	1885.6[a]	1881.7	1881.7	1884.6	1884.4	1884.4	1885.5
gdb 5587	1910.1[a]	1905.7	1905.7	1906.6	1904.7	1904.7	1906.6

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Table S73: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5588	1889.2[a]	1893.9	1893.8	1895.8	1894.5	1894.4	1896.2
gdb 5589	1889.8[a]	1894.0	1894.0	1894.5	1894.3	1894.3	1895.7
gdb 5590	1899.5[a]	1903.6	1903.6	1905.0	1906.9	1906.8	1906.8
gdb 5591	1865.0[a]	1856.4	1856.3	1858.5	1857.1	1857.1	1859.0
gdb 5592	1866.2[a]	1854.0	1853.9	1855.3	1854.7	1854.6	1856.5
gdb 5593	1864.6[a]	1861.1	1861.1	1862.4	1860.6	1860.6	1863.0
gdb 5594	1874.1[a]	1871.1	1871.1	1873.3	1873.5	1873.5	1874.5
gdb 5595	1879.3[a]	1876.3	1876.3	1879.0	1875.5	1875.5	1877.9
gdb 5596	1883.2[a]	1878.0	1877.9	1880.3	1876.6	1876.6	1880.3
gdb 5597	1889.4[a]	1884.0	1884.0	1887.2	1886.8	1886.8	1888.8
gdb 5598	1876.1[a]	1879.6	1879.6	1882.2	1872.6	1872.6	1877.2
gdb 5599	1885.3[a]	1888.0	1888.0	1891.7	1884.9	1884.9	1888.4
gdb 5600	1871.7[a]	1871.6	1871.6	1874.2	1870.6	1870.6	1873.0
gdb 5601	1874.7[a]	1874.1	1874.1	1876.9	1873.3	1873.3	1876.0
gdb 5602	1866.3[a]	1875.2	1875.2	1877.4	1873.0	1873.0	1875.8
gdb 5603	1880.0[a]	1885.1	1885.1	1888.6	1886.8	1886.8	1888.6
gdb 5604	1863.5[a]	1862.9	1862.9	1864.5	1859.3	1859.3	1863.2
gdb 5605	1873.3[a]	1873.1	1873.1	1875.7	1872.7	1872.7	1875.4
gdb 5606	1881.3[a]	1879.2	1879.2	1878.5	1874.9	1874.9	1872.9
gdb 5607	1871.3[a]	1869.8	1869.8	1867.7	1861.8	1861.8	1860.8
gdb 5608	1910.8[a]	1917.7	1917.7	1919.5	1919.4	1919.4	1920.3
gdb 5609	1896.8[a]	1904.7	1904.7	1906.1	1902.9	1902.9	1905.4
gdb 5610	1909.8[a]	1912.9	1912.9	1915.3	1914.1	1914.1	1915.6
gdb 5611	1910.3[a]	1913.5	1913.5	1914.8	1914.5	1914.5	1915.1
gdb 5612	1900.7[a]	1905.2	1905.2	1906.2	1902.8	1902.7	1905.4
gdb 5613	1908.0[a]	1915.0	1914.9	1917.1	1915.7	1915.7	1917.0
gdb 5614	1905.8[a]	1911.8	1911.7	1912.8	1912.8	1912.8	1913.3
gdb 5615	1894.0[a]	1901.7	1901.7	1903.7	1899.1	1899.0	1901.9
gdb 5616	1882.9[a]	1878.4	1878.4	1876.6	1873.3	1873.3	1871.2
gdb 5617	1870.6[a]	1867.0	1867.0	1865.2	1858.8	1858.8	1858.3
gdb 5618	1874.1[a]	1872.6	1872.6	1874.4	1871.0	1870.9	1873.3
gdb 5619	1882.8[a]	1879.2	1879.2	1882.3	1881.5	1881.4	1882.8
gdb 5620	1873.2[a]	1872.4	1872.4	1873.9	1870.7	1870.6	1873.0
gdb 5621	1882.7[a]	1879.9	1879.9	1882.9	1882.1	1882.1	1883.5
gdb 5622	1882.3[a]	1878.3	1878.3	1878.1	1873.7	1873.6	1872.4
gdb 5623	1874.2[a]	1873.6	1873.6	1875.5	1871.8	1871.8	1874.2
gdb 5624	1869.7[a]	1867.0	1866.9	1865.3	1858.5	1858.4	1858.2
gdb 5625	1884.7[a]	1882.4	1882.4	1885.5	1884.4	1884.4	1885.7
gdb 5626	1867.7[a]	1867.1	1867.1	1868.8	1859.8	1859.8	1863.2
gdb 5627	1878.1[a]	1876.0	1876.0	1879.1	1872.4	1872.4	1874.8
gdb 5628	1872.0[a]	1870.4	1870.4	1872.6	1864.6	1864.6	1868.8
gdb 5629	1871.0[a]	1869.3	1869.3	1871.4	1863.6	1863.6	1868.0
gdb 5630	1880.8[a]	1877.9	1877.9	1880.0	1875.1	1875.1	1877.7
gdb 5631	1879.7[a]	1876.9	1876.9	1880.4	1874.8	1874.7	1878.0
gdb 5632	1868.7[a]	1869.7	1869.6	1867.9	1861.4	1861.4	1860.8
gdb 5633	1881.6[a]	1881.8	1881.8	1881.6	1877.1	1877.1	1875.3
gdb 5634	1890.3[a]	1897.2	1897.2	1898.5	1895.5	1895.4	1899.0
gdb 5635	1900.1[a]	1904.8	1904.7	1905.7	1906.4	1906.4	1907.8
gdb 5636	1873.4[a]	1869.8	1869.5	1868.7	1862.8	1862.6	1861.9
gdb 5637	1885.1[a]	1878.4	1878.3	1877.9	1875.3	1875.2	1873.4
gdb 5638	1912.1[a]	1912.8	1912.8	1913.7	1909.5	1909.5	1912.5
gdb 5639	1896.4[a]	1903.5	1903.5	1903.8	1901.3	1901.2	1903.3
gdb 5640	1906.3[a]	1912.6	1912.6	1912.9	1913.9	1913.9	1914.3
gdb 5641	1913.5[a]	1924.2	1924.2	1923.8	1927.7	1927.7	1927.5
gdb 5642	1913.0[a]	1915.4	1915.4	1917.1	1917.4	1917.4	1918.2
gdb 5643	1925.7[a]	1919.5	1919.5	1920.4	1917.3	1917.3	1919.4
gdb 5644	1904.0[a]	1907.6	1907.6	1907.9	1906.0	1906.0	1907.9
gdb 5645	1875.4[a]	1877.6	1877.6	1876.0	1874.2	1874.1	1871.2
gdb 5646	1897.8[a]	1884.7	1884.6	1885.3	1883.4	1883.4	1884.2
gdb 5647	1872.3[a]	1877.9	1877.9	1879.4	1876.6	1876.6	1878.3
gdb 5648	1881.6[a]	1884.9	1884.9	1886.1	1886.9	1886.8	1886.6
gdb 5649	1898.4[a]	1904.9	1904.9	1906.5	1908.1	1908.1	1909.9
gdb 5650	1895.0[a]	1896.9	1896.9	1894.6	1893.5	1893.5	1890.4
gdb 5651	1912.1[a]	1909.3	1909.3	1909.9	1907.2	1907.2	1908.7
gdb 5652	1891.9[a]	1898.3	1898.3	1898.6	1897.0	1897.0	1898.3

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5653	1900.6[a]	1905.0	1904.9	1905.3	1907.0	1907.0	1906.5
gdb 5654	1912.8[a]	1916.2	1916.2	1918.0	1918.1	1918.1	1919.0
gdb 5655	1925.8[a]	1920.3	1920.3	1921.3	1918.1	1918.1	1920.4
gdb 5656	1904.7[a]	1909.0	1909.0	1909.4	1907.3	1907.3	1909.3
gdb 5657	1920.6[a]	1934.9	1934.9	1935.0	1938.6	1938.6	1938.9
gdb 5658	1915.5[a]	1915.4	1915.4	1916.4	1912.6	1912.6	1915.6
gdb 5659	1898.2[a]	1904.0	1904.0	1904.2	1902.4	1902.4	1904.7
gdb 5660	1908.4[a]	1911.4	1911.4	1913.2	1913.4	1913.4	1914.6
gdb 5661	1854.0[a]	1851.7	1851.7	1855.6	1849.1	1849.1	1851.6
gdb 5662	1851.7[a]	1849.1	1849.0	1852.5	1845.9	1845.8	1848.3
gdb 5663	1850.9[a]	1853.9	1853.9	1858.2	1849.9	1849.9	1853.4
gdb 5664	1857.7[a]	1860.5	1860.5	1864.4	1860.1	1860.1	1861.6
gdb 5665	1857.3[a]	1855.2	1855.2	1859.0	1851.9	1851.8	1854.1
gdb 5666	1850.9[a]	1857.7	1857.7	1860.6	1852.5	1852.5	1855.3
gdb 5667	1858.7[a]	1864.6	1864.6	1868.8	1863.3	1863.2	1864.6
gdb 5668	1914.0[a]	1917.2	1917.2	1919.0	1919.0	1919.0	1919.7
gdb 5669	1902.3[a]	1908.5	1908.5	1909.0	1906.5	1906.5	1908.0
gdb 5670	1857.2[a]	1853.0	1853.0	1856.9	1850.7	1850.6	1853.3
gdb 5671	1851.1[a]	1855.6	1855.6	1859.9	1851.9	1851.9	1855.3
gdb 5672	1858.6[a]	1860.3	1860.3	1864.6	1860.0	1859.9	1861.8
gdb 5673	1855.9[a]	1853.6	1853.5	1856.9	1852.2	1852.2	1853.8
gdb 5674	1895.1[a]	1903.2	1903.2	1905.0	1901.4	1901.4	1903.9
gdb 5675	1890.8[a]	1896.7	1896.4	1897.1	1895.0	1894.9	1898.0
gdb 5676	1899.1[a]	1904.2	1904.1	1904.9	1905.7	1905.7	1907.0
gdb 5677	1854.2[a]	1848.7	1848.6	1852.7	1847.5	1847.5	1850.2
gdb 5678	1857.8[a]	1852.8	1852.8	1852.7	1848.7	1848.6	1846.1
gdb 5679	1857.7[a]	1855.8	1855.8	1858.6	1858.5	1858.5	1858.1
gdb 5680	1847.3[a]	1844.6	1844.6	1846.9	1844.4	1844.4	1845.9
gdb 5681	1855.3[a]	1850.0	1849.9	1850.1	1845.9	1845.9	1844.1
gdb 5682	1846.6[a]	1842.2	1842.2	1845.0	1842.0	1841.9	1844.6
gdb 5683	1857.8[a]	1854.2	1854.2	1857.3	1856.8	1856.7	1857.4
gdb 5684	1894.0[a]	1899.8	1899.8	1899.9	1901.6	1901.6	1901.8
gdb 5685	1853.3[a]	1847.8	1847.8	1848.0	1842.4	1842.4	1840.6
gdb 5686	1853.2[a]	1847.8	1847.7	1847.8	1842.6	1842.6	1840.6
gdb 5687	1843.7[a]	1840.6	1840.6	1843.9	1838.8	1838.7	1841.3
gdb 5688	1845.1[a]	1842.1	1842.1	1844.5	1840.0	1840.0	1842.2
gdb 5689	1831.7[a]	1829.5	1829.4	1831.5	1824.6	1824.5	1828.4
gdb 5690	1856.9[a]	1852.3	1852.2	1855.7	1852.9	1852.8	1853.8
gdb 5691	1827.8[a]	1810.5	1810.5	1809.0	1804.0	1804.0	1799.9
gdb 5692	1815.2[a]	1803.0	1803.0	1803.9	1800.2	1800.2	1800.9
gdb 5693	1827.8[a]	1814.8	1814.8	1816.5	1814.7	1814.6	1813.8
gdb 5694	1839.2[a]	1816.1	1816.1	1818.5	1814.7	1814.7	1813.8
gdb 5695	1893.6[a]	1875.3	1875.2	1876.9	1876.8	1876.8	1879.1
gdb 5696	1878.9[a]	1878.3	1878.3	1877.5	1876.5	1876.5	1874.7
gdb 5697	1868.1[a]	1870.9	1870.9	1872.5	1871.7	1871.7	1874.3
gdb 5698	1878.0[a]	1881.2	1881.2	1883.9	1884.7	1884.7	1885.9
gdb 5699	1847.5[a]	1835.6	1835.6	1831.9	1827.2	1827.2	1821.8
gdb 5700	1836.6[a]	1829.5	1829.5	1828.3	1824.0	1823.9	1823.0
gdb 5701	1829.9[a]	1814.9	1814.9	1817.0	1814.3	1814.2	1816.8
gdb 5702	1846.7[a]	1840.1	1840.1	1840.0	1837.1	1837.1	1834.8
gdb 5703	1844.5[a]	1829.5	1829.5	1832.8	1831.6	1831.5	1832.7
gdb 5704	1852.8[a]	1842.8	1842.7	1842.9	1839.5	1839.4	1836.7
gdb 5705	1880.6[a]	1880.0	1879.9	1879.7	1876.1	1876.1	1874.2
gdb 5706	1894.5[a]	1879.5	1879.4	1880.1	1878.8	1878.8	1880.0
gdb 5707	1873.1[a]	1867.7	1867.7	1869.8	1869.2	1869.2	1870.2
gdb 5708	1878.3[a]	1879.0	1879.0	1878.0	1875.9	1875.8	1873.1
gdb 5709	1870.7[a]	1873.0	1873.0	1874.5	1873.2	1873.2	1875.0
gdb 5710	1881.5[a]	1883.8	1883.8	1886.4	1886.6	1886.6	1887.1
gdb 5711	1862.4[a]	1861.5	1861.4	1863.7	1858.7	1858.7	1862.3
gdb 5712	1875.8[a]	1874.7	1874.6	1877.7	1874.7	1874.7	1876.7
gdb 5713	1881.6[a]	1878.4	1878.3	1877.9	1874.3	1874.3	1872.1
gdb 5714	1893.3[a]	1898.5	1898.5	1898.3	1900.9	1900.8	1900.0
gdb 5715	1850.7[a]	1848.4	1848.4	1848.4	1843.6	1843.6	1841.5
gdb 5716	1850.4[a]	1849.9	1849.9	1850.1	1844.3	1844.3	1842.1
gdb 5717	1841.5[a]	1844.1	1844.1	1846.9	1841.7	1841.7	1843.7

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5718	1851.8[a]	1854.5	1854.4	1858.4	1854.7	1854.6	1855.5
gdb 5719	1852.8[a]	1850.4	1850.4	1849.9	1847.5	1847.5	1844.6
gdb 5720	1830.0[a]	1829.0	1829.0	1832.3	1825.6	1825.6	1828.9
gdb 5721	1841.6[a]	1841.6	1841.6	1845.3	1840.3	1840.1	1843.3
gdb 5722	1849.9[a]	1845.9	1845.9	1845.7	1842.4	1842.3	1840.2
gdb 5723	1870.6[a]	1866.6	1866.6	1865.2	1863.1	1863.0	1860.8
gdb 5724	1869.2[a]	1860.4	1860.4	1862.3	1861.2	1861.2	1862.6
gdb 5725	1867.6[a]	1865.2	1865.2	1866.3	1864.0	1864.0	1866.2
gdb 5726	1876.9[a]	1872.4	1872.4	1873.3	1874.4	1874.4	1874.8
gdb 5727	1874.6[a]	1877.5	1877.5	1875.8	1874.0	1874.0	1870.9
gdb 5728	1875.5[a]	1872.8	1872.8	1874.6	1873.6	1873.5	1873.7
gdb 5729	1869.0[a]	1875.5	1875.5	1876.6	1874.0	1873.9	1875.1
gdb 5730	1881.8[a]	1885.6	1885.6	1887.9	1887.7	1887.7	1887.7
gdb 5731	1871.0[a]	1870.0	1870.0	1868.0	1862.3	1862.3	1861.6
gdb 5732	1873.0[a]	1873.2	1873.2	1875.8	1866.8	1866.8	1870.9
gdb 5733	1880.2[a]	1877.7	1877.7	1875.7	1873.1	1873.1	1870.5
gdb 5734	1877.7[a]	1878.0	1878.0	1880.9	1877.4	1877.4	1878.9
gdb 5735	1784.2[a]	1769.9	1769.9	1772.4	1767.3	1767.3	1769.4
gdb 5736	1796.2[a]	1777.7	1777.7	1781.2	1779.0	1779.0	1779.7
gdb 5737	1804.6[a]	1778.3	1778.3	1784.0	1780.3	1780.3	1783.5
gdb 5738	1853.7[a]	1856.2	1856.2	1859.0	1851.1	1851.1	1855.4
gdb 5739	1865.4[a]	1866.4	1866.4	1869.1	1864.5	1864.5	1867.0
gdb 5740	1866.4[a]	1857.0	1857.0	1859.2	1858.2	1858.2	1860.3
gdb 5741	1864.5[a]	1863.2	1863.2	1865.0	1862.5	1862.5	1865.3
gdb 5742	1873.0[a]	1870.2	1870.2	1873.1	1873.3	1873.3	1874.9
gdb 5743	1896.2[a]	1883.2	1883.2	1885.6	1881.8	1881.8	1884.9
gdb 5744	1875.5[a]	1874.6	1874.6	1877.3	1873.9	1873.9	1876.3
gdb 5745	1871.9[a]	1878.1	1878.1	1880.7	1876.6	1876.5	1879.9
gdb 5746	1879.7[a]	1884.4	1884.4	1888.2	1886.6	1886.6	1888.8
gdb 5747	1858.1[a]	1847.7	1847.7	1850.8	1844.7	1844.7	1847.9
gdb 5748	1855.8[a]	1845.5	1845.5	1847.3	1841.8	1841.8	1845.1
gdb 5749	1863.6[a]	1859.6	1859.6	1861.4	1852.6	1852.6	1856.9
gdb 5750	1866.2[a]	1855.1	1855.1	1858.4	1855.2	1855.2	1857.3
gdb 5751	1868.3[a]	1862.7	1862.7	1866.1	1862.0	1861.9	1864.4
gdb 5752	1849.5[a]	1836.1	1836.1	1839.4	1832.0	1832.0	1833.6
gdb 5753	1845.0[a]	1831.9	1831.9	1833.8	1827.9	1827.9	1830.2
gdb 5754	1859.2[a]	1842.9	1842.9	1847.0	1836.8	1836.8	1842.4
gdb 5755	1853.2[a]	1838.7	1838.7	1840.6	1838.0	1838.0	1838.5
gdb 5756	1863.4[a]	1846.0	1846.0	1852.0	1845.9	1845.9	1849.6
gdb 5757	1842.7[a]	1833.8	1833.8	1834.0	1826.6	1826.5	1825.7
gdb 5758	1837.3[a]	1836.7	1836.7	1836.7	1828.8	1828.8	1828.7
gdb 5759	1845.6[a]	1842.6	1842.6	1842.4	1837.8	1837.8	1836.0
gdb 5760	1856.5[a]	1844.3	1844.3	1848.4	1843.3	1843.3	1845.7
gdb 5761	1884.3[a]	1880.4	1880.4	1883.8	1878.8	1878.8	1881.4
gdb 5762	1896.4[a]	1883.1	1883.1	1885.5	1881.7	1881.6	1884.8
gdb 5763	1878.6[a]	1876.6	1876.6	1879.8	1876.0	1876.0	1879.0
gdb 5764	1872.7[a]	1878.5	1878.5	1881.4	1876.7	1876.6	1880.3
gdb 5765	1879.0[a]	1884.3	1884.3	1888.1	1886.2	1886.2	1888.4
gdb 5766	1870.2[a]	1866.8	1866.8	1865.5	1862.8	1862.8	1860.7
gdb 5767	1868.9[a]	1859.1	1859.1	1860.6	1859.5	1859.5	1861.1
gdb 5768	1869.9[a]	1867.7	1867.6	1868.9	1866.0	1865.9	1868.2
gdb 5769	1875.4[a]	1873.5	1873.5	1875.5	1875.7	1875.6	1876.4
gdb 5770	1883.2[a]	1880.7	1880.7	1881.7	1878.5	1878.5	1878.8
gdb 5771	1881.9[a]	1880.0	1880.0	1882.8	1879.2	1879.2	1881.6
gdb 5772	1883.5[a]	1880.1	1880.0	1882.3	1878.8	1878.8	1882.4
gdb 5773	1890.7[a]	1885.8	1885.8	1887.9	1887.8	1887.8	1889.6
gdb 5774	1886.7[a]	1895.3	1895.3	1896.5	1885.0	1885.0	1888.7
gdb 5775	1879.3[a]	1884.2	1884.2	1885.6	1876.6	1876.6	1880.0
gdb 5776	1885.0[a]	1888.8	1888.8	1890.6	1880.0	1880.0	1885.1
gdb 5777	1888.9[a]	1892.6	1892.6	1894.0	1888.3	1888.3	1889.9
gdb 5778	1889.3[a]	1892.0	1892.0	1895.5	1888.8	1888.8	1891.9
gdb 5779	1895.4[a]	1897.1	1897.1	1894.8	1893.5	1893.5	1890.3
gdb 5780	1891.4[a]	1897.4	1897.4	1899.3	1896.9	1896.9	1898.3
gdb 5781	1888.7[a]	1896.2	1896.2	1896.5	1894.4	1894.4	1895.2
gdb 5782	1900.2[a]	1904.8	1904.8	1905.1	1906.5	1906.5	1905.9

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5783	1871.0[a]	1868.1	1868.1	1867.5	1861.3	1861.2	1860.9
gdb 5784	1872.6[a]	1873.9	1873.9	1875.7	1866.8	1866.8	1871.2
gdb 5785	1883.1[a]	1878.5	1878.4	1877.9	1874.4	1874.4	1872.5
gdb 5786	1877.0[a]	1877.5	1877.5	1879.5	1876.1	1876.1	1878.4
gdb 5787	1856.1[a]	1846.9	1846.9	1848.5	1843.4	1843.4	1846.7
gdb 5788	1867.1[a]	1865.8	1865.8	1867.7	1858.3	1858.3	1862.5
gdb 5789	1865.8[a]	1855.5	1855.5	1858.9	1855.8	1855.8	1858.0
gdb 5790	1870.2[a]	1868.0	1868.0	1871.7	1866.5	1866.5	1868.7
gdb 5791	1885.2[a]	1881.7	1881.6	1885.1	1880.1	1880.0	1882.7
gdb 5792	1854.6[a]	1852.9	1852.9	1854.5	1847.5	1847.5	1850.9
gdb 5793	1864.0[a]	1865.8	1865.8	1867.6	1857.9	1857.9	1862.3
gdb 5794	1863.6[a]	1860.1	1860.1	1861.6	1858.2	1858.2	1859.8
gdb 5795	1868.4[a]	1870.1	1870.1	1873.7	1868.1	1868.1	1870.7
gdb 5796	1856.5[a]	1858.8	1858.8	1861.6	1853.7	1853.6	1857.8
gdb 5797	1865.2[a]	1866.5	1866.5	1868.9	1864.4	1864.3	1866.6
gdb 5798	1867.0[a]	1863.3	1863.3	1866.0	1862.0	1862.0	1863.6
gdb 5799	1913.3[a]	1915.7	1915.7	1917.5	1917.5	1917.5	1918.2
gdb 5800	1901.7[a]	1907.1	1907.1	1907.5	1904.9	1904.9	1906.4
gdb 5801	1895.5[a]	1900.1	1900.1	1900.5	1898.7	1898.7	1901.0
gdb 5802	1903.7[a]	1905.6	1905.6	1905.9	1907.4	1907.3	1908.0
gdb 5803	1851.1[a]	1848.8	1848.8	1850.3	1843.8	1843.7	1847.2
gdb 5804	1863.5[a]	1859.9	1859.9	1862.2	1858.1	1858.1	1859.8
gdb 5805	1919.2[a]	1915.2	1915.2	1915.6	1912.1	1912.1	1914.9
gdb 5806	1902.2[a]	1906.2	1906.2	1906.7	1904.0	1904.0	1906.3
gdb 5807	1911.2[a]	1913.0	1913.0	1913.6	1914.1	1914.0	1914.7
gdb 5808	1869.6[a]	1869.7	1869.7	1868.1	1861.5	1861.5	1860.7
gdb 5809	1880.6[a]	1878.2	1878.2	1876.6	1873.6	1873.6	1871.2
gdb 5810	1890.4[a]	1898.4	1898.3	1899.7	1896.7	1896.7	1900.0
gdb 5811	1899.5[a]	1904.7	1904.7	1905.7	1906.4	1906.4	1908.0
gdb 5812	1869.7[a]	1867.4	1867.4	1865.4	1860.0	1860.0	1859.2
gdb 5813	1881.8[a]	1877.9	1877.9	1877.3	1873.8	1873.8	1871.8
gdb 5814	1897.9[a]	1902.6	1902.6	1903.1	1900.8	1900.8	1902.7
gdb 5815	1908.2[a]	1912.6	1912.6	1912.8	1914.1	1914.0	1914.4
gdb 5816	1913.3[a]	1924.2	1924.2	1923.8	1927.2	1927.2	1926.6
gdb 5817	1915.3[a]	1910.4	1910.3	1911.6	1907.3	1907.2	1910.5
gdb 5818	1902.2[a]	1906.6	1906.6	1907.6	1904.2	1904.1	1906.4
gdb 5819	1898.0[a]	1901.6	1901.6	1903.2	1899.6	1899.6	1901.8
gdb 5820	1909.1[a]	1910.5	1910.5	1911.3	1911.6	1911.5	1912.0
gdb 5821	1864.1[a]	1874.1	1874.1	1877.1	1864.4	1864.3	1868.4
gdb 5822	1866.2[a]	1875.0	1874.9	1878.4	1865.7	1865.6	1869.9
gdb 5823	1866.8[a]	1871.2	1871.2	1873.1	1863.2	1863.2	1867.4
gdb 5824	1866.1[a]	1873.4	1873.3	1873.6	1864.7	1864.7	1867.7
gdb 5825	1856.2[a]	1863.8	1863.7	1866.2	1857.5	1857.5	1861.1
gdb 5826	1869.9[a]	1873.1	1873.1	1876.5	1870.8	1870.6	1873.1
gdb 5827	1869.5[a]	1875.0	1874.9	1878.1	1872.1	1872.1	1874.0
gdb 5828	1865.9[a]	1871.4	1871.4	1873.9	1868.2	1868.1	1870.3
gdb 5829	1897.2[a]	1902.1	1902.1	1903.5	1900.5	1900.5	1902.8
gdb 5830	1894.3[a]	1898.1	1898.1	1898.4	1896.5	1896.5	1898.8
gdb 5831	1902.9[a]	1905.4	1905.4	1907.1	1907.5	1907.5	1908.6
gdb 5832	1854.6[a]	1852.1	1852.1	1855.9	1848.7	1848.6	1851.4
gdb 5833	1852.5[a]	1851.7	1851.7	1855.5	1848.1	1848.1	1850.8
gdb 5834	1853.8[a]	1855.0	1855.0	1858.2	1850.2	1850.2	1852.2
gdb 5835	1850.0[a]	1856.2	1856.2	1859.3	1850.9	1850.9	1853.4
gdb 5836	1844.9[a]	1845.3	1845.3	1847.9	1837.4	1837.4	1841.1
gdb 5837	1857.9[a]	1864.1	1864.1	1866.9	1861.9	1861.8	1862.6
gdb 5838	1855.5[a]	1852.3	1852.3	1855.6	1851.3	1851.3	1853.0
gdb 5839	1851.7[a]	1850.2	1850.1	1853.4	1848.7	1848.7	1850.7
gdb 5840	1844.0[a]	1843.7	1843.7	1845.9	1838.3	1838.2	1841.3
gdb 5841	1843.5[a]	1840.3	1840.3	1843.5	1834.5	1834.4	1839.0
gdb 5842	1850.8[a]	1845.8	1845.8	1848.4	1844.2	1844.2	1846.7
gdb 5843	1851.7[a]	1846.9	1846.9	1851.1	1844.7	1844.6	1848.0
gdb 5844	1894.8[a]	1903.0	1903.0	1904.5	1901.5	1901.5	1903.8
gdb 5845	1894.0[a]	1899.1	1899.1	1899.8	1897.2	1897.1	1899.7
gdb 5846	1900.7[a]	1906.4	1906.4	1908.1	1908.5	1908.4	1909.6
gdb 5847	1902.1[a]	1906.8	1906.8	1907.7	1904.1	1904.1	1906.1

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5848	1900.7[a]	1904.1	1904.1	1904.5	1901.2	1901.2	1902.7
gdb 5849	1910.1[a]	1912.6	1912.6	1914.5	1913.9	1913.9	1914.8
gdb 5850	1878.9[a]	1878.6	1878.6	1879.3	1870.9	1870.9	1875.6
gdb 5851	1884.8[a]	1883.1	1883.1	1885.6	1881.3	1881.2	1884.1
gdb 5852	1865.3[a]	1873.2	1873.2	1875.4	1863.6	1863.5	1867.5
gdb 5853	1856.6[a]	1865.0	1865.0	1867.3	1858.0	1858.0	1861.6
gdb 5854	1857.2[a]	1862.7	1862.6	1865.1	1856.5	1856.5	1860.5
gdb 5855	1866.5[a]	1872.1	1872.1	1873.9	1863.7	1863.6	1867.8
gdb 5856	1865.8[a]	1871.3	1871.3	1873.6	1868.0	1868.0	1870.0
gdb 5857	1866.6[a]	1869.6	1869.6	1873.4	1867.3	1867.2	1870.2
gdb 5858	1869.7[a]	1873.3	1873.0	1876.7	1870.7	1870.7	1873.2
gdb 5859	1876.0[a]	1882.8	1882.8	1883.1	1884.3	1884.2	1883.0
gdb 5860	1862.2[a]	1870.0	1869.9	1870.0	1868.5	1868.4	1869.2
gdb 5861	1874.1[a]	1881.3	1881.3	1883.2	1883.2	1883.2	1882.9
gdb 5862	1884.1[a]	1879.8	1879.8	1881.6	1878.5	1878.5	1880.2
gdb 5863	1872.7[a]	1878.0	1878.0	1878.4	1879.8	1879.8	1879.7
gdb 5864	1870.4[a]	1877.7	1877.7	1879.9	1879.7	1879.7	1880.6
gdb 5865	1859.9[a]	1866.4	1866.4	1866.6	1865.1	1865.1	1866.8
gdb 5866	1852.3[a]	1849.0	1848.8	1848.7	1845.7	1845.6	1842.6
gdb 5867	1839.8[a]	1837.6	1837.6	1835.2	1830.7	1830.7	1828.8
gdb 5868	1842.0[a]	1842.5	1842.5	1843.4	1841.2	1841.2	1841.8
gdb 5869	1854.6[a]	1853.7	1853.7	1856.4	1856.4	1856.4	1855.8
gdb 5870	1852.1[a]	1848.4	1848.4	1848.0	1845.7	1845.7	1842.8
gdb 5871	1841.8[a]	1841.1	1841.1	1842.7	1840.9	1840.8	1841.7
gdb 5872	1839.5[a]	1837.1	1837.1	1834.9	1830.8	1830.8	1829.1
gdb 5873	1854.1[a]	1852.2	1852.2	1855.0	1855.6	1855.6	1855.3
gdb 5874	1836.2[a]	1836.6	1836.6	1838.0	1831.9	1831.9	1834.6
gdb 5875	1836.2[a]	1835.4	1835.4	1837.3	1830.8	1830.8	1834.4
gdb 5876	1848.9[a]	1848.1	1848.1	1851.2	1846.9	1846.9	1848.4
gdb 5877	1848.8[a]	1846.7	1846.7	1850.0	1845.8	1845.8	1848.3
gdb 5878	1878.1[a]	1883.6	1883.4	1885.5	1886.8	1886.7	1887.6
gdb 5879	1865.8[a]	1872.7	1872.7	1873.0	1872.3	1872.3	1873.6
gdb 5880	1836.6[a]	1835.6	1835.6	1833.2	1829.7	1829.7	1827.9
gdb 5881	1849.2[a]	1846.9	1846.9	1846.2	1844.6	1844.6	1841.6
gdb 5882	1882.0[a]	1878.3	1878.3	1879.0	1877.1	1877.0	1878.6
gdb 5883	1858.4[a]	1863.7	1863.7	1863.9	1864.2	1864.2	1866.1
gdb 5884	1870.9[a]	1874.9	1874.9	1876.8	1879.0	1879.0	1879.8
gdb 5885	1874.7[a]	1882.0	1881.6	1883.4	1883.9	1883.8	1883.5
gdb 5886	1863.3[a]	1870.6	1870.6	1871.4	1869.3	1869.3	1870.2
gdb 5887	1872.8[a]	1881.2	1881.2	1882.6	1882.8	1882.8	1882.3
gdb 5888	1886.5[a]	1883.4	1883.4	1885.3	1881.9	1881.9	1883.4
gdb 5889	1874.9[a]	1880.8	1880.7	1883.2	1881.7	1881.7	1882.7
gdb 5890	1871.9[a]	1880.6	1880.5	1883.0	1880.4	1880.4	1880.9
gdb 5891	1887.0[a]	1885.2	1885.2	1886.8	1882.0	1882.0	1884.9
gdb 5892	1864.5[a]	1870.7	1870.6	1871.4	1867.6	1867.5	1869.7
gdb 5893	1877.9[a]	1883.1	1883.1	1885.1	1886.3	1886.3	1886.5
gdb 5894	1889.8[a]	1887.4	1887.3	1888.7	1886.5	1886.5	1889.2
gdb 5895	1866.9[a]	1872.9	1872.8	1873.2	1871.9	1871.8	1873.3
gdb 5896	1884.2[a]	1882.7	1882.7	1883.8	1880.3	1880.3	1882.8
gdb 5897	1888.8[a]	1884.8	1884.8	1886.3	1882.9	1882.8	1885.6
gdb 5898	1863.3[a]	1869.3	1869.3	1870.1	1867.3	1867.3	1869.4
gdb 5899	1875.2[a]	1878.5	1878.5	1880.6	1881.0	1880.9	1881.6
gdb 5900	1875.5[a]	1880.7	1880.7	1883.3	1882.0	1882.0	1883.0
gdb 5901	1866.3[a]	1876.0	1873.5	1873.9	1870.7	1870.7	1872.4
gdb 5902	1866.4[a]	1871.6	1871.6	1872.5	1868.9	1868.9	1871.4
gdb 5903	1839.0[a]	1839.3	1839.3	1837.3	1830.8	1830.8	1829.5
gdb 5904	1837.9[a]	1836.1	1836.1	1834.3	1827.7	1827.6	1827.0
gdb 5905	1847.9[a]	1845.1	1845.1	1843.7	1840.3	1840.3	1837.9
gdb 5906	1870.5[a]	1875.6	1875.6	1876.8	1874.9	1874.9	1876.2
gdb 5907	1870.9[a]	1879.2	1879.2	1881.0	1878.1	1878.1	1879.0
gdb 5908	1863.8[a]	1872.6	1872.6	1873.4	1868.1	1868.1	1870.4
gdb 5909	1861.6[a]	1867.0	1867.0	1867.9	1863.0	1862.9	1866.0
gdb 5910	1870.2[a]	1875.4	1875.4	1877.5	1877.9	1877.9	1878.6
gdb 5911	1869.4[a]	1877.5	1877.5	1879.6	1879.2	1879.2	1879.5
gdb 5912	1863.7[a]	1871.7	1871.7	1871.4	1869.8	1869.8	1871.1

... *continued on next page* ...

Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5913	1860.8[a]	1866.7	1866.7	1867.1	1865.3	1865.3	1867.2
gdb 5914	1872.0[a]	1877.7	1877.6	1880.6	1878.3	1878.2	1879.7
gdb 5915	1872.1[a]	1879.4	1879.4	1881.0	1879.3	1879.3	1879.6
gdb 5916	1866.5[a]	1873.1	1873.1	1873.8	1869.7	1869.7	1871.7
gdb 5917	1863.4[a]	1869.3	1869.3	1870.5	1866.2	1866.1	1868.6
gdb 5918	1872.2[a]	1877.0	1877.0	1879.9	1879.6	1879.6	1881.2
gdb 5919	1863.5[a]	1872.1	1869.5	1869.5	1868.3	1868.3	1869.7
gdb 5920	1863.7[a]	1868.1	1868.1	1868.7	1867.0	1867.0	1869.2
gdb 5921	1861.3[a]	1866.5	1866.5	1867.2	1864.6	1864.6	1867.3
gdb 5922	1860.9[a]	1864.5	1864.5	1865.5	1862.7	1862.7	1865.7
gdb 5923	1869.3[a]	1871.9	1871.9	1873.5	1873.6	1873.6	1875.3
gdb 5924	1881.4[a]	1878.5	1878.5	1879.7	1875.4	1875.4	1878.8
gdb 5925	1862.4[a]	1869.3	1869.3	1869.8	1867.1	1867.1	1869.8
gdb 5926	1859.2[a]	1863.3	1863.3	1864.3	1861.8	1861.8	1865.2
gdb 5927	1870.3[a]	1872.3	1872.2	1875.1	1874.6	1874.5	1876.7
gdb 5928	1852.5[a]	1846.9	1846.8	1847.3	1842.6	1842.5	1841.3
gdb 5929	1843.3[a]	1837.8	1837.8	1836.4	1829.5	1829.4	1829.0
gdb 5930	1847.0[a]	1843.1	1843.1	1845.0	1840.7	1840.7	1842.6
gdb 5931	1856.2[a]	1851.3	1851.3	1854.8	1853.2	1853.2	1854.2
gdb 5932	1841.6[a]	1837.1	1837.1	1835.2	1829.0	1829.0	1828.2
gdb 5933	1850.1[a]	1845.1	1845.1	1845.3	1841.4	1841.3	1839.8
gdb 5934	1852.7[a]	1848.9	1848.9	1848.5	1845.5	1845.4	1842.7
gdb 5935	1841.4[a]	1837.0	1837.0	1834.8	1830.0	1830.0	1828.5
gdb 5936	1853.1[a]	1847.2	1847.2	1846.1	1842.4	1842.4	1840.2
gdb 5937	1845.5[a]	1841.1	1841.1	1844.1	1839.9	1839.8	1842.1
gdb 5938	1845.4[a]	1842.0	1842.0	1843.6	1839.8	1839.8	1841.8
gdb 5939	1842.6[a]	1838.3	1838.3	1836.8	1829.9	1829.9	1829.2
gdb 5940	1858.3[a]	1852.6	1852.6	1855.0	1853.7	1853.7	1854.1
gdb 5941	1841.7[a]	1843.1	1843.1	1845.2	1835.3	1835.3	1838.9
gdb 5942	1839.3[a]	1839.7	1839.6	1843.0	1832.5	1832.4	1836.5
gdb 5943	1839.1[a]	1836.6	1836.6	1838.5	1829.7	1829.7	1833.9
gdb 5944	1850.6[a]	1849.5	1849.5	1853.3	1846.2	1846.2	1848.8
gdb 5945	1848.6[a]	1846.3	1846.3	1848.6	1842.8	1842.8	1845.3
gdb 5946	1834.1[a]	1818.7	1818.7	1820.4	1816.4	1816.3	1818.7
gdb 5947	1832.8[a]	1816.8	1816.7	1817.8	1814.3	1814.3	1817.0
gdb 5948	1842.6[a]	1826.4	1826.4	1828.0	1827.1	1827.1	1828.1
gdb 5949	1855.8[a]	1844.5	1844.5	1845.0	1844.0	1844.0	1842.4
gdb 5950	1863.0[a]	1844.2	1844.2	1847.0	1845.2	1845.2	1848.0
gdb 5951	1858.0[a]	1840.4	1840.4	1842.6	1841.6	1841.6	1844.5
gdb 5952	1867.6[a]	1849.6	1849.6	1853.7	1854.5	1854.5	1856.5
gdb 5953	1849.2[a]	1848.2	1848.2	1848.5	1841.2	1841.2	1842.8
gdb 5954	1859.9[a]	1858.0	1858.0	1860.2	1855.2	1855.2	1856.3
gdb 5955	1874.1[a]	1868.6	1868.6	1867.3	1866.6	1866.6	1864.1
gdb 5956	1889.6[a]	1866.9	1866.9	1868.3	1868.4	1868.4	1870.2
gdb 5957	1872.2[a]	1866.6	1866.6	1868.0	1867.9	1867.9	1869.9
gdb 5958	1870.6[a]	1864.7	1864.7	1865.3	1865.7	1865.7	1867.6
gdb 5959	1880.1[a]	1874.4	1874.4	1877.0	1878.3	1878.3	1879.2
gdb 5960	1827.7[a]	1817.9	1817.9	1813.4	1809.5	1809.5	1803.5
gdb 5961	1826.1[a]	1818.6	1818.6	1816.7	1813.2	1813.1	1811.4
gdb 5962	1825.0[a]	1817.1	1817.1	1814.7	1810.7	1810.7	1809.1
gdb 5963	1825.8[a]	1818.4	1818.4	1816.0	1811.9	1811.8	1809.8
gdb 5964	1833.8[a]	1826.0	1826.0	1825.5	1823.5	1823.4	1820.7
gdb 5965	1836.8[a]	1828.6	1828.6	1826.8	1825.5	1825.5	1821.9
gdb 5966	1870.4[a]	1866.3	1866.2	1864.0	1858.6	1858.6	1858.1
gdb 5967	1880.7[a]	1876.1	1876.1	1875.7	1872.5	1872.4	1870.9
gdb 5968	1887.1[a]	1865.5	1865.5	1866.6	1866.7	1866.7	1868.3
gdb 5969	1874.6[a]	1869.3	1869.3	1867.8	1867.0	1866.9	1864.2
gdb 5970	1872.1[a]	1867.0	1867.0	1868.1	1867.8	1867.8	1869.3
gdb 5971	1870.6[a]	1866.3	1866.3	1867.0	1866.1	1866.1	1867.8
gdb 5972	1880.8[a]	1875.1	1875.1	1877.6	1878.7	1878.7	1879.4
gdb 5973	1869.5[a]	1866.9	1866.9	1864.4	1859.2	1859.2	1858.5
gdb 5974	1880.3[a]	1876.2	1876.2	1874.2	1871.9	1871.9	1869.7
gdb 5975	1834.9[a]	1819.7	1819.7	1821.2	1816.5	1816.5	1818.8
gdb 5976	1845.4[a]	1829.9	1829.9	1833.1	1830.7	1830.7	1832.2
gdb 5977	1820.3[a]	1800.6	1800.6	1803.1	1797.1	1797.1	1796.7

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 5978	1825.1[a]	1801.9	1801.9	1805.0	1798.9	1798.8	1801.2
gdb 5979	1819.2[a]	1796.1	1796.1	1798.4	1793.6	1793.6	1796.1
gdb 5980	1819.9[a]	1796.7	1796.7	1799.5	1794.1	1794.0	1797.1
gdb 5981	1829.2[a]	1806.2	1806.2	1809.1	1807.0	1807.0	1808.1
gdb 5982	1831.4[a]	1807.3	1807.3	1811.8	1808.8	1808.8	1810.4
gdb 5983	1834.6[a]	1817.3	1817.3	1819.5	1815.6	1815.6	1818.5
gdb 5984	1832.5[a]	1817.2	1817.2	1818.8	1814.4	1814.4	1817.3
gdb 5985	1833.5[a]	1817.8	1817.8	1819.5	1815.2	1815.2	1817.9
gdb 5986	1842.1[a]	1825.7	1825.6	1829.1	1826.8	1826.8	1828.7
gdb 5987	1844.9[a]	1827.7	1827.7	1831.2	1829.1	1829.0	1830.8
gdb 5988	1920.4[a]	1915.0	1915.0	1915.9	1913.8	1913.7	1916.0
gdb 5989	1900.5[a]	1905.3	1905.3	1905.2	1904.2	1904.2	1905.9
gdb 5990	1910.3[a]	1914.1	1914.1	1915.7	1916.6	1916.6	1917.2
gdb 5991	1847.3[a]	1847.5	1847.5	1847.6	1841.4	1841.4	1843.3
gdb 5992	1857.7[a]	1857.0	1857.0	1857.4	1854.2	1854.2	1854.4
gdb 5993	1869.4[a]	1867.3	1867.3	1864.8	1860.1	1860.1	1859.4
gdb 5994	1879.0[a]	1876.6	1876.6	1875.7	1873.1	1873.1	1871.2
gdb 5995	1896.6[a]	1904.7	1904.7	1904.7	1903.9	1903.9	1906.1
gdb 5996	1906.5[a]	1913.9	1913.9	1914.1	1916.4	1916.4	1916.8
gdb 5997	1868.7[a]	1867.3	1867.3	1864.7	1859.8	1859.8	1858.8
gdb 5998	1879.4[a]	1877.0	1877.0	1874.7	1873.0	1872.9	1870.3
gdb 5999	1920.9[a]	1914.6	1914.6	1915.6	1913.0	1913.0	1915.1
gdb 6000	1901.0[a]	1905.0	1905.0	1904.8	1903.9	1903.9	1905.4
gdb 6001	1910.6[a]	1913.4	1913.4	1915.1	1915.8	1915.8	1916.3
gdb 6002	1845.0[a]	1840.2	1840.2	1842.8	1839.5	1839.5	1841.4
gdb 6003	1843.1[a]	1839.3	1839.3	1840.9	1838.4	1838.4	1840.4
gdb 6004	1853.4[a]	1848.5	1848.5	1851.9	1851.3	1851.3	1852.2
gdb 6005	1837.2[a]	1818.8	1818.8	1822.9	1816.0	1815.9	1818.9
gdb 6006	1831.4[a]	1816.2	1816.2	1818.2	1813.5	1813.4	1816.8
gdb 6007	1840.6[a]	1825.0	1825.0	1827.4	1825.7	1825.7	1827.3
gdb 6008	1821.8[a]	1797.7	1797.7	1800.6	1795.5	1795.5	1798.6
gdb 6009	1816.8[a]	1793.6	1793.6	1796.5	1791.5	1791.4	1794.7
gdb 6010	1825.8[a]	1802.2	1802.2	1807.0	1804.0	1804.0	1806.2
gdb 6011	1824.0[a]	1817.5	1817.5	1815.5	1811.9	1811.9	1810.3
gdb 6012	1822.4[a]	1815.0	1815.0	1813.1	1808.8	1808.8	1807.5
gdb 6013	1832.1[a]	1824.7	1824.7	1824.7	1822.4	1822.4	1820.1
gdb 6014	1885.7[a]	1863.3	1863.3	1865.0	1864.8	1864.8	1867.1
gdb 6015	1871.0[a]	1865.9	1865.9	1867.0	1866.7	1866.7	1868.7
gdb 6016	1869.0[a]	1863.8	1863.8	1865.1	1864.0	1864.0	1866.2
gdb 6017	1878.3[a]	1872.8	1872.8	1875.9	1877.0	1877.0	1878.2
gdb 6018	1850.8[a]	1839.1	1839.1	1839.9	1839.0	1839.0	1838.0
gdb 6019	1861.8[a]	1842.6	1842.6	1845.6	1844.0	1844.0	1847.7
gdb 6020	1856.5[a]	1838.6	1838.6	1841.5	1840.0	1839.9	1843.5
gdb 6021	1865.8[a]	1847.1	1847.1	1851.9	1852.5	1852.5	1855.0
gdb 6022	1850.2[a]	1849.0	1849.0	1849.3	1841.7	1841.7	1843.9
gdb 6023	1846.6[a]	1846.0	1846.0	1846.5	1839.6	1839.6	1842.2
gdb 6024	1855.5[a]	1854.4	1854.4	1855.3	1851.3	1851.3	1852.1
gdb 6025	1869.7[a]	1866.6	1866.6	1865.5	1864.0	1864.0	1861.6
gdb 6026	1871.6[a]	1869.6	1869.6	1870.3	1868.8	1868.7	1870.1
gdb 6027	1869.4[a]	1865.9	1865.9	1867.0	1865.4	1865.4	1867.3
gdb 6028	1878.5[a]	1874.9	1874.9	1877.8	1878.3	1878.2	1879.0
gdb 6029	1867.9[a]	1865.6	1865.6	1863.0	1857.6	1857.6	1856.7
gdb 6030	1868.3[a]	1865.7	1865.7	1863.5	1857.7	1857.7	1857.4
gdb 6031	1876.4[a]	1873.4	1873.4	1873.0	1869.6	1869.6	1868.2
gdb 6032	1895.8[a]	1904.2	1904.2	1904.0	1902.5	1902.5	1904.3
gdb 6033	1895.4[a]	1903.0	1903.0	1903.3	1901.5	1901.5	1904.0
gdb 6034	1904.2[a]	1911.6	1911.5	1912.4	1913.3	1913.3	1914.2
gdb 6035	1920.4[a]	1914.3	1914.3	1915.5	1912.5	1912.5	1915.2
gdb 6036	1901.8[a]	1905.8	1905.8	1905.8	1904.3	1904.3	1906.3
gdb 6037	1899.2[a]	1902.5	1902.5	1902.8	1900.9	1900.9	1903.3
gdb 6038	1907.5[a]	1910.1	1910.1	1912.2	1912.6	1912.6	1914.0
gdb 6039	1840.4[a]	1838.9	1838.8	1841.1	1832.7	1832.6	1836.3
gdb 6040	1850.3[a]	1848.1	1848.0	1852.1	1846.1	1846.0	1848.8
gdb 6041	1853.1[a]	1847.2	1847.2	1847.5	1843.2	1843.2	1841.6
gdb 6042	1844.4[a]	1841.2	1841.2	1843.0	1840.2	1840.2	1842.0

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Table S73: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
gdb 6043	1844.6[a]	1841.8	1841.8	1843.4	1839.9	1839.9	1841.7
gdb 6044	1842.5[a]	1837.7	1837.7	1836.4	1829.6	1829.6	1829.1
gdb 6045	1856.5[a]	1852.0	1852.0	1854.5	1853.4	1853.4	1853.6
gdb 6046	1852.2[a]	1848.1	1848.1	1847.9	1845.7	1845.7	1843.0
gdb 6047	1841.6[a]	1838.6	1838.6	1836.6	1831.9	1831.9	1830.3
gdb 6048	1840.2[a]	1836.2	1836.2	1834.7	1829.0	1829.0	1828.3
gdb 6049	1850.8[a]	1846.0	1846.0	1844.7	1842.4	1842.4	1839.9
gdb 6050	1899.6[a]	1905.6	1905.6	1905.6	1903.6	1903.6	1905.1
gdb 6051	1899.6[a]	1902.9	1902.9	1903.3	1901.2	1901.2	1903.5
gdb 6052	1907.4[a]	1910.9	1910.9	1913.1	1912.9	1912.9	1914.1
gdb 6053	1842.4[a]	1841.5	1841.5	1843.4	1835.2	1835.1	1838.6
gdb 6054	1838.3[a]	1836.5	1836.5	1838.6	1830.5	1830.5	1834.6
gdb 6055	1840.3[a]	1837.7	1837.7	1839.9	1831.7	1831.7	1835.6
gdb 6056	1847.7[a]	1845.5	1845.5	1847.9	1843.0	1842.9	1845.3
gdb 6057	1851.0[a]	1847.5	1847.4	1849.9	1845.1	1845.1	1847.4
gdb 6058	1875.7[a]	1882.0	1882.0	1883.9	1884.9	1884.9	1884.6
gdb 6059	1866.5[a]	1873.8	1873.8	1873.2	1872.8	1872.8	1873.3
gdb 6060	1867.4[a]	1874.1	1874.1	1874.3	1873.0	1873.0	1873.7
gdb 6061	1837.5[a]	1836.2	1836.2	1833.0	1829.8	1829.7	1827.5
gdb 6062	1838.3[a]	1836.6	1836.6	1834.1	1830.0	1829.9	1828.0
gdb 6063	1846.8[a]	1844.5	1844.5	1842.3	1841.5	1841.5	1837.9
gdb 6064	1861.4[a]	1866.9	1866.9	1866.3	1867.0	1866.9	1868.4
gdb 6065	1862.1[a]	1866.9	1866.9	1867.1	1867.0	1867.0	1868.8
gdb 6066	1870.5[a]	1874.9	1874.9	1876.8	1879.0	1879.0	1879.8
gdb 6067	1876.1[a]	1881.8	1881.7	1882.3	1883.8	1883.8	1883.1
gdb 6068	1886.9[a]	1883.2	1883.2	1883.8	1881.7	1881.7	1883.7
gdb 6069	1866.9[a]	1873.4	1873.3	1873.1	1872.3	1872.2	1873.1
gdb 6070	1866.5[a]	1873.3	1873.3	1873.6	1872.0	1872.0	1873.0
gdb 6071	1885.4[a]	1882.3	1882.3	1883.8	1880.4	1880.4	1882.9
gdb 6072	1865.5[a]	1870.4	1870.4	1870.4	1869.3	1869.3	1871.1
gdb 6073	1865.1[a]	1869.9	1869.9	1870.6	1868.7	1868.7	1870.9
gdb 6074	1871.9[a]	1878.0	1878.0	1880.6	1880.7	1880.2	1881.5
gdb 6075	1858.9[a]	1866.8	1866.8	1867.1	1863.8	1863.8	1866.1
gdb 6076	1862.1[a]	1866.1	1866.1	1866.3	1864.0	1864.0	1866.7
gdb 6077	1859.0[a]	1863.8	1863.8	1864.8	1861.8	1861.8	1864.9
gdb 6078	1868.2[a]	1871.7	1871.7	1873.0	1873.1	1873.1	1874.5
gdb 6079	1840.1[a]	1837.5	1837.5	1834.9	1829.0	1829.0	1827.6
gdb 6080	1839.3[a]	1835.4	1835.4	1833.6	1827.5	1827.5	1826.7
gdb 6081	1848.3[a]	1843.4	1843.4	1843.4	1839.4	1839.4	1837.6
gdb 6082	1845.8[a]	1843.1	1843.0	1845.1	1841.4	1841.4	1843.1
gdb 6083	1839.9[a]	1836.3	1836.3	1833.9	1828.6	1828.6	1827.5
gdb 6084	1838.7[a]	1834.6	1834.6	1833.0	1827.5	1827.5	1826.8
gdb 6085	1847.5[a]	1842.5	1842.5	1842.6	1839.4	1839.4	1837.6
gdb 6086	1845.2[a]	1842.1	1842.1	1843.8	1841.2	1841.2	1842.8
gdb 6087	1858.3[a]	1864.7	1864.7	1864.1	1864.1	1864.1	1865.3
gdb 6088	1862.8[a]	1868.0	1868.0	1867.4	1867.4	1867.4	1868.5
gdb 6089	1859.3[a]	1864.5	1864.4	1865.2	1864.1	1864.1	1866.4
gdb 6090	1868.9[a]	1873.2	1873.2	1874.3	1876.3	1876.3	1876.2
gdb 6091	1880.8[a]	1876.0	1875.9	1878.0	1873.9	1873.9	1876.7
gdb 6092	1860.6[a]	1867.2	1867.2	1867.4	1865.1	1865.1	1866.9
gdb 6093	1864.7[a]	1870.3	1870.3	1870.4	1868.5	1868.5	1870.0
gdb 6094	1861.2[a]	1867.1	1867.1	1867.8	1865.2	1865.1	1867.1
gdb 6095	1870.1[a]	1875.3	1875.3	1877.8	1877.3	1877.3	1878.2

a R.Ramakrishnan, P.O.Dral, M.Rupp, O.A. von Lilienfeld, Sci.Data 1, 140022 (2014)

Table S74: Benchmark Results for the A24-CHNOF Set. Interaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Single point calculations							
Dimer water-ammonia	−6.5[a]	−4.5	−5.0	−4.5	−5.4	−6.0	−6.4
Dimer water-water	−5.0[a]	−4.0	−4.3	−4.5	−4.1	−4.6	−4.3
Dimer HCN-HCN	−4.7[a]	−3.4	−3.8	−4.4	−3.8	−4.3	−4.8
Dimer HF-HF	−4.6[a]	−1.2	−1.4	−2.2	0.5	0.2	0.4
Dimer ammonia-ammonia	−3.2[a]	−2.0	−2.5	−2.6	−1.9	−2.6	−2.7
Dimer HF-methane	−1.7[a]	−0.6	−1.0	−1.0	0.1	−0.6	−0.2
Dimer ammonia-methane	−0.8[a]	−0.5	−0.8	−0.8	−0.5	−0.8	−0.8
Dimer water-methane	−0.7[a]	−0.4	−0.6	−0.7	−0.4	−0.7	−0.7
Dimer formaldehyde-formaldehyde	−4.5[a]	−3.2	−4.1	−4.5	−2.3	−3.5	−3.4
Dimer water-ethene	−2.6[a]	−1.7	−2.4	−2.3	−1.2	−2.0	−1.8
Dimer formaldehyde-ethene	−1.6[a]	−0.7	−1.5	−1.5	−0.4	−1.4	−1.3
Dimer ethyne-ethyne	−1.5[a]	−1.2	−1.7	−1.6	−0.7	−1.3	−1.2
Dimer ammonia-ethene	−1.4[a]	−0.7	−1.3	−1.3	−0.4	−1.2	−1.2
Dimer ethene-ethene	−1.1[a]	−0.2	−1.1	−1.1	−0.0	−1.1	−1.1
Dimer methane-ethene	−0.5[a]	−0.1	−0.6	−0.6	−0.1	−0.6	−0.6
Dimer methane-ethane	−0.8[a]	0.1	−0.8	−0.8	0.3	−0.8	−0.7
Dimer methane-ethane	−0.6[a]	0.1	−0.6	−0.6	0.2	−0.6	−0.6
Dimer methane-methane	−0.5[a]	0.1	−0.5	−0.5	0.2	−0.5	−0.5
Dimer ethene-ethyne	0.8[a]	0.6	−0.2	−0.3	0.5	−0.5	−0.5
Dimer ethene-ethene	0.9[a]	0.7	−0.3	−0.4	0.6	−0.6	−0.7
Dimer ethyne-ethyne	1.1[a]	1.0	0.3	0.1	0.8	−0.1	−0.2
Full optimizations of dimers and monomers							
Dimer water-ammonia	−6.5[a]	−4.9	−5.5	−4.6	−6.9	−7.8	−9.1
Dimer water-water	−5.0[a]	−4.3	−4.7	−5.1	−4.5	−5.1	−4.6
Dimer HCN-HCN	−4.7[a]	−3.5	−4.0	−4.5	−4.5	−5.2	−6.4
Dimer HF-HF	−4.6[a]	−2.2	−2.4	−2.6	−1.6	−1.9	−1.9
Dimer ammonia-ammonia	−3.2[a]	−2.0	−2.5	−2.5	−1.9	−2.5	−2.7
Dimer HF-methane	−1.7[a]	−0.7	−1.1	−1.0	−0.3	−0.7	−0.6
Dimer ammonia-methane	−0.8[a]	−0.6	−1.0	−0.9	−0.6	−1.1	−1.2
Dimer water-methane	−0.7[a]	−0.6	−1.0	−1.1	−0.4	−0.8	−0.8
Dimer formaldehyde-formaldehyde	−4.5[a]	−3.8	−4.8	−5.3	−2.7	−3.9	−3.8
Dimer water-ethene	−2.6[a]	−2.4	−3.3	−3.2	−1.4	−2.5	−2.2
Dimer formaldehyde-ethene	−1.6[a]	−1.2	−2.1	−2.0	−0.6	−2.4	−2.2
Dimer ethyne-ethyne	−1.5[a]	−1.9	−2.6	−2.4	−0.8	−1.7	−1.3
Dimer ammonia-ethene	−1.4[a]	−1.0	−1.8	−1.9	−0.6	−1.7	−1.6
Dimer ethene-ethene	−1.1[a]	−0.3	−1.5	−1.3	−0.1	−1.2	−1.1
Dimer methane-ethene	−0.5[a]	−0.3	−1.0	−1.0	−0.1	−0.8	−0.7
Dimer methane-ethane	−0.8[a]	−0.4	−1.0	−0.8	−0.0	−0.8	−0.7
Dimer methane-ethane	−0.6[a]	−0.0	−0.6	−0.6	−0.0	−0.6	−0.6
Dimer methane-methane	−0.5[a]	−0.0	−0.8	−0.5	0.0	−0.5	−0.5
Full optimizations of dimers, single point calculations on fragments (monomers)							
Dimer water-ammonia	−6.5[a]	−5.0	−5.6	−4.7	−7.2	−8.1	−9.6
Dimer water-water	−5.0[a]	−4.4	−4.8	−5.1	−4.5	−5.1	−4.6
Dimer HCN-HCN	−4.7[a]	−3.5	−4.0	−4.5	−4.5	−5.3	−6.6
Dimer HF-HF	−4.6[a]	−2.2	−2.4	−2.6	−1.6	−1.9	−1.9
Dimer ammonia-ammonia	−3.2[a]	−2.0	−2.5	−2.5	−1.9	−2.5	−2.7
Dimer HF-methane	−1.7[a]	−0.7	−1.1	−1.0	−0.3	−0.8	−0.6
Dimer ammonia-methane	−0.8[a]	−0.6	−1.0	−1.0	−0.6	−1.1	−1.2
Dimer water-methane	−0.7[a]	−0.6	−1.0	−1.1	−0.4	−0.8	−0.8
Dimer formaldehyde-formaldehyde	−4.5[a]	−3.9	−4.9	−5.4	−2.7	−3.9	−3.9
Dimer water-ethene	−2.6[a]	−2.5	−3.3	−3.3	−1.5	−2.6	−2.3
Dimer formaldehyde-ethene	−1.6[a]	−1.2	−2.1	−2.1	−0.6	−2.4	−2.3
Dimer ethyne-ethyne	−1.5[a]	−1.9	−2.7	−2.4	−0.8	−1.7	−1.3
Dimer ammonia-ethene	−1.4[a]	−1.0	−1.8	−1.9	−0.6	−1.7	−1.6
Dimer ethene-ethene	−1.1[a]	−0.3	−1.5	−1.4	−0.1	−1.2	−1.1
Dimer methane-ethene	−0.5[a]	−0.3	−1.0	−1.0	−0.1	−0.8	−0.7
Dimer methane-ethane	−0.8[a]	−0.4	−1.0	−0.8	−0.0	−0.8	−0.7
Dimer methane-ethane	−0.6[a]	−0.0	−0.6	−0.6	−0.0	−0.6	−0.6
Dimer methane-methane	−0.5[a]	−0.0	−0.8	−0.5	0.0	−0.5	−0.5

a J.Rezac and P.Hobza, J.Chem.Theory Comput. 9, 2151 (2013).

Table S75: Benchmark Results for the S22 Set. Interaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Single point calculations							
ammonia dimer -3.17	-3.2^a	-2.0	-2.5	-2.6	-1.9	-2.6	-2.7
water dimer -5.02	-5.0^a	-4.0	-4.3	-4.6	-4.1	-4.6	-4.2
formic acid dimer -18.61	-18.8^a	-13.6	-14.8	-15.6	-11.5	-13.3	-12.9
formamide dimer -15.96	-16.1^a	-13.0	-14.3	-15.1	-11.7	-13.5	-13.8
uracil dimer -20.47	-20.7^a	-17.5	-19.5	-19.6	-16.2	-18.7	-18.7
2-pyridoxine 2-aminopyridine -17.0	-17.0^a	-11.0	-13.4	-13.2	-11.3	-14.3	-16.1
adenine thymine -16.37	-16.7^a	-11.1	-13.6	-13.4	-11.3	-14.5	-16.4
methane dimer -0.53	-0.5^a	0.1	-0.5	-0.5	0.1	-0.5	-0.5
ethene dimer -1.51	-1.5^a	-0.4	-1.5	-1.4	0.1	-1.3	-1.1
benzene methane -1.50	-1.4^a	-0.2	-1.4	-1.4	0.1	-1.4	-1.3
benzene dimer -2.73	-2.6^a	1.3	-2.2	-2.7	1.1	-3.1	-3.3
pyrazine dimer -4.42	-4.2^a	-0.9	-4.3	-5.0	-0.7	-5.0	-5.3
uracil dimer -9.88	-9.7^a	-4.3	-9.1	-9.3	-3.9	-9.8	-9.7
indole benzene -5.22	-4.6^a	1.5	-3.3	-3.9	1.4	-4.5	-4.6
adenine thymine -12.23	-11.7^a	-4.0	-10.6	-11.1	-3.3	-11.5	-11.2
ethene ethyne -1.53	-1.5^a	-1.1	-1.7	-1.6	-0.7	-1.4	-1.3
benzene water -3.28	-3.3^a	-2.3	-3.5	-3.4	-1.7	-3.2	-3.0
benzene ammonia -2.35	-2.3^a	-1.2	-2.5	-2.5	-0.8	-2.3	-2.3
benzene hcn cs -4.46	-4.5^a	-3.1	-4.5	-4.5	-1.7	-3.6	-3.3
benzene dimer -2.74	-2.7^a	-0.6	-2.7	-2.6	0.1	-2.4	-2.3
indole benzene -5.73	-5.6^a	-2.4	-5.2	-5.0	-1.2	-4.6	-4.2
phenol dimer -7.05	-7.1^a	-3.8	-6.1	-6.2	-3.2	-6.0	-5.6
Full optimizations of dimers and monomers							
ammonia dimer -3.17	-3.2^a	-2.0	-2.5	-2.5	-1.9	-2.5	-2.7
water dimer -5.02	-5.0^a	-4.3	-4.7	-5.1	-4.5	-5.1	-4.6
formic acid dimer -18.61	-18.8^a	-14.6	-15.9	-16.1	-16.7	-18.6	-18.3
formamide dimer -15.96	-16.1^a	-13.0	-14.5	-15.1	-12.4	-14.6	-15.2
uracil dimer -20.47	-20.7^a	-18.8	-20.9	-20.6	-19.5	-22.4	-22.9
2-pyridoxine 2-aminopyridine -17.0	-17.0^a	-11.4	-13.9	-13.3	-14.8	-18.2	-22.2
adenine thymine -16.37	-16.7^a	-11.5	-14.3	-14.0	-15.1	-18.9	-22.4
methane dimer -0.53	-0.5^a	0.0	-0.5	-0.5	0.0	-0.5	-0.5
ethene dimer -1.51	-1.5^a	-0.4	-1.5	-1.4	-0.1	-1.3	-1.2
benzene methane -1.50	-1.4^a	-0.2	-1.5	-1.5	-0.1	-1.4	-1.3
benzene dimer -2.73	-2.6^a	-0.6	-2.9	-3.1	-0.0	-3.5	-3.6
pyrazine dimer -4.42	-4.2^a	-1.0	-5.2	-6.1	-0.8	-5.7	-5.8
uracil dimer -9.88	-9.7^a	-4.6	-10.6	-10.8	-3.9	-10.8	-10.0
indole benzene -5.22	-4.6^a	-2.5	-5.4	-5.4	-1.5	-5.5	-5.0
adenine thymine -12.23	-11.7^a	-11.6	-11.8	-12.4	-14.6	-12.1	-11.2
ethene ethyne -1.53	-1.5^a	-2.2	-3.1	-2.8	-0.8	-1.9	-1.5
benzene water -3.28	-3.3^a	-2.9	-4.7	-4.5	-1.9	-3.9	-3.5
benzene ammonia -2.35	-2.3^a	-1.4	-3.3	-3.4	-1.2	-3.4	-3.2
benzene hcn cs -4.46	-4.5^a	-3.3	-4.8	-4.8	-1.8	-3.6	-3.3
benzene dimer -2.74	-2.7^a	-0.7	-3.3	-3.1	-0.3	-3.5	-3.6
indole benzene -5.73	-5.6^a	-2.5	-5.7	-5.4	-1.5	-5.5	-5.0
phenol dimer -7.05	-7.1^a	-4.7	-7.1	-7.2	-4.1	-6.6	-6.0
Full optimizations of dimers, single point calculations on fragments (monomers)							
ammonia dimer -3.17	-3.2^a	-2.0	-2.5	-2.5	-1.9	-2.5	-2.7
water dimer -5.02	-5.0^a	-4.4	-4.8	-5.1	-4.5	-5.1	-4.6
formic acid dimer -18.61	-18.8^a	-18.6	-20.0	-20.4	-57.2	-58.9	-60.6
formamide dimer -15.96	-16.1^a	-14.3	-15.8	-16.8	-15.2	-17.6	-21.5
uracil dimer -20.47	-20.7^a	-21.1	-23.3	-23.2	-27.6	-30.8	-36.7
2-pyridoxine 2-aminopyridine -17.0	-17.0^a	-12.8	-15.4	-14.7	-22.5	-25.7	-38.2
adenine thymine -16.37	-16.7^a	-13.0	-16.1	-15.8	-23.4	-26.8	-36.6
methane dimer -0.53	-0.5^a	0.0	-0.5	-0.5	0.0	-0.5	-0.5
ethene dimer -1.51	-1.5^a	-0.4	-1.5	-1.4	-0.1	-1.3	-1.2
benzene methane -1.50	-1.4^a	-0.2	-1.5	-1.6	-0.1	-1.4	-1.3
benzene dimer -2.73	-2.6^a	-0.6	-2.9	-3.1	-0.0	-3.5	-3.6
pyrazine dimer -4.42	-4.2^a	-1.0	-5.2	-6.1	-0.8	-5.7	-5.9
uracil dimer -9.88	-9.7^a	-5.6	-11.9	-12.0	-4.6	-11.9	-10.8
indole benzene -5.22	-4.6^a	-2.5	-5.7	-5.7	-1.5	-5.7	-5.2
adenine thymine -12.23	-11.7^a	-12.7	-12.7	-13.3	-19.0	-12.8	-11.9
ethene ethyne -1.53	-1.5^a	-2.2	-3.2	-2.8	-0.8	-1.9	-1.5

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Table S75: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
benzene water -3.28	-3.3^a	-3.0	-4.7	-4.5	-1.9	-3.9	-3.5
benzene ammonia -2.35	-2.3^a	-1.4	-3.4	-3.5	-1.2	-3.4	-3.2
benzene hcn cs -4.46	-4.5^a	-3.4	-4.9	-4.8	-1.8	-3.6	-3.3
benzene dimer -2.74	-2.7^a	-0.7	-3.3	-3.2	-0.3	-3.5	-3.6
indole benzene -5.73	-5.6^a	-2.5	-5.7	-5.4	-1.5	-5.7	-5.2
phenol dimer -7.05	-7.1^a	-4.8	-7.3	-7.5	-4.3	-6.9	-6.2

a P.Jurecka, J.Sponer, J.Cerny, and P.Hobza, Phys.Chem.Chem.Phys. 8, 1985 (2006) ; T.Takatani, E.G.Hohenstein, M.Malagoli, M.S.Marshall, and C.D.Sherrill, J.Chem.Phys. 132, 144104 (2010).

Table S76: Benchmark Results for the S66 Set. Interaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Single point calculations							
Dimer Water-Water	−5.0[a]	−4.0	−4.3	−4.5	−4.2	−4.7	−4.3
Dimer Water-MeOH	−5.7[a]	−3.9	−4.5	−4.8	−3.7	−4.5	−4.1
Dimer Water-MeNH2	−7.0[a]	−4.4	−5.0	−4.5	−5.2	−6.0	−6.6
Dimer Water-Peptide	−8.2[a]	−6.2	−7.1	−7.3	−5.8	−7.0	−6.5
Dimer MeOH-MeOH	−5.9[a]	−3.3	−4.1	−4.4	−3.1	−4.1	−3.8
Dimer MeOH-MeNH2	−7.7[a]	−3.8	−4.9	−4.3	−4.6	−6.1	−6.7
Dimer MeOH-Peptide	−8.3[a]	−5.0	−6.2	−6.4	−4.6	−6.2	−5.7
Dimer MeOH-Water	−5.1[a]	−3.4	−3.8	−4.0	−3.5	−4.1	−3.8
Dimer MeNH2-MeOH	−3.1[a]	−1.4	−2.4	−2.6	−1.2	−2.4	−2.5
Dimer MeNH2-MeNH2	−4.2[a]	−1.5	−2.7	−2.7	−1.2	−2.8	−3.0
Dimer MeNH2-Peptide	−5.5[a]	−2.8	−4.5	−4.8	−2.2	−4.3	−4.4
Dimer MeNH2-Water	−7.4[a]	−4.3	−5.1	−4.6	−5.0	−6.0	−6.5
Dimer Peptide-MeOH	−6.3[a]	−3.9	−5.2	−5.3	−3.4	−5.0	−4.9
Dimer Peptide-MeNH2	−7.6[a]	−4.1	−5.7	−5.5	−4.2	−6.2	−6.9
Dimer Peptide-Peptide	−8.7[a]	−5.3	−7.3	−7.4	−4.5	−6.9	−6.9
Dimer Peptide-Water	−5.2[a]	−3.8	−4.4	−4.5	−3.7	−4.6	−4.5
Dimer Uracil-Uracil_BP	−17.4[a]	−13.8	−15.8	−15.9	−12.7	−15.1	−15.3
Dimer Water-Pyridine	−7.0[a]	−3.7	−4.5	−4.3	−4.5	−5.5	−6.3
Dimer MeOH-Pyridine	−7.5[a]	−3.2	−4.3	−4.0	−4.1	−5.5	−6.4
Dimer AcOH-AcOH	−19.4[a]	−13.8	−15.2	−16.0	−11.9	−13.8	−13.3
Dimer AcNH2-AcNH2	−16.5[a]	−12.9	−14.5	−14.6	−11.8	−13.8	−13.8
Dimer AcOH-Uracil	−19.8[a]	−15.4	−17.0	−17.5	−13.8	−16.0	−15.8
Dimer AcNH2-Uracil	−19.5[a]	−16.1	−17.8	−18.0	−14.9	−17.1	−17.3
Dimer Benzene-Benzene_pi-pi	−2.7[a]	1.2	−1.9	−2.3	1.0	−2.7	−2.9
Dimer Pyridine-Pyridine_pi-pi	−3.8[a]	−0.2	−3.5	−4.0	−0.2	−4.1	−4.4
Dimer Uracil-Uracil_pi-pi	−9.8[a]	−4.4	−9.2	−9.4	−3.9	−10.0	−9.8
Dimer Benzene-Pyridine_pi-pi	−3.3[a]	0.5	−2.8	−3.2	0.3	−3.5	−3.7
Dimer Benzene-Uracil_pi-pi	−5.6[a]	−1.1	−5.2	−5.6	−0.9	−5.9	−5.6
Dimer Pyridine-Uracil_pi-pi	−6.7[a]	−2.4	−6.4	−7.0	−2.2	−7.1	−7.1
Dimer Benzene-Ethene	−1.4[a]	1.0	−0.8	−1.1	0.8	−1.4	−1.5
Dimer Uracil-Ethene	−3.3[a]	−0.9	−3.1	−3.4	−0.7	−3.5	−3.3
Dimer Uracil-Ethyne	−3.7[a]	−1.7	−3.6	−3.8	−1.5	−3.9	−3.6
Dimer Pyridine-Ethene	−1.8[a]	0.5	−1.4	−1.7	0.3	−1.9	−2.0
Dimer Pentane-Pentane	−3.8[a]	−0.2	−3.9	−3.7	1.1	−3.4	−3.0
Dimer Neopentane-Pentane	−2.6[a]	−0.4	−3.1	−2.9	0.5	−2.6	−2.4
Dimer Neopentane-Neopentane	−1.8[a]	−0.5	−2.5	−2.4	0.1	−2.2	−2.1
Dimer Cyclopentane-Neopentane	−2.4[a]	−0.6	−3.1	−3.0	0.3	−2.6	−2.4
Dimer Cyclopentane-Cyclopentan	−3.0[a]	−0.4	−3.2	−3.1	0.7	−2.7	−2.4
Dimer Benzene-Cyclopentane	−3.5[a]	0.3	−2.8	−3.0	0.8	−3.0	−3.0
Dimer Benzene-Neopentane	−2.8[a]	−0.1	−2.7	−2.7	0.3	−2.7	−2.7
Dimer Uracil-Pentane	−4.8[a]	−0.6	−4.6	−4.8	−0.0	−4.9	−4.7
Dimer Uracil-Cyclopentane	−4.1[a]	−0.3	−3.8	−4.0	0.2	−4.1	−3.9
Dimer Uracil-Neopentane	−3.7[a]	−0.4	−3.3	−3.5	0.0	−3.5	−3.4
Dimer Ethene-Pentane	−2.0[a]	−0.2	−2.1	−2.0	0.5	−1.9	−1.6
Dimer Ethyne-Pentane	−1.7[a]	0.1	−1.5	−1.6	0.3	−1.6	−1.6
Dimer Peptide-Pentane	−4.3[a]	−0.4	−3.7	−3.8	0.6	−3.6	−3.3
Dimer Benzene-Benzene_TS	−2.8[a]	−0.6	−2.7	−2.7	0.0	−2.6	−2.5
Dimer Pyridine-Pyridine_TS	−3.5[a]	−1.2	−3.3	−3.4	−0.5	−3.1	−3.1
Dimer Benzene-Pyridine_TS	−3.3[a]	−1.0	−3.2	−3.2	−0.3	−3.0	−2.9
Dimer Benzene-Ethyne_CH-pi	−2.9[a]	−1.8	−3.1	−2.9	−0.8	−2.5	−2.2
Dimer Ethyne-Ethyne_TS	−1.5[a]	−1.2	−1.7	−1.6	−0.7	−1.3	−1.2
Dimer Benzene-AcOH_OH-pi	−4.7[a]	−2.7	−4.5	−4.5	−1.6	−4.0	−3.7
Dimer Benzene-AcNH2_NH-pi	−4.4[a]	−3.0	−4.7	−4.6	−2.1	−4.2	−4.0
Dimer Benzene-Water_OH-pi	−3.3[a]	−2.4	−3.6	−3.5	−1.7	−3.3	−3.1
Dimer Benzene-MeOH_OH-pi	−4.2[a]	−1.8	−3.7	−3.7	−1.1	−3.6	−3.3
Dimer Benzene-MeNH2_NH-pi	−3.2[a]	−0.8	−2.9	−3.0	−0.3	−2.8	−2.8
Dimer Benzene-Peptide_NH-pi	−5.3[a]	−1.9	−4.7	−4.7	−0.9	−4.4	−4.2
Dimer Pyridine-Pyridine_CH-N	−4.2[a]	−2.6	−3.9	−4.0	−1.8	−3.4	−3.7
Dimer Ethyne-Water_CH-O	−2.9[a]	−3.1	−3.4	−3.3	−2.7	−3.2	−2.9
Dimer Ethyne-AcOH_OH-pi	−5.0[a]	−4.0	−5.0	−4.9	−2.9	−4.2	−3.8
Dimer Pentane-AcOH	−2.9[a]	−0.6	−3.1	−3.2	−0.0	−3.1	−3.0
Dimer Pentane-AcNH2	−3.5[a]	−0.8	−3.5	−3.6	−0.1	−3.4	−3.2
Dimer Benzene-AcOH	−3.7[a]	−1.5	−3.9	−4.0	−0.7	−3.7	−3.6

