Supporting information for: Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Theory, Implementation, and Parameters

Pavlo O. Dral, Xin Wu, Lasse Spörkel, Axel Koslowski, Wolfgang Weber,[†] Rainer Steiger,[‡] Mirjam Scholten,[¶] and Walter Thiel[*]

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

E-mail: thiel@kofo.mpg.de

Contents

[*]To whom correspondence should be addressed
[†]Current address: BASF, Rue Marie de Bourgogne 58, 1000 Brussels, Belgium
[‡]Current address: Arbentalstrasse 204, 8045 Zürich, Switzerland
[¶]Current address: Leberberg 11, 65193 Wiesbaden, Germany

List of Tables

List of Figures

1 Tables: Numerical Results for Individual Molecules and Properties

Table S1: Benchmark Results for the CHNO Data Set. Heats of Formation (kcal/mol)

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Hydrogen	0.0[a]	0.7	−5.2	−13.4	−25.7	−32.0	2.6	−3.4	−3.5	−3.5	−3.5	−0.0	−0.0	−0.1	−0.1
Methane	−17.9[b]	−11.9	−8.8	−13.0	−12.3	−14.4	−13.8	−19.2	−19.8	−19.9	−19.9	−18.0	−18.4	−19.1	−19.1
Ethane	−20.0[b]	−19.7	−17.4	−18.1	−15.8	−18.2	−20.3	−21.2	−22.8	−22.9	−22.9	−20.8	−21.9	−23.6	−23.6
Ethylene	12.5[b]	15.4	16.5	16.6	15.7	13.9	11.9	12.9	12.0	11.7	11.7	13.9	13.4	12.0	12.0
Acetylene	54.5[b]	57.9	54.8	50.7	56.7	57.1	53.6	54.2	53.9	53.6	53.6	54.7	54.6	53.7	53.7
Propane	−25.0[b]	−24.9	−24.3	−23.6	−21.0	−23.1	−25.2	−25.5	−28.7	−28.7	−28.7	−25.4	−27.9	−30.4	−30.4
Propene ecl	4.8[b]	5.0	6.6	6.4	5.6	4.2	4.4	4.7	2.6	2.3	2.3	5.0	3.5	1.1	1.1
Propyne	44.2[b]	41.4	43.4	40.2	45.4	46.0	45.0	44.5	43.3	42.9	42.9	44.1	43.5	41.5	41.5
Allene	45.5[b]	43.9	46.1	47.1	37.5	36.9	45.4	45.9	44.7	44.3	44.3	45.5	44.9	42.9	42.9
n-Butane	−30.0[b]	−29.7	−31.1	−29.1	−26.0	−28.2	−30.4	−30.1	−34.9	−34.8	−34.8	−30.3	−34.1	−37.5	−37.5
Isobutane	−32.1[b]	−26.8	−29.4	−29.5	−27.5	−28.9	−28.3	−31.8	−37.0	−36.7	−36.7	−31.3	−35.5	−38.8	−38.8
But-1-ene H-ecl	0.0[b]	−0.2	0.2	1.4	1.2	−0.4	−0.7	0.1	−3.6	−3.8	−3.8	0.3	−2.4	−5.7	−5.7
trans-2-Butene	−2.7[b]	−5.1	−3.3	−3.8	−3.5	−5.1	−3.1	−3.8	−7.2	−7.5	−7.5	−4.0	−6.4	−9.8	−9.8
cis-2-Butene	−1.7[b]	−3.9	−2.2	−3.6	−2.5	−3.9	−1.1	−1.9	−5.5	−5.8	−5.8	−2.2	−4.8	−8.3	−8.2
Isobutene	−4.0[b]	−2.0	−1.2	−3.3	−5.1	−5.6	−0.4	−4.3	−8.0	−8.2	−8.2	−3.9	−6.7	−10.1	−10.0
1,2-Butadiene	38.8[b]	33.5	37.1	38.0	30.1	29.0	38.4	38.1	35.8	35.2	35.2	37.6	36.1	33.0	33.0
1,3-s-tr-Butadiene	26.3[b]	29.0	29.9	31.0	28.5	27.2	28.2	29.4	26.8	26.3	26.3	30.3	28.6	25.5	25.5
1-Butyne	39.5[b]	36.1	37.5	35.7	41.2	41.7	39.9	39.5	36.8	36.5	36.5	39.2	37.5	34.6	34.6
2-Butyne	34.8[b]	24.9	32.0	29.8	35.1	35.3	36.5	35.1	33.0	32.4	32.4	33.8	32.6	29.6	29.6
Vinylacetylene	73.0[c]	65.6	67.9	66.4	69.1	69.7	70.6	71.2	69.5	69.0	69.0	71.2	70.3	67.6	67.6
Butatriene	83.0[c]	71.3	76.1	78.6	76.8	76.0	81.6	81.9	80.4	79.8	79.8	80.7	79.9	77.3	77.3
n-Pentane	−35.1[b]	−34.4	−38.0	−34.5	−31.0	−33.3	−35.5	−34.7	−41.1	−40.8	−40.8	−35.2	−40.3	−44.6	−44.6
Neopentane	−40.2[b]	−24.6	−32.8	−35.8	−35.0	−35.5	−29.3	−39.6	−47.2	−46.5	−46.4	−37.6	−44.1	−48.1	−48.1
n-Hexane	−39.9[b]	−39.1	−44.8	−39.9	−36.0	−38.4	−40.7	−39.2	−47.3	−46.9	−46.9	−40.0	−46.5	−51.6	−51.6
tr-1,3-Pentadiene	18.2[b]	18.8	19.8	20.7	18.6	17.3	20.2	20.5	16.6	16.1	16.1	20.9	18.2	14.0	14.0
cis-1,3-Pentadiene	19.5[b]	20.1	20.9	21.1	19.5	18.4	22.2	22.4	18.3	17.8	17.8	22.8	19.8	15.6	15.6
1,4-Pentadiene	25.2[b]	26.0	25.3	27.2	23.7	22.8	24.4	26.9	22.8	22.4	22.4	26.8	23.9	19.7	19.7
Cyclopropane	12.7[b]	11.2	17.8	16.3	11.2	12.0	7.2	9.9	7.6	7.6	7.6	10.1	8.7	6.3	6.3
cis-Dimethylcyclopropane	1.3[d]	−2.1	4.8	1.4	−2.2	−0.2	−0.1	0.6	−5.4	−5.0	−5.0	0.1	−4.4	−8.4	−8.4
Cyclopropene	66.2[b]	68.3	74.8	68.2	60.9	63.2	62.8	67.4	65.9	65.7	65.7	65.5	64.7	62.8	62.8
1-Methylcyclopropene	58.2[b]	53.7	64.7	57.4	50.0	53.0	56.6	59.6	57.0	56.7	56.7	57.1	55.6	52.6	52.6
1,2-Dimethylcyclopropene	46.4[d]	39.2	54.6	46.7	40.0	43.2	50.5	51.8	48.1	47.7	47.7	48.9	46.5	42.4	42.5
Methylenecyclopropane	47.9[b]	37.9	47.7	44.5	35.8	38.1	42.2	45.0	42.3	42.0	42.0	43.7	42.2	39.1	39.1
Cyclobutane	6.8[b]	−11.9	−1.0	−3.8	−3.5	−2.3	−1.9	3.0	−1.1	−1.0	−1.0	2.9	−0.0	−3.3	−3.3
Cyclobutene plan	37.5[b]	31.0	45.8	37.7	33.8	37.2	39.0	41.3	38.4	38.2	38.2	40.8	38.9	35.8	35.8
1,2-Dimethylcyclobutene	19.8[d]	6.4	26.9	16.2	12.0	16.5	25.4	21.4	15.5	15.3	15.3	20.9	16.7	11.6	11.7
Methylenecyclobutane	29.0[b]	10.9	25.1	19.7	15.1	18.4	24.2	25.4	20.9	20.7	20.8	25.6	22.4	18.3	18.3
Cyclopentane envelope	−18.3[b]	−30.5	−28.8	−23.9	−20.1	−20.0	−24.8	−19.7	−25.8	−25.5	−25.5	−20.8	−25.2	−29.8	−29.8
Cyclopentene	8.1[b]	−0.3	3.0	3.0	5.1	5.4	3.5	6.8	2.1	1.9	1.9	5.7	2.7	−2.0	−2.0
Cyclopentadiene	32.1[b]	32.1	37.1	31.8	32.1	32.3	33.3	33.3	29.9	29.3	29.3	32.6	30.7	26.2	26.2
Cyclohexane chair (AMP)	−29.5[b]	−34.8	−38.5	−31.0	−27.5	−27.4	−31.2	−27.1	−35.9	−35.0	−35.0	−28.5	−35.1	−40.6	−40.5
Cyclohexene half-chair	−1.2[b]	−9.9	−10.1	−4.9	−4.0	−3.4	−3.7	0.4	−6.6	−6.5	−6.4	−1.1	−5.9	−11.7	−11.6

... continued on next page ...

Table S1: ... *continued from previous page* ...

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
1,3-Cyclohexadiene	25.4[b]	14.5	17.5	20.4	19.3	20.2	22.3	25.9	20.4	20.0	20.0	24.8	21.4	15.6	15.6
Benzene	19.7[b]	21.3	22.0	23.5	24.2	23.0	17.1	18.8	14.6	13.8	13.8	18.5	16.4	10.6	10.6
Toluene ecl	12.0[b]	13.6	14.4	14.1	14.2	13.2	12.2	9.5	3.6	2.9	2.9	9.6	6.1	−0.6	−0.6
Ethylbenzene stag	7.1[b]	8.8	8.7	9.5	10.2	8.5	7.1	4.8	−2.9	−3.5	−3.5	5.0	−0.0	−7.7	−7.7
Styrene	35.3[b]	37.6	38.7	39.2	37.9	36.7	36.6	34.7	28.2	27.3	27.3	35.6	31.6	24.1	24.1
Cycloheptatriene	43.2[b]	33.8	38.3	42.5	37.4	38.6	44.0	46.7	40.1	39.7	39.8	46.1	42.0	35.3	35.4
Bicyclobutane	51.9[b]	64.1	78.1	69.2	59.5	65.5	59.0	62.0	58.9	59.0	59.0	59.9	57.9	55.2	55.2
Spirocyclopentane	44.3[b]	33.7	50.5	43.1	33.2	38.5	38.4	42.8	38.2	38.4	38.4	41.0	38.1	34.3	34.3
trans-Bicyclopropyl	30.9[b]	28.6	39.5	36.1	25.0	29.5	26.9	30.7	24.2	24.7	24.7	30.2	25.6	21.0	21.0
Bicyclo[2.1.0]pentane	37.8[c]	30.2	46.1	37.8	31.5	36.9	37.3	40.1	35.1	35.4	35.4	39.0	35.5	31.6	31.6
Norbornane	−13.1[b]	−10.4	−14.4	−13.7	−10.6	−9.3	−10.8	−12.5	−22.5	−21.6	−21.5	−12.4	−19.7	−26.3	−26.3
Norbornadiene	58.8[b]	62.9	67.7	58.8	57.0	59.1	59.5	51.8	45.0	44.8	44.8	52.0	48.0	41.1	41.1
Bicyclo[2.2.2]octane	−23.7[b]	−26.3	−36.0	−27.8	−25.5	−23.3	−24.3	−22.2	−35.1	−33.7	−33.6	−23.4	−32.8	−40.6	−40.5
Naphthalene	35.9[b]	38.3	40.6	40.7	40.1	39.7	40.2	34.8	26.4	25.3	25.3	35.7	31.0	21.0	21.0
Adamantane	−32.2[b]	−26.4	−43.2	−34.6	−33.0	−28.4	−26.2	−30.4	−48.4	−45.8	−45.6	−30.2	−43.7	−53.3	−53.1
Cubane	148.7[b]	99.1	151.2	113.8	106.5	125.6	147.6	144.6	136.6	137.2	137.2	146.4	141.3	134.8	134.8
Nitrogen	0.0[a]	8.3	11.2	17.6	40.6	33.0	−4.4	2.8	2.8	2.6	2.6	2.6	2.6	2.2	2.2
Ammonia	−11.0[b]	−6.4	−7.3	−3.1	−3.1	−4.3	−3.8	−5.9	−6.1	−6.3	−6.3	−11.2	−11.3	−12.0	−12.0
Methylamine	−5.5[b]	−7.5	−7.4	−5.2	−2.4	−3.4	−4.7	−4.1	−5.3	−5.6	−5.6	−5.8	−6.6	−8.1	−8.1
Dimethylamine	−4.4[b]	−6.6	−5.6	−7.9	−3.1	−4.2	−4.7	−5.1	−7.7	−7.9	−7.9	−2.2	−4.3	−6.5	−6.5
Trimethylamine	−5.7[b]	−2.8	−1.7	−10.9	−4.4	−6.2	−3.5	−8.0	−12.4	−12.4	−12.4	−0.1	−3.8	−6.7	−6.7
Ethylamine	−11.3[b]	−13.2	−15.1	−12.5	−11.2	−11.3	−9.3	−8.9	−11.5	−11.7	−11.7	−12.1	−14.1	−16.5	−16.5
n-Propylamine	−16.8[b]	−18.2	−22.1	−17.9	−15.7	−16.2	−14.6	−13.5	−17.8	−17.8	−17.8	−16.9	−20.3	−23.5	−23.5
Isopropylamine	−20.0[b]	−16.4	−17.5	−17.3	−15.5	−15.3	−14.2	−14.5	−19.0	−18.9	−18.9	−17.4	−21.0	−24.2	−24.2
tert-Butylamine	−28.9[b]	−15.5	−21.3	−25.2	−26.1	−24.2	−14.7	−22.3	−29.1	−28.7	−28.7	−24.6	−30.4	−34.3	−34.3
Aziridine	30.2[b]	25.1	33.1	31.6	29.6	32.3	30.6	36.3	34.5	34.3	34.3	35.4	34.3	32.2	32.3
Pyrrole	25.9[b]	32.5	39.9	27.1	25.8	26.5	37.2	33.7	31.0	30.2	30.2	32.0	30.5	26.3	26.3
Pyridine	33.6[b]	28.8	32.0	30.4	33.9	31.7	33.0	30.8	27.1	26.3	26.3	29.4	27.6	22.2	22.3
Pyridazine (1,2)	66.5[b]	43.6	55.3	56.0	55.2	53.2	58.2	48.4	45.2	44.3	44.3	51.1	49.5	44.6	44.6
Pyrimidine (1,3)	46.8[b]	35.0	43.9	38.0	45.1	40.2	47.3	44.5	41.4	40.4	40.4	41.9	40.4	35.4	35.4
Pyrazine (1,4)	46.9[b]	37.8	44.2	39.3	47.6	44.3	51.7	44.9	41.9	40.9	40.9	42.0	40.4	35.5	35.5
Aniline	20.8[b]	21.7	20.5	21.3	21.4	21.2	25.6	25.2	19.9	19.0	19.0	22.3	19.2	12.7	12.7
Hydrogen cyanide	32.3[e]	35.3	31.0	33.0	33.2	29.8	24.5	26.1	25.9	25.7	25.7	25.3	25.2	24.7	24.7
Acetonitrile	18.0[c]	19.2	19.3	23.3	20.5	18.2	16.5	17.5	16.5	16.2	16.2	15.3	14.8	13.2	13.2
Methylisocyanide	39.1[b]	60.3	50.4	54.7	45.5	38.9	27.8	38.3	37.3	36.9	36.9	26.7	26.1	24.4	24.4
Propionitrile	12.3[b]	13.8	13.0	18.5	16.0	13.6	10.8	12.3	9.9	9.6	9.6	10.2	8.6	6.0	6.0
Acrylonitrile	43.2[b]	43.8	45.0	50.2	46.0	43.8	43.3	45.6	44.2	43.6	43.6	43.7	42.9	40.5	40.5
Fumaronitrile	81.0[b]	74.7	76.0	86.0	79.7	77.6	76.4	79.7	77.6	76.9	76.9	75.2	74.0	70.8	70.8
Maleonitrile	81.3[b]	75.0	76.6	86.9	80.6	78.1	78.0	81.2	78.9	78.2	78.2	76.2	75.0	71.6	71.6
Dicyanoacetylene	126.5[b]	111.4	119.8	128.1	128.2	126.6	134.8	138.0	136.8	136.1	136.1	128.3	127.8	125.3	125.3
Cyanogen	73.3[b]	66.6	67.9	77.5	74.2	71.5	72.3	74.9	74.3	73.9	73.9	68.2	68.0	66.7	66.7
Benzonitrile	51.6[b]	52.0	53.4	58.5	55.3	53.5	51.1	49.7	44.7	43.7	43.7	48.0	45.3	38.6	38.6
Hydrazine	22.8[e]	14.2	13.7	20.7	15.2	15.3	16.1	18.5	17.7	17.4	17.4	16.5	15.9	14.7	14.7
Methylhydrazine	22.6[b]	14.4	17.3	17.9	14.1	14.4	15.8	18.2	16.2	15.8	15.8	20.1	18.5	16.5	16.5

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

Table S1: ... *continued from previous page* ...

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
1,1-Dimethylhydrazine	20.1[b]	18.3	23.7	15.1	13.3	12.8	17.5	14.8	11.1	10.8	10.8	21.4	18.2	15.4	15.4
1,2-Dimethylhydrazine	22.0[b]	15.0	21.5	15.6	14.0	13.5	16.2	17.1	13.5	13.2	13.2	22.8	19.7	16.9	16.9
trans-Azodiisopropane	8.6[b]	1.5	16.6	5.6	8.9	6.7	4.7	4.5	−4.1	−4.5	−4.5	5.8	−1.3	−7.8	−7.7
Hydrogen azide	70.3[c]	73.1	75.9	75.3	74.1	73.3	71.2	72.6	72.2	71.8	71.8	69.2	69.0	67.9	67.9
Oxygen Triplet	0.0[a]	−15.3	−27.0	−4.2	−16.8	−8.5	−7.1	2.0	2.0	1.9	1.9	−2.6	−2.6	−2.8	−2.8
Ozone	34.0[c]	48.5	37.8	51.1	43.5	34.5	48.4	37.9	37.7	37.5	37.5	48.7	48.7	48.1	48.1
Water	−57.8[b]	−60.9	−59.2	−53.4	−54.3	−57.8	−56.7	−56.5	−56.6	−56.7	−56.7	−58.5	−58.5	−58.8	−58.8
Methanol	−48.2[b]	−57.4	−57.0	−51.9	−48.3	−48.9	−51.0	−49.3	−50.2	−50.3	−50.3	−49.8	−50.4	−51.4	−51.4
Ethanol	−56.2[b]	−63.0	−62.7	−56.9	−54.9	−55.9	−59.5	−56.9	−59.0	−59.1	−59.1	−57.2	−58.8	−60.8	−60.8
Propanol	−61.0[b]	−67.7	−69.5	−62.2	−60.1	−61.1	−64.9	−61.9	−65.6	−65.6	−65.6	−62.2	−65.1	−67.9	−67.9
Isopropanol	−65.2[b]	−65.1	−69.5	−65.8	−67.2	−67.2	−63.8	−66.7	−70.6	−70.5	−70.5	−67.2	−70.3	−73.1	−73.1
tert-Butanol	−74.7[b]	−64.3	−71.6	−71.3	−75.1	−74.8	−68.2	−76.8	−82.9	−82.5	−82.4	−75.9	−80.9	−84.5	−84.5
Dimethylether	−44.0[b]	−51.2	−53.2	−48.3	−45.8	−45.0	−43.8	−45.6	−47.7	−47.7	−47.7	−42.8	−44.5	−46.2	−46.2
Diethylether	−60.3[b]	−62.0	−64.4	−57.4	−58.5	−58.9	−61.4	−61.1	−65.9	−65.9	−65.9	−58.4	−62.2	−65.7	−65.7
Oxirane	−12.6[b]	−15.5	−9.0	−8.1	−10.1	−11.3	−15.7	−13.3	−14.6	−14.8	−14.8	−8.8	−9.7	−11.2	−11.2
Furan	−8.3[b]	−8.6	3.0	−4.0	−8.3	−5.7	−1.8	−2.9	−5.2	−5.9	−5.9	−2.7	−3.8	−7.4	−7.4
Phenol	−23.0[b]	−26.7	−22.2	−21.7	−21.2	−22.2	−23.1	−21.7	−26.5	−27.2	−27.2	−23.6	−26.2	−32.3	−32.3
Anisole plan	−16.2[b]	−17.7	−15.8	−14.6	−16.9	−17.2	−14.0	−16.0	−22.4	−23.0	−23.0	−14.1	−18.1	−25.0	−25.0
Hydrogen peroxide	−32.5[e]	−38.2	−35.3	−40.8	−24.0	−30.2	−36.4	−35.3	−35.6	−35.8	−35.8	−36.9	−37.0	−37.6	−37.6
Dimethylperoxide	−30.0[b]	−28.3	−25.7	−34.1	−22.9	−27.7	−27.5	−33.6	−35.7	−36.0	−36.0	−29.0	−30.7	−32.7	−32.7
Diethylperoxide	−46.1[b]	−39.1	−38.4	−40.0	−36.5	−41.6	−46.8	−52.6	−57.8	−57.8	−57.8	−46.0	−50.0	−53.8	−53.8
Diethylperoxide	−46.1[b]	−38.9	−36.7	−40.0	−35.7	−41.1	−45.7	−49.5	−54.3	−54.4	−54.4	−44.6	−48.3	−52.2	−52.2
Carbon monoxide	−26.4[b]	−5.9	−5.7	−19.7	−13.7	−18.3	−30.5	−20.3	−20.4	−20.5	−20.5	−21.5	−21.5	−21.8	−21.8
Carbon dioxide	−94.1[b]	−75.1	−79.8	−85.0	−84.8	−84.5	−90.1	−80.5	−80.7	−80.9	−80.9	−87.7	−87.7	−88.4	−88.4
Carbon suboxide	−22.0[c]	−23.5	−14.6	−24.0	−42.9	−41.0	−15.4	−3.2	−4.0	−4.4	−4.4	−16.9	−17.2	−18.9	−18.9
Formaldehyde	−26.0[b]	−32.9	−31.5	−34.1	−20.7	−25.5	−34.3	−30.3	−30.7	−30.9	−30.9	−31.9	−32.1	−32.8	−32.8
Acetaldehyde free	−39.7[b]	−42.3	−41.6	−44.2	−38.2	−41.1	−45.2	−44.2	−45.5	−45.8	−45.8	−46.5	−47.3	−49.1	−49.1
Propionaldehyde ecl	−44.4[b]	−47.5	−47.7	−48.6	−41.2	−44.8	−50.5	−48.2	−51.2	−51.3	−51.3	−50.5	−52.6	−55.3	−55.3
Acetone ecl	−51.9[b]	−49.4	−49.2	−53.3	−54.4	−55.5	−52.4	−57.4	−60.1	−60.4	−60.4	−59.3	−61.2	−63.9	−63.9
Ketene	−11.4[b]	−6.8	−5.7	−9.2	−18.5	−18.8	−9.9	−5.1	−5.7	−6.1	−6.1	−11.0	−11.3	−12.6	−12.6
Acrolein free	−18.0[c]	−17.9	−16.5	−18.3	−11.8	−15.0	−20.1	−18.1	−19.9	−20.3	−20.3	−19.1	−20.2	−22.7	−22.7
Glyoxal free	−50.7[b]	−62.5	−58.7	−64.4	−45.9	−52.7	−64.0	−59.1	−60.3	−60.6	−60.6	−62.6	−63.2	−65.0	−65.0
Biacetyl	−78.2[b]	−78.8	−74.9	−83.4	−79.0	−82.9	−82.6	−89.2	−93.1	−93.5	−93.4	−91.6	−94.3	−98.2	−98.2
Biacetyl	−78.2[b]	−75.6	−74.1	−81.4	−77.8	−82.1	−81.6	−88.8	−92.7	−93.0	−93.0	−90.7	−93.4	−97.3	−97.3
Acetylacetone	−91.0[b]	−84.3	−85.6	−91.6	−94.8	−96.0	−91.0	−99.2	−105.0	−105.2	−105.2	−101.8	−106.2	−111.0	−111.0
p-Quinone	−29.4[b]	−32.9	−25.1	−31.5	−27.7	−28.4	−26.1	−32.5	−37.2	−37.9	−37.9	−32.9	−35.3	−41.3	−41.3
Benzaldehyde	−8.8[b]	−9.9	−8.9	−10.6	−3.0	−6.1	−14.0	−14.5	−20.1	−20.9	−20.9	−15.6	−18.7	−25.6	−25.6
Formic acid (Z)	−90.5[b]	−92.6	−97.4	−94.4	−87.9	−89.5	−91.7	−86.9	−87.5	−87.8	−87.8	−88.2	−88.6	−89.7	−89.7
Acetic acid stag (Z)	−103.4[b]	−101.1	−103.0	−102.0	−101.1	−102.2	−101.3	−100.9	−102.7	−103.0	−103.0	−102.7	−103.8	−105.9	−105.9
Propionic acid C-ecl	−108.4[b]	−105.6	−109.0	−106.3	−105.2	−106.7	−107.0	−106.3	−109.7	−109.8	−109.8	−107.5	−109.8	−112.9	−112.9
Oxalic acid 4-ring	−173.0[b]	−175.1	−172.4	−174.0	−159.6	−164.5	−169.5	−165.0	−166.9	−167.3	−167.3	−166.4	−167.5	−170.2	−170.2
Benzoic acid	−70.3[b]	−67.7	−68.0	−66.2	−64.7	−66.1	−69.0	−71.1	−77.2	−78.0	−78.0	−71.0	−74.5	−81.8	−81.8
Methyl formiate (Z)	−85.0[b]	−85.5	−91.0	−87.0	−84.4	−84.0	−83.5	−81.4	−83.3	−83.5	−83.5	−79.4	−80.6	−82.6	−82.6
Methyl acetate ecl (Z)	−98.5[b]	−93.7	−96.4	−94.1	−97.3	−96.7	−93.1	−95.6	−98.6	−98.8	−98.8	−93.8	−96.0	−99.0	−99.0

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

Table S1: ... *continued from previous page* ...

