Supporting Information

Electron Redistribution within the Nitrogenase Active Site FeMo-cofactor During Reductive Elimination of H_2 to Achieve N≡N Triple-Bond Activation

Dmitriy A. Lukoyanov, Zhi-Yong Yang, Dennis R. Dean,
Lance C. Seefeldt, Simone Raugei, Brian M. Hoffman

EPR Linebroadening

As the first probe of the ^{95}Mo hyperfine coupling in the two-electron reduced cofactor of E_4(2H)*, we looked for EPR line-broadening in ^{95}Mo enriched samples, as observed for E_4(4H). The weak ^{95}Mo coupling in the E_4(4H) state causes a slight broadening of the X-band EPR spectrum (**Fig S1**), while the clearest evidence of the ^{95}Mo broadening in E_4(4H) is that enrichment obscures g_3 features generated by strong hyperfine interaction with the two bridging hydrides (**Fig S1**). EPR simulations confirm that this effect is produced by the small ^{95}Mo hyperfine coupling measured in the ENDOR experiment. The loss of the hydrides in E_4(2H)* eliminates the hydride hyperfine features at g_3, and thus this indicator of ^{95}Mo hyperfine broadening. However, but nonetheless, comparison between natural-abundance and ^{95}Mo-enriched enzyme shows that the spectrum of E_4(2H)* does not exhibit noticeable broadening upon the ^{95}Mo enrichment (**Fig S1**), demonstrating that any coupling must be small: there is no appreciable increase in the ^{95}Mo coupling in the two-electron reduced state E_4(2H)*.

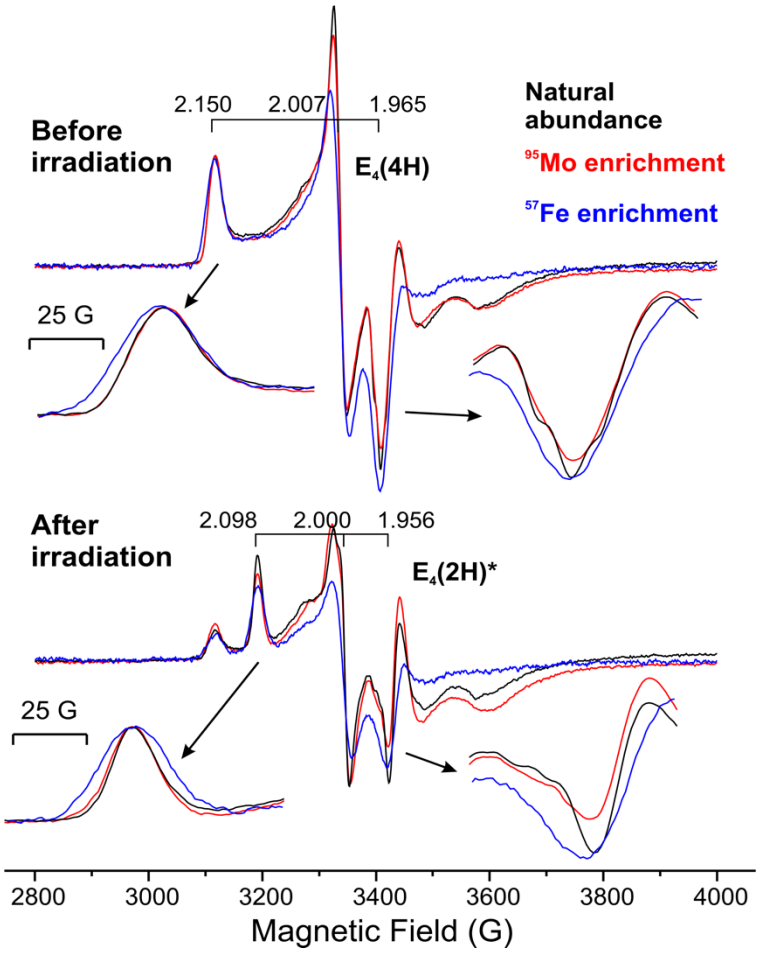

Figure S1. X-band EPR spectra of the natural abundance, 95Mo and ^{57}Fe enriched V70I trapped during turnover under Ar taken before (top) and after (low) irradiation with 450 nm laser diode at 12 K. *EPR conditions: microwave frequency, 9.36 GHz; temperature, 12 K; microwave power 10 mW; modulation amplitude, 2 G; time constant, 160 ms; scan time, 2 min; 4 scans accumulation.*

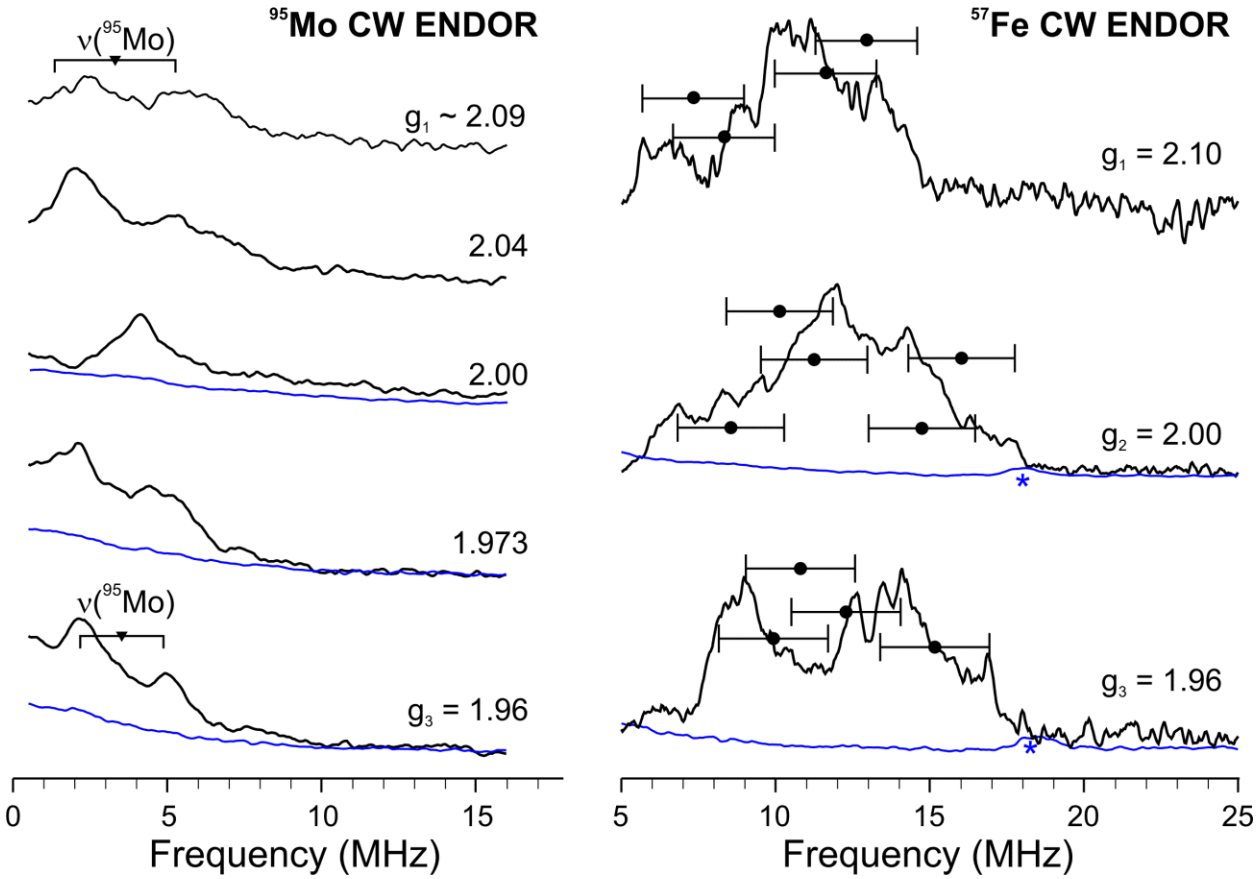

Figure S2. 35 GHz CW ENDOR ^{95}Mo and ^{57}Fe signals for E_4(2H)* state prepared with ^{95}Mo (left) and ^{57}Fe (right) enriched MoFe proteins. Meanings of the 'goalposts' for ^{95}Mo and ^{57}Fe signals are explained in legends of **Fig 4** and **Fig 5** correspondingly. Blue lines represent spectra obtained for natural abundance sample and compared with spectra of isotopically enriched samples by normalization to the same E_4(2H)* EPR signal intensity; (*) at ~18 MHz denotes intensity associated with 3rd harmonics of the matrix ^{1}H signal. *Conditions: T = 2 K; microwave frequency, 34.8 GHz (^{95}Mo and natural abundance samples) and 35.1 GHz (^{57}Fe sample); microwave power, 0.1 μW and 0.04 μW; modulation amplitude, 1 G and 4 G; RF sweep speed, 2 MHz/s and 1 MHz/s; time constant, 64 ms; RF bandwidth-broaden to 100 kHz.*