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Table S76: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Peptide-Ethene	-3.0^a	−1.2	−2.9	−3.0	−0.7	−2.8	−2.7
Dimer Pyridine-Ethyne	-4.1^a	−3.4	−4.1	−4.1	−2.9	−3.9	−4.0
Dimer MeNH2-Pyridine	-4.0^a	−1.0	−2.8	−3.0	−0.6	−2.9	−3.1
Full optimizations of dimers and monomers							
Dimer Water-Water	-5.0^a	−4.3	−4.7	−5.1	−4.5	−5.1	−4.6
Dimer Water-MeOH	-5.7^a	−4.0	−4.7	−4.9	−3.9	−4.8	−4.4
Dimer Water-MeNH2	-7.0^a	−4.3	−5.1	−4.5	−6.1	−7.2	−8.7
Dimer Water-Peptide	-8.2^a	−6.9	−7.8	−8.1	−6.4	−7.5	−7.0
Dimer MeOH-MeOH	-5.9^a	−3.4	−4.3	−4.5	−3.3	−4.3	−3.9
Dimer MeOH-MeNH2	-7.7^a	−4.1	−5.4	−4.2	−6.5	−8.2	−9.7
Dimer MeOH-Peptide	-8.3^a	−6.4	−7.6	−7.6	−6.0	−7.5	−6.8
Dimer MeOH-Water	-5.1^a	−3.9	−4.4	−4.7	−4.1	−4.8	−4.3
Dimer MeNH2-MeOH	-3.1^a	−4.1	−2.9	−3.0	−6.5	−2.7	−2.6
Dimer MeNH2-MeNH2	-4.2^a	−1.7	−2.9	−2.9	−1.7	−3.0	−3.7
Dimer MeNH2-Peptide	-5.5^a	−3.5	−4.9	−5.3	−2.7	−4.5	−4.6
Dimer MeNH2-Water	-7.4^a	−4.3	−5.1	−4.5	−6.1	−7.2	−8.7
Dimer Peptide-MeOH	-6.3^a	−3.6	−5.1	−5.2	−3.0	−4.7	−4.5
Dimer Peptide-MeNH2	-7.6^a	−3.7	−5.4	−5.0	−4.0	−6.0	−7.4
Dimer Peptide-Peptide	-8.7^a	−5.7	−8.5	−9.4	−4.6	−7.0	−6.8
Dimer Peptide-Water	-5.2^a	−4.0	−4.9	−5.1	−3.5	−4.5	−4.4
Dimer Uracil-Uracil_BP	-17.4^a	−15.5	−17.6	−17.1	−15.6	−18.6	−19.1
Dimer Water-Pyridine	-7.0^a	−4.0	−4.9	−5.0	−5.5	−6.7	−8.4
Dimer MeOH-Pyridine	-7.5^a	−3.4	−4.7	−4.2	−5.6	−7.3	−9.1
Dimer AcOH-AcOH	-19.4^a	−15.2	−16.8	−17.0	−18.2	−20.2	−19.7
Dimer AcNH2-AcNH2	-16.5^a	−13.3	−14.8	−14.6	−13.0	−15.4	−15.5
Dimer AcOH-Uracil	-19.8^a	−16.8	−18.6	−18.4	−18.4	−20.9	−21.0
Dimer AcNH2-Uracil	-19.5^a	−16.8	−18.7	−18.5	−17.1	−19.8	−20.3
Dimer Benzene-Benzene_pi-pi	-2.7^a	−0.6	−2.9	−3.1	−0.0	−3.5	−3.6
Dimer Pyridine-Pyridine_pi-pi	-3.8^a	−2.7	−4.3	−5.0	−1.9	−5.0	−5.1
Dimer Uracil-Uracil_pi-pi	-9.8^a	−4.6	−10.6	−10.8	−3.9	−10.8	−10.0
Dimer Benzene-Pyridine_pi-pi	-3.3^a	−1.3	−3.5	−4.1	−1.2	−4.3	−4.4
Dimer Benzene-Uracil_pi-pi	-5.6^a	−3.4	−6.6	−7.1	−3.1	−7.3	−6.6
Dimer Pyridine-Uracil_pi-pi	-6.7^a	−9.2	−7.8	−8.5	−10.1	−8.0	−7.7
Dimer Benzene-Ethene	-1.4^a	0.0	−1.1	−1.5	0.0	−1.8	−1.9
Dimer Uracil-Ethene	-3.3^a	−3.9	−3.9	−4.2	−2.3	−4.0	−3.6
Dimer Uracil-Ethyne	-3.7^a	−5.8	−4.7	−4.8	−3.5	−4.4	−3.8
Dimer Pyridine-Ethene	-1.8^a	−0.9	−2.2	−2.2	−0.3	−2.4	−2.4
Dimer Pentane-Pentane	-3.8^a	−0.5	−4.5	−4.0	0.0	−3.5	−3.2
Dimer Neopentane-Pentane	-2.6^a	−1.2	−4.0	−3.4	−0.0	−2.9	−2.6
Dimer Neopentane-Neopentane	-1.8^a	−1.5	−3.7	−3.1	−0.0	−2.6	−2.2
Dimer Cyclopentane-Neopentane	-2.4^a	−1.4	−3.9	−3.4	−0.0	−2.9	−2.5
Dimer Cyclopentane-Cyclopentan	-3.0^a	−1.2	−4.4	−3.8	−0.2	−3.2	−2.9
Dimer Benzene-Cyclopentane	-3.5^a	−0.0	−3.5	−3.5	−0.0	−3.3	−3.2
Dimer Benzene-Neopentane	-2.8^a	−0.4	−3.7	−3.5	−0.1	−3.2	−3.0
Dimer Uracil-Pentane	-4.8^a	−1.4	−4.9	−5.0	−0.7	−4.9	−4.5
Dimer Uracil-Cyclopentane	-4.1^a	−1.7	−4.3	−4.3	−0.5	−4.2	−3.9
Dimer Uracil-Neopentane	-3.7^a	−1.3	−3.7	−3.7	−0.5	−3.6	−3.3
Dimer Ethene-Pentane	-2.0^a	−0.8	−2.4	−2.1	−0.1	−1.9	−1.7
Dimer Ethyne-Pentane	-1.7^a	−0.7	−1.7	−1.8	0.0	−1.7	−1.6
Dimer Peptide-Pentane	-4.3^a	−0.9	−4.3	−4.2	−0.4	−3.7	−3.4
Dimer Benzene-Benzene_TS	-2.8^a	−0.7	−3.3	−3.1	−0.3	−3.5	−3.6
Dimer Pyridine-Pyridine_TS	-3.5^a	−2.0	−3.5	−5.0	−1.9	−5.0	−3.2
Dimer Benzene-Pyridine_TS	-3.3^a	−1.1	−3.8	−3.6	−0.6	−3.2	−3.0
Dimer Benzene-Ethyne_CH-pi	-2.9^a	−2.0	−3.5	−3.2	−0.9	−2.5	−2.2
Dimer Ethyne-Ethyne_TS	-1.5^a	−1.9	−2.6	−2.4	−0.8	−1.7	−1.3
Dimer Benzene-AcOH_OH-pi	-4.7^a	−4.3	−6.3	−6.1	−2.4	−4.9	−4.4
Dimer Benzene-AcNH2_NH-pi	-4.4^a	−3.8	−5.8	−5.5	−2.3	−4.6	−4.0
Dimer Benzene-Water_OH-pi	-3.3^a	−2.9	−4.7	−4.5	−1.9	−3.9	−3.5
Dimer Benzene-MeOH_OH-pi	-4.2^a	−2.5	−4.7	−4.6	−1.5	−4.1	−3.7
Dimer Benzene-MeNH2_NH-pi	-3.2^a	−1.2	−3.5	−3.7	−0.7	−3.3	−3.2
Dimer Benzene-Peptide_NH-pi	-5.3^a	−2.3	−5.4	−5.4	−1.3	−4.5	−4.3
Dimer Pyridine-Pyridine_CH-N	-4.2^a	−2.7	−4.3	−4.2	−2.1	−4.0	−4.3
Dimer Ethyne-Water_CH-O	-2.9^a	−4.3	−4.8	−4.8	−3.2	−3.9	−3.1
Dimer Ethyne-AcOH_OH-pi	-5.0^a	−6.1	−7.3	−7.0	−3.5	−5.1	−4.5
Dimer Pentane-AcOH	-2.9^a	−1.0	−3.8	−3.7	−0.4	−3.4	−3.1

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Table S76: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Pentane-AcNH2	-3.5^a	-0.8	-3.9	-3.8	-0.6	-3.4	-3.1
Dimer Benzene-AcOH	-3.7^a	-2.5	-4.7	-4.8	-1.4	-4.3	-4.1
Dimer Peptide-Ethene	-3.0^a	-2.1	-3.5	-3.6	-1.2	-3.1	-2.9
Dimer Pyridine-Ethyne	-4.1^a	-4.1	-5.1	-4.5	-4.4	-5.8	-6.1
Dimer MeNH2-Pyridine	-4.0^a	-2.1	-3.3	-3.2	-1.7	-3.1	-3.8
Full optimizations of dimers, single point calculations on fragments (monomers)							
Dimer Water-Water	-5.0^a	-4.4	-4.8	-5.1	-4.5	-5.1	-4.6
Dimer Water-MeOH	-5.7^a	-4.0	-4.7	-4.9	-3.9	-4.8	-4.4
Dimer Water-MeNH2	-7.0^a	-4.4	-5.2	-4.6	-6.4	-7.5	-9.2
Dimer Water-Peptide	-8.2^a	-7.0	-8.0	-8.2	-6.7	-8.0	-7.3
Dimer MeOH-MeOH	-5.9^a	-3.5	-4.4	-4.6	-3.3	-4.4	-4.0
Dimer MeOH-MeNH2	-7.7^a	-4.4	-5.6	-4.3	-7.4	-9.1	-10.9
Dimer MeOH-Peptide	-8.3^a	-6.6	-7.8	-7.9	-6.5	-8.1	-7.3
Dimer MeOH-Water	-5.1^a	-4.0	-4.5	-4.8	-4.2	-4.9	-4.4
Dimer MeNH2-MeOH	-3.1^a	-4.4	-3.0	-3.0	-7.4	-2.7	-2.6
Dimer MeNH2-MeNH2	-4.2^a	-1.8	-2.9	-2.9	-1.7	-3.0	-3.8
Dimer MeNH2-Peptide	-5.5^a	-3.6	-5.0	-5.5	-2.7	-4.7	-4.8
Dimer MeNH2-Water	-7.4^a	-4.4	-5.1	-4.5	-6.4	-7.5	-9.2
Dimer Peptide-MeOH	-6.3^a	-3.8	-5.2	-5.4	-3.2	-4.8	-4.6
Dimer Peptide-MeNH2	-7.6^a	-3.9	-5.5	-5.1	-4.2	-6.3	-8.0
Dimer Peptide-Peptide	-8.7^a	-6.0	-9.4	-10.0	-4.9	-7.5	-7.1
Dimer Peptide-Water	-5.2^a	-4.1	-4.9	-5.1	-3.7	-4.7	-4.5
Dimer Uracil-Uracil_BP	-17.4^a	-17.4	-19.6	-19.2	-22.2	-25.6	-31.3
Dimer Water-Pyridine	-7.0^a	-4.0	-4.9	-5.0	-5.6	-6.9	-8.8
Dimer MeOH-Pyridine	-7.5^a	-3.5	-4.8	-4.3	-6.1	-7.9	-10.0
Dimer AcOH-AcOH	-19.4^a	-20.0	-21.7	-21.9	-59.8	-61.7	-63.2
Dimer AcNH2-AcNH2	-16.5^a	-14.5	-16.2	-16.2	-16.1	-18.8	-22.3
Dimer AcOH-Uracil	-19.8^a	-20.2	-22.1	-22.0	-35.2	-37.0	-43.1
Dimer AcNH2-Uracil	-19.5^a	-18.7	-20.7	-20.6	-22.9	-25.9	-31.0
Dimer Benzene-Benzene_pi-pi	-2.7^a	-0.7	-2.9	-3.2	-0.0	-3.5	-3.6
Dimer Pyridine-Pyridine_pi-pi	-3.8^a	-2.8	-4.3	-5.0	-1.9	-5.1	-5.1
Dimer Uracil-Uracil_pi-pi	-9.8^a	-5.6	-11.9	-12.0	-4.6	-11.9	-10.8
Dimer Benzene-Pyridine_pi-pi	-3.3^a	-1.3	-3.5	-4.1	-1.2	-4.3	-4.4
Dimer Benzene-Uracil_pi-pi	-5.6^a	-3.5	-6.9	-7.4	-3.2	-7.5	-6.8
Dimer Pyridine-Uracil_pi-pi	-6.7^a	-9.7	-8.0	-8.8	-12.1	-8.2	-7.8
Dimer Benzene-Ethene	-1.4^a	0.0	-1.1	-1.5	0.0	-1.8	-1.9
Dimer Uracil-Ethene	-3.3^a	-4.0	-4.0	-4.3	-2.4	-4.1	-3.7
Dimer Uracil-Ethyne	-3.7^a	-6.0	-4.8	-5.0	-3.6	-4.5	-3.9
Dimer Pyridine-Ethene	-1.8^a	-1.0	-2.2	-2.2	-0.4	-2.4	-2.4
Dimer Pentane-Pentane	-3.8^a	-0.5	-4.5	-4.0	0.0	-3.5	-3.2
Dimer Neopentane-Pentane	-2.6^a	-1.2	-4.0	-3.4	-0.0	-2.9	-2.6
Dimer Neopentane-Neopentane	-1.8^a	-1.5	-3.7	-3.1	-0.0	-2.6	-2.2
Dimer Cyclopentane-Neopentane	-2.4^a	-1.4	-3.9	-3.4	-0.0	-2.9	-2.5
Dimer Cyclopentane-Cyclopentan	-3.0^a	-1.2	-4.4	-3.8	-0.2	-3.2	-2.9
Dimer Benzene-Cyclopentane	-3.5^a	-0.0	-3.6	-3.5	-0.0	-3.3	-3.2
Dimer Benzene-Neopentane	-2.8^a	-0.4	-3.7	-3.6	-0.1	-3.2	-3.0
Dimer Uracil-Pentane	-4.8^a	-1.5	-5.1	-5.2	-0.8	-5.0	-4.6
Dimer Uracil-Cyclopentane	-4.1^a	-1.8	-4.4	-4.4	-0.5	-4.3	-4.0
Dimer Uracil-Neopentane	-3.7^a	-1.3	-3.7	-3.8	-0.5	-3.6	-3.4
Dimer Ethene-Pentane	-2.0^a	-0.8	-2.4	-2.2	-0.1	-1.9	-1.7
Dimer Ethyne-Pentane	-1.7^a	-0.7	-1.8	-1.8	0.0	-1.7	-1.6
Dimer Peptide-Pentane	-4.3^a	-0.9	-4.4	-4.3	-0.4	-3.7	-3.5
Dimer Benzene-Benzene_TS	-2.8^a	-0.7	-3.3	-3.1	-0.3	-3.5	-3.6
Dimer Pyridine-Pyridine_TS	-3.5^a	-2.1	-3.5	-5.0	-1.9	-5.1	-3.2
Dimer Benzene-Pyridine_TS	-3.3^a	-1.1	-3.8	-3.7	-0.6	-3.2	-3.0
Dimer Benzene-Ethyne_CH-pi	-2.9^a	-2.1	-3.5	-3.2	-0.9	-2.5	-2.2
Dimer Ethyne-Ethyne_TS	-1.5^a	-1.9	-2.7	-2.4	-0.8	-1.7	-1.3
Dimer Benzene-AcOH_OH-pi	-4.7^a	-4.4	-6.5	-6.3	-2.5	-5.0	-4.5
Dimer Benzene-AcNH2_NH-pi	-4.4^a	-3.8	-5.9	-5.6	-2.3	-4.6	-4.1
Dimer Benzene-Water_OH-pi	-3.3^a	-3.0	-4.7	-4.5	-1.9	-3.9	-3.5
Dimer Benzene-MeOH_OH-pi	-4.2^a	-2.5	-4.7	-4.7	-1.5	-4.1	-3.8
Dimer Benzene-MeNH2_NH-pi	-3.2^a	-1.2	-3.6	-3.7	-0.7	-3.3	-3.2
Dimer Benzene-Peptide_NH-pi	-5.3^a	-2.4	-5.4	-5.5	-1.3	-4.6	-4.3
Dimer Pyridine-Pyridine_CH-N	-4.2^a	-2.8	-4.3	-4.2	-2.1	-4.1	-4.4
Dimer Ethyne-Water_CH-O	-2.9^a	-4.4	-4.8	-4.8	-3.3	-3.9	-3.2

... *continued on next page* ...

Table S76: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Ethyne-AcOH_OH-pi	-5.0^a	-6.3	-7.5	-7.2	-3.6	-5.2	-4.7
Dimer Pentane-AcOH	-2.9^a	-1.1	-3.9	-3.8	-0.4	-3.4	-3.2
Dimer Pentane-AcNH2	-3.5^a	-0.9	-4.0	-3.9	-0.6	-3.5	-3.2
Dimer Benzene-AcOH	-3.7^a	-2.6	-4.8	-4.9	-1.4	-4.4	-4.2
Dimer Peptide-Ethene	-3.0^a	-2.2	-3.6	-3.7	-1.2	-3.1	-2.9
Dimer Pyridine-Ethyne	-4.1^a	-4.1	-5.1	-4.6	-4.7	-6.2	-6.5
Dimer MeNH2-Pyridine	-4.0^a	-2.1	-3.3	-3.2	-1.7	-3.1	-3.8

a J.Rezac, K.E.Riley, and P.Hobza, J.Chem.Theory Comput. 7, 2427 (2011) ; 7, 3466 (2011).

Table S77: Benchmark Results for the S66×8 Set. Interaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Water-Water_0.90	-4.6^a	-4.3	-4.7	-5.0	-4.4	-4.9	-4.5
Dimer Water-Water_0.95	-4.9^a	-4.1	-4.5	-4.7	-4.3	-4.8	-4.4
Dimer Water-Water_1.00	-4.9^a	-3.8	-4.2	-4.3	-4.0	-4.5	-4.2
Dimer Water-Water_1.05	-4.7^a	-3.5	-3.8	-3.9	-3.8	-4.3	-4.0
Dimer Water-Water_1.10	-4.5^a	-3.2	-3.5	-3.6	-3.6	-4.0	-3.7
Dimer Water-Water_1.25	-3.5^a	-2.4	-2.7	-2.7	-2.8	-3.2	-3.0
Dimer Water-Water_1.50	-2.1^a	-1.6	-1.8	-1.8	-1.9	-2.1	-2.0
Dimer Water-Water_2.00	-0.9^a	-0.8	-0.8	-0.8	-1.0	-1.0	-0.9
Dimer Water-MeOH_0.90	-5.2^a	-4.0	-4.7	-5.0	-3.5	-4.5	-4.0
Dimer Water-MeOH_0.95	-5.5^a	-4.0	-4.6	-4.9	-3.7	-4.5	-4.1
Dimer Water-MeOH_1.00	-5.6^a	-3.8	-4.4	-4.6	-3.6	-4.4	-4.1
Dimer Water-MeOH_1.05	-5.4^a	-3.5	-4.1	-4.3	-3.5	-4.2	-3.9
Dimer Water-MeOH_1.10	-5.1^a	-3.3	-3.8	-3.9	-3.3	-4.0	-3.8
Dimer Water-MeOH_1.25	-3.9^a	-2.5	-2.9	-3.0	-2.8	-3.3	-3.1
Dimer Water-MeOH_1.50	-2.4^a	-1.7	-1.9	-2.0	-1.9	-2.2	-2.1
Dimer Water-MeOH_2.00	-1.0^a	-0.8	-0.9	-0.9	-0.9	-1.0	-1.0
Dimer Water-MeNH2_0.90	-6.5^a	-4.5	-5.3	-4.3	-5.7	-6.7	-7.5
Dimer Water-MeNH2_0.95	-6.9^a	-4.5	-5.2	-4.5	-5.4	-6.3	-6.9
Dimer Water-MeNH2_1.00	-6.9^a	-4.3	-4.9	-4.4	-5.0	-5.8	-6.3
Dimer Water-MeNH2_1.05	-6.6^a	-4.0	-4.6	-4.3	-4.5	-5.3	-5.6
Dimer Water-MeNH2_1.10	-6.3^a	-3.7	-4.2	-4.1	-4.1	-4.8	-5.1
Dimer Water-MeNH2_1.25	-4.9^a	-2.8	-3.3	-3.3	-3.1	-3.6	-3.8
Dimer Water-MeNH2_1.50	-3.0^a	-1.8	-2.1	-2.2	-2.0	-2.3	-2.4
Dimer Water-MeNH2_2.00	-1.1^a	-0.8	-0.9	-1.0	-0.9	-1.0	-1.1
Dimer Water-Peptide_0.90	-7.6^a	-6.5	-7.5	-7.7	-6.0	-7.3	-6.7
Dimer Water-Peptide_0.95	-8.1^a	-6.4	-7.3	-7.5	-5.9	-7.2	-6.6
Dimer Water-Peptide_1.00	-8.1^a	-6.0	-6.9	-7.1	-5.7	-6.9	-6.3
Dimer Water-Peptide_1.05	-7.8^a	-5.6	-6.4	-6.6	-5.4	-6.5	-6.0
Dimer Water-Peptide_1.10	-7.5^a	-5.2	-6.0	-6.1	-5.1	-6.1	-5.7
Dimer Water-Peptide_1.25	-6.0^a	-4.1	-4.7	-4.8	-4.2	-5.0	-4.7
Dimer Water-Peptide_1.50	-3.8^a	-2.8	-3.2	-3.2	-3.0	-3.5	-3.3
Dimer Water-Peptide_2.00	-1.4^a	-1.3	-1.4	-1.4	-1.4	-1.5	-1.5
Dimer MeOH-MeOH_0.90	-5.3^a	-3.3	-4.2	-4.5	-2.9	-4.1	-3.7
Dimer MeOH-MeOH_0.95	-5.7^a	-3.4	-4.2	-4.5	-3.1	-4.2	-3.8
Dimer MeOH-MeOH_1.00	-5.7^a	-3.3	-4.1	-4.3	-3.1	-4.1	-3.8
Dimer MeOH-MeOH_1.05	-5.6^a	-3.1	-3.8	-4.0	-3.0	-3.9	-3.7
Dimer MeOH-MeOH_1.10	-5.3^a	-2.8	-3.5	-3.7	-2.9	-3.7	-3.5
Dimer MeOH-MeOH_1.25	-4.1^a	-2.2	-2.7	-2.8	-2.4	-3.1	-2.9
Dimer MeOH-MeOH_1.50	-2.5^a	-1.4	-1.8	-1.8	-1.7	-2.0	-2.0
Dimer MeOH-MeOH_2.00	-1.0^a	-0.7	-0.8	-0.8	-0.8	-0.9	-0.9
Dimer MeOH-MeNH2_0.90	-7.0^a	-3.8	-5.1	-4.0	-5.1	-6.8	-7.7
Dimer MeOH-MeNH2_0.95	-7.5^a	-3.9	-5.1	-4.2	-4.9	-6.4	-7.1
Dimer MeOH-MeNH2_1.00	-7.5^a	-3.7	-4.8	-4.3	-4.5	-5.9	-6.5
Dimer MeOH-MeNH2_1.05	-7.3^a	-3.5	-4.5	-4.2	-4.1	-5.4	-5.8
Dimer MeOH-MeNH2_1.10	-7.0^a	-3.3	-4.2	-4.0	-3.8	-4.9	-5.2
Dimer MeOH-MeNH2_1.25	-5.5^a	-2.5	-3.2	-3.3	-2.8	-3.7	-3.8
Dimer MeOH-MeNH2_1.50	-3.3^a	-1.6	-2.0	-2.1	-1.8	-2.3	-2.4
Dimer MeOH-MeNH2_2.00	-1.3^a	-0.7	-0.9	-0.9	-0.8	-1.0	-1.0
Dimer MeOH-Peptide_0.90	-7.6^a	-5.2	-6.6	-6.7	-4.7	-6.4	-5.8
Dimer MeOH-Peptide_0.95	-8.1^a	-5.2	-6.5	-6.6	-4.7	-6.4	-5.8
Dimer MeOH-Peptide_1.00	-8.2^a	-4.9	-6.1	-6.3	-4.5	-6.1	-5.6
Dimer MeOH-Peptide_1.05	-8.0^a	-4.6	-5.7	-5.8	-4.3	-5.8	-5.3
Dimer MeOH-Peptide_1.10	-7.7^a	-4.2	-5.3	-5.4	-4.1	-5.4	-5.0
Dimer MeOH-Peptide_1.25	-6.2^a	-3.2	-4.1	-4.2	-3.3	-4.4	-4.1
Dimer MeOH-Peptide_1.50	-3.6^a	-2.0	-2.5	-2.6	-2.1	-2.8	-2.7
Dimer MeOH-Peptide_2.00	-1.1^a	-0.7	-0.9	-0.9	-0.8	-1.0	-0.9
Dimer MeOH-Water_0.90	-4.6^a	-3.6	-4.2	-4.5	-3.6	-4.4	-4.0
Dimer MeOH-Water_0.95	-5.0^a	-3.5	-4.0	-4.3	-3.6	-4.3	-3.9
Dimer MeOH-Water_1.00	-5.0^a	-3.3	-3.7	-3.9	-3.4	-4.1	-3.8
Dimer MeOH-Water_1.05	-4.8^a	-3.0	-3.4	-3.6	-3.3	-3.8	-3.6
Dimer MeOH-Water_1.10	-4.6^a	-2.7	-3.2	-3.2	-3.1	-3.6	-3.4
Dimer MeOH-Water_1.25	-3.6^a	-2.1	-2.4	-2.4	-2.5	-2.9	-2.7
Dimer MeOH-Water_1.50	-2.2^a	-1.4	-1.6	-1.6	-1.7	-1.9	-1.8
Dimer MeOH-Water_2.00	-0.9^a	-0.7	-0.7	-0.7	-0.8	-0.9	-0.8

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Table S77: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer MeNH2-MeOH_0.90	−2.8[a]	−1.5	−2.5	−2.8	−0.9	−2.3	−2.5
Dimer MeNH2-MeOH_0.95	−3.0[a]	−1.5	−2.5	−2.7	−1.2	−2.4	−2.5
Dimer MeNH2-MeOH_1.00	−3.0[a]	−1.4	−2.3	−2.5	−1.2	−2.3	−2.5
Dimer MeNH2-MeOH_1.05	−2.9[a]	−1.3	−2.1	−2.2	−1.2	−2.2	−2.3
Dimer MeNH2-MeOH_1.10	−2.7[a]	−1.2	−1.9	−2.0	−1.2	−2.0	−2.2
Dimer MeNH2-MeOH_1.25	−2.0[a]	−0.8	−1.4	−1.4	−0.9	−1.5	−1.6
Dimer MeNH2-MeOH_1.50	−1.1[a]	−0.5	−0.8	−0.8	−0.6	−0.9	−0.9
Dimer MeNH2-MeOH_2.00	−0.4[a]	−0.2	−0.3	−0.3	−0.3	−0.3	−0.4
Dimer MeNH2-MeNH2_0.90	−3.7[a]	−0.8	−2.1	−2.0	−0.4	−2.2	−2.6
Dimer MeNH2-MeNH2_0.95	−4.1[a]	−1.3	−2.6	−2.5	−1.0	−2.7	−2.9
Dimer MeNH2-MeNH2_1.00	−4.2[a]	−1.5	−2.7	−2.7	−1.3	−2.8	−3.0
Dimer MeNH2-MeNH2_1.05	−4.0[a]	−1.6	−2.7	−2.8	−1.4	−2.7	−3.0
Dimer MeNH2-MeNH2_1.10	−3.8[a]	−1.6	−2.5	−2.7	−1.4	−2.6	−2.9
Dimer MeNH2-MeNH2_1.25	−2.8[a]	−1.2	−1.9	−2.1	−1.2	−2.0	−2.2
Dimer MeNH2-MeNH2_1.50	−1.3[a]	−0.6	−1.0	−1.0	−0.6	−1.0	−1.1
Dimer MeNH2-MeNH2_2.00	−0.4[a]	−0.2	−0.3	−0.3	−0.2	−0.3	−0.4
Dimer MeNH2-Peptide_0.90	−4.9[a]	−2.8	−4.7	−5.0	−1.7	−4.2	−4.2
Dimer MeNH2-Peptide_0.95	−5.4[a]	−2.9	−4.6	−4.9	−2.0	−4.3	−4.4
Dimer MeNH2-Peptide_1.00	−5.4[a]	−2.8	−4.4	−4.7	−2.2	−4.3	−4.4
Dimer MeNH2-Peptide_1.05	−5.2[a]	−2.6	−4.2	−4.4	−2.2	−4.1	−4.3
Dimer MeNH2-Peptide_1.10	−4.9[a]	−2.5	−3.9	−4.1	−2.2	−3.9	−4.1
Dimer MeNH2-Peptide_1.25	−3.2[a]	−1.6	−2.5	−2.7	−1.6	−2.6	−2.8
Dimer MeNH2-Peptide_1.50	−1.4[a]	−0.8	−1.2	−1.3	−0.8	−1.2	−1.4
Dimer MeNH2-Peptide_2.00	−0.5[a]	−0.3	−0.5	−0.5	−0.3	−0.5	−0.5
Dimer MeNH2-Water_0.90	−6.7[a]	−4.2	−5.1	−4.1	−5.2	−6.4	−7.1
Dimer MeNH2-Water_0.95	−7.2[a]	−4.4	−5.2	−4.5	−5.1	−6.2	−6.8
Dimer MeNH2-Water_1.00	−7.2[a]	−4.3	−5.0	−4.6	−4.9	−5.9	−6.3
Dimer MeNH2-Water_1.05	−7.0[a]	−4.1	−4.8	−4.5	−4.5	−5.5	−5.8
Dimer MeNH2-Water_1.10	−6.7[a]	−3.8	−4.5	−4.3	−4.2	−5.1	−5.3
Dimer MeNH2-Water_1.25	−5.2[a]	−3.0	−3.6	−3.6	−3.3	−3.9	−4.1
Dimer MeNH2-Water_1.50	−3.2[a]	−2.0	−2.3	−2.4	−2.2	−2.5	−2.6
Dimer MeNH2-Water_2.00	−1.2[a]	−0.9	−1.0	−1.1	−1.0	−1.1	−1.2
Dimer Peptide-MeOH_0.90	−5.7[a]	−3.8	−5.3	−5.4	−2.9	−4.8	−4.7
Dimer Peptide-MeOH_0.95	−6.1[a]	−3.9	−5.3	−5.4	−3.3	−5.0	−4.9
Dimer Peptide-MeOH_1.00	−6.2[a]	−3.9	−5.1	−5.2	−3.4	−5.0	−4.9
Dimer Peptide-MeOH_1.05	−6.0[a]	−3.7	−4.9	−5.0	−3.4	−4.9	−4.8
Dimer Peptide-MeOH_1.10	−5.7[a]	−3.5	−4.6	−4.6	−3.3	−4.7	−4.6
Dimer Peptide-MeOH_1.25	−4.6[a]	−2.8	−3.7	−3.7	−2.9	−3.9	−3.8
Dimer Peptide-MeOH_1.50	−2.9[a]	−2.0	−2.5	−2.5	−2.1	−2.6	−2.6
Dimer Peptide-MeOH_2.00	−1.3[a]	−1.1	−1.3	−1.3	−1.1	−1.3	−1.3
Dimer Peptide-MeNH2_0.90	−6.8[a]	−3.7	−5.6	−5.2	−4.0	−6.3	−7.5
Dimer Peptide-MeNH2_0.95	−7.3[a]	−4.1	−5.8	−5.5	−4.2	−6.3	−7.2
Dimer Peptide-MeNH2_1.00	−7.5[a]	−4.1	−5.7	−5.5	−4.2	−6.1	−6.8
Dimer Peptide-MeNH2_1.05	−7.3[a]	−4.0	−5.5	−5.4	−4.0	−5.8	−6.4
Dimer Peptide-MeNH2_1.10	−7.0[a]	−3.8	−5.2	−5.2	−3.8	−5.5	−5.9
Dimer Peptide-MeNH2_1.25	−5.6[a]	−3.1	−4.2	−4.3	−3.2	−4.3	−4.6
Dimer Peptide-MeNH2_1.50	−3.6[a]	−2.1	−2.8	−2.9	−2.2	−2.9	−3.1
Dimer Peptide-MeNH2_2.00	−1.5[a]	−1.1	−1.3	−1.4	−1.1	−1.4	−1.4
Dimer Peptide-Peptide_0.90	−8.0[a]	−5.4	−7.6	−7.8	−4.2	−7.0	−7.1
Dimer Peptide-Peptide_0.95	−8.5[a]	−5.4	−7.5	−7.7	−4.4	−7.0	−7.0
Dimer Peptide-Peptide_1.00	−8.6[a]	−5.2	−7.2	−7.3	−4.5	−6.9	−6.8
Dimer Peptide-Peptide_1.05	−8.4[a]	−4.9	−6.8	−6.8	−4.4	−6.6	−6.5
Dimer Peptide-Peptide_1.10	−8.1[a]	−4.6	−6.3	−6.3	−4.2	−6.2	−6.1
Dimer Peptide-Peptide_1.25	−6.7[a]	−3.7	−5.0	−5.0	−3.6	−5.1	−5.1
Dimer Peptide-Peptide_1.50	−4.4[a]	−2.6	−3.4	−3.4	−2.6	−3.5	−3.5
Dimer Peptide-Peptide_2.00	−1.8[a]	−1.2	−1.5	−1.5	−1.3	−1.6	−1.5
Dimer Peptide-Water_0.90	−4.7[a]	−4.0	−4.8	−5.0	−3.7	−4.7	−4.7
Dimer Peptide-Water_0.95	−5.1[a]	−3.9	−4.6	−4.7	−3.8	−4.7	−4.6
Dimer Peptide-Water_1.00	−5.1[a]	−3.7	−4.4	−4.4	−3.7	−4.5	−4.4
Dimer Peptide-Water_1.05	−5.0[a]	−3.5	−4.1	−4.1	−3.6	−4.3	−4.2
Dimer Peptide-Water_1.10	−4.7[a]	−3.2	−3.8	−3.8	−3.4	−4.1	−4.0
Dimer Peptide-Water_1.25	−3.8[a]	−2.6	−3.0	−3.0	−2.8	−3.3	−3.2
Dimer Peptide-Water_1.50	−2.4[a]	−1.8	−2.1	−2.0	−2.0	−2.3	−2.2
Dimer Peptide-Water_2.00	−1.1[a]	−1.0	−1.1	−1.1	−1.1	−1.2	−1.1
Dimer Uracil-Uracil_BP_0.90	−15.7[a]	−14.8	−17.0	−17.3	−13.8	−16.6	−17.4

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Table S77: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Uracil-Uracil_BP_0.95	-16.9^a	−14.5	−16.6	−16.8	−13.3	−15.9	−16.4
Dimer Uracil-Uracil_BP_1.00	-17.2^a	−13.7	−15.7	−15.8	−12.6	−15.0	−15.2
Dimer Uracil-Uracil_BP_1.05	-16.9^a	−12.7	−14.5	−14.6	−11.7	−14.0	−14.0
Dimer Uracil-Uracil_BP_1.10	-16.2^a	−11.5	−13.2	−13.3	−10.8	−12.9	−12.8
Dimer Uracil-Uracil_BP_1.25	-13.2^a	−8.6	−10.0	−10.0	−8.4	−10.1	−9.9
Dimer Uracil-Uracil_BP_1.50	-8.4^a	−5.4	−6.4	−6.3	−5.6	−6.7	−6.6
Dimer Uracil-Uracil_BP_2.00	-3.3^a	−2.5	−2.9	−2.9	−2.6	−3.0	−3.0
Dimer Water-Pyridine_0.90	-6.4^a	−3.5	−4.4	−4.0	−4.9	−6.0	−7.3
Dimer Water-Pyridine_0.95	-6.8^a	−3.7	−4.5	−4.2	−4.7	−5.8	−6.7
Dimer Water-Pyridine_1.00	-6.8^a	−3.7	−4.5	−4.3	−4.4	−5.3	−6.1
Dimer Water-Pyridine_1.05	-6.6^a	−3.5	−4.2	−4.2	−4.0	−4.9	−5.5
Dimer Water-Pyridine_1.10	-6.3^a	−3.3	−4.0	−4.0	−3.7	−4.5	−4.9
Dimer Water-Pyridine_1.25	-4.9^a	−2.6	−3.1	−3.3	−2.8	−3.4	−3.6
Dimer Water-Pyridine_1.50	-3.0^a	−1.7	−2.0	−2.2	−1.8	−2.2	−2.3
Dimer Water-Pyridine_2.00	-1.2^a	−0.8	−0.9	−1.0	−0.9	−1.0	−1.1
Dimer MeOH-Pyridine_0.90	-6.8^a	−2.7	−4.0	−3.5	−4.3	−6.0	−7.3
Dimer MeOH-Pyridine_0.95	-7.3^a	−3.1	−4.3	−3.8	−4.2	−5.8	−6.8
Dimer MeOH-Pyridine_1.00	-7.4^a	−3.2	−4.3	−4.0	−4.0	−5.4	−6.2
Dimer MeOH-Pyridine_1.05	-7.2^a	−3.1	−4.1	−4.0	−3.7	−5.0	−5.6
Dimer MeOH-Pyridine_1.10	-6.9^a	−2.9	−3.9	−3.8	−3.4	−4.6	−5.0
Dimer MeOH-Pyridine_1.25	-5.5^a	−2.3	−3.1	−3.2	−2.6	−3.5	−3.7
Dimer MeOH-Pyridine_1.50	-3.4^a	−1.5	−2.0	−2.2	−1.7	−2.2	−2.3
Dimer MeOH-Pyridine_2.00	-1.3^a	−0.7	−0.9	−1.0	−0.8	−1.0	−1.0
Dimer AcOH-AcOH_0.90	-17.4^a	−14.8	−16.3	−17.1	−13.2	−15.4	−14.9
Dimer AcOH-AcOH_0.95	-18.8^a	−14.5	−16.0	−16.8	−12.7	−14.7	−14.3
Dimer AcOH-AcOH_1.00	-19.1^a	−13.6	−15.0	−15.8	−11.8	−13.7	−13.2
Dimer AcOH-AcOH_1.05	-18.7^a	−12.4	−13.8	−14.5	−10.7	−12.5	−12.0
Dimer AcOH-AcOH_1.10	-17.9^a	−11.2	−12.5	−13.1	−9.6	−11.3	−10.8
Dimer AcOH-AcOH_1.25	-14.6^a	−7.9	−9.0	−9.4	−7.1	−8.5	−8.1
Dimer AcOH-AcOH_1.50	-9.2^a	−4.7	−5.5	−5.7	−4.6	−5.5	−5.3
Dimer AcOH-AcOH_2.00	-3.6^a	−2.1	−2.4	−2.5	−2.0	−2.4	−2.3
Dimer AcNH2-AcNH2_0.90	-14.9^a	−14.0	−15.7	−16.1	−12.7	−15.0	−15.6
Dimer AcNH2-AcNH2_0.95	-16.0^a	−13.6	−15.2	−15.5	−12.3	−14.5	−14.7
Dimer AcNH2-AcNH2_1.00	-16.3^a	−12.8	−14.3	−14.4	−11.7	−13.6	−13.6
Dimer AcNH2-AcNH2_1.05	-15.9^a	−11.8	−13.2	−13.2	−10.9	−12.7	−12.6
Dimer AcNH2-AcNH2_1.10	-15.3^a	−10.8	−12.1	−12.1	−10.1	−11.8	−11.6
Dimer AcNH2-AcNH2_1.25	-12.4^a	−8.1	−9.2	−9.1	−8.1	−9.4	−9.1
Dimer AcNH2-AcNH2_1.50	-8.0^a	−5.3	−6.0	−5.9	−5.5	−6.3	−6.1
Dimer AcNH2-AcNH2_2.00	-3.0^a	−2.4	−2.6	−2.5	−2.5	−2.7	−2.6
Dimer AcOH-Uracil_0.90	-17.9^a	−16.4	−18.2	−18.8	−15.2	−17.7	−17.8
Dimer AcOH-Uracil_0.95	-19.2^a	−16.1	−17.9	−18.4	−14.7	−17.0	−16.9
Dimer AcOH-Uracil_1.00	-19.5^a	−15.3	−16.9	−17.4	−13.7	−15.9	−15.6
Dimer AcOH-Uracil_1.05	-19.2^a	−14.1	−15.6	−16.0	−12.7	−14.7	−14.3
Dimer AcOH-Uracil_1.10	-18.4^a	−12.8	−14.3	−14.7	−11.6	−13.5	−13.1
Dimer AcOH-Uracil_1.25	-15.1^a	−9.5	−10.8	−11.0	−9.0	−10.5	−10.1
Dimer AcOH-Uracil_1.50	-9.9^a	−6.1	−7.0	−7.1	−6.0	−7.1	−6.8
Dimer AcOH-Uracil_2.00	-4.1^a	−3.0	−3.3	−3.4	−2.9	−3.3	−3.2
Dimer AcNH2-Uracil_0.90	-17.7^a	−17.1	−19.0	−19.4	−16.1	−18.6	−19.5
Dimer AcNH2-Uracil_0.95	-18.9^a	−16.8	−18.7	−18.9	−15.6	−18.0	−18.5
Dimer AcNH2-Uracil_1.00	-19.2^a	−16.0	−17.7	−17.9	−14.8	−17.1	−17.2
Dimer AcNH2-Uracil_1.05	-18.9^a	−14.9	−16.6	−16.7	−13.9	−16.0	−15.9
Dimer AcNH2-Uracil_1.10	-18.2^a	−13.8	−15.3	−15.4	−13.0	−14.9	−14.7
Dimer AcNH2-Uracil_1.25	-15.2^a	−10.7	−12.0	−11.9	−10.5	−12.0	−11.7
Dimer AcNH2-Uracil_1.50	-10.2^a	−7.3	−8.1	−8.1	−7.4	−8.4	−8.1
Dimer AcNH2-Uracil_2.00	-4.7^a	−3.8	−4.2	−4.2	−3.9	−4.3	−4.1
Dimer Benzene-Benzene_pi-pi_0.	-0.2^a	2.3	−2.3	−2.9	2.6	−3.3	−3.4
Dimer Benzene-Benzene_pi-pi_0.	-2.1^a	1.7	−2.3	−2.9	1.7	−3.3	−3.5
Dimer Benzene-Benzene_pi-pi_1.	-2.7^a	1.3	−2.1	−2.6	1.2	−3.0	−3.2
Dimer Benzene-Benzene_pi-pi_1.	-2.8^a	1.1	−1.8	−2.2	0.9	−2.5	−2.8
Dimer Benzene-Benzene_pi-pi_1.	-2.6^a	1.0	−1.5	−1.8	0.7	−2.1	−2.3
Dimer Benzene-Benzene_pi-pi_1.	-1.5^a	0.6	−0.8	−0.9	0.5	−1.1	−1.2
Dimer Benzene-Benzene_pi-pi_1.	-0.5^a	0.3	−0.2	−0.2	0.2	−0.3	−0.3
Dimer Benzene-Benzene_pi-pi_2.	-0.1^a	0.1	0.0	0.0	0.1	−0.0	−0.0
Dimer Pyridine-Pyridine_pi-pi_	-1.3^a	0.4	−4.3	−5.0	1.1	−5.0	−5.0
Dimer Pyridine-Pyridine_pi-pi_	-3.2^a	−0.0	−4.1	−4.8	0.3	−4.9	−5.0