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Acetic anhydride ecl	−136.8[b]	−132.6	−131.7	−135.0	−138.8	−140.3	−136.7	−139.5	−143.4	−143.9	−143.9	−138.8	−141.4	−145.7	−145.7
Maleic anhydride	−95.2[b]	−88.5	−76.4	−90.1	−84.4	−82.4	−85.6	−87.1	−89.8	−90.4	−90.4	−87.2	−88.4	−92.5	−92.5
Formamide	−44.0[c]	−40.2	−44.8	−41.8	−40.6	−44.1	−41.2	−39.8	−40.7	−41.1	−41.1	−46.3	−46.9	−48.4	−48.4
Dimethylformamide	−45.8[b]	−37.4	−36.9	−44.6	−40.9	−43.9	−43.2	−43.5	−47.3	−47.6	−47.6	−41.4	−44.5	−47.8	−47.7
Nitrous oxide	19.6[e]	31.0	28.5	25.4	27.9	28.0	19.7	21.2	21.0	20.8	20.8	20.7	20.7	19.9	19.9
Dinitrotetroxide free	2.2[b]	29.9	24.9	8.3	10.5	7.0	8.6	13.2	12.0	11.5	11.5	9.5	8.7	6.7	6.7
Nitrous acid trans	−18.3[e]	−40.7	−39.4	−14.9	−18.4	−23.6	−30.3	−19.7	−20.0	−20.3	−20.3	−26.8	−26.9	−27.8	−27.8
Nitric acid	−32.1[e]	−17.5	−37.5	−38.0	−37.1	−34.3	−28.2	−33.6	−34.3	−34.6	−34.6	−33.4	−33.7	−35.1	−35.1
Methylnitrite	−15.9[b]	−36.7	−31.8	−9.1	−16.5	−19.2	−24.4	−16.8	−18.0	−18.4	−18.4	−20.0	−20.9	−22.6	−22.6
Nitromethane	−17.8[b]	3.3	−9.9	−15.9	−16.3	−17.2	−6.9	−17.3	−18.8	−19.1	−19.1	−15.7	−16.7	−18.5	−18.5

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 S2: Benchmark Results for the CHNO Data Set. Ionization Potentials (eV)

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Hydrogen	15.98[a]	15.75	14.92	16.11	15.04	15.03	15.96	15.68	15.68	15.68	15.68	15.65	15.65	15.65	15.65
Methane	14.00[a]	13.87	13.31	13.64	13.68	13.73	14.28	13.64	13.64	13.64	13.64	14.17	14.16	14.17	14.17
Ethane	12.10[b]	12.70	11.77	11.98	11.92	11.97	12.44	11.92	11.92	11.92	11.92	12.30	12.30	12.30	12.30
Ethylene	10.51[a]	10.17	10.55	10.64	10.68	10.75	10.79	10.74	10.74	10.74	10.74	11.05	11.05	11.05	11.05
Acetylene	11.40[a]	11.01	11.50	11.61	11.59	11.62	11.49	11.55	11.55	11.55	11.55	11.79	11.79	11.79	11.79
Propane	11.50[a]	12.34	11.32	11.51	11.34	11.39	11.84	11.39	11.40	11.39	11.39	11.69	11.70	11.69	11.69
Propene ecl	9.88[b]	9.96	9.99	10.10	10.04	10.12	10.08	9.99	9.99	9.99	9.99	10.28	10.29	10.29	10.29
Propyne	10.37[a]	10.72	10.74	10.89	10.73	10.76	10.66	10.64	10.64	10.64	10.64	10.88	10.88	10.88	10.88
Allene	10.07[c]	10.02	10.14	10.18	10.37	10.40	10.19	10.16	10.16	10.16	10.16	10.44	10.44	10.45	10.45
Isobutane	11.40[a]	12.12	11.29	11.59	11.21	11.28	11.54	11.06	11.07	11.07	11.07	11.41	11.42	11.41	11.41
1,3-s-tr-Butadiene	9.08[a]	9.14	9.33	9.47	9.58	9.61	9.29	9.32	9.32	9.32	9.32	9.61	9.61	9.61	9.61
Diacetylene	10.17[a]	9.99	10.37	10.47	10.58	10.53	10.06	10.30	10.30	10.30	10.30	10.47	10.46	10.47	10.47
Butatriene	9.15[d]	9.01	9.34	9.34	9.62	9.65	9.19	9.35	9.35	9.35	9.35	9.60	9.60	9.60	9.60
Neopentane	11.30[a]	12.12	11.53	12.06	11.34	11.38	11.30	10.82	10.82	10.82	10.82	11.31	11.31	11.31	11.31
Cyclopropane	11.00[b]	11.43	11.48	11.78	11.42	11.59	11.61	10.88	10.88	10.88	10.88	11.47	11.46	11.47	11.47
Cyclopropene	9.86[a]	9.88	9.82	9.88	10.08	10.16	9.97	9.84	9.84	9.84	9.84	10.13	10.13	10.13	10.13
Cyclobutane	11.00[c]	11.81	10.99	11.02	11.02	11.07	11.06	10.38	10.37	10.38	10.38	10.98	10.97	10.98	10.98
Cyclobutene plan	9.43[a]	9.77	9.72	9.82	9.81	9.93	9.78	9.65	9.65	9.64	9.64	9.93	9.93	9.93	9.93
Cyclopentene	9.18[a]	9.72	9.44	9.52	9.43	9.50	9.41	9.22	9.22	9.22	9.22	9.51	9.51	9.51	9.51
Cyclopentadiene	8.57[a]	9.04	9.08	9.23	9.20	9.31	8.92	8.82	8.82	8.82	8.82	9.10	9.10	9.10	9.10
Benzene	9.24[a]	9.39	9.65	9.75	9.64	9.82	9.66	9.59	9.59	9.59	9.59	9.91	9.91	9.91	9.91
Toluene ecl	8.82[b]	9.28	9.33	9.44	9.24	9.43	9.26	9.17	9.16	9.17	9.17	9.46	9.46	9.46	9.46
Naphthalene	8.15[a]	8.57	8.71	8.84	8.88	8.95	8.48	8.51	8.51	8.51	8.51	8.79	8.79	8.79	8.79
Nitrogen	15.60[b]	14.87	14.32	13.80	12.86	13.66	15.19	15.46	15.46	15.46	15.46	14.51	14.51	14.51	14.51
Ammonia	10.85[b]	11.19	10.42	9.70	10.10	10.15	11.08	10.67	10.67	10.67	10.67	11.23	11.23	11.23	11.23
Methylamine	9.45[c]	10.56	9.76	9.40	9.41	9.48	10.14	9.75	9.75	9.75	9.75	10.00	10.01	10.01	10.01
Dimethylamine	8.93[c]	10.04	9.39	9.22	8.96	9.07	9.45	9.23	9.24	9.23	9.23	9.24	9.26	9.25	9.25
Trimethylamine	8.54[c]	9.59	9.12	9.07	8.65	8.83	8.90	8.84	8.86	8.85	8.85	8.67	8.70	8.69	8.69
Aziridine	9.80[b]	10.68	10.31	9.92	9.97	10.16	10.39	10.13	10.13	10.13	10.13	10.39	10.39	10.39	10.39
Pyrrole	8.21[d]	8.56	8.66	8.93	8.90	9.02	8.40	8.46	8.46	8.47	8.47	8.65	8.65	8.65	8.65
Pyridine	9.67[e]	9.69	9.93	10.10	10.10	10.24	9.99	9.96	9.96	9.96	9.96	10.13	10.13	10.13	10.13
Hydrogen cyanide	13.60[b]	13.41	13.68	12.60	13.13	13.80	13.56	13.91	13.91	13.91	13.91	13.94	13.94	13.94	13.94
Acetonitrile	12.21[d]	12.79	12.46	12.33	12.77	12.77	12.45	12.50	12.50	12.50	12.50	12.63	12.63	12.63	12.63
Acrylonitrile	10.91[d]	10.61	10.86	10.89	11.25	11.28	10.85	10.88	10.88	10.88	10.88	11.09	11.09	11.09	11.09
Cyanoacetylene	11.60[c]	11.35	11.65	11.58	11.99	11.95	11.37	11.58	11.58	11.58	11.58	11.67	11.67	11.67	11.67
Cyanogen	13.36[d]	13.20	13.31	12.87	13.58	13.79	12.94	13.27	13.27	13.27	13.27	13.22	13.22	13.22	13.22
Ozone	12.75[c]	12.70	13.10	12.69	11.53	12.64	12.13	12.85	12.85	12.85	12.85	13.27	13.27	13.27	13.27
Water	12.62[b]	12.19	12.46	12.32	11.91	12.12	12.29	12.91	12.91	12.91	12.91	13.12	13.12	13.12	13.12
Methanol	10.96[a]	11.42	11.13	11.14	10.53	10.73	11.22	11.22	11.22	11.22	11.22	11.60	11.60	11.60	11.60
Dimethylether	10.04[a]	11.04	10.61	10.69	9.76	9.95	10.67	10.51	10.52	10.51	10.51	10.94	10.94	10.94	10.94
Oxirane	10.57[a]	11.49	11.33	11.34	10.27	10.55	11.40	11.31	11.31	11.31	11.31	11.79	11.79	11.79	11.79
Furan	8.88[a]	9.14	9.32	9.38	9.54	9.55	9.12	9.03	9.03	9.03	9.03	9.45	9.45	9.45	9.45
Carbon monoxide	14.01[a]	13.43	13.31	13.03	12.02	12.33	13.32	13.60	13.60	13.60	13.60	13.68	13.68	13.68	13.68

... continued on next page ...

Table S2: ... *continued from previous page* ...

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Carbon dioxide	13.78[a]	12.79	13.21	12.73	12.99	12.76	12.67	13.27	13.27	13.27	13.27	13.57	13.57	13.57	13.57
Formaldehyde	10.88[b]	11.04	10.78	10.63	10.20	10.35	10.85	11.03	11.03	11.03	11.03	11.26	11.26	11.26	11.26
Acetaldehyde free	10.21[a]	10.88	10.72	10.71	10.24	10.30	10.51	10.62	10.62	10.62	10.62	10.94	10.94	10.94	10.94
Acetone ecl	9.72[a]	10.76	10.67	10.77	10.26	10.24	10.18	10.31	10.31	10.31	10.31	10.67	10.67	10.67	10.67
Ketene	9.64[a]	9.29	9.60	9.46	9.86	9.89	9.39	9.75	9.74	9.75	9.75	9.97	9.97	9.97	9.97
Acrolein free	10.11[b]	10.69	10.69	10.69	10.22	10.30	10.46	10.59	10.59	10.59	10.59	10.87	10.87	10.87	10.87
trans-Glyoxal	10.59[a]	10.75	10.66	10.57	10.09	10.26	10.22	10.57	10.57	10.57	10.57	10.77	10.77	10.77	10.77
Formic acid (Z)	11.51[a]	11.74	11.82	11.56	11.58	11.53	11.52	11.72	11.72	11.72	11.72	12.12	12.12	12.12	12.12
Methyl formiate (Z)	11.02[a]	11.61	11.57	11.35	11.19	11.13	11.27	11.24	11.24	11.24	11.24	11.70	11.70	11.70	11.70

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 S3: Benchmark Results for the CHNO Data Set. Relative Energies (kcal/mol)

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Isobutane	−2.1[a]	2.9	1.8	−0.5	−1.5	−0.7	2.0	−1.7	−2.0	−1.9	−1.9	−1.0	−1.4	−1.3	−1.3
trans-2-Butene	−2.7[a]	−4.8	−3.5	−5.2	−4.6	−4.6	−2.5	−3.9	−3.6	−3.7	−3.7	−4.3	−4.0	−4.1	−4.1
cis-2-Butene	−1.7[a]	−3.6	−2.4	−5.0	−3.7	−3.4	−0.5	−2.0	−2.0	−2.0	−2.0	−2.5	−2.5	−2.6	−2.6
cis-2-Butene	1.0[a]	1.2	1.1	0.2	0.9	1.2	2.0	1.8	1.6	1.7	1.7	1.8	1.5	1.5	1.5
Isobutene	−4.0[a]	−1.8	−1.3	−4.8	−6.2	−5.2	0.3	−4.4	−4.5	−4.5	−4.5	−4.2	−4.4	−4.4	−4.4
2-Butyne	−4.7[a]	−11.2	−5.5	−5.9	−6.0	−6.3	−3.3	−4.4	−3.8	−4.0	−4.1	−5.4	−4.9	−4.9	−4.9
2-Methylbutane	−1.6[a]	4.4	2.6	0.1	−0.7	−0.2	2.9	−1.2	−1.9	−1.6	−1.6	−0.3	−1.1	−0.9	−0.9
Neopentane	−5.1[a]	9.8	5.2	−1.4	−4.0	−2.2	6.2	−4.9	−6.0	−5.7	−5.6	−2.5	−3.8	−3.5	−3.5
cis-1,3-Pentadiene	1.3[a]	1.2	1.1	0.4	0.9	1.1	2.0	1.9	1.7	1.7	1.7	1.9	1.6	1.6	1.6
Isopropylamine	−3.2[a]	1.8	4.6	0.5	0.2	1.0	0.4	−1.0	−1.2	−1.1	−1.1	−0.6	−0.8	−0.7	−0.7
Methylisocyanide	21.1[a]	41.1	31.1	31.4	25.0	20.7	11.3	20.8	20.8	20.7	20.7	11.4	11.3	11.2	11.2
cis-Diimine	5.2[b]	1.8	0.9	5.1	3.8	3.2	0.5	−4.6	−4.6	−4.6	−4.6	0.7	0.5	0.6	0.6
Oxygen Singlet	22.5[c]	18.3	18.5	15.0	39.0	22.8	19.4	18.3	18.3	18.3	18.3	19.0	19.0	19.0	19.0
Isopropanol	−4.2[a]	2.6	−0.0	−3.6	−7.1	−6.1	1.1	−4.7	−5.0	−4.9	−4.9	−5.0	−5.2	−5.3	−5.3
Acetylacetone Enol	−4.0[d]	0.3	0.7	2.9	−2.3	−1.7	5.9	5.2	5.9	5.5	5.5	4.6	5.7	5.0	5.0
Acetylacetone Enol TS	6.9[e]	35.4	21.4	27.3	−1.0	0.9	11.6	5.8	6.4	6.1	6.1	4.6	5.7	5.0	5.0
Nitromethane	−1.9[a]	40.0	21.9	−6.8	0.2	2.0	17.5	−0.6	−0.8	−0.7	−0.7	4.3	4.2	4.1	4.1

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). d N.S.Hush, M.K.Livett, J.B.Peel, and G.D.Willett, Austr.J.Chem. 40, 599 (1987). e M.A.Rios and J.Rodriguez, J.Mol.Struct.: THEOCHEM 204, 137 (1990).

Table S4: Benchmark Results for the CHNO Data Set. Barriers (kcal/mol)

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Ethane ecl	2.9[a]	1.0	1.2	1.4	1.0	1.0	1.8	2.8	2.8	2.8	2.8	2.4	2.4	2.5	2.5
Ethylene ort	65.0[b]	29.7	36.8	36.1	34.2	37.5	57.4	57.4	57.4	57.4	57.4	55.9	55.9	56.0	56.0
Propene stag	2.0[b]	0.2	0.6	0.7	0.3	0.3	0.2	0.8	0.8	0.8	0.8	0.7	0.7	0.7	0.7
n-Butane cis-Barrier	6.0[c]	3.2	3.3	4.0	3.5	3.8	4.2	5.1	4.8	4.9	4.9	5.0	4.6	4.7	4.7
But-1-ene C-ecl	0.4[c]	1.3	0.7	0.9	1.0	1.1	1.1	1.4	1.1	1.2	1.2	1.2	1.0	1.0	1.0
1,3-s-cis-Butadiene	3.8[b]	0.5	0.8	0.7	0.9	1.0	0.7	1.1	0.9	1.0	1.0	1.0	0.8	0.8	0.8
1,3-gauche-Butadiene (FREE)	2.9[b]	0.3	0.8	0.7	0.6	0.6	0.6	0.9	0.7	0.8	0.8	0.8	0.7	0.6	0.6
1,3-Butadiene ort	6.0[b]	0.3	2.0	1.5	0.8	0.8	0.6	0.9	0.7	0.8	0.8	0.8	0.7	0.6	0.7
Cyclobutane plan	1.4[a]	0.0	0.0	0.0	−0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Cyclopentane planar	4.8[c]	0.0	0.1	0.5	0.4	0.8	0.7	2.6	2.8	2.7	2.7	1.9	2.1	2.0	2.0
Cyclopentene plan	0.7[e]	0.0	0.0	0.0	−0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.0	0.0	0.0	0.0
Cyclohexane twist (AMP)	4.8[c]	2.4	3.2	4.1	3.2	3.4	3.7	5.2	5.3	5.2	5.2	5.0	5.0	5.0	5.0
Cyclohexene plan	13.4[f]	2.5	5.5	6.1	5.6	7.0	7.1	11.9	12.3	12.1	12.1	9.8	10.1	10.2	10.2
Cyclohexadiene plan	3.2[g]	0.0	0.2	0.3	0.4	0.8	0.4	2.0	2.1	2.1	2.1	1.3	1.4	1.4	1.4
Toluene stag	0.1[c]	0.0	−0.0	−0.0	0.0	0.0	0.0	−0.0	−0.0	−0.0	−0.0	0.0	−0.0	0.0	0.0
Styrene plan	0.0[b]	1.4	0.0	0.0	0.3	0.5	0.4	0.2	0.2	0.2	0.2	0.1	0.1	0.1	0.1
Styrene ort	3.1[b]	−1.4	1.4	1.3	0.0	−0.1	0.3	0.8	1.1	0.9	0.9	0.7	1.0	0.9	0.9
Ammonia planar	5.8[h]	11.6	4.2	10.0	5.9	3.8	13.0	3.5	3.4	3.5	3.5	6.7	6.7	6.7	6.7
Methylamine ecl (TS rot)	2.0[i]	1.1	1.3	1.2	0.9	1.0	1.6	2.2	2.2	2.2	2.2	2.3	2.3	2.3	2.3
Methylamine planar (TS inv)	4.8[h]	7.6	4.2	9.1	7.2	5.3	7.7	3.6	3.6	3.6	3.6	4.2	4.2	4.2	4.2
Dimethylamine planar	4.4[h]	4.0	4.1	8.4	8.5	7.5	4.2	3.5	3.6	3.5	3.5	2.8	2.8	2.8	2.8
Trimethylamine planar (C3h inv)	6.0[h]	1.7	4.6	8.4	11.7	11.5	2.2	4.2	4.5	4.3	4.3	2.6	2.8	2.7	2.7
Trimethylamine (C3 inv)	6.0[h]	1.7	4.6	8.4	11.7	11.5	2.2	4.2	4.5	4.3	4.3	0.0	2.8	2.7	2.7
Aziridine planar (inv)	11.6[h]	19.6	15.7	19.5	20.3	18.8	15.9	13.4	13.4	13.4	13.4	11.5	11.5	11.5	11.5
Aniline planar	1.5[b]	4.2	1.0	4.5	0.8	0.2	3.5	0.5	0.5	0.6	0.6	0.6	0.6	0.7	0.7
Hydrazine trans	2.5[j]	0.0	0.0	0.0	−0.0	−0.0	−0.9	8.0	8.1	8.0	8.0	1.8	1.8	1.8	1.8
Hydrazine cis	8.3[j]	7.9	8.2	8.0	11.2	11.4	5.9	10.8	10.8	10.8	10.8	8.7	8.6	8.7	8.7
Methanol ecl	1.1[i]	0.7	1.0	0.9	0.7	0.7	1.3	1.8	1.8	1.8	1.8	1.6	1.6	1.6	1.6
Phenol plan	0.0[k]	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Phenol ort	3.5[b]	1.9	2.4	2.4	3.8	3.2	1.9	1.4	1.5	1.4	1.4	2.0	2.0	2.0	2.0
Anisole ort	3.0[l]	−0.5	1.6	1.1	3.1	2.5	0.5	0.1	0.2	0.1	0.1	0.5	0.5	0.5	0.5
Hydrogen peroxide cis	7.0[i]	6.9	7.0	7.3	8.3	7.5	9.4	8.5	8.5	8.5	8.5	10.5	10.4	10.5	10.5
Hydrogen peroxide trans	1.1[i]	−0.0	0.1	−0.0	0.0	−0.0	2.1	2.5	2.5	2.5	2.5	1.1	1.1	1.1	1.1
Diethylperoxide	0.0[i]	0.2	1.7	0.0	0.8	0.5	1.1	3.2	3.5	3.4	3.4	1.4	1.7	1.6	1.6
Acetaldehyde ecl	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Acetaldehyde stag	1.1[c]	0.2	0.4	0.6	0.2	0.2	0.0	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3
Propionaldehyde stag	1.5[c]	0.2	−0.6	−0.6	−1.3	−1.1	−0.2	−0.8	−0.8	−0.8	−0.8	−0.7	−0.7	−0.6	−0.6
Acrolein s-trans	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Acrolein s-cis	1.7[b]	−0.4	0.2	0.4	0.2	−0.0	−0.7	0.0	−0.0	−0.0	−0.0	−0.2	−0.1	−0.2	−0.2
Acrolein ort (TS rot)	4.7[m]	0.2	1.8	1.1	1.0	0.8	1.4	2.6	2.7	2.6	2.6	2.0	2.1	2.0	2.0
trans-Glyoxal	0.0[k]	1.1	0.0	0.1	0.0	0.1	1.0	0.0	0.0	0.0	0.0	0.8	0.7	0.8	0.8
cis-Glyoxal	4.8[n]	0.5	2.5	2.1	4.4	3.6	1.6	3.8	3.8	3.8	3.8	2.9	2.9	2.9	2.9

... continued on next page ...

Table S4: ... *continued from previous page* ...

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Glyoxal ort (TS)	5.9[n]	−1.1	0.0	−0.1	−0.0	−0.1	−1.0	0.0	0.0	0.0	0.0	−0.8	−0.7	−0.8	−0.8
Biacetyl	0.0[i]	3.2	0.8	2.0	1.2	0.8	1.0	0.5	0.4	0.5	0.5	0.9	0.9	0.9	0.9
Benzaldehyde ort	4.6[b]	−0.4	2.7	1.6	2.2	1.9	2.3	3.6	3.8	3.7	3.7	3.3	3.4	3.3	3.3
Formic acid (E)	3.9[o]	3.7	7.4	4.3	8.4	8.7	4.1	6.1	6.1	6.1	6.1	6.2	6.1	6.2	6.2
Formic acid ort (TS)	12.4[o]	7.7	11.9	8.9	12.9	11.4	9.4	10.5	10.5	10.5	10.5	11.3	11.3	11.3	11.3
Acetic acid stag (E)	5.8[p]	4.5	5.8	2.6	5.8	6.8	6.2	5.6	5.5	5.6	5.6	5.8	5.7	5.7	5.7
Acetic acid stag ort (TS)	12.6[o]	7.7	10.5	7.4	10.6	9.9	10.8	10.1	10.1	10.1	10.1	10.9	10.8	10.8	10.8
Benzoic acid plan	0.0[k]	1.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Benzoic acid ort	5.0[q]	−1.9	2.8	0.7	2.2	2.1	2.7	4.0	4.1	4.0	4.1	3.5	3.6	3.6	3.6
Methyl formiate (E)	4.8[o]	2.9	5.6	1.9	7.0	7.5	2.9	4.0	4.1	4.1	4.1	4.1	4.1	4.2	4.2
Methyl formiate (Z) ECL	1.2[o]	1.0	0.6	1.0	−0.0	0.4	0.8	−0.0	0.1	0.0	0.0	0.1	0.3	0.2	0.2
Methyl acetate ecl (E)	8.5[o]	5.2	5.3	1.2	6.0	7.3	6.6	5.1	4.7	4.8	4.8	5.9	5.4	5.6	5.6
Formamide plan	0.0[r]	0.8	0.0	1.3	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Formamide rot	16.0[s]	4.5	10.1	4.8	10.5	10.3	8.3	13.7	13.7	13.7	13.7	14.9	14.9	14.9	14.9
Formamide rot LP cis	18.7[t]	7.0	15.1	8.1	17.1	17.0	10.2	16.7	16.7	16.7	16.7	17.8	17.8	17.8	17.8
Dinitrotetroxide plan	0.0[u]	2.1	0.0	2.9	−0.0	0.2	0.5	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Dinitrotetroxide ort	2.9[u]	−2.1	0.2	−2.9	0.0	−0.1	−0.5	−0.1	−0.1	−0.1	−0.1	−0.1	−0.1	−0.1	−0.1

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 S5: Benchmark Results for the FLUOR Data Set. Heats of Formation (kcal/mol)

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Fluorine	0.0[a]	7.3	−22.5	−21.7	0.3	−15.9	12.3	0.6	0.6	0.5	0.5	−1.7	−1.7	−1.8	−1.8
Hydrogen fluoride	−65.1[a]	−59.7	−74.3	−62.7	−63.6	−61.9	−69.7	−63.3	−63.3	−63.4	−63.4	−64.9	−64.9	−65.0	−65.0
Methylfluoride	−56.0[a]	−60.9	−61.0	−53.8	−53.6	−49.4	−54.8	−60.4	−61.0	−61.1	−61.1	−57.3	−57.7	−58.5	−58.5
Difluoromethane	−108.1[b]	−111.8	−116.1	−103.8	−104.7	−97.8	−104.7	−110.9	−111.6	−111.6	−111.6	−106.6	−107.0	−107.8	−107.8
Trifluoromethane	−166.2[b]	−163.8	−172.5	−162.0	−162.7	−157.1	−160.6	−166.8	−167.6	−167.6	−167.6	−162.0	−162.4	−163.3	−163.3
Tetrafluoromethane	−223.1[b]	−214.2	−225.7	−225.1	−219.1	−215.9	−217.2	−220.5	−221.4	−221.4	−221.4	−215.8	−216.2	−217.3	−217.3
Fluoroethane	−63.0[c]	−65.1	−66.3	−60.2	−61.9	−59.3	−65.6	−67.5	−69.4	−69.4	−69.4	−65.8	−67.2	−68.8	−68.8
1,1-Difluoroethane	−118.8[b]	−113.4	−118.6	−111.9	−117.1	−113.3	−119.0	−121.8	−123.8	−123.6	−123.6	−119.4	−120.8	−122.4	−122.4
1,1,1-Trifluoroethane	−178.0[b]	−164.4	−172.6	−172.3	−176.6	−174.8	−176.9	−178.4	−180.6	−180.4	−180.4	−176.3	−177.7	−179.4	−179.4
Hexafluoroethane	−321.3[b]	−299.6	−313.2	−317.8	−314.4	−311.9	−316.2	−317.5	−320.4	−319.7	−319.7	−310.5	−312.4	−314.0	−314.0
i-Propylfluoride	−70.1[b]	−66.6	−69.8	−66.8	−71.3	−69.7	−74.5	−76.2	−79.6	−79.4	−79.4	−75.1	−77.8	−80.2	−80.2
Octafluorocyclobutane	−368.7[b]	−363.7	−367.2	−379.2	−380.3	−375.3	−379.9	−379.9	−386.5	−384.6	−384.6	−372.9	−377.6	−380.1	−380.1
Fluoroethene	−33.2[b]	−34.5	−34.0	−28.6	−33.3	−32.3	−33.1	−32.3	−33.3	−33.5	−33.5	−32.2	−32.7	−34.1	−34.1
1,2-Difluoroethene cis	−71.0[c]	−83.6	−82.7	−73.0	−76.6	−73.6	−73.0	−72.2	−73.4	−73.5	−73.5	−71.7	−72.3	−73.7	−73.7
1,2-Difluoroethene trans	−70.0[c]	−83.1	−82.7	−71.5	−77.5	−73.7	−74.7	−74.3	−75.5	−75.6	−75.6	−72.7	−73.4	−74.8	−74.8
1,1-Difluoroethene	−80.1[b]	−84.1	−84.3	−79.6	−85.1	−84.4	−80.3	−78.4	−79.5	−79.6	−79.6	−79.9	−80.5	−81.9	−81.9
Trifluoroethene	−117.2[b]	−131.1	−130.6	−121.5	−125.0	−122.0	−117.6	−116.4	−117.7	−117.7	−117.7	−115.9	−116.6	−118.0	−118.0
Tetrafluoroethene	−157.5[b]	−175.7	−175.1	−168.2	−169.1	−166.5	−157.6	−156.3	−157.7	−157.7	−157.7	−155.9	−156.7	−158.2	−158.2
Fluorobenzene	−27.7[b]	−25.2	−23.3	−20.2	−24.3	−24.6	−28.8	−27.3	−31.8	−32.3	−32.3	−28.0	−30.3	−35.9	−35.9
1,2-Difluorobenzene	−70.2[b]	−70.6	−66.4	−63.1	−68.3	−68.5	−70.5	−69.1	−73.8	−74.2	−74.1	−69.9	−72.4	−78.0	−77.9
1,3-Difluorobenzene	−73.9[b]	−70.9	−67.9	−63.3	−72.5	−71.5	−74.2	−72.9	−77.6	−78.0	−78.0	−74.0	−76.5	−82.0	−82.0
1,4-Difluorobenzene	−73.3[b]	−71.0	−68.0	−63.3	−71.3	−70.9	−73.9	−72.6	−77.2	−77.6	−77.6	−73.5	−76.0	−81.5	−81.5
Pentafluorobenzene	−192.8[b]	−201.7	−192.0	−188.6	−197.9	−196.9	−192.6	−191.8	−197.3	−197.1	−197.1	−192.7	−195.8	−201.0	−201.0
Hexafluorobenzene	−228.3[b]	−243.4	−231.2	−229.3	−237.1	−236.2	−229.0	−228.4	−234.2	−233.7	−233.7	−228.8	−232.1	−237.2	−237.2
Fluoroacetylene	25.1[d]	15.7	15.2	18.1	21.4	23.5	26.7	26.9	26.4	26.2	26.2	23.9	23.8	22.9	22.9
Difluoroacetylene	1.4[d]	−21.0	−19.6	−11.6	−9.2	−5.7	4.0	4.4	3.9	3.8	3.8	−2.6	−2.8	−3.7	−3.7
Hypofluorous acid	−23.5[a]	−18.6	−22.6	−29.2	−17.3	−17.3	−15.8	−19.6	−19.7	−19.8	−19.8	−20.3	−20.4	−20.7	−20.7
Fluoroethanol gauche	−100.0[c]	−107.8	−111.5	−99.8	−99.4	−96.2	−101.0	−100.7	−103.2	−103.1	−103.1	−100.1	−101.9	−103.8	−103.8
1,1,1-Trifluoroethanol	−212.3[a]	−207.2	−214.1	−209.1	−206.8	−207.3	−212.4	−209.2	−211.9	−211.6	−211.6	−206.4	−208.3	−210.2	−210.2
Trifluoromethylhypofluorite	−182.8[a]	−163.3	−177.7	−187.3	−180.8	−177.4	−167.0	−174.0	−175.5	−175.3	−175.3	−166.3	−167.1	−168.4	−168.4
Difluorine monoxide	5.9[a]	18.2	10.5	−4.8	4.3	3.5	16.2	5.3	5.1	5.1	5.1	7.2	7.1	6.7	6.7
Formyl fluoride	−90.0[a]	−88.8	−92.9	−88.8	−84.4	−84.5	−87.3	−86.3	−86.8	−86.9	−86.9	−88.2	−88.4	−89.2	−89.2
Acetyl fluoride	−105.7[b]	−96.5	−98.8	−98.7	−100.7	−100.9	−99.8	−100.0	−101.5	−101.6	−101.6	−103.0	−104.0	−105.7	−105.7
Carbonyl fluoride	−145.9[e]	−138.6	−146.3	−141.6	−139.7	−138.8	−137.1	−136.5	−137.0	−137.1	−137.1	−138.7	−138.8	−139.7	−139.7
Trifluoroacetic acid trans	−246.5[b]	−238.1	−242.7	−244.0	−239.1	−241.3	−244.7	−242.3	−244.6	−244.6	−244.6	−239.7	−241.1	−243.3	−243.3
p-Fluorobenzoic acid	−118.2[b]	−111.8	−113.0	−109.5	−113.0	−113.5	−114.8	−116.9	−123.2	−123.9	−123.9	−117.4	−121.0	−128.3	−128.3
Trifluoroamine	−29.8[b]	−34.2	−40.0	−24.4	−29.2	−28.2	−36.1	−30.1	−30.6	−30.7	−30.7	−35.9	−36.1	−36.9	−36.9
(Z)-Difluorodiazene	16.4[a]	−2.3	20.8	28.0	26.9	23.2	4.5	13.5	13.0	12.8	12.8	11.7	11.4	10.5	10.5
(E)-Difluorodiazene	19.4[a]	2.4	31.3	29.2	35.7	33.6	6.0	22.7	22.3	22.0	22.0	22.4	22.2	21.3	21.3
Tetrafluorohydrazine gauche	−8.0[c]	−19.7	5.8	−0.5	−8.5	−8.3	−26.7	−6.3	−7.7	−7.7	−7.7	−6.4	−7.3	−8.6	−8.6
Fluorocyanide	8.6[a]	−2.3	−4.4	6.5	−0.3	−0.4	2.2	1.9	1.7	1.5	1.5	−1.5	−1.7	−2.2	−2.2
Trifluoroacetonitrile	−119.0[b]	−113.2	−119.5	−115.0	−120.9	−118.4	−126.7	−125.5	−126.9	−127.0	−127.0	−125.1	−125.7	−127.5	−127.5

... continued on next page ...