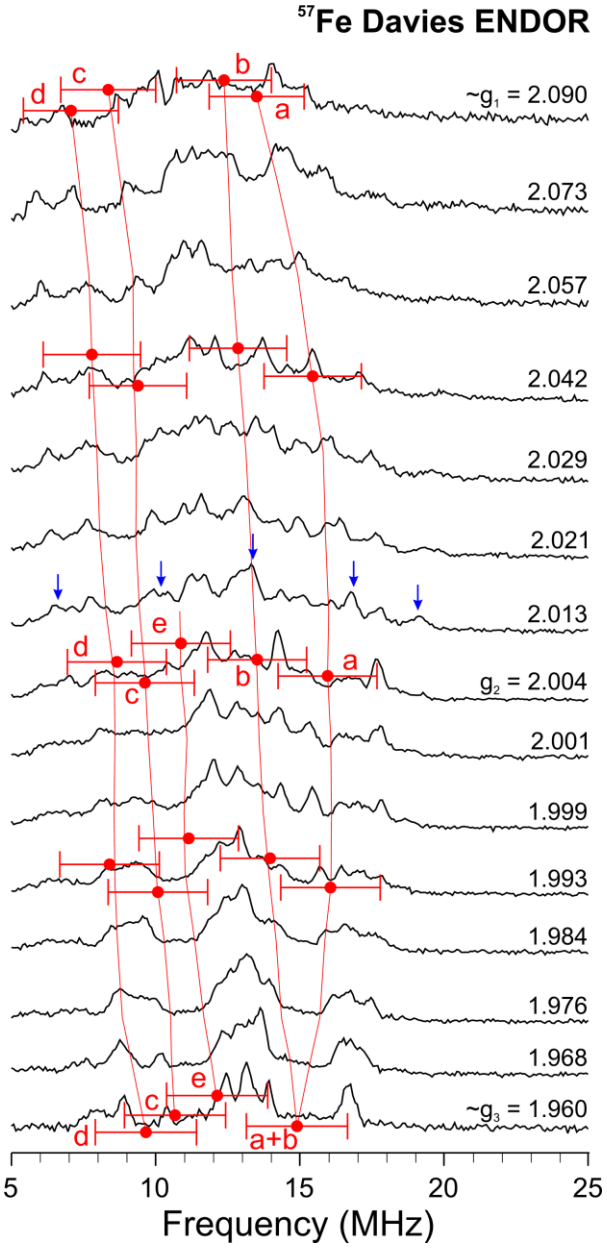

Figure S3. Field dependence of ^{57}Fe random-hop Davies ENDOR collected for ^{57}Fe enriched V70I Ar turnover after irradiation of E_4(4H) with 450 nm laser diode at 12 K to generate E_4(2H)*. Red 'goalposts' indicate response from one E_4(2H)* ^{57}Fe centered at half of its hyperfine coupling and split by 2ν(^{57}Fe). Arrows indicate signals originating from ^{57}Fe of E_4(4H) that is present in the sample due to incomplete photolysis. Red lines that connect E_4(2H)* ^{57}Fe hyperfine doublets at magnetic fields across the EPR envelope, are drawn with consideration of peaks known to arise from the E_4(4H) residual background.[12] Because some signals split as the field changes, or broaden into near-undetectability at some fields, then narrow again and reappear, these correspondences of signals across the EPR envelope are overall successful, but nevertheless do not support attempts to obtain hyperfine tensors to high precision. *ENDOR conditions: microwave frequency, 34.90 GHz; temperature, 2 K; $t(\pi/2)$ = 40 ns, τ = 600 ns; T_{RF} = 35 μs; repetition time, 25 ms; 200-400 scans.*

DFT Model adopted in the QM/MM molecular dynamics simulation

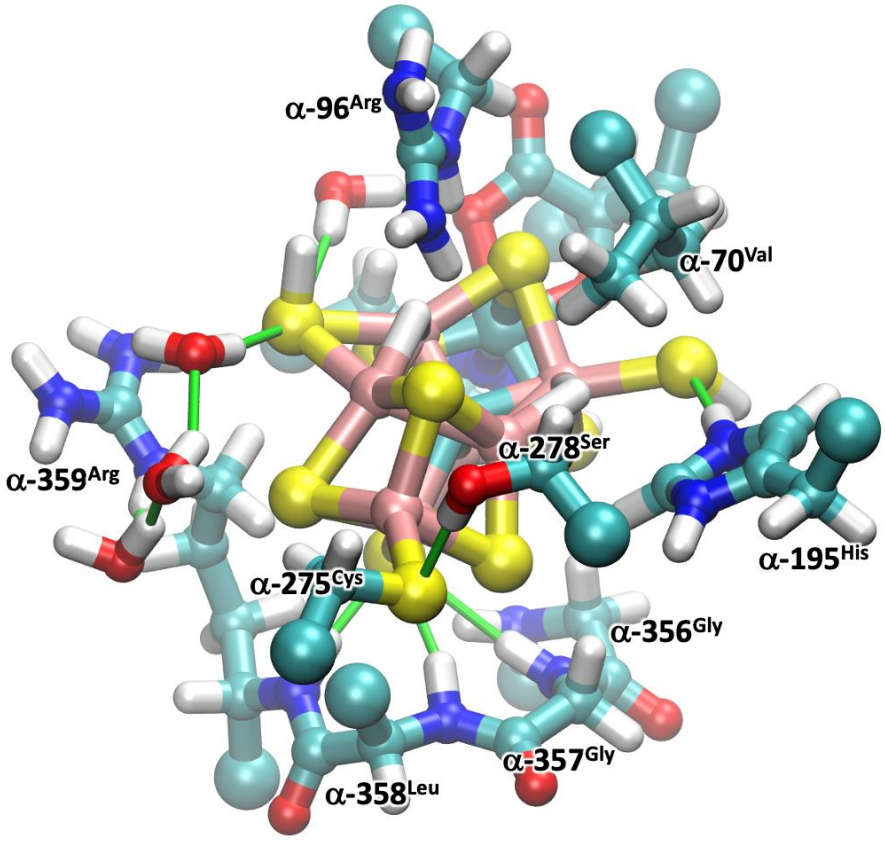

Figure S4. Ball and stick representation of the cofactor and protein environment treated at DFT level in the metadynamics QM/MM simulation. Protein residues and ligands are labelled except α-442^{His} and homocitrate which are located on the back of the cofactor. Fe atoms are shown in rust, S atoms in yellow, C atoms in cyan, O atoms in red, N atoms in blue, and H atoms in light gray. Relevant H-bonds are shown as thin green sticks. The C atoms in the molecular mechanics part of the system linked to the QM atoms are shown as large spheres.