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Table S77: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Pyridine-Pyridine_pi-pi_	−3.8[a]	−0.1	−3.7	−4.3	−0.1	−4.4	−4.6
Dimer Pyridine-Pyridine_pi-pi_	−3.9[a]	−0.2	−3.2	−3.7	−0.2	−3.8	−4.1
Dimer Pyridine-Pyridine_pi-pi_	−3.6[a]	−0.2	−2.8	−3.2	−0.2	−3.3	−3.5
Dimer Pyridine-Pyridine_pi-pi_	−2.4[a]	−0.2	−1.7	−1.9	−0.2	−1.9	−2.1
Dimer Pyridine-Pyridine_pi-pi_	−1.0[a]	−0.1	−0.7	−0.8	−0.2	−0.8	−0.9
Dimer Pyridine-Pyridine_pi-pi_	−0.2[a]	−0.1	−0.2	−0.2	−0.1	−0.2	−0.2
Dimer Uracil-Uracil_pi-pi_0.90	−7.9[a]	−4.6	−10.4	−10.8	−2.9	−10.5	−10.0
Dimer Uracil-Uracil_pi-pi_0.95	−9.5[a]	−4.6	−9.9	−10.2	−3.8	−10.5	−10.2
Dimer Uracil-Uracil_pi-pi_1.00	−9.8[a]	−4.3	−9.1	−9.3	−3.9	−9.8	−9.7
Dimer Uracil-Uracil_pi-pi_1.05	−9.4[a]	−4.0	−8.2	−8.3	−3.8	−8.9	−8.8
Dimer Uracil-Uracil_pi-pi_1.10	−8.7[a]	−3.6	−7.3	−7.4	−3.5	−8.0	−7.9
Dimer Uracil-Uracil_pi-pi_1.25	−6.1[a]	−2.6	−5.1	−5.0	−2.7	−5.5	−5.4
Dimer Uracil-Uracil_pi-pi_1.50	−3.1[a]	−1.6	−2.8	−2.7	−1.7	−2.9	−2.9
Dimer Uracil-Uracil_pi-pi_2.00	−1.0[a]	−0.7	−0.9	−0.9	−0.8	−1.0	−1.0
Dimer Benzene-Pyridine_pi-pi_0	−0.7[a]	1.3	−3.4	−4.0	1.8	−4.2	−4.2
Dimer Benzene-Pyridine_pi-pi_0	−2.7[a]	0.8	−3.3	−3.9	0.9	−4.2	−4.3
Dimer Benzene-Pyridine_pi-pi_1	−3.4[a]	0.5	−3.0	−3.5	0.5	−3.8	−4.0
Dimer Benzene-Pyridine_pi-pi_1	−3.4[a]	0.4	−2.6	−3.0	0.3	−3.3	−3.5
Dimer Benzene-Pyridine_pi-pi_1	−3.1[a]	0.3	−2.2	−2.5	0.2	−2.7	−2.9
Dimer Benzene-Pyridine_pi-pi_1	−2.0[a]	0.2	−1.3	−1.4	0.1	−1.5	−1.7
Dimer Benzene-Pyridine_pi-pi_1	−0.7[a]	0.1	−0.5	−0.5	0.0	−0.5	−0.6
Dimer Benzene-Pyridine_pi-pi_2	−0.1[a]	−0.0	−0.1	−0.1	−0.0	−0.1	−0.1
Dimer Benzene-Uracil_pi-pi_0.9	−3.5[a]	−1.1	−6.4	−7.0	0.0	−6.9	−6.1
Dimer Benzene-Uracil_pi-pi_0.9	−5.2[a]	−1.2	−6.0	−6.5	−0.7	−6.7	−6.2
Dimer Benzene-Uracil_pi-pi_1.0	−5.7[a]	−1.1	−5.3	−5.7	−0.9	−6.0	−5.7
Dimer Benzene-Uracil_pi-pi_1.0	−5.5[a]	−1.0	−4.6	−5.0	−0.9	−5.3	−5.1
Dimer Benzene-Uracil_pi-pi_1.1	−5.1[a]	−0.8	−4.0	−4.3	−0.8	−4.5	−4.4
Dimer Benzene-Uracil_pi-pi_1.2	−3.3[a]	−0.5	−2.5	−2.6	−0.5	−2.7	−2.7
Dimer Benzene-Uracil_pi-pi_1.5	−1.4[a]	−0.2	−1.0	−1.1	−0.2	−1.1	−1.1
Dimer Benzene-Uracil_pi-pi_2.0	−0.3[a]	0.0	−0.1	−0.2	−0.0	−0.2	−0.2
Dimer Pyridine-Uracil_pi-pi_0.	−3.7[a]	−2.3	−7.7	−8.4	−1.0	−8.0	−7.4
Dimer Pyridine-Uracil_pi-pi_0.	−6.2[a]	−2.6	−7.3	−8.0	−1.9	−7.9	−7.7
Dimer Pyridine-Uracil_pi-pi_1.	−6.8[a]	−2.4	−6.5	−7.1	−2.2	−7.2	−7.2
Dimer Pyridine-Uracil_pi-pi_1.	−6.6[a]	−2.2	−5.7	−6.2	−2.1	−6.3	−6.4
Dimer Pyridine-Uracil_pi-pi_1.	−6.0[a]	−2.0	−5.0	−5.4	−2.0	−5.5	−5.5
Dimer Pyridine-Uracil_pi-pi_1.	−3.9[a]	−1.4	−3.2	−3.5	−1.5	−3.4	−3.5
Dimer Pyridine-Uracil_pi-pi_1.	−1.8[a]	−0.9	−1.6	−1.7	−0.9	−1.7	−1.7
Dimer Pyridine-Uracil_pi-pi_2.	−0.5[a]	−0.4	−0.5	−0.5	−0.4	−0.5	−0.5
Dimer Benzene-Ethene_0.90	−0.3[a]	1.6	−1.1	−1.4	1.6	−1.8	−1.8
Dimer Benzene-Ethene_0.95	−1.1[a]	1.3	−1.0	−1.4	1.1	−1.7	−1.8
Dimer Benzene-Ethene_1.00	−1.4[a]	1.1	−0.9	−1.2	0.9	−1.5	−1.6
Dimer Benzene-Ethene_1.05	−1.4[a]	0.9	−0.7	−1.0	0.7	−1.2	−1.4
Dimer Benzene-Ethene_1.10	−1.3[a]	0.8	−0.6	−0.8	0.6	−1.0	−1.1
Dimer Benzene-Ethene_1.25	−0.7[a]	0.6	−0.2	−0.3	0.4	−0.4	−0.5
Dimer Benzene-Ethene_1.50	−0.2[a]	0.3	0.0	−0.0	0.2	−0.1	−0.1
Dimer Benzene-Ethene_2.00	0.0[a]	0.1	0.1	0.1	0.1	0.0	0.0
Dimer Uracil-Ethene_0.90	−2.6[a]	−0.9	−3.6	−3.9	−0.2	−3.8	−3.4
Dimer Uracil-Ethene_0.95	−3.2[a]	−0.9	−3.4	−3.7	−0.6	−3.7	−3.5
Dimer Uracil-Ethene_1.00	−3.4[a]	−0.9	−3.1	−3.3	−0.7	−3.4	−3.3
Dimer Uracil-Ethene_1.05	−3.2[a]	−0.8	−2.7	−2.9	−0.7	−3.0	−2.9
Dimer Uracil-Ethene_1.10	−3.0[a]	−0.7	−2.4	−2.6	−0.7	−2.7	−2.6
Dimer Uracil-Ethene_1.25	−2.0[a]	−0.5	−1.6	−1.7	−0.5	−1.7	−1.7
Dimer Uracil-Ethene_1.50	−0.9[a]	−0.3	−0.8	−0.8	−0.3	−0.8	−0.8
Dimer Uracil-Ethene_2.00	−0.3[a]	−0.1	−0.2	−0.2	−0.1	−0.2	−0.2
Dimer Uracil-Ethyne_0.90	−2.8[a]	−2.0	−4.4	−4.6	−1.3	−4.4	−3.8
Dimer Uracil-Ethyne_0.95	−3.6[a]	−1.9	−4.0	−4.2	−1.5	−4.3	−3.8
Dimer Uracil-Ethyne_1.00	−3.7[a]	−1.7	−3.6	−3.8	−1.5	−3.9	−3.5
Dimer Uracil-Ethyne_1.05	−3.6[a]	−1.5	−3.2	−3.3	−1.4	−3.4	−3.2
Dimer Uracil-Ethyne_1.10	−3.3[a]	−1.3	−2.8	−2.9	−1.3	−3.0	−2.8
Dimer Uracil-Ethyne_1.25	−2.2[a]	−0.9	−1.8	−1.9	−0.9	−1.9	−1.8
Dimer Uracil-Ethyne_1.50	−1.0[a]	−0.5	−0.9	−0.9	−0.5	−0.9	−0.9
Dimer Uracil-Ethyne_2.00	−0.3[a]	−0.2	−0.3	−0.3	−0.2	−0.3	−0.2
Dimer Pyridine-Ethene_0.90	−0.9[a]	0.8	−1.8	−2.2	1.0	−2.4	−2.3
Dimer Pyridine-Ethene_0.95	−1.6[a]	0.6	−1.7	−2.0	0.6	−2.3	−2.3
Dimer Pyridine-Ethene_1.00	−1.9[a]	0.5	−1.5	−1.8	0.4	−2.0	−2.1

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Table S77: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Pyridine-Ethene_1.05	−1.8[a]	0.5	−1.2	−1.5	0.3	−1.7	−1.8
Dimer Pyridine-Ethene_1.10	−1.7[a]	0.4	−1.0	−1.2	0.2	−1.5	−1.6
Dimer Pyridine-Ethene_1.25	−1.0[a]	0.3	−0.6	−0.7	0.2	−0.8	−0.9
Dimer Pyridine-Ethene_1.50	−0.4[a]	0.2	−0.2	−0.2	0.1	−0.3	−0.3
Dimer Pyridine-Ethene_2.00	−0.0[a]	0.1	0.0	−0.0	0.0	−0.0	−0.0
Dimer Pentane-Pentane_0.90	−2.9[a]	0.7	−3.8	−3.0	3.5	−2.3	−1.2
Dimer Pentane-Pentane_0.95	−3.6[a]	0.0	−4.1	−3.7	1.9	−3.2	−2.6
Dimer Pentane-Pentane_1.00	−3.8[a]	−0.2	−3.8	−3.7	1.0	−3.4	−3.0
Dimer Pentane-Pentane_1.05	−3.6[a]	−0.2	−3.4	−3.4	0.6	−3.2	−3.1
Dimer Pentane-Pentane_1.10	−3.3[a]	−0.2	−3.0	−3.0	0.3	−3.0	−2.9
Dimer Pentane-Pentane_1.25	−2.2[a]	−0.0	−1.9	−2.0	0.0	−2.0	−2.1
Dimer Pentane-Pentane_1.50	−1.1[a]	−0.0	−0.9	−0.9	0.0	−1.0	−1.0
Dimer Pentane-Pentane_2.00	−0.3[a]	0.0	−0.3	−0.3	0.0	−0.3	−0.3
Dimer Neopentane-Pentane_0.90	−1.9[a]	0.1	−3.3	−2.7	2.1	−2.1	−1.3
Dimer Neopentane-Pentane_0.95	−2.5[a]	−0.4	−3.3	−3.0	1.0	−2.6	−2.2
Dimer Neopentane-Pentane_1.00	−2.6[a]	−0.4	−3.0	−2.9	0.4	−2.6	−2.4
Dimer Neopentane-Pentane_1.05	−2.5[a]	−0.4	−2.6	−2.6	0.2	−2.4	−2.3
Dimer Neopentane-Pentane_1.10	−2.3[a]	−0.3	−2.2	−2.2	0.1	−2.1	−2.1
Dimer Neopentane-Pentane_1.25	−1.5[a]	−0.1	−1.3	−1.4	−0.0	−1.4	−1.4
Dimer Neopentane-Pentane_1.50	−0.7[a]	−0.0	−0.6	−0.7	−0.0	−0.7	−0.7
Dimer Neopentane-Pentane_2.00	−0.2[a]	−0.0	−0.2	−0.2	−0.0	−0.2	−0.2
Dimer Neopentane-Neopentane_0.	−1.5[a]	−0.8	−3.3	−3.0	0.4	−2.6	−2.2
Dimer Neopentane-Neopentane_0.	−1.7[a]	−0.7	−2.8	−2.7	0.2	−2.4	−2.2
Dimer Neopentane-Neopentane_1.	−1.8[a]	−0.5	−2.4	−2.3	0.0	−2.1	−2.0
Dimer Neopentane-Neopentane_1.	−1.7[a]	−0.3	−2.0	−2.0	−0.0	−1.8	−1.8
Dimer Neopentane-Neopentane_1.	−1.5[a]	−0.2	−1.6	−1.6	−0.0	−1.6	−1.6
Dimer Neopentane-Neopentane_1.	−1.0[a]	−0.1	−1.0	−1.0	−0.0	−1.0	−1.0
Dimer Neopentane-Neopentane_1.	−0.5[a]	−0.0	−0.5	−0.5	−0.0	−0.5	−0.5
Dimer Neopentane-Neopentane_2.	−0.1[a]	−0.0	−0.1	−0.1	−0.0	−0.1	−0.1
Dimer Cyclopentane-Neopentane_	−1.6[a]	−0.2	−3.5	−2.8	1.8	−2.3	−1.5
Dimer Cyclopentane-Neopentane_	−2.2[a]	−0.6	−3.5	−3.1	0.8	−2.7	−2.3
Dimer Cyclopentane-Neopentane_	−2.4[a]	−0.6	−3.1	−3.0	0.3	−2.6	−2.4
Dimer Cyclopentane-Neopentane_	−2.3[a]	−0.5	−2.7	−2.6	0.1	−2.4	−2.3
Dimer Cyclopentane-Neopentane_	−2.1[a]	−0.4	−2.2	−2.3	0.0	−2.1	−2.1
Dimer Cyclopentane-Neopentane_	−1.5[a]	−0.1	−1.4	−1.4	−0.0	−1.4	−1.4
Dimer Cyclopentane-Neopentane_	−0.7[a]	−0.0	−0.6	−0.7	−0.0	−0.7	−0.7
Dimer Cyclopentane-Neopentane_	−0.2[a]	−0.0	−0.2	−0.2	−0.0	−0.2	−0.2
Dimer Cyclopentane-Cyclopentan	−2.2[a]	0.2	−3.4	−2.7	2.4	−2.1	−1.3
Dimer Cyclopentane-Cyclopentan	−2.8[a]	−0.3	−3.5	−3.1	1.3	−2.6	−2.1
Dimer Cyclopentane-Cyclopentan	−3.0[a]	−0.4	−3.2	−3.0	0.7	−2.7	−2.4
Dimer Cyclopentane-Cyclopentan	−2.9[a]	−0.3	−2.8	−2.7	0.4	−2.5	−2.4
Dimer Cyclopentane-Cyclopentan	−2.6[a]	−0.2	−2.3	−2.4	0.2	−2.3	−2.2
Dimer Cyclopentane-Cyclopentan	−1.7[a]	−0.0	−1.4	−1.5	0.0	−1.5	−1.5
Dimer Cyclopentane-Cyclopentan	−0.8[a]	−0.0	−0.7	−0.7	0.0	−0.7	−0.7
Dimer Cyclopentane-Cyclopentan	−0.2[a]	0.0	−0.2	−0.2	0.0	−0.2	−0.2
Dimer Benzene-Cyclopentane_0.9	−2.2[a]	1.3	−2.8	−2.8	2.7	−2.5	−2.1
Dimer Benzene-Cyclopentane_0.9	−3.2[a]	0.6	−3.0	−3.1	1.5	−3.0	−2.8
Dimer Benzene-Cyclopentane_1.0	−3.6[a]	0.3	−2.9	−3.0	0.9	−3.0	−3.0
Dimer Benzene-Cyclopentane_1.0	−3.5[a]	0.2	−2.5	−2.7	0.5	−2.8	−2.8
Dimer Benzene-Cyclopentane_1.1	−3.2[a]	0.1	−2.2	−2.4	0.3	−2.4	−2.5
Dimer Benzene-Cyclopentane_1.2	−2.1[a]	0.1	−1.4	−1.5	0.1	−1.5	−1.6
Dimer Benzene-Cyclopentane_1.5	−0.9[a]	0.0	−0.6	−0.6	0.0	−0.6	−0.7
Dimer Benzene-Cyclopentane_2.0	−0.2[a]	0.0	−0.1	−0.1	0.0	−0.1	−0.1
Dimer Benzene-Neopentane_0.90	−1.9[a]	0.4	−3.0	−2.9	1.6	−2.6	−2.4
Dimer Benzene-Neopentane_0.95	−2.7[a]	−0.0	−3.0	−3.0	0.7	−2.9	−2.8
Dimer Benzene-Neopentane_1.00	−2.9[a]	−0.1	−2.7	−2.8	0.3	−2.7	−2.7
Dimer Benzene-Neopentane_1.05	−2.8[a]	−0.2	−2.4	−2.5	0.1	−2.5	−2.5
Dimer Benzene-Neopentane_1.10	−2.6[a]	−0.2	−2.0	−2.1	−0.0	−2.1	−2.2
Dimer Benzene-Neopentane_1.25	−1.7[a]	−0.1	−1.3	−1.3	−0.1	−1.3	−1.4
Dimer Benzene-Neopentane_1.50	−0.8[a]	−0.1	−0.6	−0.6	−0.0	−0.6	−0.6
Dimer Benzene-Neopentane_2.00	−0.2[a]	−0.0	−0.1	−0.1	−0.0	−0.1	−0.1
Dimer Uracil-Pentane_0.90	−3.8[a]	0.2	−4.7	−4.8	1.6	−4.7	−3.8
Dimer Uracil-Pentane_0.95	−4.7[a]	−0.4	−4.8	−5.0	0.4	−5.0	−4.6
Dimer Uracil-Pentane_1.00	−4.8[a]	−0.6	−4.5	−4.7	−0.1	−4.9	−4.7
Dimer Uracil-Pentane_1.05	−4.6[a]	−0.6	−4.0	−4.3	−0.4	−4.5	−4.4

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Table S77: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Uracil-Pentane_1.10	-4.1^a	−0.5	−3.5	−3.7	−0.4	−3.9	−3.8
Dimer Uracil-Pentane_1.25	-2.4^a	−0.3	−2.1	−2.2	−0.3	−2.2	−2.3
Dimer Uracil-Pentane_1.50	-1.0^a	−0.1	−0.9	−0.9	−0.1	−0.9	−0.9
Dimer Uracil-Pentane_2.00	-0.2^a	−0.0	−0.2	−0.2	−0.0	−0.2	−0.2
Dimer Uracil-Cyclopentane_0.90	-3.0^a	0.5	−3.8	−3.9	1.8	−3.8	−3.1
Dimer Uracil-Cyclopentane_0.95	-4.0^a	−0.1	−3.9	−4.1	0.6	−4.2	−3.9
Dimer Uracil-Cyclopentane_1.00	-4.1^a	−0.3	−3.7	−3.9	0.1	−4.0	−3.9
Dimer Uracil-Cyclopentane_1.05	-3.9^a	−0.3	−3.3	−3.5	−0.1	−3.7	−3.6
Dimer Uracil-Cyclopentane_1.10	-3.5^a	−0.3	−2.9	−3.1	−0.2	−3.2	−3.2
Dimer Uracil-Cyclopentane_1.25	-2.3^a	−0.2	−1.9	−2.0	−0.2	−2.0	−2.1
Dimer Uracil-Cyclopentane_1.50	-1.0^a	−0.1	−0.9	−0.9	−0.1	−0.9	−0.9
Dimer Uracil-Cyclopentane_2.00	-0.2^a	−0.0	−0.2	−0.2	−0.0	−0.2	−0.2
Dimer Uracil-Neopentane_0.90	-2.9^a	0.1	−3.6	−3.6	1.2	−3.4	−2.9
Dimer Uracil-Neopentane_0.95	-3.6^a	−0.3	−3.5	−3.7	0.3	−3.6	−3.4
Dimer Uracil-Neopentane_1.00	-3.7^a	−0.4	−3.2	−3.4	−0.1	−3.5	−3.3
Dimer Uracil-Neopentane_1.05	-3.5^a	−0.4	−2.9	−3.0	−0.2	−3.1	−3.1
Dimer Uracil-Neopentane_1.10	-3.1^a	−0.4	−2.5	−2.6	−0.3	−2.7	−2.7
Dimer Uracil-Neopentane_1.25	-2.0^a	−0.2	−1.6	−1.7	−0.2	−1.7	−1.7
Dimer Uracil-Neopentane_1.50	-0.9^a	−0.1	−0.7	−0.7	−0.1	−0.8	−0.8
Dimer Uracil-Neopentane_2.00	-0.2^a	−0.0	−0.2	−0.2	−0.0	−0.2	−0.2
Dimer Ethene-Pentane_0.90	-1.7^a	0.1	−2.1	−1.8	1.5	−1.5	−0.9
Dimer Ethene-Pentane_0.95	-2.0^a	−0.2	−2.2	−2.0	0.7	−1.8	−1.5
Dimer Ethene-Pentane_1.00	-2.0^a	−0.2	−2.0	−2.0	0.3	−1.8	−1.7
Dimer Ethene-Pentane_1.05	-1.9^a	−0.2	−1.8	−1.8	0.1	−1.7	−1.7
Dimer Ethene-Pentane_1.10	-1.7^a	−0.2	−1.6	−1.6	0.0	−1.6	−1.5
Dimer Ethene-Pentane_1.25	-1.1^a	−0.1	−1.0	−1.0	−0.0	−1.0	−1.1
Dimer Ethene-Pentane_1.50	-0.5^a	−0.0	−0.5	−0.5	−0.0	−0.5	−0.5
Dimer Ethene-Pentane_2.00	-0.1^a	−0.0	−0.1	−0.1	−0.0	−0.1	−0.1
Dimer Ethyne-Pentane_0.90	-1.1^a	0.3	−1.7	−1.7	1.0	−1.6	−1.4
Dimer Ethyne-Pentane_0.95	-1.6^a	0.1	−1.6	−1.7	0.5	−1.7	−1.6
Dimer Ethyne-Pentane_1.00	-1.7^a	0.1	−1.5	−1.6	0.3	−1.6	−1.6
Dimer Ethyne-Pentane_1.05	-1.7^a	0.1	−1.3	−1.4	0.2	−1.4	−1.4
Dimer Ethyne-Pentane_1.10	-1.5^a	0.0	−1.1	−1.2	0.1	−1.2	−1.2
Dimer Ethyne-Pentane_1.25	-1.0^a	0.0	−0.7	−0.7	0.1	−0.7	−0.7
Dimer Ethyne-Pentane_1.50	-0.4^a	0.0	−0.3	−0.3	0.0	−0.3	−0.3
Dimer Ethyne-Pentane_2.00	-0.1^a	0.0	−0.1	−0.1	0.0	−0.1	−0.1
Dimer Peptide-Pentane_0.90	-3.8^a	0.2	−3.8	−3.6	1.9	−3.2	−2.4
Dimer Peptide-Pentane_0.95	-4.2^a	−0.3	−3.8	−3.8	0.9	−3.6	−3.1
Dimer Peptide-Pentane_1.00	-4.2^a	−0.4	−3.7	−3.7	0.4	−3.6	−3.3
Dimer Peptide-Pentane_1.05	-4.0^a	−0.4	−3.3	−3.5	0.1	−3.4	−3.3
Dimer Peptide-Pentane_1.10	-3.7^a	−0.4	−3.0	−3.1	−0.0	−3.1	−3.1
Dimer Peptide-Pentane_1.25	-2.6^a	−0.3	−2.1	−2.2	−0.1	−2.2	−2.2
Dimer Peptide-Pentane_1.50	-1.2^a	−0.1	−1.0	−1.0	−0.1	−1.0	−1.0
Dimer Peptide-Pentane_2.00	-0.3^a	−0.0	−0.2	−0.2	−0.0	−0.2	−0.2
Dimer Benzene-Benzene_TS_0.90	-1.6^a	0.2	−2.7	−2.5	1.6	−2.0	−1.6
Dimer Benzene-Benzene_TS_0.95	-2.6^a	−0.4	−2.9	−2.8	0.6	−2.5	−2.3
Dimer Benzene-Benzene_TS_1.00	-2.9^a	−0.6	−2.8	−2.8	0.1	−2.6	−2.5
Dimer Benzene-Benzene_TS_1.05	-2.8^a	−0.6	−2.5	−2.5	−0.1	−2.5	−2.4
Dimer Benzene-Benzene_TS_1.10	-2.6^a	−0.6	−2.3	−2.3	−0.2	−2.2	−2.2
Dimer Benzene-Benzene_TS_1.25	-1.8^a	−0.4	−1.5	−1.5	−0.3	−1.5	−1.5
Dimer Benzene-Benzene_TS_1.50	-0.8^a	−0.3	−0.8	−0.7	−0.2	−0.7	−0.7
Dimer Benzene-Benzene_TS_2.00	-0.2^a	−0.1	−0.2	−0.2	−0.1	−0.2	−0.2
Dimer Pyridine-Pyridine_TS_0.9	-2.5^a	−0.6	−3.3	−3.2	0.7	−2.8	−2.5
Dimer Pyridine-Pyridine_TS_0.9	-3.3^a	−1.0	−3.4	−3.5	−0.1	−3.1	−3.0
Dimer Pyridine-Pyridine_TS_1.0	-3.5^a	−1.2	−3.3	−3.4	−0.5	−3.1	−3.1
Dimer Pyridine-Pyridine_TS_1.0	-3.5^a	−1.1	−3.1	−3.2	−0.6	−3.0	−3.0
Dimer Pyridine-Pyridine_TS_1.1	-3.2^a	−1.1	−2.8	−2.9	−0.7	−2.7	−2.8
Dimer Pyridine-Pyridine_TS_1.2	-2.3^a	−0.8	−2.0	−2.1	−0.6	−1.9	−2.0
Dimer Pyridine-Pyridine_TS_1.5	-1.2^a	−0.5	−1.1	−1.1	−0.4	−1.0	−1.0
Dimer Pyridine-Pyridine_TS_2.0	-0.4^a	−0.2	−0.4	−0.4	−0.2	−0.3	−0.3
Dimer Benzene-Pyridine_TS_0.90	-2.1^a	−0.3	−3.2	−3.0	1.3	−2.4	−2.0
Dimer Benzene-Pyridine_TS_0.95	-3.0^a	−0.9	−3.4	−3.4	0.3	−2.9	−2.7
Dimer Benzene-Pyridine_TS_1.00	-3.3^a	−1.0	−3.3	−3.3	−0.2	−3.0	−2.9
Dimer Benzene-Pyridine_TS_1.05	-3.3^a	−1.0	−3.0	−3.0	−0.5	−2.8	−2.8
Dimer Benzene-Pyridine_TS_1.10	-3.0^a	−1.0	−2.7	−2.7	−0.6	−2.6	−2.6

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Table S77: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Benzene-Pyridine_TS_1.25	-2.1^a	−0.8	−1.8	−1.9	−0.5	−1.8	−1.8
Dimer Benzene-Pyridine_TS_1.50	-1.0^a	−0.5	−1.0	−1.0	−0.4	−0.9	−0.9
Dimer Benzene-Pyridine_TS_2.00	-0.3^a	−0.2	−0.3	−0.3	−0.2	−0.3	−0.3
Dimer Benzene-Ethyne_CH-pi_0.9	-1.9^a	−1.5	−3.2	−2.9	0.4	−1.9	−1.3
Dimer Benzene-Ethyne_CH-pi_0.9	-2.6^a	−1.8	−3.3	−3.1	−0.4	−2.4	−2.0
Dimer Benzene-Ethyne_CH-pi_1.0	-2.9^a	−1.8	−3.2	−3.0	−0.7	−2.5	−2.2
Dimer Benzene-Ethyne_CH-pi_1.0	-2.8^a	−1.6	−2.9	−2.7	−0.9	−2.4	−2.2
Dimer Benzene-Ethyne_CH-pi_1.1	-2.6^a	−1.5	−2.5	−2.4	−0.9	−2.2	−2.1
Dimer Benzene-Ethyne_CH-pi_1.2	-1.8^a	−1.1	−1.8	−1.7	−0.7	−1.5	−1.5
Dimer Benzene-Ethyne_CH-pi_1.5	-0.9^a	−0.6	−1.0	−0.9	−0.5	−0.8	−0.8
Dimer Benzene-Ethyne_CH-pi_2.0	-0.3^a	−0.2	−0.3	−0.3	−0.2	−0.3	−0.2
Dimer Ethyne-Ethyne_TS_0.90	-1.2^a	−1.6	−2.3	−2.1	−0.8	−1.6	−1.3
Dimer Ethyne-Ethyne_TS_0.95	-1.5^a	−1.4	−1.9	−1.8	−0.7	−1.5	−1.3
Dimer Ethyne-Ethyne_TS_1.00	-1.5^a	−1.1	−1.7	−1.6	−0.7	−1.3	−1.2
Dimer Ethyne-Ethyne_TS_1.05	-1.5^a	−1.0	−1.4	−1.3	−0.6	−1.2	−1.1
Dimer Ethyne-Ethyne_TS_1.10	-1.3^a	−0.8	−1.2	−1.2	−0.5	−1.0	−1.0
Dimer Ethyne-Ethyne_TS_1.25	-0.9^a	−0.5	−0.8	−0.8	−0.4	−0.7	−0.7
Dimer Ethyne-Ethyne_TS_1.50	-0.5^a	−0.3	−0.4	−0.4	−0.2	−0.4	−0.3
Dimer Ethyne-Ethyne_TS_2.00	-0.1^a	−0.1	−0.1	−0.1	−0.1	−0.1	−0.1
Dimer Benzene-AcOH_OH-pi_0.90	-4.0^a	−2.8	−5.0	−5.0	−1.1	−4.0	−3.6
Dimer Benzene-AcOH_OH-pi_0.95	-4.6^a	−2.8	−4.8	−4.8	−1.5	−4.1	−3.8
Dimer Benzene-AcOH_OH-pi_1.00	-4.7^a	−2.6	−4.5	−4.4	−1.7	−4.0	−3.7
Dimer Benzene-AcOH_OH-pi_1.05	-4.5^a	−2.4	−4.0	−3.9	−1.6	−3.7	−3.5
Dimer Benzene-AcOH_OH-pi_1.10	-4.2^a	−2.1	−3.6	−3.5	−1.6	−3.4	−3.2
Dimer Benzene-AcOH_OH-pi_1.25	-3.1^a	−1.5	−2.5	−2.5	−1.2	−2.4	−2.3
Dimer Benzene-AcOH_OH-pi_1.50	-1.7^a	−0.9	−1.4	−1.4	−0.8	−1.4	−1.3
Dimer Benzene-AcOH_OH-pi_2.00	-0.6^a	−0.3	−0.5	−0.5	−0.3	−0.5	−0.4
Dimer Benzene-AcNH2_NH-pi_0.90	-3.8^a	−3.2	−5.3	−5.1	−1.8	−4.4	−3.9
Dimer Benzene-AcNH2_NH-pi_0.95	-4.3^a	−3.2	−5.0	−4.9	−2.0	−4.4	−4.0
Dimer Benzene-AcNH2_NH-pi_1.00	-4.4^a	−3.0	−4.7	−4.5	−2.1	−4.2	−3.9
Dimer Benzene-AcNH2_NH-pi_1.05	-4.2^a	−2.7	−4.2	−4.1	−2.0	−3.9	−3.7
Dimer Benzene-AcNH2_NH-pi_1.10	-4.0^a	−2.4	−3.8	−3.7	−1.9	−3.6	−3.4
Dimer Benzene-AcNH2_NH-pi_1.25	-3.0^a	−1.7	−2.7	−2.6	−1.5	−2.6	−2.5
Dimer Benzene-AcNH2_NH-pi_1.50	-1.6^a	−1.0	−1.5	−1.5	−0.9	−1.4	−1.4
Dimer Benzene-AcNH2_NH-pi_2.00	-0.5^a	−0.4	−0.5	−0.5	−0.3	−0.4	−0.4
Dimer Benzene-Water_OH-pi_0.90	-2.8^a	−2.6	−4.0	−3.9	−1.5	−3.4	−3.0
Dimer Benzene-Water_OH-pi_0.95	-3.2^a	−2.5	−3.8	−3.7	−1.7	−3.4	−3.1
Dimer Benzene-Water_OH-pi_1.00	-3.3^a	−2.3	−3.5	−3.4	−1.7	−3.2	−3.0
Dimer Benzene-Water_OH-pi_1.05	-3.1^a	−2.1	−3.1	−3.1	−1.7	−3.0	−2.8
Dimer Benzene-Water_OH-pi_1.10	-2.9^a	−1.9	−2.8	−2.7	−1.6	−2.7	−2.6
Dimer Benzene-Water_OH-pi_1.25	-2.1^a	−1.4	−2.0	−2.0	−1.3	−2.0	−1.9
Dimer Benzene-Water_OH-pi_1.50	-1.2^a	−0.9	−1.2	−1.2	−0.8	−1.2	−1.1
Dimer Benzene-Water_OH-pi_2.00	-0.4^a	−0.4	−0.5	−0.5	−0.4	−0.5	−0.4
Dimer Benzene-MeOH_OH-pi_0.90	-3.5^a	−1.7	−4.0	−4.0	−0.3	−3.4	−3.1
Dimer Benzene-MeOH_OH-pi_0.95	-4.0^a	−1.8	−4.0	−4.0	−0.8	−3.6	−3.3
Dimer Benzene-MeOH_OH-pi_1.00	-4.2^a	−1.8	−3.7	−3.7	−1.1	−3.5	−3.3
Dimer Benzene-MeOH_OH-pi_1.05	-4.1^a	−1.6	−3.4	−3.4	−1.2	−3.3	−3.2
Dimer Benzene-MeOH_OH-pi_1.10	-3.8^a	−1.5	−3.1	−3.0	−1.2	−3.1	−3.0
Dimer Benzene-MeOH_OH-pi_1.25	-2.8^a	−1.1	−2.2	−2.2	−1.0	−2.2	−2.2
Dimer Benzene-MeOH_OH-pi_1.50	-1.5^a	−0.7	−1.3	−1.2	−0.7	−1.3	−1.2
Dimer Benzene-MeOH_OH-pi_2.00	-0.5^a	−0.3	−0.5	−0.4	−0.3	−0.4	−0.4
Dimer Benzene-MeNH2_NH-pi_0.90	-2.5^a	−0.4	−3.0	−3.1	0.8	−2.5	−2.3
Dimer Benzene-MeNH2_NH-pi_0.95	-3.1^a	−0.7	−3.0	−3.2	0.1	−2.8	−2.7
Dimer Benzene-MeNH2_NH-pi_1.00	-3.2^a	−0.8	−2.9	−3.0	−0.3	−2.8	−2.8
Dimer Benzene-MeNH2_NH-pi_1.05	-3.1^a	−0.8	−2.6	−2.7	−0.5	−2.6	−2.6
Dimer Benzene-MeNH2_NH-pi_1.10	-2.9^a	−0.8	−2.3	−2.4	−0.5	−2.4	−2.4
Dimer Benzene-MeNH2_NH-pi_1.25	-1.9^a	−0.6	−1.6	−1.6	−0.5	−1.6	−1.6
Dimer Benzene-MeNH2_NH-pi_1.50	-0.9^a	−0.4	−0.8	−0.8	−0.3	−0.8	−0.8
Dimer Benzene-MeNH2_NH-pi_2.00	-0.3^a	−0.1	−0.2	−0.2	−0.1	−0.2	−0.2
Dimer Benzene-Peptide_NH-pi_0.	-3.7^a	−1.0	−4.7	−4.7	1.1	−3.7	−3.0
Dimer Benzene-Peptide_NH-pi_0.	-5.0^a	−1.7	−5.0	−5.0	−0.3	−4.4	−3.9
Dimer Benzene-Peptide_NH-pi_1.	-5.3^a	−1.9	−4.8	−4.8	−0.9	−4.5	−4.2
Dimer Benzene-Peptide_NH-pi_1.	-5.1^a	−1.8	−4.4	−4.4	−1.1	−4.2	−4.0
Dimer Benzene-Peptide_NH-pi_1.	-4.8^a	−1.7	−3.9	−3.9	−1.2	−3.9	−3.7
Dimer Benzene-Peptide_NH-pi_1.	-3.4^a	−1.3	−2.8	−2.7	−1.1	−2.7	−2.7