Table S5: ... *continued from previous page* ...

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Fluorocarbene	34.2[f]	21.5	20.9	35.3	27.3	25.3	26.1	24.9	24.7	24.6	24.6	24.4	24.4	23.9	23.9
Difluorocarbene	−43.8[g]	−65.2	−68.0	−49.1	−63.0	−69.6	−56.0	−57.8	−58.0	−58.1	−58.1	−55.7	−55.8	−56.3	−56.3
Nitrosyl fluoride	−15.7[a]	−24.8	−26.5	−3.3	−3.0	−7.8	−20.9	−10.4	−10.5	−10.7	−10.7	−21.6	−21.6	−22.2	−22.2
Nitryl fluoride	−26.0[a]	0.7	−21.3	−25.6	−28.5	−21.4	−22.6	−25.7	−26.1	−26.4	−26.4	−29.3	−29.4	−30.4	−30.4
Fluorine nitrate	2.5[b]	28.0	13.7	−6.1	−5.2	−1.3	12.4	2.6	1.8	1.5	1.5	4.3	3.9	2.5	2.5
Nitrosyl trifluoride	−39.0[a]	22.8	−14.6	−26.6	−42.2	−29.9	−36.3	−50.0	−50.8	−51.0	−51.0	−50.7	−50.9	−52.3	−52.3

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.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 S6: Benchmark Results for the FLUOR Data Set. Ionization Potentials (eV)

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Fluorine	15.83[a]	15.25	14.28	15.35	15.74	16.10	15.92	16.32	16.32	16.32	16.32	16.36	16.36	16.36	16.36
Hydrogen fluoride	16.03[a]	14.82	14.09	16.14	15.82	15.80	15.87	16.45	16.45	16.45	16.45	17.03	17.03	17.03	17.03
Methylfluoride	13.31[a]	13.05	12.10	12.92	13.27	13.17	13.40	13.07	13.07	13.07	13.07	13.41	13.40	13.41	13.41
Difluoromethane	13.17[a]	13.09	12.02	12.86	13.39	13.23	13.30	12.98	12.98	12.98	12.98	13.23	13.23	13.23	13.23
Trifluoromethane	14.67[a]	14.57	13.31	14.36	14.54	14.46	14.43	14.17	14.17	14.17	14.17	14.45	14.45	14.45	14.45
Tetrafluoromethane	16.23[a]	16.81	15.32	16.79	16.04	16.09	16.48	16.27	16.27	16.27	16.27	16.89	16.89	16.89	16.89
Fluoroethane	12.43[a]	12.61	11.58	12.07	12.16	12.11	12.46	12.01	12.02	12.01	12.01	12.28	12.29	12.28	12.28
1,1-Difluoroethane	12.80[a]	12.73	11.93	12.82	12.96	12.85	12.91	12.30	12.30	12.30	12.30	12.69	12.69	12.69	12.69
1,1,1-Trifluoroethane	13.80[a]	14.01	13.12	14.38	14.13	14.06	13.96	13.23	13.22	13.23	13.23	13.78	13.77	13.78	13.78
Hexafluoroethane	14.60[a]	14.50	13.23	14.48	14.37	14.26	14.24	13.67	13.66	13.67	13.67	13.92	13.90	13.91	13.91
Fluoroethene	10.58[a]	10.17	10.24	10.60	10.81	10.84	10.66	10.59	10.59	10.59	10.59	10.85	10.85	10.85	10.85
1,2-Difluoroethene cis	10.43[a]	10.18	9.99	10.54	10.79	10.80	10.46	10.38	10.38	10.38	10.38	10.56	10.56	10.56	10.56
1,2-Difluoroethene trans	10.38[a]	10.19	10.01	10.54	10.83	10.84	10.52	10.43	10.43	10.43	10.43	10.61	10.61	10.61	10.61
1,1-Difluoroethene	10.72[a]	10.45	10.33	10.76	11.04	11.07	10.71	10.62	10.62	10.62	10.62	10.84	10.84	10.84	10.84
Trifluoroethene	10.53[a]	10.46	10.09	10.68	10.95	10.98	10.51	10.40	10.40	10.40	10.40	10.53	10.53	10.53	10.53
Tetrafluoroethene	10.52[a]	10.74	10.19	10.80	11.01	11.09	10.50	10.38	10.38	10.38	10.38	10.45	10.45	10.45	10.45
Fluorobenzene	9.19[a]	9.47	9.54	9.81	9.78	9.94	9.68	9.58	9.58	9.58	9.58	9.85	9.85	9.85	9.85
1,2-Difluorobenzene	9.68[a]	9.69	9.63	9.98	9.97	10.13	9.83	9.71	9.71	9.71	9.71	9.92	9.92	9.92	9.92
1,3-Difluorobenzene	9.68[a]	9.73	9.72	10.02	10.09	10.22	9.91	9.79	9.79	9.79	9.79	10.02	10.02	10.02	10.02
1,4-Difluorobenzene	9.15[a]	9.56	9.49	9.87	9.89	10.04	9.71	9.58	9.58	9.58	9.58	9.80	9.80	9.80	9.80
Hexafluorobenzene	10.12[a]	10.77	10.37	10.85	10.88	11.04	10.69	10.50	10.50	10.50	10.50	10.60	10.60	10.60	10.60
Fluoroacetylene	11.30[a]	11.06	11.15	11.56	11.59	11.65	11.31	11.33	11.33	11.33	11.33	11.52	11.52	11.52	11.52
Hypofluorous acid	13.00[a]	12.75	12.55	12.98	11.31	11.78	12.79	13.23	13.23	13.23	13.23	13.44	13.44	13.44	13.44
1,1,1-Trifluoroethanol	11.74[a]	12.44	12.05	12.04	11.36	11.60	12.06	12.04	12.04	12.04	12.04	12.34	12.34	12.34	12.34
Trifluoromethylhypofluorite	13.64[a]	14.23	13.67	14.18	12.63	13.03	13.90	14.01	14.01	14.01	14.01	14.20	14.20	14.20	14.20
Difluorine monoxide	13.26[a]	13.52	12.90	13.47	11.20	11.87	13.25	13.56	13.56	13.56	13.56	13.78	13.78	13.78	13.78
Acetyl fluoride	11.80[a]	12.21	11.99	12.06	11.69	11.68	11.79	11.86	11.86	11.86	11.86	12.30	12.29	12.30	12.30
Carbonyl fluoride	13.60[a]	13.61	13.39	13.30	12.95	13.01	13.21	13.39	13.39	13.39	13.39	13.86	13.86	13.86	13.86
Hexafluoroacetone	12.09[a]	13.00	12.34	12.71	12.06	12.17	12.11	12.03	12.03	12.03	12.03	12.16	12.15	12.16	12.16
Trifluoroamine	13.73[a]	13.93	13.18	12.24	12.82	13.40	13.25	13.29	13.29	13.29	13.29	13.68	13.67	13.68	13.68
(E)-Difluorodiazene	12.80[b]	13.00	12.25	11.91	11.53	12.13	12.46	12.47	12.46	12.47	12.47	12.45	12.45	12.45	12.45
Tetrafluorohydrazine gauche	12.84[a]	13.04	12.47	12.46	12.27	12.92	12.90	12.87	12.88	12.87	12.87	12.59	12.60	12.59	12.59
Difluorodiazacyclopropane	11.78[a]	12.05	11.68	11.58	12.09	12.27	11.67	11.41	11.41	11.41	11.41	11.58	11.58	11.58	11.58
Hexafluorodimethyldiimine cis	11.35[a]	12.27	11.73	11.37	11.40	11.78	10.96	11.20	11.20	11.20	11.20	10.98	10.98	10.99	10.99
2,4,6-Trifluorotriazine	12.00[a]	12.70	12.27	12.09	12.15	12.39	12.33	12.29	12.29	12.29	12.29	12.15	12.15	12.15	12.15
Pentafluoropyridine	10.27[a]	10.72	10.34	10.87	11.00	11.12	10.65	10.59	10.58	10.59	10.59	10.65	10.64	10.65	10.65
Difluorocarbene	12.27[a]	12.18	11.59	11.58	12.29	12.62	11.93	12.18	12.18	12.18	12.18	12.12	12.12	12.12	12.12
Nitrosyl fluoride	12.94[a]	12.93	12.52	11.54	11.41	11.81	12.23	12.80	12.79	12.80	12.80	13.00	13.00	13.00	13.00
Nitryl fluoride	13.51[a]	12.99	13.39	13.37	12.84	12.74	12.84	13.69	13.69	13.69	13.69	14.08	14.08	14.08	14.08

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 S7: Mean Absolute Errors of the Interaction Energies (kcal/mol) for the S22 and S66x8 Benchmark Sets from Single-Point MNDO, AM1, PM3, PM6, and OMx Calculations at the Reference Geometries

Subset	N	Method						
		MNDO	AM1	PM3	PM6	OM1	OM2	OM3
S22								
Overall	22	16.74	6.78	5.90	3.35	5.09	3.07	3.58
H-bonded	7	28.16	10.74	7.42	5.03	7.82	3.63	4.20
Mixed	7	9.96	3.27	2.79	2.03	3.34	1.80	2.57
Dispersion	8	12.68	6.40	7.28	3.04	4.23	3.68	3.92
S66x8								
Overall	528	9.48	3.76	3.32	1.98	2.96	1.93	2.23
Electrostatic	184	13.40	5.24	4.42	2.50	3.77	2.27	2.39
Mixed	160	6.82	2.60	2.34	1.55	2.30	1.31	1.78
Dispersion	184	7.88	3.30	3.08	1.84	2.72	2.13	2.45

Table S8: Mean Absolute Errors in Selected Interatomic Distances (Å) and Angles (degree) from MNDO, AM1, PM3, PM6, and OMx Optimizations for the S22 Set

Subset	N	Method						
		MNDO	AM1	PM3	PM6	OM1	OM2	OM3
Selected interatomic distances								
Overall	105	3.117	3.635	1.557	0.383	2.336	0.708	1.996
Selected angles								
Overall	14	36.12	16.52	7.51	9.33	21.51	2.50	1.76

Table S9: Benchmark Results for the S22 Data Set. Interaction Energies (kcal/mol)

Complex	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Single point calculations															
ammonia dimer -3.17	−3.2[a]	4.5	−0.8	0.8	−2.3	−4.3	−1.5	−2.0	−2.6	−2.5	−2.5	−1.9	−2.7	−2.6	−2.6
water dimer -5.02 WH	−5.0[a]	6.8	−2.9	−2.8	−3.9	−4.9	−2.7	−4.0	−4.4	−4.3	−4.3	−4.1	−4.6	−4.6	−4.6
formic acid dimer -1	−18.8[a]	25.0	1.5	−9.9	−11.1	−18.6	−6.1	−13.6	−14.9	−14.8	−14.8	−11.5	−12.9	−13.3	−13.3
formamide dimer -15.	−16.1[a]	16.4	−5.7	−8.1	−12.6	−16.6	−7.9	−13.0	−14.3	−14.3	−14.3	−11.7	−13.2	−13.5	−13.5
uracil dimer -20.47	−20.7[a]	16.5	−5.8	−11.3	−13.3	−19.0	−11.0	−17.5	−19.1	−19.4	−19.5	−16.2	−18.1	−18.6	−18.7
2-pyridoxine 2-amino	−17.0[a]	15.1	−4.5	−7.5	−10.0	−17.9	−7.1	−11.0	−13.0	−13.3	−13.4	−11.3	−13.7	−14.2	−14.3
adenine thymine -16.	−16.7[a]	15.4	−4.3	−6.8	−9.1	−17.3	−6.6	−11.1	−13.2	−13.5	−13.6	−11.3	−13.8	−14.4	−14.5
methane dimer -0.53	−0.5[a]	1.2	0.2	−0.3	−0.1	−0.4	0.0	0.1	−0.3	−0.5	−0.5	0.1	−0.4	−0.5	−0.5
ethene dimer -1.51 W	−1.5[a]	4.0	−0.1	−1.1	−0.4	−1.1	0.4	−0.4	−1.4	−1.5	−1.5	0.1	−1.1	−1.3	−1.3
benzene methane -1.5	−1.4[a]	3.2	0.4	−0.2	−0.5	−1.8	0.4	−0.2	−1.2	−1.4	−1.4	0.1	−1.2	−1.4	−1.4
benzene dimer -2.73	−2.6[a]	6.4	3.5	2.4	0.1	−4.2	0.9	1.3	−1.5	−2.4	−2.2	1.1	−2.2	−3.2	−3.1
pyrazine dimer -4.42	−4.2[a]	7.8	2.5	3.9	−1.8	−5.7	−0.5	−0.9	−3.9	−4.4	−4.3	−0.7	−4.3	−5.1	−5.0
uracil dimer -9.88 W	−9.7[a]	13.5	0.1	5.8	−4.5	−8.6	−2.7	−4.3	−8.6	−9.3	−9.1	−3.9	−9.2	−10.0	−9.8
indole benzene -5.22	−4.6[a]	10.4	5.4	4.0	0.1	−6.0	1.3	1.5	−2.6	−3.5	−3.3	1.4	−3.6	−4.7	−4.5
adenine thymine -12.	−11.7[a]	18.7	2.9	7.4	−4.9	−11.4	−2.1	−4.0	−10.3	−10.9	−10.6	−3.3	−11.0	−11.8	−11.5
ethene ethyne -1.53	−1.5[a]	1.6	−0.3	−0.8	−0.5	−1.0	−0.2	−1.1	−1.6	−1.7	−1.7	−0.7	−1.3	−1.4	−1.4
benzene water -3.28	−3.3[a]	4.5	−0.7	−1.5	−2.3	−2.8	−0.9	−2.3	−3.4	−3.5	−3.5	−1.7	−3.1	−3.3	−3.2
benzene ammonia -2.3	−2.3[a]	3.5	−0.3	−0.6	−1.5	−2.9	−0.4	−1.2	−2.3	−2.5	−2.5	−0.8	−2.1	−2.3	−2.3
benzene hcn cs -4.46	−4.5[a]	6.0	−0.8	−1.6	−2.0	−3.1	−0.7	−3.1	−4.4	−4.5	−4.5	−1.7	−3.4	−3.6	−3.6
benzene dimer -2.74	−2.7[a]	5.4	0.4	−0.4	−0.8	−3.3	0.6	−0.6	−2.3	−2.7	−2.7	0.1	−2.0	−2.5	−2.4
indole benzene -5.73	−5.6[a]	8.8	−1.0	−1.3	−2.4	−6.0	−0.2	−2.4	−4.8	−5.3	−5.2	−1.2	−4.1	−4.7	−4.6
phenol dimer -7.05 W	−7.1[a]	12.8	−1.4	−1.4	−3.4	−6.3	−2.0	−3.8	−5.8	−6.2	−6.1	−3.2	−5.6	−6.1	−6.0
Full optimizations of dimers and monomers															
ammonia dimer -3.17	−3.2[a]	−0.8	−2.0	−0.7	−2.4	−5.8	−3.6	−2.0	−2.5	−2.5	−2.5	−1.9	−2.6	−2.5	−2.5
water dimer -5.02 WH	−5.0[a]	−1.0	−5.5	−3.5	−4.9	−6.6	−4.3	−4.3	−4.8	−4.7	−4.7	−4.5	−5.0	−5.1	−5.1
formic acid dimer -1	−18.8[a]	−1.7	−6.4	−8.6	−10.0	−17.2	−6.7	−14.6	−15.9	−15.9	−15.9	−16.7	−18.2	−18.6	−18.6
formamide dimer -15.	−16.1[a]	−1.5	−8.1	−6.1	−10.8	−15.2	−7.4	−13.0	−14.5	−14.5	−14.5	−12.4	−14.0	−14.6	−14.6
uracil dimer -20.47	−20.7[a]	−2.7	−10.2	−9.6	−12.5	−18.6	−9.8	−18.8	−20.6	−20.9	−20.9	−19.5	−21.6	−22.4	−22.4
2-pyridoxine 2-amino	−17.0[a]	−1.4	−6.0	−5.9	−9.6	−17.4	−6.7	−11.4	−13.5	−13.9	−13.9	−14.8	−17.5	−18.2	−18.2
adenine thymine -16.	−16.7[a]	−1.0	−5.0	−5.7	−9.0	−17.4	−6.2	−11.5	−13.9	−14.3	−14.3	−15.1	−18.1	−18.8	−18.9
methane dimer -0.53	−0.5[a]	−0.0	−0.0	−0.9	−0.2	−0.5	0.0	0.0	−0.7	−0.5	−0.5	0.0	−0.4	−0.5	−0.5
ethene dimer -1.51 W	−1.5[a]	−0.0	−0.1	−1.1	−0.4	−1.1	−0.0	−0.4	−1.6	−1.5	−1.5	−0.1	−1.2	−1.3	−1.3
benzene methane -1.5	−1.4[a]	−0.0	−0.0	−2.4	−0.5	−1.8	−0.0	−0.2	−1.3	−1.5	−1.5	−0.1	−1.2	−1.4	−1.4
benzene dimer -2.73	−2.6[a]	−0.0	−0.0	−2.4	−0.9	−4.8	−0.0	−0.6	−2.5	−2.9	−2.9	−0.0	−2.6	−3.6	−3.5
pyrazine dimer -4.42	−4.2[a]	−0.4	−1.4	−2.5	−2.1	−6.7	−1.8	−1.0	−5.2	−5.3	−5.2	−0.8	−4.9	−5.8	−5.7
uracil dimer -9.88 W	−9.7[a]	−1.2	−5.9	−4.2	−4.4	−15.6	−3.0	−4.6	−11.0	−10.8	−10.6	−3.9	−10.2	−11.0	−10.8
indole benzene -5.22	−4.6[a]	−0.1	−0.0	−2.7	−2.6	−6.4	−0.0	−2.5	−5.3	−5.5	−5.4	−1.5	−4.8	−5.6	−5.5
adenine thymine -12.	−11.7[a]	−2.3	−5.1	−5.7	−5.2	−11.8	−7.0	−11.6	−12.4	−12.1	−11.8	−14.6	−11.5	−12.5	−12.1
ethene ethyne -1.53	−1.5[a]	0.0	−0.6	−1.2	−0.5	−1.0	−0.3	−2.2	−3.1	−3.1	−3.1	−0.8	−1.6	−1.9	−1.9
benzene water -3.28	−3.3[a]	−0.1	−1.3	−1.8	−2.6	−3.0	−1.3	−2.9	−4.9	−4.7	−4.7	−1.9	−3.8	−3.9	−3.9
benzene ammonia -2.3	−2.3[a]	−0.1	−1.0	−1.0	−2.0	−3.0	−1.1	−1.4	−3.3	−3.3	−3.3	−1.2	−3.2	−3.4	−3.4
benzene hcn cs -4.46	−4.5[a]	−0.1	−0.9	−1.9	−2.0	−3.0	−1.1	−3.3	−4.8	−4.8	−4.8	−1.8	−3.3	−3.6	−3.6

... continued on next page ...

Table S9: ... *continued from previous page* ...

Complex	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
benzene dimer -2.74	−2.7[a]	−0.0	−0.4	−3.8	−0.8	−4.8	−0.1	−0.7	−2.4	−2.8	−3.3	−0.3	−2.6	−3.6	−3.5
indole benzene -5.73	−5.6[a]	−0.2	−1.3	−2.9	−2.6	−6.0	−1.0	−2.5	−5.3	−5.7	−5.7	−1.5	−4.8	−5.6	−5.5
phenol dimer -7.05 W	−7.1[a]	−0.5	−3.3	−2.6	−4.3	−7.3	−3.1	−4.7	−7.0	−7.1	−7.1	−4.1	−6.3	−6.6	−6.6
Full optimizations of dimers, single-point calculations on fragments (monomers)															
ammonia dimer -3.17	−3.2[a]	−0.8	−2.0	−0.7	−2.4	−5.9	−3.6	−2.0	−2.5	−2.5	−2.5	−1.9	−2.6	−2.5	−2.5
water dimer -5.02 WH	−5.0[a]	−1.0	−5.5	−3.6	−5.1	−6.6	−4.3	−4.4	−4.8	−4.8	−4.8	−4.5	−5.1	−5.1	−5.1
formic acid dimer -1	−18.8[a]	−1.7	−6.6	−9.6	−12.5	−19.3	−7.1	−18.6	−20.2	−20.0	−20.0	−57.2	−58.5	−58.9	−58.9
formamide dimer -15.	−16.1[a]	−1.5	−8.4	−7.0	−11.8	−16.0	−7.7	−14.3	−15.7	−15.8	−15.8	−15.2	−16.9	−17.6	−17.6
uracil dimer -20.47	−20.7[a]	−2.7	−10.5	−10.7	−13.6	−19.7	−10.3	−21.1	−23.0	−23.3	−23.3	−27.6	−30.0	−30.8	−30.8
2-pyridoxine 2-amino	−17.0[a]	−1.5	−6.2	−7.1	−10.4	−18.1	−7.0	−12.8	−15.1	−15.4	−15.4	−22.5	−25.5	−25.7	−25.7
adenine thymine -16.	−16.7[a]	−1.0	−5.1	−6.9	−9.6	−18.1	−6.5	−13.0	−15.8	−16.0	−16.1	−23.4	−26.8	−26.8	−26.8
methane dimer -0.53	−0.5[a]	−0.0	−0.0	−0.9	−0.2	−0.5	0.0	0.0	−0.7	−0.5	−0.5	0.0	−0.4	−0.5	−0.5
ethene dimer -1.51 W	−1.5[a]	−0.0	−0.1	−1.1	−0.4	−1.1	−0.0	−0.4	−1.6	−1.5	−1.5	−0.1	−1.2	−1.3	−1.3
benzene methane -1.5	−1.4[a]	−0.0	−0.0	−2.4	−0.5	−1.8	−0.0	−0.2	−1.4	−1.5	−1.5	−0.1	−1.2	−1.4	−1.4
benzene dimer -2.73	−2.6[a]	−0.0	−0.0	−2.5	−0.9	−4.8	−0.0	−0.6	−2.5	−3.0	−2.9	−0.0	−2.7	−3.6	−3.5
pyrazine dimer -4.42	−4.2[a]	−0.4	−1.4	−2.5	−2.2	−6.7	−1.8	−1.0	−5.3	−5.3	−5.2	−0.8	−5.0	−5.8	−5.7
uracil dimer -9.88 W	−9.7[a]	−1.2	−6.0	−4.3	−4.9	−16.4	−3.7	−5.6	−12.4	−12.1	−11.9	−4.6	−11.3	−12.1	−11.9
indole benzene -5.22	−4.6[a]	−0.1	−0.0	−2.8	−2.6	−6.4	−0.0	−2.5	−5.6	−5.8	−5.7	−1.5	−5.0	−5.8	−5.7
adenine thymine -12.	−11.7[a]	−2.4	−5.2	−6.5	−5.9	−12.7	−7.2	−12.7	−13.4	−13.1	−12.7	−19.0	−12.2	−13.2	−12.8
ethene ethyne -1.53	−1.5[a]	0.0	−0.6	−1.2	−0.5	−1.0	−0.3	−2.2	−3.1	−3.2	−3.2	−0.8	−1.7	−1.9	−1.9
benzene water -3.28	−3.3[a]	−0.1	−1.3	−1.8	−2.7	−3.0	−1.3	−3.0	−4.9	−4.7	−4.7	−1.9	−3.8	−3.9	−3.9
benzene ammonia -2.3	−2.3[a]	−0.1	−1.0	−1.0	−2.1	−3.0	−1.1	−1.4	−3.4	−3.4	−3.4	−1.2	−3.2	−3.4	−3.4
benzene hcn cs -4.46	−4.5[a]	−0.1	−0.9	−1.9	−2.0	−3.0	−1.1	−3.4	−4.8	−4.9	−4.9	−1.8	−3.3	−3.6	−3.6
benzene dimer -2.74	−2.7[a]	−0.0	−0.4	−3.9	−0.9	−4.8	−0.1	−0.7	−2.4	−2.8	−3.3	−0.3	−2.7	−3.6	−3.5
indole benzene -5.73	−5.6[a]	−0.1	−1.3	−2.8	−2.6	−6.1	−1.0	−2.5	−5.3	−5.8	−5.7	−1.5	−5.0	−5.8	−5.7
phenol dimer -7.05 W	−7.1[a]	−0.5	−3.4	−2.7	−4.4	−7.6	−3.1	−4.8	−7.2	−7.4	−7.3	−4.3	−6.5	−6.9	−6.9

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 S10: Benchmark Results for the S66x8 Data Set. Interaction Energies (kcal/mol)

