Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Exhaustive exploration of the conformational landscape of mono- and disubstituted five-membered rings by DFT and MP2 calculations

Carlos A. Stortz[a,*] and Ariel M. Sarotti[b,*]

a) Universidad de Buenos Aires, Facultad de Ciencias Exactas, Departamento de Química Orgánica and Centro de Investigaciones en Hidratos de Carbono (CIHIDECAR), Ciudad Universitaria, Pab. 2, 1428 Buenos Aires, Argentina
stortz@go.fcen.uba.ar

b) Instituto de Química Rosario (CONICET), Facultad de Ciencias Bioquímicas y Farmacéuticas, Universidad Nacio-nal de Rosario, Suipacha 531, 2000 Rosario, Argentina.
sarotti@iquir-conicet.gov.ar

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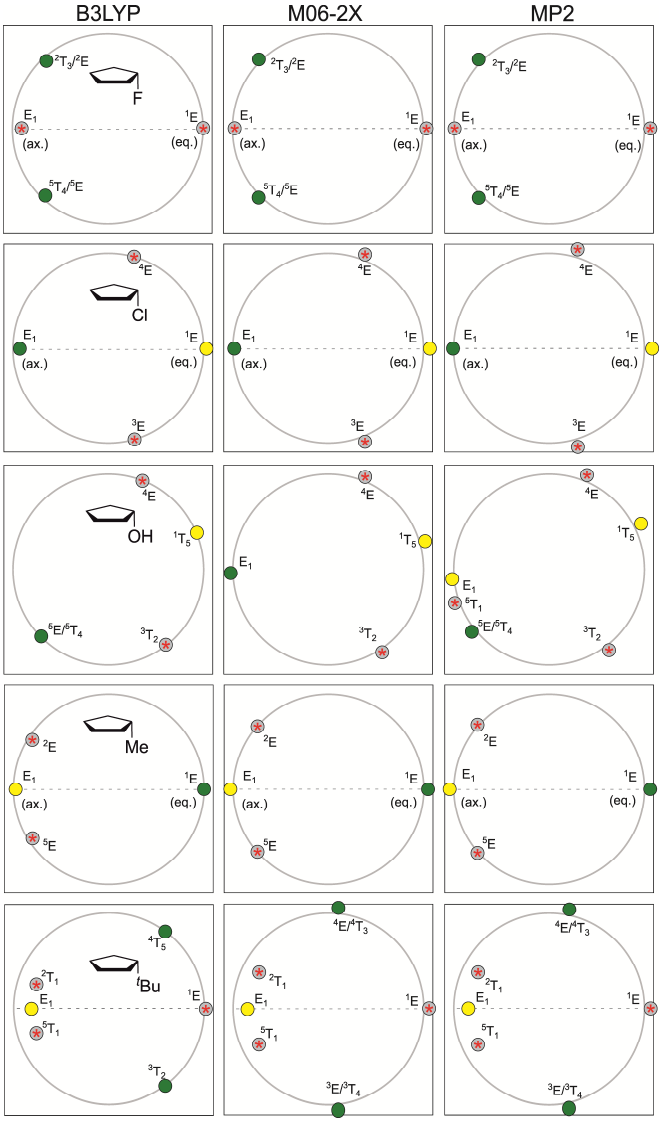

Figure *S*1. Geometry representations of the Cremer-Pople puckering parameters of minima (green, global minima; yellow, local minima) and transition states (grey circle with red star) computed for compounds **2-6** at the three levels of theory under study.

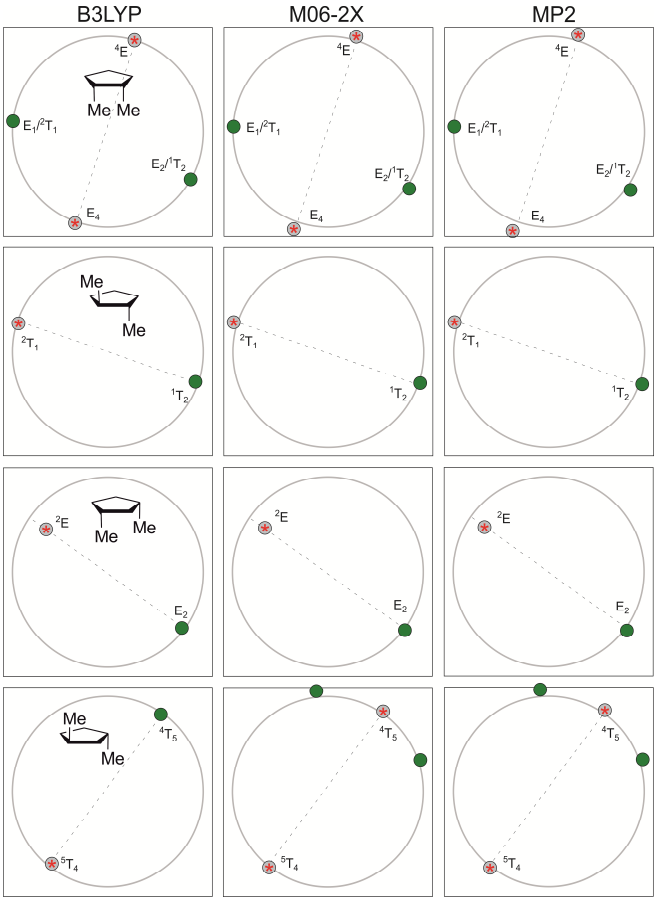

Figure *S*2. Geometry representations of the Cremer-Pople puckering parameters of minima (green, global minima; yellow, local minima) and transition states (grey circle with red star) computed for compounds **10-13** at the three levels of theory under study.

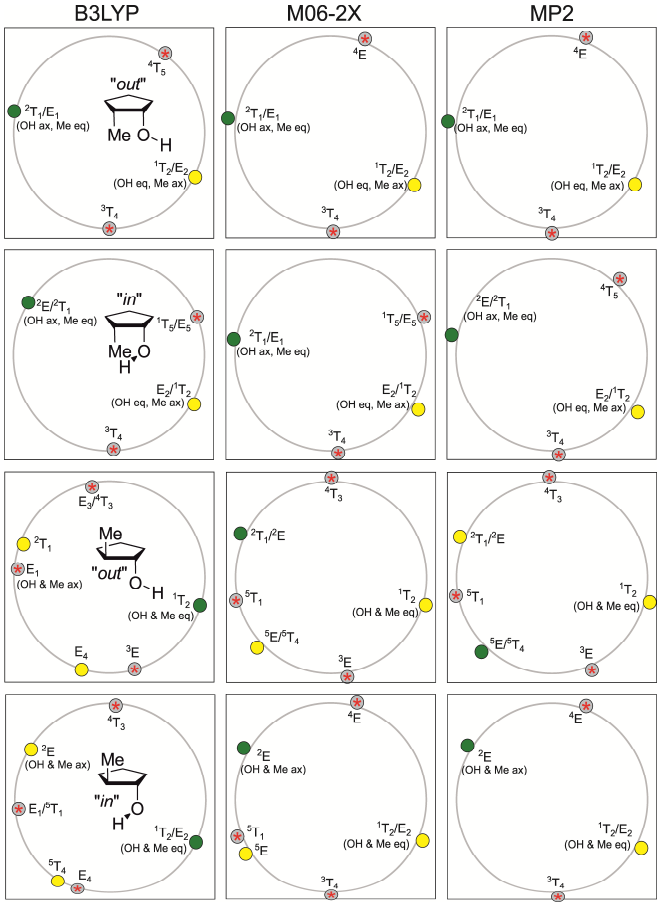

Figure *S*3. Geometry representations of the Cremer-Pople puckering parameters of minima (green, global minima; yellow, local minima) and transition states (grey circle with red star) computed for compounds **14-15** at the three levels of theory under study.

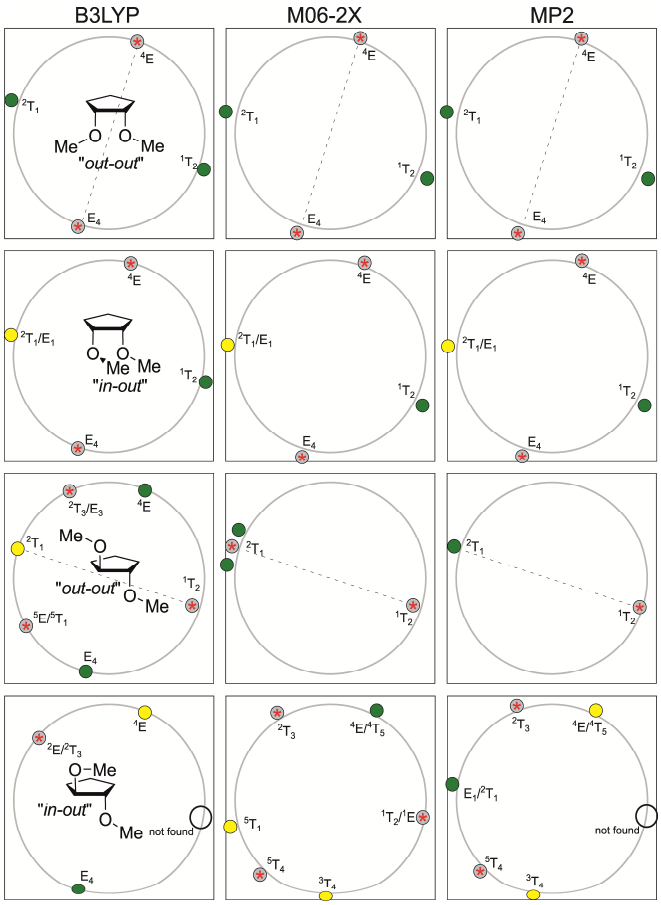

Figure *S*4. Geometry representations of the Cremer-Pople puckering parameters of minima (green, global minima; yellow, local minima) and transition states (grey circle with red star) computed for compounds **16-17** at the three levels of theory under study.

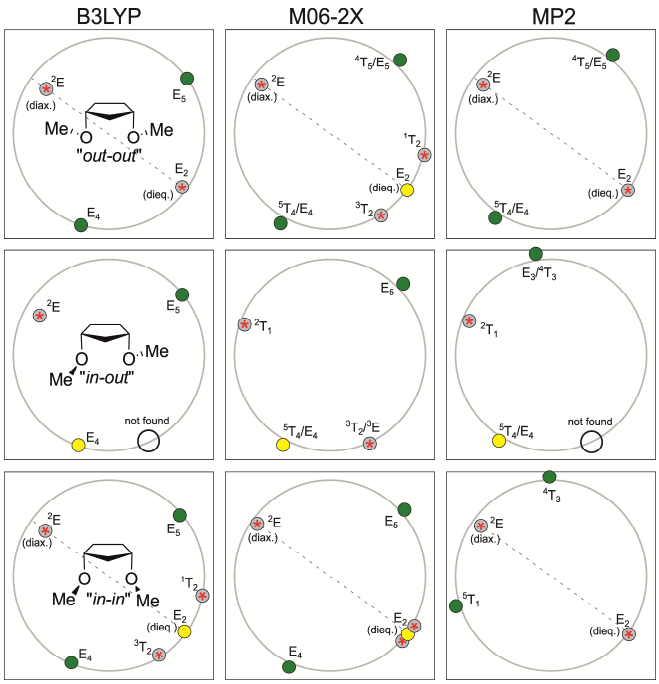

Figure *S*5. Geometry representations of the Cremer-Pople puckering parameters of minima (green, global minima; yellow, local minima) and transition states (grey circle with red star) computed for compound **18** at the three levels of theory under study.

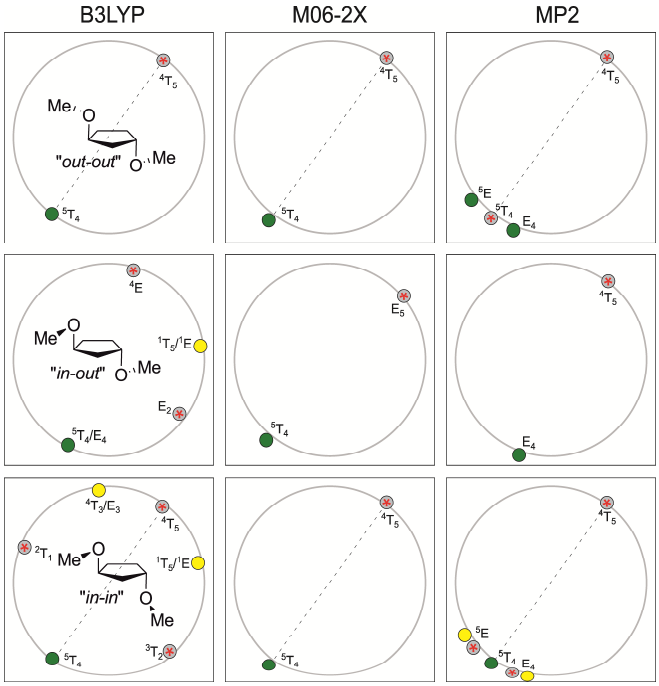

Figure *S*6. Geometry representations of the Cremer-Pople puckering parameters of minima (green, global minima; yellow, local minima) and transition states (grey circle with red star) computed for compound **19** at the three levels of theory under study.

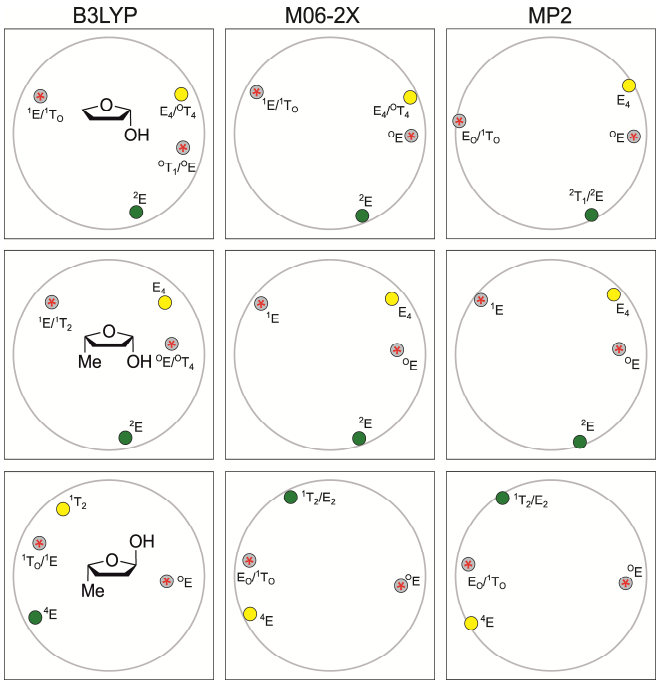

Figure *S*7. Geometry representations of the Cremer-Pople puckering parameters of minima (green, global minima; yellow, local minima) and transition states (grey circle with red star) computed for compounds **20-22** at the three levels of theory under study.