Coordination Numbers as Order Parameters to Follow the Hydrogen Reorganization

We have performed metadynamics simulations to explore the hydride reorganization on the Fe2,3,6,7 face. Metadynamics is an adaptive biasing potential technique, which disfavors configurations that have been already explored, and consequently favors situations that would have been poorly explored thermally. The bias can be applied to any physical quantity describing the process being studied. The history-dependent potential is constructed as a sum of Gaussians centered on each value of the collective variable previously explored. The potential fills the minima of the free energy surface in time, and as the simulation proceeds, its sum converges to the free energy landscape as a function of the collective variables. In the present case, we chose the coordination numbers Fe-to-H described in the text.

Coordination numbers are very useful order parameters to study chemical processes with biased molecular dynamics simulations. In the present study, we used the coordination numbers to identify the location of the two hydridic hydrogen atoms on the $Fe_2/Fe_3/Fe_6/Fe_7$ face of FeMo-co and characterize the type of E_4 isomer that a given arrangement of hydrogen atoms gives rise.

Specifically, we adopted coordination numbers that quantify and characterize the number of hydrogen atoms coordinated to each Fe atom of the Fe_2/Fe_6 and Fe_3/Fe_7 either pairs.

A coordination number can be defined using different functional forms. However, all definitions rely on a distance cutoff, r_0. The following definition of coordination number was adopted:

$$n = \frac{1}{2}\sum_k n'(r_k)$$

With (**S1**)

$$n'_k(r) = \frac{1-\left(\frac{r_k}{r_0}\right)^6}{1-\left(\frac{r_k}{r_0}\right)^{12}}$$

where r_k is the distance between a given Fe-H pair and the summation runs over all of the possible Fe-H distances. For instance, for the coordination number $n(\mathrm{Fe_2/Fe_6})$ the sum runs over *k* = Fe_2-H_1, Fe_2-H_2, Fe_6-H_1, and Fe_6-H_1. A value of the cutoff distance r_0 = 1.85 Å was used, which yields the $n'(r)$ reported in Figure S4. For this choice of r_0, we are able to distinguish between different E_4 isomers. For example, $n(\mathrm{Fe_2/Fe_6})$ assumes the value of about 1.4, 2.1 and 2.6 for $E_4(2H;H_2)$, $E_4(4H)^{(b)}$ and $E_4(4H)^{(c)}$.

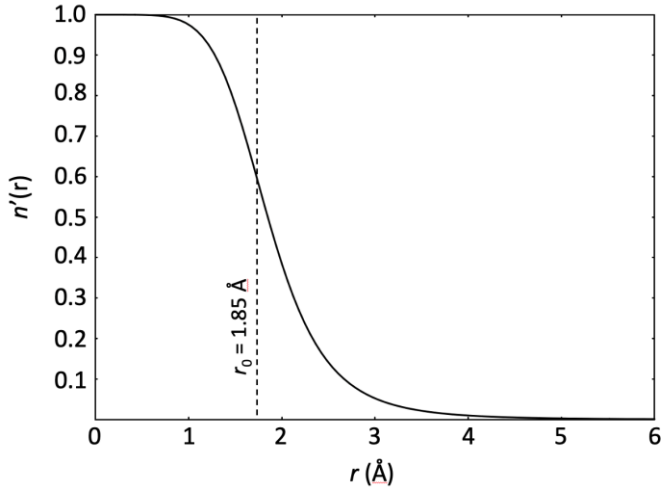

Figure S5. Graphical representation of the function $n'(r)$ for r_0 = 1.85 Å.

Natural Bond Orbital Analysis of the Electron Density

The mechanistic model put forward in the main text requires that as H_2 is formed and released via reductive elimination, two electrons are first stored in and then depart with the H_2 molecule. This process leaves two electrons on the FeMo-co, likely on the Fe center and not on the Mo center.

The electronic redistribution that follows the H atoms reorganization should be in principle quantifiable by DFT analysis. However, the reorganization of electrons highlighted above cannot be appreciated from a simple analysis of the charge of each individual Fe center obtained by traditional partitioning schemes, such Mulliken population analysis. As can be seen from **Table**

S1, the Mulliken charges on the metal centers atoms do not change with the location of the hydrogen atoms and they are all close to +0.5*e* (with variations within 0.4 *e*).

To obtain quantitative information on the charge redistribution, we performed a natural bond orbital (NBO) analysis. The NBO theory was originally developed to study hybridization and covalency in molecules in terms of concepts similar to Lewis chemical structures. Then it was extended to the analysis of intermolecular charge transfer due to localized orbital interactions. The NBO, ϕ, associated to a bond between two atoms A and B is formed by a linear combination of two orthonormal hybrid orbitals, h_A and h_B, defined in terms of atomic orbitals centered on A and B:

$$\phi(\text{A-B}) = c_A h_A + c_B h_B$$

where $|c_A|^2 + |c_B|^2 = 1$. The relative magnitude of the coefficients c_A and c_B can be taken as a measure of the bond polarization due to the different electronegativity of A and B. For a perfectly apolar bond $c_A = c_B = 2^{-1/2} \approx 0.707$. Non-bonded orbitals, such as lone pairs or localized *d*-orbitals, are given by only one hybrid (i.e., $c_A = 1$ and $c_B = 0$). In principle, from the occupancy of a given NBO ϕ and the cofficients c of the linear combition that defines ϕ one can obtaine the total fractional charge on a given atomic center. However, as for the Mulliken analysis, charges obtained in this way are not informative as they are all close to +1*e* (with variations within 0.15 *e*; see **Table S2**). Instead, the analysis of non-bonded orbitals localized on the Fe atoms (3*d* and 4*s* orbitals) provides values which can clearly discriminate among different H atoms arrangements. We consider non-bonded electrons those electrons that either belong to orbitals classified as non-bonded according to the NBO analysis ("lone pairs"), or that are in highly polarized σ□, or that $c_{Fe}h_{Fe} + c_X h_X$ for which $|c_{Fe}|^2>0.9$. As can be seen from the data reported in **Table S3**, the different Fe atoms have an appreciably different number of electrons in non-bonded orbitals, and this number has a rather large variability in the various E_4 isomers.

All NBO calculations were performed using the NBO7 program (nbo7.chem.wisc.edu) on the truncated models reported in PNAS **2018**, *115*, E10521. These models were optimized at DFT/BP86 level using the Ahlrichs VTZ for all Fe atoms, the LANL2TZ basis set with an effective core potential for the Mo atom, the 6-311++G** basis set for all atoms coordinated to metal atoms, including protic and hydridic hydrogen atoms and all of the atoms with which they interact via a covalent bond or a hydrogen bond, and finally the 6-31G* basis set for all other atoms. The wavefunction of the lowest-energy broken symmetry state of each model was then recalculated using the 6-31G basis and employed as an input for the NBO code. All DFT calculation were performed with NWChem (*Comput Phys Commun* **2010,** *181*, 1477).

	$E_4(4H)^{(a)}$	$E_4(4H)^{(b)}$	$E_4(4H)^{(c)}$	$E_4(2H;H_2)$	$E_4(2H)^*$
Fe_1	0.6	0.7	0.5	0.6	0.6
Fe_2	0.1	-0.2	-0.1	-0.1	-0.1
Fe_3	0.1	0.1	0.1	0.0	0.0
Fe_4	-0.1	-0.1	0.3	0.2	0.3
Fe_5	0.6	0.6	0.6	0.6	0.6
Fe_6	1.0	1.1	0.8	0.9	0.9
Fe_7	0.5	0.4	0.1	0.2	0.3

Table S1. Mulliken charges (*e*) of the Fe atoms of FeMo-co for different E_4 isomers.