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Water-Water_0.90	−4.6[a]	10.0	−1.2	−3.5	−3.8	−5.6	−1.8	−4.3	−4.8	−4.7	−4.7	−4.4	−4.9	−4.9	−4.9
Water-Water_0.95	−4.9[a]	7.4	−2.5	−3.1	−3.9	−4.9	−2.5	−4.1	−4.5	−4.5	−4.5	−4.3	−4.7	−4.8	−4.8
Water-Water_1.00	−4.9[a]	5.4	−3.1	−2.3	−3.9	−4.9	−2.9	−3.8	−4.2	−4.2	−4.2	−4.0	−4.5	−4.5	−4.5
Water-Water_1.05	−4.7[a]	3.8	−3.2	−1.8	−3.7	−4.8	−3.1	−3.5	−3.8	−3.8	−3.8	−3.8	−4.2	−4.3	−4.3
Water-Water_1.10	−4.5[a]	2.6	−3.1	−1.6	−3.4	−4.6	−3.1	−3.2	−3.5	−3.5	−3.5	−3.6	−3.9	−4.0	−4.0
Water-Water_1.25	−3.5[a]	0.5	−2.3	−1.6	−2.6	−3.9	−2.7	−2.4	−2.6	−2.7	−2.7	−2.8	−3.1	−3.2	−3.2
Water-Water_1.50	−2.1[a]	−0.5	−1.2	−1.1	−1.6	−2.8	−1.8	−1.6	−1.7	−1.8	−1.8	−1.9	−2.0	−2.1	−2.1
Water-Water_2.00	−0.9[a]	−0.5	−0.6	−0.5	−0.8	−1.5	−0.9	−0.8	−0.8	−0.8	−0.8	−1.0	−1.0	−1.0	−1.0
Water-MeOH_0.90	−5.2[a]	13.6	0.3	−2.7	−3.9	−6.3	−0.6	−4.0	−4.7	−4.7	−4.7	−3.5	−4.4	−4.5	−4.5
Water-MeOH_0.95	−5.5[a]	10.3	−1.5	−2.8	−4.2	−5.2	−1.6	−4.0	−4.6	−4.6	−4.6	−3.7	−4.4	−4.5	−4.5
Water-MeOH_1.00	−5.6[a]	7.7	−2.5	−2.2	−4.2	−5.0	−2.3	−3.8	−4.4	−4.4	−4.4	−3.6	−4.3	−4.4	−4.4
Water-MeOH_1.05	−5.4[a]	5.7	−2.9	−1.7	−4.1	−5.0	−2.6	−3.5	−4.1	−4.1	−4.1	−3.5	−4.1	−4.2	−4.2
Water-MeOH_1.10	−5.1[a]	4.1	−2.9	−1.4	−3.8	−4.8	−2.8	−3.3	−3.8	−3.8	−3.8	−3.3	−3.9	−4.0	−4.0
Water-MeOH_1.25	−3.9[a]	1.3	−2.2	−1.5	−3.0	−4.2	−2.6	−2.5	−2.9	−2.9	−2.9	−2.8	−3.2	−3.3	−3.3
Water-MeOH_1.50	−2.4[a]	−0.3	−1.2	−1.1	−1.8	−3.0	−1.8	−1.7	−1.9	−1.9	−1.9	−1.9	−2.1	−2.2	−2.2
Water-MeOH_2.00	−1.0[a]	−0.5	−0.6	−0.5	−0.9	−1.6	−0.9	−0.8	−0.9	−0.9	−0.9	−0.9	−1.0	−1.0	−1.0
Water-MeNH2_0.90	−6.5[a]	10.6	1.2	−2.6	−3.2	−5.9	−0.8	−4.5	−5.2	−5.3	−5.3	−5.7	−6.6	−6.7	−6.7
Water-MeNH2_0.95	−6.9[a]	7.9	−0.0	−2.5	−3.9	−6.6	−1.9	−4.5	−5.1	−5.2	−5.2	−5.4	−6.2	−6.3	−6.3
Water-MeNH2_1.00	−6.9[a]	5.9	−0.7	−1.9	−4.2	−6.9	−2.6	−4.3	−4.9	−4.9	−4.9	−5.0	−5.7	−5.8	−5.8
Water-MeNH2_1.05	−6.6[a]	4.3	−1.0	−1.5	−4.3	−6.9	−3.0	−4.0	−4.5	−4.6	−4.6	−4.5	−5.1	−5.3	−5.3
Water-MeNH2_1.10	−6.3[a]	3.0	−1.3	−1.4	−4.3	−6.8	−3.2	−3.7	−4.2	−4.2	−4.2	−4.1	−4.7	−4.8	−4.8
Water-MeNH2_1.25	−4.9[a]	0.7	−1.7	−1.4	−3.7	−5.7	−3.0	−2.8	−3.2	−3.3	−3.3	−3.1	−3.6	−3.6	−3.6
Water-MeNH2_1.50	−3.0[a]	−0.5	−1.3	−1.0	−2.4	−4.0	−2.1	−1.8	−2.0	−2.1	−2.1	−2.0	−2.2	−2.3	−2.3
Water-MeNH2_2.00	−1.1[a]	−0.5	−0.6	−0.5	−1.1	−2.1	−1.0	−0.8	−0.9	−0.9	−0.9	−0.9	−1.0	−1.0	−1.0
Water-Peptide_0.90	−7.6[a]	16.7	0.3	−3.8	−5.8	−9.0	−2.4	−6.5	−7.5	−7.5	−7.5	−6.0	−7.1	−7.3	−7.3
Water-Peptide_0.95	−8.1[a]	13.0	−2.0	−4.6	−6.2	−8.3	−3.3	−6.4	−7.3	−7.3	−7.3	−5.9	−7.0	−7.1	−7.2
Water-Peptide_1.00	−8.1[a]	10.0	−3.3	−4.2	−6.3	−7.4	−3.8	−6.0	−6.9	−6.9	−6.9	−5.7	−6.8	−6.9	−6.9
Water-Peptide_1.05	−7.8[a]	7.6	−3.9	−3.5	−6.1	−7.1	−4.1	−5.6	−6.5	−6.4	−6.4	−5.4	−6.4	−6.5	−6.5
Water-Peptide_1.10	−7.5[a]	5.6	−4.1	−3.0	−5.8	−6.9	−4.2	−5.2	−6.0	−6.0	−6.0	−5.1	−6.0	−6.1	−6.1
Water-Peptide_1.25	−6.0[a]	2.0	−3.4	−2.8	−4.7	−5.9	−3.9	−4.1	−4.6	−4.7	−4.7	−4.2	−4.9	−5.0	−5.0
Water-Peptide_1.50	−3.8[a]	−0.3	−2.0	−2.1	−3.0	−4.2	−2.8	−2.8	−3.1	−3.2	−3.2	−3.0	−3.4	−3.5	−3.5
Water-Peptide_2.00	−1.4[a]	−0.7	−0.9	−0.9	−1.3	−2.2	−1.3	−1.3	−1.3	−1.4	−1.4	−1.4	−1.5	−1.5	−1.5
MeOH-MeOH_0.90	−5.3[a]	14.2	1.4	−2.3	−2.9	−5.9	−0.5	−3.3	−4.2	−4.2	−4.2	−2.9	−3.9	−4.1	−4.1
MeOH-MeOH_0.95	−5.7[a]	10.8	−0.7	−2.7	−3.4	−4.9	−1.5	−3.4	−4.2	−4.2	−4.2	−3.1	−4.0	−4.2	−4.2
MeOH-MeOH_1.00	−5.7[a]	8.2	−2.0	−2.2	−3.5	−4.6	−2.1	−3.3	−4.0	−4.1	−4.1	−3.1	−4.0	−4.1	−4.1
MeOH-MeOH_1.05	−5.6[a]	6.1	−2.5	−1.6	−3.5	−4.7	−2.5	−3.1	−3.7	−3.8	−3.8	−3.0	−3.8	−3.9	−3.9
MeOH-MeOH_1.10	−5.3[a]	4.5	−2.7	−1.3	−3.3	−4.6	−2.7	−2.8	−3.4	−3.5	−3.5	−2.9	−3.6	−3.7	−3.7
MeOH-MeOH_1.25	−4.1[a]	1.4	−2.2	−1.4	−2.6	−4.1	−2.5	−2.2	−2.6	−2.7	−2.7	−2.4	−3.0	−3.1	−3.1
MeOH-MeOH_1.50	−2.5[a]	−0.3	−1.2	−1.0	−1.6	−3.0	−1.7	−1.4	−1.7	−1.8	−1.8	−1.7	−1.9	−2.0	−2.0
MeOH-MeOH_2.00	−1.0[a]	−0.5	−0.5	−0.5	−0.8	−1.6	−0.8	−0.7	−0.8	−0.8	−0.8	−0.8	−0.9	−0.9	−0.9
MeOH-MeNH2_0.90	−7.0[a]	13.1	2.1	−2.5	−1.7	−4.5	−0.6	−3.8	−5.1	−5.1	−5.1	−5.1	−6.6	−6.8	−6.8
MeOH-MeNH2_0.95	−7.5[a]	10.0	0.6	−2.7	−2.7	−5.6	−1.7	−3.9	−5.0	−5.1	−5.1	−4.9	−6.2	−6.4	−6.4
MeOH-MeNH2_1.00	−7.5[a]	7.5	−0.2	−2.2	−3.2	−6.2	−2.5	−3.7	−4.7	−4.9	−4.8	−4.5	−5.7	−5.9	−5.9
MeOH-MeNH2_1.05	−7.3[a]	5.6	−0.6	−1.7	−3.5	−6.4	−2.9	−3.5	−4.4	−4.5	−4.5	−4.1	−5.2	−5.4	−5.4

... continued on next page ...

Table S10: *... continued from previous page ...*

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
MeOH-MeNH2_1.10	−7.0[a]	4.1	−0.9	−1.4	−3.6	−6.4	−3.2	−3.3	−4.0	−4.2	−4.2	−3.8	−4.7	−4.9	−4.9
MeOH-MeNH2_1.25	−5.5[a]	1.2	−1.4	−1.4	−3.2	−5.7	−3.1	−2.5	−3.1	−3.2	−3.2	−2.8	−3.5	−3.7	−3.7
MeOH-MeNH2_1.50	−3.3[a]	−0.4	−1.3	−1.0	−2.1	−4.1	−2.1	−1.6	−1.9	−2.0	−2.0	−1.8	−2.2	−2.3	−2.3
MeOH-MeNH2_2.00	−1.3[a]	−0.5	−0.6	−0.5	−0.9	−2.1	−1.0	−0.7	−0.8	−0.9	−0.9	−0.8	−0.9	−1.0	−1.0
MeOH-Peptide_0.90	−7.6[a]	18.2	2.0	−2.8	−4.1	−7.8	−1.6	−5.2	−6.5	−6.6	−6.6	−4.7	−6.2	−6.4	−6.4
MeOH-Peptide_0.95	−8.1[a]	14.3	−0.6	−4.0	−4.7	−7.6	−2.5	−5.2	−6.4	−6.5	−6.5	−4.7	−6.2	−6.4	−6.4
MeOH-Peptide_1.00	−8.2[a]	11.2	−2.2	−3.9	−5.0	−6.6	−3.0	−4.9	−6.1	−6.1	−6.1	−4.5	−5.9	−6.1	−6.1
MeOH-Peptide_1.05	−8.0[a]	8.7	−3.1	−3.2	−4.9	−6.4	−3.4	−4.6	−5.6	−5.7	−5.7	−4.3	−5.6	−5.8	−5.8
MeOH-Peptide_1.10	−7.7[a]	6.6	−3.4	−2.7	−4.7	−6.3	−3.5	−4.2	−5.2	−5.3	−5.3	−4.1	−5.2	−5.4	−5.4
MeOH-Peptide_1.25	−6.2[a]	2.6	−3.0	−2.4	−3.8	−5.5	−3.3	−3.2	−4.0	−4.1	−4.1	−3.3	−4.2	−4.4	−4.4
MeOH-Peptide_1.50	−3.6[a]	−0.1	−1.6	−1.8	−2.2	−3.8	−2.2	−2.0	−2.3	−2.5	−2.5	−2.1	−2.6	−2.8	−2.8
MeOH-Peptide_2.00	−1.1[a]	−0.5	−0.5	−0.6	−0.8	−1.6	−0.8	−0.7	−0.8	−0.9	−0.9	−0.8	−0.9	−1.0	−1.0
MeOH-Water_0.90	−4.6[a]	10.7	−0.2	−3.2	−2.8	−5.1	−1.6	−3.6	−4.2	−4.2	−4.2	−3.6	−4.3	−4.4	−4.4
MeOH-Water_0.95	−5.0[a]	8.0	−1.8	−3.0	−3.1	−4.3	−2.3	−3.5	−4.0	−4.0	−4.0	−3.6	−4.2	−4.3	−4.3
MeOH-Water_1.00	−5.0[a]	5.9	−2.6	−2.2	−3.2	−4.3	−2.7	−3.3	−3.7	−3.7	−3.7	−3.4	−4.0	−4.1	−4.1
MeOH-Water_1.05	−4.8[a]	4.2	−2.9	−1.7	−3.1	−4.4	−2.9	−3.0	−3.4	−3.4	−3.4	−3.3	−3.7	−3.8	−3.8
MeOH-Water_1.10	−4.6[a]	2.9	−2.9	−1.5	−3.0	−4.3	−3.0	−2.7	−3.1	−3.2	−3.2	−3.1	−3.5	−3.6	−3.6
MeOH-Water_1.25	−3.6[a]	0.7	−2.2	−1.5	−2.3	−3.7	−2.6	−2.1	−2.4	−2.4	−2.4	−2.5	−2.8	−2.9	−2.9
MeOH-Water_1.50	−2.2[a]	−0.5	−1.2	−1.0	−1.4	−2.7	−1.8	−1.4	−1.5	−1.6	−1.6	−1.7	−1.8	−1.9	−1.9
MeOH-Water_2.00	−0.9[a]	−0.5	−0.5	−0.5	−0.7	−1.5	−0.8	−0.7	−0.7	−0.7	−0.7	−0.8	−0.9	−0.9	−0.9
MeNH2-MeOH_0.90	−2.8[a]	8.6	−1.5	0.1	−2.3	−4.5	−0.5	−1.5	−2.5	−2.6	−2.5	−0.9	−2.2	−2.3	−2.3
MeNH2-MeOH_0.95	−3.0[a]	6.2	−1.8	0.1	−2.3	−4.6	−1.1	−1.5	−2.3	−2.5	−2.5	−1.2	−2.2	−2.4	−2.4
MeNH2-MeOH_1.00	−3.0[a]	4.4	−1.8	−0.2	−2.2	−4.5	−1.4	−1.4	−2.1	−2.3	−2.3	−1.2	−2.2	−2.4	−2.3
MeNH2-MeOH_1.05	−2.9[a]	3.1	−1.6	−0.5	−2.0	−4.3	−1.4	−1.3	−1.9	−2.1	−2.1	−1.2	−2.1	−2.2	−2.2
MeNH2-MeOH_1.10	−2.7[a]	2.1	−1.4	−0.6	−1.7	−4.1	−1.4	−1.2	−1.7	−1.9	−1.9	−1.2	−1.9	−2.1	−2.0
MeNH2-MeOH_1.25	−2.0[a]	0.5	−0.8	−0.6	−1.1	−3.3	−1.1	−0.8	−1.2	−1.4	−1.4	−0.9	−1.4	−1.5	−1.5
MeNH2-MeOH_1.50	−1.1[a]	−0.2	−0.4	−0.4	−0.6	−2.2	−0.7	−0.5	−0.7	−0.8	−0.8	−0.6	−0.8	−0.9	−0.9
MeNH2-MeOH_2.00	−0.4[a]	−0.2	−0.2	−0.2	−0.3	−1.0	−0.3	−0.2	−0.3	−0.3	−0.3	−0.3	−0.3	−0.3	−0.3
MeNH2-MeNH2_0.90	−3.7[a]	12.3	1.4	2.1	−0.4	−4.4	1.1	−0.8	−2.2	−2.2	−2.1	−0.4	−2.2	−2.2	−2.2
MeNH2-MeNH2_0.95	−4.1[a]	9.1	0.5	1.3	−1.4	−5.1	−0.2	−1.3	−2.6	−2.6	−2.6	−1.0	−2.6	−2.7	−2.7
MeNH2-MeNH2_1.00	−4.2[a]	6.7	−0.1	0.6	−2.0	−5.4	−0.9	−1.5	−2.7	−2.7	−2.7	−1.3	−2.7	−2.8	−2.8
MeNH2-MeNH2_1.05	−4.0[a]	4.9	−0.5	0.1	−2.2	−5.4	−1.3	−1.6	−2.6	−2.7	−2.7	−1.4	−2.7	−2.8	−2.7
MeNH2-MeNH2_1.10	−3.8[a]	3.5	−0.7	−0.3	−2.2	−5.2	−1.5	−1.6	−2.4	−2.5	−2.5	−1.4	−2.5	−2.6	−2.6
MeNH2-MeNH2_1.25	−2.8[a]	1.1	−0.8	−0.5	−1.7	−4.2	−1.4	−1.2	−1.7	−1.9	−1.9	−1.2	−1.8	−2.0	−2.0
MeNH2-MeNH2_1.50	−1.3[a]	−0.1	−0.4	−0.3	−0.8	−2.5	−0.7	−0.6	−0.8	−1.0	−1.0	−0.6	−0.9	−1.0	−1.0
MeNH2-MeNH2_2.00	−0.4[a]	−0.2	−0.2	−0.1	−0.3	−1.1	−0.3	−0.2	−0.3	−0.3	−0.3	−0.2	−0.3	−0.3	−0.3
MeNH2-Peptide_0.90	−4.9[a]	14.8	−0.6	1.9	−3.4	−5.9	−0.6	−2.8	−4.7	−4.7	−4.7	−1.7	−4.0	−4.2	−4.2
MeNH2-Peptide_0.95	−5.4[a]	11.1	−1.6	1.2	−3.8	−6.2	−1.4	−2.9	−4.6	−4.7	−4.6	−2.0	−4.2	−4.4	−4.3
MeNH2-Peptide_1.00	−5.4[a]	8.4	−2.0	0.4	−3.8	−6.2	−1.9	−2.8	−4.3	−4.5	−4.4	−2.2	−4.2	−4.3	−4.3
MeNH2-Peptide_1.05	−5.2[a]	6.2	−2.0	−0.3	−3.7	−6.0	−2.2	−2.6	−4.0	−4.2	−4.2	−2.2	−4.0	−4.1	−4.1
MeNH2-Peptide_1.10	−4.9[a]	4.5	−1.9	−0.7	−3.4	−5.7	−2.2	−2.5	−3.7	−3.9	−3.9	−2.2	−3.7	−3.9	−3.9
MeNH2-Peptide_1.25	−3.2[a]	0.8	−1.2	−1.0	−2.1	−4.1	−1.7	−1.6	−2.3	−2.6	−2.5	−1.6	−2.4	−2.6	−2.6
MeNH2-Peptide_1.50	−1.4[a]	−0.3	−0.6	−0.6	−1.0	−2.3	−0.9	−0.8	−1.1	−1.2	−1.2	−0.8	−1.1	−1.3	−1.2
MeNH2-Peptide_2.00	−0.5[a]	−0.3	−0.3	−0.3	−0.4	−0.8	−0.4	−0.3	−0.4	−0.5	−0.5	−0.3	−0.4	−0.5	−0.5
MeNH2-Water_0.90	−6.7[a]	14.0	2.1	−1.8	−2.5	−5.1	0.1	−4.2	−5.1	−5.1	−5.1	−5.2	−6.2	−6.4	−6.4

... continued on next page ...

Table S10: *... continued from previous page ...*

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
MeNH2-Water_0.95	−7.2[a]	10.7	0.5	−2.2	−3.5	−6.1	−1.2	−4.4	−5.2	−5.2	−5.2	−5.1	−6.1	−6.2	−6.2
MeNH2-Water_1.00	−7.2[a]	8.2	−0.4	−1.9	−4.0	−6.6	−2.1	−4.3	−5.1	−5.0	−5.0	−4.9	−5.8	−5.9	−5.9
MeNH2-Water_1.05	−7.0[a]	6.1	−0.9	−1.5	−4.3	−6.8	−2.7	−4.1	−4.8	−4.8	−4.8	−4.5	−5.4	−5.5	−5.5
MeNH2-Water_1.10	−6.7[a]	4.5	−1.1	−1.3	−4.4	−6.7	−3.0	−3.8	−4.5	−4.5	−4.5	−4.2	−5.0	−5.1	−5.1
MeNH2-Water_1.25	−5.2[a]	1.5	−1.6	−1.4	−3.9	−5.8	−3.0	−3.0	−3.5	−3.6	−3.6	−3.3	−3.9	−3.9	−3.9
MeNH2-Water_1.50	−3.2[a]	−0.2	−1.3	−1.0	−2.5	−4.1	−2.1	−2.0	−2.2	−2.3	−2.3	−2.2	−2.4	−2.5	−2.5
MeNH2-Water_2.00	−1.2[a]	−0.5	−0.6	−0.5	−1.1	−2.2	−1.0	−0.9	−1.0	−1.0	−1.0	−1.0	−1.1	−1.1	−1.1
Peptide-MeOH_0.90	−5.7[a]	14.0	0.1	−1.1	−3.6	−5.8	−1.2	−3.8	−5.1	−5.3	−5.3	−2.9	−4.6	−4.8	−4.8
Peptide-MeOH_0.95	−6.1[a]	10.6	−1.8	−1.2	−4.1	−6.3	−2.1	−3.9	−5.2	−5.3	−5.3	−3.3	−4.8	−5.0	−5.0
Peptide-MeOH_1.00	−6.2[a]	7.9	−2.8	−0.9	−4.2	−6.5	−2.6	−3.9	−5.0	−5.2	−5.1	−3.4	−4.8	−5.0	−5.0
Peptide-MeOH_1.05	−6.0[a]	5.8	−3.1	−0.8	−4.2	−6.5	−2.9	−3.7	−4.7	−4.9	−4.9	−3.4	−4.6	−4.9	−4.9
Peptide-MeOH_1.10	−5.7[a]	4.2	−3.0	−1.0	−4.0	−6.3	−3.0	−3.5	−4.4	−4.6	−4.6	−3.3	−4.4	−4.7	−4.7
Peptide-MeOH_1.25	−4.6[a]	1.2	−2.3	−1.5	−3.1	−5.4	−2.7	−2.8	−3.5	−3.7	−3.7	−2.9	−3.7	−3.9	−3.9
Peptide-MeOH_1.50	−2.9[a]	−0.4	−1.4	−1.2	−2.0	−3.8	−2.0	−2.0	−2.3	−2.5	−2.5	−2.1	−2.5	−2.7	−2.6
Peptide-MeOH_2.00	−1.3[a]	−0.6	−0.7	−0.7	−1.1	−2.0	−1.1	−1.1	−1.2	−1.3	−1.3	−1.1	−1.3	−1.3	−1.3
Peptide-MeNH2_0.90	−6.8[a]	12.3	0.0	−2.1	−2.7	−8.1	−1.3	−3.7	−5.4	−5.6	−5.6	−4.0	−6.1	−6.4	−6.3
Peptide-MeNH2_0.95	−7.3[a]	9.3	−0.9	−1.9	−3.7	−9.0	−2.4	−4.1	−5.6	−5.8	−5.8	−4.2	−6.1	−6.4	−6.3
Peptide-MeNH2_1.00	−7.5[a]	7.0	−1.3	−1.5	−4.2	−9.4	−3.0	−4.1	−5.5	−5.7	−5.7	−4.2	−5.8	−6.2	−6.1
Peptide-MeNH2_1.05	−7.3[a]	5.1	−1.6	−1.4	−4.5	−9.4	−3.4	−4.0	−5.2	−5.5	−5.5	−4.0	−5.5	−5.8	−5.8
Peptide-MeNH2_1.10	−7.0[a]	3.6	−1.7	−1.4	−4.5	−9.2	−3.6	−3.8	−4.9	−5.2	−5.2	−3.8	−5.2	−5.5	−5.5
Peptide-MeNH2_1.25	−5.6[a]	0.9	−2.0	−1.6	−3.9	−7.8	−3.3	−3.1	−3.9	−4.2	−4.2	−3.2	−4.1	−4.4	−4.3
Peptide-MeNH2_1.50	−3.6[a]	−0.6	−1.5	−1.2	−2.6	−5.5	−2.3	−2.1	−2.5	−2.8	−2.8	−2.2	−2.7	−2.9	−2.9
Peptide-MeNH2_2.00	−1.5[a]	−0.7	−0.9	−0.7	−1.3	−2.8	−1.2	−1.1	−1.2	−1.3	−1.3	−1.1	−1.3	−1.4	−1.4
Peptide-Peptide_0.90	−8.0[a]	16.0	0.1	−2.9	−5.4	−9.0	−2.3	−5.4	−7.4	−7.7	−7.6	−4.2	−6.6	−7.1	−7.0
Peptide-Peptide_0.95	−8.5[a]	12.4	−2.2	−3.1	−5.8	−9.4	−3.1	−5.4	−7.2	−7.6	−7.5	−4.4	−6.6	−7.1	−7.0
Peptide-Peptide_1.00	−8.6[a]	9.5	−3.3	−2.7	−5.9	−9.4	−3.6	−5.2	−6.9	−7.2	−7.2	−4.5	−6.5	−6.9	−6.9
Peptide-Peptide_1.05	−8.4[a]	7.1	−3.7	−2.2	−5.7	−9.3	−3.8	−4.9	−6.4	−6.8	−6.8	−4.4	−6.2	−6.6	−6.6
Peptide-Peptide_1.10	−8.1[a]	5.3	−3.7	−2.1	−5.4	−8.9	−3.8	−4.6	−5.9	−6.3	−6.3	−4.2	−5.8	−6.3	−6.2
Peptide-Peptide_1.25	−6.7[a]	1.8	−2.9	−2.4	−4.3	−7.6	−3.5	−3.7	−4.7	−5.0	−5.0	−3.6	−4.8	−5.1	−5.1
Peptide-Peptide_1.50	−4.4[a]	−0.4	−1.8	−1.9	−2.8	−5.5	−2.5	−2.6	−3.1	−3.4	−3.4	−2.6	−3.2	−3.5	−3.5
Peptide-Peptide_2.00	−1.8[a]	−0.7	−0.9	−0.9	−1.3	−2.7	−1.2	−1.2	−1.4	−1.5	−1.5	−1.3	−1.5	−1.6	−1.6
Peptide-Water_0.90	−4.7[a]	9.1	−1.8	−2.2	−3.6	−5.8	−2.4	−4.0	−4.7	−4.8	−4.8	−3.7	−4.6	−4.8	−4.7
Peptide-Water_0.95	−5.1[a]	6.6	−3.0	−1.7	−3.8	−6.1	−2.9	−3.9	−4.5	−4.6	−4.6	−3.8	−4.5	−4.7	−4.7
Peptide-Water_1.00	−5.1[a]	4.7	−3.4	−1.3	−3.8	−6.1	−3.2	−3.7	−4.3	−4.4	−4.4	−3.7	−4.4	−4.6	−4.5
Peptide-Water_1.05	−5.0[a]	3.2	−3.3	−1.2	−3.7	−6.0	−3.3	−3.5	−4.0	−4.1	−4.1	−3.6	−4.2	−4.3	−4.3
Peptide-Water_1.10	−4.7[a]	2.1	−3.1	−1.4	−3.4	−5.7	−3.2	−3.2	−3.7	−3.8	−3.8	−3.4	−4.0	−4.1	−4.1
Peptide-Water_1.25	−3.8[a]	0.1	−2.3	−1.6	−2.7	−4.8	−2.8	−2.6	−2.9	−3.0	−3.0	−2.8	−3.2	−3.3	−3.3
Peptide-Water_1.50	−2.4[a]	−0.8	−1.3	−1.2	−1.8	−3.4	−1.9	−1.8	−2.0	−2.1	−2.1	−2.0	−2.2	−2.3	−2.3
Peptide-Water_2.00	−1.1[a]	−0.6	−0.7	−0.7	−1.0	−1.8	−1.1	−1.0	−1.0	−1.1	−1.1	−1.1	−1.1	−1.2	−1.2
Uracil-Uracil_BP_0.90	−15.7[a]	27.5	6.5	−3.1	−9.0	−14.5	−6.7	−14.8	−16.6	−16.9	−17.0	−13.8	−15.8	−16.5	−16.6
Uracil-Uracil_BP_0.95	−16.9[a]	21.9	0.1	−7.3	−10.7	−15.7	−7.6	−14.5	−16.3	−16.5	−16.6	−13.3	−15.3	−15.9	−15.9
Uracil-Uracil_BP_1.00	−17.2[a]	17.1	−4.2	−8.3	−11.4	−16.1	−8.1	−13.7	−15.3	−15.6	−15.7	−12.6	−14.4	−15.0	−15.0
Uracil-Uracil_BP_1.05	−16.9[a]	13.2	−6.8	−7.3	−11.4	−16.0	−8.4	−12.7	−14.1	−14.4	−14.5	−11.7	−13.4	−13.9	−14.0
Uracil-Uracil_BP_1.10	−16.2[a]	9.9	−8.0	−5.8	−10.9	−15.6	−8.4	−11.5	−12.9	−13.2	−13.2	−10.8	−12.4	−12.9	−12.9
Uracil-Uracil_BP_1.25	−13.2[a]	3.4	−7.3	−3.8	−8.8	−13.5	−7.5	−8.6	−9.6	−9.9	−10.0	−8.4	−9.7	−10.1	−10.1

... continued on next page ...