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Table S77: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Benzene-Peptide_NH-pi_1.	-1.8^{a}	−0.8	−1.5	−1.5	−0.7	−1.5	−1.4
Dimer Benzene-Peptide_NH-pi_2.	-0.6^{a}	−0.4	−0.6	−0.5	−0.4	−0.5	−0.5
Dimer Pyridine-Pyridine_CH-N_0	-2.8^{a}	−1.8	−3.5	−3.0	−0.7	−2.9	−3.2
Dimer Pyridine-Pyridine_CH-N_0	-3.8^{a}	−2.4	−4.0	−3.8	−1.4	−3.4	−3.6
Dimer Pyridine-Pyridine_CH-N_1	-4.1^{a}	−2.6	−3.9	−4.0	−1.8	−3.4	−3.7
Dimer Pyridine-Pyridine_CH-N_1	-3.9^{a}	−2.4	−3.5	−3.7	−1.7	−3.1	−3.4
Dimer Pyridine-Pyridine_CH-N_1	-3.4^{a}	−2.1	−3.1	−3.3	−1.6	−2.8	−3.0
Dimer Pyridine-Pyridine_CH-N_1	-2.2^{a}	−1.3	−1.9	−2.1	−1.0	−1.8	−1.9
Dimer Pyridine-Pyridine_CH-N_1	-1.0^{a}	−0.6	−1.0	−1.0	−0.5	−0.8	−0.9
Dimer Pyridine-Pyridine_CH-N_2	-0.3^{a}	−0.2	−0.3	−0.3	−0.1	−0.2	−0.3
Dimer Ethyne-Water_CH-O_0.90	-2.5^{a}	−3.7	−4.1	−4.0	−3.1	−3.6	−3.1
Dimer Ethyne-Water_CH-O_0.95	-2.8^{a}	−3.4	−3.7	−3.6	−2.9	−3.4	−3.0
Dimer Ethyne-Water_CH-O_1.00	-2.8^{a}	−3.0	−3.3	−3.2	−2.7	−3.1	−2.8
Dimer Ethyne-Water_CH-O_1.05	-2.8^{a}	−2.7	−3.0	−2.9	−2.5	−2.9	−2.6
Dimer Ethyne-Water_CH-O_1.10	-2.6^{a}	−2.4	−2.7	−2.6	−2.3	−2.6	−2.4
Dimer Ethyne-Water_CH-O_1.25	-2.0^{a}	−1.8	−2.0	−1.9	−1.7	−2.0	−1.8
Dimer Ethyne-Water_CH-O_1.50	-1.2^{a}	−1.1	−1.2	−1.2	−1.1	−1.2	−1.1
Dimer Ethyne-Water_CH-O_2.00	-0.5^{a}	−0.5	−0.5	−0.5	−0.5	−0.5	−0.5
Dimer Ethyne-AcOH_OH-pi_0.90	-4.3^{a}	−4.8	−6.0	−5.9	−3.1	−4.7	−4.2
Dimer Ethyne-AcOH_OH-pi_0.95	-4.8^{a}	−4.4	−5.4	−5.4	−3.0	−4.5	−4.1
Dimer Ethyne-AcOH_OH-pi_1.00	-4.9^{a}	−3.9	−4.8	−4.8	−2.8	−4.1	−3.8
Dimer Ethyne-AcOH_OH-pi_1.05	-4.7^{a}	−3.4	−4.2	−4.2	−2.5	−3.7	−3.4
Dimer Ethyne-AcOH_OH-pi_1.10	-4.4^{a}	−2.9	−3.7	−3.7	−2.2	−3.3	−3.1
Dimer Ethyne-AcOH_OH-pi_1.25	-3.3^{a}	−1.9	−2.5	−2.5	−1.6	−2.3	−2.2
Dimer Ethyne-AcOH_OH-pi_1.50	-1.8^{a}	−1.0	−1.4	−1.4	−0.9	−1.3	−1.2
Dimer Ethyne-AcOH_OH-pi_2.00	-0.6^{a}	−0.4	−0.5	−0.5	−0.3	−0.4	−0.4
Dimer Pentane-AcOH_0.90	-2.7^{a}	−0.6	−3.4	−3.4	0.4	−3.2	−2.9
Dimer Pentane-AcOH_0.95	-2.9^{a}	−0.6	−3.2	−3.2	0.0	−3.1	−3.0
Dimer Pentane-AcOH_1.00	-2.9^{a}	−0.6	−2.9	−3.0	−0.1	−3.0	−2.9
Dimer Pentane-AcOH_1.05	-2.7^{a}	−0.5	−2.6	−2.7	−0.2	−2.7	−2.7
Dimer Pentane-AcOH_1.10	-2.5^{a}	−0.5	−2.3	−2.4	−0.3	−2.5	−2.5
Dimer Pentane-AcOH_1.25	-1.8^{a}	−0.3	−1.6	−1.7	−0.2	−1.7	−1.8
Dimer Pentane-AcOH_1.50	-0.8^{a}	−0.1	−0.8	−0.8	−0.1	−0.8	−0.8
Dimer Pentane-AcOH_2.00	-0.2^{a}	−0.0	−0.2	−0.2	−0.0	−0.2	−0.2
Dimer Pentane-AcNH2_0.90	-3.2^{a}	−0.7	−3.8	−3.8	0.6	−3.4	−3.0
Dimer Pentane-AcNH2_0.95	-3.5^{a}	−0.8	−3.6	−3.7	0.1	−3.5	−3.2
Dimer Pentane-AcNH2_1.00	-3.5^{a}	−0.8	−3.3	−3.4	−0.2	−3.3	−3.2
Dimer Pentane-AcNH2_1.05	-3.3^{a}	−0.7	−3.0	−3.1	−0.3	−3.0	−3.0
Dimer Pentane-AcNH2_1.10	-3.0^{a}	−0.6	−2.6	−2.7	−0.3	−2.7	−2.7
Dimer Pentane-AcNH2_1.25	-2.1^{a}	−0.4	−1.7	−1.8	−0.3	−1.8	−1.9
Dimer Pentane-AcNH2_1.50	-1.0^{a}	−0.2	−0.9	−0.9	−0.1	−0.9	−0.9
Dimer Pentane-AcNH2_2.00	-0.3^{a}	−0.0	−0.2	−0.2	−0.0	−0.2	−0.2
Dimer Benzene-AcOH_0.90	-2.7^{a}	−1.3	−4.3	−4.4	0.2	−3.8	−3.5
Dimer Benzene-AcOH_0.95	-3.6^{a}	−1.5	−4.2	−4.3	−0.4	−3.9	−3.7
Dimer Benzene-AcOH_1.00	-3.8^{a}	−1.5	−3.9	−4.0	−0.7	−3.7	−3.6
Dimer Benzene-AcOH_1.05	-3.7^{a}	−1.3	−3.5	−3.6	−0.8	−3.4	−3.3
Dimer Benzene-AcOH_1.10	-3.3^{a}	−1.2	−3.1	−3.1	−0.8	−3.0	−3.0
Dimer Benzene-AcOH_1.25	-2.2^{a}	−0.9	−2.0	−2.1	−0.6	−1.9	−2.0
Dimer Benzene-AcOH_1.50	-1.0^{a}	−0.5	−1.0	−1.0	−0.4	−0.9	−0.9
Dimer Benzene-AcOH_2.00	-0.3^{a}	−0.2	−0.3	−0.3	−0.1	−0.2	−0.2
Dimer Peptide-Ethene_0.90	-2.6^{a}	−1.3	−3.3	−3.3	−0.3	−2.9	−2.7
Dimer Peptide-Ethene_0.95	-2.9^{a}	−1.3	−3.1	−3.2	−0.6	−2.9	−2.8
Dimer Peptide-Ethene_1.00	-3.0^{a}	−1.2	−2.8	−2.9	−0.7	−2.7	−2.7
Dimer Peptide-Ethene_1.05	-2.9^{a}	−1.0	−2.5	−2.6	−0.7	−2.5	−2.5
Dimer Peptide-Ethene_1.10	-2.6^{a}	−0.9	−2.2	−2.3	−0.7	−2.3	−2.3
Dimer Peptide-Ethene_1.25	-1.9^{a}	−0.6	−1.6	−1.6	−0.5	−1.6	−1.6
Dimer Peptide-Ethene_1.50	-0.9^{a}	−0.3	−0.8	−0.8	−0.3	−0.8	−0.8
Dimer Peptide-Ethene_2.00	-0.2^{a}	−0.1	−0.2	−0.2	−0.1	−0.2	−0.2
Dimer Pyridine-Ethyne_0.90	-3.5^{a}	−4.0	−4.9	−4.5	−3.6	−4.7	−5.0
Dimer Pyridine-Ethyne_0.95	-3.9^{a}	−3.7	−4.5	−4.3	−3.2	−4.3	−4.4
Dimer Pyridine-Ethyne_1.00	-4.0^{a}	−3.3	−4.1	−4.0	−2.9	−3.8	−4.0
Dimer Pyridine-Ethyne_1.05	-3.9^{a}	−3.0	−3.7	−3.7	−2.6	−3.4	−3.6
Dimer Pyridine-Ethyne_1.10	-3.7^{a}	−2.7	−3.3	−3.4	−2.3	−3.1	−3.2
Dimer Pyridine-Ethyne_1.25	-2.8^{a}	−2.0	−2.4	−2.5	−1.7	−2.2	−2.3
Dimer Pyridine-Ethyne_1.50	-1.7^{a}	−1.2	−1.4	−1.5	−1.0	−1.3	−1.4

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Table S77: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Pyridine-Ethyne_2.00	-0.6^{a}	-0.5	-0.6	-0.6	-0.4	-0.5	-0.6
Dimer MeNH2-Pyridine_0.90	-3.4^{a}	-0.2	-2.4	-2.6	0.3	-2.5	-2.7
Dimer MeNH2-Pyridine_0.95	-3.9^{a}	-0.8	-2.8	-3.0	-0.3	-2.9	-3.1
Dimer MeNH2-Pyridine_1.00	-4.0^{a}	-1.0	-2.8	-3.0	-0.6	-2.9	-3.1
Dimer MeNH2-Pyridine_1.05	-3.9^{a}	-1.1	-2.7	-2.9	-0.8	-2.8	-3.1
Dimer MeNH2-Pyridine_1.10	-3.6^{a}	-1.0	-2.6	-2.8	-0.8	-2.7	-2.9
Dimer MeNH2-Pyridine_1.25	-2.7^{a}	-0.8	-1.9	-2.1	-0.7	-2.0	-2.2
Dimer MeNH2-Pyridine_1.50	-1.5^{a}	-0.5	-1.1	-1.2	-0.5	-1.1	-1.2
Dimer MeNH2-Pyridine_2.00	-0.5^{a}	-0.2	-0.4	-0.4	-0.2	-0.4	-0.4

a J.Rezac, K.E.Riley, and P.Hobza, J.Chem.Theory Comput. 7, 2427 (2011) ; 7, 3466 (2011).

Table S78: Benchmark Results for the S66a8 Set. Interaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Water-Water_1_y_-30	−4.1[a]	−3.2	−3.6	−3.6	−3.6	−4.0	−3.7
Dimer Water-Water_1_y_+30	−4.1[a]	−3.2	−3.6	−3.6	−3.6	−4.0	−3.7
Dimer Water-Water_1_z_-30	−4.3[a]	−3.5	−3.9	−4.0	−3.9	−4.4	−4.1
Dimer Water-Water_1_z_+30	−4.2[a]	−3.2	−3.5	−3.6	−3.4	−3.9	−3.6
Dimer Water-Water_2_y_-30	−3.9[a]	−3.2	−3.6	−3.7	−3.2	−3.7	−3.3
Dimer Water-Water_2_y_+30	−3.9[a]	−3.2	−3.6	−3.7	−3.2	−3.7	−3.3
Dimer Water-Water_2_z_-30	−4.5[a]	−3.3	−3.7	−3.9	−3.3	−3.8	−3.4
Dimer Water-Water_2_z_+30	−4.7[a]	−3.7	−4.0	−4.0	−3.9	−4.3	−4.0
Dimer Water-MeOH_1_y_-30	−4.7[a]	−3.4	−3.9	−4.0	−3.4	−4.1	−3.8
Dimer Water-MeOH_1_y_+30	−4.8[a]	−3.2	−3.8	−4.0	−3.2	−4.0	−3.7
Dimer Water-MeOH_1_z_-30	−4.8[a]	−3.6	−4.2	−4.3	−3.7	−4.4	−4.1
Dimer Water-MeOH_1_z_+30	−4.9[a]	−3.1	−3.7	−3.9	−3.0	−3.8	−3.5
Dimer Water-MeOH_2_y_-30	−4.4[a]	−3.0	−3.4	−3.7	−2.6	−3.2	−2.9
Dimer Water-MeOH_2_y_+30	−3.3[a]	−2.7	−3.3	−3.2	−2.3	−3.2	−2.7
Dimer Water-MeOH_2_z_-30	−4.7[a]	−3.0	−3.7	−3.8	−2.4	−3.4	−2.9
Dimer Water-MeOH_2_z_+30	−5.3[a]	−3.6	−4.1	−4.3	−3.5	−4.1	−3.8
Dimer Water-MeNH2_1_y_-30	−5.6[a]	−3.6	−4.1	−4.0	−4.0	−4.7	−5.0
Dimer Water-MeNH2_1_y_+30	−5.6[a]	−3.5	−4.1	−3.9	−3.9	−4.7	−4.9
Dimer Water-MeNH2_1_z_-30	−5.8[a]	−4.1	−4.7	−4.5	−4.6	−5.4	−5.7
Dimer Water-MeNH2_1_z_+30	−5.8[a]	−3.3	−3.8	−3.6	−3.6	−4.4	−4.6
Dimer Water-MeNH2_2_y_-30	−5.6[a]	−3.1	−3.8	−3.3	−3.5	−4.4	−4.6
Dimer Water-MeNH2_2_y_+30	−5.6[a]	−3.1	−3.8	−3.4	−3.5	−4.4	−4.6
Dimer Water-MeNH2_2_z_-30	−5.6[a]	−3.3	−3.9	−3.5	−3.8	−4.6	−4.7
Dimer Water-MeNH2_2_z_+30	−5.6[a]	−2.7	−3.5	−3.1	−2.8	−3.9	−4.1
Dimer MeOH-Water_1_y_-30	−4.3[a]	−2.8	−3.2	−3.3	−3.0	−3.6	−3.4
Dimer MeOH-Water_1_y_+30	−4.3[a]	−2.8	−3.2	−3.3	−3.0	−3.6	−3.4
Dimer MeOH-Water_1_z_-30	−4.5[a]	−2.7	−3.2	−3.4	−3.0	−3.7	−3.5
Dimer MeOH-Water_1_z_+30	−4.4[a]	−2.9	−3.3	−3.4	−3.1	−3.6	−3.4
Dimer MeOH-Water_2_y_-30	−4.0[a]	−2.7	−3.2	−3.3	−2.6	−3.2	−2.9
Dimer MeOH-Water_2_y_+30	−4.0[a]	−2.7	−3.2	−3.3	−2.6	−3.2	−2.9
Dimer MeOH-Water_2_z_-30	−4.7[a]	−2.8	−3.3	−3.6	−2.8	−3.4	−3.1
Dimer MeOH-Water_2_z_+30	−4.8[a]	−3.2	−3.6	−3.7	−3.4	−3.9	−3.6
Dimer MeNH2-Water_1_y_-30	−6.1[a]	−3.4	−4.1	−3.8	−3.6	−4.6	−4.8
Dimer MeNH2-Water_1_y_+30	−6.1[a]	−3.3	−4.0	−3.7	−3.5	−4.5	−4.7
Dimer MeNH2-Water_1_z_-30	−4.3[a]	−2.9	−3.7	−3.6	−2.6	−3.6	−3.5
Dimer MeNH2-Water_1_z_+30	−6.0[a]	−3.0	−3.6	−3.3	−3.5	−4.2	−4.5
Dimer MeNH2-Water_2_y_-30	−5.9[a]	−3.6	−4.4	−4.1	−4.0	−5.0	−5.3
Dimer MeNH2-Water_2_y_+30	−5.8[a]	−3.8	−4.5	−4.2	−4.2	−5.2	−5.4
Dimer MeNH2-Water_2_z_-30	−6.0[a]	−4.3	−5.0	−4.8	−4.8	−5.8	−6.1
Dimer MeNH2-Water_2_z_+30	−6.0[a]	−3.1	−3.8	−3.6	−3.3	−4.4	−4.5
Dimer MeOH-MeOH_1_y_-30	−4.9[a]	−2.8	−3.5	−3.7	−2.9	−3.7	−3.5
Dimer MeOH-MeOH_1_y_+30	−5.0[a]	−2.8	−3.6	−3.8	−2.7	−3.8	−3.5
Dimer MeOH-MeOH_1_z_-30	−5.2[a]	−2.9	−3.7	−3.9	−2.8	−4.0	−3.7
Dimer MeOH-MeOH_1_z_+30	−5.1[a]	−2.9	−3.5	−3.7	−2.8	−3.7	−3.4
Dimer MeOH-MeOH_2_y_-30	−4.8[a]	−2.7	−3.3	−3.5	−2.4	−3.2	−2.9
Dimer MeOH-MeOH_2_y_+30	−3.3[a]	−2.0	−2.8	−2.7	−1.5	−2.6	−2.2
Dimer MeOH-MeOH_2_z_-30	−5.4[a]	−2.8	−3.7	−3.9	−2.4	−3.5	−3.1
Dimer MeOH-MeOH_2_z_+30	−5.6[a]	−3.2	−3.9	−4.0	−2.9	−3.9	−3.6
Dimer MeOH-MeNH2_1_y_-30	−6.3[a]	−3.1	−4.1	−3.8	−3.5	−4.8	−5.1
Dimer MeOH-MeNH2_1_y_+30	−6.3[a]	−3.1	−4.1	−3.8	−3.5	−4.8	−5.1
Dimer MeOH-MeNH2_1_z_-30	−5.6[a]	−2.5	−3.7	−3.6	−2.4	−4.0	−4.0
Dimer MeOH-MeNH2_1_z_+30	−6.4[a]	−3.2	−4.0	−3.5	−3.7	−4.7	−5.1
Dimer MeOH-MeNH2_2_y_-30	−6.2[a]	−2.6	−3.7	−3.2	−3.0	−4.4	−4.7
Dimer MeOH-MeNH2_2_y_+30	−6.2[a]	−2.6	−3.7	−3.2	−3.0	−4.4	−4.6
Dimer MeOH-MeNH2_2_z_-30	−6.3[a]	−2.9	−3.7	−3.2	−3.5	−4.5	−4.8
Dimer MeOH-MeNH2_2_z_+30	−4.8[a]	−1.8	−3.1	−2.8	−1.3	−3.0	−2.8
Dimer MeNH2-MeOH_1_y_-30	−2.6[a]	−1.3	−2.2	−2.3	−1.3	−2.3	−2.4
Dimer MeNH2-MeOH_1_y_+30	−2.6[a]	−1.0	−1.9	−2.0	−1.0	−2.0	−2.1
Dimer MeNH2-MeOH_1_z_-30	−2.1[a]	−0.7	−1.6	−1.7	−0.5	−1.7	−1.7
Dimer MeNH2-MeOH_1_z_+30	−2.6[a]	−1.4	−2.0	−2.1	−1.3	−2.1	−2.2
Dimer MeNH2-MeOH_2_y_-30	−2.9[a]	−1.1	−2.1	−2.2	−0.9	−2.0	−2.1
Dimer MeNH2-MeOH_2_y_+30	−2.7[a]	−1.3	−2.3	−2.4	−1.1	−2.2	−2.3
Dimer MeNH2-MeOH_2_z_-30	−2.7[a]	−1.5	−2.1	−2.3	−1.3	−2.1	−2.2
Dimer MeNH2-MeOH_2_z_+30	−2.1[a]	−0.7	−1.8	−1.8	−0.4	−1.7	−1.6

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Table S78: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer MeNH2-MeNH2_1_y_-30	-3.1^a	-1.2	-2.3	-2.4	-0.8	-2.3	-2.3
Dimer MeNH2-MeNH2_1_y_+30	-3.7^a	-1.5	-2.5	-2.6	-1.3	-2.5	-2.7
Dimer MeNH2-MeNH2_1_z_-30	-3.2^a	-1.1	-2.3	-2.3	-0.7	-2.2	-2.1
Dimer MeNH2-MeNH2_1_z_+30	-3.4^a	-1.7	-2.7	-2.8	-1.7	-2.8	-3.2
Dimer MeNH2-MeNH2_2_y_-30	-3.2^a	-1.2	-2.4	-2.4	-0.7	-2.2	-2.2
Dimer MeNH2-MeNH2_2_y_+30	-3.3^a	-1.2	-2.2	-2.2	-1.0	-2.3	-2.4
Dimer MeNH2-MeNH2_2_z_-30	-3.1^a	-0.9	-1.7	-1.7	-0.9	-1.8	-2.1
Dimer MeNH2-MeNH2_2_z_+30	-1.6^a	-1.0	-1.8	-1.8	-0.7	-1.7	-1.7
Dimer Water-Peptide_1_y_-30	-6.8^a	-5.1	-6.0	-6.1	-5.0	-6.1	-5.6
Dimer Water-Peptide_1_y_+30	-6.8^a	-5.2	-6.0	-6.1	-5.0	-6.1	-5.7
Dimer Water-Peptide_1_z_-30	-6.8^a	-5.4	-6.2	-6.2	-5.3	-6.3	-5.9
Dimer Water-Peptide_1_z_+30	-6.3^a	-4.8	-5.7	-5.8	-4.4	-5.6	-5.2
Dimer Water-Peptide_2_y_-30	-7.8^a	-5.9	-6.8	-6.9	-5.5	-6.6	-6.1
Dimer Water-Peptide_2_y_+30	-7.7^a	-5.9	-6.8	-6.9	-5.4	-6.6	-6.0
Dimer Water-Peptide_2_z_-30	-1.8^a	-1.5	-2.1	-2.0	-1.2	-2.0	-1.7
Dimer Water-Peptide_2_z_+30	-6.7^a	-5.0	-5.5	-5.6	-4.7	-5.5	-5.1
Dimer Peptide-Water_1_y_-30	-4.5^a	-3.2	-3.9	-3.9	-3.3	-4.1	-4.0
Dimer Peptide-Water_1_y_+30	-4.5^a	-3.2	-3.9	-3.9	-3.3	-4.1	-4.0
Dimer Peptide-Water_1_z_-30	-3.9^a	-3.1	-3.7	-3.7	-3.2	-3.9	-3.8
Dimer Peptide-Water_1_z_+30	-4.5^a	-3.1	-3.7	-3.7	-3.1	-3.9	-3.8
Dimer Peptide-Water_2_y_-30	-4.4^a	-3.1	-3.8	-3.9	-3.0	-3.8	-3.7
Dimer Peptide-Water_2_y_+30	-4.4^a	-3.2	-3.9	-3.9	-3.0	-3.9	-3.7
Dimer Peptide-Water_2_z_-30	-5.0^a	-3.5	-4.2	-4.3	-3.5	-4.3	-4.3
Dimer Peptide-Water_2_z_+30	-5.0^a	-3.5	-4.1	-4.2	-3.5	-4.3	-4.2
Dimer MeOH-Peptide_1_y_-30	-7.3^a	-4.3	-5.8	-5.9	-4.0	-5.8	-5.4
Dimer MeOH-Peptide_1_y_+30	-7.0^a	-3.8	-4.8	-4.9	-3.6	-4.8	-4.4
Dimer MeOH-Peptide_1_z_-30	-6.7^a	-4.2	-5.5	-5.6	-3.7	-5.4	-4.9
Dimer MeOH-Peptide_1_z_+30	-7.0^a	-3.8	-4.9	-5.0	-3.7	-5.1	-4.7
Dimer MeOH-Peptide_2_y_-30	-6.9^a	-3.9	-5.3	-5.2	-3.0	-4.9	-4.3
Dimer MeOH-Peptide_2_y_+30	-7.4^a	-4.6	-5.6	-5.7	-4.3	-5.6	-5.2
Dimer MeOH-Peptide_2_z_-30	-6.9^a	-4.3	-5.1	-5.1	-4.1	-5.1	-4.8
Dimer MeOH-Peptide_2_z_+30	-1.2^a	-1.0	-1.7	-1.6	-0.7	-1.5	-1.3
Dimer MeNH2-Peptide_1_y_-30	-4.5^a	-2.0	-3.8	-4.1	-1.6	-3.9	-4.0
Dimer MeNH2-Peptide_1_y_+30	-4.5^a	-2.6	-3.9	-4.0	-2.3	-3.9	-4.1
Dimer MeNH2-Peptide_1_z_-30	-4.4^a	-2.1	-3.8	-4.0	-1.6	-3.8	-3.9
Dimer MeNH2-Peptide_1_z_+30	-4.6^a	-2.7	-3.9	-4.1	-2.1	-3.7	-3.8
Dimer MeNH2-Peptide_2_y_-30	-4.5^a	-1.9	-3.5	-3.8	-1.4	-3.4	-3.5
Dimer MeNH2-Peptide_2_y_+30	-2.0^a	-1.2	-2.2	-2.1	-0.8	-2.0	-1.9
Dimer MeNH2-Peptide_2_z_-30	-4.2^a	-2.1	-3.2	-3.4	-1.8	-3.1	-3.3
Dimer MeNH2-Peptide_2_z_+30	-3.0^a	-1.5	-3.0	-3.1	-1.1	-3.0	-3.0
Dimer Peptide-MeOH_1_y_-30	-5.5^a	-3.3	-4.7	-4.7	-3.1	-4.7	-4.5
Dimer Peptide-MeOH_1_y_+30	-5.4^a	-3.4	-4.6	-4.6	-3.2	-4.6	-4.5
Dimer Peptide-MeOH_1_z_-30	-4.7^a	-2.9	-4.3	-4.3	-2.6	-4.3	-4.1
Dimer Peptide-MeOH_1_z_+30	-5.6^a	-3.5	-4.5	-4.6	-3.2	-4.5	-4.3
Dimer Peptide-MeOH_2_y_-30	-4.1^a	-2.4	-3.8	-3.6	-1.8	-3.6	-3.2
Dimer Peptide-MeOH_2_y_+30	-5.5^a	-3.4	-4.5	-4.6	-3.1	-4.3	-4.2
Dimer Peptide-MeOH_2_z_-30	-5.8^a	-3.8	-4.8	-5.0	-3.4	-4.7	-4.7
Dimer Peptide-MeOH_2_z_+30	-5.3^a	-3.0	-4.5	-4.5	-2.3	-4.3	-4.0
Dimer Peptide-MeNH2_1_y_-30	-6.5^a	-3.5	-5.2	-5.2	-3.5	-5.5	-5.9
Dimer Peptide-MeNH2_1_y_+30	-6.4^a	-3.8	-5.2	-5.1	-3.6	-5.4	-5.7
Dimer Peptide-MeNH2_1_z_-30	-5.6^a	-2.9	-4.5	-4.4	-2.4	-4.4	-4.4
Dimer Peptide-MeNH2_1_z_+30	-6.5^a	-3.6	-5.0	-4.9	-3.7	-5.3	-5.7
Dimer Peptide-MeNH2_2_y_-30	-4.6^a	-2.4	-4.1	-4.0	-1.7	-3.8	-3.8
Dimer Peptide-MeNH2_2_y_+30	-6.3^a	-3.3	-4.6	-4.4	-3.4	-5.0	-5.5
Dimer Peptide-MeNH2_2_z_-30	-6.2^a	-3.4	-4.7	-4.6	-3.4	-5.1	-5.6
Dimer Peptide-MeNH2_2_z_+30	-5.7^a	-2.6	-4.4	-4.1	-2.0	-4.2	-4.3
Dimer Peptide-Peptide_1_y_-30	-7.6^a	-4.5	-6.6	-6.7	-3.8	-6.5	-6.3
Dimer Peptide-Peptide_1_y_+30	-7.5^a	-4.3	-6.0	-6.0	-3.7	-5.8	-5.6
Dimer Peptide-Peptide_1_z_-30	-6.4^a	-3.9	-5.9	-5.7	-3.1	-5.6	-5.3
Dimer Peptide-Peptide_1_z_+30	-7.6^a	-4.3	-5.9	-6.0	-3.8	-5.7	-5.6
Dimer Peptide-Peptide_2_y_-30	-3.0^a	-1.4	-3.0	-2.8	-0.8	-2.8	-2.4
Dimer Peptide-Peptide_2_y_+30	-7.9^a	-5.2	-6.6	-6.5	-4.7	-6.3	-6.1
Dimer Peptide-Peptide_2_z_-30	-8.0^a	-5.3	-6.8	-6.9	-4.6	-6.4	-6.3
Dimer Peptide-Peptide_2_z_+30	-7.2^a	-3.7	-6.0	-5.8	-2.5	-5.5	-5.0
Dimer Water-Pyridine_1_y_-30	-5.8^a	-2.6	-3.3	-3.2	-3.0	-3.9	-4.4

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Table S78: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Water-Pyridine_1_y_+30	-5.9^a	−3.8	−4.5	−4.6	−4.2	−5.1	−5.6
Dimer Water-Pyridine_1_z_-30	-5.8^a	−3.2	−3.9	−3.9	−3.6	−4.5	−4.9
Dimer Water-Pyridine_1_z_+30	-5.8^a	−3.2	−3.9	−3.9	−3.6	−4.5	−4.9
Dimer Water-Pyridine_2_y_-30	-6.0^a	−3.3	−4.1	−4.0	−3.8	−4.8	−5.5
Dimer Water-Pyridine_2_y_+30	-6.2^a	−3.1	−3.8	−3.6	−3.5	−4.5	−5.1
Dimer Water-Pyridine_2_z_-30	-5.3^a	−2.5	−3.3	−3.1	−2.5	−3.5	−3.8
Dimer Water-Pyridine_2_z_+30	-5.3^a	−2.5	−3.3	−3.1	−2.5	−3.5	−3.8
Dimer MeOH-Pyridine_1_y_-30	-6.5^a	−2.8	−3.9	−3.8	−3.3	−4.6	−5.1
Dimer MeOH-Pyridine_1_y_+30	-6.5^a	−2.8	−3.9	−3.8	−3.3	−4.6	−5.1
Dimer MeOH-Pyridine_1_z_-30	-6.5^a	−2.8	−4.1	−4.1	−3.2	−4.9	−5.3
Dimer MeOH-Pyridine_1_z_+30	-6.4^a	−2.6	−3.5	−3.2	−3.2	−4.3	−4.9
Dimer MeOH-Pyridine_2_y_-30	-6.0^a	−1.9	−3.1	−2.8	−2.0	−3.5	−3.8
Dimer MeOH-Pyridine_2_y_+30	-6.0^a	−1.9	−3.1	−2.8	−1.9	−3.5	−3.8
Dimer MeOH-Pyridine_2_z_-30	-6.7^a	−2.8	−3.9	−3.7	−3.4	−4.8	−5.5
Dimer MeOH-Pyridine_2_z_+30	-6.7^a	−2.6	−3.8	−3.5	−3.2	−4.7	−5.4
Dimer AcOH-AcOH_1_y_-30	-16.2^a	−11.1	−12.5	−13.2	−9.3	−11.1	−10.6
Dimer AcOH-AcOH_1_y_+30	-16.2^a	−11.1	−12.5	−13.2	−9.3	−11.1	−10.6
Dimer AcOH-AcOH_1_z_-30	-11.1^a	−7.7	−8.7	−8.9	−6.7	−7.9	−7.5
Dimer AcOH-AcOH_1_z_+30	-9.8^a	−5.5	−6.5	−6.8	−4.5	−5.7	−5.5
Dimer AcOH-AcOH_2_y_-30	-16.0^a	−11.3	−12.7	−13.4	−9.4	−11.2	−10.7
Dimer AcOH-AcOH_2_y_+30	-16.0^a	−11.3	−12.7	−13.4	−9.4	−11.2	−10.7
Dimer AcOH-AcOH_2_z_-30	-10.5^a	−8.0	−9.0	−9.1	−7.0	−8.2	−7.7
Dimer AcOH-AcOH_2_z_+30	-7.1^a	−3.3	−4.4	−4.6	−2.1	−3.4	−3.2
Dimer AcNH2-AcNH2_1_y_-30	-14.1^a	−10.8	−12.2	−12.3	−9.9	−11.8	−11.4
Dimer AcNH2-AcNH2_1_y_+30	-14.1^a	−10.8	−12.2	−12.3	−9.9	−11.8	−11.4
Dimer AcNH2-AcNH2_1_z_-30	-10.1^a	−7.9	−8.9	−8.8	−7.4	−8.6	−8.5
Dimer AcNH2-AcNH2_1_z_+30	-9.3^a	−7.0	−8.1	−8.1	−6.6	−7.9	−7.6
Dimer AcNH2-AcNH2_2_y_-30	-13.9^a	−10.9	−12.4	−12.4	−10.0	−11.9	−11.5
Dimer AcNH2-AcNH2_2_y_+30	-13.9^a	−10.9	−12.4	−12.4	−10.0	−11.9	−11.5
Dimer AcNH2-AcNH2_2_z_-30	-9.6^a	−7.6	−8.6	−8.4	−7.0	−8.2	−8.0
Dimer AcNH2-AcNH2_2_z_+30	-7.8^a	−6.0	−7.2	−7.1	−5.4	−6.9	−6.4
Dimer AcOH-Uracil_1_y_-30	-16.7^a	−12.7	−14.3	−14.7	−11.1	−13.2	−12.9
Dimer AcOH-Uracil_1_y_+30	-16.7^a	−12.7	−14.2	−14.6	−11.1	−13.1	−12.8
Dimer AcOH-Uracil_1_z_-30	-11.9^a	−9.6	−10.8	−10.9	−8.5	−9.9	−9.9
Dimer AcOH-Uracil_1_z_+30	-10.3^a	−6.4	−7.5	−7.7	−5.8	−7.2	−6.8
Dimer AcOH-Uracil_2_y_-30	-17.2^a	−13.4	−15.0	−15.5	−12.0	−14.1	−13.5
Dimer AcOH-Uracil_2_y_+30	-17.2^a	−13.4	−15.0	−15.5	−12.0	−14.1	−13.5
Dimer AcOH-Uracil_2_z_-30	-11.4^a	−9.0	−10.0	−9.9	−8.4	−9.7	−8.9
Dimer AcOH-Uracil_2_z_+30	-9.7^a	−7.2	−8.5	−8.8	−5.7	−7.4	−7.2
Dimer AcNH2-Uracil_1_y_-30	-17.3^a	−14.3	−16.0	−16.1	−13.2	−15.4	−15.2
Dimer AcNH2-Uracil_1_y_+30	-17.2^a	−14.1	−15.8	−15.9	−13.0	−15.2	−15.0
Dimer AcNH2-Uracil_1_z_-30	-13.8^a	−11.6	−12.9	−12.8	−11.0	−12.5	−12.4
Dimer AcNH2-Uracil_1_z_+30	-10.1^a	−7.8	−9.0	−9.0	−7.2	−8.7	−8.4
Dimer AcNH2-Uracil_2_y_-30	-16.3^a	−13.6	−15.3	−15.4	−12.5	−14.7	−14.3
Dimer AcNH2-Uracil_2_y_+30	-16.3^a	−13.6	−15.3	−15.4	−12.5	−14.7	−14.3
Dimer AcNH2-Uracil_2_z_-30	-10.2^a	−8.6	−9.7	−9.5	−8.0	−9.3	−9.0
Dimer AcNH2-Uracil_2_z_+30	-11.2^a	−9.2	−10.7	−10.8	−8.4	−10.2	−9.6
Dimer Uracil-Uracil_BP_1_y_-30	-15.3^a	−12.0	−13.9	−14.0	−11.0	−13.4	−13.2
Dimer Uracil-Uracil_BP_1_y_+30	-15.3^a	−12.0	−13.9	−14.0	−11.0	−13.4	−13.2
Dimer Uracil-Uracil_BP_1_z_-30	-8.2^a	−5.1	−6.5	−6.6	−4.6	−6.3	−6.3
Dimer Uracil-Uracil_BP_1_z_+30	-11.5^a	−9.5	−10.8	−10.7	−9.0	−10.6	−10.4
Dimer Uracil-Uracil_BP_2_y_-30	-14.9^a	−11.9	−13.8	−13.9	−10.8	−13.2	−13.0
Dimer Uracil-Uracil_BP_2_y_+30	-14.9^a	−11.9	−13.8	−13.9	−10.8	−13.2	−13.0
Dimer Uracil-Uracil_BP_2_z_-30	-9.6^a	−7.5	−9.0	−9.2	−6.8	−8.8	−8.4
Dimer Uracil-Uracil_BP_2_z_+30	-9.6^a	−7.7	−9.0	−8.7	−6.9	−8.5	−8.2
Dimer Benzene-Ethene_1_y_-30	-0.7^a	0.7	−0.5	−0.6	0.5	−0.8	−0.9
Dimer Benzene-Ethene_1_y_+30	-0.7^a	0.7	−0.5	−0.6	0.5	−0.8	−0.9
Dimer Benzene-Ethene_1_z_-30	-0.7^a	0.7	−0.5	−0.6	0.5	−0.8	−0.9
Dimer Benzene-Ethene_1_z_+30	-0.7^a	0.7	−0.5	−0.6	0.5	−0.8	−0.9
Dimer Benzene-Ethene_2_y_-30	-1.5^a	0.7	−1.1	−1.3	0.6	−1.6	−1.6
Dimer Benzene-Ethene_2_y_+30	-1.5^a	0.7	−1.1	−1.3	0.6	−1.6	−1.6
Dimer Benzene-Ethene_2_z_-30	-1.3^a	0.6	−0.9	−1.1	0.5	−1.3	−1.4
Dimer Benzene-Ethene_2_z_+30	-1.3^a	0.6	−0.9	−1.1	0.5	−1.3	−1.4
Dimer Pyridine-Ethene_1_y_-30	-1.0^a	0.4	−0.8	−0.9	0.3	−1.1	−1.2
Dimer Pyridine-Ethene_1_y_+30	-1.0^a	0.4	−0.8	−0.9	0.3	−1.1	−1.2

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Table S78: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Pyridine-Ethene_1_z_-30	-1.0^a	0.5	-0.8	-1.0	0.3	-1.1	-1.2
Dimer Pyridine-Ethene_1_z_+30	-1.1^a	0.4	-0.9	-1.0	0.2	-1.2	-1.3
Dimer Pyridine-Ethene_2_y_-30	-1.6^a	0.3	-1.3	-1.5	0.2	-1.6	-1.7
Dimer Pyridine-Ethene_2_y_+30	-1.6^a	0.3	-1.3	-1.5	0.2	-1.6	-1.7
Dimer Pyridine-Ethene_2_z_-30	-1.8^a	0.2	-1.6	-1.7	0.2	-1.9	-1.9
Dimer Pyridine-Ethene_2_z_+30	-1.6^a	0.6	-1.3	-1.5	0.5	-1.8	-1.9
Dimer Uracil-Ethene_1_y_-30	-2.4^a	-1.0	-2.3	-2.4	-0.8	-2.4	-2.3
Dimer Uracil-Ethene_1_y_+30	-2.3^a	-0.8	-2.2	-2.3	-0.6	-2.3	-2.3
Dimer Uracil-Ethene_1_z_-30	-2.7^a	-0.8	-2.5	-2.6	-0.7	-2.7	-2.6
Dimer Uracil-Ethene_1_z_+30	-2.1^a	-0.5	-2.0	-2.2	-0.5	-2.3	-2.2
Dimer Uracil-Ethene_2_y_-30	-2.4^a	-0.4	-2.1	-2.3	-0.2	-2.3	-2.2
Dimer Uracil-Ethene_2_y_+30	-2.4^a	-0.4	-2.1	-2.3	-0.3	-2.4	-2.3
Dimer Uracil-Ethene_2_z_-30	-3.0^a	-0.6	-2.7	-3.0	-0.6	-3.1	-3.0
Dimer Uracil-Ethene_2_z_+30	-2.9^a	-0.7	-2.7	-2.8	-0.4	-2.8	-2.7
Dimer Uracil-Ethyne_1_y_-30	-2.5^a	-1.0	-2.4	-2.5	-1.0	-2.7	-2.5
Dimer Uracil-Ethyne_1_y_+30	-3.1^a	-1.6	-3.1	-3.2	-1.4	-3.3	-3.0
Dimer Uracil-Ethyne_1_z_-30	-3.0^a	-2.0	-3.0	-3.1	-1.7	-3.0	-2.8
Dimer Uracil-Ethyne_1_z_+30	-2.1^a	-0.6	-2.0	-2.1	-0.5	-2.2	-2.1
Dimer Uracil-Ethyne_2_y_-30	-3.7^a	-1.7	-3.6	-3.8	-1.5	-3.9	-3.6
Dimer Uracil-Ethyne_2_y_+30	-3.7^a	-1.7	-3.6	-3.8	-1.5	-3.9	-3.5
Dimer Uracil-Ethyne_2_z_-30	-2.9^a	-1.0	-2.8	-2.9	-0.9	-3.1	-2.8
Dimer Uracil-Ethyne_2_z_+30	-2.8^a	-1.1	-2.6	-2.7	-0.7	-2.5	-2.3
Dimer Benzene-Benzene_pi-pi_1_y_-30	-1.8^a	1.1	-1.4	-1.7	0.9	-2.0	-2.2
Dimer Benzene-Benzene_pi-pi_1_y_+30	-2.1^a	0.6	-1.9	-2.1	0.6	-2.3	-2.4
Dimer Benzene-Benzene_pi-pi_1_z_-30	-2.5^a	0.4	-2.2	-2.5	0.5	-2.6	-2.7
Dimer Benzene-Benzene_pi-pi_1_z_+30	-1.7^a	1.2	-1.1	-1.4	1.0	-1.8	-1.9
Dimer Benzene-Benzene_pi-pi_2_y_-30	-2.1^a	0.4	-2.0	-2.2	0.5	-2.4	-2.4
Dimer Benzene-Benzene_pi-pi_2_y_+30	-1.8^a	1.1	-1.4	-1.7	0.9	-2.0	-2.2
Dimer Benzene-Benzene_pi-pi_2_z_-30	-2.4^a	0.1	-2.4	-2.5	0.3	-2.6	-2.7
Dimer Benzene-Benzene_pi-pi_2_z_+30	-1.6^a	1.3	-1.1	-1.4	1.1	-1.7	-1.9
Dimer Pyridine-Pyridine_pi-pi_1_y_-30	-2.6^a	0.1	-2.7	-3.0	0.2	-3.1	-3.2
Dimer Pyridine-Pyridine_pi-pi_1_y_+30	-2.9^a	-0.5	-2.9	-3.3	-0.3	-3.2	-3.4
Dimer Pyridine-Pyridine_pi-pi_1_z_-30	-2.7^a	0.0	-2.5	-2.9	-0.1	-3.0	-3.2
Dimer Pyridine-Pyridine_pi-pi_1_z_+30	-3.1^a	-0.5	-3.1	-3.4	-0.2	-3.3	-3.4
Dimer Pyridine-Pyridine_pi-pi_2_y_-30	-2.5^a	0.2	-2.5	-2.9	0.2	-3.0	-3.1
Dimer Pyridine-Pyridine_pi-pi_2_y_+30	-2.9^a	-0.5	-3.0	-3.3	-0.2	-3.2	-3.4
Dimer Pyridine-Pyridine_pi-pi_2_z_-30	-2.5^a	0.0	-2.4	-2.8	-0.1	-3.0	-3.2
Dimer Pyridine-Pyridine_pi-pi_2_z_+30	-2.8^a	-0.5	-3.0	-3.3	-0.2	-3.2	-3.3
Dimer Benzene-Pyridine_pi-pi_1_y_-30	-2.4^a	0.4	-2.2	-2.5	0.4	-2.7	-2.8
Dimer Benzene-Pyridine_pi-pi_1_y_+30	-2.4^a	0.3	-2.2	-2.5	0.3	-2.6	-2.8
Dimer Benzene-Pyridine_pi-pi_1_z_-30	-2.0^a	0.8	-1.6	-1.9	0.6	-2.2	-2.4
Dimer Benzene-Pyridine_pi-pi_1_z_+30	-2.8^a	-0.2	-2.7	-3.0	0.0	-3.0	-3.1
Dimer Benzene-Pyridine_pi-pi_2_y_-30	-2.3^a	0.5	-2.2	-2.5	0.5	-2.7	-2.9
Dimer Benzene-Pyridine_pi-pi_2_y_+30	-2.6^a	-0.2	-2.6	-2.8	0.0	-2.8	-2.9
Dimer Benzene-Pyridine_pi-pi_2_z_-30	-2.1^a	0.7	-1.8	-2.1	0.4	-2.4	-2.5
Dimer Benzene-Pyridine_pi-pi_2_z_+30	-2.9^a	-0.3	-2.9	-3.1	-0.0	-3.2	-3.2
Dimer Benzene-Uracil_pi-pi_1_y_-30	-4.0^a	-0.9	-3.8	-4.0	-0.6	-4.2	-4.0
Dimer Benzene-Uracil_pi-pi_1_y_+30	-4.1^a	-1.1	-4.1	-4.3	-0.9	-4.4	-4.2
Dimer Benzene-Uracil_pi-pi_1_z_-30	-4.2^a	-1.3	-4.2	-4.4	-1.0	-4.5	-4.2
Dimer Benzene-Uracil_pi-pi_1_z_+30	-3.8^a	-0.3	-3.5	-3.8	-0.1	-4.0	-3.8
Dimer Benzene-Uracil_pi-pi_2_y_-30	-2.2^a	0.3	-1.9	-2.1	0.2	-2.3	-2.3
Dimer Benzene-Uracil_pi-pi_2_y_+30	-2.4^a	0.3	-2.0	-2.2	0.3	-2.4	-2.5
Dimer Benzene-Uracil_pi-pi_2_z_-30	-3.0^a	-0.2	-3.0	-3.2	-0.2	-3.5	-3.4
Dimer Benzene-Uracil_pi-pi_2_z_+30	-5.2^a	-1.6	-5.0	-5.1	-1.0	-5.1	-4.8
Dimer Pyridine-Uracil_pi-pi_1_y_-30	-4.8^a	-2.0	-4.8	-5.2	-1.7	-5.1	-5.1
Dimer Pyridine-Uracil_pi-pi_1_y_+30	-4.6^a	-1.9	-4.8	-5.0	-1.7	-5.1	-5.0
Dimer Pyridine-Uracil_pi-pi_1_z_-30	-4.8^a	-1.9	-5.0	-5.3	-1.6	-5.3	-5.2
Dimer Pyridine-Uracil_pi-pi_1_z_+30	-5.9^a	-2.4	-5.5	-6.1	-2.5	-6.2	-6.2
Dimer Pyridine-Uracil_pi-pi_2_y_-30	-3.5^a	-1.2	-3.2	-3.6	-1.2	-3.6	-3.8
Dimer Pyridine-Uracil_pi-pi_2_y_+30	-3.9^a	-1.1	-3.8	-4.2	-1.1	-4.3	-4.4
Dimer Pyridine-Uracil_pi-pi_2_z_-30	-5.4^a	-2.6	-5.4	-5.9	-2.5	-5.9	-6.0
Dimer Pyridine-Uracil_pi-pi_2_z_+30	-4.7^a	-1.7	-4.7	-5.1	-1.4	-5.0	-5.0
Dimer Uracil-Uracil_pi-pi_1_y_-30	-8.3^a	-4.0	-7.4	-7.5	-3.6	-7.7	-7.3
Dimer Uracil-Uracil_pi-pi_1_y_+30	-7.4^a	-3.6	-7.3	-7.3	-3.4	-7.8	-7.6
Dimer Uracil-Uracil_pi-pi_1_z_-30	-6.8^a	-3.6	-6.2	-6.2	-3.2	-6.4	-6.3