SCF and Gibbs free energies (in Hartress), amplitudes (Q), phase coordinates (ϕ), relative energies (in kcal/mol) and lower frequencies computed for all shapes found for compounds 1-22 at the B3LYP, M06-2X and MP2 levels of theory.

Compound 1: cyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
E (^{1}E)	B3LYP/6-311+G**	-196.611648	0.399	0.4	**0.000**	+24.7
	idem Ultrafine / Tight	-196.611644	0.399	0.0	0.003	**-12.9**
	idem Superfine / Tight	-196.611645	0.399	0.5	0.001	**-8.3**
	M06-2X/6-311+G**	-196.502249	0.419	0.5	0.003	**-40.9**
	idem Ultrafine / Tight	-196.502265	0.419	0.5	0.002	**-16.4**
	idem Superfine / Tight	-196.502267	0.419	0.0	0.001	**-12.2**
	MP2/6-311+G**	-195.964900	0.427	0.4	**0.000**	+7.9
	idem Tight	-195.964900	0.426	0.4	**0.000**	**-2.5**
	G (B3LYP/6-311+G**)	-196.500820			**0.000**	
	idem Ultrafine / Tight	-196.498843			2.046	
	idem Superfine / Tight	-196.498835			1.779	
	G (M06-2X/6-311+G**)	-196.388231			1.824	
	idem Ultrafine / Tight	-196.387885			2.304	
	idem Superfine / Tight	-196.387870			2.523	
	G (MP2/6-311+G**)	-195.852896			**0.000**	
	idem Tight	-195.849809			0.002	
T (^{1}T$_5$)	B3LYP/6-311+G**	-196.611636	0.399	345.1	0.008	**-22.4**
	idem Ultrafine / Tight	-196.611649	0.399	346.7	**0.000**	+10.9
	idem Superfine / Tight	-196.611646	0.399	342.0	0.000	+10.3
	M06-2X/6-311+G**	-196.502240	0.419	345.0	0.008	**-43.5**
	idem Ultrafine / Tight	-196.502269	0.419	344.6	**0.000**	+4.3
	idem Superfine / Tight	-196.502268	0.419	344.6	0.000	+2.9
	MP2/6-311+G**	-195.964900	0.427	345.1	**0.000**	+8.1
	idem Tight	-195.964900	0.426	345.1	**0.000**	**-0.5**
	G (B3LYP/6-311+G**)	-196.498804			1.265	
	idem Ultrafine / Tight	-196.501625			0.301	
	idem Superfine / Tight	-196.501670			**0.000**	
	G (M06-2X/6-311+G**)	-196.388262			1.804	
	idem Ultrafine / Tight	-196.391556			**0.000**	
	idem Superfine / Tight	-196.391890			**0.000**	
	G (MP2/6-311+G**)	-195.852870			0.016	
	idem Tight	-195.849812			**0.000**	
E/T (^{1}T$_5$/^{1}E)	B3LYP/6-311+G**	-196.611648	0.399	352.7	0.000	**-21.1**
	idem Ultrafine / Tight	-196.611645	0.399	352.7	0.003	+6.6
	M06-2X/6-311+G**	-196.502253	0.419	352.5	**0.000**	+23.2
	idem Ultrafine / Tight	-196.502267	0.419	352.5	0.001	+12.4
	idem Superfine / Tight	-196.502267	0.419	348.3	0.001	+9.0
	MP2/6-311+G**	-195.964900	0.427	352.7	**0.000**	+8.1
	idem Tight	-195.964900	0.426	352.7	**0.000**	**-2.1**
	G (B3LYP/6-311+G**)	-196.498815			1.258	
	idem Ultrafine / Tight	-196.502104			**0.000**	
	G (M06-2X/6-311+G**)	-196.391137			**0.000**	
	idem Ultrafine / Tight	-196.390561			0.624	
	idem Superfine / Tight	-196.390826			0.668	
	G (MP2/6-311+G**)	-195.852874			0.014	
	idem Tight	-195.849810			0.001	

Compound 2: fluorocyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
^{5}T$_4$/^{5}E	B3LYP/6-311+G**	-295.885200	0.387	133.1	**0.00**	+51.9
(=^{2}T$_3$/^{2}E)	M06-2X/6-311+G**	-295.749442	0.412	135.0	**0.00**	+54.8
	MP2/6-311+G**	-295.048299	0.416	135.5	**0.00**	+62.2
	G (B3LYP/6-311+G**)	-295.782647			**0.00**	
	G (M06-2X/6-311+G**)	-295.645115			**0.00**	
	G(MP2/6-311+G**)	-294.943139			**0.00**	
E_1	B3LYP/6-311+G**	-295.884951	0.366	180.0	0.16	-44.2
	M06-2X/6-311+G**	-295.749195	0.394	180.0	0.15	-39.0
	MP2/6-311+G**	-295.047958	0.399	180.0	0.21	-48.8
	G (B3LYP/6-311+G**)	-295.781188			0.92	
	G (M06-2X/6-311+G**)	-295.643719			0.88	
	G(MP2/6-311+G**)	-294.941863			0.80	
^{1}E	B3LYP/6-311+G**	-295.882831	0.395	0.0	1.49	**-34.8**
	M06-2X/6-311+G**	-295.746684	0.415	0.0	1.73	**-32.6**
	MP2/6-311+G**	-295.045425	0.426	0.0	1.80	**-27.5**
	G (B3LYP/6-311+G**)	-295.779044			2.26	
	G (M06-2X/6-311+G**)	-295.641194			2.46	
	G(MP2/6-311+G**)	-294.939311			2.40	

Compound 3: chlorocyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
E_1	B3LYP/6-311+G**	-656.239554	0.371	180.0	**0.00**	+61.9
	M06-2X/6-311+G**	-656.110253	0.396	180.0	**0.00**	+86.0
	MP2/6-311+G**	-655.030234	0.405	180.0	**0.00**	+78.7

	G (B3LYP/6-311+G**)	-656.138981			**0.00**	
	G (M06-2X/6-311+G**)	-656.007630			**0.00**	
	G(MP2/6-311+G**)	-654.927005			**0.00**	
^{1}E	B3LYP/6-311+G**	-656.238772	0.410	0.0	0.49	+34.7
	M06-2X/6-311+G**	-656.108325	0.428	0.0	1.21	+43.8
	MP2/6-311+G**	-655.028563	0.433	0.0	1.05	+33.8
	G (B3LYP/6-311+G**)	-656.138831			0.09	
	G (M06-2X/6-311+G**)	-656.006547			0.68	
	G(MP2/6-311+G**)	-654.926332			0.42	
^{3}E(=^{4}E)	B3LYP/6-311+G**	-656.238121	0.405	72.8	0.90	**-34.6**
	M06-2X/6-311+G**	-656.107497	0.426	68.7	1.73	**-49.3**
	MP2/6-311+G**	-655.027259	0.434	74.0	1.87	**-53.3**
	G (B3LYP/6-311+G**)	-656.136164			1.77	
	G (M06-2X/6-311+G**)	-656.003998			2.28	
	G(MP2/6-311+G**)	-654.923024			2.50	

Compound 4: cyclopentanol

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
^{1}T$_5$	B3LYP/6-311+G**	-271.854158	0.402	337.1	0.64	+31.6
	M06-2X/6-311+G**	-271.722418	0.422	340.9	1.12	+33.7
	MP2/6-311+G**	-271.043388	0.431	333.6	1.33	+26.9
	G (B3LYP/6-311+G**)	-271.740353			0.30	
	G (M06-2X/6-311+G**)	-271.606769			0.59	
	G (MP2/6-311+G**)	-270.927360			0.84	
^{5}E/^{5}T$_4$	B3LYP/6-311+G**	-271.855181	0.397	135.3	**0.00**	+39.2[a]
	MP2/6-311+G**	-271.045515	0.418	141.1	**0.00**	+43.1
	G (B3LYP/6-311+G**)	-271.740839			**0.00**	
	G (MP2/6-311+G**)	-270.928409			0.18	
E$_1$	M06-2X/6-311+G**	-271.724204	0.413	177.8	**0.00**	+51.9
	MP2/6-311+G**	-271.045496	0.416	176.9	0.01	+41.9
	G (M06-2X/6-311+G**)	-271.607712			**0.00**	
	G (MP2/6-311+G**)	-270.928693			**0.00**	
^{5}T$_1$	MP2/6-311+G**	-271.045479	0.413	161.5	0.02	**-33.5**
	G (MP2/6-311+G**)	-270.927041			1.04	
^{3}T$_2$	B3LYP/6-311+G**	-271.853846	0.395	52.5	0.84	**-45.2**
	M06-2X/6-311+G**	-271.721964	0.416	56.9	1.41	**-49.7**
	MP2/6-311+G**	-271.042941	0.424	53.5	1.62	**-52.7**
	G (B3LYP/6-311+G**)	-271.738161			1.68	
	G (M06-2X/6-311+G**)	-271.604486			2.02	
	G (MP2/6-311+G**)	-270.924846			2.41	
^{4}E	B3LYP/6-311+G**	-271.853964	0.399	291.0	0.76	**-38.3**
	M06-2X/6-311+G**	-271.722086	0.420	291.7	1.33	**-43.7**
	MP2/6-311+G**	-271.043170	0.429	291.9	1.47	**-44.8**
	G (B3LYP/6-311+G**)	-271.738150			1.69	
	G (M06-2X/6-311+G**)	-271.604484			2.03	
	G (MP2/6-311+G**)	-270.924848			2.41	

a) B3PW91 is 0.404/135.8/+40.8 (only). PBE1PBE is 0.409/134.8/+44.8 (only)

Compound 5: methylcyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
E$_1$	B3LYP/6-311+G**	-235.935865	0.394	180.0	1.16	+68.7
	M06-2X/6-311+G**	-235.807909	0.415	180.0	0.31	+98.4
	MP2/6-311+G**	-235.163719	0.420	180.0	0.33	+94.3
	G (B3LYP/6-311+G**)	-235.797975			1.86	
	G (M06-2X/6-311+G**)	-235.667698			1.21	
	G(MP2/6-311+G**)	-235.022728			1.16	
^{1}E	B3LYP/6-311+G**	-235.937711	0.401	0.0	**0.00**	+28.5
	M06-2X/6-311+G**	-235.808405	0.418	0.0	**0.00**	+33.6
	MP2/6-311+G**	-235.164241	0.425	0.0	**0.00**	+35.3
	G (B3LYP/6-311+G**)	-235.800941			**0.00**	
	G (M06-2X/6-311+G**)	-235.669632			**0.00**	
	G(MP2/6-311+G**)	-235.024572			**0.00**	
^{5}E(=^{2}E)	B3LYP/6-311+G**	-235.935642	0.385	146.9	1.30	**-60.2**
	M06-2X/6-311+G**	-235.807145	0.402	138.3	0.79	**-68.5**
	MP2/6-311+G**	-235.162980	0.408	138.0	0.79	**-68.8**
	G (B3LYP/6-311+G**)	-235.796573			2.74	
	G (M06-2X/6-311+G**)	-235.666089			2.22	
	G(MP2/6-311+G**)	-235.021080			2.19	

Compound 6: t-butylcyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
^{3}T$_2$ (=^{4}T$_5$)	B3LYP/6-311+G**	-353.905924	0.403	53.9	**0.00**	+29.6
^{3}E/^{3}T$_4$	M06-2X/6-311+G**	-353.722523	0.425	84.5	**0.00**	+61.6
	MP2/6-31+G*	-352.502553	0.425	78.6	**0.00**	+51.6
	MP2/6-311+G**//	-352.758144			**0.00**	
	G (B3LYP/6-311+G**)	-353.689318			**0.00**	
	G (M06-2X/6-311+G**)	-353.501821			**0.00**	
	G (MP2/6-31+G*)	-352.278197			**0.00**	

^{1}E	B3LYP/6-311+G**	-353.905718	0.407	0.0	0.13	**-33.4**
	M06-2X/6-311+G**	-353.721612	0.423	0.0	0.57	**-55.4**
	MP2/6-311+G*	-352.501771	0.427	0.0	0.49	**-46.5**
	MP2/6-311+G**//	-352.757065			0.68	
	G (B3LYP/6-311+G**)	-353.688131			0.74	
	G (M06-2X/6-311+G**)	-353.501475			0.22	
	G (MP2/6-31+G*)	-352.277558			0.40	
E_1	B3LYP/6-311+G**	-353.901303	0.330	180.0	2.90	+30.5
	M06-2X/6-311+G**	-353.718466	0.344	179.4	2.55	+34.9
	MP2/6-31+G*	-352.497819	0.344	180.0	2.97	+21.9
	MP2/6-311+G**//	-352.753703			2.79	
	G (B3LYP/6-311+G**)	-353.684952			2.74	
	G (M06-2X/6-311+G**)	-353.499200			1.64	
	G (MP2/6-31+G*)	-352.274508			2.31	
$^5T_1$ (=$^2T_1$)	B3LYP/6-311+G**	-353.901273	0.326	161.5	2.92	**-65.2**
	M06-2X/6-311+G**	-353.718312	0.333	152.5	2.64	**-85.2**
	MP2/6-31+G*	-352.497653	0.339	153.1	3.08	**-85.3**
	MP2/6-311+G**//	-352.753522			2.90	
	G (B3LYP/6-311+G**)	-353.683149			3.87	
	G (M06-2X/6-311+G**)	-353.496971			3.04	
	G (MP2/6-31+G*)	-352.272401			3.64	

Compound 7: oxolane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
E (^{1}E)	B3LYP/6-311+G**	-232.518663	0.367	0.0	0.02	+24.5
	M06-2X/6-311+G**	-232.406246	0.380	0.7	0.07	**-15.1**
	MP2/6-311+G**	-231.830787	0.394	0.0	0.20	**-78.7**
	G (B3LYP/6-311+G**)	-232.431315			**0.00**	
	G (M06-2X/6-311+G**)	-232.315234			1.02	
	G (MP2/6-311+G**)	-231.739332			1.12	
T ($^3T_4$)	B3LYP/6-311+G**	-232.518693	0.367	90.0	**0.00**	+46.8
	M06-2X/6-311+G**	-232.406358	0.386	89.9	**0.00**	+60.0
	MP2/6-311+G**	-231.831046	0.398	90.0	0.04	**-23.5**
	G (B3LYP/6-311+G**)	-232.431031			0.18	
	G (M06-2X/6-311+G**)	-232.316867			**0.00**	
	G (MP2/6-311+G**)	-231.739731			0.87	
Int (E_2/$^3T_2$)	B3LYP/6-311+G**	-232.518581	0.365	44.6	0.07	**-46.2**
	M06-2X/6-311+G**	-232.406192	0.383	47.6	0.10	**-59.6**
	MP2/6-311+G**	-231.831107	0.401	42.3	**0.00**	+42.0
	G (B3LYP/6-311+G**)	-232.429357			1.05	
	G (M06-2X/6-311+G**)	-232.315334			0.96	
	G (MP2/6-311+G**)	-231.741113			**0.00**	