Table S10: *... continued from previous page ...*

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Uracil-Uracil_BP_1.50	−8.4[a]	−0.8	−4.3	−3.3	−5.4	−9.6	−5.2	−5.4	−6.1	−6.3	−6.4	−5.6	−6.4	−6.6	−6.7
Uracil-Uracil_BP_2.00	−3.3[a]	−1.4	−1.7	−1.5	−2.4	−4.9	−2.4	−2.5	−2.7	−2.9	−2.9	−2.6	−2.9	−3.0	−3.0
Water-Pyridine_0.90	−6.4[a]	10.8	2.8	−2.1	−1.8	−4.8	−0.2	−3.5	−4.3	−4.4	−4.4	−4.9	−5.7	−6.0	−6.0
Water-Pyridine_0.95	−6.8[a]	8.1	1.3	−2.1	−2.8	−5.8	−1.4	−3.7	−4.4	−4.5	−4.5	−4.7	−5.5	−5.7	−5.8
Water-Pyridine_1.00	−6.8[a]	6.0	0.4	−1.6	−3.3	−6.3	−2.1	−3.7	−4.3	−4.4	−4.5	−4.4	−5.1	−5.3	−5.3
Water-Pyridine_1.05	−6.6[a]	4.3	−0.1	−1.3	−3.6	−6.5	−2.6	−3.5	−4.1	−4.2	−4.2	−4.0	−4.7	−4.9	−4.9
Water-Pyridine_1.10	−6.3[a]	3.0	−0.5	−1.2	−3.7	−6.4	−2.9	−3.3	−3.8	−4.0	−4.0	−3.7	−4.3	−4.5	−4.5
Water-Pyridine_1.25	−4.9[a]	0.7	−1.3	−1.4	−3.3	−5.5	−2.9	−2.6	−3.0	−3.1	−3.1	−2.8	−3.3	−3.4	−3.4
Water-Pyridine_1.50	−3.0[a]	−0.6	−1.2	−1.1	−2.2	−3.9	−2.0	−1.7	−1.9	−2.0	−2.0	−1.8	−2.1	−2.2	−2.2
Water-Pyridine_2.00	−1.2[a]	−0.6	−0.6	−0.6	−1.0	−2.2	−1.0	−0.8	−0.9	−0.9	−0.9	−0.9	−0.9	−1.0	−1.0
MeOH-Pyridine_0.90	−6.8[a]	12.2	3.8	−1.7	−0.3	−3.6	−0.0	−2.7	−3.8	−4.0	−4.0	−4.3	−5.6	−6.0	−6.0
MeOH-Pyridine_0.95	−7.3[a]	9.3	2.0	−2.1	−1.5	−4.9	−1.2	−3.1	−4.1	−4.3	−4.3	−4.2	−5.4	−5.8	−5.8
MeOH-Pyridine_1.00	−7.4[a]	6.9	0.9	−1.7	−2.3	−5.7	−2.0	−3.2	−4.1	−4.3	−4.3	−4.0	−5.1	−5.4	−5.4
MeOH-Pyridine_1.05	−7.2[a]	5.1	0.2	−1.3	−2.8	−6.0	−2.6	−3.1	−3.9	−4.1	−4.1	−3.7	−4.7	−5.0	−5.0
MeOH-Pyridine_1.10	−6.9[a]	3.7	−0.2	−1.1	−3.0	−6.1	−2.9	−2.9	−3.7	−3.9	−3.9	−3.4	−4.3	−4.6	−4.6
MeOH-Pyridine_1.25	−5.5[a]	1.0	−1.1	−1.3	−2.9	−5.5	−2.9	−2.3	−2.9	−3.1	−3.1	−2.6	−3.3	−3.5	−3.5
MeOH-Pyridine_1.50	−3.4[a]	−0.5	−1.2	−1.1	−2.0	−3.9	−2.1	−1.5	−1.8	−2.0	−2.0	−1.7	−2.0	−2.2	−2.2
MeOH-Pyridine_2.00	−1.3[a]	−0.6	−0.6	−0.6	−0.9	−2.2	−1.0	−0.7	−0.8	−0.9	−0.9	−0.8	−0.9	−1.0	−1.0
AcOH-AcOH_0.90	−17.4[a]	36.0	10.8	0.1	−8.3	−16.5	−5.0	−14.8	−16.3	−16.3	−16.3	−13.2	−14.8	−15.3	−15.4
AcOH-AcOH_0.95	−18.8[a]	29.4	5.1	−6.9	−10.3	−18.2	−5.9	−14.5	−15.9	−16.0	−16.0	−12.7	−14.2	−14.7	−14.7
AcOH-AcOH_1.00	−19.1[a]	23.8	0.4	−10.8	−11.2	−18.7	−6.4	−13.6	−15.0	−15.0	−15.0	−11.8	−13.2	−13.6	−13.7
AcOH-AcOH_1.05	−18.7[a]	19.0	−3.1	−11.6	−11.2	−16.2	−6.7	−12.4	−13.7	−13.8	−13.8	−10.7	−12.1	−12.5	−12.5
AcOH-AcOH_1.10	−17.9[a]	15.1	−5.4	−10.3	−10.9	−14.1	−6.8	−11.2	−12.4	−12.4	−12.5	−9.6	−11.0	−11.3	−11.3
AcOH-AcOH_1.25	−14.6[a]	6.7	−7.1	−5.4	−9.0	−12.2	−6.6	−7.9	−8.9	−9.0	−9.0	−7.1	−8.2	−8.5	−8.5
AcOH-AcOH_1.50	−9.2[a]	0.6	−4.6	−4.0	−5.6	−9.1	−4.8	−4.7	−5.3	−5.5	−5.5	−4.6	−5.3	−5.5	−5.5
AcOH-AcOH_2.00	−3.6[a]	−1.1	−1.6	−1.7	−2.3	−4.8	−2.1	−2.1	−2.2	−2.4	−2.4	−2.0	−2.2	−2.4	−2.4
AcNH2-AcNH2_0.90	−14.9[a]	25.8	2.9	−6.1	−10.9	−15.7	−6.2	−14.0	−15.5	−15.7	−15.7	−12.7	−14.5	−15.0	−15.0
AcNH2-AcNH2_0.95	−16.0[a]	20.1	−2.8	−8.6	−12.1	−16.5	−7.2	−13.6	−15.1	−15.2	−15.2	−12.3	−14.0	−14.4	−14.5
AcNH2-AcNH2_1.00	−16.3[a]	15.4	−6.3	−8.3	−12.4	−16.7	−7.8	−12.8	−14.2	−14.3	−14.3	−11.7	−13.3	−13.6	−13.6
AcNH2-AcNH2_1.05	−15.9[a]	11.5	−8.1	−6.7	−12.1	−16.4	−8.1	−11.8	−13.0	−13.2	−13.2	−10.9	−12.4	−12.7	−12.7
AcNH2-AcNH2_1.10	−15.3[a]	8.4	−8.6	−5.4	−11.5	−15.8	−8.1	−10.8	−11.9	−12.1	−12.1	−10.1	−11.5	−11.8	−11.8
AcNH2-AcNH2_1.25	−12.4[a]	2.3	−7.2	−4.4	−9.0	−13.4	−7.3	−8.1	−9.0	−9.2	−9.2	−8.1	−9.2	−9.4	−9.4
AcNH2-AcNH2_1.50	−8.0[a]	−1.3	−4.2	−3.6	−5.6	−9.4	−5.1	−5.3	−5.8	−6.0	−6.0	−5.5	−6.1	−6.3	−6.3
AcNH2-AcNH2_2.00	−3.0[a]	−1.5	−1.7	−1.7	−2.4	−4.4	−2.2	−2.4	−2.5	−2.6	−2.6	−2.5	−2.6	−2.7	−2.7
AcOH-Uracil_0.90	−17.9[a]	30.9	7.9	−2.7	−9.4	−16.3	−7.5	−16.4	−18.1	−18.2	−18.2	−15.2	−17.0	−17.6	−17.7
AcOH-Uracil_0.95	−19.2[a]	24.8	1.8	−8.5	−11.3	−17.7	−8.3	−16.1	−17.7	−17.8	−17.9	−14.7	−16.4	−16.9	−17.0
AcOH-Uracil_1.00	−19.5[a]	19.7	−2.8	−10.9	−12.1	−18.2	−8.7	−15.3	−16.7	−16.9	−16.9	−13.7	−15.4	−15.8	−15.9
AcOH-Uracil_1.05	−19.2[a]	15.4	−5.9	−10.8	−12.1	−16.8	−8.9	−14.1	−15.4	−15.6	−15.6	−12.7	−14.2	−14.6	−14.7
AcOH-Uracil_1.10	−18.4[a]	11.8	−7.7	−9.3	−11.8	−15.7	−8.9	−12.8	−14.1	−14.3	−14.3	−11.6	−13.1	−13.5	−13.5
AcOH-Uracil_1.25	−15.1[a]	4.4	−8.2	−5.5	−9.8	−13.9	−8.2	−9.5	−10.5	−10.7	−10.8	−9.0	−10.1	−10.5	−10.5
AcOH-Uracil_1.50	−9.9[a]	−0.7	−5.2	−4.5	−6.3	−10.3	−6.0	−6.1	−6.7	−7.0	−7.0	−6.0	−6.8	−7.0	−7.1
AcOH-Uracil_2.00	−4.1[a]	−1.7	−2.1	−2.2	−2.8	−5.6	−2.8	−3.0	−3.2	−3.3	−3.3	−2.9	−3.2	−3.3	−3.3
AcNH2-Uracil_0.90	−17.7[a]	25.6	3.3	−5.4	−12.0	−17.7	−8.9	−17.1	−18.8	−19.0	−19.0	−16.1	−18.0	−18.6	−18.6
AcNH2-Uracil_0.95	−18.9[a]	20.2	−2.5	−9.3	−13.5	−18.7	−9.7	−16.8	−18.4	−18.6	−18.7	−15.6	−17.5	−18.0	−18.0
AcNH2-Uracil_1.00	−19.2[a]	15.6	−6.5	−10.3	−14.1	−18.9	−10.2	−16.0	−17.5	−17.7	−17.7	−14.8	−16.6	−17.0	−17.1

... continued on next page ...

Table S10: *... continued from previous page ...*

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
AcNH2-Uracil_1.05	−18.9[a]	11.8	−8.8	−9.5	−13.9	−18.7	−10.3	−14.9	−16.3	−16.5	−16.6	−13.9	−15.6	−16.0	−16.0
AcNH2-Uracil_1.10	−18.2[a]	8.7	−9.9	−8.2	−13.4	−18.2	−10.3	−13.8	−15.1	−15.3	−15.3	−13.0	−14.5	−14.9	−14.9
AcNH2-Uracil_1.25	−15.2[a]	2.3	−9.2	−5.9	−11.0	−15.8	−9.3	−10.7	−11.7	−11.9	−12.0	−10.5	−11.7	−12.0	−12.0
AcNH2-Uracil_1.50	−10.2[a]	−1.8	−5.8	−4.9	−7.2	−11.5	−6.8	−7.3	−7.9	−8.1	−8.1	−7.4	−8.2	−8.4	−8.4
AcNH2-Uracil_2.00	−4.7[a]	−2.3	−2.7	−2.7	−3.6	−6.3	−3.6	−3.8	−4.0	−4.2	−4.2	−3.9	−4.1	−4.3	−4.3
Benzene-Benzene_pi-pi_0.90	−0.2[a]	15.1	7.6	6.3	1.5	−2.8	2.6	2.3	−2.1	−2.5	−2.3	2.6	−2.5	−3.5	−3.3
Benzene-Benzene_pi-pi_0.95	−2.1[a]	9.6	5.2	3.8	0.5	−3.8	1.4	1.7	−1.8	−2.5	−2.3	1.7	−2.5	−3.5	−3.3
Benzene-Benzene_pi-pi_1.00	−2.7[a]	6.1	3.4	2.3	0.1	−4.3	0.9	1.3	−1.4	−2.3	−2.1	1.2	−2.2	−3.1	−3.0
Benzene-Benzene_pi-pi_1.05	−2.8[a]	3.9	2.2	1.4	0.0	−4.4	0.6	1.1	−1.0	−2.0	−1.8	0.9	−1.7	−2.7	−2.5
Benzene-Benzene_pi-pi_1.10	−2.6[a]	2.4	1.4	0.8	0.0	−4.3	0.4	1.0	−0.7	−1.6	−1.5	0.7	−1.4	−2.2	−2.1
Benzene-Benzene_pi-pi_1.25	−1.5[a]	0.6	0.4	0.2	0.1	−3.3	0.2	0.6	−0.3	−0.9	−0.8	0.5	−0.6	−1.2	−1.1
Benzene-Benzene_pi-pi_1.50	−0.5[a]	0.0	0.1	0.0	0.1	−1.2	0.1	0.3	−0.0	−0.3	−0.2	0.2	−0.2	−0.4	−0.3
Benzene-Benzene_pi-pi_2.00	−0.1[a]	0.0	0.0	−0.0	0.0	−0.2	0.0	0.1	0.0	−0.0	0.0	0.1	−0.0	−0.1	−0.0
Pyridine-Pyridine_pi-pi_0.90	−1.3[a]	17.3	7.0	7.7	0.5	−3.4	1.6	0.4	−4.1	−4.4	−4.3	1.1	−4.1	−5.1	−5.0
Pyridine-Pyridine_pi-pi_0.95	−3.2[a]	11.1	4.7	4.6	−0.6	−4.6	0.5	−0.0	−3.7	−4.2	−4.1	0.3	−4.1	−5.0	−4.9
Pyridine-Pyridine_pi-pi_1.00	−3.8[a]	7.1	3.1	2.7	−1.0	−5.2	−0.1	−0.1	−3.1	−3.8	−3.7	−0.1	−3.6	−4.6	−4.4
Pyridine-Pyridine_pi-pi_1.05	−3.9[a]	4.5	1.9	1.5	−1.0	−5.3	−0.3	−0.2	−2.5	−3.4	−3.2	−0.2	−3.1	−4.0	−3.8
Pyridine-Pyridine_pi-pi_1.10	−3.6[a]	2.8	1.1	0.8	−0.9	−5.2	−0.4	−0.2	−2.1	−2.9	−2.8	−0.2	−2.5	−3.4	−3.3
Pyridine-Pyridine_pi-pi_1.25	−2.4[a]	0.6	0.1	−0.0	−0.6	−4.2	−0.3	−0.2	−1.2	−1.9	−1.7	−0.2	−1.4	−2.1	−1.9
Pyridine-Pyridine_pi-pi_1.50	−1.0[a]	−0.1	−0.2	−0.2	−0.3	−1.7	−0.2	−0.1	−0.5	−0.8	−0.7	−0.2	−0.6	−0.9	−0.8
Pyridine-Pyridine_pi-pi_2.00	−0.2[a]	−0.1	−0.1	−0.1	−0.1	−0.4	−0.1	−0.1	−0.2	−0.2	−0.2	−0.1	−0.2	−0.2	−0.2
Uracil-Uracil_pi-pi_0.90	−7.9[a]	29.7	2.8	15.0	−1.2	−5.6	−0.7	−4.6	−10.5	−10.6	−10.4	−2.9	−9.9	−10.8	−10.5
Uracil-Uracil_pi-pi_0.95	−9.5[a]	20.1	0.8	9.4	−3.5	−7.6	−2.2	−4.6	−9.7	−10.1	−9.9	−3.8	−9.9	−10.7	−10.5
Uracil-Uracil_pi-pi_1.00	−9.8[a]	13.5	0.1	5.8	−4.5	−8.6	−2.7	−4.3	−8.6	−9.3	−9.1	−3.9	−9.2	−10.0	−9.8
Uracil-Uracil_pi-pi_1.05	−9.4[a]	8.9	−0.1	3.5	−4.7	−8.9	−2.8	−4.0	−7.5	−8.4	−8.2	−3.8	−8.2	−9.1	−8.9
Uracil-Uracil_pi-pi_1.10	−8.7[a]	5.8	−0.3	2.0	−4.5	−8.9	−2.7	−3.6	−6.5	−7.5	−7.3	−3.5	−7.2	−8.2	−8.0
Uracil-Uracil_pi-pi_1.25	−6.1[a]	1.2	−0.8	−0.0	−3.3	−7.7	−2.1	−2.6	−4.3	−5.3	−5.1	−2.7	−4.8	−5.7	−5.5
Uracil-Uracil_pi-pi_1.50	−3.1[a]	−0.4	−1.0	−0.6	−1.9	−4.6	−1.3	−1.6	−2.4	−2.9	−2.8	−1.7	−2.6	−3.1	−2.9
Uracil-Uracil_pi-pi_2.00	−1.0[a]	−0.4	−0.5	−0.4	−0.8	−1.4	−0.6	−0.7	−0.9	−1.1	−0.9	−0.8	−1.0	−1.1	−1.0
Benzene-Pyridine_pi-pi_0.90	−0.7[a]	16.8	7.4	7.1	1.0	−3.1	2.1	1.3	−3.2	−3.5	−3.4	1.8	−3.4	−4.3	−4.2
Benzene-Pyridine_pi-pi_0.95	−2.7[a]	10.6	5.0	4.2	−0.1	−4.3	0.9	0.8	−2.8	−3.4	−3.3	0.9	−3.4	−4.3	−4.2
Benzene-Pyridine_pi-pi_1.00	−3.4[a]	6.6	3.2	2.4	−0.5	−4.8	0.3	0.5	−2.3	−3.1	−3.0	0.5	−3.0	−3.9	−3.8
Benzene-Pyridine_pi-pi_1.05	−3.4[a]	4.2	2.0	1.4	−0.6	−4.9	0.1	0.4	−1.8	−2.7	−2.6	0.3	−2.5	−3.4	−3.3
Benzene-Pyridine_pi-pi_1.10	−3.1[a]	2.6	1.2	0.8	−0.5	−4.8	−0.0	0.3	−1.4	−2.3	−2.2	0.2	−2.0	−2.9	−2.7
Benzene-Pyridine_pi-pi_1.25	−2.0[a]	0.6	0.2	0.0	−0.3	−3.7	−0.1	0.2	−0.7	−1.4	−1.3	0.1	−1.1	−1.6	−1.5
Benzene-Pyridine_pi-pi_1.50	−0.7[a]	−0.0	−0.1	−0.1	−0.1	−1.4	−0.1	0.1	−0.3	−0.6	−0.5	0.0	−0.4	−0.6	−0.5
Benzene-Pyridine_pi-pi_2.00	−0.1[a]	−0.0	−0.0	−0.0	−0.0	−0.3	−0.0	−0.0	−0.1	−0.1	−0.1	−0.0	−0.1	−0.1	−0.1
Benzene-Uracil_pi-pi_0.90	−3.5[a]	23.0	8.1	9.9	0.4	−3.2	1.3	−1.1	−6.4	−6.6	−6.4	0.0	−6.1	−7.0	−6.9
Benzene-Uracil_pi-pi_0.95	−5.2[a]	15.4	5.8	6.2	−1.1	−4.7	0.1	−1.2	−5.6	−6.1	−6.0	−0.7	−5.9	−6.8	−6.7
Benzene-Uracil_pi-pi_1.00	−5.7[a]	10.2	4.1	3.8	−1.6	−5.4	−0.4	−1.1	−4.8	−5.5	−5.3	−0.9	−5.3	−6.2	−6.0
Benzene-Uracil_pi-pi_1.05	−5.5[a]	6.8	2.8	2.2	−1.7	−5.7	−0.6	−1.0	−3.9	−4.8	−4.6	−0.9	−4.5	−5.5	−5.3
Benzene-Uracil_pi-pi_1.10	−5.1[a]	4.5	1.9	1.3	−1.5	−5.8	−0.6	−0.8	−3.2	−4.2	−4.0	−0.8	−3.8	−4.7	−4.5
Benzene-Uracil_pi-pi_1.25	−3.3[a]	1.2	0.4	0.1	−0.9	−5.0	−0.5	−0.5	−1.8	−2.6	−2.5	−0.5	−2.2	−2.9	−2.7
Benzene-Uracil_pi-pi_1.50	−1.4[a]	0.1	−0.1	−0.2	−0.4	−2.4	−0.2	−0.2	−0.7	−1.2	−1.0	−0.2	−0.9	−1.3	−1.1
Benzene-Uracil_pi-pi_2.00	−0.3[a]	−0.0	−0.0	−0.1	−0.1	−0.5	−0.0	0.0	−0.1	−0.2	−0.1	−0.0	−0.2	−0.3	−0.2

... continued on next page ...

Table S10: *... continued from previous page ...*

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Pyridine-Uracil_pi-pi_0.90	−3.7[a]	24.8	6.4	11.8	−0.0	−3.6	0.5	−2.3	−7.8	−7.8	−7.7	−1.0	−7.2	−8.1	−8.0
Pyridine-Uracil_pi-pi_0.95	−6.2[a]	15.2	4.1	6.6	−2.4	−5.8	−1.2	−2.6	−7.0	−7.4	−7.3	−1.9	−7.2	−8.1	−7.9
Pyridine-Uracil_pi-pi_1.00	−6.8[a]	9.2	2.5	3.4	−3.2	−6.8	−1.7	−2.4	−6.0	−6.7	−6.5	−2.2	−6.5	−7.4	−7.2
Pyridine-Uracil_pi-pi_1.05	−6.6[a]	5.4	1.4	1.5	−3.3	−7.1	−1.9	−2.2	−5.1	−5.9	−5.7	−2.1	−5.6	−6.5	−6.3
Pyridine-Uracil_pi-pi_1.10	−6.0[a]	3.0	0.6	0.4	−3.0	−7.1	−1.8	−2.0	−4.2	−5.1	−5.0	−2.0	−4.7	−5.6	−5.5
Pyridine-Uracil_pi-pi_1.25	−3.9[a]	0.1	−0.5	−0.7	−2.1	−5.7	−1.5	−1.4	−2.6	−3.4	−3.2	−1.5	−2.9	−3.6	−3.4
Pyridine-Uracil_pi-pi_1.50	−1.8[a]	−0.6	−0.7	−0.7	−1.1	−2.7	−0.9	−0.9	−1.3	−1.7	−1.6	−0.9	−1.5	−1.8	−1.7
Pyridine-Uracil_pi-pi_2.00	−0.5[a]	−0.3	−0.3	−0.4	−0.5	−0.6	−0.4	−0.4	−0.5	−0.6	−0.5	−0.4	−0.5	−0.6	−0.5
Benzene-Ethene_0.90	−0.3[a]	8.7	4.0	3.2	0.8	−1.2	1.4	1.6	−0.9	−1.1	−1.1	1.6	−1.2	−1.8	−1.8
Benzene-Ethene_0.95	−1.1[a]	5.5	2.8	1.9	0.3	−1.7	0.8	1.3	−0.7	−1.1	−1.0	1.1	−1.2	−1.8	−1.7
Benzene-Ethene_1.00	−1.4[a]	3.5	1.9	1.2	0.2	−2.0	0.5	1.1	−0.4	−1.0	−0.9	0.9	−1.0	−1.6	−1.5
Benzene-Ethene_1.05	−1.4[a]	2.2	1.3	0.7	0.1	−2.2	0.4	0.9	−0.2	−0.8	−0.7	0.7	−0.7	−1.3	−1.2
Benzene-Ethene_1.10	−1.3[a]	1.4	0.8	0.4	0.1	−2.3	0.3	0.8	−0.1	−0.6	−0.6	0.6	−0.5	−1.0	−1.0
Benzene-Ethene_1.25	−0.7[a]	0.3	0.3	0.1	0.1	−1.8	0.2	0.6	0.1	−0.3	−0.2	0.4	−0.2	−0.5	−0.4
Benzene-Ethene_1.50	−0.2[a]	0.0	0.1	0.0	0.1	−0.8	0.1	0.3	0.1	−0.0	0.0	0.2	0.0	−0.1	−0.1
Benzene-Ethene_2.00	0.0[a]	0.0	0.0	0.0	0.0	−0.1	0.0	0.1	0.1	0.0	0.1	0.1	0.0	0.0	0.0
Uracil-Ethene_0.90	−2.6[a]	12.9	2.9	4.3	−0.4	−1.8	0.9	−0.9	−3.6	−3.7	−3.6	−0.2	−3.4	−3.9	−3.8
Uracil-Ethene_0.95	−3.2[a]	8.7	2.1	2.6	−0.9	−2.4	0.1	−0.9	−3.2	−3.5	−3.4	−0.6	−3.3	−3.8	−3.7
Uracil-Ethene_1.00	−3.4[a]	5.9	1.5	1.6	−1.0	−2.8	−0.2	−0.9	−2.7	−3.2	−3.1	−0.7	−3.0	−3.5	−3.4
Uracil-Ethene_1.05	−3.2[a]	3.9	1.1	0.9	−1.0	−2.9	−0.4	−0.8	−2.3	−2.8	−2.7	−0.7	−2.6	−3.1	−3.0
Uracil-Ethene_1.10	−3.0[a]	2.6	0.7	0.5	−0.9	−2.9	−0.4	−0.7	−2.0	−2.5	−2.4	−0.7	−2.2	−2.7	−2.7
Uracil-Ethene_1.25	−2.0[a]	0.7	0.1	−0.0	−0.6	−2.6	−0.4	−0.5	−1.2	−1.7	−1.6	−0.5	−1.4	−1.8	−1.7
Uracil-Ethene_1.50	−0.9[a]	0.0	−0.1	−0.1	−0.3	−1.4	−0.2	−0.3	−0.6	−0.8	−0.8	−0.3	−0.7	−0.9	−0.8
Uracil-Ethene_2.00	−0.3[a]	−0.0	−0.1	−0.1	−0.1	−0.4	−0.1	−0.1	−0.2	−0.3	−0.2	−0.1	−0.2	−0.3	−0.2
Uracil-Ethyne_0.90	−2.8[a]	10.7	2.6	3.9	−0.2	−1.2	−0.3	−2.0	−4.3	−4.4	−4.4	−1.3	−4.0	−4.5	−4.4
Uracil-Ethyne_0.95	−3.6[a]	7.0	1.7	2.3	−0.9	−2.0	−0.9	−1.9	−3.8	−4.1	−4.0	−1.5	−3.8	−4.3	−4.3
Uracil-Ethyne_1.00	−3.7[a]	4.6	1.2	1.2	−1.1	−2.4	−1.0	−1.7	−3.3	−3.7	−3.6	−1.5	−3.4	−3.9	−3.9
Uracil-Ethyne_1.05	−3.6[a]	3.0	0.7	0.6	−1.1	−2.5	−1.0	−1.5	−2.8	−3.2	−3.2	−1.4	−3.0	−3.5	−3.4
Uracil-Ethyne_1.10	−3.3[a]	1.9	0.4	0.2	−1.0	−2.6	−1.0	−1.3	−2.4	−2.8	−2.8	−1.3	−2.6	−3.0	−3.0
Uracil-Ethyne_1.25	−2.2[a]	0.3	−0.1	−0.3	−0.7	−2.3	−0.7	−0.9	−1.5	−1.9	−1.8	−0.9	−1.6	−2.0	−1.9
Uracil-Ethyne_1.50	−1.0[a]	−0.1	−0.2	−0.3	−0.3	−1.3	−0.4	−0.5	−0.7	−1.0	−0.9	−0.5	−0.8	−1.0	−0.9
Uracil-Ethyne_2.00	−0.3[a]	−0.1	−0.1	−0.1	−0.1	−0.3	−0.1	−0.2	−0.2	−0.3	−0.3	−0.2	−0.2	−0.3	−0.3
Pyridine-Ethene_0.90	−0.9[a]	9.4	3.4	3.5	0.3	−1.4	1.0	0.8	−1.6	−1.8	−1.8	1.0	−1.9	−2.4	−2.4
Pyridine-Ethene_0.95	−1.6[a]	6.2	2.5	2.2	−0.1	−2.0	0.4	0.6	−1.4	−1.7	−1.7	0.6	−1.8	−2.3	−2.3
Pyridine-Ethene_1.00	−1.9[a]	4.1	1.8	1.4	−0.2	−2.2	0.2	0.5	−1.0	−1.5	−1.5	0.4	−1.5	−2.1	−2.0
Pyridine-Ethene_1.05	−1.8[a]	2.7	1.2	0.8	−0.2	−2.4	0.1	0.5	−0.8	−1.3	−1.2	0.3	−1.3	−1.8	−1.7
Pyridine-Ethene_1.10	−1.7[a]	1.7	0.8	0.5	−0.2	−2.4	0.0	0.4	−0.6	−1.1	−1.0	0.2	−1.0	−1.5	−1.5
Pyridine-Ethene_1.25	−1.0[a]	0.4	0.2	0.1	−0.1	−2.1	0.0	0.3	−0.2	−0.6	−0.6	0.2	−0.5	−0.8	−0.8
Pyridine-Ethene_1.50	−0.4[a]	0.0	0.0	−0.0	−0.0	−1.0	0.0	0.2	−0.0	−0.2	−0.2	0.1	−0.2	−0.3	−0.3
Pyridine-Ethene_2.00	−0.0[a]	−0.0	0.0	−0.0	0.0	−0.1	0.0	0.1	0.0	−0.0	0.0	0.0	−0.0	−0.1	−0.0
Pentane-Pentane_0.90	−2.9[a]	21.0	0.4	−2.3	−0.0	−3.5	4.8	0.7	−4.1	−4.0	−3.8	3.5	−2.9	−2.5	−2.3
Pentane-Pentane_0.95	−3.6[a]	14.6	−0.2	−3.2	−0.5	−4.0	2.6	0.0	−4.0	−4.2	−4.1	1.9	−3.3	−3.3	−3.2
Pentane-Pentane_1.00	−3.8[a]	10.2	−0.3	−3.4	−0.6	−4.1	1.3	−0.2	−3.5	−4.0	−3.8	1.0	−3.1	−3.5	−3.4
Pentane-Pentane_1.05	−3.6[a]	7.1	−0.2	−3.0	−0.6	−3.9	0.6	−0.2	−2.9	−3.6	−3.4	0.6	−2.8	−3.4	−3.2
Pentane-Pentane_1.10	−3.3[a]	5.0	−0.1	−2.4	−0.6	−3.7	0.3	−0.2	−2.4	−3.1	−3.0	0.3	−2.4	−3.1	−3.0

... continued on next page ...