	$E_4(4H)^{(a)}$	$E_4(4H)^{(b)}$	$E_4(4H)^{(c)}$	$E_4(2H;H_2)$	$E_4(2H)$*
Fe_1	1.1	1.1	1.1	1.1	1.1
Fe_2	0.9	0.9	0.8	0.8	0.8
Fe_3	1.0	0.9	0.8	0.9	0.9
Fe_4	1.1	1.0	1.0	1.0	1.0
Fe_5	1.0	1.0	1.1	1.0	1.0
Fe_6	1.1	1.1	1.0	1.1	0.9
Fe_7	0.8	0.8	0.8	0.8	0.8

Table S2. Natural charges (*e*) of the Fe atoms of FeMo-co for different E_4 isomers.

	$E_4(4H)^{(a)}$	$E_4(4H)^{(b)}$	$E_4(4H)^{(c)}$	$E_4(2H;H_2)$	$E_4(2H)$*
Fe_1	4.8	5.0	5.0	5.1	5.0
Fe_2	3.8	4.0	2.4	4.9	4.8
Fe_3	4.4	3.5	2.8	3.8	4.3
Fe_4	4.7	2.8	3.1	4.2	4.1
Fe_5	3.4	4.1	4.5	4.4	3.9
Fe_6	3.3	3.0	1.8	3.5	2.8
Fe_7	1.7	2.5	1.3	2.9	3.3

Table S3. Total number of electron in non-bonded orbitals localized on the Fe atoms of FeMo-co for different E_4 isomers.

Coordinates of QM core of selected structures on the free energy surface reported in Figure 7

The coordinates of the QM region for representative structures discussed in Figure 7 as obtained from the QM/MM simulations are reported below. It is important to point out that these coordinates do not correspond to equilibrium structures on a potential energy surface but rather they belong to an ensemble of structures as obtained from non-equilibrium biased molecular dynamics. Nevertheless, the comparison between these non-equilibrium coordinates and the coordinates of the corresponding stationary points on the potential energy surface of the truncated models reported in PNAS 115, 2018, E10521 might provide useful insights for the interested reader. Please note that the QM/MM covalent boundary is marked by a bare C atom. The full QM/MM trajectories are available upon request.

Structure A (close to $E_4(4H)^{(a)}$)

C	11.168	9.709	19.152
C	12.651	10.192	18.900
H	13.130	10.244	19.942
C	13.439	9.254	17.935
H	14.496	9.333	18.141
H	13.041	8.141	18.056
H	13.301	9.658	16.943
C	12.632	11.690	18.376
H	12.073	12.323	19.069
H	13.628	12.054	18.186
H	11.984	11.685	17.430
C	6.004	10.988	16.885
C	7.439	11.047	17.341
H	7.786	12.047	17.430
H	7.454	10.519	18.320
N	8.378	10.371	16.393
H	8.767	11.022	15.756
C	8.943	9.176	16.577
N	8.320	8.143	17.255
H	7.685	8.395	17.970
H	8.908	7.380	17.563
N	10.006	8.918	15.809
H	10.445	9.669	15.216
H	10.388	7.990	15.737
C	18.620	10.199	19.349
C	18.682	10.791	17.960
H	19.414	11.624	17.934
H	19.189	10.023	17.376
C	17.450	11.438	17.326
N	17.018	11.018	16.044
C	16.048	11.840	15.593
H	15.497	11.830	14.613
N	15.766	12.680	16.549
H	14.913	13.331	16.524
C	16.502	12.451	17.658
H	16.282	12.903	18.567
C	15.896	6.340	9.812
C	15.026	6.962	10.868
H	14.899	6.183	11.674
H	14.009	7.022	10.465
S	15.581	8.608	11.501
C	17.757	7.877	15.167
C	16.120	7.494	15.225
H	15.820	7.045	16.148
H	15.663	8.525	15.176
O	15.772	6.720	14.109
H	15.634	7.295	13.289
C	12.696	19.179	9.012
N	12.565	17.788	9.810
H	11.606	17.780	10.077
C	13.484	17.743	11.008
H	13.544	18.751	11.402
H	13.094	17.027	11.707
C	14.870	17.227	10.690
O	15.917	17.917	10.868
N	14.887	15.881	10.387
H	13.922	15.431	10.476
C	15.954	14.977	10.728
H	16.926	15.500	10.840
H	15.642	14.463	11.648
C	16.266	13.857	9.705
O	17.449	13.485	9.570
N	15.185	13.439	9.017
H	14.322	13.736	9.453
C	15.159	12.302	8.120
H	16.152	12.164	7.657
C	14.917	10.917	8.667

C	14.167	12.546	6.930
O	14.676	12.635	5.790
N	12.870	12.807	7.208
H	12.498	12.846	8.185
C	11.916	13.155	6.269
H	11.625	12.397	5.592
C	10.637	13.754	6.972
C	9.143	12.498	7.392
C	9.490	11.643	8.649
H	10.613	11.580	8.862
H	9.090	12.181	9.531
N	9.039	10.287	8.501
H	9.746	9.578	8.219
C	7.807	9.852	8.697
N	6.838	10.537	9.282
H	7.051	11.529	9.550
H	5.960	10.484	8.796
N	7.595	8.577	8.336
H	8.202	8.102	7.726
H	6.723	8.088	8.508
C	12.633	14.362	5.058
C	6.273	15.493	10.396
C	6.448	16.309	11.734
H	5.586	16.925	11.980
H	6.657	15.540	12.539
C	7.723	17.128	11.851
N	8.816	16.852	12.647
C	9.650	17.864	12.584
H	10.578	17.967	13.047
N	9.158	18.782	11.727
H	9.573	19.758	11.624
C	7.949	18.399	11.332
H	7.276	18.897	10.673
Fe	13.542	9.704	11.853
Mo	9.490	15.012	13.953
Fe	13.047	11.502	13.674
Fe	11.156	10.429	12.653
Fe	12.583	12.032	11.243
Fe	11.112	14.081	12.104
Fe	11.998	13.690	14.553
Fe	9.749	12.276	13.422
C	11.617	12.480	12.978
S	14.669	11.750	12.211
S	11.737	15.671	13.448
S	12.515	9.303	13.883
S	13.166	14.309	16.432
S	11.911	13.834	10.043
S	9.837	13.113	15.450
S	11.783	9.938	10.494
S	8.838	13.825	12.120
S	8.819	10.450	12.218
C	8.232	16.216	18.962
C	9.130	16.427	17.529
H	9.697	17.300	17.667
H	9.894	15.639	17.409
C	8.422	16.596	16.175
C	7.354	15.562	15.974
O	7.472	14.958	14.768
O	6.482	15.253	16.802
O	9.410	16.539	15.245
C	7.625	18.002	16.120
H	6.794	18.003	16.795
H	8.361	18.770	16.370
C	7.036	18.355	14.816
H	12.995	12.322	15.017
H	10.300	10.928	14.038
H	13.533	15.615	16.127
H	8.304	9.667	13.230
O	6.946	6.133	10.239
H	6.440	6.300	9.331

H	7.388	5.242	10.098
O	6.155	12.923	13.581
H	6.935	12.539	13.092
H	6.639	13.517	14.200
O	9.513	7.414	11.268
H	8.650	7.176	10.898
H	9.423	8.345	11.523
O	10.906	8.387	7.529
H	10.397	7.659	7.003
H	11.370	7.926	8.305
O	11.518	6.369	9.628
H	10.836	6.777	10.258
H	12.155	5.850	10.199
H	17.543	10.426	15.441