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Table S78: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Uracil-Uracil_pi-pi_1_z_+30	-6.7^{a}	−3.6	−6.9	−7.0	−3.9	−7.8	−7.4
Dimer Uracil-Uracil_pi-pi_2_y_-30	-6.3^{a}	−3.2	−5.9	−5.9	−2.9	−6.2	−6.1
Dimer Uracil-Uracil_pi-pi_2_y_+30	-6.4^{a}	−3.6	−6.5	−6.6	−3.9	−7.4	−6.9
Dimer Uracil-Uracil_pi-pi_2_z_-30	-6.8^{a}	−3.2	−6.9	−6.9	−3.0	−7.5	−7.3
Dimer Uracil-Uracil_pi-pi_2_z_+30	-7.9^{a}	−3.4	−6.9	−7.0	−2.7	−7.0	−6.6
Dimer Pentane-Pentane_1_y_-30	-1.7^{a}	−0.1	−1.7	−1.7	0.3	−1.6	−1.5
Dimer Pentane-Pentane_1_y_+30	-1.7^{a}	−0.1	−1.7	−1.7	0.3	−1.6	−1.5
Dimer Pentane-Pentane_1_z_-30	-2.9^{a}	−0.4	−3.1	−3.0	0.4	−2.8	−2.6
Dimer Pentane-Pentane_1_z_+30	-2.6^{a}	−0.4	−3.1	−3.0	0.4	−2.7	−2.5
Dimer Pentane-Pentane_2_y_-30	-1.6^{a}	−0.1	−1.7	−1.7	0.2	−1.6	−1.5
Dimer Pentane-Pentane_2_y_+30	-1.6^{a}	−0.1	−1.7	−1.7	0.2	−1.6	−1.5
Dimer Pentane-Pentane_2_z_-30	-2.7^{a}	−0.4	−3.0	−2.9	0.4	−2.7	−2.5
Dimer Pentane-Pentane_2_z_+30	-2.7^{a}	−0.4	−3.1	−3.0	0.5	−2.7	−2.5
Dimer Neopentane-Pentane_1_y_-30	-1.2^{a}	−0.2	−1.4	−1.4	0.1	−1.3	−1.3
Dimer Neopentane-Pentane_1_y_+30	-1.2^{a}	−0.2	−1.4	−1.4	0.1	−1.3	−1.3
Dimer Neopentane-Pentane_1_z_-30	-1.8^{a}	−0.4	−2.2	−2.1	0.0	−1.9	−1.9
Dimer Neopentane-Pentane_1_z_+30	-1.6^{a}	−0.4	−2.0	−2.0	−0.0	−1.8	−1.8
Dimer Neopentane-Pentane_2_y_-30	-1.9^{a}	−0.2	−2.0	−2.0	0.2	−1.9	−1.8
Dimer Neopentane-Pentane_2_y_+30	-1.9^{a}	−0.2	−2.0	−2.0	0.2	−1.9	−1.8
Dimer Neopentane-Pentane_2_z_-30	-1.8^{a}	−0.2	−2.0	−1.9	0.2	−1.8	−1.7
Dimer Neopentane-Pentane_2_z_+30	-2.0^{a}	−0.3	−2.3	−2.3	0.2	−2.1	−2.0
Dimer Neopentane-Neopentane_1_y_-30	-1.3^{a}	−0.3	−1.6	−1.5	0.0	−1.4	−1.4
Dimer Neopentane-Neopentane_1_y_+30	-1.3^{a}	−0.3	−1.6	−1.5	0.0	−1.4	−1.4
Dimer Neopentane-Neopentane_1_z_-30	-1.2^{a}	−0.3	−1.5	−1.5	0.0	−1.4	−1.3
Dimer Neopentane-Neopentane_1_z_+30	-1.4^{a}	−0.3	−1.7	−1.7	−0.0	−1.5	−1.5
Dimer Neopentane-Neopentane_2_y_-30	-1.2^{a}	−0.3	−1.5	−1.5	0.0	−1.4	−1.4
Dimer Neopentane-Neopentane_2_y_+30	-1.2^{a}	−0.3	−1.5	−1.5	0.0	−1.4	−1.4
Dimer Neopentane-Neopentane_2_z_-30	-1.2^{a}	−0.2	−1.5	−1.5	0.1	−1.4	−1.3
Dimer Neopentane-Neopentane_2_z_+30	-1.3^{a}	−0.3	−1.6	−1.6	−0.0	−1.5	−1.5
Dimer Cyclopentane-Neopentane_1_y_-30	-1.8^{a}	−0.4	−2.1	−2.0	0.1	−1.8	−1.8
Dimer Cyclopentane-Neopentane_1_y_+30	-1.8^{a}	−0.4	−2.2	−2.1	0.1	−1.9	−1.8
Dimer Cyclopentane-Neopentane_1_z_-30	-1.6^{a}	−0.4	−1.9	−1.9	−0.0	−1.7	−1.7
Dimer Cyclopentane-Neopentane_1_z_+30	-1.3^{a}	−0.3	−1.7	−1.6	0.0	−1.5	−1.5
Dimer Cyclopentane-Neopentane_2_y_-30	-1.4^{a}	−0.3	−1.8	−1.7	0.1	−1.6	−1.6
Dimer Cyclopentane-Neopentane_2_y_+30	-1.4^{a}	−0.3	−1.8	−1.7	0.1	−1.6	−1.6
Dimer Cyclopentane-Neopentane_2_z_-30	-1.8^{a}	−0.4	−2.1	−2.1	0.1	−1.9	−1.9
Dimer Cyclopentane-Neopentane_2_z_+30	-1.6^{a}	−0.3	−1.8	−1.8	0.1	−1.6	−1.6
Dimer Cyclopentane-Cyclopentane_1_y_-30	-1.9^{a}	−0.3	−2.1	−2.0	0.3	−1.8	−1.7
Dimer Cyclopentane-Cyclopentane_1_y_+30	-1.8^{a}	−0.2	−2.0	−1.9	0.3	−1.8	−1.7
Dimer Cyclopentane-Cyclopentane_1_z_-30	-1.9^{a}	−0.2	−2.0	−1.9	0.4	−1.8	−1.6
Dimer Cyclopentane-Cyclopentane_1_z_+30	-1.8^{a}	−0.4	−2.3	−2.2	0.2	−2.0	−1.9
Dimer Cyclopentane-Cyclopentane_2_y_-30	-1.8^{a}	−0.3	−2.1	−2.1	0.2	−1.9	−1.8
Dimer Cyclopentane-Cyclopentane_2_y_+30	-1.9^{a}	−0.4	−2.2	−2.2	0.1	−2.0	−1.9
Dimer Cyclopentane-Cyclopentane_2_z_-30	-2.0^{a}	−0.5	−2.5	−2.4	0.1	−2.2	−2.1
Dimer Cyclopentane-Cyclopentane_2_z_+30	-1.9^{a}	−0.4	−2.2	−2.1	0.2	−1.9	−1.8
Dimer Ethene-Pentane_1_y_-30	-1.9^{a}	0.1	−1.6	−1.7	0.4	−1.7	−1.6
Dimer Ethene-Pentane_1_y_+30	-1.9^{a}	−0.4	−2.1	−2.0	0.2	−1.9	−1.7
Dimer Ethene-Pentane_1_z_-30	-1.4^{a}	−0.2	−1.6	−1.5	0.2	−1.4	−1.3
Dimer Ethene-Pentane_1_z_+30	-1.4^{a}	−0.2	−1.6	−1.5	0.2	−1.4	−1.3
Dimer Ethene-Pentane_2_y_-30	-1.0^{a}	−0.3	−1.3	−1.3	−0.0	−1.2	−1.2
Dimer Ethene-Pentane_2_y_+30	-1.2^{a}	−0.2	−1.4	−1.4	0.2	−1.2	−1.2
Dimer Ethene-Pentane_2_z_-30	-0.8^{a}	−0.1	−1.0	−1.0	0.1	−0.9	−0.8
Dimer Ethene-Pentane_2_z_+30	-0.8^{a}	−0.1	−1.0	−1.0	0.1	−0.9	−0.9
Dimer Ethyne-Pentane_1_y_-30	-1.8^{a}	0.1	−1.5	−1.5	0.3	−1.6	−1.6
Dimer Ethyne-Pentane_1_y_+30	-1.8^{a}	0.1	−1.5	−1.5	0.3	−1.6	−1.6
Dimer Ethyne-Pentane_1_z_-30	-1.6^{a}	−0.2	−1.5	−1.5	0.2	−1.4	−1.3
Dimer Ethyne-Pentane_1_z_+30	-1.6^{a}	−0.2	−1.5	−1.5	0.2	−1.4	−1.3
Dimer Ethyne-Pentane_2_y_-30	-1.1^{a}	0.1	−0.9	−1.0	0.2	−1.0	−1.0
Dimer Ethyne-Pentane_2_y_+30	-1.1^{a}	−0.1	−1.0	−1.0	0.1	−1.0	−1.0
Dimer Ethyne-Pentane_2_z_-30	-1.2^{a}	0.1	−0.9	−1.0	0.2	−1.0	−0.9
Dimer Ethyne-Pentane_2_z_+30	-1.2^{a}	0.1	−0.9	−1.0	0.2	−1.0	−0.9
Dimer Peptide-Pentane_1_y_-30	-1.8^{a}	−0.1	−1.6	−1.5	0.3	−1.4	−1.2
Dimer Peptide-Pentane_1_y_+30	-2.4^{a}	−0.5	−2.5	−2.4	0.1	−2.2	−2.0
Dimer Peptide-Pentane_1_z_-30	-3.0^{a}	−0.2	−2.9	−2.9	0.4	−2.8	−2.7
Dimer Peptide-Pentane_1_z_+30	-3.2^{a}	−0.4	−2.7	−2.8	0.0	−2.7	−2.6

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Table S78: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Peptide-Pentane_2_y_-30	−1.9[a]	−0.1	−1.7	−1.8	0.2	−1.7	−1.7
Dimer Peptide-Pentane_2_y_+30	−1.6[a]	−0.3	−1.6	−1.6	0.0	−1.4	−1.4
Dimer Peptide-Pentane_2_z_-30	−2.6[a]	−0.4	−2.6	−2.7	0.1	−2.6	−2.5
Dimer Peptide-Pentane_2_z_+30	−2.6[a]	−0.1	−2.4	−2.4	0.4	−2.2	−2.1
Dimer Benzene-Cyclopentane_1_y_-30	−2.6[a]	0.1	−2.3	−2.3	0.5	−2.3	−2.2
Dimer Benzene-Cyclopentane_1_y_+30	−2.4[a]	0.0	−2.2	−2.3	0.4	−2.2	−2.2
Dimer Benzene-Cyclopentane_1_z_-30	−2.1[a]	0.1	−1.9	−2.0	0.3	−2.0	−2.0
Dimer Benzene-Cyclopentane_1_z_+30	−2.4[a]	0.0	−2.3	−2.3	0.5	−2.2	−2.1
Dimer Benzene-Cyclopentane_2_y_-30	−2.3[a]	0.0	−2.1	−2.1	0.4	−2.1	−2.1
Dimer Benzene-Cyclopentane_2_y_+30	−2.5[a]	0.0	−2.4	−2.4	0.4	−2.4	−2.4
Dimer Benzene-Cyclopentane_2_z_-30	−2.2[a]	0.0	−2.0	−2.0	0.4	−2.0	−1.9
Dimer Benzene-Cyclopentane_2_z_+30	−2.1[a]	0.1	−2.1	−2.1	0.4	−2.1	−2.1
Dimer Benzene-Neopentane_1_y_-30	−2.0[a]	−0.2	−2.0	−2.1	0.1	−2.0	−2.0
Dimer Benzene-Neopentane_1_y_+30	−2.0[a]	−0.2	−2.0	−2.1	0.1	−2.0	−2.0
Dimer Benzene-Neopentane_1_z_-30	−1.7[a]	−0.2	−1.8	−1.8	0.0	−1.8	−1.8
Dimer Benzene-Neopentane_1_z_+30	−2.1[a]	−0.2	−2.2	−2.2	0.2	−2.1	−2.1
Dimer Benzene-Neopentane_2_y_-30	−2.3[a]	−0.1	−2.2	−2.3	0.2	−2.3	−2.3
Dimer Benzene-Neopentane_2_y_+30	−2.3[a]	−0.1	−2.2	−2.3	0.2	−2.3	−2.3
Dimer Benzene-Neopentane_2_z_-30	−2.2[a]	−0.3	−2.2	−2.2	0.0	−2.2	−2.2
Dimer Benzene-Neopentane_2_z_+30	−2.2[a]	0.1	−2.0	−2.1	0.4	−2.1	−2.1
Dimer Uracil-Pentane_1_y_-30	−2.8[a]	−0.6	−2.9	−3.0	−0.4	−3.1	−3.0
Dimer Uracil-Pentane_1_y_+30	−3.1[a]	−0.6	−3.3	−3.3	−0.1	−3.3	−3.0
Dimer Uracil-Pentane_1_z_-30	−2.9[a]	−0.4	−3.0	−3.1	−0.2	−3.2	−3.2
Dimer Uracil-Pentane_1_z_+30	−3.0[a]	−0.6	−2.9	−3.0	−0.4	−3.0	−3.0
Dimer Uracil-Pentane_2_y_-30	−2.0[a]	−0.1	−2.0	−2.1	−0.0	−2.2	−2.1
Dimer Uracil-Pentane_2_y_+30	−2.3[a]	−0.2	−2.1	−2.2	0.0	−2.2	−2.1
Dimer Uracil-Pentane_2_z_-30	−2.7[a]	−0.2	−2.7	−2.8	0.0	−2.9	−2.9
Dimer Uracil-Pentane_2_z_+30	−3.1[a]	0.1	−2.8	−3.0	0.4	−3.0	−3.0
Dimer Uracil-Cyclopentane_1_y_-30	−2.6[a]	−0.3	−2.3	−2.4	−0.1	−2.5	−2.5
Dimer Uracil-Cyclopentane_1_y_+30	−2.6[a]	−0.3	−2.3	−2.5	−0.1	−2.5	−2.5
Dimer Uracil-Cyclopentane_1_z_-30	−2.4[a]	−0.2	−2.4	−2.5	0.0	−2.5	−2.5
Dimer Uracil-Cyclopentane_1_z_+30	−3.4[a]	−0.5	−3.3	−3.3	0.0	−3.3	−3.1
Dimer Uracil-Cyclopentane_2_y_-30	−2.5[a]	−0.0	−2.3	−2.4	0.2	−2.5	−2.4
Dimer Uracil-Cyclopentane_2_y_+30	−2.8[a]	0.0	−2.5	−2.6	0.3	−2.7	−2.7
Dimer Uracil-Cyclopentane_2_z_-30	−2.5[a]	−0.2	−2.4	−2.4	−0.0	−2.5	−2.4
Dimer Uracil-Cyclopentane_2_z_+30	−2.7[a]	−0.1	−2.4	−2.5	0.2	−2.6	−2.6
Dimer Uracil-Neopentane_1_y_-30	−2.5[a]	−0.4	−2.2	−2.3	−0.2	−2.3	−2.3
Dimer Uracil-Neopentane_1_y_+30	−2.8[a]	−0.4	−2.4	−2.5	−0.2	−2.5	−2.5
Dimer Uracil-Neopentane_1_z_-30	−2.2[a]	−0.3	−2.1	−2.1	−0.1	−2.2	−2.2
Dimer Uracil-Neopentane_1_z_+30	−3.2[a]	−0.6	−2.9	−2.9	−0.1	−2.8	−2.6
Dimer Uracil-Neopentane_2_y_-30	−2.3[a]	0.1	−2.0	−2.1	0.3	−2.2	−2.1
Dimer Uracil-Neopentane_2_y_+30	−2.6[a]	−0.0	−2.4	−2.5	0.2	−2.5	−2.5
Dimer Uracil-Neopentane_2_z_-30	−2.1[a]	−0.2	−1.9	−2.0	−0.0	−2.1	−2.0
Dimer Uracil-Neopentane_2_z_+30	−2.2[a]	−0.2	−2.0	−2.1	−0.0	−2.1	−2.1
Dimer Ethyne-Ethyne_TS_1_y_-30	−1.5[a]	−1.1	−1.7	−1.6	−0.7	−1.3	−1.2
Dimer Ethyne-Ethyne_TS_1_y_+30	−1.5[a]	−1.1	−1.7	−1.6	−0.7	−1.3	−1.2
Dimer Ethyne-Ethyne_TS_1_z_-30	−1.0[a]	−0.7	−1.2	−1.1	−0.4	−1.0	−0.9
Dimer Ethyne-Ethyne_TS_1_z_+30	−1.0[a]	−0.7	−1.2	−1.1	−0.4	−1.0	−0.9
Dimer Ethyne-Ethyne_TS_2_y_-30	−1.3[a]	−0.9	−1.4	−1.3	−0.5	−1.2	−1.1
Dimer Ethyne-Ethyne_TS_2_y_+30	−1.3[a]	−0.9	−1.4	−1.3	−0.5	−1.2	−1.1
Dimer Ethyne-Ethyne_TS_2_z_-30	−1.4[a]	−0.9	−1.5	−1.4	−0.6	−1.2	−1.1
Dimer Ethyne-Ethyne_TS_2_z_+30	−1.4[a]	−0.9	−1.5	−1.4	−0.6	−1.2	−1.1
Dimer Benzene-Water_OH-pi_1_y_-30	−2.6[a]	−2.0	−3.0	−2.9	−1.6	−2.8	−2.6
Dimer Benzene-Water_OH-pi_1_y_+30	−2.6[a]	−2.0	−3.0	−2.9	−1.6	−2.8	−2.6
Dimer Benzene-Water_OH-pi_1_z_-30	−2.4[a]	−1.7	−2.7	−2.6	−1.4	−2.6	−2.5
Dimer Benzene-Water_OH-pi_1_z_+30	−2.6[a]	−2.1	−3.0	−2.9	−1.6	−2.7	−2.5
Dimer Benzene-Water_OH-pi_2_y_-30	−2.8[a]	−1.8	−3.0	−2.9	−1.4	−2.9	−2.7
Dimer Benzene-Water_OH-pi_2_y_+30	−2.8[a]	−1.8	−3.0	−2.9	−1.4	−2.9	−2.7
Dimer Benzene-Water_OH-pi_2_z_-30	−3.0[a]	−1.6	−2.7	−2.7	−1.1	−2.6	−2.4
Dimer Benzene-Water_OH-pi_2_z_+30	−3.1[a]	−2.4	−3.6	−3.5	−1.9	−3.5	−3.3
Dimer Benzene-Ethyne_CH-pi_1_y_-30	−2.1[a]	−1.6	−2.6	−2.5	−0.9	−2.2	−2.0
Dimer Benzene-Ethyne_CH-pi_1_y_+30	−2.1[a]	−1.6	−2.6	−2.5	−0.9	−2.2	−2.0
Dimer Benzene-Ethyne_CH-pi_1_z_-30	−2.1[a]	−1.6	−2.6	−2.5	−0.9	−2.2	−2.0
Dimer Benzene-Ethyne_CH-pi_1_z_+30	−2.1[a]	−1.6	−2.6	−2.5	−0.9	−2.2	−2.0
Dimer Benzene-Ethyne_CH-pi_2_y_-30	−2.7[a]	−1.5	−2.9	−2.8	−0.6	−2.4	−2.2

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Table S78: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Benzene-Ethyne_CH-pi_2_y_+30	-2.7^a	−1.5	−2.9	−2.8	−0.6	−2.4	−2.2
Dimer Benzene-Ethyne_CH-pi_2_z_-30	-2.7^a	−1.5	−2.9	−2.8	−0.6	−2.4	−2.2
Dimer Benzene-Ethyne_CH-pi_2_z_+30	-2.7^a	−1.5	−2.9	−2.8	−0.6	−2.4	−2.2
Dimer Benzene-MeOH_OH-pi_1_y_-30	-3.5^a	−1.7	−3.3	−3.2	−1.2	−3.1	−2.9
Dimer Benzene-MeOH_OH-pi_1_y_+30	-3.5^a	−1.7	−3.3	−3.3	−1.2	−3.1	−2.9
Dimer Benzene-MeOH_OH-pi_1_z_-30	-3.3^a	−2.0	−3.3	−3.2	−1.4	−3.0	−2.8
Dimer Benzene-MeOH_OH-pi_1_z_+30	-3.1^a	−1.0	−2.7	−2.6	−0.7	−2.7	−2.5
Dimer Benzene-MeOH_OH-pi_2_y_-30	-3.5^a	−1.3	−3.1	−3.1	−0.8	−3.1	−3.0
Dimer Benzene-MeOH_OH-pi_2_y_+30	-3.5^a	−1.3	−3.1	−3.1	−0.8	−3.1	−3.0
Dimer Benzene-MeOH_OH-pi_2_z_-30	-2.6^a	−1.0	−2.6	−2.7	−0.8	−2.7	−2.7
Dimer Benzene-MeOH_OH-pi_2_z_+30	-3.3^a	−1.1	−2.6	−2.6	−0.6	−2.5	−2.3
Dimer Benzene-MeNH2_NH-pi_1_y_-30	-2.5^a	−0.9	−2.5	−2.5	−0.4	−2.3	−2.3
Dimer Benzene-MeNH2_NH-pi_1_y_+30	-2.3^a	−0.7	−2.3	−2.3	−0.4	−2.2	−2.2
Dimer Benzene-MeNH2_NH-pi_1_z_-30	-2.2^a	−0.5	−2.1	−2.1	−0.2	−2.1	−2.0
Dimer Benzene-MeNH2_NH-pi_1_z_+30	-2.3^a	−1.1	−2.4	−2.4	−0.6	−2.2	−2.2
Dimer Benzene-MeNH2_NH-pi_2_y_-30	-2.4^a	−0.3	−2.1	−2.2	−0.0	−2.2	−2.1
Dimer Benzene-MeNH2_NH-pi_2_y_+30	-3.0^a	−1.1	−3.1	−3.2	−0.6	−3.0	−3.0
Dimer Benzene-MeNH2_NH-pi_2_z_-30	-2.4^a	−0.4	−2.0	−2.1	0.1	−1.9	−1.8
Dimer Benzene-MeNH2_NH-pi_2_z_+30	-1.9^a	−0.5	−2.0	−2.1	−0.4	−2.1	−2.1
Dimer Benzene-AcOH_OH-pi_1_y_-30	-3.9^a	−2.4	−4.0	−3.9	−1.7	−3.6	−3.3
Dimer Benzene-AcOH_OH-pi_1_y_+30	-3.9^a	−2.5	−4.0	−4.0	−1.7	−3.6	−3.4
Dimer Benzene-AcOH_OH-pi_1_z_-30	-3.6^a	−1.8	−3.3	−3.2	−1.2	−3.1	−2.9
Dimer Benzene-AcOH_OH-pi_1_z_+30	-4.2^a	−2.9	−4.3	−4.2	−2.0	−3.8	−3.5
Dimer Benzene-AcOH_OH-pi_2_y_-30	-4.2^a	−2.1	−4.0	−4.0	−1.4	−3.7	−3.5
Dimer Benzene-AcOH_OH-pi_2_y_+30	-4.3^a	−2.2	−4.1	−4.1	−1.4	−3.8	−3.6
Dimer Benzene-AcOH_OH-pi_2_z_-30	-2.1^a	−0.6	−2.0	−2.0	−0.6	−2.1	−2.1
Dimer Benzene-AcOH_OH-pi_2_z_+30	-2.6^a	−0.7	−2.0	−2.0	−0.4	−2.0	−1.9
Dimer Benzene-AcNH2_NH-pi_1_y_-30	-3.7^a	−2.4	−3.9	−3.8	−1.7	−3.5	−3.3
Dimer Benzene-AcNH2_NH-pi_1_y_+30	-3.7^a	−2.5	−4.0	−3.8	−1.8	−3.6	−3.4
Dimer Benzene-AcNH2_NH-pi_1_z_-30	-4.4^a	−2.4	−4.4	−4.3	−1.5	−4.0	−3.7
Dimer Benzene-AcNH2_NH-pi_1_z_+30	-3.7^a	−1.9	−3.3	−3.2	−1.3	−3.1	−2.9
Dimer Benzene-AcNH2_NH-pi_2_y_-30	-4.0^a	−2.6	−4.3	−4.1	−1.9	−3.9	−3.7
Dimer Benzene-AcNH2_NH-pi_2_y_+30	-4.0^a	−2.6	−4.3	−4.1	−1.9	−3.9	−3.7
Dimer Benzene-AcNH2_NH-pi_2_z_-30	-2.1^a	−1.2	−2.2	−2.1	−0.9	−2.1	−2.0
Dimer Benzene-AcNH2_NH-pi_2_z_+30	-3.5^a	−2.4	−3.8	−3.7	−1.7	−3.3	−3.1
Dimer Benzene-Peptide_NH-pi_1_y_-30	-4.1^a	−1.7	−4.0	−3.9	−1.0	−3.6	−3.5
Dimer Benzene-Peptide_NH-pi_1_y_+30	-4.1^a	−1.7	−4.0	−4.0	−1.0	−3.8	−3.6
Dimer Benzene-Peptide_NH-pi_1_z_-30	-3.9^a	−1.6	−3.8	−3.7	−0.8	−3.4	−3.2
Dimer Benzene-Peptide_NH-pi_1_z_+30	-3.8^a	−1.5	−3.6	−3.6	−0.8	−3.4	−3.2
Dimer Benzene-Peptide_NH-pi_2_y_-30	-4.9^a	−1.9	−4.6	−4.6	−1.0	−4.3	−4.0
Dimer Benzene-Peptide_NH-pi_2_y_+30	-4.6^a	−1.4	−4.3	−4.3	−0.8	−4.2	−4.0
Dimer Benzene-Peptide_NH-pi_2_z_-30	-3.1^a	−1.1	−3.0	−3.0	−0.7	−3.0	−2.9
Dimer Benzene-Peptide_NH-pi_2_z_+30	-3.2^a	−1.5	−3.4	−3.3	−0.9	−3.2	−3.0
Dimer Benzene-Benzene_TS_1_y_-30	-2.0^a	−0.6	−2.2	−2.2	−0.2	−2.1	−2.0
Dimer Benzene-Benzene_TS_1_y_+30	-2.1^a	−0.6	−2.3	−2.3	−0.2	−2.2	−2.2
Dimer Benzene-Benzene_TS_1_z_-30	-1.8^a	−0.6	−2.1	−2.0	−0.3	−1.9	−1.9
Dimer Benzene-Benzene_TS_1_z_+30	-2.1^a	−0.5	−2.2	−2.2	−0.0	−2.1	−2.0
Dimer Benzene-Benzene_TS_2_y_-30	-2.8^a	−0.5	−2.7	−2.7	0.1	−2.6	−2.5
Dimer Benzene-Benzene_TS_2_y_+30	-2.7^a	−0.3	−2.6	−2.7	0.2	−2.7	−2.6
Dimer Benzene-Benzene_TS_2_z_-30	-1.9^a	−0.5	−2.2	−2.1	−0.1	−2.0	−2.0
Dimer Benzene-Benzene_TS_2_z_+30	-2.8^a	−0.6	−2.7	−2.7	0.1	−2.5	−2.3
Dimer Pyridine-Pyridine_TS_1_y_-30	-2.6^a	−1.1	−2.8	−2.8	−0.5	−2.6	−2.6
Dimer Pyridine-Pyridine_TS_1_y_+30	-2.6^a	−1.1	−2.8	−2.8	−0.5	−2.6	−2.6
Dimer Pyridine-Pyridine_TS_1_z_-30	-1.9^a	−0.7	−2.3	−2.2	−0.3	−2.1	−2.0
Dimer Pyridine-Pyridine_TS_1_z_+30	-3.1^a	−1.5	−3.0	−3.1	−1.1	−2.9	−3.0
Dimer Pyridine-Pyridine_TS_2_y_-30	-3.3^a	−1.0	−3.2	−3.3	−0.4	−3.1	−3.1
Dimer Pyridine-Pyridine_TS_2_y_+30	-3.3^a	−1.0	−3.2	−3.3	−0.4	−3.1	−3.1
Dimer Pyridine-Pyridine_TS_2_z_-30	-2.4^a	−1.1	−2.5	−2.5	−0.6	−2.3	−2.4
Dimer Pyridine-Pyridine_TS_2_z_+30	-2.9^a	−0.7	−2.7	−2.7	0.1	−2.3	−2.3
Dimer Benzene-Pyridine_TS_1_y_-30	-2.4^a	−1.0	−2.6	−2.6	−0.5	−2.4	−2.4
Dimer Benzene-Pyridine_TS_1_y_+30	-2.4^a	−1.0	−2.6	−2.6	−0.5	−2.4	−2.4
Dimer Benzene-Pyridine_TS_1_z_-30	-2.4^a	−0.8	−2.5	−2.5	−0.3	−2.4	−2.3
Dimer Benzene-Pyridine_TS_1_z_+30	-2.1^a	−1.0	−2.5	−2.4	−0.5	−2.2	−2.2
Dimer Benzene-Pyridine_TS_2_y_-30	-3.2^a	−0.9	−3.2	−3.2	−0.2	−3.0	−3.0
Dimer Benzene-Pyridine_TS_2_y_+30	-3.2^a	−0.9	−3.2	−3.2	−0.2	−3.0	−3.0

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Table S78: *... continued from previous page ...*

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Benzene-Pyridine_TS_2_z_-30	-3.2^a	−1.1	−3.2	−3.1	−0.2	−2.8	−2.7
Dimer Benzene-Pyridine_TS_2_z_+30	-2.2^a	−0.9	−2.5	−2.5	−0.4	−2.3	−2.3
Dimer Ethyne-Water_CH-O_1_y_-30	-2.4^a	−2.5	−2.8	−2.7	−2.3	−2.7	−2.5
Dimer Ethyne-Water_CH-O_1_y_+30	-2.4^a	−2.4	−2.7	−2.6	−2.2	−2.6	−2.4
Dimer Ethyne-Water_CH-O_1_z_-30	-2.5^a	−2.5	−2.8	−2.7	−2.3	−2.7	−2.4
Dimer Ethyne-Water_CH-O_1_z_+30	-2.5^a	−2.4	−2.8	−2.7	−2.2	−2.6	−2.4
Dimer Ethyne-Water_CH-O_2_y_-30	-2.8^a	−2.7	−3.1	−3.0	−2.4	−2.9	−2.6
Dimer Ethyne-Water_CH-O_2_y_+30	-2.8^a	−3.0	−3.3	−3.2	−2.6	−3.1	−2.8
Dimer Ethyne-Water_CH-O_2_z_-30	-2.4^a	−2.6	−2.9	−2.8	−2.2	−2.6	−2.3
Dimer Ethyne-Water_CH-O_2_z_+30	-2.4^a	−2.5	−2.9	−2.8	−2.1	−2.6	−2.3
Dimer Ethyne-AcOH_OH-pi_1_y_-30	-4.8^a	−3.8	−4.8	−4.7	−2.7	−4.0	−3.7
Dimer Ethyne-AcOH_OH-pi_1_y_+30	-4.8^a	−3.8	−4.8	−4.7	−2.7	−4.0	−3.7
Dimer Ethyne-AcOH_OH-pi_1_z_-30	-3.1^a	−2.2	−3.0	−2.9	−1.6	−2.6	−2.4
Dimer Ethyne-AcOH_OH-pi_1_z_+30	-3.9^a	−3.0	−3.8	−3.7	−2.0	−3.1	−2.8
Dimer Ethyne-AcOH_OH-pi_2_y_-30	-4.3^a	−3.4	−4.3	−4.3	−2.4	−3.7	−3.4
Dimer Ethyne-AcOH_OH-pi_2_y_+30	-4.3^a	−3.4	−4.3	−4.3	−2.4	−3.7	−3.4
Dimer Ethyne-AcOH_OH-pi_2_z_-30	-2.6^a	−2.2	−2.9	−2.9	−1.8	−2.6	−2.4
Dimer Ethyne-AcOH_OH-pi_2_z_+30	-3.4^a	−2.3	−3.1	−3.0	−1.6	−2.6	−2.4
Dimer Peptide-Ethene_1_y_-30	-2.2^a	−0.9	−1.9	−1.9	−0.7	−1.8	−1.8
Dimer Peptide-Ethene_1_y_+30	-1.9^a	−0.6	−2.0	−2.0	−0.3	−1.9	−1.9
Dimer Peptide-Ethene_1_z_-30	-1.3^a	−0.6	−1.5	−1.5	−0.2	−1.4	−1.3
Dimer Peptide-Ethene_1_z_+30	-2.0^a	−0.9	−2.0	−2.0	−0.6	−1.9	−1.8
Dimer Peptide-Ethene_2_y_-30	-2.0^a	−0.7	−1.9	−1.9	−0.4	−1.8	−1.7
Dimer Peptide-Ethene_2_y_+30	-2.3^a	−0.6	−2.1	−2.2	−0.3	−2.1	−2.1
Dimer Peptide-Ethene_2_z_-30	-2.5^a	−1.2	−2.4	−2.5	−0.9	−2.4	−2.3
Dimer Peptide-Ethene_2_z_+30	-1.8^a	−0.3	−1.6	−1.6	0.1	−1.6	−1.5
Dimer Pyridine-Ethyne_1_y_-30	-3.7^a	−2.9	−3.7	−3.6	−2.5	−3.4	−3.5
Dimer Pyridine-Ethyne_1_y_+30	-3.6^a	−2.8	−3.6	−3.6	−2.4	−3.3	−3.4
Dimer Pyridine-Ethyne_1_z_-30	-3.5^a	−2.5	−3.3	−3.2	−1.9	−2.9	−2.9
Dimer Pyridine-Ethyne_1_z_+30	-3.5^a	−2.5	−3.3	−3.2	−1.9	−2.9	−2.9
Dimer Pyridine-Ethyne_2_y_-30	-3.4^a	−2.7	−3.5	−3.5	−2.3	−3.2	−3.3
Dimer Pyridine-Ethyne_2_y_+30	-3.3^a	−2.7	−3.4	−3.4	−2.3	−3.2	−3.3
Dimer Pyridine-Ethyne_2_z_-30	-3.4^a	−2.8	−3.5	−3.5	−2.4	−3.3	−3.4
Dimer Pyridine-Ethyne_2_z_+30	-3.4^a	−2.8	−3.5	−3.6	−2.4	−3.3	−3.4
Dimer Pentane-AcOH_1_y_-30	-1.5^a	−0.4	−1.8	−1.8	−0.0	−1.7	−1.6
Dimer Pentane-AcOH_1_y_+30	-1.4^a	−0.3	−1.5	−1.5	−0.2	−1.5	−1.5
Dimer Pentane-AcOH_1_z_-30	-1.8^a	−0.1	−1.8	−1.8	0.1	−1.8	−1.8
Dimer Pentane-AcOH_1_z_+30	-1.6^a	−0.3	−1.8	−1.8	0.0	−1.8	−1.7
Dimer Pentane-AcOH_2_y_-30	-1.7^a	−0.4	−2.1	−2.1	0.0	−1.9	−1.8
Dimer Pentane-AcOH_2_y_+30	-2.4^a	−0.6	−2.4	−2.4	−0.3	−2.4	−2.4
Dimer Pentane-AcOH_2_z_-30	-2.3^a	−0.5	−2.4	−2.4	0.0	−2.3	−2.3
Dimer Pentane-AcOH_2_z_+30	-2.1^a	−0.3	−1.8	−1.9	−0.1	−1.9	−2.0
Dimer Pentane-AcNH2_1_y_-30	-1.8^a	−0.3	−1.6	−1.7	−0.1	−1.7	−1.6
Dimer Pentane-AcNH2_1_y_+30	-1.5^a	−0.5	−1.6	−1.6	−0.1	−1.5	−1.4
Dimer Pentane-AcNH2_1_z_-30	-2.2^a	−0.2	−2.1	−2.1	0.2	−2.0	−1.9
Dimer Pentane-AcNH2_1_z_+30	-2.2^a	−0.5	−2.2	−2.3	−0.2	−2.2	−2.2
Dimer Pentane-AcNH2_2_y_-30	-2.6^a	−0.7	−2.6	−2.6	−0.1	−2.5	−2.3
Dimer Pentane-AcNH2_2_y_+30	-2.2^a	−0.6	−2.4	−2.3	0.0	−2.1	−2.0
Dimer Pentane-AcNH2_2_z_-30	-2.5^a	−0.3	−1.9	−2.0	−0.1	−1.9	−1.9
Dimer Pentane-AcNH2_2_z_+30	-2.6^a	−0.5	−2.8	−2.8	0.1	−2.8	−2.6
Dimer Benzene-AcOH_1_y_-30	-2.9^a	−1.4	−3.2	−3.2	−0.9	−3.0	−3.0
Dimer Benzene-AcOH_1_y_+30	-2.4^a	−1.0	−2.7	−2.7	−0.6	−2.5	−2.4
Dimer Benzene-AcOH_1_z_-30	-2.9^a	−1.3	−3.1	−3.2	−0.7	−3.0	−2.9
Dimer Benzene-AcOH_1_z_+30	-2.2^a	−0.9	−2.5	−2.5	−0.5	−2.3	−2.3
Dimer Benzene-AcOH_2_y_-30	-2.4^a	−0.7	−2.5	−2.6	−0.5	−2.5	−2.6
Dimer Benzene-AcOH_2_y_+30	-3.0^a	−1.2	−3.2	−3.2	−0.4	−2.9	−2.8
Dimer Benzene-AcOH_2_z_-30	-2.8^a	−1.3	−3.2	−3.2	−0.7	−2.9	−2.8
Dimer Benzene-AcOH_2_z_+30	-2.1^a	−0.5	−2.2	−2.4	−0.3	−2.3	−2.4
Dimer Pyridine-Pyridine_CH-N_1_y_-30	-3.8^a	−2.3	−3.6	−3.8	−1.6	−3.2	−3.5
Dimer Pyridine-Pyridine_CH-N_1_y_+30	-3.8^a	−2.3	−3.6	−3.7	−1.6	−3.2	−3.5
Dimer Pyridine-Pyridine_CH-N_1_z_-30	-2.8^a	−1.8	−2.8	−2.9	−1.4	−2.6	−2.8
Dimer Pyridine-Pyridine_CH-N_1_z_+30	-2.9^a	−1.8	−2.8	−2.9	−1.2	−2.5	−2.7
Dimer Pyridine-Pyridine_CH-N_2_y_-30	-3.8^a	−2.3	−3.6	−3.8	−1.6	−3.2	−3.5
Dimer Pyridine-Pyridine_CH-N_2_y_+30	-3.8^a	−2.3	−3.6	−3.8	−1.6	−3.2	−3.5
Dimer Pyridine-Pyridine_CH-N_2_z_-30	-2.6^a	−1.6	−2.6	−2.6	−1.2	−2.4	−2.6

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Table S78: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer Pyridine-Pyridine_CH-N_2_z_+30	-2.6^{a}	-1.6	-2.7	-2.7	-0.9	-2.2	-2.4
Dimer MeNH2-Pyridine_1_y_-30	-3.3^{a}	-1.1	-2.3	-2.4	-0.9	-2.3	-2.6
Dimer MeNH2-Pyridine_1_y_+30	-2.6^{a}	-0.5	-2.2	-2.3	-0.1	-2.2	-2.2
Dimer MeNH2-Pyridine_1_z_-30	-3.5^{a}	-1.0	-2.8	-3.1	-0.7	-3.0	-3.2
Dimer MeNH2-Pyridine_1_z_+30	-3.5^{a}	-1.0	-2.5	-2.7	-0.7	-2.6	-2.8
Dimer MeNH2-Pyridine_2_y_-30	-3.9^{a}	-1.2	-2.6	-2.7	-1.0	-2.7	-3.0
Dimer MeNH2-Pyridine_2_y_+30	-2.7^{a}	-0.7	-2.5	-2.6	-0.3	-2.5	-2.6
Dimer MeNH2-Pyridine_2_z_-30	-2.6^{a}	-1.2	-2.6	-2.7	-0.7	-2.4	-2.5
Dimer MeNH2-Pyridine_2_z_+30	-3.1^{a}	-0.3	-2.1	-2.2	0.0	-2.3	-2.3

a J.Rezac, K.E.Riley, and P.Hobza, J.Chem.Theory Comput. 7, 2427 (2011) ; 7, 3466 (2011).