Table S10: *... continued from previous page ...*

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Pentane-Pentane_1.25	−2.2[a]	1.8	0.1	−1.1	−0.2	−2.9	0.0	−0.0	−1.3	−2.0	−1.9	0.0	−1.5	−2.1	−2.0
Pentane-Pentane_1.50	−1.1[a]	0.3	0.1	−0.3	−0.1	−1.7	0.0	−0.0	−0.6	−1.0	−0.9	0.0	−0.7	−1.0	−1.0
Pentane-Pentane_2.00	−0.3[a]	0.0	−0.0	−0.0	−0.0	−0.5	0.0	0.0	−0.2	−0.3	−0.3	0.0	−0.2	−0.3	−0.3
Neopentane-Pentane_0.90	−1.9[a]	14.1	−0.5	−2.5	−0.4	−3.4	3.6	0.1	−3.3	−3.5	−3.3	2.1	−2.4	−2.2	−2.1
Neopentane-Pentane_0.95	−2.5[a]	9.4	−0.8	−3.1	−0.7	−3.6	1.8	−0.4	−3.1	−3.5	−3.3	1.0	−2.5	−2.7	−2.6
Neopentane-Pentane_1.00	−2.6[a]	6.3	−0.7	−2.9	−0.7	−3.4	0.8	−0.4	−2.6	−3.1	−3.0	0.4	−2.3	−2.7	−2.6
Neopentane-Pentane_1.05	−2.5[a]	4.3	−0.5	−2.5	−0.6	−3.2	0.4	−0.4	−2.1	−2.7	−2.6	0.2	−2.0	−2.5	−2.4
Neopentane-Pentane_1.10	−2.3[a]	2.9	−0.3	−1.9	−0.5	−2.9	0.1	−0.3	−1.7	−2.3	−2.2	0.1	−1.7	−2.2	−2.1
Neopentane-Pentane_1.25	−1.5[a]	1.0	−0.0	−0.8	−0.2	−2.0	−0.0	−0.1	−0.9	−1.4	−1.3	−0.0	−1.0	−1.5	−1.4
Neopentane-Pentane_1.50	−0.7[a]	0.2	0.0	−0.2	−0.1	−1.1	−0.0	−0.0	−0.4	−0.7	−0.6	−0.0	−0.5	−0.7	−0.7
Neopentane-Pentane_2.00	−0.2[a]	0.0	−0.0	−0.0	−0.0	−0.4	−0.0	−0.0	−0.1	−0.2	−0.2	−0.0	−0.1	−0.2	−0.2
Neopentane-Neopentane_0.90	−1.5[a]	7.3	−0.8	−3.0	−0.7	−3.1	1.6	−0.8	−3.0	−3.4	−3.3	0.4	−2.4	−2.7	−2.6
Neopentane-Neopentane_0.95	−1.7[a]	5.0	−0.8	−2.9	−0.6	−2.9	0.8	−0.7	−2.4	−2.9	−2.8	0.2	−2.1	−2.5	−2.4
Neopentane-Neopentane_1.00	−1.8[a]	3.4	−0.7	−2.5	−0.5	−2.7	0.4	−0.5	−1.9	−2.4	−2.4	0.0	−1.8	−2.2	−2.1
Neopentane-Neopentane_1.05	−1.7[a]	2.4	−0.5	−2.0	−0.4	−2.4	0.2	−0.3	−1.5	−2.0	−2.0	−0.0	−1.4	−1.9	−1.8
Neopentane-Neopentane_1.10	−1.5[a]	1.6	−0.4	−1.5	−0.4	−2.2	0.1	−0.2	−1.2	−1.7	−1.6	−0.0	−1.2	−1.6	−1.6
Neopentane-Neopentane_1.25	−1.0[a]	0.6	−0.1	−0.6	−0.2	−1.5	−0.0	−0.1	−0.6	−1.0	−1.0	−0.0	−0.7	−1.0	−1.0
Neopentane-Neopentane_1.50	−0.5[a]	0.1	0.0	−0.1	−0.0	−0.8	−0.0	−0.0	−0.3	−0.5	−0.5	−0.0	−0.3	−0.5	−0.5
Neopentane-Neopentane_2.00	−0.1[a]	0.0	−0.0	−0.0	−0.0	−0.3	−0.0	−0.0	−0.1	−0.1	−0.1	−0.0	−0.1	−0.1	−0.1
Cyclopentane-Neopentane_0.90	−1.6[a]	14.2	−0.4	−2.7	−0.6	−3.4	3.6	−0.2	−3.5	−3.6	−3.5	1.8	−2.6	−2.4	−2.3
Cyclopentane-Neopentane_0.95	−2.2[a]	9.5	−0.7	−2.9	−0.7	−3.5	1.9	−0.6	−3.3	−3.6	−3.5	0.8	−2.7	−2.8	−2.7
Cyclopentane-Neopentane_1.00	−2.4[a]	6.4	−0.7	−2.9	−0.7	−3.3	0.9	−0.6	−2.7	−3.2	−3.1	0.3	−2.4	−2.7	−2.6
Cyclopentane-Neopentane_1.05	−2.3[a]	4.4	−0.6	−2.5	−0.6	−3.1	0.4	−0.5	−2.2	−2.8	−2.7	0.1	−2.1	−2.5	−2.4
Cyclopentane-Neopentane_1.10	−2.1[a]	3.1	−0.4	−2.1	−0.5	−2.8	0.2	−0.4	−1.8	−2.3	−2.2	0.0	−1.7	−2.2	−2.1
Cyclopentane-Neopentane_1.25	−1.5[a]	1.0	−0.1	−0.9	−0.3	−2.0	−0.0	−0.1	−0.9	−1.4	−1.4	−0.0	−1.0	−1.5	−1.4
Cyclopentane-Neopentane_1.50	−0.7[a]	0.2	0.0	−0.2	−0.1	−1.1	−0.0	−0.0	−0.4	−0.7	−0.6	−0.0	−0.5	−0.7	−0.7
Cyclopentane-Neopentane_2.00	−0.2[a]	0.0	−0.0	−0.0	−0.0	−0.4	−0.0	−0.0	−0.1	−0.2	−0.2	−0.0	−0.1	−0.2	−0.2
Cyclopentane-Cyclopentane_0.90	−2.2[a]	16.0	0.2	−2.2	0.0	−3.0	4.3	0.2	−3.5	−3.5	−3.4	2.4	−2.6	−2.2	−2.1
Cyclopentane-Cyclopentane_0.95	−2.8[a]	11.4	−0.3	−2.8	−0.3	−3.4	2.4	−0.3	−3.4	−3.6	−3.5	1.3	−2.8	−2.7	−2.6
Cyclopentane-Cyclopentane_1.00	−3.0[a]	7.8	−0.5	−3.0	−0.4	−3.4	1.2	−0.4	−2.9	−3.3	−3.2	0.7	−2.6	−2.8	−2.7
Cyclopentane-Cyclopentane_1.05	−2.9[a]	5.3	−0.5	−2.7	−0.4	−3.3	0.6	−0.3	−2.4	−2.9	−2.8	0.4	−2.2	−2.6	−2.5
Cyclopentane-Cyclopentane_1.10	−2.6[a]	3.6	−0.3	−2.2	−0.4	−3.0	0.3	−0.2	−1.9	−2.5	−2.3	0.2	−1.9	−2.4	−2.3
Cyclopentane-Cyclopentane_1.25	−1.7[a]	1.2	−0.0	−0.9	−0.2	−2.2	0.0	−0.0	−1.0	−1.5	−1.4	0.0	−1.1	−1.6	−1.5
Cyclopentane-Cyclopentane_1.50	−0.8[a]	0.2	0.0	−0.2	−0.0	−1.2	0.0	−0.0	−0.4	−0.7	−0.7	0.0	−0.5	−0.8	−0.7
Cyclopentane-Cyclopentane_2.00	−0.2[a]	0.0	−0.0	−0.0	−0.0	−0.4	0.0	0.0	−0.1	−0.2	−0.2	0.0	−0.1	−0.2	−0.2
Benzene-Cyclopentane_0.90	−2.2[a]	16.7	2.4	0.5	0.4	−3.8	3.5	1.3	−2.9	−3.0	−2.8	2.7	−2.3	−2.6	−2.5
Benzene-Cyclopentane_0.95	−3.2[a]	11.3	1.6	−0.3	−0.4	−4.3	1.8	0.6	−2.8	−3.2	−3.0	1.5	−2.7	−3.1	−3.0
Benzene-Cyclopentane_1.00	−3.6[a]	7.6	1.3	−0.4	−0.5	−4.2	0.9	0.3	−2.4	−3.0	−2.9	0.9	−2.5	−3.1	−3.0
Benzene-Cyclopentane_1.05	−3.5[a]	5.1	1.1	−0.4	−0.5	−4.0	0.5	0.2	−2.0	−2.7	−2.5	0.5	−2.2	−2.9	−2.8
Benzene-Cyclopentane_1.10	−3.2[a]	3.4	0.9	−0.4	−0.3	−3.7	0.2	0.1	−1.6	−2.3	−2.2	0.3	−1.9	−2.6	−2.4
Benzene-Cyclopentane_1.25	−2.1[a]	1.0	0.3	−0.2	−0.1	−2.7	0.0	0.1	−0.9	−1.5	−1.4	0.1	−1.1	−1.6	−1.5
Benzene-Cyclopentane_1.50	−0.9[a]	0.1	0.0	−0.1	−0.0	−1.4	0.0	0.0	−0.4	−0.7	−0.6	0.0	−0.4	−0.7	−0.6
Benzene-Cyclopentane_2.00	−0.2[a]	−0.0	−0.0	−0.0	−0.0	−0.3	0.0	0.0	−0.1	−0.2	−0.1	0.0	−0.1	−0.2	−0.1
Benzene-Neopentane_0.90	−1.9[a]	11.8	0.9	−0.6	−0.4	−4.1	2.4	0.4	−2.7	−3.1	−3.0	1.6	−2.3	−2.8	−2.6
Benzene-Neopentane_0.95	−2.7[a]	7.8	0.7	−0.8	−0.8	−4.2	1.1	−0.0	−2.5	−3.1	−3.0	0.7	−2.5	−3.0	−2.9

... continued on next page ...

Table S10: *... continued from previous page ...*

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Benzene-Neopentane_1.00	−2.9[a]	5.2	0.6	−0.7	−0.7	−3.9	0.5	−0.1	−2.2	−2.8	−2.7	0.3	−2.2	−2.9	−2.7
Benzene-Neopentane_1.05	−2.8[a]	3.4	0.6	−0.5	−0.6	−3.6	0.2	−0.2	−1.8	−2.5	−2.4	0.1	−1.9	−2.6	−2.5
Benzene-Neopentane_1.10	−2.6[a]	2.3	0.5	−0.4	−0.4	−3.2	0.1	−0.2	−1.5	−2.2	−2.0	−0.0	−1.6	−2.3	−2.1
Benzene-Neopentane_1.25	−1.7[a]	0.7	0.2	−0.2	−0.2	−2.2	−0.0	−0.1	−0.9	−1.4	−1.3	−0.1	−1.0	−1.4	−1.3
Benzene-Neopentane_1.50	−0.8[a]	0.1	−0.0	−0.1	−0.1	−1.1	−0.0	−0.1	−0.4	−0.7	−0.6	−0.0	−0.4	−0.7	−0.6
Benzene-Neopentane_2.00	−0.2[a]	−0.0	−0.0	−0.0	−0.0	−0.3	−0.0	−0.0	−0.1	−0.2	−0.1	−0.0	−0.1	−0.2	−0.1
Uracil-Pentane_0.90	−3.8[a]	26.5	3.0	5.4	−0.9	−4.2	3.5	0.2	−4.9	−4.9	−4.7	1.6	−4.8	−4.9	−4.7
Uracil-Pentane_0.95	−4.7[a]	18.6	1.9	3.1	−1.7	−5.0	1.6	−0.4	−4.6	−5.0	−4.8	0.4	−4.9	−5.2	−5.0
Uracil-Pentane_1.00	−4.8[a]	13.0	1.4	1.9	−1.8	−5.1	0.6	−0.6	−4.1	−4.7	−4.5	−0.1	−4.5	−5.1	−4.9
Uracil-Pentane_1.05	−4.6[a]	9.0	1.2	1.1	−1.6	−4.9	0.1	−0.6	−3.5	−4.2	−4.0	−0.4	−3.9	−4.7	−4.5
Uracil-Pentane_1.10	−4.1[a]	5.8	1.0	0.6	−1.3	−4.6	−0.2	−0.5	−2.8	−3.7	−3.5	−0.4	−3.2	−4.0	−3.9
Uracil-Pentane_1.25	−2.4[a]	1.6	0.4	0.0	−0.6	−3.5	−0.2	−0.3	−1.5	−2.2	−2.1	−0.3	−1.8	−2.4	−2.2
Uracil-Pentane_1.50	−1.0[a]	0.2	0.0	−0.1	−0.2	−1.8	−0.1	−0.1	−0.6	−1.0	−0.9	−0.1	−0.7	−1.0	−0.9
Uracil-Pentane_2.00	−0.2[a]	−0.0	−0.0	−0.0	−0.1	−0.4	−0.0	−0.0	−0.1	−0.2	−0.2	−0.0	−0.2	−0.2	−0.2
Uracil-Cyclopentane_0.90	−3.0[a]	23.4	3.6	4.9	−0.2	−3.6	3.7	0.5	−3.9	−4.0	−3.8	1.8	−3.8	−4.0	−3.8
Uracil-Cyclopentane_0.95	−4.0[a]	15.9	2.0	2.6	−1.1	−4.4	1.7	−0.1	−3.8	−4.1	−3.9	0.6	−4.0	−4.4	−4.2
Uracil-Cyclopentane_1.00	−4.1[a]	10.9	1.4	1.5	−1.2	−4.5	0.7	−0.3	−3.3	−3.9	−3.7	0.1	−3.7	−4.2	−4.0
Uracil-Cyclopentane_1.05	−3.9[a]	7.4	1.1	0.8	−1.1	−4.3	0.2	−0.3	−2.8	−3.5	−3.3	−0.1	−3.2	−3.8	−3.7
Uracil-Cyclopentane_1.10	−3.5[a]	5.1	0.9	0.5	−0.9	−4.0	0.0	−0.3	−2.3	−3.1	−2.9	−0.2	−2.7	−3.4	−3.2
Uracil-Cyclopentane_1.25	−2.3[a]	1.6	0.4	0.1	−0.4	−3.1	−0.1	−0.2	−1.3	−2.0	−1.9	−0.2	−1.6	−2.2	−2.0
Uracil-Cyclopentane_1.50	−1.0[a]	0.2	0.0	−0.0	−0.2	−1.7	−0.1	−0.1	−0.6	−1.0	−0.9	−0.1	−0.7	−1.0	−0.9
Uracil-Cyclopentane_2.00	−0.2[a]	0.0	−0.0	−0.0	−0.0	−0.5	−0.0	−0.0	−0.2	−0.3	−0.2	−0.0	−0.2	−0.3	−0.2
Uracil-Neopentane_0.90	−2.9[a]	18.0	2.1	3.9	−0.4	−3.1	2.5	0.1	−3.5	−3.7	−3.6	1.2	−3.3	−3.6	−3.4
Uracil-Neopentane_0.95	−3.6[a]	12.2	1.4	2.2	−1.0	−3.5	1.1	−0.3	−3.3	−3.7	−3.5	0.3	−3.4	−3.8	−3.6
Uracil-Neopentane_1.00	−3.7[a]	8.2	1.1	1.3	−1.0	−3.6	0.4	−0.4	−2.8	−3.4	−3.2	−0.1	−3.0	−3.6	−3.5
Uracil-Neopentane_1.05	−3.5[a]	5.6	1.0	0.8	−0.9	−3.4	0.1	−0.4	−2.3	−3.0	−2.9	−0.2	−2.6	−3.2	−3.1
Uracil-Neopentane_1.10	−3.1[a]	3.8	0.8	0.5	−0.7	−3.2	−0.0	−0.4	−1.9	−2.6	−2.5	−0.3	−2.2	−2.8	−2.7
Uracil-Neopentane_1.25	−2.0[a]	1.2	0.4	0.1	−0.4	−2.5	−0.1	−0.2	−1.1	−1.7	−1.6	−0.2	−1.3	−1.8	−1.7
Uracil-Neopentane_1.50	−0.9[a]	0.2	0.0	0.0	−0.2	−1.4	−0.1	−0.1	−0.5	−0.8	−0.7	−0.1	−0.6	−0.8	−0.8
Uracil-Neopentane_2.00	−0.2[a]	0.0	−0.0	−0.0	−0.0	−0.4	−0.0	−0.0	−0.1	−0.2	−0.2	−0.0	−0.2	−0.2	−0.2
Ethene-Pentane_0.90	−1.7[a]	10.1	0.1	−1.3	−0.2	−1.9	2.0	0.1	−2.1	−2.2	−2.1	1.5	−1.6	−1.5	−1.5
Ethene-Pentane_0.95	−2.0[a]	6.9	−0.1	−1.7	−0.4	−2.1	1.0	−0.2	−2.0	−2.2	−2.2	0.7	−1.7	−1.9	−1.8
Ethene-Pentane_1.00	−2.0[a]	4.8	−0.1	−1.7	−0.5	−2.1	0.5	−0.2	−1.7	−2.1	−2.0	0.3	−1.6	−1.9	−1.8
Ethene-Pentane_1.05	−1.9[a]	3.3	−0.1	−1.4	−0.4	−2.0	0.2	−0.2	−1.4	−1.8	−1.8	0.1	−1.4	−1.8	−1.7
Ethene-Pentane_1.10	−1.7[a]	2.3	−0.0	−1.1	−0.3	−1.9	0.1	−0.2	−1.2	−1.6	−1.6	0.0	−1.2	−1.6	−1.6
Ethene-Pentane_1.25	−1.1[a]	0.8	0.1	−0.5	−0.2	−1.5	−0.0	−0.1	−0.6	−1.0	−1.0	−0.0	−0.7	−1.1	−1.0
Ethene-Pentane_1.50	−0.5[a]	0.1	0.0	−0.1	−0.0	−0.9	−0.0	−0.0	−0.3	−0.5	−0.5	−0.0	−0.3	−0.5	−0.5
Ethene-Pentane_2.00	−0.1[a]	0.0	−0.0	−0.0	−0.0	−0.2	−0.0	−0.0	−0.1	−0.1	−0.1	−0.0	−0.1	−0.1	−0.1
Ethyne-Pentane_0.90	−1.1[a]	7.5	1.2	−0.0	−0.1	−1.5	1.2	0.3	−1.6	−1.7	−1.7	1.0	−1.4	−1.6	−1.6
Ethyne-Pentane_0.95	−1.6[a]	5.0	0.9	−0.3	−0.3	−1.7	0.6	0.1	−1.4	−1.7	−1.6	0.5	−1.4	−1.7	−1.7
Ethyne-Pentane_1.00	−1.7[a]	3.3	0.7	−0.3	−0.3	−1.7	0.3	0.1	−1.1	−1.5	−1.5	0.3	−1.2	−1.6	−1.6
Ethyne-Pentane_1.05	−1.7[a]	2.2	0.6	−0.3	−0.2	−1.6	0.1	0.1	−0.9	−1.3	−1.3	0.2	−1.0	−1.4	−1.4
Ethyne-Pentane_1.10	−1.5[a]	1.4	0.4	−0.2	−0.2	−1.5	0.1	0.0	−0.7	−1.1	−1.1	0.1	−0.8	−1.2	−1.2
Ethyne-Pentane_1.25	−1.0[a]	0.4	0.1	−0.1	−0.0	−1.2	0.0	0.0	−0.4	−0.7	−0.7	0.1	−0.4	−0.7	−0.7
Ethyne-Pentane_1.50	−0.4[a]	0.0	0.0	−0.0	−0.0	−0.6	0.0	0.0	−0.1	−0.3	−0.3	0.0	−0.2	−0.3	−0.3

... continued on next page ...