Transition state from A to B

C	11.026	9.991	19.566
C	12.410	10.678	19.191
H	13.139	10.591	19.966
C	12.877	9.874	17.888
H	13.905	10.208	17.575
H	12.937	8.811	18.012
H	12.134	10.026	17.125
C	12.319	12.140	18.858
H	11.816	12.741	19.631
H	13.287	12.666	18.691
H	11.786	12.342	17.907
C	5.978	11.138	17.497
C	7.389	11.595	17.510
H	7.503	12.643	17.284
H	7.788	11.371	18.496
N	8.234	10.954	16.549
H	8.732	11.552	15.899
C	8.744	9.740	16.693
N	8.280	8.813	17.560
H	7.817	9.187	18.428
H	9.031	8.222	17.865
N	9.835	9.385	15.984
H	10.233	9.983	15.221
H	10.132	8.416	15.868
C	18.630	10.602	19.703
C	18.625	10.922	18.124
H	19.378	11.647	17.846
H	18.855	9.929	17.670
C	17.330	11.464	17.483
N	17.079	11.250	16.174
C	15.942	11.915	15.781
H	15.439	11.827	14.824
N	15.483	12.519	16.857
H	14.534	12.933	16.855
C	16.332	12.320	17.993
H	15.970	12.682	18.998
C	15.860	6.232	10.016
C	14.892	6.723	11.075
H	14.967	6.121	11.993
H	13.844	6.679	10.665
S	15.486	8.552	11.452
C	17.752	7.863	15.208
C	16.244	7.396	15.365
H	16.248	6.819	16.339
H	15.691	8.341	15.469
O	15.744	6.665	14.194
H	15.722	7.311	13.429
C	12.813	19.333	9.299
N	12.663	18.013	10.037
H	11.695	17.859	10.265
C	13.504	17.779	11.156
H	13.633	18.703	11.756
H	12.923	17.043	11.664
C	14.939	17.291	10.840
O	15.842	18.120	10.699
N	15.119	15.953	10.724
H	14.295	15.344	11.044
C	16.435	15.291	10.756
H	17.137	16.066	10.431
H	16.701	14.960	11.719
C	16.511	14.174	9.824
O	17.658	13.794	9.516
N	15.407	13.654	9.293
H	14.501	14.034	9.645
C	15.434	12.635	8.304
H	16.458	12.445	8.007
C	14.990	11.171	8.759

C	14.608	13.091	7.081
O	15.026	13.066	5.865
N	13.305	13.354	7.335
H	12.911	13.544	8.293
C	12.362	13.676	6.275
H	12.009	12.736	5.728
C	11.135	14.419	6.774
C	9.470	13.443	8.254
C	9.834	12.233	8.972
H	10.863	11.987	8.660
H	9.819	12.399	10.035
N	9.143	10.956	8.672
H	9.648	10.268	8.168
C	7.956	10.618	9.141
N	7.079	11.521	9.609
H	7.394	12.426	9.926
H	6.087	11.296	9.729
N	7.606	9.300	8.963
H	8.187	8.668	8.415
H	6.686	8.921	8.885
C	13.085	14.584	5.034
C	6.152	15.535	10.840
C	6.546	16.283	12.069
H	5.622	16.887	12.365
H	6.719	15.560	12.862
C	7.758	17.178	11.963
N	8.957	16.995	12.636
C	9.662	18.158	12.528
H	10.578	18.318	12.993
N	8.994	18.992	11.727
H	9.287	19.984	11.639
C	7.807	18.451	11.341
H	7.095	19.095	10.818
Fe	13.742	9.846	12.172
Mo	9.555	15.261	14.098
Fe	12.760	11.616	13.861
Fe	11.163	10.465	12.427
Fe	12.812	12.250	11.484
Fe	11.186	14.327	12.009
Fe	11.988	13.922	14.742
Fe	10.115	12.668	13.570
C	11.906	12.918	12.966
S	14.630	11.943	12.756
S	11.728	15.813	13.497
S	12.420	9.368	13.950
S	13.130	14.655	16.570
S	12.377	14.086	10.135
S	9.965	13.491	15.661
S	12.128	10.248	10.513
S	8.940	13.963	12.192
S	8.996	10.918	12.721
C	7.595	16.479	18.988
C	8.751	16.623	17.753
H	9.377	17.501	17.946
H	9.314	15.703	17.813
C	8.186	16.798	16.307
C	7.241	15.717	15.883
O	7.541	15.113	14.758
O	6.276	15.287	16.539
O	9.276	16.713	15.435
C	7.414	18.173	16.224
H	6.572	18.152	16.941
H	8.016	18.969	16.687
C	6.915	18.562	14.860
H	13.371	11.793	15.251
H	11.324	11.755	14.680
H	13.990	15.510	16.051
H	8.936	9.805	13.567
O	7.467	5.979	10.602
H	7.027	6.297	9.768

H	7.704	5.016	10.328
O	6.569	12.450	14.587
H	7.306	12.102	14.061
H	6.873	13.364	14.797
O	9.658	7.283	11.602
H	8.797	7.094	11.188
H	9.800	8.246	11.696
O	10.407	8.855	7.826
H	9.877	8.213	7.224
H	10.960	8.223	8.431
O	11.614	6.593	9.349
H	11.276	6.703	10.313
H	12.547	6.359	9.521
H	17.749	10.746	15.568

Structure B (close to $E_4(4H)^{(b)}$)

C	11.226	10.119	19.309
C	12.666	10.641	18.994
H	13.156	10.592	20.000
C	13.348	9.795	18.015
H	14.394	10.086	18.001
H	13.317	8.730	18.292
H	13.015	9.891	16.971
C	12.656	12.125	18.475
H	12.366	12.841	19.218
H	13.606	12.372	18.034
H	11.896	12.214	17.641
C	5.989	11.185	17.273
C	7.471	11.492	17.391
H	7.540	12.478	16.950
H	7.801	11.591	18.416
N	8.437	10.652	16.630
H	8.975	11.230	15.887
C	8.979	9.479	16.967
N	8.424	8.751	17.948
H	7.651	9.026	18.512
H	8.908	7.937	18.353
N	10.001	8.906	16.236
H	10.601	9.455	15.567
H	10.585	8.282	16.766
C	18.526	10.375	19.706
C	18.692	10.801	18.243
H	19.669	11.287	18.081
H	18.780	9.862	17.543
C	17.559	11.557	17.594
N	17.514	11.581	16.243
C	16.495	12.448	15.899
H	16.097	12.522	14.918
N	15.890	12.885	16.998
H	14.987	13.535	16.978
C	16.561	12.372	18.035
H	16.364	12.542	19.051
C	15.783	6.225	9.964
C	14.766	6.775	10.960
H	14.577	6.052	11.769
H	13.897	7.077	10.375
S	15.423	8.436	11.612
C	17.484	7.901	15.249
C	15.888	7.364	15.221
H	15.628	6.751	16.096
H	15.323	8.286	15.270
O	15.505	6.566	14.169
H	15.377	7.254	13.403
C	12.731	19.313	9.004
N	12.861	17.861	9.713
H	11.926	17.460	9.688
C	13.624	17.830	10.915
H	13.711	18.754	11.437
H	13.057	17.223	11.662
C	15.035	17.306	10.817
O	15.977	18.078	10.984
N	15.201	15.987	10.555
H	14.302	15.435	10.664
C	16.427	15.247	10.748
H	17.255	15.934	10.589
H	16.563	14.793	11.791
C	16.652	14.041	9.818
O	17.802	13.610	9.549
N	15.515	13.446	9.328
H	14.607	13.646	9.817
C	15.458	12.504	8.238
H	16.498	12.526	7.874
C	14.962	11.086	8.651