Compound 8: pyrrolidine

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
^{1}E (H eq)	B3LYP/6-311+G**	-212.646344	0.420	0.0	**0.00**	+76.5
	M06-2X/6-311+G**	-212.536770	0.436	0.0	**0.00**	+71.7
	MP2/6-311+G**	-211.982186	0.449	0.0	**0.00**	+70.2
	G (B3LYP/6-311+G**)	-212.545361			0.47	
	G (M06-2X/6-311+G**)	-212.434211			0.40	
	G (MP2/6-311+G**)	-211.879120			**0.00**	
E_1 (H ax)	B3LYP/6-311+G**	-212.646038	0.342	180.0	0.19	+24.1
	M06-2X/6-311+G**	-212.536631	0.360	180.0	0.09	**-23.6**
	MP2/6-311+G**	-211.981964	0.365	180.0	0.14	**-65.5**
	G (B3LYP/6-311+G**)	-212.546103			**0.00**	
	G (M06-2X/6-311+G**)	-212.433096			1.10	
	G (MP2/6-311+G**)	-211.877852			0.80	
$^3T_4$	B3LYP/6-311+G**	-212.645217	0.381	89.3	0.71	**-60.5**
	M06-2X/6-311+G**	-212.535809	0.398	93.6	0.60	**-58.7**
	MP2/6-311+G**	-211.981208	0.414	84.9	0.61	**-49.6**
	G (B3LYP/6-311+G**)	-212.543597			1.57	
	G (M06-2X/6-311+G**)	-212.432556			1.44	
	G (MP2/6-311+G**)	-211.877304			1.14	
E_1/$^5T_1$	M06-2X/6-311+G**	-212.536632	0.361	172.9	0.09	+31.6
^{5}E	MP2/6-311+G**	-211.982117	0.379	150.0	0.04	+71.1
	G (M06-2X/6-311+G**)	-212.434849			**0.00**	
	G (MP2/6-311+G**)	-211.878969			0.09	
Inversion TS	B3LYP/6-311+G**	-212.640904	0.363	90.0	3.41	**-473.0**
	M06-2X/6-311+G**	-212.531150	0.389	90.0	3.53	**-497.3**
	MP2/6-311+G**	-211.975243	0.404	90.0	4.36	**-533.5**
	G (B3LYP/6-311+G**)	-212.540944			3.24	
	G (M06-2X/6-311+G**)	-212.429520			2.24	
	G (MP2/6-311+G**)	-211.872975			3.86	

Compound 9: cyclopentanone

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
$^3T_4$ (=$^4T_3$)	B3LYP/6-311+G**	-270.652704	0.361	90.0	**0.00**	+99.6

	M06-2X/6-311+G**	-270.524551	0.383	90.0	**0.00**	+100.9
	MP2/6-311+G**	-269.856359	0.338	90.0	**0.00**	+94.8
	G (B3LYP/6-311+G**)	-270.561030			**0.00**	
	G (M06-2X/6-311+G**)	-270.431385			**0.00**	
	G (MP2/6-311+G**)	-269.762905			**0.00**	
^1E (=E_1)	B3LYP/6-311+G**	-270.648465	0.192	0.0	2.66	**-151.2**
	M06-2X/6-311+G**	-270.519467	0.238	0.0	3.19	**-149.6**
	MP2/6-311+G**	-269.850670	0.280	0.0	3.57	**-149.3**
	G (B3LYP/6-311+G**)	-270.556906			2.59	
	G (M06-2X/6-311+G**)	-270.426289			3.20	
	G (MP2/6-311+G**)	-269.757038			3.68	

Compound 10: *cis*-1,2-dimethylcyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
$^1T_2/E_2$ (=$^2T_1/^2E$)	B3LYP/6-311+G**	-275.260095	0.412	28.7	**0.00**	+80.4
	M06-2X/6-311+G**	-275.113348	0.425	34.1	**0.00**	+100.3
	MP2/6-311+G**	-274.362108	0.431	34.4	**0.00**	+101.1
	G (B3LYP/6-311+G**)	-275.095772			**0.00**	
	G (M06-2X/6-311+G**)	-274.946385			**0.00**	
	G (MP2/6-311+G**)	-274.194280			**0.00**	
^4E	B3LYP/6-311+G**	-275.259256	0.405	288.0	0.53	**-36.1**
	M06-2X/6-311+G**	-275.111380	0.421	288.0	1.24	**-54.5**
	MP2/6-311+G**	-274.359885	0.427	288.0	1.39	**-63.7**
	G (B3LYP/6-311+G**)	-275.093495			1.43	
	G (M06-2X/6-311+G**)	-274.943356			1.90	
	G (MP2/6-311+G**)	-274.191056			2.02	
E_4	B3LYP/6-311+G**	-275.256516	0.406	108.0	2.25	**-59.4**
	M06-2X/6-311+G**	-275.109664	0.432	108.0	2.31	**-54.1**
	MP2/6-311+G**	-274.358036	0.437	108.0	2.56	**-62.0**
	G (B3LYP/6-311+G**)	-275.090468			3.33	
	G (M06-2X/6-311+G**)	-274.941265			3.21	
	G (MP2/6-311+G**)	-274.188854			3.40	

Compound 11: *trans*-1,2-dimethylcyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
$^1T_2$	B3LYP/6-311+G**	-275.263308	0.402	18.0	**0.00**	+46.3
	M06-2X/6-311+G**	-275.114866	0.420	18.0	**0.00**	+54.2
	MP2/6-311+G**	-274.363919	0.425	18.0	**0.00**	+51.1
	G (B3LYP/6-311+G**)	-275.100090			**0.00**	
	G (M06-2X/6-311+G**)	-274.949369			**0.00**	
	G (MP2/6-311+G**)	-274.197546			**0.00**	
$^2T_1$	B3LYP/6-311+G**	-275.259822	0.384	198.0	2.19	**-15.7**
	M06-2X/6-311+G**	-275.113121	0.405	198.0	1.09	+55.4[a]
	MP2/6-311+G**	-274.362212	0.408	198.0	1.07	+49.7[a]
	G (B3LYP/6-311+G**)	-275.094663			3.41	
	G (M06-2X/6-311+G**)	-274.946877			1.56	
	G (MP2/6-311+G**)	-274.195224			1.46	

a) All efforts to find the TS were unsuccessful

Compound 12: *cis*-1,3-dimethylcyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
E_2	B3LYP/6-311+G**	-275.263431	0.403	36.0	**0.00**	+44.9
	M06-2X/6-311+G**	-275.114146	0.418	36.0	**0.00**	+49.1
	MP2/6-311+G**	-274.363204	0.423	36.0	**0.00**	+31.3
	G (B3LYP/6-311+G**)	-275.100144			**0.00**	
	G (M06-2X/6-311+G**)	-274.948663			**0.00**	
	G (MP2/6-311+G**)	-274.197160			**0.00**	
^2E	B3LYP/6-311+G**	-275.257044	0.308	216.0	4.01	**-112.8**
	M06-2X/6-311+G**	-275.108347	0.318	216.0	3.64	**-128.7**
	MP2/6-311+G**	-274.357211	0.323	216.0	3.76	**-128.4**
	G (B3LYP/6-311+G**)	-275.091805			5.23	
	G (M06-2X/6-311+G**)	-274.941022			4.79	
	G (MP2/6-311+G**)	-274.188878			5.20	

Compound 13: *trans*-1,3-dimethylcyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
$^4T_5$	B3LYP/6-311+G**	-275.262981	0.403	306.0	**0.00**	+25.6
	M06-2X/6-311+G**	-275.113674	0.418	306.0	0.11	**-13.6**
	MP2/6-311+G**	-274.362888	0.424	306.0	0.06	**-8.0**
	G (B3LYP/6-311+G**)	-275.099773			**0.00**	
	G (M06-2X/6-311+G**)	-274.946401			1.04	
	G (MP2/6-311+G**)	-274.194534			0.06	
$^5T_4$	B3LYP/6-311+G**	-275.260061	0.382	126.0	1.83	**-39.0**
	M06-2X/6-311+G**	-275.112248	0.399	126.0	1.00	**-46.4**
	MP2/6-311+G**	-274.361278	0.402	126.0	1.07	**-45.7**
	G (B3LYP/6-311+G**)	-275.094525			3.29	

	G (M06-2X/6-311+G**)	-274.944341			2.33	
	G (MP2/6-311+G**)	-274.192458			1.36	
$^4T_3$	M06-2X/6-311+G**	-275.113845	0.423	265.3	**0.00**	+39.0
	MP2/6-311+G**	-274.362979	0.428	266.8	**0.00**	+32.9
	G (M06-2X/6-311+G**)	-274.948052			**0.00**	
	G (MP2/6-311+G**)	-274.194625			**0.00**	

Compound 14: *cis*-2-methylcyclopentanol

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
$^2T_1/E_1$ out	B3LYP/6-311+G**	-311.180157	0.404	192.6	0.13	+59.2
	M06-2X/6-311+G**	-311.030116	0.422	187.9	0.07	+71.9
	MP2/6-311+G**	-310.244401	0.425	185.5	**0.00**	+60.1
	G (B3LYP/6-311+G**)	-311.039549			0.41	
	G (M06-2X/6-311+G**)	-310.887113			0.19	
	G (MP2/6-311+G**)	-310.100678			0.27	
$^3T_4$ out	B3LYP/6-311+G**	-311.175757	0.402	89.1	2.89	**-52.9**
	M06-2X/6-311+G**	-311.025809	0.417	86.6	2.77	**-61.8**
	MP2/6-311+G**	-310.239611	0.426	88.2	3.01	**-62.5**
	G (B3LYP/6-311+G**)	-311.033347			4.30	
	G (M06-2X/6-311+G**)	-310.881087			3.97	
	G (MP2/6-311+G**)	-310.094162			4.36	
$^1T_2/E_2$ out	B3LYP/6-311+G**	-311.177572	0.411	26.9	1.75	+77.1
	M06-2X/6-311+G**	-311.028071	0.426	31.0	1.35	+95.5
	MP2/6-311+G**	-310.242099	0.433	31.3	1.44	+96.1
	G (B3LYP/6-311+G**)	-311.036635			2.24	
	G (M06-2X/6-311+G**)	-310.884515			1.82	
	G (MP2/6-311+G**)	-310.097905			2.01	
$^4T_5$ out	B3LYP/6-311+G**	-311.177215	0.409	305.9	1.97	**-28.4**
^4E out	M06-2X/6-311+G**	-311.026682	0.422	292.1	2.23	**-48.4**
	MP2/6-311+G**	-310.240394	0.430	292.1	2.51	**-58.2**
	G (B3LYP/6-311+G**)	-311.034894			3.33	
	G (M06-2X/6-311+G**)	-310.882146			3.31	
	G (MP2/6-311+G**)	-310.095303			3.65	
$^2E/^2T_1$ in	B3LYP/6-311+G**	-311.180362	0.401	212.7	**0.00**	+32.7
$^2T_1/E_1$ in	M06-2X/6-311+G**	-311.030230	0.416	189.2	**0.00**	+51.0
	MP2/6-311+G**	-310.244250	0.421	190.5	0.09	+38.1
	G (B3LYP/6-311+G**)	-311.040204			**0.00**	
	G (M06-2X/6-311+G**)	-310.887421			**0.00**	
	G (MP2/6-311+G**)	-310.101113			**0.00**	
$^3T_4$ in	B3LYP/6-311+G**	-311.175700	0.396	87.4	2.93	**-61.2**
	M06-2X/6-311+G**	-311.025659	0.415	86.2	2.87	**-66.6**
	MP2/6-311+G**	-310.239260	0.422	85.2	3.23	**-72.3**
	G (B3LYP/6-311+G**)	-311.033297			4.33	
	G (M06-2X/6-311+G**)	-310.880794			4.16	
	G (MP2/6-311+G**)	-310.093828			4.57	
E_2 in	B3LYP/6-311+G**	-311.177666	0.416	29.9	1.69	+89.2
	M06-2X/6-311+G**	-311.028140	0.431	32.3	1.31	+100.8
	MP2/6-311+G**	-310.242051	0.439	32.5	1.47	+105.8
	G (B3LYP/6-311+G**)	-311.036620			2.25	
	G (M06-2X/6-311+G**)	-310.884680			1.72	
	G (MP2/6-311+G**)	-310.097947			1.99	
$^1T_5/E_5$ in	B3LYP/6-311+G**	-311.176985	0.404	336.9	2.12	**-28.8**
	M06-2X/6-311+G**	-311.026862	0.418	338.2	2.11	**-50.5**
$^4T_5$ in	MP2/6-311+G**	-310.240334	0.432	312.6	2.55	**-40.0**
	G (B3LYP/6-311+G**)	-311.034937			3.31	
	G (M06-2X/6-311+G**)	-310.882929			2.82	
	G (MP2/6-311+G**)	-310.095332			3.63	
$^2T_1$ (TS between in/out)	B3LYP/6-311+G**	-311.178488	0.411	200.5	1.18	**-264.7**
	M06-2X/6-311+G**	-311.028116	0.431	190.7	1.33	**-261.0**
	MP2/6-311+G**	-310.242303	0.435	188.9	1.32	**-263.2**
	G (B3LYP/6-311+G**)	-311.038484			1.08	
	G (M06-2X/6-311+G**)	-310.885701			1.08	
	G (MP2/6-311+G**)	-310.099335			1.12	
$^1T_2$ (TS between in/out)	B3LYP/6-311+G**	-311.176596	0.409	29.1	2.36	**-232.7**
	M06-2X/6-311+G**	-311.026813	0.424	32.0	2.14	**-256.7**
	MP2/6-311+G**	-310.240898	0.431	30.9	2.20	**-228.9**
	G (B3LYP/6-311+G**)	-311.035727			2.81	
	G (M06-2X/6-311+G**)	-310.883499			2.46	
	G (MP2/6-311+G**)	-310.096943			2.62	

Compound 15: *trans*-2-methylcyclopentanol

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
$^1T_2$ out	B3LYP/6-311+G**	-311.180566	0.404	16.6	**0.00**	+49.7
	M06-2X/6-311+G**	-311.029403	0.422	15.9	0.41	+54.1
	MP2/6-311+G**	-310.243522	0.430	14.4	0.71	+51.7
	G (B3LYP/6-311+G**)	-311.040476			**0.00**	
	G (M06-2X/6-311+G**)	-310.887032			**0.00**	
	G (MP2/6-311+G**)	-310.100658			**0.00**	
^3E out	B3LYP/6-311+G**	-311.180151	0.399	74.0	0.26	**-26.2**
	M06-2X/6-311+G**	-311.028644	0.420	80.1	0.89	**-30.0**