Table S79: Benchmark Results for the JSCH2005-CHNOF Set. Interaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer G...C WC(1)	−32.1[a]	−23.8	−26.7	−27.1	−22.9	−26.7	−28.7
Dimer mG...mC WC	−31.6[a]	−24.2	−27.3	−27.9	−23.4	−27.3	−29.8
Dimer A...T WC	−16.9[a]	−11.1	−13.6	−13.4	−11.3	−14.5	−16.4
Dimer mA...mT H	−18.2[a]	−11.8	−14.4	−14.6	−12.6	−15.9	−18.2
Dimer 8-oxoG...C WC	−33.3[a]	−26.0	−29.1	−29.6	−25.3	−29.2	−31.6
Dimer I...C WC	−24.9[a]	−19.5	−22.1	−22.4	−19.4	−22.8	−25.4
Dimer G...U wobble	−19.1[a]	−14.2	−16.5	−16.9	−12.5	−15.4	−15.9
Dimer C...C H+	−51.4[a]	−44.9	−48.1	−48.9	−45.7	−49.7	−52.8
Dimer U...U “calcutta”	−10.3[a]	−8.4	−10.1	−10.2	−7.1	−9.2	−9.0
Dimer U...U pl	−13.7[a]	−10.1	−12.0	−12.1	−8.6	−11.1	−11.2
Dimer 2-aminoA...T	−19.5[a]	−14.2	−17.3	−17.3	−13.8	−17.8	−20.1
Dimer 2-aminoA...T pl	−19.7[a]	−14.3	−17.3	−17.2	−13.6	−17.5	−19.5
Dimer A...difluorotoluene WC	−5.2[a]	−3.0	−4.7	−4.7	−2.2	−4.2	−4.3
Dimer A...C	−17.6[a]	−11.3	−13.8	−13.3	−12.6	−15.8	−18.8
Dimer G...G H-bond	−21.3[a]	−15.3	−17.8	−18.2	−15.6	−18.8	−20.5
Dimer G...A1	−19.4[a]	−12.9	−15.8	−15.9	−12.8	−16.5	−18.6
Dimer G...A1 pl	−18.9[a]	−12.8	−15.6	−15.5	−12.5	−16.0	−17.5
Dimer G...A2	−14.4[a]	−7.5	−10.0	−10.0	−8.4	−11.5	−14.2
Dimer GA2pl	−12.8[a]	−7.3	−9.9	−9.9	−8.4	−11.5	−14.4
Dimer G...A3	−18.8[a]	−12.1	−15.0	−15.3	−12.4	−16.0	−18.3
Dimer G...A4	−13.5[a]	−7.9	−10.4	−10.2	−9.0	−12.1	−15.0
Dimer A...A1	−14.5[a]	−8.6	−10.9	−10.5	−9.8	−12.8	−15.6
Dimer A...A2	−13.7[a]	−7.4	−9.8	−9.5	−8.7	−11.7	−14.4
Dimer A...A3	−12.2[a]	−5.9	−8.4	−8.2	−6.9	−9.9	−12.3
Dimer 8-oxoG...G	−22.8[a]	−17.4	−19.9	−20.4	−15.7	−18.9	−19.3
Dimer mA...mT WC(AT)	−16.4[a]	−11.0	−13.6	−13.4	−11.4	−14.7	−16.8
Dimer mG...mC WC*	−35.8[a]	−27.5	−30.6	−31.3	−26.5	−30.5	−33.4
Dimer mA...mT WC(AC)	−18.4[a]	−12.1	−14.7	−14.5	−12.6	−15.9	−18.0
Dimer G...A HB	−11.3[a]	−7.6	−10.5	−10.5	−9.0	−12.6	−16.3
Dimer C...G WC	−30.7[a]	−26.6	−29.7	−30.2	−25.8	−29.8	−32.3
Dimer G...C WC(2)	−31.4[a]	−26.4	−29.5	−29.8	−25.5	−29.5	−31.8
Dimer GG0/3.36CGis036	−3.7[a]	−1.9	−3.2	−3.2	−2.0	−3.3	−3.2
Dimer GG0/3.36GCis036	−4.8[a]	−3.9	−4.5	−4.6	−3.9	−4.6	−4.5
Dimer AA20/3.05ATis2005	−2.3[a]	−1.1	−2.2	−2.2	−1.0	−2.3	−2.1
Dimer AA20/3.05TAis2005	−2.2[a]	−1.0	−2.4	−2.4	−0.6	−2.2	−2.3
Dimer GC0/3.25C//Cis	3.1[a]	3.8	3.5	3.6	3.8	3.5	3.4
Dimer GC0/3.25G//Gis	1.9[a]	5.0	3.2	3.2	5.3	3.3	2.7
Dimer CG0/3.19G//Gis	−3.9[a]	2.2	1.6	1.7	2.2	1.6	1.5
Dimer CG0/3.19C//Cis	1.2[a]	−0.1	−3.9	−3.9	0.7	−3.8	−4.4
Dimer GA10/3.15A//Cis	−0.3[a]	1.2	0.2	0.1	1.3	0.1	0.1
Dimer GA10/3.15T//Gis	0.6[a]	2.0	1.2	1.2	2.1	1.3	1.1
Dimer AG08/3.19T//Gis	−0.5[a]	1.0	−0.7	−0.7	1.3	−0.6	−0.8
Dimer AG08/3.19A//Cis	−0.2[a]	0.9	−0.1	−0.0	1.0	−0.1	−0.1
Dimer TG03.19A//Gis	−4.2[a]	−1.2	−4.3	−4.3	−0.8	−4.4	−4.3
Dimer TG03.19T//Cis	−1.1[a]	−0.6	−1.0	−1.0	−0.6	−1.1	−1.0
Dimer GT10/3.15T//Cis	0.3[a]	1.0	0.7	0.7	0.9	0.6	0.5
Dimer GT10/3.15A//Gis	−4.1[a]	−1.7	−3.5	−3.6	−1.8	−3.8	−3.6
Dimer AT10/3.26T//Tis	0.9[a]	1.7	1.1	1.1	1.7	1.1	0.9
Dimer AT10/3.26A//Ais	−0.9[a]	0.4	−0.9	−0.9	0.5	−1.0	−1.1
Dimer TA08/3.16A//Ais	−1.6[a]	0.9	−1.7	−2.0	1.1	−2.1	−2.0
Dimer TA08/3.16T//Tis	0.7[a]	1.4	1.0	1.0	1.5	1.1	1.0
Dimer AA0/3.24A//Tis	−1.7[a]	−0.4	−1.3	−1.4	−0.4	−1.4	−1.4
Dimer AA0/3.24T//Ais	−1.3[a]	−0.3	−1.1	−1.1	−0.3	−1.2	−1.1
Dimer A...A	−0.7[a]	0.6	−1.0	−1.0	0.6	−1.2	−1.2
Dimer T...T	1.0[a]	1.9	1.3	1.3	1.9	1.3	1.1
Dimer G...G interstrand	−4.5[a]	−0.2	−4.3	−4.4	0.4	−4.4	−4.8
Dimer C...C	1.4[a]	2.4	1.5	1.7	2.4	1.4	1.4
Dimer A...G	−4.8[a]	−2.3	−4.0	−3.9	−2.2	−4.1	−3.9
Dimer T...C	−0.1[a]	0.7	0.3	0.3	0.7	0.3	0.2
Dimer C...A	−3.0[a]	0.2	−1.2	−1.0	0.5	−1.1	−0.8
Dimer G...G 9	−5.2[a]	−4.2	−5.3	−5.5	−4.1	−5.4	−5.5
Dimer G...G 10	0.8[a]	4.3	1.8	1.9	4.7	1.9	1.2

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Table S79: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer C...C 11	3.1^{a}	3.8	3.5	3.7	3.8	3.5	3.5
Dimer G...C S	-19.0^{a}	−11.7	−17.8	−18.8	−10.8	−18.4	−18.5
Dimer mG...mC S	-20.4^{a}	−11.2	−19.1	−20.5	−10.0	−20.1	−20.1
Dimer A...T S1	-12.3^{a}	−4.0	−10.6	−11.1	−3.3	−11.5	−11.2
Dimer mA...mT S	-14.6^{a}	−4.3	−12.8	−13.4	−2.9	−13.6	−13.0
Dimer CC 1	2.5^{a}	6.7	2.2	2.1	6.8	1.5	1.3
Dimer CC 2	-3.9^{a}	1.9	−2.8	−3.1	1.9	−3.8	−3.6
Dimer CC 3	-8.9^{a}	−3.1	−7.8	−8.5	−3.0	−8.8	−8.6
Dimer CC 4	-9.9^{a}	−4.2	−8.8	−9.9	−3.8	−9.5	−9.9
Dimer CC 5	0.3^{a}	5.8	1.2	1.0	5.9	0.4	0.2
Dimer CC 6	0.6^{a}	6.1	1.5	1.4	6.4	0.8	0.5
Dimer CC 7	-1.0^{a}	3.3	0.2	0.1	3.1	−0.5	−0.3
Dimer CC 8	-9.1^{a}	−3.2	−7.3	−8.4	−3.3	−8.2	−8.3
Dimer CC 9	-9.1^{a}	−4.4	−9.1	−10.0	−3.8	−9.5	−9.9
Dimer CC 10	-8.3^{a}	−3.6	−8.1	−9.1	−3.2	−8.7	−9.0
Dimer CC 11	-9.4^{a}	−4.6	−9.0	−10.1	−4.3	−9.6	−10.0
Dimer CC 12	-7.4^{a}	−3.1	−5.7	−6.6	−3.9	−7.0	−6.6
Dimer CC 13	-8.8^{a}	−3.5	−7.6	−8.4	−3.0	−7.9	−8.3
Dimer CC 14	-9.1^{a}	−4.0	−8.8	−9.8	−3.8	−9.6	−9.6
Dimer A...A S	-8.6^{a}	−0.8	−6.1	−6.9	−0.7	−7.1	−7.2
Dimer GGst	-12.7^{a}	−4.4	−10.3	−11.1	−4.3	−11.4	−11.3
Dimer ACst	-10.2^{a}	−3.4	−8.4	−9.0	−3.0	−9.1	−9.1
Dimer GAst	-11.4^{a}	−2.8	−8.4	−9.3	−2.7	−9.5	−9.4
Dimer CCst	-10.0^{a}	−5.0	−9.6	−10.5	−4.4	−9.9	−10.4
Dimer AUst	-9.8^{a}	−3.3	−8.4	−8.9	−3.0	−9.1	−9.0
Dimer GCst	-10.6^{a}	−5.2	−10.1	−10.6	−4.6	−10.6	−10.8
Dimer CUst	-10.4^{a}	−5.1	−9.6	−10.1	−5.1	−10.5	−10.1
Dimer UUst	-7.5^{a}	−3.3	−7.4	−7.7	−3.2	−8.2	−7.8
Dimer GUst	-12.1^{a}	−5.7	−10.9	−11.3	−5.5	−11.8	−11.4
Dimer GG0/3.36GGs036	-3.5^{a}	3.7	0.0	−0.1	3.4	−1.0	−0.6
Dimer GG0/3.36CCs036	-1.6^{a}	4.6	−0.7	−1.3	4.6	−1.7	−2.0
Dimer AA20/3.05AAs2005	-6.1^{a}	1.3	−4.2	−4.9	1.3	−5.4	−5.2
Dimer AA20/3.05TTs2005	-4.2^{a}	1.7	−3.1	−3.5	2.0	−3.8	−4.0
Dimer GC0/3.25G//Cs	-10.8^{a}	−4.0	−9.5	−10.3	−4.0	−10.7	−10.3
Dimer CG0/3.19G//Cs	-7.9^{a}	−1.8	−5.3	−6.3	−2.7	−7.0	−6.4
Dimer GA10/3.15A//Gs	-9.1^{a}	−1.2	−7.3	−7.8	−1.1	−8.5	−8.2
Dimer GA10/3.15T//Cs	-4.7^{a}	0.6	−3.6	−3.8	0.6	−4.4	−4.2
Dimer AG08/3.19A//Gs	-7.6^{a}	0.3	−4.4	−5.1	−0.1	−5.7	−5.5
Dimer AG08/3.19T//Cs	-6.1^{a}	−0.7	−4.6	−5.1	−1.0	−5.6	−5.1
Dimer TG03.19T//Gs	-5.7^{a}	−0.0	−3.7	−4.3	−0.4	−4.8	−4.4
Dimer TG03.19A//Cs	-5.0^{a}	1.3	−2.7	−3.6	0.6	−4.3	−4.1
Dimer GT10/3.15T//Gs	-5.0^{a}	1.7	−3.9	−4.3	2.3	−4.5	−4.5
Dimer GT10/3.15A//Cs	-5.4^{a}	0.9	−4.0	−4.5	1.0	−4.9	−4.9
Dimer AT10/3.26A//Ts	-6.6^{a}	−0.0	−5.1	−5.4	0.3	−5.8	−5.7
Dimer TA08/3.16A//Ts	-6.1^{a}	1.4	−4.9	−5.4	2.2	−5.8	−5.5
Dimer AA0/3.24A//As	-6.2^{a}	1.1	−4.2	−4.9	1.0	−5.4	−5.2
Dimer AA0/3.24T//Ts	-3.9^{a}	1.3	−3.6	−3.9	1.8	−4.2	−3.9
Dimer A...T S2	-8.1^{a}	0.5	−5.5	−6.0	0.8	−6.4	−6.4
Dimer G...C S1	-7.9^{a}	−1.7	−4.9	−5.8	−2.6	−6.2	−5.8
Dimer A...C S	-6.7^{a}	1.4	−4.0	−4.8	1.2	−5.1	−5.4
Dimer T...G S	-6.2^{a}	1.7	−3.9	−4.3	2.0	−4.6	−4.9
Dimer G...C S2	-7.7^{a}	−2.3	−7.2	−7.8	−1.8	−7.7	−7.8
Dimer A...G S	-6.5^{a}	−0.4	−6.0	−6.8	−0.3	−7.0	−7.2
Dimer C...G S	-12.4^{a}	−3.6	−8.6	−9.3	−3.8	−9.8	−9.3
Dimer G...C S3	-11.6^{a}	−4.3	−9.1	−9.7	−4.1	−9.9	−9.7
Dimer F30-K46	-3.1^{a}	−1.0	−3.0	−3.0	−0.6	−2.9	−2.9
Dimer F30-L33	-5.0^{a}	−0.9	−4.7	−4.8	−0.2	−4.7	−4.7
Dimer F30-Y13	-3.9^{a}	−1.0	−3.9	−4.0	−0.6	−3.9	−4.0
Dimer F30-F49	-3.3^{a}	−0.7	−3.0	−3.0	−0.2	−2.9	−2.8
Dimer F30-Y4	-7.0^{a}	0.5	−4.3	−4.6	0.7	−4.8	−5.0
Dimer F49-K46	-4.8^{a}	−2.0	−4.9	−5.1	−1.0	−4.5	−4.5
Dimer F49-V5	-6.7^{a}	−4.0	−8.4	−8.7	−2.4	−7.7	−7.7
Dimer F49-W37	-2.5^{a}	−0.3	−2.0	−2.1	−0.0	−2.0	−2.0
Dimer F49-Y4	-3.1^{a}	0.0	−3.9	−3.6	1.2	−3.3	−3.0
Dimer F49-PB(Y4-V5)	-2.8^{a}	−0.4	−2.6	−2.7	−0.0	−2.5	−2.6

... *continued on next page* ...

Table S79: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer F49-PB(V5_C6)	-8.2^a	-4.4	-8.6	-8.9	-3.5	-8.4	-8.3
Dimer E47-K6(1IU5)	-80.7^a	-71.4	-74.7	-74.5	-69.7	-73.6	-72.9
Dimer E49-K6(1BQ9)	-113.3^a	-98.5	-101.7	-102.6	-97.3	-101.1	-101.8
Dimer E54-K2(1SMM)	-88.3^a	-85.8	-87.2	-87.8	-85.2	-86.9	-87.2
Dimer E50-K30(1BRF)	-60.4^a	-58.5	-58.8	-58.7	-58.5	-58.7	-58.5
Dimer E50-K52(1BRF)	-97.1^a	-84.0	-87.5	-88.0	-83.3	-87.4	-87.7
Dimer E49-K6(1BRF)	-74.2^a	-64.8	-68.0	-67.1	-63.8	-67.7	-66.6

a P.Jurecka, J.Sponer, J.Cerny, and P.Hobza, Phys.Chem.Chem.Phys. 8, 1985 (2006).

Table S80: Benchmark Results for the S7L Set. Interaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Single point calculations							
Dimer Naphthalene-Naphthalene (sandwich)	−4.0[a]	2.3	−2.4	−3.0	1.7	−3.6	−4.0
Dimer Naphthalene-Naphthalene (displaced)	−6.0[a]	1.7	−4.0	−4.7	1.4	−5.3	−5.7
Dimer Naphthalene-Naphthalene (displaced, rotated)	−6.1[a]	2.2	−3.9	−4.7	1.8	−5.4	−5.8
Dimer Naphthalene-Naphthalene (cross)	−5.5[a]	2.0	−3.7	−4.4	1.6	−5.0	−5.5
Dimer Coronene-Coronene	−20.0[a]	3.6	−13.9	−15.9	3.3	−17.4	−18.4
Dimer Decalin-Decalin (haDZ)	−4.8[a]	−1.0	−5.7	−5.6	0.2	−5.1	−4.9
Dimer Perhydrocoronene-Perhydrocoronene	−13.6[a]	−2.8	−15.7	−15.3	0.8	−14.0	−13.5
Full optimizations							
Dimer Naphthalene-Naphthalene (sandwich)	−4.0[a]	0.0	−4.2	−6.4	0.0	−6.2	−6.6
Dimer Naphthalene-Naphthalene (displaced)	−6.0[a]	−1.3	−5.7	−6.4	−0.0	−7.0	−7.2
Dimer Naphthalene-Naphthalene (displaced, rotated)	−6.1[a]	−0.0	−5.7	−6.6	−0.3	−7.3	−7.5
Dimer Naphthalene-Naphthalene (cross)	−5.5[a]	0.0	−5.5	−6.6	0.0	−7.3	−7.5
Dimer Coronene-Coronene	−20.0[a]	−0.0	−17.2	−19.8	−0.7	−21.2	−21.6
Dimer Decalin-Decalin (haDZ)	−4.8[a]	−2.0	−8.2	−7.0	−0.0	−6.1	−5.5
Dimer Perhydrocoronene-Perhydrocoronene	−13.6[a]	−5.0	−22.2	−19.0	−0.1	−16.2	−14.3

a T.Janowski and P.Pulay, J.Am.Chem.Soc. 134, 17520 (2012).

Table S81: Benchmark Results for the S30L-CHNOF Set. Interaction Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
# 1	−29.0[a]	−8.1	−30.5	−32.4	−3.1	−30.1	−30.5
# 2	−20.8[a]	−2.9	−19.2	−20.5	0.3	−19.3	−19.5
# 3	−23.5[a]	−4.0	−23.0	−23.5	−4.6	−27.6	−26.9
# 5	−29.0[a]	−8.1	−32.4	−34.8	−6.0	−35.1	−35.1
# 6	−25.5[a]	1.2	−21.6	−24.7	3.1	−24.5	−25.2
# 7	−35.1[a]	7.4	−28.1	−31.7	8.1	−34.1	−35.7
# 8	−36.8[a]	8.4	−31.7	−35.8	9.0	−38.5	−40.4
# 9	−28.4[a]	1.9	−29.4	−31.5	4.2	−32.8	−33.2
# 10	−29.8[a]	3.3	−30.1	−32.3	5.7	−33.7	−34.1
# 13	−30.8[a]	−3.7	−22.5	−24.3	−1.5	−23.7	−24.5
# 17	−33.4[a]	−20.7	−35.4	−34.2	−13.7	−31.8	−29.7
# 18	−23.3[a]	−12.1	−25.6	−25.2	−7.0	−23.5	−21.7
# 19	−17.5[a]	−2.6	−13.8	−13.9	−0.0	−13.0	−12.2
# 20	−19.2[a]	−2.4	−18.4	−18.2	1.6	−17.0	−15.7
# 21	−24.2[a]	1.0	−20.4	−21.8	4.0	−20.9	−22.6
# 22	−42.6[a]	−25.4	−34.9	−33.3	−25.0	−36.6	−36.1
# 23	−61.3[a]	−43.8	−50.6	−52.5	−46.7	−54.9	−63.4
# 24	−135.5[a]	−121.2	−156.3	−158.5	−106.9	−148.2	−151.3
# 25	−26.0[a]	1.9	−24.4	−26.3	4.1	−26.4	−27.6
# 26	−25.8[a]	2.1	−24.2	−26.2	4.2	−26.3	−27.5
# 27	−82.2[a]	−77.5	−92.7	−94.3	−71.1	−88.9	−92.5
# 28	−80.1[a]	−76.5	−89.3	−90.6	−70.0	−84.9	−88.7
# 29	−53.5[a]	−38.0	−47.1	−45.4	−39.6	−50.9	−47.9
# 30	−49.3[a]	−30.7	−42.7	−41.8	−32.5	−47.0	−44.8

a R.Sure and S.Grimme, J.Chem.Theory Comput. 11, 3785 (2015). Correction see: J.Chem.Theory Comput. 11, 5990 (2015).

Table S82: Benchmark Results for the AF6 Set. Folding Energies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Single point calculations							
c8 n-alkane bowl G+G+TG+G+ mp2	1.6[a]	3.7	2.4	3.8	4.7	3.0	4.8
c10 n-alkane hairpin mp2/vtz	1.4[a]	3.4	1.8	3.3	4.7	2.7	4.5
c12 n-alkane hairpin mp2/vtz	1.0[a]	3.5	1.5	3.0	4.8	2.3	4.2
c14 n-alkane hairpin mp2/vtz	0.1[a]	4.4	0.2	1.9	6.3	1.1	3.3
c16 n-alkane hairpin mp2/vtz	−0.6[a]	4.1	−0.8	1.0	6.2	0.2	2.4
c18 n-alkane hairpin mp2/vtz	−1.6[a]	4.1	−1.7	0.1	6.7	−0.5	1.8
Full optimizations							
c8 n-alkane bowl G+G+TG+G+ mp2	1.6[a]	3.1	2.0	3.3	3.4	2.2	3.5
c10 n-alkane hairpin mp2/vtz	1.4[a]	3.0	1.7	3.0	3.4	2.0	3.3
c12 n-alkane hairpin mp2/vtz	1.0[a]	3.0	0.8	2.6	3.4	1.4	3.2
c14 n-alkane hairpin mp2/vtz	0.1[a]	3.0	−0.0	1.8	3.4	0.6	2.4
c16 n-alkane hairpin mp2/vtz	−0.6[a]	3.0	−1.1	0.8	3.4	−0.2	1.7
c18 n-alkane hairpin mp2/vtz	−1.6[a]	3.0	−2.1	−0.1	3.4	−1.0	0.9

a J.N.Byrd, R.J.Barlett, and J.A.Montgomery Jr., J.Phys.Chem.A 118, 1706 (2014).

Table S83: Benchmark Results for the AF6 Set. Folding Enthalpies (kcal/mol)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Full optimizations							
c8 n-alkane bowl G+G+TG+G+ mp2	1.8[a]	3.1	2.0	3.2	3.4	2.2	3.4
c10 n-alkane hairpin mp2/vtz	1.5[a]	3.0	1.7	2.9	3.4	2.0	3.2
c12 n-alkane hairpin mp2/vtz	1.1[a]	3.0	0.8	2.5	3.4	1.4	2.4
c14 n-alkane hairpin mp2/vtz	0.3[a]	3.0	−0.0	1.7	3.4	0.6	2.3
c16 n-alkane hairpin mp2/vtz	−0.5[a]	3.0	−1.1	0.7	3.4	−0.2	1.5
c18 n-alkane hairpin mp2/vtz	−1.4[a]	3.0	−2.1	−0.2	3.4	−1.0	0.8

a J.N.Byrd, R.J.Barlett, and J.A.Montgomery Jr., J.Phys.Chem.A 118, 1706 (2014).

Table S84: Benchmark Results for the X40×10-CHNOF Set. Interaction Energies (kcal/mol)

Molecule	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer methane-F2_0.80	0.3[a]	0.1	−0.2	−0.3	0.7	0.3	0.5
Dimer methane-F2_0.85	−0.3[a]	0.0	−0.3	−0.3	0.4	−0.0	0.1
Dimer methane-F2_0.90	−0.5[a]	−0.0	−0.3	−0.3	0.2	−0.2	−0.1
Dimer methane-F2_0.95	−0.5[a]	−0.0	−0.2	−0.3	0.1	−0.2	−0.2
Dimer methane-F2_1.00	−0.5[a]	−0.0	−0.2	−0.2	0.0	−0.2	−0.2
Dimer methane-F2_1.05	−0.4[a]	−0.0	−0.2	−0.2	0.0	−0.2	−0.2
Dimer methane-F2_1.10	−0.3[a]	−0.0	−0.2	−0.2	−0.0	−0.2	−0.2
Dimer methane-F2_1.25	−0.2[a]	−0.0	−0.1	−0.1	−0.0	−0.1	−0.1
Dimer methane-F2_1.50	−0.1[a]	−0.0	−0.0	−0.0	−0.0	−0.0	—[b]
Dimer methane-F2_2.00	−0.0[a]	0.0	−0.0	−0.0	—[b]	—[b]	—[b]
Dimer fluoromethane-methane_0.80	0.7[a]	1.2	0.2	0.5	2.2	0.9	1.4
Dimer fluoromethane-methane_0.85	−0.3[a]	0.4	−0.5	−0.4	1.0	−0.2	0.1
Dimer fluoromethane-methane_0.90	−0.7[a]	0.1	−0.7	−0.6	0.4	−0.6	−0.4
Dimer fluoromethane-methane_0.95	−0.8[a]	0.0	−0.7	−0.7	0.2	−0.7	−0.6
Dimer fluoromethane-methane_1.00	−0.7[a]	−0.0	−0.6	−0.6	0.1	−0.6	−0.6
Dimer fluoromethane-methane_1.05	−0.6[a]	−0.0	−0.5	−0.5	0.0	−0.6	−0.6
Dimer fluoromethane-methane_1.10	−0.5[a]	−0.0	−0.4	−0.5	−0.0	−0.5	−0.5
Dimer fluoromethane-methane_1.25	−0.3[a]	−0.0	−0.3	−0.3	−0.0	−0.3	−0.3
Dimer fluoromethane-methane_1.50	−0.1[a]	−0.0	−0.1	−0.1	−0.0	−0.1	−0.1
Dimer fluoromethane-methane_2.00	−0.0[a]	−0.0	−0.0	−0.0	−0.0	−0.0	−0.0
Dimer trifluoromethane-methane_0.80	0.3[a]	0.0	−0.8	−0.9	0.5	−0.7	−0.5
Dimer trifluoromethane-methane_0.85	−0.5[a]	−0.0	−0.8	−0.9	0.2	−0.8	−0.8
Dimer trifluoromethane-methane_0.90	−0.7[a]	−0.0	−0.7	−0.8	0.0	−0.8	−0.8
Dimer trifluoromethane-methane_0.95	−0.7[a]	−0.0	−0.6	−0.6	0.0	−0.7	−0.7
Dimer trifluoromethane-methane_1.00	−0.6[a]	−0.0	−0.5	−0.5	0.0	−0.5	−0.5
Dimer trifluoromethane-methane_1.05	−0.5[a]	−0.0	−0.4	−0.4	0.0	−0.4	−0.4
Dimer trifluoromethane-methane_1.10	−0.4[a]	0.0	−0.3	−0.3	0.0	−0.3	−0.4
Dimer trifluoromethane-methane_1.25	−0.2[a]	0.0	−0.2	−0.2	0.0	−0.2	−0.2
Dimer trifluoromethane-methane_1.50	−0.1[a]	0.0	−0.1	−0.1	0.0	−0.1	−0.1
Dimer trifluoromethane-methane_2.00	−0.0[a]	0.0	−0.0	−0.0	0.0	−0.0	−0.0
Dimer fluoromethane-fluoromethane_0.80	0.6[a]	−0.0	−0.6	−0.5	1.2	0.4	0.8
Dimer fluoromethane-fluoromethane_0.85	−0.9[a]	−0.5	−1.0	−1.1	0.1	−0.6	−0.3
Dimer fluoromethane-fluoromethane_0.90	−1.5[a]	−0.7	−1.1	−1.2	−0.4	−1.0	−0.9
Dimer fluoromethane-fluoromethane_0.95	−1.7[a]	−0.7	−1.1	−1.2	−0.6	−1.1	−1.1
Dimer fluoromethane-fluoromethane_1.00	−1.6[a]	−0.7	−1.0	−1.1	−0.6	−1.1	−1.1
Dimer fluoromethane-fluoromethane_1.05	−1.5[a]	−0.6	−0.9	−1.0	−0.6	−1.0	−1.0
Dimer fluoromethane-fluoromethane_1.10	−1.3[a]	−0.6	−0.9	−0.9	−0.6	−0.9	−1.0
Dimer fluoromethane-fluoromethane_1.25	−0.9[a]	−0.5	−0.6	−0.7	−0.5	−0.7	−0.7
Dimer fluoromethane-fluoromethane_1.50	−0.6[a]	−0.3	−0.4	−0.5	−0.4	−0.4	−0.5
Dimer fluoromethane-fluoromethane_2.00	−0.3[a]	−0.2	−0.2	−0.2	−0.2	−0.2	−0.2
Dimer benF3-ben_0.80	9.1[a]	4.3	−1.7	−1.9	7.1	−1.1	−0.6
Dimer benF3-ben_0.85	1.9[a]	1.8	−3.7	−4.1	3.3	−4.0	−3.7
Dimer benF3-ben_0.90	−1.9[a]	0.7	−4.3	−4.8	1.4	−4.9	−4.9
Dimer benF3-ben_0.95	−3.7[a]	0.2	−4.2	−4.7	0.5	−5.0	−5.0
Dimer benF3-ben_1.00	−4.3[a]	0.0	−3.8	−4.3	0.1	−4.6	−4.7
Dimer benF3-ben_1.05	−4.3[a]	−0.0	−3.4	−3.8	−0.0	−4.0	−4.2
Dimer benF3-ben_1.10	−4.0[a]	−0.0	−2.9	−3.2	−0.1	−3.5	−3.6
Dimer benF3-ben_1.25	−2.6[a]	0.0	−1.8	−1.9	−0.1	−2.0	−2.2
Dimer benF3-ben_1.50	−1.1[a]	0.0	−0.7	−0.8	−0.0	−0.8	−0.9
Dimer benF3-ben_2.00	−0.2[a]	0.0	−0.1	−0.1	−0.0	−0.1	−0.1
Dimer benF6-ben_0.80	12.5[a]	3.7	−3.0	−3.0	7.6	−1.6	−0.9
Dimer benF6-ben_0.85	2.2[a]	0.2	−5.8	−6.2	2.5	−5.6	−5.2
Dimer benF6-ben_0.90	−3.1[a]	−1.1	−6.5	−7.0	0.1	−6.9	−6.7
Dimer benF6-ben_0.95	−5.4[a]	−1.5	−6.2	−6.8	−0.8	−6.9	−6.8
Dimer benF6-ben_1.00	−6.0[a]	−1.5	−5.7	−6.1	−1.2	−6.3	−6.3
Dimer benF6-ben_1.05	−5.9[a]	−1.4	−5.0	−5.4	−1.2	−5.5	−5.6
Dimer benF6-ben_1.10	−5.4[a]	−1.3	−4.3	−4.6	−1.2	−4.7	−4.8
Dimer benF6-ben_1.25	−3.5[a]	−0.9	−2.7	−2.9	−0.8	−2.9	−2.9
Dimer benF6-ben_1.50	−1.5[a]	−0.5	−1.2	−1.3	−0.5	−1.2	−1.2
Dimer benF6-ben_2.00	−0.4[a]	−0.2	−0.3	−0.3	−0.2	−0.3	−0.3
Dimer trifluorometOH-wat_0.80	−5.2[a]	−6.8	−7.6	−8.4	−8.4	−9.5	−8.7
Dimer trifluorometOH-wat_0.85	−7.7[a]	−7.8	−8.6	−9.3	−9.1	−10.2	−9.5
Dimer trifluorometOH-wat_0.90	−9.0[a]	−8.1	−8.8	−9.4	−9.1	−10.1	−9.5
Dimer trifluorometOH-wat_0.95	−9.6[a]	−7.8	−8.5	−9.0	−8.7	−9.6	−9.0

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Table S84: ... *continued from previous page* ...

Molecule	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Dimer trifluorometOH-wat_1.00	−9.7[a]	−7.4	−8.0	−8.4	−8.1	−8.9	−8.4
Dimer trifluorometOH-wat_1.05	−9.5[a]	−6.8	−7.4	−7.7	−7.5	−8.3	−7.8
Dimer trifluorometOH-wat_1.10	−9.1[a]	−6.2	−6.7	−7.0	−6.9	−7.6	−7.2
Dimer trifluorometOH-wat_1.25	−7.4[a]	−4.6	−5.1	−5.2	−5.4	−5.9	−5.7
Dimer trifluorometOH-wat_1.50	−4.7[a]	−3.1	−3.4	−3.4	−3.7	−4.0	−3.9
Dimer trifluorometOH-wat_2.00	−2.0[a]	−1.5	−1.6	−1.7	−1.8	−2.0	−1.9
Dimer HF-mOH_0.80	−5.5[a]	0.1	−0.4	−2.9	−0.5	−1.3	−1.8
Dimer HF-mOH_0.85	−7.9[a]	−2.4	−2.9	−4.8	−2.6	−3.3	−3.7
Dimer HF-mOH_0.90	−9.1[a]	−3.8	−4.3	−5.8	−3.6	−4.4	−4.6
Dimer HF-mOH_0.95	−9.6[a]	−4.5	−5.0	−6.1	−4.1	−4.8	−4.9
Dimer HF-mOH_1.00	−9.6[a]	−4.7	−5.2	−6.0	−4.3	−4.9	−5.0
Dimer HF-mOH_1.05	−9.3[a]	−4.7	−5.1	−5.7	−4.2	−4.8	−4.9
Dimer HF-mOH_1.10	−8.9[a]	−4.5	−4.9	−5.3	−4.1	−4.7	−4.7
Dimer HF-mOH_1.25	−7.1[a]	−3.6	−4.0	−4.2	−3.5	−4.0	−4.0
Dimer HF-mOH_1.50	−4.6[a]	−2.5	−2.7	−2.8	−2.6	−2.9	−2.9
Dimer HF-mOH_2.00	−2.0[a]	−1.3	−1.4	−1.4	−1.4	−1.5	−1.5
Dimer HF-mNH2_0.80	−3.0[a]	−1.6	−2.3	−6.2	−6.5	−7.5	−12.5
Dimer HF-mNH2_0.85	−4.8[a]	−4.5	−5.2	−8.0	−8.6	−9.6	−13.8
Dimer HF-mNH2_0.90	−5.8[a]	−6.0	−6.7	−8.7	−9.3	−10.3	−13.8
Dimer HF-mNH2_0.95	−6.2[a]	−6.7	−7.3	−8.7	−9.3	−10.2	−13.1
Dimer HF-mNH2_1.00	−6.4[a]	−6.7	−7.4	−8.3	−8.7	−9.6	−12.0
Dimer HF-mNH2_1.05	−6.2[a]	−6.5	−7.1	−7.7	−8.0	−8.8	−10.8
Dimer HF-mNH2_1.10	−6.0[a]	−6.1	−6.7	−7.1	−7.2	−8.0	−9.6
Dimer HF-mNH2_1.25	−4.8[a]	−4.9	−5.3	−5.5	−5.2	−5.9	−6.7
Dimer HF-mNH2_1.50	−3.1[a]	−3.2	−3.6	−3.8	−3.3	−3.8	−4.2
Dimer HF-mNH2_2.00	−1.3[a]	−1.6	−1.7	−1.8	−1.6	−1.8	−2.0
Dimer methanol-fluoromethane_0.80	−1.7[a]	1.1	0.4	−0.5	4.0	2.9	3.6
Dimer methanol-fluoromethane_0.85	−3.0[a]	−0.2	−0.9	−1.4	2.0	1.0	1.6
Dimer methanol-fluoromethane_0.90	−3.7[a]	−0.9	−1.6	−1.9	0.7	−0.2	0.3
Dimer methanol-fluoromethane_0.95	−3.9[a]	−1.3	−2.0	−2.1	−0.2	−1.0	−0.6
Dimer methanol-fluoromethane_1.00	−3.9[a]	−1.5	−2.1	−2.2	−0.7	−1.5	−1.2
Dimer methanol-fluoromethane_1.05	−3.7[a]	−1.5	−2.1	−2.2	−1.0	−1.8	−1.5
Dimer methanol-fluoromethane_1.10	−3.5[a]	−1.5	−2.0	−2.1	−1.2	−1.9	−1.7
Dimer methanol-fluoromethane_1.25	−2.6[a]	−1.2	−1.6	−1.7	−1.2	−1.7	−1.7
Dimer methanol-fluoromethane_1.50	−1.6[a]	−0.8	−1.1	−1.1	−0.9	−1.2	−1.2
Dimer methanol-fluoromethane_2.00	−0.6[a]	−0.4	−0.5	−0.5	−0.5	−0.5	−0.5

a J.Rezac, K.E.Riley, and P.Hobza, J.Chem.Theory Comput. 8, 4285-4292 (2012); M.K.Kesharwani, D.Manna, N.Sylvetsky, J.M.L.Martin, J.Phys.Chem.A, 122, 2184-2197 (2018). b Calculation could not be converged.