C	14.612	13.001	7.017
O	15.104	13.205	5.888
N	13.295	13.222	7.299
H	13.037	13.140	8.317
C	12.298	13.630	6.344
H	11.788	12.770	5.897
C	11.266	14.578	6.992
C	9.425	12.706	7.410
C	9.472	12.298	8.910
H	10.500	12.197	9.140
H	9.172	13.136	9.595
N	8.860	11.039	9.061
H	9.427	10.163	9.026
C	7.563	10.858	9.386
N	6.711	11.907	9.388
H	7.023	12.846	9.111
H	5.747	11.842	9.779
N	7.137	9.566	9.648
H	7.840	8.837	9.465
H	6.236	9.462	9.119
C	13.035	14.428	5.000
C	5.677	15.106	11.100
C	6.088	16.081	12.228
H	5.331	16.753	12.664
H	6.276	15.491	13.137
C	7.283	16.987	12.025
N	8.493	16.862	12.717
C	9.177	17.975	12.397
H	10.112	18.247	12.764
N	8.415	18.810	11.660
H	8.766	19.700	11.205
C	7.243	18.170	11.328
H	6.431	18.766	10.877
Fe	13.720	9.732	12.050
Mo	9.442	15.032	14.114
Fe	13.350	11.700	13.852
Fe	11.281	10.490	12.616
Fe	12.664	12.223	11.342
Fe	11.132	14.142	12.048
Fe	11.977	13.800	14.740
Fe	10.006	12.345	13.529
C	11.734	12.612	13.059
S	14.791	11.841	12.208
S	11.635	15.809	13.705
S	12.699	9.605	14.067
S	13.331	14.606	16.579
S	12.416	14.165	10.159
S	9.998	13.308	15.597
S	12.036	10.197	10.537
S	8.959	13.762	12.240
S	9.123	10.443	12.881
C	7.483	16.182	18.927
C	8.557	16.352	17.712
H	9.142	17.241	17.898
H	9.240	15.515	17.716
C	7.958	16.597	16.341
C	7.034	15.376	15.866
O	7.450	14.650	14.842
O	5.862	15.292	16.267
O	9.143	16.512	15.390
C	7.188	17.986	16.233
H	6.537	18.026	17.141
H	7.943	18.746	16.336
C	6.359	18.410	14.978
H	13.345	12.952	14.757
H	14.186	11.310	15.151
H	13.983	15.725	16.098
H	9.185	9.503	13.880
O	7.031	6.244	10.466
H	6.622	6.515	9.606

H	7.368	5.300	10.212
O	6.140	12.583	13.823
H	6.901	12.233	13.402
H	6.527	13.305	14.373
O	9.872	7.147	11.464
H	8.930	7.106	11.246
H	10.012	8.098	11.765
O	10.149	8.703	8.483
H	9.769	7.931	8.013
H	10.896	8.400	9.004
O	11.576	6.187	9.784
H	10.893	6.475	10.422
H	12.183	5.538	10.255
H	18.053	11.043	15.598

Structure C (close to $E_4(4H)^{(c)}$)

C	11.292	10.094	19.171
C	12.661	10.791	18.958
H	13.058	10.667	20.014
C	13.601	10.036	17.893
H	14.639	10.379	18.106
H	13.669	8.917	18.007
H	13.258	10.326	16.880
C	12.551	12.233	18.537
H	12.003	12.924	19.198
H	13.546	12.683	18.368
H	12.019	12.233	17.562
C	6.173	11.299	17.119
C	7.626	11.543	17.288
H	7.798	12.583	17.167
H	7.870	11.351	18.332
N	8.456	10.827	16.328
H	9.126	11.360	15.769
C	8.889	9.600	16.571
N	8.352	8.839	17.592
H	8.093	9.318	18.424
H	9.112	8.199	17.871
N	9.887	9.056	15.887
H	10.325	9.625	15.167
H	10.508	8.321	16.225
C	18.428	10.640	19.633
C	18.552	10.942	18.109
H	19.532	11.291	17.845
H	18.596	9.896	17.605
C	17.521	11.694	17.425
N	17.274	11.624	16.048
C	16.155	12.254	15.657
H	15.766	12.302	14.614
N	15.715	12.872	16.754
H	14.778	13.404	16.774
C	16.479	12.434	17.892
H	16.298	12.954	18.827
C	15.781	6.432	9.585
C	14.795	6.936	10.591
H	14.890	6.148	11.386
H	13.757	6.880	10.102
S	15.352	8.501	11.217
C	17.564	7.920	15.023
C	16.006	7.548	15.069
H	15.759	7.072	16.139
H	15.614	8.557	15.063
O	15.547	6.726	14.067
H	15.234	7.185	13.217
C	12.805	19.609	9.140
N	12.915	18.220	9.725
H	11.948	17.930	9.968
C	13.720	18.033	10.940
H	13.830	18.840	11.577
H	13.108	17.387	11.494
C	15.131	17.523	10.828
O	16.129	18.206	10.902
N	15.267	16.106	10.816
H	14.412	15.548	10.840
C	16.550	15.368	10.824
H	17.404	16.010	10.955
H	16.600	14.659	11.754
C	16.710	14.230	9.757
O	17.838	13.718	9.514
N	15.578	13.956	9.096
H	14.659	14.127	9.600
C	15.530	12.885	8.099
H	16.593	12.767	7.819
C	15.167	11.522	8.620

C	14.593	13.219	6.934
O	14.934	13.115	5.738
N	13.304	13.412	7.278
H	13.038	13.592	8.256
C	12.328	13.743	6.349
H	11.855	12.984	5.743
C	11.137	14.516	6.950
C	9.404	13.248	7.911
C	9.954	11.992	8.603
H	10.931	11.803	8.034
H	10.274	12.341	9.642
N	9.057	10.908	8.497
H	9.520	10.064	8.122
C	7.846	10.832	9.154
N	7.450	11.789	10.034
H	8.004	12.643	10.143
H	6.478	11.965	10.251
N	7.176	9.676	8.991
H	7.262	9.015	8.187
H	6.287	9.488	9.497
C	12.937	14.763	4.986
C	6.073	15.292	10.769
C	6.410	16.233	12.017
H	5.468	16.789	12.349
H	6.528	15.606	12.918
C	7.618	17.114	11.912
N	8.828	16.836	12.498
C	9.547	17.960	12.370
H	10.520	18.095	12.778
N	8.948	18.894	11.655
H	9.287	19.867	11.579
C	7.667	18.414	11.307
H	6.918	18.937	10.776
Fe	13.817	9.986	12.079
Mo	9.498	15.046	13.980
Fe	13.180	11.760	13.985
Fe	11.437	10.726	12.464
Fe	12.803	12.433	11.266
Fe	11.201	14.243	12.016
Fe	11.899	13.744	14.632
Fe	9.833	12.449	13.396
C	11.665	12.518	12.910
S	14.780	12.083	12.395
S	11.673	15.795	13.537
S	12.609	9.424	13.926
S	13.146	14.784	16.745
S	12.354	14.281	10.111
S	9.956	13.245	15.477
S	12.154	10.365	10.398
S	8.917	13.979	11.942
S	9.132	10.493	12.746
C	7.344	15.907	18.863
C	8.480	16.378	17.735
H	9.021	17.278	18.025
H	9.245	15.626	17.690
C	8.062	16.497	16.229
C	7.069	15.481	15.711
O	7.492	14.788	14.652
O	5.986	15.306	16.247
O	9.271	16.513	15.363
C	7.352	17.954	16.165
H	6.507	18.016	16.854
H	8.093	18.720	16.418
C	6.837	18.295	14.770
H	13.557	13.175	14.713
H	12.319	12.328	15.308
H	13.696	15.732	15.960
H	8.890	9.559	13.621
O	7.423	6.083	10.158
H	6.852	6.229	9.322

H	7.692	5.133	10.025
O	6.547	12.466	13.561
H	7.270	12.040	13.085
H	7.043	13.225	13.883
O	9.645	7.511	11.237
H	8.824	7.154	10.696
H	9.644	8.490	11.458
O	10.527	8.720	7.397
H	9.877	8.032	7.305
H	11.143	8.518	8.113
O	11.550	5.908	9.609
H	11.125	6.493	10.312
H	11.972	5.218	10.220
H	17.855	11.191	15.369

Structure D (close to $E_4(2H; H_2)$)