	MP2/6-311+G**	-310.242968	0.422	66.2	1.05	**-41.9**
	G (B3LYP/6-311+G**)	-311.038318			1.35	
	G (M06-2X/6-311+G**)	-310.884677			1.48	
	G (MP2/6-311+G**)	-310.098416			1.41	
E_4 out	B3LYP/6-311+G**	-311.180213	0.406	105.9	0.22	+18.4
$^5E/^5T_4$	M06-2X/6-311+G**	-311.029485	0.425	135.7	0.36	+42.6
	MP2/6-311+G**	-310.244204	0.427	133.2	0.28	+46.5
	G (B3LYP/6-311+G**)	-311.040322			0.10	
	G (M06-2X/6-311+G**)	-310.886491			0.34	
	G (MP2/6-311+G**)	-310.100154			0.32	
E_1 out	B3LYP/6-311+G**	-311.179151	0.383	185.1	0.89	**-46.1**
$^5T_1$	M06-2X/6-311+G**	-311.029275	0.405	165.7	0.49	**-48.8**
	MP2/6-311+G**	-310.243801	0.405	169.2	0.53	**-55.5**
	G (B3LYP/6-311+G**)	-311.037173			2.07	
	G (M06-2X/6-311+G**)	-310.884838			1.38	
	G (MP2/6-311+G**)	-310.098628			1.27	
$^2T_1$ out	B3LYP/6-311+G**	-311.179175	0.386	201.1	0.87	+44.5
$^2T_1/^2E$	M06-2X/6-311+G**	-311.029762	0.417	206.4	0.19	+78.1
	MP2/6-311+G**	-310.244125	0.418	204.1	0.33	+71.5
	G (B3LYP/6-311+G**)	-311.038784			1.06	
	G (M06-2X/6-311+G**)	-310.886383			0.41	
	G (MP2/6-311+G**)	-310.100310			0.22	
$E_3/^4T_3$ out	B3LYP/6-311+G**	-311.178078	0.387	260.0	1.56	**-48.2**
$^4T_3$	M06-2X/6-311+G**	-311.027279	0.412	271.6	1.75	**-49.0**
	MP2/6-311+G**	-310.241628	0.416	269.5	1.90	**-53.5**
	G (B3LYP/6-311+G**)	-311.035939			2.85	
	G (M06-2X/6-311+G**)	-310.882787			2.66	
	G (MP2/6-311+G**)	-310.096486			2.62	
$^1T_2$ in	B3LYP/6-311+G**	-311.180456	0.408	26.1	0.07	+54.9
	M06-2X/6-311+G**	-311.029323	0.426	23.9	0.46	+59.8
	MP2/6-311+G**	-310.243356	0.432	27.8	0.81	+55.4
	G (B3LYP/6-311+G**)	-311.040274			0.13	
	G (M06-2X/6-311+G**)	-310.886949			0.05	
	G (MP2/6-311+G**)	-310.100390			0.17	
E_4 in	B3LYP/6-311+G**	-311.179567	0.402	109.7	0.63	**-19.2**
$^3T_4$	M06-2X/6-311+G**	-311.028201	0.420	89.3	1.17	**-33.8**
	MP2/6-311+G**	-310.242517	0.427	86.3	1.34	**-36.4**
	G (B3LYP/6-311+G**)	-311.037529			1.85	
	G (M06-2X/6-311+G**)	-310.883980			1.92	
	G (MP2/6-311+G**)	-310.097656			1.88	
$^5T_4$ in	B3LYP/6-311+G**	-311.179581	0.403	122.0	0.62	+20.5
^5E	M06-2X/6-311+G**	-311.029296	0.419	146.8	0.48	+35.7
	G (B3LYP/6-311+G**)	-311.039670			0.51	
	G (M06-2X/6-311+G**)	-310.886589			0.28	
$E_1/^5T_1$ in	B3LYP/6-311+G**	-311.179193	0.382	174.0	0.86	**-49.3**
$^5T_1$	M06-2X/6-311+G**	-311.029284	0.411	157.8	0.49	**-29.6**
	G (B3LYP/6-311+G**)	-311.037150			2.09	
	G (M06-2X/6-311+G**)	-310.884894			1.34	
^2E in	B3LYP/6-311+G**	-311.179471	0.393	213.4	0.69	+65.2
	M06-2X/6-311+G**	-311.030060	0.416	211.3	**0.00**	+80.3
	MP2/6-311+G**	-310.244648	0.417	213.1	**0.00**	+85.1
	G (B3LYP/6-311+G**)	-311.038581			1.19	
	G (M06-2X/6-311+G**)	-310.886532			0.31	
	G (MP2/6-311+G**)	-310.100318			0.21	
$^4T_3$ in	B3LYP/6-311+G**	-311.178507	0.393	273.8	1.29	**-27.3**
^4E	M06-2X/6-311+G**	-311.027537	0.418	286.7	1.58	**-29.8**
	MP2/6-311+G**	-310.241827	0.425	290.6	1.77	**-30.4**
	G (B3LYP/6-311+G**)	-311.036290			2.63	
	G (M06-2X/6-311+G**)	-310.883132			2.45	
	G (MP2/6-311+G**)	-310.096773			2.44	
^2E (TS between	B3LYP/6-311+G**	-311.177181	0.402	209.7	2.12	**-279.8**
in/out)	M06-2X/6-311+G**	-311.027518	0.427	209.8	1.60	**-314.8**
	MP2/6-311+G**	-310.241960	0.428	209.8	1.69	**-273.4**
	G (B3LYP/6-311+G**)	-311.036861			2.27	
	G (M06-2X/6-311+G**)	-310.884632			1.51	
	G (MP2/6-311+G**)	-310.098421			1.40	
$^1T_2$ (TS between	B3LYP/6-311+G**	-311.179443	0.401	25.0	0.70	**-235.2**
in/out)	M06-2X/6-311+G**	-311.028080	0.419	24.3	1.24	**-273.5**
	MP2/6-311+G**	-310.242286	0.425	22.8	1.48	**-221.1**
	G (B3LYP/6-311+G**)	-311.039467			0.63	
	G (M06-2X/6-311+G**)	-310.885920			0.70	
	G (MP2/6-311+G**)	-310.099452			0.76	
$^5T_4$ (TS between	M06-2X/6-311+G**	-311.027023	0.434	138.9	1.91	**-301.5**[a]
in/out)	G (M06-2X/6-311+G**)	-310.884480			1.60	

a) With B3LYP, the TS falls into $^1T_2$

Compound 16: *cis*-1,2-dimethoxycyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
$^2T_1$ sym	B3LYP/6-311+G**	-425.712042	0.430	198.9	1.34	+64.1
(=$^1T_2$)	M06-2X/6-311+G**	-425.518092	0.446	191.8	1.62	+63.3
	MP2/6-31+G*	-424.208130	0.447	192.1	1.83	+69.2
	MP2/6-311+G**//	-424.474889			1.50	
	G (B3LYP/6-311+G**)	-425.543308			1.44	
	G (M06-2X/6-311+G**)	-425.345832			1.50	

	G (MP2/6-31+G*)	-424.033475			1.57	
^{4}E sym	B3LYP/6-311+G**	-425.707902	0.401	288.0	3.94	**-60.3**
	M06-2X/6-311+G**	-425.513442	0.419	288.0	4.54	**-62.1**
	MP2/6-31+G*	-424.202266	0.419	288.0	5.51	**-72.8**
	MP2/6-311+G**//	-424.469609			4.81	
	G (B3LYP/6-311+G**)	-425.537501			5.09	
	G (M06-2X/6-311+G**)	-425.339473			5.49	
	G (MP2/6-31+G*)	-424.025983			6.27	
E_4 sym	B3LYP/6-311+G**	-425.706901	0.412	108.0	4.57	**-64.1**
	M06-2X/6-311+G**	-425.512180	0.439	108.0	5.33	**-64.9**
	MP2/6-31+G*	-424.201479	0.437	108.0	6.01	**-71.1**
	MP2/6-311+G**//	-424.469003			5.19	
	G (B3LYP/6-311+G**)	-425.536285			5.85	
	G (M06-2X/6-311+G**)	-425.338091			6.36	
	G (MP2/6-31+G*)	-424.025253			6.73	
$^2T_1/E_1$ asym	B3LYP/6-311+G**	-425.713331	0.416	192.3	0.53	+50.5
	M06-2X/6-311+G**	-425.519935	0.429	185.9	0.46	+48.2
	MP2/6-31+G*	-424.209818	0.433	185.3	0.77	+56.5
	MP2/6-311+G**//	-424.476620			0.41	
	G (B3LYP/6-311+G**)	-425.544721			0.56	
	G (M06-2X/6-311+G**)	-425.347646			0.37	
	G (MP2/6-31+G*)	-424.035114			0.54	
^{4}E asym	B3LYP/6-311+G**	-425.711848	0.399	283.7	1.46	**-40.7**
	M06-2X/6-311+G**	-425.517599	0.419	290.5	1.93	**-46.6**
	MP2/6-31+G*	-424.206880	0.419	287.5	2.62	**-49.9**
	MP2/6-311+G**//	-424.473759			2.21	
	G (B3LYP/6-311+G**)	-425.540714			3.07	
	G (M06-2X/6-311+G**)	-425.343092			3.22	
	G (MP2/6-31+G*)	-424.029986			3.76	
$^1T_2$ asym	B3LYP/6-311+G**	-425.714182	0.426	14.6	**0.00**	+43.8
	M06-2X/6-311+G**	-425.520672	0.443	28.3	**0.00**	+61.5
	MP2/6-31+G*	-424.211051	0.444	27.7	**0.00**	+72.5
	MP2/6-311+G**//	-424.477276			**0.00**	
	G (B3LYP/6-311+G**)	-425.545608			**0.00**	
	G (M06-2X/6-311+G**)	-425.348229			**0.00**	
	G (MP2/6-31+G*)	-424.035982			**0.00**	
E_4 asym	B3LYP/6-311+G**	-425.710560	0.408	107.6	2.27	**-45.9**
	M06-2X/6-311+G**	-425.516566	0.437	104.9	2.58	**-48.1**
	MP2/6-31+G*	-424.206000	0.435	106.0	3.17	**-56.0**
	MP2/6-311+G**//	-424.472999			2.68	
	G (B3LYP/6-311+G**)	-425.539363			3.92	
	G (M06-2X/6-311+G**)	-425.342014			3.90	
	G (MP2/6-31+G*)	-424.029229			4.24	
$^2T_1$ (TS between in/out)	B3LYP/6-311+G**	-425.710159	0.428	199.7	2.52	**-84.6**
	M06-2X/6-311+G**	-425.515102	0.444	197.0	3.49	**-95.7**
	MP2/6-31+G*	-424.205563	0.446	196.8	3.44	**-90.1**
	MP2/6-311+G**//	-424.472318			3.11	
	G (B3LYP/6-311+G**)	-425.540690			3.09	
	G (M06-2X/6-311+G**)	-425.342294			3.72	
	G (MP2/6-31+G*)	-424.030326			3.55	
$^1T_2$ (TS between in/out)	B3LYP/6-311+G**	-425.711393	0.431	18.3	1.75	**-78.3**
	M06-2X/6-311+G**	-425.517170	0.446	24.7	2.20	**-87.9**
	MP2/6-31+G*	-424.207435	0.447	24.8	2.27	**-85.1**
	MP2/6-311+G**//	-424.474069			2.01	
	G (B3LYP/6-311+G**)	-425.541895			2.33	
	G (M06-2X/6-311+G**)	-425.344004			2.65	
	G (MP2/6-31+G*)	-424.031800			2.62	

Compound 17: *trans*-1,2-dimethoxycyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
$^2T_1$ sym	B3LYP/6-311+G**	-425.716533	0.399	198.0	0.52	+44.6
	M06-2X/6-311+G**	-425.522635	0.428	198.0	0.16	**-10.2**
	MP2/6-31+G*	-424.213129	0.424	198.0	**0.00**	+43.9
	MP2/6-311+G**//	-424.479547			**0.00**	
	G (B3LYP/6-311+G**)	-425.548025			0.26	
	G (M06-2X/6-311+G**)	-425.349467			1.28	
	G (MP2/6-31+G*)	-424.039086			0.44	
$^2T_3/E_3$ sym	B3LYP/6-311+G**	-425.716254	0.396	246.2	0.70	**-35.1**
	G (B3LYP/6-311+G**)	-425.545805			1.65	
^{4}E sym (=E_4)	B3LYP/6-311+G**	-425.716568	0.402	292.9	0.50	+22.2
	G (B3LYP/6-311+G**)	-425.548022			0.26	
$^2T_1$ sym (min)	M06-2X/6-311+G**	-425.522636	0.428	201.4	0.16	+22.8
	G (M06-2X/6-311+G**)	-425.351505			**0.00**	
$^1T_2$ sym	B3LYP/6-311+G**	-425.715095	0.374	18.0	1.43	**-59.7**
	M06-2X/6-311+G**	-425.519927	0.392	18.0	1.86	**-51.9**
	MP2/6-31+G*	-424.209570	0.395	18.0	2.23	**-59.2**
	MP2/6-311+G**//	-424.476126			2.15	
	G (B3LYP/6-311+G**)	-425.545739			1.69	
	G (M06-2X/6-311+G**)	-425.346474			3.16	
	G (MP2/6-31+G*)	-424.034519			3.31	
E_4 asym	B3LYP/6-311+G**	-425.717369	0.400	108.3	**0.00**	+26.0
$^3T_4$ asym	M06-2X/6-311+G**	-425.522792	0.421	92.1	0.06	+39.6
	MP2/6-31+G*	-424.212940	0.421	100.0	0.12	+29.3