Table S10: *... continued from previous page ...*

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Ethyne-Pentane_2.00	−0.1[a]	−0.0	0.0	−0.0	0.0	−0.1	0.0	0.0	−0.0	−0.1	−0.1	0.0	−0.0	−0.1	−0.1
Peptide-Pentane_0.90	−3.8[a]	20.5	1.0	1.3	−0.9	−3.3	2.9	0.2	−4.0	−3.9	−3.8	1.9	−3.4	−3.3	−3.2
Peptide-Pentane_0.95	−4.2[a]	15.0	0.5	0.1	−1.2	−3.7	1.5	−0.3	−3.8	−4.0	−3.8	0.9	−3.5	−3.7	−3.6
Peptide-Pentane_1.00	−4.2[a]	11.0	0.4	−0.5	−1.2	−3.8	0.7	−0.4	−3.4	−3.8	−3.7	0.4	−3.3	−3.7	−3.6
Peptide-Pentane_1.05	−4.0[a]	8.0	0.4	−0.6	−1.1	−3.7	0.3	−0.4	−2.9	−3.5	−3.3	0.1	−3.0	−3.5	−3.4
Peptide-Pentane_1.10	−3.7[a]	5.8	0.4	−0.7	−0.9	−3.5	0.0	−0.4	−2.5	−3.1	−3.0	−0.0	−2.6	−3.3	−3.1
Peptide-Pentane_1.25	−2.6[a]	2.2	0.4	−0.4	−0.5	−2.9	−0.1	−0.3	−1.5	−2.2	−2.1	−0.1	−1.7	−2.3	−2.2
Peptide-Pentane_1.50	−1.2[a]	0.3	0.1	−0.1	−0.1	−1.8	−0.1	−0.1	−0.6	−1.1	−1.0	−0.1	−0.7	−1.1	−1.0
Peptide-Pentane_2.00	−0.3[a]	−0.0	−0.0	−0.0	−0.0	−0.5	−0.0	−0.0	−0.2	−0.3	−0.2	−0.0	−0.2	−0.3	−0.2
Benzene-Benzene_TS_0.90	−1.6[a]	12.4	1.8	0.8	0.3	−2.7	2.7	0.2	−2.5	−2.7	−2.7	1.6	−1.6	−2.1	−2.0
Benzene-Benzene_TS_0.95	−2.6[a]	8.3	0.9	−0.1	−0.6	−3.2	1.3	−0.4	−2.6	−2.9	−2.9	0.6	−2.1	−2.6	−2.5
Benzene-Benzene_TS_1.00	−2.9[a]	5.5	0.6	−0.3	−0.8	−3.2	0.5	−0.6	−2.4	−2.8	−2.8	0.1	−2.2	−2.7	−2.6
Benzene-Benzene_TS_1.05	−2.8[a]	3.7	0.5	−0.4	−0.8	−3.1	0.2	−0.6	−2.1	−2.6	−2.5	−0.1	−2.0	−2.5	−2.5
Benzene-Benzene_TS_1.10	−2.6[a]	2.5	0.4	−0.4	−0.6	−2.8	−0.0	−0.6	−1.8	−2.3	−2.3	−0.2	−1.7	−2.3	−2.2
Benzene-Benzene_TS_1.25	−1.8[a]	0.7	0.1	−0.2	−0.3	−2.1	−0.1	−0.4	−1.1	−1.5	−1.5	−0.3	−1.1	−1.5	−1.5
Benzene-Benzene_TS_1.50	−0.8[a]	0.1	−0.1	−0.1	−0.2	−1.1	−0.1	−0.3	−0.5	−0.8	−0.8	−0.2	−0.5	−0.7	−0.7
Benzene-Benzene_TS_2.00	−0.2[a]	−0.0	−0.0	−0.0	−0.1	−0.4	−0.0	−0.1	−0.2	−0.2	−0.2	−0.1	−0.2	−0.2	−0.2
Pyridine-Pyridine_TS_0.90	−2.5[a]	14.0	3.1	3.2	0.1	−2.5	2.3	−0.6	−3.1	−3.3	−3.3	0.7	−2.5	−2.8	−2.8
Pyridine-Pyridine_TS_0.95	−3.3[a]	9.7	1.7	1.6	−0.9	−3.2	0.9	−1.0	−3.2	−3.5	−3.4	−0.1	−2.8	−3.2	−3.1
Pyridine-Pyridine_TS_1.00	−3.5[a]	6.7	0.9	0.8	−1.2	−3.3	0.2	−1.2	−3.0	−3.4	−3.3	−0.5	−2.8	−3.2	−3.1
Pyridine-Pyridine_TS_1.05	−3.5[a]	4.7	0.5	0.4	−1.2	−3.2	−0.2	−1.1	−2.7	−3.1	−3.1	−0.6	−2.5	−3.0	−3.0
Pyridine-Pyridine_TS_1.10	−3.2[a]	3.2	0.3	0.1	−1.1	−3.1	−0.3	−1.1	−2.3	−2.8	−2.8	−0.7	−2.2	−2.7	−2.7
Pyridine-Pyridine_TS_1.25	−2.3[a]	1.0	−0.0	−0.1	−0.7	−2.4	−0.4	−0.8	−1.6	−2.0	−2.0	−0.6	−1.5	−1.9	−1.9
Pyridine-Pyridine_TS_1.50	−1.2[a]	0.1	−0.2	−0.2	−0.4	−1.4	−0.3	−0.5	−0.9	−1.1	−1.1	−0.4	−0.8	−1.0	−1.0
Pyridine-Pyridine_TS_2.00	−0.4[a]	−0.0	−0.1	−0.1	−0.2	−0.5	−0.1	−0.2	−0.3	−0.4	−0.4	−0.2	−0.3	−0.4	−0.3
Benzene-Pyridine_TS_0.90	−2.1[a]	12.9	1.6	0.7	0.0	−2.9	2.5	−0.3	−3.0	−3.2	−3.2	1.3	−1.9	−2.4	−2.4
Benzene-Pyridine_TS_0.95	−3.0[a]	8.6	0.7	−0.3	−0.9	−3.5	1.0	−0.9	−3.1	−3.5	−3.4	0.3	−2.5	−3.0	−2.9
Benzene-Pyridine_TS_1.00	−3.3[a]	5.7	0.4	−0.5	−1.2	−3.5	0.3	−1.0	−2.9	−3.3	−3.3	−0.2	−2.6	−3.0	−3.0
Benzene-Pyridine_TS_1.05	−3.3[a]	3.8	0.3	−0.6	−1.1	−3.3	−0.1	−1.0	−2.5	−3.0	−3.0	−0.5	−2.4	−2.9	−2.8
Benzene-Pyridine_TS_1.10	−3.0[a]	2.5	0.2	−0.5	−1.0	−3.1	−0.3	−1.0	−2.2	−2.7	−2.7	−0.6	−2.1	−2.6	−2.6
Benzene-Pyridine_TS_1.25	−2.1[a]	0.7	−0.1	−0.4	−0.6	−2.3	−0.3	−0.8	−1.4	−1.9	−1.8	−0.5	−1.4	−1.8	−1.8
Benzene-Pyridine_TS_1.50	−1.0[a]	0.0	−0.2	−0.2	−0.3	−1.3	−0.2	−0.5	−0.8	−1.0	−1.0	−0.4	−0.7	−0.9	−0.9
Benzene-Pyridine_TS_2.00	−0.3[a]	−0.0	−0.1	−0.1	−0.1	−0.4	−0.1	−0.2	−0.3	−0.4	−0.3	−0.2	−0.3	−0.3	−0.3
Benzene-Ethyne_CH-pi_0.90	−1.9[a]	10.8	0.8	0.2	0.2	−1.1	1.7	−1.5	−3.3	−3.3	−3.2	0.4	−1.6	−1.9	−1.9
Benzene-Ethyne_CH-pi_0.95	−2.6[a]	7.3	0.1	−0.7	−0.7	−1.9	0.6	−1.8	−3.3	−3.4	−3.3	−0.4	−2.2	−2.4	−2.4
Benzene-Ethyne_CH-pi_1.00	−2.9[a]	4.9	−0.1	−0.8	−1.0	−2.1	−0.0	−1.8	−3.0	−3.2	−3.2	−0.7	−2.3	−2.5	−2.5
Benzene-Ethyne_CH-pi_1.05	−2.8[a]	3.3	−0.1	−0.8	−1.0	−2.0	−0.3	−1.6	−2.6	−2.9	−2.9	−0.9	−2.1	−2.4	−2.4
Benzene-Ethyne_CH-pi_1.10	−2.6[a]	2.2	−0.1	−0.7	−0.8	−1.9	−0.4	−1.5	−2.3	−2.6	−2.5	−0.9	−1.9	−2.2	−2.2
Benzene-Ethyne_CH-pi_1.25	−1.8[a]	0.6	−0.1	−0.4	−0.5	−1.4	−0.4	−1.1	−1.5	−1.8	−1.8	−0.7	−1.3	−1.6	−1.5
Benzene-Ethyne_CH-pi_1.50	−0.9[a]	0.0	−0.2	−0.2	−0.2	−0.7	−0.3	−0.6	−0.8	−1.0	−1.0	−0.5	−0.7	−0.8	−0.8
Benzene-Ethyne_CH-pi_2.00	−0.3[a]	−0.0	−0.1	−0.1	−0.1	−0.2	−0.1	−0.2	−0.3	−0.3	−0.3	−0.2	−0.2	−0.3	−0.3
Ethyne-Ethyne_TS_0.90	−1.2[a]	3.3	−0.4	−1.1	−0.2	−0.7	0.1	−1.6	−2.2	−2.3	−2.3	−0.8	−1.4	−1.6	−1.6
Ethyne-Ethyne_TS_0.95	−1.5[a]	2.3	−0.5	−1.0	−0.4	−0.8	−0.2	−1.4	−1.9	−1.9	−1.9	−0.7	−1.3	−1.5	−1.5
Ethyne-Ethyne_TS_1.00	−1.5[a]	1.5	−0.4	−0.8	−0.5	−0.8	−0.3	−1.1	−1.6	−1.6	−1.7	−0.7	−1.2	−1.3	−1.3
Ethyne-Ethyne_TS_1.05	−1.5[a]	1.0	−0.3	−0.6	−0.4	−0.7	−0.3	−1.0	−1.3	−1.4	−1.4	−0.6	−1.0	−1.2	−1.2

... continued on next page ...

Table S10: *... continued from previous page ...*

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Ethyne-Ethyne_TS_1.10	−1.3[a]	0.7	−0.2	−0.5	−0.3	−0.7	−0.3	−0.8	−1.1	−1.2	−1.2	−0.5	−0.9	−1.0	−1.0
Ethyne-Ethyne_TS_1.25	−0.9[a]	0.2	−0.1	−0.2	−0.2	−0.5	−0.2	−0.5	−0.7	−0.8	−0.8	−0.4	−0.6	−0.7	−0.7
Ethyne-Ethyne_TS_1.50	−0.5[a]	−0.0	−0.1	−0.1	−0.1	−0.3	−0.1	−0.3	−0.4	−0.4	−0.4	−0.2	−0.3	−0.4	−0.4
Ethyne-Ethyne_TS_2.00	−0.1[a]	−0.0	−0.0	−0.0	−0.0	−0.1	−0.0	−0.1	−0.1	−0.1	−0.1	−0.1	−0.1	−0.1	−0.1
Benzene-AcOH_OH-pi_0.90	−4.0[a]	14.8	1.4	0.4	−1.3	−3.1	0.8	−2.8	−5.0	−5.1	−5.0	−1.1	−3.6	−4.1	−4.0
Benzene-AcOH_OH-pi_0.95	−4.6[a]	10.6	0.1	−0.9	−2.3	−3.8	−0.1	−2.8	−4.7	−4.9	−4.8	−1.5	−3.8	−4.2	−4.1
Benzene-AcOH_OH-pi_1.00	−4.7[a]	7.6	−0.5	−1.4	−2.6	−3.9	−0.6	−2.6	−4.3	−4.5	−4.5	−1.7	−3.7	−4.0	−4.0
Benzene-AcOH_OH-pi_1.05	−4.5[a]	5.4	−0.6	−1.5	−2.5	−3.8	−0.9	−2.4	−3.8	−4.0	−4.0	−1.6	−3.4	−3.7	−3.7
Benzene-AcOH_OH-pi_1.10	−4.2[a]	3.8	−0.6	−1.3	−2.3	−3.5	−1.0	−2.1	−3.3	−3.6	−3.6	−1.6	−3.1	−3.4	−3.4
Benzene-AcOH_OH-pi_1.25	−3.1[a]	1.3	−0.4	−0.8	−1.5	−2.7	−0.9	−1.5	−2.2	−2.5	−2.5	−1.2	−2.1	−2.5	−2.4
Benzene-AcOH_OH-pi_1.50	−1.7[a]	0.1	−0.3	−0.4	−0.8	−1.6	−0.6	−0.9	−1.2	−1.4	−1.4	−0.8	−1.2	−1.4	−1.4
Benzene-AcOH_OH-pi_2.00	−0.6[a]	−0.1	−0.2	−0.1	−0.3	−0.5	−0.2	−0.3	−0.4	−0.5	−0.5	−0.3	−0.4	−0.5	−0.5
Benzene-AcNH2_NH-pi_0.90	−3.8[a]	11.5	−0.7	0.5	−1.7	−3.2	−0.2	−3.2	−5.1	−5.3	−5.3	−1.8	−4.0	−4.4	−4.4
Benzene-AcNH2_NH-pi_0.95	−4.3[a]	8.3	−1.2	−0.6	−2.3	−3.7	−0.9	−3.2	−4.9	−5.1	−5.0	−2.0	−4.1	−4.4	−4.4
Benzene-AcNH2_NH-pi_1.00	−4.4[a]	5.9	−1.2	−1.0	−2.4	−3.7	−1.2	−3.0	−4.4	−4.7	−4.7	−2.1	−3.9	−4.2	−4.2
Benzene-AcNH2_NH-pi_1.05	−4.2[a]	4.2	−1.0	−1.0	−2.3	−3.5	−1.3	−2.7	−3.9	−4.2	−4.2	−2.0	−3.6	−3.9	−3.9
Benzene-AcNH2_NH-pi_1.10	−4.0[a]	3.0	−0.8	−1.0	−2.0	−3.2	−1.3	−2.4	−3.5	−3.8	−3.8	−1.9	−3.2	−3.6	−3.6
Benzene-AcNH2_NH-pi_1.25	−3.0[a]	1.0	−0.5	−0.7	−1.4	−2.5	−1.0	−1.7	−2.4	−2.7	−2.7	−1.5	−2.3	−2.6	−2.6
Benzene-AcNH2_NH-pi_1.50	−1.6[a]	0.0	−0.4	−0.4	−0.8	−1.6	−0.6	−1.0	−1.3	−1.6	−1.5	−0.9	−1.3	−1.5	−1.4
Benzene-AcNH2_NH-pi_2.00	−0.5[a]	−0.1	−0.2	−0.2	−0.3	−0.5	−0.2	−0.4	−0.4	−0.5	−0.5	−0.3	−0.4	−0.5	−0.4
Benzene-Water_OH-pi_0.90	−2.8[a]	9.4	−0.1	−1.1	−1.9	−2.6	0.1	−2.6	−4.0	−4.0	−4.0	−1.5	−3.2	−3.4	−3.4
Benzene-Water_OH-pi_0.95	−3.2[a]	6.6	−0.6	−1.5	−2.3	−2.8	−0.5	−2.5	−3.8	−3.8	−3.8	−1.7	−3.2	−3.4	−3.4
Benzene-Water_OH-pi_1.00	−3.3[a]	4.6	−0.7	−1.5	−2.3	−2.8	−0.9	−2.3	−3.4	−3.5	−3.5	−1.7	−3.1	−3.3	−3.2
Benzene-Water_OH-pi_1.05	−3.1[a]	3.2	−0.6	−1.3	−2.1	−2.6	−1.0	−2.1	−3.0	−3.2	−3.1	−1.7	−2.8	−3.0	−3.0
Benzene-Water_OH-pi_1.10	−2.9[a]	2.2	−0.5	−1.1	−1.8	−2.4	−1.0	−1.9	−2.6	−2.8	−2.8	−1.6	−2.5	−2.8	−2.7
Benzene-Water_OH-pi_1.25	−2.1[a]	0.6	−0.4	−0.6	−1.2	−1.9	−0.9	−1.4	−1.8	−2.1	−2.0	−1.3	−1.8	−2.0	−2.0
Benzene-Water_OH-pi_1.50	−1.2[a]	−0.0	−0.4	−0.3	−0.7	−1.2	−0.6	−0.9	−1.1	−1.2	−1.2	−0.8	−1.0	−1.2	−1.2
Benzene-Water_OH-pi_2.00	−0.4[a]	−0.1	−0.2	−0.1	−0.3	−0.4	−0.3	−0.4	−0.4	−0.5	−0.5	−0.4	−0.4	−0.5	−0.5
Benzene-MeOH_OH-pi_0.90	−3.5[a]	13.9	1.5	0.3	−0.9	−2.5	1.2	−1.7	−4.1	−4.1	−4.0	−0.3	−3.1	−3.5	−3.4
Benzene-MeOH_OH-pi_0.95	−4.0[a]	10.0	0.4	−0.8	−1.7	−3.2	0.2	−1.8	−3.9	−4.0	−4.0	−0.8	−3.3	−3.7	−3.6
Benzene-MeOH_OH-pi_1.00	−4.2[a]	7.2	−0.0	−1.1	−1.9	−3.3	−0.4	−1.8	−3.6	−3.8	−3.7	−1.1	−3.3	−3.6	−3.5
Benzene-MeOH_OH-pi_1.05	−4.1[a]	5.1	−0.2	−1.1	−1.9	−3.3	−0.7	−1.6	−3.2	−3.4	−3.4	−1.2	−3.1	−3.4	−3.3
Benzene-MeOH_OH-pi_1.10	−3.8[a]	3.6	−0.2	−1.0	−1.7	−3.1	−0.8	−1.5	−2.8	−3.1	−3.1	−1.2	−2.8	−3.1	−3.1
Benzene-MeOH_OH-pi_1.25	−2.8[a]	1.2	−0.2	−0.6	−1.1	−2.6	−0.8	−1.1	−1.9	−2.2	−2.2	−1.0	−1.9	−2.3	−2.2
Benzene-MeOH_OH-pi_1.50	−1.5[a]	0.1	−0.3	−0.3	−0.6	−1.6	−0.5	−0.7	−1.0	−1.3	−1.3	−0.7	−1.1	−1.3	−1.3
Benzene-MeOH_OH-pi_2.00	−0.5[a]	−0.1	−0.2	−0.1	−0.3	−0.5	−0.2	−0.3	−0.4	−0.5	−0.5	−0.3	−0.4	−0.5	−0.4
Benzene-MeNH2_NH-pi_0.90	−2.5[a]	11.7	0.7	0.5	−0.8	−3.0	1.5	−0.4	−2.9	−3.0	−3.0	0.8	−2.2	−2.6	−2.5
Benzene-MeNH2_NH-pi_0.95	−3.1[a]	8.3	0.3	−0.2	−1.3	−3.5	0.5	−0.7	−2.9	−3.1	−3.0	0.1	−2.5	−2.9	−2.8
Benzene-MeNH2_NH-pi_1.00	−3.2[a]	5.8	0.2	−0.4	−1.4	−3.6	−0.0	−0.8	−2.6	−2.9	−2.9	−0.3	−2.5	−2.9	−2.8
Benzene-MeNH2_NH-pi_1.05	−3.1[a]	4.0	0.1	−0.5	−1.3	−3.5	−0.3	−0.8	−2.3	−2.7	−2.6	−0.5	−2.3	−2.7	−2.6
Benzene-MeNH2_NH-pi_1.10	−2.9[a]	2.7	0.1	−0.4	−1.1	−3.3	−0.4	−0.8	−2.0	−2.4	−2.3	−0.5	−2.0	−2.4	−2.4
Benzene-MeNH2_NH-pi_1.25	−1.9[a]	0.8	−0.1	−0.3	−0.7	−2.5	−0.4	−0.6	−1.2	−1.6	−1.6	−0.5	−1.3	−1.6	−1.6
Benzene-MeNH2_NH-pi_1.50	−0.9[a]	0.0	−0.2	−0.2	−0.3	−1.4	−0.3	−0.4	−0.6	−0.8	−0.8	−0.3	−0.6	−0.8	−0.8
Benzene-MeNH2_NH-pi_2.00	−0.3[a]	−0.0	−0.1	−0.1	−0.1	−0.3	−0.1	−0.1	−0.2	−0.3	−0.2	−0.1	−0.2	−0.2	−0.2
Benzene-Peptide_NH-pi_0.90	−3.7[a]	18.2	1.1	1.3	−0.6	−4.1	2.3	−1.0	−4.6	−4.8	−4.7	1.1	−3.2	−3.8	−3.7

... continued on next page ...

Table S10: *... continued from previous page ...*

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Benzene-Peptide_NH-pi_0.95	−5.0[a]	12.3	0.1	−0.4	−1.9	−5.2	0.6	−1.7	−4.7	−5.1	−5.0	−0.3	−4.0	−4.5	−4.4
Benzene-Peptide_NH-pi_1.00	−5.3[a]	8.3	−0.1	−0.9	−2.3	−5.4	−0.3	−1.9	−4.4	−4.9	−4.8	−0.9	−4.0	−4.6	−4.5
Benzene-Peptide_NH-pi_1.05	−5.1[a]	5.6	−0.2	−1.0	−2.2	−5.2	−0.7	−1.8	−3.9	−4.5	−4.4	−1.1	−3.8	−4.3	−4.2
Benzene-Peptide_NH-pi_1.10	−4.8[a]	3.8	−0.2	−0.9	−1.9	−4.8	−0.9	−1.7	−3.4	−4.0	−3.9	−1.2	−3.4	−3.9	−3.9
Benzene-Peptide_NH-pi_1.25	−3.4[a]	1.1	−0.3	−0.6	−1.2	−3.7	−0.8	−1.3	−2.3	−2.8	−2.8	−1.1	−2.3	−2.8	−2.7
Benzene-Peptide_NH-pi_1.50	−1.8[a]	0.0	−0.4	−0.4	−0.7	−2.2	−0.5	−0.8	−1.3	−1.6	−1.5	−0.7	−1.2	−1.5	−1.5
Benzene-Peptide_NH-pi_2.00	−0.6[a]	−0.1	−0.2	−0.2	−0.3	−0.7	−0.3	−0.4	−0.5	−0.6	−0.6	−0.4	−0.5	−0.6	−0.5
Pyridine-Pyridine_CH-N_0.90	−2.8[a]	14.1	3.9	3.1	−0.1	−1.5	2.1	−1.8	−3.3	−3.4	−3.5	−0.7	−2.5	−2.9	−2.9
Pyridine-Pyridine_CH-N_0.95	−3.8[a]	9.7	1.8	1.5	−1.7	−3.0	0.1	−2.4	−3.8	−3.9	−4.0	−1.4	−3.1	−3.3	−3.4
Pyridine-Pyridine_CH-N_1.00	−4.1[a]	5.5	−0.1	−0.1	−2.5	−3.6	−1.2	−2.6	−3.7	−3.9	−3.9	−1.8	−3.2	−3.4	−3.4
Pyridine-Pyridine_CH-N_1.05	−3.9[a]	3.2	−1.0	−0.7	−2.5	−3.4	−1.5	−2.4	−3.3	−3.5	−3.5	−1.7	−2.9	−3.1	−3.1
Pyridine-Pyridine_CH-N_1.10	−3.4[a]	1.8	−1.1	−0.8	−2.2	−3.1	−1.5	−2.1	−2.8	−3.0	−3.1	−1.6	−2.5	−2.7	−2.8
Pyridine-Pyridine_CH-N_1.25	−2.2[a]	0.2	−0.7	−0.7	−1.3	−2.2	−1.0	−1.3	−1.7	−1.9	−1.9	−1.0	−1.5	−1.7	−1.8
Pyridine-Pyridine_CH-N_1.50	−1.0[a]	−0.2	−0.4	−0.3	−0.6	−1.4	−0.5	−0.6	−0.8	−0.9	−1.0	−0.5	−0.7	−0.8	−0.8
Pyridine-Pyridine_CH-N_2.00	−0.3[a]	−0.1	−0.1	−0.1	−0.2	−0.7	−0.1	−0.2	−0.2	−0.3	−0.3	−0.1	−0.2	−0.2	−0.2
Ethyne-Water_CH-O_0.90	−2.5[a]	6.8	−1.2	−0.9	−1.7	−1.0	−1.4	−3.7	−4.1	−4.1	−4.1	−3.1	−3.5	−3.6	−3.6
Ethyne-Water_CH-O_0.95	−2.8[a]	4.9	−1.7	−0.6	−1.8	−1.3	−1.7	−3.4	−3.7	−3.7	−3.7	−2.9	−3.2	−3.4	−3.4
Ethyne-Water_CH-O_1.00	−2.8[a]	3.4	−1.8	−0.6	−1.7	−1.5	−1.8	−3.0	−3.3	−3.3	−3.3	−2.7	−3.0	−3.1	−3.1
Ethyne-Water_CH-O_1.05	−2.8[a]	2.4	−1.7	−0.8	−1.6	−1.5	−1.8	−2.7	−2.9	−3.0	−3.0	−2.5	−2.8	−2.9	−2.9
Ethyne-Water_CH-O_1.10	−2.6[a]	1.6	−1.5	−0.9	−1.4	−1.4	−1.7	−2.4	−2.6	−2.7	−2.7	−2.3	−2.6	−2.6	−2.6
Ethyne-Water_CH-O_1.25	−2.0[a]	0.3	−1.0	−0.8	−0.9	−1.1	−1.3	−1.8	−1.9	−2.0	−2.0	−1.7	−1.9	−2.0	−2.0
Ethyne-Water_CH-O_1.50	−1.2[a]	−0.2	−0.5	−0.5	−0.5	−0.6	−0.8	−1.1	−1.2	−1.2	−1.2	−1.1	−1.2	−1.2	−1.2
Ethyne-Water_CH-O_2.00	−0.5[a]	−0.2	−0.2	−0.2	−0.2	−0.2	−0.4	−0.5	−0.5	−0.5	−0.5	−0.5	−0.5	−0.5	−0.5
Ethyne-AcOH_OH-pi_0.90	−4.3[a]	11.6	0.1	−0.2	−0.7	−1.1	−0.7	−4.8	−6.0	−6.0	−6.0	−3.1	−4.3	−4.7	−4.7
Ethyne-AcOH_OH-pi_0.95	−4.8[a]	8.3	−1.0	−1.3	−1.5	−2.0	−1.2	−4.4	−5.4	−5.4	−5.4	−3.0	−4.2	−4.4	−4.5
Ethyne-AcOH_OH-pi_1.00	−4.9[a]	5.9	−1.5	−1.9	−1.9	−2.3	−1.5	−3.9	−4.8	−4.8	−4.8	−2.8	−3.9	−4.1	−4.1
Ethyne-AcOH_OH-pi_1.05	−4.7[a]	4.2	−1.6	−2.0	−1.9	−2.3	−1.6	−3.4	−4.2	−4.2	−4.2	−2.5	−3.5	−3.7	−3.7
Ethyne-AcOH_OH-pi_1.10	−4.4[a]	2.9	−1.4	−1.9	−1.8	−2.2	−1.6	−2.9	−3.6	−3.7	−3.7	−2.2	−3.1	−3.3	−3.3
Ethyne-AcOH_OH-pi_1.25	−3.3[a]	0.9	−0.8	−1.2	−1.2	−1.6	−1.2	−1.9	−2.3	−2.5	−2.5	−1.6	−2.1	−2.3	−2.3
Ethyne-AcOH_OH-pi_1.50	−1.8[a]	−0.0	−0.4	−0.5	−0.6	−1.0	−0.7	−1.0	−1.2	−1.4	−1.4	−0.9	−1.1	−1.3	−1.3
Ethyne-AcOH_OH-pi_2.00	−0.6[a]	−0.1	−0.2	−0.2	−0.2	−0.3	−0.3	−0.4	−0.4	−0.5	−0.5	−0.3	−0.4	−0.4	−0.4
Pentane-AcOH_0.90	−2.7[a]	13.0	0.3	0.2	−1.5	−2.7	1.1	−0.6	−3.3	−3.5	−3.4	0.4	−3.1	−3.3	−3.2
Pentane-AcOH_0.95	−2.9[a]	9.8	0.2	−0.2	−1.4	−2.8	0.5	−0.6	−3.0	−3.3	−3.2	0.0	−2.9	−3.2	−3.1
Pentane-AcOH_1.00	−2.9[a]	7.3	0.2	−0.5	−1.2	−2.7	0.1	−0.6	−2.6	−3.0	−2.9	−0.1	−2.6	−3.0	−3.0
Pentane-AcOH_1.05	−2.7[a]	5.4	0.2	−0.5	−1.0	−2.6	−0.1	−0.5	−2.2	−2.7	−2.6	−0.2	−2.3	−2.8	−2.7
Pentane-AcOH_1.10	−2.5[a]	4.1	0.2	−0.5	−0.9	−2.5	−0.1	−0.5	−1.9	−2.4	−2.3	−0.3	−2.0	−2.5	−2.5
Pentane-AcOH_1.25	−1.8[a]	1.7	0.2	−0.3	−0.5	−2.1	−0.2	−0.3	−1.2	−1.7	−1.6	−0.2	−1.3	−1.8	−1.7
Pentane-AcOH_1.50	−0.8[a]	0.3	0.0	−0.1	−0.2	−1.3	−0.1	−0.1	−0.5	−0.8	−0.8	−0.1	−0.6	−0.8	−0.8
Pentane-AcOH_2.00	−0.2[a]	0.0	−0.0	−0.0	−0.1	−0.4	−0.0	−0.0	−0.1	−0.2	−0.2	−0.0	−0.1	−0.2	−0.2
Pentane-AcNH2_0.90	−3.2[a]	16.3	0.3	0.9	−1.6	−3.3	1.7	−0.7	−3.8	−3.9	−3.8	0.6	−3.5	−3.6	−3.4
Pentane-AcNH2_0.95	−3.5[a]	11.7	0.1	−0.0	−1.6	−3.5	0.7	−0.8	−3.5	−3.7	−3.6	0.1	−3.3	−3.6	−3.5
Pentane-AcNH2_1.00	−3.5[a]	8.5	0.1	−0.4	−1.4	−3.4	0.2	−0.8	−3.0	−3.4	−3.3	−0.2	−3.0	−3.4	−3.3
Pentane-AcNH2_1.05	−3.3[a]	6.1	0.1	−0.6	−1.2	−3.2	−0.1	−0.7	−2.5	−3.1	−3.0	−0.3	−2.6	−3.1	−3.0
Pentane-AcNH2_1.10	−3.0[a]	4.4	0.2	−0.6	−1.0	−3.0	−0.2	−0.6	−2.1	−2.7	−2.6	−0.3	−2.3	−2.8	−2.7
Pentane-AcNH2_1.25	−2.1[a]	1.6	0.2	−0.4	−0.5	−2.4	−0.2	−0.4	−1.3	−1.8	−1.7	−0.3	−1.4	−1.9	−1.8

... continued on next page ...

Table S10: ... *continued from previous page* ...