C	10.826	9.959	19.461
C	12.109	10.819	19.092
H	12.729	10.903	19.943
C	12.832	10.143	17.965
H	13.755	10.606	17.620
H	13.179	9.095	18.132
H	12.132	10.075	17.125
C	11.970	12.268	18.589
H	11.612	12.904	19.389
H	12.931	12.598	18.348
H	11.364	12.396	17.714
C	5.787	10.882	17.603
C	7.265	11.364	17.585
H	7.262	12.449	17.469
H	7.681	11.150	18.626
N	8.090	10.686	16.596
H	8.407	11.363	15.903
C	8.753	9.511	16.715
N	8.185	8.380	17.278
H	7.532	8.716	17.942
H	8.847	7.731	17.717
N	9.846	9.416	15.976
H	10.460	10.201	15.665
H	10.373	8.522	15.996
C	18.753	10.490	19.769
C	18.701	10.804	18.228
H	19.703	11.213	17.970
H	18.660	9.869	17.735
C	17.593	11.604	17.578
N	17.579	11.811	16.176
C	16.506	12.530	15.803
H	16.111	12.565	14.759
N	15.834	12.809	16.923
H	14.857	13.269	16.812
C	16.495	12.238	18.031
H	16.054	12.293	19.031
C	15.691	6.387	10.095
C	14.724	6.978	11.069
H	14.658	6.128	11.805
H	13.773	7.073	10.565
S	15.283	8.550	11.780
C	17.467	8.173	15.120
C	15.848	7.704	15.341
H	15.675	7.437	16.413
H	15.261	8.665	15.257
O	15.522	6.705	14.547
H	15.184	6.954	13.651
C	12.456	19.357	9.078
N	12.414	18.013	9.694
H	11.371	17.832	9.855
C	13.229	17.791	10.843
H	13.377	18.732	11.416
H	12.696	17.059	11.508
C	14.637	17.223	10.560
O	15.590	17.967	10.768
N	14.665	15.920	10.314
H	13.779	15.353	10.347
C	15.935	15.200	10.503
H	16.721	15.951	10.533
H	15.870	14.539	11.381
C	16.270	14.135	9.368
O	17.300	14.008	8.742
N	15.165	13.289	9.187
H	14.407	13.255	9.945
C	15.098	12.246	8.116
H	16.117	12.335	7.713
C	14.752	10.921	8.605

C	14.068	12.780	7.070
O	14.376	12.943	5.887
N	12.809	13.126	7.460
H	12.601	13.469	8.410
C	11.762	13.439	6.525
H	11.298	12.572	6.084
C	10.586	14.221	7.100
C	8.964	12.394	7.757
C	8.909	12.034	9.274
H	9.812	12.355	9.844
H	8.085	12.639	9.746
N	8.757	10.591	9.393
H	9.624	10.086	9.278
C	7.573	9.985	9.144
N	6.366	10.595	9.390
H	6.179	11.530	9.769
H	5.558	10.081	9.032
N	7.623	8.741	8.650
H	8.526	8.461	8.213
H	6.833	8.099	8.697
C	12.467	14.310	5.057
C	6.332	15.310	10.769
C	6.327	16.279	12.066
H	5.297	16.857	12.163
H	6.392	15.674	12.976
C	7.565	17.092	12.008
N	8.777	16.710	12.658
C	9.552	17.792	12.599
H	10.502	18.052	13.101
N	8.882	18.781	11.999
H	9.389	19.697	11.858
C	7.664	18.341	11.544
H	7.099	18.909	10.778
Fe	13.606	10.034	12.145
Mo	9.170	15.003	14.260
Fe	13.084	11.587	13.981
Fe	11.037	10.527	12.844
Fe	12.606	12.352	11.707
Fe	10.873	14.130	12.310
Fe	11.438	13.767	14.931
Fe	9.695	12.405	13.838
C	11.421	12.525	13.336
S	14.735	12.110	12.389
S	11.346	15.753	13.741
S	12.588	9.457	14.105
S	13.039	14.620	16.607
S	11.959	14.180	10.416
S	9.547	13.363	15.934
S	11.873	10.330	10.747
S	8.808	13.630	12.277
S	8.687	10.483	13.030
C	6.741	15.563	18.977
C	7.974	15.996	17.892
H	8.502	16.833	18.321
H	8.634	15.157	17.934
C	7.575	16.245	16.486
C	6.736	15.119	15.893
O	7.183	14.605	14.715
O	5.729	14.707	16.476
O	8.690	16.453	15.584
C	6.666	17.496	16.442
H	5.684	17.156	16.812
H	7.050	18.240	17.203
C	6.345	18.088	15.129
H	13.558	11.991	15.408
H	12.682	11.483	15.516
H	13.975	14.815	15.542
H	8.634	9.496	13.978
O	6.968	6.113	10.635
H	6.574	6.485	9.831

H	7.404	5.303	10.340
O	5.786	12.428	13.773
H	6.380	11.694	13.611
H	6.229	13.108	14.301
O	9.381	7.251	11.916
H	8.491	7.132	11.543
H	9.548	8.201	12.037
O	10.263	8.196	7.958
H	9.946	7.575	7.254
H	10.704	7.607	8.603
O	11.339	6.573	9.997
H	10.645	6.807	10.597
H	11.873	5.951	10.503
H	18.230	11.338	15.581

Transition state from B to E

C	10.425	10.211	19.213
C	11.526	11.310	19.000
H	12.091	11.524	19.964
C	12.578	10.786	18.004
H	13.391	11.533	17.845
H	13.113	9.869	18.306
H	12.158	10.557	17.036
C	10.870	12.601	18.443
H	10.298	13.067	19.277
H	11.502	13.413	18.086
H	10.303	12.373	17.522
C	5.809	11.122	17.279
C	7.284	11.505	17.200
H	7.367	12.553	16.922
H	7.683	11.341	18.182
N	7.957	10.688	16.170
H	8.199	11.257	15.364
C	8.496	9.485	16.345
N	8.082	8.684	17.338
H	7.623	9.138	18.120
H	8.699	7.976	17.736
N	9.531	9.125	15.575
H	10.030	9.869	14.969
H	10.075	8.264	15.715
C	18.654	10.605	19.542
C	18.706	10.928	17.994
H	19.657	11.360	17.777
H	18.640	9.951	17.439
C	17.570	11.715	17.459
N	17.441	11.743	16.040
C	16.232	12.282	15.708
H	15.902	12.433	14.624
N	15.668	12.654	16.859
H	14.696	13.100	16.764
C	16.425	12.267	17.912
H	16.053	12.411	18.917
C	15.813	6.473	10.000
C	14.774	7.057	10.895
H	14.634	6.392	11.833
H	13.798	7.308	10.372
S	15.432	8.659	11.531
C	17.581	8.193	15.173
C	16.047	7.807	15.322
H	15.994	7.084	16.168
H	15.520	8.718	15.717
O	15.397	7.172	14.225
H	15.250	7.828	13.498
C	12.377	19.314	8.950
N	12.472	17.772	9.492
H	11.469	17.576	9.585
C	13.149	17.787	10.825
H	13.101	18.778	11.316
H	12.703	16.969	11.475
C	14.609	17.471	10.594
O	15.517	18.294	10.418
N	14.871	16.104	10.703
H	14.052	15.491	10.749
C	16.157	15.587	10.502
H	16.837	16.489	10.209
H	16.462	15.137	11.498
C	16.317	14.475	9.478
O	17.436	14.185	9.000
N	15.148	13.837	9.175
H	14.275	13.876	9.819
C	15.163	12.822	8.100
H	16.111	12.795	7.603
C	15.059	11.430	8.781