	MP2/6-311+G**//	-424.479468			0.05	
	G (B3LYP/6-311+G**)	-425.548437			**0.00**	
	G (M06-2X/6-311+G**)	-425.350114			0.87	
	G (MP2/6-31+G*)	-424.037882			1.20	
$^5T_4$ asym	M06-2X/6-311+G**	-425.522297	0.426	133.2	0.37	**-23.1**
	MP2/6-31+G*	-424.212682	0.420	134.5	0.28	**-20.9**
	MP2/6-311+G**//	-424.479452			0.06	
	G (M06-2X/6-311+G**)	-425.348539			1.86	
	G (MP2/6-31+G*)	-424.036461			2.09	
$^5T_1$ asym	M06-2X/6-311+G**	-425.522482	0.430	165.1	0.26	+34.8
	MP2/6-31+G*	-424.212971	0.418	188.5	0.10	+24.2
	MP2/6-311+G**//	-424.479432			0.07	
	G (M06-2X/6-311+G**)	-425.351005			0.31	
	G (MP2/6-31+G*)	-424.039788			**0.00**	
$^2E/^2T_3$ asym	B3LYP/6-311+G**	-425.716440	0.392	222.0	0.58	**-20.8**
	M06-2X/6-311+G**	-425.522258	0.423	238.8	0.40	**-30.2**
	MP2/6-31+G*	-424.212399	0.416	248.9	0.46	**-36.9**
	MP2/6-311+G**//	-424.478998			0.34	
	G (B3LYP/6-311+G**)	-425.546319			1.33	
	G (M06-2X/6-311+G**)	-425.348466			1.91	
	G (MP2/6-31+G*)	-424.036127			2.30	
^4E asym	B3LYP/6-311+G**	-425.716978	0.399	293.0	0.25	+25.9
$^4E/^4T_5$	M06-2X/6-311+G**	-425.522889	0.422	298.2	**0.00**	+34.6
	MP2/6-31+G*	-424.212893	0.423	297.0	0.15	+29.3
	MP2/6-311+G**//	-424.479363			0.12	
	G (B3LYP/6-311+G**)	-425.548061			0.24	
	G (M06-2X/6-311+G**)	-425.350231			0.80	
	G (MP2/6-31+G*)	-424.038095			1.06	
$^1T_2/^1E$ asym	M06-2X/6-311+G**	-425.521410	0.402	10.3	0.93	**-33.9**[a]
	G (M06-2X/6-311+G**)	-425.348726			1.74	
$^2T_1$ (TS between	B3LYP/6-311+G**	-425.714652	0.403	197.8	1.70	**-85.2**
in/out)	MP2/6-31+G*	-424.211135	0.424	196.6	1.25	**-88.0**
	MP2/6-311+G**//	-424.477419			1.34	
	G (B3LYP/6-311+G**)	-425.545520			1.83	
	G (MP2/6-31+G*)	-424.036248			2.22	
$^3E/^3T_4$ (TS between	B3LYP/6-311+G**	-425.714871	0.401	79.2	1.57	**-76.1**
in/out)	G (B3LYP/6-311+G**)	-425.545539			1.82	
E_5 (TS between	M06-2X/6-311+G**	-425.518434	0.415	332.6	2.80	**-85.0**
in/out)	G (M06-2X/6-311+G**)	-425.346547			3.11	

a) All efforts to find this TS with B3LYP or MP2 were unsuccessful

Compound 18: *cis*-1,3-dimethoxycyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
E_4 out	B3LYP/6-311+G**	-425.717026	0.405	106.2	0.09	+25.7
(=E_5)	M06-2X/6-311+G**	-425.521788	0.427	118.2	0.35	+21.7
	MP2/6-31+G*	-424.211715	0.423	122.9	0.63	+11.4
	MP2/6-311+G**//	-424.478604			0.48	
	G (B3LYP/6-311+G**)	-425.548321			0.19	
	G (M06-2X/6-311+G**)	-425.349910			0.29	
	G (MP2/6-31+G*)	-424.038110			0.08	
^2E out	B3LYP/6-311+G**	-425.713330	0.321	216.0	2.41	**-87.2**
	M06-2X/6-311+G**	-425.517865	0.351	216.0	2.81	**-95.4**
	MP2/6-31+G*	-424.208111	0.350	216.0	2.89	**-98.4**
	MP2/6-311+G**//	-424.474616			2.98	
	G (B3LYP/6-311+G**)	-425.543358			3.30	
	G (M06-2X/6-311+G**)	-425.344409			3.74	
	G (MP2/6-31+G*)	-424.032635			3.52	
$^3T_2$ out	M06-2X/6-311+G**	-425.521012	0.408	57.3	0.83	**-32.8**
(=$^1T_2$)	G (M06-2X/6-311+G**)	-425.347390			1.87	
E_2 out	B3LYP/6-311+G**	-425.716148	0.387	36.0	0.64	**-41.8**
	M06-2X/6-311+G**	-425.521046	0.409	36.0	0.81	+29.7
	MP2/6-31+G*	-424.210526	0.406	36.0	1.38	**-39.5**
	MP2/6-311+G**//	-424.477162			1.39	
	G (B3LYP/6-311+G**)	-425.546142			1.55	
	G (M06-2X/6-311+G**)	-425.349388			0.62	
	G (MP2/6-31+G*)	-424.034655			2.25	
E_4 io	B3LYP/6-311+G**	-425.716923	0.397	108.1	0.16	+22.9
	M06-2X/6-311+G**	-425.521794	0.423	116.7	0.34	+29.5
	MP2/6-31+G*	-424.211611	0.418	120.6	0.70	+11.5
	MP2/6-311+G**//	-424.478511			0.54	
	G (B3LYP/6-311+G**)	-425.548378			0.15	
	G (M06-2X/6-311+G**)	-425.349613			0.48	
	G (MP2/6-31+G*)	-424.038069			0.11	
^2E io	B3LYP/6-311+G**	-425.714349	0.334	210.1	1.77	**-74.1**
$^2T_1$ io	M06-2X/6-311+G**	-425.519201	0.377	200.1	1.97	**-63.2**
	MP2/6-31+G*	-424.209617	0.370	203.1	1.95	**-71.0**
	MP2/6-311+G**//	-424.476390			1.87	
	G (B3LYP/6-311+G**)	-425.544346			2.68	
	G (M06-2X/6-311+G**)	-425.346027			2.73	
	G (MP2/6-31+G*)	-424.034153			2.57	
E_5 io	B3LYP/6-311+G**	-425.717175	0.403	321.5	**0.00**	+21.4
	M06-2X/6-311+G**	-425.522338	0.426	315.7	**0.00**	+20.1
$E_3/^4T_3$ io	MP2/6-31+G*	-424.212723	0.428	262.2	**0.00**	+37.5
	MP2/6-311+G**//	-424.479372			**0.00**	

	G (B3LYP/6-311+G**)	-425.548567			0.03	
	G (M06-2X/6-311+G**)	-425.350374			**0.00**	
	G (MP2/6-31+G*)	-424.037584			0.41	
$^3T_2/^3E$ io	M06-2X/6-311+G**	-425.521138	0.409	65.1	0.75	**-34.2**[a]
	G (M06-2X/6-311+G**)	-425.347552			1.77	
E_5 in	B3LYP/6-311+G**	-425.716816	0.397	320.4	0.23	+18.9
(=^5E)	M06-2X/6-311+G**	-425.522045	0.422	319.4	0.18	+29.5
$^4T_3$ in	MP2/6-31+G*	-424.211943	0.417	270.2	0.49	+13.2
	MP2/6-311+G**//	-424.478623			0.47	
	G (B3LYP/6-311+G**)	-425.548458			0.10	
	G (M06-2X/6-311+G**)	-425.349868			0.32	
	G (MP2/6-31+G*)	-424.038241			**0.00**	
^2E in	B3LYP/6-311+G**	-425.714169	0.328	216.0	1.89	**-78.3**
	M06-2X/6-311+G**	-425.519303	0.374	216.0	1.90	**-80.3**
	MP2/6-31+G*	-424.209469	0.360	216.0	2.04	**-83.1**
	MP2/6-311+G**//	-424.476395			1.87	
	G (B3LYP/6-311+G**)	-425.544189			2.78	
	G (M06-2X/6-311+G**)	-425.346162			2.64	
	G (MP2/6-31+G*)	-424.034169			2.56	
$^3T_2$ in	B3LYP/6-311+G**	-425.716500	0.396	57.1	0.42	**-26.6**
(=$^1T_2$)	M06-2X/6-311+G**	-425.521139	0.413	41.3	0.75	**-23.7**
	G (B3LYP/6-311+G**)	-425.546392			1.40	
	G (M06-2X/6-311+G**)	-425.347819			1.60	
E_2 in	B3LYP/6-311+G**	-425.716523	0.400	36.0	0.41	+22.3
	M06-2X/6-311+G**	-425.521141	0.414	36.0	0.75	+26.2
	MP2/6-31+G*	-424.210836	0.413	36.0	1.18	**-28.3**
	MP2/6-311+G**//	-424.477440			1.21	
	G (B3LYP/6-311+G**)	-425.548617			**0.00**	
	G (M06-2X/6-311+G**)	-425.349761			0.38	
	G (MP2/6-31+G*)	-424.035072			1.99	
E_4 (TS between	B3LYP/6-311+G**	-425.713942	0.403	127.9	2.03	**-97.6**
in/in-out)	M06-2X/6-311+G**	-425.518317	0.430	129.8	2.52	**-111.0**
	G (B3LYP/6-311+G**)	-425.545022			2.26	
	G (M06-2X/6-311+G**)	-425.345718			2.92	
E_4 (TS between	B3LYP/6-311+G**	-425.714600	0.402	98.1	1.62	**-85.5**
in-out/out)	M06-2X/6-311+G**	-425.518273	0.425	105.1	2.55	**-96.4**
	MP2/6-31+G*	-424.208520	0.422	100.6	2.64	**-91.6**
	MP2/6-311+G**//	-424.475081			2.69	
	G (B3LYP/6-311+G**)	-425.545255			2.11	
	G (M06-2X/6-311+G**)	-425.345674			2.95	
	G (MP2/6-31+G*)	-424.033551			2.94	
E_5 (TS between	B3LYP/6-311+G**	-425.714689	0.401	335.3	1.56	**-84.2**
in/in-out)	M06-2X/6-311+G**	-425.518809	0.424	331.2	2.21	**-96.8**
E_3 (TS between	MP2/6-31+G*	-424.208778	0.427	257.5	2.48	**-108.8**
in/in-out)	MP2/6-311+G**//	-424.475294			2.56	
	G (B3LYP/6-311+G**)	-425.545280			2.09	
	G (M06-2X/6-311+G**)	-425.345937			2.78	
	G (MP2/6-31+G*)	-424.033296			3.10	
E_5 (TS between	B3LYP/6-311+G**	-425.714090	0.410	312.8	1.94	**-97.5**
in-out/out)	M06-2X/6-311+G**	-425.518523	0.431	296.4	2.39	**-110.8**
	G (B3LYP/6-311+G**)	-425.545221			2.13	
	G (M06-2X/6-311+G**)	-425.345886			2.82	

a) All efforts to find this TS with B3LYP or MP2 were unsuccessful

Compound 19: *trans*-1,3-dimethoxycyclopentane

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
$^5T_4$ out	B3LYP/6-311+G**	-425.718710	0.396	126.0	**0.00**	+19.8
	M06-2X/6-311+G**	-425.523894	0.428	126.0	**0.00**	+22.7
	MP2/6-31+G*	-424.214271	0.420	126.0	0.00	**-6.7**
	MP2/6-311+G**//	-424.480935			**0.00**	
	G (B3LYP/6-311+G**)	-425.550220			**0.00**	
	G (M06-2X/6-311+G**)	-425.352135			**0.00**	
	G (MP2/6-31+G*)	-424.038169			1.80	
E_4 out	MP2/6-31+G*	-424.214276	0.420	111.5	**0.00**	+9.4
	MP2/6-311+G**//	-424.480830			0.07	
	G (MP2/6-31+G*)	-424.041042			**0.00**	
$^4T_5$ out	B3LYP/6-311+G**	-425.717116	0.394	306.0	1.00	**-14.4**
	M06-2X/6-311+G**	-425.521886	0.411	306.0	1.26	**-10.7**
	MP2/6-31+G*	-424.211549	0.412	306.0	1.71	**-26.7**
	MP2/6-311+G**//	-424.478118			1.77	
	G (B3LYP/6-311+G**)	-425.546596			2.27	
	G (M06-2X/6-311+G**)	-425.347860			2.68	
	G (MP2/6-31+G*)	-424.035081			3.74	
$^5T_4/E_4$ io	B3LYP/6-311+G**	-425.718412	0.394	115.0	0.19	+20.3
	M06-2X/6-311+G**	-425.523750	0.426	127.7	0.09	+21.1
E_4 io	MP2/6-31+G*	-424.214011	0.417	107.6	0.17	+13.6
	MP2/6-311+G**//	-424.480443	0.412	306.0	0.31	
	G (B3LYP/6-311+G**)	-425.549855			0.23	
	G (M06-2X/6-311+G**)	-425.351901			0.15	
	G (MP2/6-31+G*)	-424.040221			0.52	
^4E io	B3LYP/6-311+G**	-425.717346	0.389	286.3	0.86	**-16.1**
E_5 io	M06-2X/6-311+G**	-425.522153	0.412	319.5	1.09	**-18.2**
$^4T_5$ io	MP2/6-31+G*	-424.211882	0.410	306.8	1.50	**-27.1**
	MP2/6-311+G**//	-424.478505			1.52	

	G (B3LYP/6-311+G**)	-425.546754			2.17	
	G (M06-2X/6-311+G**)	-425.348088			2.54	
	G (MP2/6-31+G*)	-424.035449			3.51	
$^{1}T_5$ io	B3LYP/6-311+G**	-425.717748	0.394	351.8	0.60	+15.6
	G (B3LYP/6-311+G**)	-425.549710			0.32	
E_2 io	B3LYP/6-311+G**	-425.717581	0.382	37.1	0.71	**-36.6**
	G (B3LYP/6-311+G**)	-425.547504			1.70	
$^{5}T_4$ in	B3LYP/6-311+G**	-425.717914	0.396	126.0	0.50	+17.0
	M06-2X/6-311+G**	-425.523476	0.428	126.0	0.26	+20.4
	MP2/6-31+G*	-424.213543	0.420	126.0	0.46	+8.7
	MP2/6-311+G**//	-424.480104			0.52	
	G (B3LYP/6-311+G**)	-425.549568			0.41	
	G (M06-2X/6-311+G**)	-425.351573			0.35	
	G (MP2/6-31+G*)	-424.040223			0.51	
E_4 in	MP2/6-31+G*	-424.213539	0.418	111.5	0.46	**-8.1**
	MP2/6-311+G**//	-424.480023			0.57	
	G (MP2/6-31+G*)	-424.037189			2.42	
$E_4/^{3}T_4$ in	MP2/6-31+G*	-424.213540	0.416	102.9	0.46	+10.5
	MP2/6-311+G**//	-424.479939			0.62	
	G (MP2/6-31+G*)	-424.039972			0.67	
$^{2}T_1/^{2}E$ in	B3LYP/6-311+G**	-425.717260	0.381	202.5	0.91	**-31.1**
	G (B3LYP/6-311+G**)	-425.547091			1.96	
$^{1}T_5$ in	B3LYP/6-311+G**	-425.717576	0.392	348.2	0.71	+17.2
	G (B3LYP/6-311+G**)	-425.549497			0.45	
$^{4}T_5$ in	B3LYP/6-311+G**	-425.717477	0.389	306.0	0.77	**-16.1**
	M06-2X/6-311+G**	-425.522889	0.413	306.0	0.63	**-13.6**
	MP2/6-31+G*	-424.211827	0.410	306.0	1.54	**-28.1**
	MP2/6-311+G**//	-424.478547			1.50	
	G (B3LYP/6-311+G**)	-425.546936			2.06	
	G (M06-2X/6-311+G**)	-425.348399			2.34	
	G (MP2/6-31+G*)	-424.035551			3.45	
^{5}E (TS between in/in-out)	B3LYP/6-311+G**	-425.715534	0.399	139.8	1.99	**-95.1**
	M06-2X/6-311+G**	-425.520448	0.429	140.9	2.16	**-107.3**
	MP2/6-31+G*	-424.211032	0.419	156.0	2.04	**-98.7**
	MP2/6-311+G**//	-424.477189			2.35	
	G (B3LYP/6-311+G**)	-425.546425			2.38	
	G (M06-2X/6-311+G**)	-425.347679			2.80	
	G (MP2/6-31+G*)	-424.035966			3.19	
E_4 (TS between in-out/out)	B3LYP/6-311+G**	-425.715987	0.401	108.4	1.71	**-93.9**
	M06-2X/6-311+G**	-425.520576	0.432	114.0	2.08	**-110.0**
	MP2/6-31+G*	-424.211347	0.421	101.7	1.84	**-99.0**
	MP2/6-311+G**//	-424.477550			2.12	
	G (B3LYP/6-311+G**)	-425.546734			2.19	
	G (M06-2X/6-311+G**)	-425.347965			2.62	
	G (MP2/6-31+G*)	-424.036468			2.87	
$^{1}T_5$ (TS between in/in-out)	B3LYP/6-311+G**	-425.715608	0.395	359.7	1.95	**-86.7**
	G (B3LYP/6-311+G**)	-425.546600			2.27	