Molecule	Ref.	MNDO	AM1	PM3	PM6	PM7	OM1	OM2	OM2			OM3	OM3		
									D2	D3	D3T		D2	D3	D3T
Pentane-AcNH2_1.50	−1.0[a]	0.3	0.0	−0.1	−0.2	−1.5	−0.1	−0.2	−0.6	−0.9	−0.9	−0.1	−0.7	−0.9	−0.9
Pentane-AcNH2_2.00	−0.3[a]	−0.0	−0.0	−0.0	−0.0	−0.4	−0.0	−0.0	−0.2	−0.3	−0.2	−0.0	−0.2	−0.3	−0.2
Benzene-AcOH_0.90	−2.7[a]	14.6	3.0	2.8	−0.9	−2.7	1.3	−1.3	−4.4	−4.4	−4.3	0.2	−3.5	−3.9	−3.8
Benzene-AcOH_0.95	−3.6[a]	9.8	2.0	1.4	−1.5	−3.3	0.3	−1.5	−4.1	−4.3	−4.2	−0.4	−3.6	−4.0	−3.9
Benzene-AcOH_1.00	−3.8[a]	6.5	1.3	0.7	−1.6	−3.5	−0.2	−1.5	−3.6	−4.0	−3.9	−0.7	−3.3	−3.8	−3.7
Benzene-AcOH_1.05	−3.7[a]	4.4	0.9	0.2	−1.5	−3.4	−0.4	−1.3	−3.1	−3.5	−3.5	−0.8	−2.9	−3.5	−3.4
Benzene-AcOH_1.10	−3.3[a]	2.9	0.5	0.0	−1.3	−3.3	−0.5	−1.2	−2.6	−3.1	−3.1	−0.8	−2.5	−3.1	−3.0
Benzene-AcOH_1.25	−2.2[a]	0.8	−0.0	−0.2	−0.8	−2.7	−0.4	−0.9	−1.6	−2.1	−2.0	−0.6	−1.6	−2.0	−1.9
Benzene-AcOH_1.50	−1.0[a]	0.0	−0.2	−0.2	−0.4	−1.5	−0.3	−0.5	−0.8	−1.1	−1.0	−0.4	−0.8	−1.0	−0.9
Benzene-AcOH_2.00	−0.3[a]	−0.0	−0.1	−0.1	−0.1	−0.4	−0.1	−0.2	−0.3	−0.3	−0.3	−0.1	−0.2	−0.3	−0.2
Peptide-Ethene_0.90	−2.6[a]	11.3	0.7	1.5	−1.2	−2.1	0.7	−1.3	−3.2	−3.3	−3.3	−0.3	−2.7	−3.0	−2.9
Peptide-Ethene_0.95	−2.9[a]	8.1	0.2	0.6	−1.3	−2.4	0.1	−1.3	−2.9	−3.1	−3.1	−0.6	−2.7	−2.9	−2.9
Peptide-Ethene_1.00	−3.0[a]	5.8	0.1	0.1	−1.2	−2.4	−0.2	−1.2	−2.6	−2.8	−2.8	−0.7	−2.5	−2.8	−2.7
Peptide-Ethene_1.05	−2.9[a]	4.2	0.0	−0.1	−1.1	−2.3	−0.4	−1.0	−2.2	−2.6	−2.5	−0.7	−2.2	−2.6	−2.5
Peptide-Ethene_1.10	−2.6[a]	3.0	0.0	−0.2	−0.9	−2.1	−0.4	−0.9	−1.9	−2.3	−2.2	−0.7	−1.9	−2.3	−2.3
Peptide-Ethene_1.25	−1.9[a]	1.1	0.0	−0.2	−0.5	−1.8	−0.3	−0.6	−1.2	−1.6	−1.6	−0.5	−1.2	−1.6	−1.6
Peptide-Ethene_1.50	−0.9[a]	0.1	−0.1	−0.1	−0.2	−1.1	−0.2	−0.3	−0.6	−0.8	−0.8	−0.3	−0.6	−0.8	−0.8
Peptide-Ethene_2.00	−0.2[a]	−0.0	−0.0	−0.0	−0.1	−0.2	−0.1	−0.1	−0.2	−0.2	−0.2	−0.1	−0.1	−0.2	−0.2
Pyridine-Ethyne_0.90	−3.5[a]	6.8	1.7	−0.5	−0.2	−0.5	−1.0	−4.0	−4.6	−4.8	−4.9	−3.6	−4.4	−4.7	−4.7
Pyridine-Ethyne_0.95	−3.9[a]	4.9	0.9	−0.4	−0.9	−1.4	−1.5	−3.7	−4.3	−4.5	−4.5	−3.2	−4.0	−4.3	−4.3
Pyridine-Ethyne_1.00	−4.0[a]	3.5	0.3	−0.5	−1.3	−1.8	−1.8	−3.3	−3.9	−4.1	−4.1	−2.9	−3.6	−3.8	−3.8
Pyridine-Ethyne_1.05	−3.9[a]	2.4	−0.1	−0.7	−1.5	−2.0	−1.9	−3.0	−3.5	−3.7	−3.7	−2.6	−3.2	−3.4	−3.4
Pyridine-Ethyne_1.10	−3.7[a]	1.6	−0.5	−0.8	−1.5	−2.0	−1.9	−2.7	−3.1	−3.3	−3.3	−2.3	−2.9	−3.1	−3.1
Pyridine-Ethyne_1.25	−2.8[a]	0.3	−0.9	−0.8	−1.3	−1.7	−1.5	−2.0	−2.3	−2.4	−2.4	−1.7	−2.1	−2.2	−2.2
Pyridine-Ethyne_1.50	−1.7[a]	−0.2	−0.6	−0.5	−0.7	−1.2	−0.9	−1.2	−1.3	−1.4	−1.4	−1.0	−1.2	−1.3	−1.3
Pyridine-Ethyne_2.00	−0.6[a]	−0.2	−0.3	−0.3	−0.3	−0.7	−0.4	−0.5	−0.5	−0.6	−0.6	−0.4	−0.5	−0.5	−0.5
MeNH2-Pyridine_0.90	−3.4[a]	13.1	2.9	4.1	0.4	−3.1	1.6	−0.2	−2.3	−2.5	−2.4	0.3	−2.3	−2.6	−2.5
MeNH2-Pyridine_0.95	−3.9[a]	9.7	1.7	2.8	−0.8	−4.0	0.4	−0.8	−2.6	−2.8	−2.8	−0.3	−2.6	−2.9	−2.9
MeNH2-Pyridine_1.00	−4.0[a]	7.1	0.9	1.7	−1.3	−4.3	−0.3	−1.0	−2.6	−2.9	−2.8	−0.6	−2.7	−3.0	−2.9
MeNH2-Pyridine_1.05	−3.9[a]	5.2	0.4	1.0	−1.6	−4.4	−0.7	−1.1	−2.5	−2.8	−2.7	−0.8	−2.6	−2.9	−2.8
MeNH2-Pyridine_1.10	−3.6[a]	3.7	0.1	0.5	−1.6	−4.3	−0.9	−1.0	−2.3	−2.6	−2.6	−0.8	−2.4	−2.7	−2.7
MeNH2-Pyridine_1.25	−2.7[a]	1.3	−0.3	−0.1	−1.3	−3.6	−0.9	−0.8	−1.6	−2.0	−1.9	−0.7	−1.7	−2.0	−2.0
MeNH2-Pyridine_1.50	−1.5[a]	0.0	−0.3	−0.2	−0.7	−2.4	−0.6	−0.5	−0.9	−1.2	−1.1	−0.5	−0.9	−1.2	−1.1
MeNH2-Pyridine_2.00	−0.5[a]	−0.2	−0.2	−0.1	−0.3	−0.9	−0.3	−0.2	−0.3	−0.4	−0.4	−0.2	−0.3	−0.4	−0.4

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

2 Figures: Reference and Optimized SQC Geometries of Selected Noncovalent Complexes

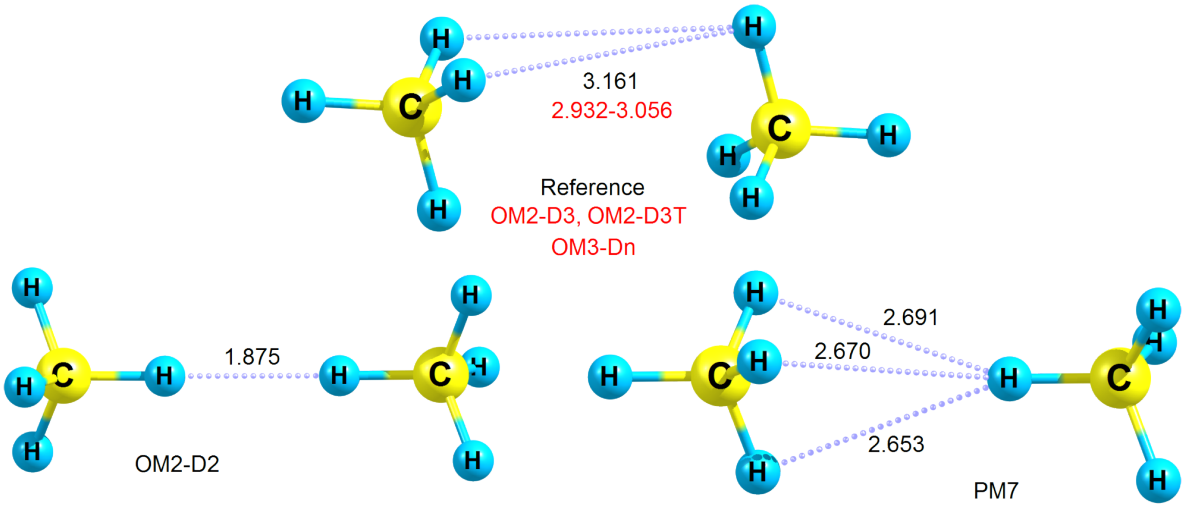

Figure S1: Reference, OM2-D3, OM2-D3T, and OM3-Dn geometries of the methane dimer from the S22 data set (top) and geometries optimized with the OM2-D2 (bottom left) and PM7 (bottom right) methods. Selected interatomic distances are given in Ångstrom.

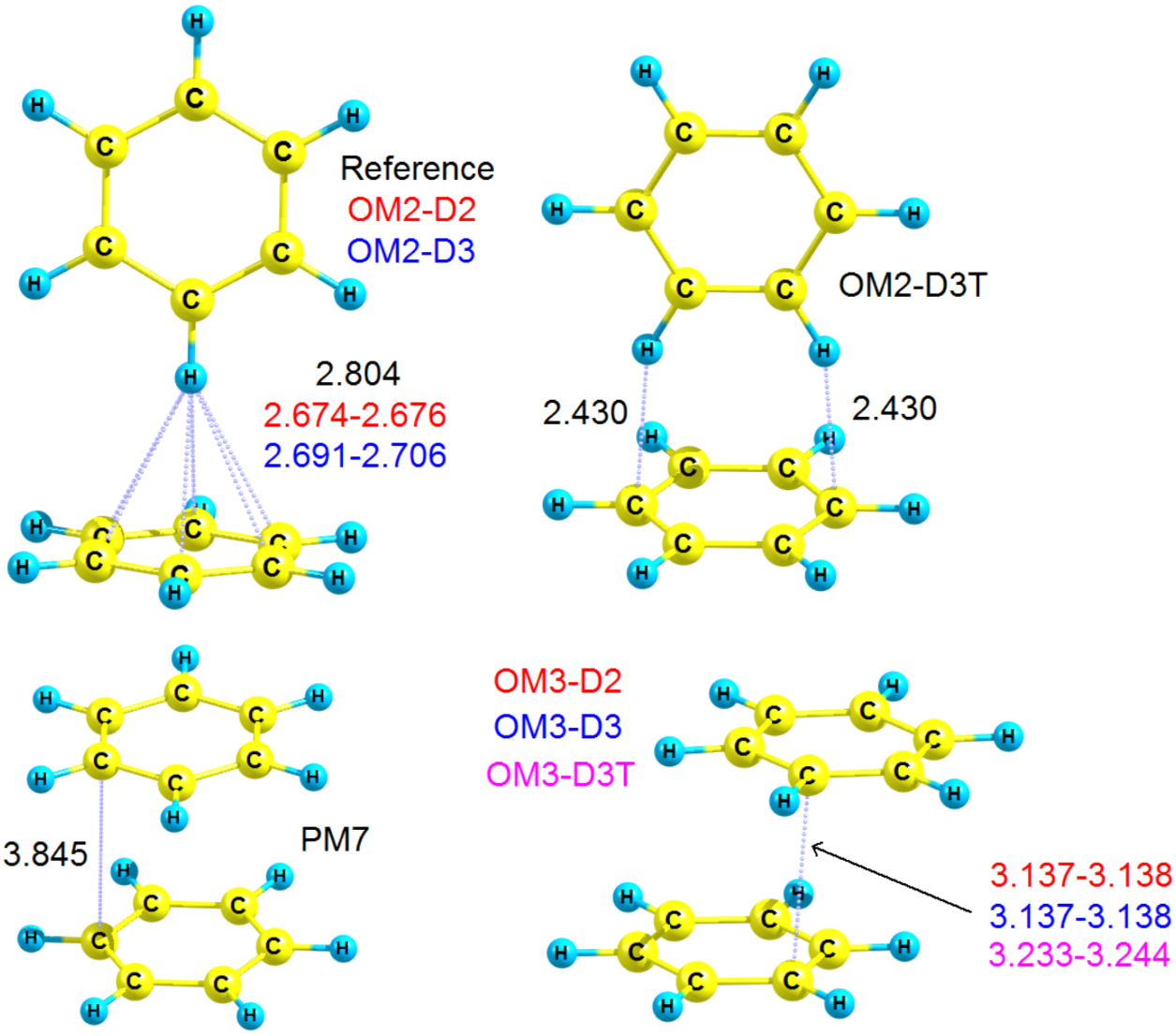

Figure S2: Reference, OM2-D2, and OM2-D3 geometries of the T-shaped benzene dimer from the S22 data set (top left) and geometries optimized with other OMx-Dn and PM7 methods. Selected interatomic distances are given in Ångstrom.

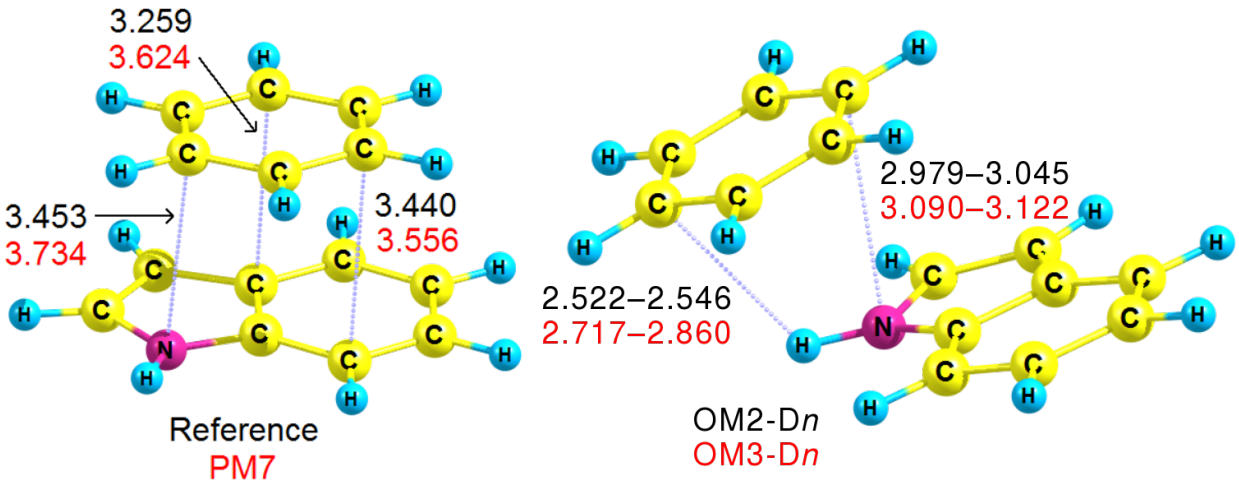

Figure S3: Reference and PM7 geometries of the indole$\cdots$benzene dimer from the S22 data set (left) and geometries optimized with OMx-Dn (right). Selected interatomic distances are given in Ångstrom.

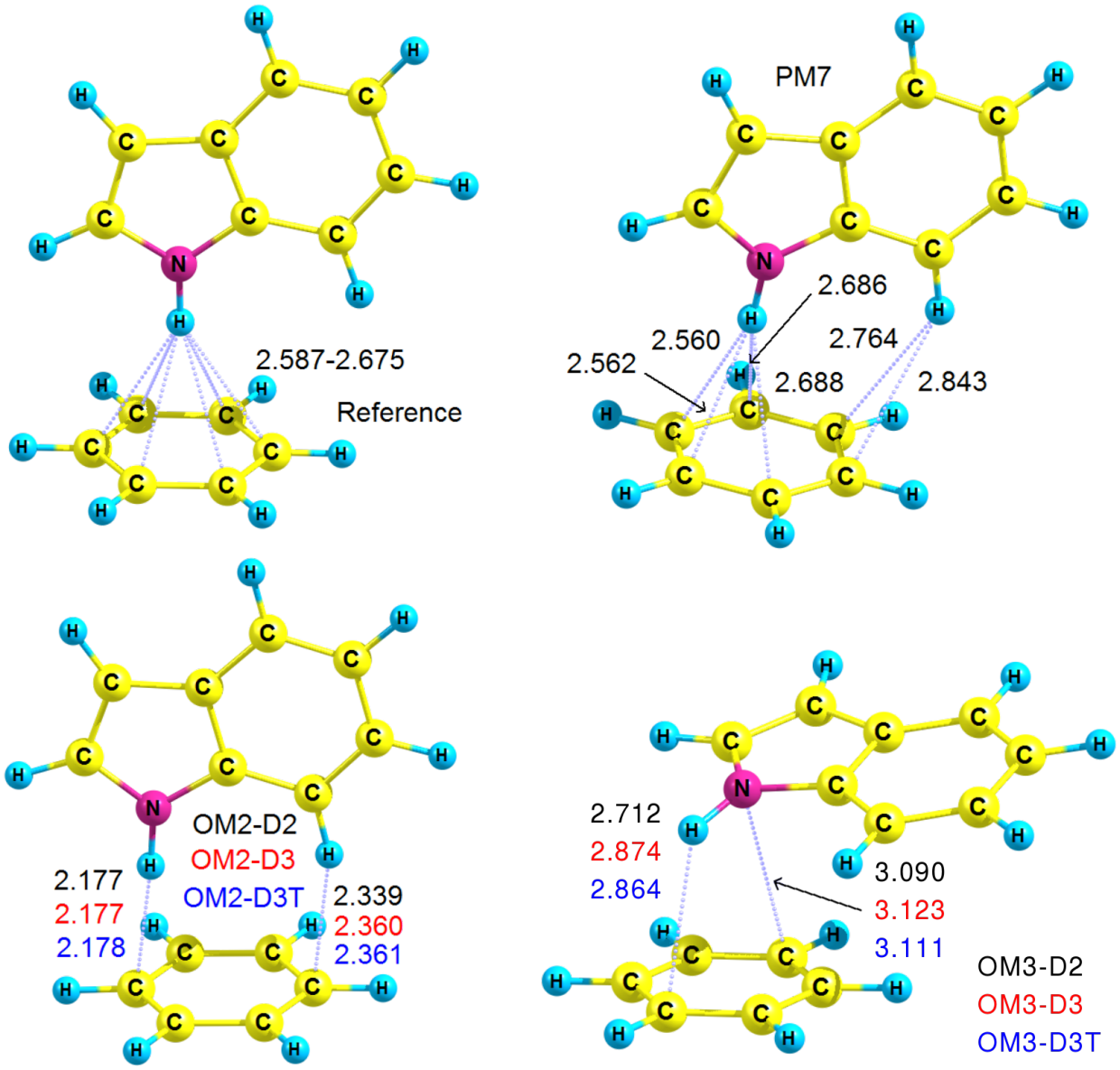

Figure S4: Reference geometry of the T-shaped indole$\cdots$benzene dimer from the S22 data set (top left) and geometries optimized with PM7 (top right), OM2-Dn (bottom left), and OM3-Dn (bottom right). Selected interatomic distances are given in Ångstrom.

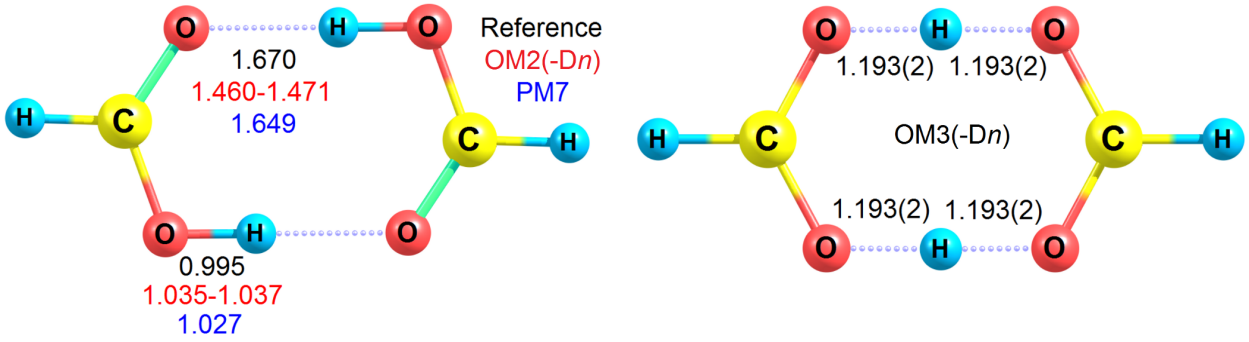

Figure S5: Reference, PM7 and OM2(-Dn) geometries of the formic acid dimer from the S22 data set (left) and geometries optimized with the OM3(-Dn) methods (right). Selected interatomic distances are given in Ångstrom.

3 Additional Statistical Evaluations for RM1

The RM1 method is a reparametrization of the AM1 method. According to the following statistical evaluations, it tends to be generally more accurate than AM1, about as accurate as the PMx methods, and somewhat less accurate than the OMx methods.

For the CHNO benchmark set (Table S11), RM1 predicts heats of formation with a mean absolute error (MAE) of 4.22 kcal/mol, similar to that of PM3 and about 1.1 kcal/mol higher than those of OM2 and OM3. The MAEs of RM1 for bond lengths and angles are similar to those of the PMx methods. For ionization potentials, RM1 performs better than the PMx methods, but not as well as OM2 (MAE 0.36 vs. 0.26 eV). Dipole moments are predicted best by RM1 (MAE 0.21 D vs. 0.23–0.26 D for the OMx methods). RM1 also gives reasonable relative energies and barriers, but is in both cases less accurate than OM2 (MAEs 2.50 vs. 1.96 kcal/mol and 2.39 vs. 1.63 kcal/mol, respectively).

For the FLUOR set (Table S12), RM1 gives larger errors for the heats of formation (MAE 6.27 kcal/mol) compared with the PMx methods (MAEs 5.21–5.87 kcal/mol) and the OMx methods (MAEs 3.70–4.92 kcal/mol). Bond lengths, bond angles, and ionization potentials are predicted by RM1 somewhat less accurately than by the OMx methods, whereas dipole moments are reproduced with similar accuracy (MAE 0.27 D vs. 0.25–0.31 D).

Table S11: Mean Absolute Errors in Calculated Heats of Formation, Relative Energies and Barriers (kcal/mol), Bond Lengths (Å), Bond Angles (degree), Ionization Potentials (eV), and Dipole Moments (D) for the CHNO Set and Its Subsets: MNDO, AM1, RM1, PMx, and OMx

Subset	N	Method								
		MNDO	AM1	RM1	PM3	PM6	PM7	OM1	OM2	OM3
Heats of formation										
Overall	140	6.34	5.51	4.22	4.17	4.80	3.80	3.46	3.10	3.05
CH	57	5.90	4.89	4.86	3.63	4.74	3.50	2.49	1.72	1.63
CHN	32	6.24	4.65	3.89	5.02	4.30	4.11	4.27	3.92	3.80
CHO	39	4.80	5.54	3.14	3.69	4.53	3.42	3.41	4.53	4.20
CHNO	4	13.52	8.36	4.66	3.00	2.59	1.48	6.18	1.96	3.24
HNO	8	13.73	11.93	6.09	7.54	9.63	7.71	5.94	3.28	4.53
Bond lengths										
Overall	242	0.014	0.017	0.013	0.011	0.012	0.011	0.012	0.016	0.019
CH	113	0.011	0.013	0.011	0.011	0.009	0.009	0.012	0.010	0.009
CHN	49	0.011	0.015	0.011	0.010	0.010	0.009	0.009	0.015	0.027
CHO	57	0.017	0.019	0.013	0.011	0.013	0.011	0.013	0.018	0.022
CHNO	5	0.015	0.017	0.010	0.016	0.011	0.010	0.013	0.018	0.033
HNO	18	0.036	0.038	0.032	0.016	0.036	0.036	0.019	0.049	0.043
Bond angles										
Overall	101	2.56	1.90	2.26	2.08	2.14	2.31	1.82	2.24	1.85
CH	38	1.81	1.36	2.06	1.57	1.64	1.88	1.45	1.46	1.23
CHN	22	2.03	1.86	2.04	2.04	1.86	2.04	1.85	2.30	1.82
CHO	31	3.11	2.17	2.44	2.43	2.38	2.69	1.95	2.45	2.03
HNO	10	4.83	3.17	2.97	3.04	3.91	3.30	2.76	4.42	3.76
Ionization potentials										
Overall	52	0.46	0.36	0.36	0.42	0.45	0.42	0.32	0.26	0.44
CH	22	0.38	0.27	0.24	0.34	0.31	0.37	0.24	0.24	0.37
CHN	13	0.54	0.37	0.48	0.52	0.53	0.52	0.33	0.22	0.39
CHO	14	0.57	0.45	0.42	0.51	0.48	0.41	0.41	0.34	0.61
HNO	3	0.24	0.52	0.50	0.16	0.96	0.52	0.33	0.23	0.45
Dipole moments										
Overall	63	0.36	0.24	0.21	0.28	0.38	0.38	0.23	0.25	0.26
CH	20	0.30	0.16	0.12	0.16	0.24	0.24	0.08	0.11	0.10
CHN	16	0.54	0.48	0.34	0.39	0.54	0.54	0.40	0.27	0.33
CHO	19	0.22	0.10	0.19	0.25	0.39	0.33	0.23	0.31	0.26
HNO	6	0.40	0.32	0.19	0.31	0.38	0.56	0.31	0.49	0.58
Relative energies										
Overall	17	9.01	5.70	2.50	4.17	2.97	1.97	5.25	1.96	2.83
CH	9	4.34	2.62	0.65	1.83	1.19	1.39	3.20	0.52	1.08
CHN	3	9.48	7.37	4.41	4.71	2.91	2.17	6.04	4.09	5.65
CHO	3	13.22	7.78	2.34	9.30	4.17	3.41	6.63	3.63	3.91
Barriers										
Overall	60	3.48	2.12	2.39	3.01	2.55	2.46	2.31	1.63	1.61
CH	20	4.27	3.31	3.42	3.25	3.65	3.32	2.37	1.69	2.01
CHN	10	3.20	1.32	2.15	3.17	3.39	3.17	3.03	1.91	1.51
CHO	25	2.42	1.42	1.72	2.07	1.46	1.56	1.61	1.50	1.45
CHNO	3	7.98	3.16	2.67	7.70	2.35	2.46	5.42	1.43	0.68

Table S12: Mean Absolute Errors in Calculated Heats of Formation (kcal/mol), Bond Lengths (Å), Bond Angles (degree), Ionization Potentials (eV), and Dipole Moments (D) for the FLUOR Set and Its Subsets: MNDO, AM1, RM1, PMx, and OMx

Subset	N	Method								
		MNDO	AM1	RM1	PM3	PM6	PM7	OM1	OM2	OM3
Heats of formation										
Overall	48	10.81	7.75	6.27	5.87	5.21	5.82	4.92	3.41	3.70
CHF	39	9.89	7.37	6.30	4.96	4.92	5.57	3.67	3.72	3.88
HNOF	9	14.79	9.42	6.12	9.81	6.48	6.90	10.32	2.08	2.93
Bond lengths										
Overall	125	0.037	0.028	0.029	0.022	0.016	0.017	0.020	0.023	0.024
CHF	104	0.030	0.026	0.023	0.020	0.014	0.015	0.018	0.019	0.021
CHNOF	3	0.029	0.052	0.038	0.021	0.013	0.017	0.024	0.020	0.014
HNOF	17	0.080	0.037	0.063	0.037	0.026	0.026	0.032	0.043	0.044
Bond angles										
Overall	69	3.00	3.16	2.60	2.75	2.76	2.55	1.97	2.23	1.78
CHF	56	2.59	2.93	2.43	2.69	2.64	2.45	1.88	2.06	1.61
CHNOF	3	2.89	3.76	2.21	3.41	3.76	2.61	1.30	2.44	1.75
HNOF	9	5.56	4.59	3.87	3.05	3.50	3.37	2.43	2.91	2.68
Ionization potentials										
Overall	39	0.34	0.53	0.33	0.39	0.50	0.46	0.23	0.26	0.32
CHF	29	0.33	0.47	0.33	0.32	0.36	0.40	0.20	0.25	0.29
HNOF	9	0.38	0.70	0.35	0.57	1.00	0.68	0.30	0.29	0.42
Dipole moments										
Overall	39	0.38	0.31	0.27	0.29	0.33	0.29	0.27	0.31	0.25
CHF	30	0.41	0.29	0.26	0.25	0.31	0.26	0.31	0.33	0.24
HNOF	8	0.29	0.44	0.32	0.47	0.42	0.41	0.15	0.26	0.29