C	14.174	13.128	6.996
O	14.483	13.160	5.802
N	12.894	13.322	7.335
H	12.544	13.359	8.308
C	11.851	13.586	6.450
H	11.301	12.724	5.950
C	10.513	14.192	7.181
C	9.149	12.991	7.876
C	9.682	11.884	8.816
H	10.756	11.689	8.468
H	9.706	12.237	9.825
N	9.072	10.536	8.656
H	9.724	9.814	8.216
C	7.754	10.178	8.787
N	7.017	11.045	9.575
H	7.513	11.967	9.717
H	6.109	11.328	9.221
N	7.292	9.055	8.317
H	7.901	8.432	7.703
H	6.388	8.768	8.574
C	12.404	14.491	5.036
C	5.860	15.583	10.395
C	6.161	16.407	11.620
H	5.343	17.202	11.686
H	6.067	15.793	12.542
C	7.441	17.193	11.707
N	8.599	16.753	12.414
C	9.358	17.838	12.462
H	10.321	17.907	12.904
N	8.863	18.877	11.801
H	9.283	19.832	12.034
C	7.658	18.472	11.260
H	7.042	19.085	10.680
Fe	13.651	9.962	12.035
Mo	9.068	15.067	13.812
Fe	12.650	11.594	13.826
Fe	11.117	10.457	12.272
Fe	12.546	12.292	11.243
Fe	10.831	14.281	11.995
Fe	11.446	13.643	14.511
Fe	9.454	12.376	13.276
C	11.313	12.365	12.788
S	14.488	12.177	12.465
S	11.273	15.755	13.713
S	12.288	9.370	13.786
S	13.013	14.333	16.215
S	12.096	14.256	10.177
S	9.516	13.227	15.309
S	12.119	10.137	10.349
S	8.658	13.840	11.832
S	8.878	10.240	12.515
C	7.051	15.722	18.577
C	8.101	15.830	17.362
H	8.865	16.476	17.699
H	8.601	14.941	17.152
C	7.577	16.350	16.012
C	6.578	15.351	15.370
O	6.990	14.882	14.188
O	5.581	14.856	15.963
O	8.740	16.417	15.188
C	6.942	17.710	16.120
H	6.087	17.501	16.729
H	7.619	18.384	16.628
C	6.566	18.420	14.810
H	13.534	12.174	15.359
H	13.930	11.459	15.528
H	13.869	15.026	15.364
H	8.713	9.524	13.777
O	7.020	6.214	10.281
H	6.487	6.531	9.433

H	7.159	5.168	10.076
O	6.013	12.422	13.517
H	6.524	12.087	12.771
H	6.379	13.349	13.601
O	9.696	6.895	11.271
H	8.722	6.716	11.049
H	9.824	7.863	11.498
O	10.625	8.542	6.961
H	10.007	7.749	6.865
H	11.342	8.330	7.604
O	11.572	6.110	9.326
H	10.958	6.421	10.062
H	12.193	5.405	9.810
H	18.067	11.259	15.421

Structure E (Representative E_4*(2H) + H_2)

C	10.420	10.164	19.246
C	11.575	11.213	19.085
H	12.192	11.230	20.028
C	12.407	10.679	17.840
H	13.348	11.221	17.839
H	12.591	9.596	17.987
H	11.910	10.938	16.929
C	10.938	12.649	18.734
H	10.408	13.127	19.555
H	11.792	13.301	18.312
H	10.121	12.463	18.016
C	5.583	10.861	17.030
C	7.062	11.150	17.011
H	7.263	12.165	16.650
H	7.357	11.093	18.048
N	7.973	10.395	16.189
H	8.646	11.106	15.758
C	8.573	9.221	16.475
N	8.002	8.335	17.311
H	7.720	8.674	18.195
H	8.378	7.401	17.398
N	9.618	8.826	15.693
H	10.068	9.493	15.041
H	10.262	8.124	16.076
C	18.704	10.433	19.450
C	18.957	10.807	17.889
H	19.830	11.608	17.867
H	19.292	9.979	17.215
C	17.713	11.359	17.276
N	17.478	11.573	15.888
C	16.340	12.167	15.662
H	15.976	12.290	14.621
N	15.790	12.439	16.880
H	14.982	13.057	16.947
C	16.684	12.027	17.913
H	16.465	12.191	18.931
C	15.632	6.587	9.977
C	14.694	7.072	11.049
H	14.715	6.339	11.898
H	13.674	7.297	10.717
S	15.491	8.653	11.722
C	17.754	8.204	15.256
C	16.207	7.806	15.496
H	16.265	7.276	16.485
H	15.686	8.804	15.578
O	15.737	6.927	14.510
H	15.514	7.500	13.719
C	12.253	19.215	9.041
N	12.306	17.775	9.566
H	11.358	17.480	9.761
C	13.075	17.481	10.800
H	13.059	18.332	11.476
H	12.617	16.652	11.390
C	14.517	17.246	10.673
O	15.342	18.197	10.644
N	14.890	15.930	10.856
H	14.202	15.177	10.896
C	16.242	15.406	10.616
H	16.847	16.276	10.307
H	16.668	15.016	11.524
C	16.307	14.403	9.457
O	17.436	14.176	9.008
N	15.135	13.755	9.086
H	14.304	13.919	9.671
C	15.058	12.725	8.077
H	16.108	12.557	7.590
C	14.626	11.364	8.770

C	14.105	13.023	6.896
O	14.401	12.872	5.678
N	12.854	13.361	7.256
H	12.588	13.612	8.314
C	11.864	13.609	6.313
H	11.423	12.734	5.773
C	10.680	14.418	6.973
C	9.411	12.880	7.516
C	9.689	11.707	8.538
H	10.741	11.401	8.585
H	9.416	12.218	9.526
N	9.021	10.419	8.247
H	9.536	9.639	7.861
C	7.792	10.088	8.720
N	6.968	10.962	9.340
H	7.209	11.917	9.421
H	5.967	10.818	9.172
N	7.333	8.829	8.447
H	7.965	8.154	8.042
H	6.351	8.485	8.603
C	12.610	14.402	4.972
C	5.989	15.430	10.352
C	6.127	16.286	11.746
H	5.170	16.859	11.808
H	6.170	15.739	12.638
C	7.295	17.212	11.759
N	8.462	16.947	12.425
C	9.190	18.057	12.379
H	10.242	18.248	12.786
N	8.586	18.975	11.617
H	8.834	19.990	11.560
C	7.364	18.499	11.250
H	6.678	19.180	10.732
Fe	13.595	9.812	12.128
Mo	9.174	14.931	13.731
Fe	12.698	11.550	13.717
Fe	10.963	10.425	12.341
Fe	12.682	12.097	11.357
Fe	10.928	14.058	12.058
Fe	11.513	13.662	14.402
Fe	9.401	12.227	13.176
C	11.340	12.338	12.796
S	14.711	11.955	12.543
S	11.402	15.786	13.438
S	12.233	9.401	13.875
S	13.229	14.002	15.979
S	12.261	13.973	10.217
S	9.510	13.047	15.187
S	12.017	9.968	10.420
S	8.818	13.716	11.721
S	8.750	10.160	12.342
C	7.179	15.618	18.584
C	8.309	16.026	17.379
H	8.958	16.871	17.553
H	8.913	15.156	17.273
C	7.793	16.431	15.953
C	6.786	15.363	15.442
O	7.152	14.731	14.306
O	5.773	15.042	16.095
O	8.808	16.441	15.093
C	6.936	17.753	16.144
H	6.157	17.471	16.868
H	7.609	18.447	16.703
C	6.431	18.268	14.874
H	14.018	11.670	15.201
H	13.963	10.927	15.196
H	13.878	14.899	15.257
H	8.384	9.137	13.227
O	6.938	5.896	10.438
H	6.460	6.228	9.616

H	7.269	5.010	10.083
O	6.180	12.096	13.845
H	6.889	11.667	13.351
H	6.520	13.048	13.992
O	9.362	7.074	10.869
H	8.458	6.714	10.691
H	9.311	8.020	10.999
O	10.701	8.597	7.056
H	10.065	7.902	6.734
H	11.220	8.200	7.759
O	11.424	6.041	9.408
H	10.911	6.608	10.028
H	11.858	5.377	9.954
H	18.074	11.180	15.112