Compound 20: 2-hydroxytetrahydrofuran

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
^{2}E	B3LYP/6-311+G**	-307.775887	0.354	69.6	**0.00**	+87.1
	M06-2X/6-311+G**	-307.642140	0.377	67.5	**0.00**	+72.5
$^{2}T_1/^{2}E$	MP2/6-311+G**	-306.926076	0.386	63.2	**0.00**	+81.2
	G (B3LYP/6-311+G**)	-307.684183			**0.00**	
	G (M06-2X/6-311+G**)	-307.548671			**0.00**	
	G (MP2/6-311+G**)	-306.831943			**0.00**	
^{0}E	B3LYP/6-311+G**	-307.775279	0.326	10.8	0.38	**-62.8**
	M06-2X/6-311+G**	-307.641317	0.350	1.7	0.52	**-60.2**
	MP2/6-311+G**	-306.924789	0.355	2.4	0.81	**-91.8**
	G (B3LYP/6-311+G**)	-307.682447			1.09	
	G (M06-2X/6-311+G**)	-307.546474			1.38	
	G (MP2/6-311+G**)	-306.829562			1.49	
E_4	B3LYP/6-311+G**	-307.775540	0.354	332.0	0.22	+62.9
	M06-2X/6-311+G**	-307.641428	0.372	335.7	0.45	+57.0
	MP2/6-311+G**	-306.925281	0.391	328.8	0.50	+81.6
	G (B3LYP/6-311+G**)	-307.683748			0.27	
	G (M06-2X/6-311+G**)	-307.547763			0.57	
	G (MP2/6-311+G**)	-306.830823			0.70	
^{1}E	B3LYP/6-311+G**	-307.770531	0.331	208.9	3.36	**-77.3**
	M06-2X/6-311+G**	-307.636007	0.360	210.8	3.85	**-65.9**
$E_0/^{1}E_0$	MP2/6-311+G**	-306.919423	0.380	188.4	4.17	**-61.9**
	G (B3LYP/6-311+G**)	-307.678524			3.55	
	G (M06-2X/6-311+G**)	-307.542118			4.11	
	G (MP2/6-311+G**)	-306.824927			4.40	

Compound 21: *cis*-2-hydroxy-5-methyloxolane (β-2,3,5-trideoxy-L-*glycero*-pentose)

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
^{2}E	B3LYP/6-311+G**	-347.106048	0.360	78.1	**0.00**	+66.1
	M06-2X/6-311+G**	-346.952092	0.377	70.1	**0.00**	+59.0
	MP2/6-311+G**	-346.129031	0.389	71.3	**0.00**	+61.4

	G (B3LYP/6-311+G**)	-346.988398			**0.00**	
	G (M06-2X/6-311+G**)	-346.832260			**0.00**	
	G (MP2/6-311+G**)	-346.008497			**0.00**	
^{O}E	B3LYP/6-311+G**	-347.103177	0.278	350.8	1.80	**-78.3**
	M06-2X/6-311+G**	-346.949274	0.294	356.0	1.77	**-96.9**
	MP2/6-311+G**	-346.125265	0.296	356.4	2.36	**-103.4**
	G (B3LYP/6-311+G**)	-346.984230			2.62	
	G (M06-2X/6-311+G**)	-346.827941			2.71	
	G (MP2/6-311+G**)	-346.003448			3.17	
E_4	B3LYP/6-311+G**	-347.103491	0.328	318.3	1.60	+73.6
	M06-2X/6-311+G**	-346.950040	0.356	318.6	1.29	+95.8
	MP2/6-311+G**	-346.126343	0.368	316.6	1.69	+101.5
	G (B3LYP/6-311+G**)	-346.985633			1.74	
	G (M06-2X/6-311+G**)	-346.829644			1.64	
	G (MP2/6-311+G**)	-346.005326			1.99	
^{1}E	B3LYP/6-311+G**	-347.100781	0.326	222.8	3.30	**-56.6**
	M06-2X/6-311+G**	-346.945861	0.358	216.8	3.91	**-57.0**
	MP2/6-311+G**	-346.122623	0.379	217.9	4.02	**-42.7**
	G (B3LYP/6-311+G**)	-346.982576			3.65	
	G (M06-2X/6-311+G**)	-346.825391			4.31	
	G (MP2/6-311+G**)	-346.001577			4.34	

Compound 22: *trans*-2-hydroxy-5-methyloxolane (α-2,3,5-trideoxy-L-*glycero*-pentose)

Shape	Level of theory	Energy (Hartrees)	Q (Å)	Φ (º)	Rel. Energy (kcal/mol)	Lower freq. (cm-1)
^{4}E	B3LYP/6-311+G**	-347.106102	0.354	149.8	**0.00**	+66.2
	M06-2X/6-311+G**	-346.951422	0.370	153.6	0.22	+65.0
	MP2/6-311+G**	-346.128529	0.387	148.8	0.17	+82.1
	G (B3LYP/6-311+G**)	-346.988543			**0.00**	
	G (M06-2X/6-311+G**)	-346.831606			0.10	
	G (MP2/6-311+G**)	-346.007912			0.20	
^{O}E	B3LYP/6-311+G**	-347.099249	0.257	5.1	4.30	**-95.0**
	M06-2X/6-311+G**	-346.944601	0.311	8.3	4.50	**-85.1**
	MP2/6-311+G**	-346.120611	0.323	4.9	5.14	**-96.9**
	G (B3LYP/6-311+G**)	-346.981405			4.48	
	G (M06-2X/6-311+G**)	-346.824096			4.82	
	G (MP2/6-311+G**)	-345.999598			5.42	
$^{1}T_2/E_2$	B3LYP/6-311+G**	-347.105645	0.339	235.7	0.29	+40.3
	M06-2X/6-311+G**	-346.951775	0.373	244.0	**0.00**	+58.5
	MP2/6-311+G**	-346.128801	0.383	239.0	**0.00**	+60.2
	G (B3LYP/6-311+G**)	-346.988366			0.11	
	G (M06-2X/6-311+G**)	-346.831772			**0.00**	
	G (MP2/6-311+G**)	-346.008229			**0.00**	
$^{1}E/^{1}T_O$	B3LYP/6-311+G**	-347.105557	0.323	206.3	0.34	**-38.1**
$^{1}T_O/E_O$	M06-2X/6-311+G**	-346.951151	0.344	190.8	0.39	**-52.8**
$E_O/^{1}E_O$	MP2/6-311+G**	-346.127866	0.349	187.9	0.59	**-76.6**
	G (B3LYP/6-311+G**)	-346.986741			1.13	
	G (M06-2X/6-311+G**)	-346.830108			1.04	
	G (MP2/6-311+G**)	-346.006308			1.21	

Cartesian coordinates of all shapes found for compounds **1-22** at the B3LYP, M06-2X and MP2 levels of theory.

COMP. 01_E-T_B3LYP
C 0.561438 -1.125731 0.259104
C -0.898154 -0.912907 -0.177305
C -1.159877 0.600157 0.041597
C 0.243976 1.274982 0.098204
C 1.259257 0.155744 -0.221782
H 1.002567 -2.038061 -0.151047
H 0.621978 -1.195025 1.351917
H -1.604050 -1.545187 0.366918
H -0.998017 -1.161664 -1.239331
H -1.779887 1.015738 -0.756313
H -1.701274 0.767194 0.976511
H 0.430746 1.670372 1.100996
H 0.328876 2.117197 -0.592549
H 2.232626 0.320897 0.247286
H 1.426596 0.095071 -1.303302

COMP. 01_E-T_M06-2X
C 0.332873 -1.202023 0.273085
C -1.048579 -0.721297 -0.184940
C -1.018659 0.807187 0.042363
C 0.483916 1.196982 0.102506
C 1.256248 -0.090941 -0.233780
H 0.592343 -2.191154 -0.108664
H 0.371299 -1.242968 1.367177
H -1.870831 -1.209357 0.340700
H -1.166668 -0.939168 -1.250583
H -1.545945 1.338075 -0.751706
H -1.516257 1.065139 0.979326
H 0.744657 1.527228 1.110976
H 0.729967 2.015772 -0.575122
H 2.252803 -0.115306 0.210479
H 1.373835 -0.187708 -1.317992

COMP. 01_E-T_MP2
C 0.460476 -1.158166 0.278302
C -0.963518 -0.830803 -0.188445
C -1.100840 0.692586 0.043754
C 0.352706 1.242587 0.103415
C 1.258230 0.043929 -0.237211
H 0.826146 -2.118227 -0.098862
H 0.500252 -1.185896 1.374880
H -1.734527 -1.406237 0.332466
H -1.047596 -1.056554 -1.258073
H -1.683267 1.166572 -0.751537
H -1.622927 0.890812 0.984938
H 0.579371 1.596157 1.114862
H 0.506939 2.085506 -0.576289
H 2.256253 0.130672 0.203030
H 1.377029 -0.043603 -1.324310

COMP. 01_E_B3LYP
C 0.000135 -1.257118 0.261966
C -1.203194 -0.420348 -0.201044
C -0.779802 1.043530 0.069742
C 0.779502 1.043749 0.069876
C 1.203359 -0.420029 -0.200745
H 0.000321 -2.272201 -0.143990
H 0.000008 -1.341216 1.355461
H -1.360189 -0.574885 -1.274400
H -2.135084 -0.689895 0.302377
H -1.192282 1.728114 -0.675150
H -1.157925 1.373227 1.041439
H 1.191912 1.728394 -0.674998
H 1.157368 1.373629 1.041610
H 1.360688 -0.574559 -1.274053
H 2.135186 -0.689308 0.302936

COMP. 01_E_M06-2X
C -0.013974 -1.246188 0.276120
C -1.198365 -0.406876 -0.212358
C -0.766038 1.045211 0.074137
C 0.788061 1.029379 0.070455
C 1.190006 -0.433182 -0.209286
H -0.024602 -2.270450 -0.101044
H -0.016121 -1.290294 1.370832
H -1.322530 -0.556466 -1.289487
H -2.143190 -0.668538 0.266926
H -1.174282 1.742704 -0.658691
H -1.136749 1.359149 1.052436
H 1.206325 1.713231 -0.669551
H 1.170180 1.343070 1.044373
H 1.316005 -0.588914 -1.285280
H 2.126823 -0.713560 0.275079

COMP. 01_E_MP2
C -0.029048 -1.245022 0.281286
C -1.202302 -0.393285 -0.215855
C -0.754213 1.054625 0.075427
C 0.801376 1.019964 0.071719
C 1.183722 -0.448447 -0.212805
H -0.052116 -2.273749 -0.091392
H -0.031542 -1.280040 1.378421
H -1.318163 -0.541947 -1.296326
H -2.156286 -0.641989 0.258753
H -1.153171 1.760057 -0.659051
H -1.122903 1.368842 1.057202
H 1.227173 1.701759 -0.669979
H 1.188906 1.324813 1.049127
H 1.297640 -0.605803 -1.292211
H 2.123256 -0.738952 0.266826

COMP. 01_T_B3LYP
C 0.861319 -0.919403 0.252855
C -0.607455 -1.133333 -0.155959
C -1.282261 0.255366 0.018099
C -0.121193 1.287903 0.121343
C 1.159117 0.505830 -0.236448
H 1.534873 -1.671218 -0.166903
H 0.960426 -0.964158 1.344017
H -1.100241 -1.915705 0.426321
H -0.650473 -1.442197 -1.205576
H -1.944668 0.477505 -0.822053
H -1.901581 0.281160 0.918281
H -0.045913 1.666271 1.145472
H -0.274323 2.155246 -0.525196
H 2.058800 0.938172 0.209148
H 1.305937 0.496748 -1.322849

COMP. 01_T_M06-2X
C 0.849216 -0.917970 0.263229
C -0.612826 -1.123835 -0.154861
C -1.273776 0.267611 0.010171
C -0.105297 1.280303 0.134543
C 1.153738 0.490442 -0.253288
H 1.518915 -1.682784 -0.134167
H 0.934115 -0.932622 1.355188
H -1.115974 -1.899639 0.424207
H -0.645110 -1.430250 -1.204160
H -1.913933 0.499132 -0.842737
H -1.907892 0.299102 0.897949
H -0.013309 1.618530 1.170101
H -0.252298 2.168242 -0.482045
H 2.068742 0.918703 0.159795
H 1.260415 0.462281 -1.342898

COMP. 01_T_MP2
C 0.886427 -0.880479 0.268893
C -0.563758 -1.148608 -0.159164
C -1.284987 0.213320 0.012606
C -0.158336 1.275417 0.134467
C 1.132247 0.537044 -0.256863
H 1.590305 -1.621434 -0.122476
H 0.964568 -0.883406 1.363611
H -1.038923 -1.949992 0.414124
H -0.574731 -1.447696 -1.213516
H -1.939171 0.420414 -0.839345
H -1.915255 0.213703 0.906926

H -0.076418 1.616962 1.172286
H -0.345768 2.157145 -0.485118
H 2.031022 1.008106 0.152830
H 1.234813 0.506040 -1.348954

COMP. 02_1E_B3LYP
C 0.785517 -0.000001 0.368668
C 0.003167 -1.204971 -0.145576
C -1.473441 -0.781816 0.019241
C -1.473442 0.781815 0.019237
C 0.003167 1.204972 -0.145573
F 2.112418 0.000000 -0.097553
H 0.851582 -0.000002 1.462008
H 0.257423 -1.340498 -1.201683
H 0.251853 -2.130162 0.377556
H -2.096771 -1.193048 -0.776800
H -1.879084 -1.160104 0.960919
H -2.096766 1.193044 -0.776810
H -1.879091 1.160108 0.960911
H 0.257427 1.340503 -1.201679
H 0.251852 2.130161 0.377564