Table S85: Benchmark Results for the VEE Set. Vertical Excitation Energies (eV)

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Ethene: 1 1B1u, $\pi \rightarrow \pi^*$	7.80[a]	7.78	7.78	7.91	7.85	7.85	7.95
Ethene: 1 3B1u, $\pi \rightarrow \pi^*$	4.50[a]	4.14	4.14	4.26	4.16	4.16	4.24
E-Butadiene: 2 1Ag, $\pi \rightarrow \pi^*$	6.55[a]	5.96	5.96	6.11	5.98	5.98	6.08
E-Butadiene: 1 1Bu, $\pi \rightarrow \pi^*$	6.18[a]	6.22	6.22	6.31	6.26	6.26	6.33
E-Butadiene: 1 3Ag, $\pi \rightarrow \pi^*$	5.08[a]	4.56	4.56	4.68	4.59	4.59	4.66
E-Butadiene: 1 3Bu, $\pi \rightarrow \pi^*$	3.20[a]	3.04	3.04	3.13	3.04	3.04	3.10
Hexatriene: 2 1Ag, $\pi \rightarrow \pi^*$	5.09[a]	4.86	4.86	4.98	4.86	4.86	4.95
Hexatriene: 1 1Bu, $\pi \rightarrow \pi^*$	5.10[a]	5.33	5.33	5.40	5.36	5.36	5.41
Hexatriene: 1 3Ag, $\pi \rightarrow \pi^*$	4.15[a]	3.80	3.80	3.90	3.81	3.81	3.88
Hexatriene: 1 3Bu, $\pi \rightarrow \pi^*$	2.40[a]	2.46	2.46	2.53	2.45	2.45	2.50
Octatetraene: 2 1Ag, $\pi \rightarrow \pi^*$	4.47[a]	4.14	4.14	4.25	4.13	4.13	4.22
Octatetraene: 1 1Bu, $\pi \rightarrow \pi^*$	4.66[a]	4.77	4.77	4.83	4.79	4.79	4.84
Octatetraene: 1 3Ag, $\pi \rightarrow \pi^*$	3.55[a]	3.23	3.23	3.32	3.24	3.24	3.30
Octatetraene: 1 3Bu, $\pi \rightarrow \pi^*$	2.20[a]	2.12	2.12	2.18	2.11	2.11	2.16
Cyclopropene: 1 1B1, $\sigma \rightarrow \pi^*$	6.67[a]	5.75	5.75	5.90	5.93	5.93	6.10
Cyclopropene: 1 1B2, $\pi \rightarrow \pi^*$	6.68[a]	6.42	6.42	6.62	6.39	6.39	6.61
Cyclopropene: 1 3B2, $\pi \rightarrow \pi^*$	4.28[a]	3.80	3.80	3.95	3.72	3.72	3.86
Cyclopropene: 1 3B1, $\sigma \rightarrow \pi^*$	6.40[a]	5.48	5.48	5.63	5.65	5.65	5.80
Cyclopentadiene: 2 1A1, $\pi \rightarrow \pi^*$	6.28[a]	5.60	5.60	5.74	5.59	5.59	5.71
Cyclopentadiene: 1 1B2, $\pi \rightarrow \pi^*$	5.55[a]	5.07	5.07	5.14	5.09	5.09	5.17
Cyclopentadiene: 1 3A1, $\pi \rightarrow \pi^*$	5.09[a]	4.30	4.30	4.42	4.31	4.31	4.40
Cyclopentadiene: 1 3B2, $\pi \rightarrow \pi^*$	3.26[a]	2.87	2.87	2.94	2.86	2.86	2.93
Norbornadiene: 1 1A2 $\pi \rightarrow \pi^*$	5.37[a]	6.00	6.00	6.07	6.06	6.06	6.15
Norbornadiene: 1 1B2 $\pi \rightarrow \pi^*$	6.21[a]	6.34	6.34	6.40	6.46	6.46	6.55
Norbornadiene: 1 3A2 $\pi \rightarrow \pi^*$	3.68[a]	4.27	4.27	4.38	4.26	4.26	4.32
Norbornadiene: 1 3B2 $\pi \rightarrow \pi^*$	4.16[a]	4.10	4.10	4.22	4.07	4.07	4.11
Benzene: 1 1B2u, $\pi \rightarrow \pi^*$	5.08[a]	4.48	4.48	4.59	4.51	4.51	4.58
Benzene: 1 1B1u, $\pi \rightarrow \pi^*$	6.54[a]	5.94	5.94	6.06	6.03	6.03	6.10
Benzene: 1 1E1u, $\pi \rightarrow \pi^*$	7.13[a]	7.16	7.16	7.27	7.20	7.20	7.27
Benzene: 1 1E2g, $\pi \rightarrow \pi^*$	8.15[a]	7.19	7.19	7.36	7.22	7.22	7.33
Benzene: 1 3B1u, $\pi \rightarrow \pi^*$	4.15[a]	3.74	3.74	3.84	3.76	3.76	3.82
Benzene: 1 3E1u, $\pi \rightarrow \pi^*$	4.86[a]	4.54	4.54	4.65	4.57	4.57	4.63
Benzene: 1 3B2u, $\pi \rightarrow \pi^*$	5.88[a]	5.80	5.80	5.90	5.85	5.85	5.91
Benzene: 1 3E2g, $\pi \rightarrow \pi^*$	7.51[a]	6.30	6.30	6.46	6.34	6.34	6.44
Naphthalene: 2 1Ag, $\pi \rightarrow \pi^*$	5.90[a]	5.23	5.23	5.36	5.27	5.27	5.35
Naphthalene: 3 1Ag, $\pi \rightarrow \pi^*$	6.49[a]	6.03	6.03	6.17	6.05	6.05	6.14
Naphthalene: 1 1B2u, $\pi \rightarrow \pi^*$	4.82[a]	4.83	4.83	4.91	4.87	4.87	4.93
Naphthalene: 2 1B2u, $\pi \rightarrow \pi^*$	6.36[a]	6.23	6.23	6.34	6.28	6.28	6.35
Naphthalene: 1 1B3u, $\pi \rightarrow \pi^*$	4.25[a]	3.81	3.81	3.91	3.84	3.84	3.90
Naphthalene: 2 1B3u, $\pi \rightarrow \pi^*$	6.11[a]	6.16	6.16	6.24	6.18	6.18	6.24
Naphthalene: 1 1B1g, $\pi \rightarrow \pi^*$	5.75[a]	5.74	5.74	5.87	5.76	5.76	5.85
Naphthalene: 2 1B1g, $\pi \rightarrow \pi^*$	6.46[a]	6.24	6.24	6.35	6.31	6.31	6.39
Naphthalene: 1 3Ag, $\pi \rightarrow \pi^*$	5.42[a]	4.90	4.90	5.02	4.93	4.93	5.00
Naphthalene: 2 3Ag, $\pi \rightarrow \pi^*$	6.17[a]	6.51	6.51	6.63	6.58	6.58	6.65
Naphthalene: 3 3Ag, $\pi \rightarrow \pi^*$	6.65[a]	5.76	5.76	5.90	5.79	5.79	5.87
Naphthalene: 1 3B2u, $\pi \rightarrow \pi^*$	3.09[a]	2.89	2.89	2.97	2.90	2.90	2.95
Naphthalene: 2 3B2u, $\pi \rightarrow \pi^*$	4.56[a]	4.28	4.28	4.38	4.31	4.31	4.37
Naphthalene: 1 3B3u, $\pi \rightarrow \pi^*$	4.09[a]	3.91	3.91	4.00	3.94	3.94	4.00
Naphthalene: 2 3B3u, $\pi \rightarrow \pi^*$	4.92[a]	4.95	4.95	5.03	4.99	4.99	5.04
Naphthalene: 1 3B1g, $\pi \rightarrow \pi^*$	4.42[a]	4.07	4.07	4.17	4.09	4.09	4.15
Naphthalene: 2 3B1g, $\pi \rightarrow \pi^*$	6.12[a]	6.49	6.49	6.60	6.52	6.52	6.59
Naphthalene: 3 3B1g, $\pi \rightarrow \pi^*$	6.67[a]	5.79	5.79	5.93	5.83	5.83	5.91
Furan: 2 1A1, $\pi \rightarrow \pi^*$	6.57[a]	5.43	5.43	5.61	5.51	5.51	5.64
Furan: 3 1A1, $\pi \rightarrow \pi^*$	8.13[a]	7.47	7.47	7.67	7.62	7.62	7.76
Furan: 1 1B2, $\pi \rightarrow \pi^*$	6.32[a]	5.82	5.82	5.93	5.88	5.88	5.93
Furan: 1 3A1, $\pi \rightarrow \pi^*$	5.43[a]	4.54	4.54	4.67	4.59	4.59	4.66
Furan: 1 3B2, $\pi \rightarrow \pi^*$	4.11[a]	3.50	3.50	3.58	3.53	3.53	3.55
Pyrrole: 2 1A1, $\pi \rightarrow \pi^*$	6.37[a]	5.28	5.28	5.43	5.29	5.29	5.44
Pyrrole: 3 1A1, $\pi \rightarrow \pi^*$	7.91[a]	7.18	7.18	7.35	7.16	7.16	7.32
Pyrrole: 2 1B2, $\pi \rightarrow \pi^*$	6.57[a]	5.86	5.86	5.99	5.94	5.94	5.96
Pyrrole: 1 3A1, $\pi \rightarrow \pi^*$	5.42[a]	4.59	4.59	4.71	4.64	4.64	4.69
Pyrrole: 1 3B2, $\pi \rightarrow \pi^*$	4.44[a]	3.76	3.76	3.80	3.89	3.89	3.82
Imidazole: 2 1A', $\pi \rightarrow \pi^*$	6.25[a]	5.59	5.59	5.73	5.85	5.85	5.80
Imidazole: 3 1A', $\pi \rightarrow \pi^*$	6.73[a]	6.04	6.04	6.19	6.16	6.16	6.17

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Table S85: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
Imidazole: 1 1A", $n \to \pi^*$	6.65[a]	6.00	6.00	6.10	6.08	6.08	6.23
Imidazole: 1 3A', $\pi \to \pi^*$	4.65[a]	3.95	3.95	4.00	4.06	4.06	4.00
Imidazole: 2 3A', $\pi \to \pi^*$	5.64[a]	4.95	4.95	5.07	5.27	5.27	5.10
Imidazole: 3 3A', $\pi \to \pi^*$	6.38[a]	5.69	5.69	5.90	5.99	5.99	6.02
Imidazole: 1 3A", $n \to \pi^*$	6.25[a]	5.60	5.60	5.71	5.70	5.70	5.81
Pyridine: 2 1A1, $\pi \to \pi^*$	6.26[a]	6.11	6.11	6.21	6.25	6.25	6.28
Pyridine: 3 1A1, $\pi \to \pi^*$	7.18[a]	7.43	7.43	7.53	7.63	7.63	7.63
Pyridine: 1 1A2, $n \to \pi^*$	5.11[a]	5.06	5.06	5.17	4.84	4.84	5.18
Pyridine: 1 1B2, $\pi \to \pi^*$	4.85[a]	4.65	4.65	4.75	4.83	4.83	4.77
Pyridine: 2 1B2, $\pi \to \pi^*$	7.27[a]	7.48	7.48	7.64	7.62	7.62	7.65
Pyridine: 1 1B1, $n \to \pi^*$	4.59[a]	4.85	4.85	4.87	4.86	4.86	4.89
Pyridine: 1 3A1, $\pi \to \pi^*$	4.06[a]	3.86	3.86	3.97	3.94	3.94	3.97
Pyridine: 2 3A1, $\pi \to \pi^*$	4.91[a]	4.74	4.74	4.85	4.97	4.97	4.91
Pyridine: 1 3A2, $n \to \pi^*$	5.28[a]	4.96	4.96	5.08	4.75	4.75	5.09
Pyridine: 1 3B2, $\pi \to \pi^*$	4.64[a]	4.66	4.66	4.73	4.83	4.83	4.76
Pyridine: 2 3B2, $\pi \to \pi^*$	6.08[a]	5.97	5.97	6.09	6.17	6.17	6.20
Pyridine: 1 3B1, $n \to \pi^*$	4.25[a]	4.48	4.48	4.50	4.47	4.47	4.52
Pyrazine: 1 1Au, $n \to \pi^*$	4.98[a]	4.12	4.12	4.25	3.89	3.89	4.34
Pyrazine: 1 1B1g, $n \to \pi^*$	6.69[a]	6.54	6.54	6.73	6.32	6.32	6.63
Pyrazine: 1 1B1u, $\pi \to \pi^*$	6.83[a]	6.22	6.22	6.33	6.35	6.35	6.38
Pyrazine: 2 1B1u, $\pi \to \pi^*$	7.86[a]	8.06	8.06	8.16	8.68	8.68	8.32
Pyrazine: 1 1B2g, $n \to \pi^*$	5.65[a]	5.78	5.78	5.79	5.86	5.86	5.73
Pyrazine: 1 1B2u, $\pi \to \pi^*$	4.97[a]	4.76	4.76	4.82	5.20	5.20	4.86
Pyrazine: 2 1B2u, $\pi \to \pi^*$	7.81[a]	7.67	7.67	7.85	8.12	8.12	7.97
Pyrazine: 1 1B3u, $n \to \pi^*$	4.13[a]	3.81	3.81	3.75	4.04	4.04	3.88
Pyrimidine: 2 1A1, $\pi \to \pi^*$	6.82[a]	6.36	6.36	6.45	6.62	6.62	6.55
Pyrimidine: 1 1A2, $n \to \pi^*$	4.85[a]	4.54	4.54	4.66	4.40	4.40	4.69
Pyrimidine: 1 1B2, $\pi \to \pi^*$	5.34[a]	4.86	4.86	4.98	5.22	5.22	5.06
Pyrimidine: 1 1B1, $n \to \pi^*$	4.43[a]	4.34	4.34	4.35	4.38	4.38	4.40
Pyridazine: 2 1A1, $\pi \to \pi^*$	5.20[a]	4.74	4.74	4.85	5.08	5.08	4.92
Pyridazine: 1 1A2, $n \to \pi^*$	4.44[a]	4.70	4.70	4.76	4.21	4.21	4.66
Pyridazine: 2 1A2, $n \to \pi^*$	5.66[a]	5.38	5.38	5.44	5.57	5.57	5.38
Pyridazine: 1 1B1, $n \to \pi^*$	3.85[a]	4.37	4.37	4.30	4.14	4.14	4.25
s-Triazine: 1 1A1", $n \to \pi^*$	4.70[a]	4.51	4.51	4.73	4.66	4.66	4.70
s-Triazine: 1 1E", $n \to \pi^*$	4.75[a]	4.40	4.40	4.66	4.58	4.58	4.59
s-Triazine: 1 1A2", $n \to \pi^*$	4.71[a]	4.24	4.24	4.52	4.43	4.43	4.43
s-Triazine: 1 1A2', $\pi \to \pi^*$	5.71[a]	5.12	5.12	5.28	5.69	5.69	5.44
s-Tetrazine: 1 1Au, $n \to \pi^*$	3.78[a]	3.55	3.55	3.67	3.08	3.08	3.59
s-Tetrazine: 2 1Au, $n \to \pi^*$	5.39[a]	4.65	4.65	4.71	5.06	5.06	4.73
s-Tetrazine: 1 1B1g, $n \to \pi^*$	4.87[a]	6.15	6.15	5.99	6.49	6.49	6.18
s-Tetrazine: 1 1B2g, $n \to \pi^*$	5.28[a]	5.33	5.33	5.25	6.11	6.11	5.41
s-Tetrazine: 1 1B2u, $\pi \to \pi^*$	5.08[a]	4.88	4.88	4.92	5.74	5.74	5.12
s-Tetrazine: 1 1B3g, $n, n \to \pi^*, \pi^*$	5.76[a]	6.28	6.28	6.21	5.88	5.88	6.24
s-Tetrazine: 1 1B3u, $n \to \pi^*$	2.46[a]	2.83	2.83	2.66	2.88	2.88	2.72
s-Tetrazine: 1 3Au, $n \to \pi^*$	3.49[a]	3.31	3.31	3.45	2.87	2.87	3.36
s-Tetrazine: 2 3Au, $n \to \pi^*$	4.96[a]	4.40	4.40	4.47	4.79	4.79	4.45
s-Tetrazine: 1 3B1g, $n \to \pi^*$	4.18[a]	4.85	4.85	4.78	4.78	4.78	4.91
s-Tetrazine: 1 3B1u, $\pi \to \pi^*$	4.36[a]	4.07	4.07	4.13	4.74	4.74	4.37
s-Tetrazine: 2 3B1u, $\pi \to \pi^*$	5.32[a]	5.07	5.07	5.18	6.00	6.00	5.36
s-Tetrazine: 1 3B2g, $n \to \pi^*$	4.89[a]	5.04	5.04	4.98	5.66	5.66	5.10
s-Tetrazine: 1 3B2u, $\pi \to \pi^*$	4.39[a]	4.76	4.76	4.68	5.62	5.62	4.89
s-Tetrazine: 1 3B3u, $n \to \pi^*$	1.87[a]	2.35	2.35	2.18	2.36	2.36	2.25
Formaldehyde: 1 1A2, $n \to \pi^*$	3.88[a]	3.55	3.55	3.70	3.59	3.59	3.73
Formaldehyde: 1 1B1, $\sigma \to \pi^*$	9.04[a]	7.93	7.93	8.21	9.01	9.01	9.27
Formaldehyde: 3 1A1, $\pi \to \pi^*$	9.29[a]	9.23	9.23	9.39	9.89	9.89	9.79
Formaldehyde: 1 3A2, $n \to \pi^*$	3.50[a]	3.23	3.23	3.39	3.24	3.24	3.39
Formaldehyde: 1 3A1, $\pi \to \pi^*$	5.87[a]	5.63	5.63	5.81	6.07	6.07	5.99
Acetone: 2 1A1, $\pi \to \pi^*$	8.90[a]	8.08	8.08	8.27	8.51	8.51	8.57
Acetone: 1 1A2, $n \to \pi^*$	4.38[a]	3.98	3.98	4.12	4.05	4.05	4.11
Acetone: 2 1B1, $\sigma \to \pi^*$	9.04[a]	7.71	7.71	8.03	8.34	8.34	8.58
Acetone: 1 3A1, $\pi \to \pi^*$	6.07[a]	5.45	5.45	5.66	5.79	5.79	5.78
Acetone: 1 3A2, $n \to \pi^*$	4.05[a]	3.74	3.74	3.89	3.79	3.79	3.86
p-Benzoquinone: 1 1Au, $n \to \pi^*$	2.86[a]	3.35	3.35	3.43	3.37	3.37	3.39
p-Benzoquinone: 1 1B1g, $n \to \pi^*$	2.74[a]	2.64	2.64	2.71	2.58	2.58	2.61
p-Benzoquinone: 1 1B1u, $\pi \to \pi^*$	5.47[a]	5.52	5.52	5.59	5.71	5.71	5.70

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Table S85: ... *continued from previous page* ...

Species	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
p-Benzoquinone: 1 1B3g, $\pi \to \pi^*$	4.44[a]	4.62	4.62	4.65	4.68	4.68	4.65
p-Benzoquinone: 2 1B3g, $\pi \to \pi^*$	7.16[a]	6.73	6.73	6.94	6.93	6.93	7.01
p-Benzoquinone: 1 1B3u, $n \to \pi^*$	5.55[a]	5.34	5.34	5.51	5.31	5.31	5.45
p-Benzoquinone: 1 3Au, $n \to \pi^*$	2.61[a]	3.21	3.21	3.29	3.23	3.23	3.25
p-Benzoquinone: 1 3B1g, $n \to \pi^*$	2.50[a]	2.50	2.50	2.57	2.42	2.42	2.46
p-Benzoquinone: 1 3B1u, $\pi \to \pi^*$	3.02[a]	2.79	2.79	2.89	2.91	2.91	2.92
p-Benzoquinone: 1 3B3g, $\pi \to \pi^*$	3.37[a]	3.32	3.32	3.37	3.34	3.34	3.36
Formamide: 1 1A", $n \to \pi^*$	5.55[a]	4.56	4.56	4.80	4.82	4.82	5.07
Formamide: 2 1A', $\pi \to \pi^*$	7.35[a]	6.71	6.71	7.08	7.07	7.07	7.14
Formamide: 1 3A", $n \to \pi^*$	5.28[a]	4.34	4.34	4.58	4.58	4.58	4.83
Formamide: 1 3A', $\pi \to \pi^*$	5.69[a]	4.77	4.77	5.15	4.98	4.98	5.18
Acetamide: 2 1A', $\pi \to \pi^*$	7.14[a]	6.63	6.63	7.00	6.95	6.95	7.01
Acetamide: 1 1A", $n \to \pi^*$	5.62[a]	4.75	4.75	5.01	4.98	4.98	5.17
Acetamide: 1 3A', $\pi \to \pi^*$	5.71[a]	4.86	4.86	5.24	5.07	5.07	5.24
Acetamide: 1 3A", $n \to \pi^*$	5.35[a]	4.54	4.54	4.80	4.76	4.76	4.95
Propanamide: 2 1A', $\pi \to \pi^*$	7.09[a]	6.64	6.64	7.00	6.94	6.94	7.01
Propanamide: 1 1A", $n \to \pi^*$	5.65[a]	4.85	4.85	5.11	5.06	5.06	5.24
Propanamide: 1 3A', $\pi \to \pi^*$	6.08[a]	4.87	4.87	5.24	5.07	5.07	5.25
Propanamide: 1 3A", $n \to \pi^*$	5.38[a]	4.61	4.61	4.87	4.81	4.81	4.99
Cytosine: 2 1A', $\pi \to \pi^*$	4.69[b]	4.21	4.21	4.44	4.39	4.39	4.56
Cytosine: 3 1A', $\pi \to \pi^*$	5.60[b]	5.00	5.00	5.30	5.05	5.05	5.33
Cytosine: 1 1A", $n \to \pi^*$	5.18[b]	4.24	4.24	4.43	4.41	4.41	4.57
Cytosine: 2 1A", $n \to \pi^*$	5.82[b]	4.84	4.84	5.13	4.96	4.96	5.27
Thymine: 2 1A', $\pi \to \pi^*$	5.15[b]	4.81	4.81	5.08	4.81	4.81	5.05
Thymine: 3 1A', $\pi \to \pi^*$	6.26[b]	5.56	5.56	5.90	5.65	5.65	5.94
Thymine: 4 1A', $\pi \to \pi^*$	6.46[b]	5.73	5.73	6.09	5.90	5.90	6.13
Thymine: 1 1A", $n \to \pi^*$	4.85[b]	4.52	4.52	4.73	4.68	4.68	4.83
Thymine: 2 1A", $n \to \pi^*$	6.27[b]	5.47	5.47	5.80	5.69	5.69	6.00
Uracil: 2 1A', $\pi \to \pi^*$	5.25[a]	4.88	4.88	5.17	4.90	4.90	5.14
Uracil: 3 1A', $\pi \to \pi^*$	6.26[a]	5.68	5.68	6.05	5.86	5.86	6.08
Uracil: 4 1A', $\pi \to \pi^*$	6.70[a]	5.85	5.85	6.20	5.97	5.97	6.26
Uracil: 1 1A", $n \to \pi^*$	5.00[a]	4.45	4.45	4.67	4.64	4.64	4.80
Uracil: 2 1A", $n \to \pi^*$	6.10[a]	5.43	5.43	5.76	5.65	5.65	5.96
Uracil: 3 1A", $n \to \pi^*$	6.56[a]	6.09	6.09	6.45	6.10	6.10	6.50
Adenine: 2 1A', $\pi \to \pi^*$	5.04[b]	4.23	4.23	4.45	4.33	4.33	4.50
Adenine: 3 1A', $\pi \to \pi^*$	5.23[b]	4.79	4.79	4.94	4.90	4.90	4.98
Adenine: 1 1A", $n \to \pi^*$	5.28[b]	4.60	4.60	4.73	4.62	4.62	4.87
Adenine: 2 1A", $n \to \pi^*$	5.84[b]	5.05	5.05	5.15	5.16	5.16	5.28

a M.R.Silva-Junior, M. Schreiber, S.P.A. Sauer, and W. Thiel, J.Chem.Phys. 133, 174318 (2010). b P.G. Szalay, T. Watson, A. Perera, V.F. Lorich, and R.J. Bartlett, J.Phys.Chem.A 116, 6702 (2012).

Table S86: C=O and C−H Bond Lengths (Å), ∠HCH Bond Angles (degree), and Out-of-Plane Bending Angles θ (degree) Calculated with the TDDFT/B3LYP, CC2, OMx/MRCI, OMx-D3T/MRCI, and ODMx/MRCI Methods for Two States of Formaldehyde in the Ex-Geom Set. Available Experimental Values Are Also Given for Comparison[a]

	Exp.	TDDFT	CC2	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
					$1\ ^1n\pi^*$				
C=O	1.323	1.296	1.361	1.279	1.279	1.292	1.276	1.276	1.285
C−H	1.098	1.095	1.089	1.113	1.113	1.111	1.126	1.126	1.119
∠HCH	118.4	117.2	121.0	113.9	113.9	114.3	107.9	107.9	109.9
θ	34.0	31.0	27.8	27.3	27.3	31.0	31.2	31.2	29.7
					$1\ ^3n\pi^*$				
C=O	1.307	1.298	1.343	1.261	1.261	1.275	1.254	1.254	1.267
C−H	1.084	1.102	1.093	1.148	1.148	1.138	1.160	1.160	1.139
∠HCH	117.9	112.1	117.6	108.1	108.1	109.8	101.7	101.7	105.8
θ	41.1	45.9	39.1	40.2	40.2	40.7	38.9	38.9	36.4

[a] Available OMx/MRCI, TDDFT, CC2, and experimental values are taken from Ref. S13.

Table S87: C=O Bond Lengths (Å) Calculated with the TDDFT/B3LYP, CC2, OMx/MRCI, OMx-D3T/MRCI, and ODMx/MRCI Methods for Various States of Acetaldehyde, Acetone, and Formaldehyde in the ExGeom Set. Available Experimental Values Are Also Given for Comparison[a]

Species	State	Exp.	TDDFT	CC2	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
acetaldehyde	$^1n\pi^*$	1.32	1.304	1.387	1.290	1.290	1.303	1.298	1.298	1.304
	$^3n\pi^*$	—	1.305	1.364	1.270	1.270	1.283	1.276	1.276	1.285
	$^3\pi\pi^*$	—	—	1.478	1.414	1.414	1.421	1.416	1.415	1.422
acetone	$^1n\pi^*$	—	1.310	1.420	1.291	1.291	1.304	1.310	1.309	1.316
	$^3n\pi^*$	—	1.312	1.387	1.266	1.266	1.277	1.284	1.283	1.291
	$^3\pi\pi^*$	—	—	1.489	1.414	1.414	1.422	1.439	1.439	1.432
formaldehyde	$^1n\pi^*$	1.323	1.296	1.361	1.279	1.279	1.292	1.276	1.276	1.285
	$^3n\pi^*$	1.307	1.298	1.343	1.261	1.261	1.275	1.254	1.254	1.267
	$^3\pi\pi^*$	1.423	—	1.469	1.398	1.398	1.410	1.424	1.424	1.420

[a] Available OMx/MRCI, TDDFT, CC2, and experimental values are taken from Ref. S13.

Table S88: Out-of-Plane Bending Angles (degree) Formed by the C=O Bond and the HCC, CCC, and HCH Planes for Various States of Acetaldehyde, Acetone, and Formaldehyde in the ExGeom Set, Respectively. Geometries Optimized at the TDDFT/B3LYP, CC2, OMx/MRCI, OMx-D3T/MRCI, and ODMx/MRCI Levels of Theory. Available Experimental Values Are Also Given for Comparison[a]

Species	State	Exp.	TDDFT	CC2	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
acetaldehyde	$^1n\pi^*$	≈ 26	31.3	31.4	31.4	31.4	32.7	31.8	31.9	28.4
	$^3n\pi^*$	42.2	41.6	38.6	40.2	40.3	40.4	38.2	38.3	34.7
	$^3\pi\pi^*$	—	—	34.2	39.1	39.2	39.3	37.4	37.5	35.0
acetone	$^1n\pi^*$	—	33.5	35.6	36.0	36.1	35.7	34.4	34.6	31.4
	$^3n\pi^*$	—	39.4	39.9	44.1	44.2	43.4	40.2	40.4	37.3
	$^3\pi\pi^*$	—	—	38.6	44.1	44.2	43.9	41.7	42.0	38.2
formaldehyde	$^1n\pi^*$	34.0	31.0	27.8	27.3	27.3	31.0	31.2	31.2	29.7
	$^3n\pi^*$	41.1	45.9	29.1	40.2	40.2	40.7	38.9	38.9	36.4
	$^3\pi\pi^*$	—	—	28.5	34.7	34.7	36.6	36.1	36.1	33.8

[a] Available OMx/MRCI, TDDFT, CC2, and experimental values are taken from Ref. S13.

Table S89: ∠CCH Bond Angles (degree) Calculated with the TDDFT/B3LYP, CC2, OMx/MRCI, OMx-D3T/MRCI, and ODMx/MRCI Methods for Various States of Acetylene in the ExGeom Set[a]

State	TDDFT	CC2	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
1 $^1A_2$	132.3	132.7	147.2	147.2	147.4	149.1	149.0	150.3
2 $^1A_2$	174.3	171.6	180.0	180.0	180.0	180.0	180.0	180.0
1 $^1B_2$	143.7	142.0	139.5	139.4	139.6	150.7	150.6	154.1
1 $^3A_2$	—	130.4	144.5	144.5	143.9	144.6	144.5	145.9
2 $^3A_2$	166.0	167.3	180.0	180.0	180.0	180.0	180.0	180.0
1 $^3B_2$	—	126.9	133.8	133.8	133.6	133.9	133.7	135.0
1 ^1A_u	122.6	122.1	125.0	125.0	124.3	125.1	125.1	127.2
2 ^1A_u	175.2	171.1	170.0	170.0	169.7	171.7	171.7	172.0
1 ^1B_u	150.2	147.0	143.2	143.2	142.0	145.4	145.3	146.1
1 ^3A_u	116.9	120.5	123.7	123.7	122.9	122.6	122.6	124.7
2 ^3A_u	162.9	164.7	163.8	163.8	163.2	164.1	164.1	164.4
1 ^3B_u	129.4	131.2	138.3	138.3	137.0	135.9	135.9	136.6
2 ^3B_u	156.5	153.8	150.5	150.5	148.5	152.8	152.8	153.1

[a] Available OMx/MRCI, TDDFT and CC2 values are taken from Ref. S13.

Table S90: Out-of-Plane Bending Angles (degree) Formed by the C−N Bond and the NH_2 Plane Calculated with the TDDFT/B3LYP, CC2, OMx/MRCI, OMx-D3T/MRCI, and ODMx/MRCI Methods for Various States of 9H-Adenine, Aniline, Cytosine, and 9H-Guanine in the ExGeom Set[a]

Species	State	TDDFT	CC2	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
9H-adenine	$^1n\pi^*$	39.6	39.3	0.4	0.4	1.2	4.6	4.6	3.0
aniline	$^1\pi\pi^*$	5.9	27.0	0.0	0.0	0.0	0.0	0.0	0.0
	$^3\pi\pi^*$	—	37.1	13.4	13.8	11.8	16.0	16.5	20.9
cytosine	$^1n\pi^*$	32.4	47.8	0.0	0.0	0.0	0.0	0.0	0.0
	$^1\pi\pi^*$	28.6	44.3	0.0	0.0	0.0	0.0	0.0	0.0
9H-guanine	$^1\pi\pi^*$	34.9	45.8	11.4	11.2	5.2	16.4	16.6	1.6

[a] Available OMx/MRCI, TDDFT, and CC2 are taken from Ref. S13.

Table S91: Benchmark Results for the SKF Set. 0−0 Transition Energies (eV)

Molecule	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
1,6-epoxy-10-annulene: 1 1B1	3.07[a]	3.22	3.22	3.33	3.24	3.25	3.42
2-cyclopenten-1-one: 2 1A	3.47[a]	3.49	3.49	—[b]	3.52	3.52	3.56
7-azaindole: 2 1A	4.41[a]	3.97	3.97	4.08	4.00	4.00	4.05
β-dinaphtyleneoxide: 2 1A	3.73[a]	3.93	3.93	3.97	3.96	3.95	3.97
acetaldehyde: 2 1A	3.76[a]	3.65	3.65	3.77	3.70	3.70	3.80
acetone: 2 1A	3.83[a]	3.81	3.81	3.92	3.84	3.84	3.93
acrolein: 1 1A”	3.29[a]	3.68	3.67	3.75	3.70	3.70	3.78
acrolein: 1 3A”	3.11[a]	3.52	3.52	3.61	3.55	3.55	3.64
aminobenzonitrile: 1 1B1	4.33[a]	3.89	3.89	4.05	3.81	3.81	3.98
aniline: 2 1A	4.39[a]	3.97	3.97	4.12	3.86	3.86	4.03
anisol: 2 1A	4.68[a]	4.15	4.15	4.28	4.16	4.17	4.27
anthracene: 1 1B2u	3.51[a]	3.87	3.87	3.92	3.88	3.88	3.92
azulene: 1 1B1	1.81[a]	1.55	1.55	1.60	1.53	1.53	1.56
benzaldehyde: 2 1A’	4.50[a]	4.18	4.19	4.28	4.19	4.19	4.26
benzaldehyde: 1 1A”	3.43[a]	3.75	3.75	3.79	3.70	3.70	3.75
benzaldehyde 1 3A”	3.21[a]	3.54	3.54	3.59	3.47	3.47	3.55
benzene: 1 1B1u	4.88[a]	4.37	4.37	4.48	4.35	4.36	4.43
benzonitrile: 1 1B1	4.68[a]	4.24	4.24	4.35	4.24	4.24	4.31
benzophenone ketyl radical: 2 2A	2.36[a]	2.72	2.70	2.74	—[b]	—[b]	—[b]
biphenyl: 1 1B1u	4.52[a]	4.83	4.83	4.91	4.85	4.85	4.91
biphenylene: 1 1B3u	3.61[a]	3.69	3.69	3.78	3.66	3.66	3.73
acetylene: 2 1A	5.32[a]	5.22	5.22	4.88	4.94	4.94	5.05
formaldehyde: 2 1A	3.58[a]	3.42	3.42	3.50	3.46	3.46	3.56
formaldehyde: 1 3A	3.22[a]	3.12	3.12	3.21	3.14	3.14	3.25
cinnoline: 1 1A”	2.90[a]	3.35	3.35	3.28	3.18	3.19	3.31
cyanoacetylene: 2 1A’	4.90[a]	5.55	5.55	4.95	5.60	5.60	5.69
cyclohexadienyl radical: 2 2A	2.33[a]	2.15	2.15	2.21	2.12	2.13	2.16
2,3-diazabicyclo[2,2,1]hept-2-ene: 2 1A	3.76[a]	3.61	3.61	3.48	—[b]	—[b]	—[b]
4-(dimethylamino)-4’-cyanostilbene: 2 1A	3.43[a]	3.78	3.78	—[b]	3.69	3.69	3.81
dimethylaminobenzonitrile: 1 1B	4.14[a]	3.92	3.92	4.06	3.80	3.80	3.99
N,N-dimethyl-p-phenylenediamine: 2 1A	3.74[a]	4.65	4.65	4.86	4.46	4.46	4.76
fluorene: 2 1A’	4.37[a]	4.24	4.24	4.35	4.22	4.22	4.29
glyoxal: 1 1Au	2.78[a]	3.00	3.00	3.10	3.00	3.00	3.11
hydrogen cyanide: 1 1A”	6.61[a]	6.78	6.78	6.81	6.31	6.31	6.25
formic acid: 2 1A	4.74[a]	4.36	4.36	4.49	4.39	4.39	4.49
hexatriene: 1 1Bu	5.06[a]	5.06	5.07	5.12	5.09	5.09	5.13
hydroquinone: 1 1Bu	4.31[a]	3.85	3.85	4.01	3.91	3.91	4.04
indole: 2 1A’	4.52[a]	3.95	3.95	4.07	3.90	3.90	4.02
methyl-4-hydroxycinnamate: 2 1A	4.12[a]	3.94	3.94	4.09	3.95	3.95	—[b]
naphthalene: 1 1B2u	4.09[a]	4.65	4.65	4.72	4.66	4.66	4.71
octatetraene: 1 1Bu	4.51[a]	4.51	4.51	4.55	4.52	4.52	4.56
o-cyanobenzyl radical: 2 2A	2.56[a]	2.37	2.37	2.45	2.37	2.37	2.43
oxalylfluoride: 1 1Au	4.12[a]	4.06	4.06	4.18	4.22	4.22	4.33
benzoquinone: 1 1B1g	4.14[a]	4.24	4.24	4.22	4.26	4.26	4.23
benzoquinone: 1 1B2g	2.64[a]	2.66	2.66	2.70	2.61	2.60	2.63
p-diethynylbenzene: 1 1B2u	4.40[a]	4.72	4.72	4.81	4.71	4.71	4.78
p-phenylenediamine: 2 1A	3.87[a]	3.53	3.53	3.71	3.35	3.35	3.58
phenol: 2 1A	4.67[a]	4.83	4.83	4.97	4.87	4.87	4.98
porphyrin: 1 1B1u	2.08[a]	1.96	1.97	2.01	2.03	1.99	1.98
propynal: 2 1A	3.33[a]	3.49	3.49	3.56	3.50	3.50	3.55
pyrene: 2 1A	3.46[a]	3.36	—[b]	—[b]	3.48	3.48	3.54
pyridine: 2 1A	4.50[a]	4.31	4.31	4.44	4.08	4.08	4.27
pyridone lactam: 3 1A	3.82[a]	4.03	4.03	4.17	4.16	4.16	4.24
pyridone lactim: 1 1A”	4.64[a]	4.68	4.69	4.74	4.56	4.56	4.62
pyrimidine: 2 1A	4.02[a]	4.04	4.04	4.13	3.83	3.83	4.06
pyrimidine: 4 1A	5.01[a]	4.71	4.71	4.82	4.90	4.90	4.81
quinoline: 1 1A”	4.12[a]	3.95	3.95	3.97	3.80	3.80	3.82
quinoline: 1 3A’	2.96[a]	2.75	2.75	2.82	2.76	2.77	2.79
quinoxaline: 2 1A1	4.06[a]	3.79	3.79	3.86	3.87	3.88	3.86
quinoxaline: 2 1A	3.51[a]	3.39	3.39	3.36	3.40	3.41	3.35
quinoxaline: 1 3A’	2.84[a]	2.81	2.81	2.85	2.85	2.86	2.85
styrene: 2 1A	4.45[a]	4.15	4.15	4.25	4.13	4.14	4.21
syn-coumarin 153: 2 1A	3.33[a]	3.68	3.68	3.83	3.49	3.49	3.63

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Table S91: . . . *continued from previous page* . . .

Molecule	Ref.	OM2	OM2-D3T	ODM2	OM3	OM3-D3T	ODM3
terylene: 2 1A'	2.53[a]	2.83	2.83	2.87	2.83	2.83	2.87
s-tetrazine: 1 1B3u	2.33[a]	2.84	2.84	2.64	2.92	2.92	2.74
toluene: 1 1A"	4.81[a]	4.28	4.29	4.40	4.26	4.27	4.35
stilbene: 2 1A	4.09[a]	4.37	4.37	4.43	4.39	4.38	4.44
vinyl radical: 2 2A	2.47[a]	2.38	2.38	2.35	2.49	2.49	2.51

a R. Send, M. Kuehn, and F. Furche, J.Chem.Theory Comput. 7, 2376 (2011). Experimental data are back-corrected with ΔZPVE values from (TD)DFT calculations for reasons described in D. Tuna, Y. Lu, A. Koslowski, W. Thiel, J.Chem.Theory Comput. 12, 4400 (2016). b Calculation could not be converged.

References

(S1) Levenberg, K. A Method for the Solution of Certain Non-Linear Problems in Least Squares. *Quart. Appl. Math.* **1944**, *2*, 164–168.

(S2) Marquardt, D. W. An Algorithm for Least-Squares Estimation of Nonlinear Parameters. *SIAM J. Appl. Math.* **1963**, *11*, 431–441.

(S3) Fletcher, R. *Practical Methods of Optimization*, 2nd ed.; John Wiley & Sons, Ltd: New York, NY, USA, 1987.

(S4) Nelder, J. A.; Mead, R. A Simplex Method for Function Minimization. *Computer J.* **1965**, *7*, 308–313.

(S5) Kaelo, P.; Ali, M. M. Some Variants of the Controlled Random Search Algorithm for Global Optimization. *J. Optim. Theory Appl.* **2006**, *130*, 253–264.

(S6) Jones, D. R.; Perttunen, C. D.; Stuckman, B. E. Lipschitzian Optimization Without the Lipschitz Constant. *J. Optim. Theory Appl.* **1993**, *79*, 157–181.

(S7) Gablonsky, J.; Kelley, C. A Locally-Biased Form of the DIRECT Algorithm. *J. Global Optim.* **2001**, *21*, 27–37.

(S8) Runarsson, T. P.; Yao, X. Search Biases in Constrained Evolutionary Optimization. *IEEE Trans. Syst. Man Cybern. C, Appl. Rev.* **2005**, *35*, 233–243.

(S9) Brent, R. P. *Algorithms for Minimization Without Derivatives*; Prentice-Hall, 1973.

(S10) Rowan, T. Functional Stability Analysis of Numerical Algorithms. Ph.D. thesis, Department of Computer Sciences, University of Texas at Austin, 1990.

(S11) Johnson, S. G. The NLopt Nonlinear-Optimization Package. `http://ab-initio.mit.edu/nlopt`, accessed on December 18, 2018.

(S12) Dral, P. O.; Wu, X.; Spörkel, L.; Koslowski, A.; Weber, W.; Steiger, R.; Scholten, M.; Thiel, W. Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Theory, Implementation, and Parameters. *J. Chem. Theory Comput.* **2016**, *12*, 1082–1096.

(S13) Tuna, D.; Lu, Y.; Koslowski, A.; Thiel, W. Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks of Electronically Excited States. *J. Chem. Theory Comput.* **2016**, *12*, 4400–4422.