COMP. 02_1E_M06-2X
C 0.780885 -0.000003 0.364161
C 0.005008 -1.196606 -0.164566
C -1.463641 -0.779398 0.029798
C -1.463644 0.779396 0.029780
C 0.005010 1.196609 -0.164551
F 2.097084 0.000000 -0.078189
H 0.815379 -0.000010 1.458941
H 0.246942 -1.300117 -1.226469
H 0.264040 -2.130282 0.335029
H -2.102844 -1.190740 -0.751337
H -1.843553 -1.156112 0.981308
H -2.102823 1.190716 -0.751387
H -1.843591 1.156132 0.981267
H 0.246961 1.300142 -1.226448
H 0.264033 2.130275 0.335066

COMP. 02_1E_MP2
C 0.777509 0.000000 0.361018
C 0.004001 -1.194959 -0.174912
C -1.465039 -0.780466 0.035915
C -1.465040 0.780466 0.035913
C 0.004001 1.194959 -0.174910
F 2.106132 0.000000 -0.067564
H 0.798685 -0.000001 1.457747
H 0.236108 -1.286301 -1.241949
H 0.267073 -2.135219 0.315801
H -2.112978 -1.191955 -0.741823
H -1.833437 -1.159177 0.994067
H -2.112976 1.191952 -0.741829
H -1.833442 1.159179 0.994062
H 0.236110 1.286304 -1.241946
H 0.267072 2.135218 0.315805

COMP. 02_5T4_B3LYP
C -0.886005 0.106022 0.474365
C 0.096068 1.269318 0.273425
C 1.438688 0.630751 -0.185378
C 1.125671 -0.864584 -0.414458
C -0.024527 -1.147909 0.565693
F -1.710303 -0.002033 -0.677705
H -1.572326 0.242581 1.312091
H -0.318303 1.959617 -0.463704
H 0.216029 1.828097 1.205221
H 1.841627 1.110637 -1.079238
H 2.191930 0.738122 0.600717
H 0.780130 -1.029344 -1.438824
H 1.992966 -1.508163 -0.251916
H -0.598009 -2.049911 0.343720
H 0.359314 -1.234929 1.589396

COMP. 02_5T4_M06-2X
C -0.888727 0.118909 0.469625
C 0.105437 1.267603 0.281647
C 1.427609 0.610944 -0.194372
C 1.085455 -0.873720 -0.418550
C -0.035194 -1.132348 0.594194
F -1.658807 -0.000702 -0.695446
H -1.594213 0.269993 1.287814
H -0.303295 1.973381 -0.442548
H 0.242331 1.805310 1.221758
H 1.826475 1.084099 -1.091715
H 2.189189 0.700329 0.584079
H 0.697973 -1.025678 -1.428675
H 1.945185 -1.531102 -0.284887
H -0.615029 -2.037141 0.408590
H 0.373164 -1.181208 1.609336

COMP. 02_5T4_MP2
C -0.888192 0.121450 0.472228
C 0.108234 1.268513 0.283785
C 1.428013 0.608743 -0.200317
C 1.081096 -0.877091 -0.420746
C -0.033813 -1.129086 0.601305
F -1.660217 -0.002487 -0.699622
H -1.595053 0.276319 1.291381
H -0.300438 1.980911 -0.437321
H 0.250429 1.800361 1.229687
H 1.820106 1.082334 -1.103821
H 2.195783 0.697210 0.575511
H 0.687430 -1.029928 -1.430281
H 1.944286 -1.535040 -0.288711
H -0.615896 -2.037530 0.426738
H 0.383272 -1.167421 1.615887

COMP. 02_E1_B3LYP
C -0.915052 0.000004 0.459442
C 0.016266 1.204015 0.506421
C 1.253031 0.779570 -0.322227
C 1.253019 -0.779580 -0.322232
C 0.016260 -1.204010 0.506431
F -1.596894 0.000000 -0.786014
H -1.692765 0.000010 1.226064
H -0.473175 2.105847 0.133961
H 0.289398 1.384569 1.551748
H 1.172213 1.158205 -1.342814
H 2.173430 1.190662 0.097625
H 1.172176 -1.158206 -1.342820
H 2.173419 -1.190689 0.097601
H -0.473186 -2.105845 0.133988
H 0.289400 -1.384550 1.551759

COMP. 02_E1_M06-2X
C -0.888728 0.118909 0.469625
C 0.105436 1.267604 0.281650
C 1.427606 0.610947 -0.194376
C 1.085456 -0.873720 -0.418548
C -0.035194 -1.132348 0.594196
F -1.658802 -0.000704 -0.695450
H -1.594218 0.269990 1.287811
H -0.303301 1.973387 -0.442538
H 0.242334 1.805302 1.221766
H 1.826466 1.084100 -1.091721
H 2.189189 0.700333 0.584071
H 0.697977 -1.025685 -1.428673
H 1.945188 -1.531098 -0.284878
H -0.615028 -2.037142 0.408594
H 0.373165 -1.181203 1.609337

COMP. 02_E1_MP2
C -0.920078 0.000002 0.453194
C 0.013493 1.195550 0.530625
C 1.226242 0.778177 -0.329182
C 1.226238 -0.778181 -0.329183
C 0.013491 -1.195548 0.530628
F -1.538015 0.000000 -0.811422
H -1.721909 0.000004 1.196464
H -0.470430 2.113299 0.187114
H 0.305850 1.333605 1.578163
H 1.110451 1.154976 -1.348352

H 2.158003 1.189384 0.067993
H 1.110439 -1.154977 -1.348354
H 2.157998 -1.189394 0.067985
H -0.470435 -2.113298 0.187123
H 0.305851 -1.333599 1.578167

COMP. 03_1E_B3LYP
C 0.341860 -0.000034 0.406239
C -0.421165 -1.205408 -0.141339
C -1.901468 -0.781235 0.002162
C -1.901464 0.781236 0.002337
C -0.421167 1.205430 -0.141136
Cl 2.106546 0.000005 -0.053679
H 0.345077 -0.000124 1.497428
H -0.156394 -1.340219 -1.194022
H -0.180995 -2.131819 0.383004
H -2.510861 -1.192770 -0.804616
H -2.319722 -1.160381 0.937830
H -2.510897 1.192959 -0.804316
H -2.319665 1.160173 0.938114
H -0.156421 1.340402 -1.193805
H -0.180982 2.131759 0.383345

COMP. 03_1E_M06-2X
C -0.343651 -0.000001 0.400545
C 0.414610 1.196889 -0.158506
C 1.887410 0.778832 0.013535
C 1.887410 -0.778833 0.013538
C 0.414610 -1.196889 -0.158509
Cl -2.086598 0.000000 -0.045294
H -0.322599 -0.000002 1.491760
H 0.160577 1.300605 -1.216982
H 0.162472 2.130904 0.343883
H 2.512556 1.190593 -0.778896
H 2.280607 1.156154 0.959305
H 2.512560 -1.190598 -0.778887
H 2.280599 -1.156150 0.959313
H 0.160581 -1.300600 -1.216986
H 0.162471 -2.130906 0.343876

COMP. 03_1E_MP2
C -0.349742 -0.000004 0.396399
C 0.411287 1.194917 -0.165137
C 1.884602 0.779739 0.018435
C 1.884597 -0.779740 0.018461
C 0.411290 -1.194913 -0.165159
Cl -2.080131 0.000000 -0.041769
H -0.310644 -0.000016 1.490509
H 0.164059 1.291569 -1.228198
H 0.159266 2.135443 0.331644
H 2.517381 1.190246 -0.772698
H 2.269631 1.158566 0.970019
H 2.517414 -1.190282 -0.772624
H 2.269574 -1.158536 0.970080
H 0.164086 -1.291530 -1.228229
H 0.159256 -2.135453 0.331588

COMP. 03_3E_B3LYP
C 0.368552 -0.061163 0.550388
C -0.461401 -1.232117 -0.003872
C -1.904621 -0.702915 0.017389
C -1.740111 0.760613 -0.426709
C -0.453444 1.227969 0.288183
Cl 2.042265 0.000181 -0.197324
H 0.574623 -0.187589 1.611117
H -0.313114 -2.150260 0.567775
H -0.160621 -1.432071 -1.035917
H -2.315050 -0.747105 1.032760
H -2.570767 -1.278304 -0.629555
H -2.603326 1.384625 -0.185399
H -1.602695 0.799390 -1.512068
H -0.693680 1.697762 1.246242
H 0.112275 1.956148 -0.292718

COMP. 03_3E_M06-2X
C 0.369973 -0.059431 0.529230
C -0.451093 -1.219632 -0.042256
C -1.890387 -0.706584 0.054289
C -1.750284 0.748863 -0.408606
C -0.445320 1.227101 0.256629
Cl 2.031411 0.000150 -0.179885
H 0.540900 -0.193953 1.595546
H -0.266486 -2.156176 0.484641
H -0.185962 -1.362095 -1.093440
H -2.237632 -0.741072 1.092234
H -2.587452 -1.287579 -0.550933
H -2.606652 1.371041 -0.146523
H -1.644706 0.770425 -1.496774
H -0.654832 1.728814 1.203684
H 0.111499 1.926150 -0.366117

COMP. 03_3E_MP2
C 0.379867 -0.063922 0.544863
C -0.454054 -1.224762 -0.017006
C -1.890473 -0.693975 0.038489
C -1.714803 0.752465 -0.441842
C -0.446538 1.222377 0.293935
Cl 2.012844 0.000103 -0.194545
H 0.560350 -0.202131 1.612649
H -0.289663 -2.154774 0.533957
H -0.176141 -1.394059 -1.063003
H -2.266092 -0.706518 1.069357
H -2.579223 -1.276303 -0.580406
H -2.578564 1.391546 -0.238267
H -1.542834 0.751698 -1.524427
H -0.713195 1.671543 1.256589
H 0.123012 1.964154 -0.269818

COMP. 03_E1_B3LYP
C 0.380374 0.000004 0.823493
C -0.531682 -1.202236 0.587973
C -1.460203 -0.779146 -0.574386
C -1.460213 0.779137 -0.574386
C -0.531683 1.202241 0.587962
Cl 1.764699 0.000000 -0.397338
H 0.879586 0.000009 1.789824
H 0.020416 -2.122718 0.396175
H -1.111905 -1.353045 1.506307
H -1.074758 -1.158000 -1.522641
H -2.463248 -1.192031 -0.449332
H -1.074788 1.157997 -1.522647
H -2.463262 1.192008 -0.449317
H 0.020415 2.122720 0.396148
H -1.111900 1.353063 1.506299

COMP. 03_E1_M06-2X
C -0.383370 0.000003 0.835758
C 0.532506 1.194996 0.604313
C 1.410791 0.776799 -0.591405
C 1.410783 -0.776806 -0.591404
C 0.532503 -1.194993 0.604321
Cl -1.716297 0.000000 -0.400353
H -0.888232 0.000007 1.798824
H -0.015897 2.122488 0.442239
H 1.142918 1.316261 1.505343
H 0.979856 1.152845 -1.519967
H 2.416147 1.190552 -0.508788
H 0.979833 -1.152847 -1.519963
H 2.416134 -1.190571 -0.508799
H -0.015901 -2.122486 0.442256
H 1.142918 -1.316250 1.505350

COMP. 03_E1_MP2
C 0.393252 0.000002 0.830437
C -0.528898 -1.193716 0.608379
C -1.404581 -0.777645 -0.591958
C -1.404586 0.777640 -0.591959
C -0.528899 1.193719 0.608374
Cl 1.704912 0.000000 -0.402142
H 0.891051 0.000005 1.801423
H 0.014522 -2.127635 0.447347
H -1.143191 -1.306950 1.510674

H -0.973438 -1.155040 -1.522622
H -2.414026 -1.189118 -0.507716
H -0.973453 1.155038 -1.522626
H -2.414034 1.189106 -0.507710
H 0.014521 2.127637 0.447334
H -1.143190 1.306959 1.510669

COMP. 04_1T5_B3LYP
C -0.791008 -0.016270 0.358437
C 0.019429 1.217827 -0.056038
C 1.501884 0.758588 -0.070168
C 1.472443 -0.788848 0.099695
C 0.020830 -1.190549 -0.205785
O -2.122104 0.096421 -0.145295
H -0.820539 -0.091222 1.455933
H -0.313305 1.506837 -1.057172
H -0.161652 2.069025 0.603021
H 1.981635 1.039596 -1.010484
H 2.081019 1.228816 0.727780
H 2.194000 -1.296881 -0.543606
H 1.722671 -1.058821 1.130685
H -0.153155 -1.238912 -1.286674
H -0.260224 -2.156760 0.224074
H -2.635082 -0.657536 0.161960

COMP. 04_1T5_M06-2X
C 0.783254 0.010719 0.355636
C -0.020680 -1.208893 -0.087573
C -1.497468 -0.754436 -0.045547
C -1.460584 0.791687 0.101748
C -0.014145 1.179719 -0.222757
O 2.112578 -0.099179 -0.118393
H 0.779689 0.079427 1.453515
H 0.182116 -2.085806 0.527692
H 0.290481 -1.442387 -1.109417
H -2.035598 -1.210568 0.786642
H -2.017847 -1.050063 -0.957521
H -1.693814 1.075236 1.131531
H -2.185193 1.292855 -0.540583
H 0.276885 2.150117 0.186986
H 0.153305 1.198062 -1.304865
H 2.607089 0.673789 0.164121

COMP. 04_1T5_MP2
C -0.783725 -0.020240 0.358060
C 0.019200 1.214236 -0.053594
C 1.497967 0.749774 -0.083508
C 1.458529 -0.787222 0.127110
C 0.021432 -1.177205 -0.233410
O -2.116695 0.101329 -0.127451
H -0.790701 -0.113755 1.455673
H -0.323492 1.502998 -1.052861
H -0.153839 2.060869 0.615483
H 1.954794 0.994000 -1.046832
H 2.097104 1.240106 0.688681
H 2.209522 -1.314146 -0.467741
H 1.647222 -1.027247 1.179859
H -0.123997 -1.173597 -1.320885
H -0.275704 -2.157438 0.155104
H -2.587761 -0.698477 0.125177

COMP. 04_3T2_B3LYP
C 0.810785 -0.051993 0.380605
C -0.054252 -1.205299 -0.133898
C -1.487427 -0.735148 0.140804
C -1.455484 0.760666 -0.240839
C -0.015836 1.234319 0.097897
O 2.084369 -0.087378 -0.268995
H 0.958355 -0.166311 1.463268
H 0.199225 -2.159477 0.332983
H 0.117161 -1.303830 -1.211691
H -1.722442 -0.850379 1.205326
H -2.237944 -1.299634 -0.417345
H -2.223466 1.341641 0.274738
H -1.641706 0.868390 -1.313294
H -0.002258 1.906950 0.959965
H 0.435409 1.771160 -0.740355
H 2.655996 0.575240 0.130949

COMP. 04_3T2_M06-2X
C 0.809024 -0.059719 0.384343
C -0.060789 -1.201170 -0.134882
C -1.482300 -0.721044 0.154112
C -1.434007 0.755912 -0.269541
C -0.014337 1.227730 0.122351
O 2.063778 -0.090149 -0.277111
H 0.963123 -0.187389 1.463679
H 0.192910 -2.160091 0.318503
H 0.100498 -1.279204 -1.215196
H -1.692307 -0.799977 1.226086
H -2.246613 -1.291708 -0.375109
H -2.221297 1.356094 0.188260
H -1.562543 0.822031 -1.352793
H -0.035533 1.865054 1.009058
H 0.456825 1.796996 -0.681710
H 2.629166 0.589133 0.097812

COMP. 04_3T2_MP2
C 0.804124 -0.058213 0.379648
C -0.058914 -1.197179 -0.154000
C -1.479708 -0.727268 0.162542
C -1.446199 0.755209 -0.251721
C -0.013117 1.228174 0.099148
O 2.078873 -0.091387 -0.259191
H 0.933750 -0.186801 1.464439
H 0.205995 -2.163087 0.284330
H 0.087623 -1.254924 -1.239692
H -1.669724 -0.816294 1.239549
H -2.252432 -1.297223 -0.361115
H -2.220518 1.352706 0.237516
H -1.608023 0.829095 -1.332325
H -0.007589 1.893990 0.968220
H 0.447141 1.766427 -0.735379
H 2.615675 0.602880 0.134285

COMP. 04_4E_B3LYP
C 0.823968 0.047477 0.409446
C -0.037612 -1.225241 0.213289
C -1.405321 -0.747999 -0.327079
C -1.493948 0.726060 0.108851
C -0.052755 1.222297 -0.076059
O 2.046268 -0.100492 -0.323974
H 1.064189 0.176069 1.472747
H 0.472824 -1.905104 -0.471199
H -0.155408 -1.751449 1.164004
H -1.419069 -0.804229 -1.420320
H -2.238796 -1.353018 0.037248
H -2.222177 1.303510 -0.466033
H -1.786188 0.792053 1.163564
H 0.151108 1.378968 -1.141189
H 0.160795 2.158116 0.448479
H 2.596590 0.673454 -0.166190

COMP. 04_4E_M06-2X
C 0.818671 0.046392 0.407399
C -0.040682 -1.221445 0.207601
C -1.400364 -0.737681 -0.332941
C -1.482427 0.724027 0.127036
C -0.049369 1.212886 -0.092193
O 2.036542 -0.102841 -0.309584
H 1.042286 0.181566 1.472762
H 0.472391 -1.896430 -0.478398
H -0.165313 -1.748074 1.155649
H -1.403037 -0.769075 -1.426067
H -2.235682 -1.346417 0.015635
H -2.225080 1.309101 -0.417601
H -1.737085 0.769386 1.191390
H 0.136503 1.333551 -1.164701
H 0.178360 2.158558 0.404922
H 2.569344 0.685496 -0.178336

COMP. 04_4E_MP2

C -0.816610 -0.049739 0.409009
C 0.039064 1.220971 0.208189
C 1.399395 0.738350 -0.336764
C 1.485062 -0.721519 0.132693
C 0.052872 -1.211955 -0.098176
O -2.043977 0.104291 -0.306497
H -1.035510 -0.190671 1.476869
H -0.477407 1.896744 -0.478624
H 0.166551 1.746736 1.159256
H 1.395190 0.760763 -1.432433
H 2.235024 1.355206 0.005900
H 2.235000 -1.308411 -0.405829
H 1.729836 -0.760330 1.201818
H -0.125767 -1.322848 -1.174975
H -0.181004 -2.162728 0.392424
H -2.548800 -0.705441 -0.182136

COMP. 04_5EB3P
C -0.873347 0.128318 0.481371
C 0.141899 1.262836 0.282126
C 1.451192 0.599717 -0.214408
C 1.104544 -0.882720 -0.430683
C -0.013980 -1.134976 0.582367
O -1.707707 0.102604 -0.679830
H -1.494287 0.282853 1.373573
H -0.266573 1.977411 -0.435588
H 0.301482 1.801359 1.220183
H 1.836805 1.070326 -1.121841
H 2.232667 0.692583 0.546961
H 0.719471 -1.037271 -1.443001
H 1.964058 -1.545004 -0.297672
H -0.586425 -2.050274 0.397636
H 0.399764 -1.207184 1.596405
H -2.307157 -0.644691 -0.602651

COMP. 04_5E_M06-2X
C 0.903431 -0.043975 0.478180
C -0.082751 -1.204034 0.518175
C -1.257903 -0.731958 -0.363369
C -1.194070 0.820119 -0.355855
C -0.009879 1.178986 0.562960
O 1.559698 -0.110279 -0.784633
H 1.639564 -0.084581 1.288659
H 0.377111 -2.127859 0.165773
H -0.407077 -1.355202 1.551356
H -1.136925 -1.107540 -1.379512
H -2.212166 -1.105122 0.010757
H -1.010525 1.191077 -1.364841
H -2.123887 1.272123 -0.008367
H 0.497164 2.103322 0.272916
H -0.342037 1.297848 1.598776
H 2.088226 0.683338 -0.898993

COMP. 04_5E_MP2
C -0.878158 0.138814 0.486942
C 0.148203 1.264053 0.312212
C 1.432582 0.592914 -0.247981
C 1.076629 -0.897743 -0.425595
C -0.024571 -1.123955 0.616690
O -1.660156 0.105839 -0.713887
H -1.532932 0.301375 1.352796
H -0.263676 2.019974 -0.361138
H 0.344412 1.744354 1.275870
H 1.758827 1.050016 -1.185646
H 2.253455 0.697715 0.469242
H 0.670042 -1.070117 -1.426110
H 1.939900 -1.555328 -0.288782
H -0.604342 -2.041061 0.461438
H 0.407743 -1.162677 1.625229
H -2.220294 -0.675466 -0.665409

COMP. 04_5T1_MP2
C 0.896042 -0.101421 0.481083
C -0.121215 -1.237288 0.429262
C -1.345955 -0.656718 -0.324749
C -1.119375 0.876970 -0.384312
C 0.018699 1.142923 0.614192
O 1.588997 -0.111545 -0.772110
H 1.610132 -0.213462 1.307523
H 0.308857 -2.115304 -0.059383
H -0.393243 -1.516512 1.452910
H -1.424647 -1.076720 -1.330354
H -2.272936 -0.899865 0.203050
H -0.799476 1.166203 -1.388624
H -2.024138 1.442826 -0.145245
H 0.564865 2.072138 0.414695
H -0.368041 1.194430 1.639865
H 2.117482 0.691832 -0.810420

COMP. 04_E1B3P
C -0.873347 0.128318 0.481371
C 0.141898 1.262836 0.282129
C 1.451190 0.599718 -0.214411
C 1.104544 -0.882720 -0.430682
C -0.013981 -1.134976 0.582367
O -1.707704 0.102604 -0.679831
H -1.494289 0.282852 1.373572
H -0.266574 1.977414 -0.435581
H 0.301484 1.801354 1.220189
H 1.836798 1.070326 -1.121847
H 2.232669 0.692587 0.546955
H 0.719473 -1.037275 -1.443000
H 1.964059 -1.545002 -0.297668
H -0.586425 -2.050274 0.397636
H 0.399763 -1.207185 1.596406
H -2.307154 -0.644691 -0.602655

COMP. 04_E1_B3LYP
C -0.875332 0.124269 0.484256
C 0.137787 1.267611 0.281949
C 1.457706 0.608149 -0.212063
C 1.119358 -0.882633 -0.430023
C -0.012164 -1.143522 0.575859
O -1.722395 0.101952 -0.678275
H -1.493242 0.273374 1.377701
H -0.272025 1.976756 -0.439178
H 0.293486 1.809080 1.218242
H 1.841406 1.079917 -1.118875
H 2.235744 0.706311 0.551099
H 0.747840 -1.041591 -1.445836
H 1.981034 -1.538548 -0.285111
H -0.583521 -2.055452 0.376077
H 0.393936 -1.227692 1.591468
H -2.329624 -0.641022 -0.599254

COMP. 04_E1_M06-2X
C 0.903431 -0.043972 0.478180
C -0.082750 -1.204032 0.518179
C -1.257900 -0.731961 -0.363371
C -1.194072 0.820117 -0.355855
C -0.009881 1.178987 0.562958
O 1.559696 -0.110279 -0.784634
H 1.639565 -0.084574 1.288658
H 0.377114 -2.127857 0.165782
H -0.407078 -1.355195 1.551360
H -1.136911 -1.107539 -1.379513
H -2.212163 -1.105130 0.010747
H -1.010530 1.191074 -1.364842
H -2.123890 1.272118 -0.008366
H 0.497160 2.103324 0.272913
H -0.342039 1.297849 1.598775
H 2.088234 0.683332 -0.898992

COMP. 04_E1_MP2
C 0.903936 -0.048015 0.480466
C -0.085209 -1.205500 0.516828
C -1.261035 -0.728179 -0.364462
C -1.186737 0.825125 -0.359735
C -0.007430 1.175415 0.570719
O 1.560082 -0.112473 -0.790351
H 1.642442 -0.092648 1.291798
H 0.371530 -2.133245 0.162141

H -0.411410 -1.355584 1.552268
H -1.146856 -1.108549 -1.382127
H -2.218234 -1.093060 0.018587
H -0.990855 1.193900 -1.369636
H -2.119036 1.283165 -0.017772
H 0.501163 2.105251 0.291191
H -0.347643 1.282673 1.607954
H 2.057092 0.704806 -0.894493

COMP. 05_1E_B3LYP
C -0.761659 -0.000043 -0.362747
C 0.054995 -1.198314 0.154375
C 1.531499 -0.779991 -0.026085
C 1.531499 0.779986 -0.026269
C 0.054994 1.198351 0.154090
C -2.231246 0.000006 0.053741
H -0.708403 -0.000174 -1.460888
H -0.170689 -1.347784 1.217608
H -0.187775 -2.132626 -0.359523
H 2.168618 -1.192332 0.759856
H 1.921274 -1.158749 -0.975003
H 2.168616 1.192510 0.759577
H 1.921276 1.158519 -0.975274
H -0.170691 1.348074 1.217286
H -0.187775 2.132540 -0.360031
H -2.754460 0.883068 -0.325824
H -2.326024 0.000136 1.145202
H -2.754460 -0.883147 -0.325613

COMP. 05_1E_M06-2X
C -0.753619 -0.000040 -0.365896
C 0.052754 -1.189578 0.166574
C 1.523208 -0.777640 -0.032410
C 1.523204 0.777635 -0.032618
C 0.052756 1.189614 0.166310
C -2.219406 0.000005 0.043672
H -0.683156 -0.000160 -1.461938
H -0.167853 -1.308018 1.233987
H -0.197993 -2.131555 -0.326165
H 2.169931 -1.190432 0.743144
H 1.893600 -1.154721 -0.988197
H 2.169959 1.190642 0.742794
H 1.893547 1.154460 -0.988525
H -0.167831 1.308276 1.233704
H -0.198003 2.131486 -0.326622
H -2.738719 0.883711 -0.335348
H -2.308147 0.000127 1.134519
H -2.738719 -0.883786 -0.335150

COMP. 05_1E_MP2
C -0.753106 0.000000 -0.365012
C 0.052637 -1.188170 0.172543
C 1.524264 -0.778556 -0.036467
C 1.524264 0.778555 -0.036466
C 0.052637 1.188170 0.172541
C -2.222393 0.000000 0.038977
H -0.678012 -0.000001 -1.463345
H -0.163453 -1.295905 1.244389
H -0.199587 -2.136276 -0.314194
H 2.176473 -1.191551 0.738480
H 1.886788 -1.157545 -0.997462
H 2.176472 1.191549 0.738484
H 1.886792 1.157547 -0.997459
H -0.163455 1.295907 1.244387
H -0.199587 2.136276 -0.314197
H -2.740056 0.886038 -0.343713
H -2.312140 0.000000 1.131650
H -2.740056 -0.886038 -0.343713

COMP. 05_5E_B3LYP
C -0.844252 0.082069 0.537327
C 0.150446 1.260463 0.355877
C 1.432779 0.666668 -0.301689
C 1.177465 -0.853765 -0.442360
C 0.078547 -1.154672 0.590929
C -1.867538 -0.001155 -0.604364
H -1.394840 0.189825 1.477364
H 0.394970 1.697779 1.327822
H -0.287697 2.061778 -0.245324
H 2.302136 0.848994 0.335880
H 1.652534 1.129334 -1.266713
H 2.080954 -1.447440 -0.282719
H 0.818940 -1.089076 -1.449148
H 0.523297 -1.237579 1.589440
H -0.453445 -2.089996 0.393793
H -2.530012 -0.863243 -0.478897
H -1.380271 -0.095340 -1.580020
H -2.491250 0.897311 -0.635788

COMP. 05_5E_M06-2X
C -0.835225 0.099045 0.543333
C 0.156080 1.266376 0.311918
C 1.451339 0.637084 -0.270203
C 1.141920 -0.859048 -0.460901
C 0.073265 -1.140899 0.600211
C -1.859989 -0.002783 -0.588010
H -1.373147 0.228324 1.485999
H 0.373002 1.779343 1.251035
H -0.273855 2.010666 -0.362555
H 2.272922 0.753547 0.440586
H 1.765363 1.115055 -1.199274
H 2.027144 -1.487798 -0.351602
H 0.736162 -1.043264 -1.459256
H 0.547921 -1.205752 1.585078
H -0.473162 -2.071955 0.430999
H -2.515697 -0.866416 -0.450955
H -1.367191 -0.103878 -1.559297
H -2.483808 0.893480 -0.628850

COMP. 05_5E_MP2
C -0.835076 0.100382 0.544669
C 0.156928 1.267630 0.311478
C 1.452728 0.634970 -0.271144
C 1.137122 -0.861171 -0.464091
C 0.073895 -1.139360 0.605219
C -1.858070 -0.003450 -0.590035
H -1.375827 0.234317 1.488792
H 0.374448 1.782477 1.252867
H -0.274624 2.011440 -0.366996
H 2.275078 0.746853 0.443432
H 1.767137 1.115753 -1.202025
H 2.024782 -1.492566 -0.360113
H 0.722483 -1.041695 -1.461717
H 0.555680 -1.198541 1.589825
H -0.476388 -2.072547 0.442338
H -2.508598 -0.874494 -0.455369
H -1.361384 -0.096734 -1.561869
H -2.487948 0.891724 -0.625734

COMP. 05_E1_B3LYP
C 0.855994 0.000002 0.545057
C -0.114529 -1.200035 0.535394
C -1.272205 -0.778783 -0.402815
C -1.272213 0.778777 -0.402811
C -0.114533 1.200039 0.535388
C 1.803697 0.000001 -0.662628
H 1.461707 0.000005 1.457399
H 0.366351 -2.130821 0.221427
H -0.496595 -1.362067 1.548903
H -1.108361 -1.160884 -1.413748
H -2.227344 -1.189681 -0.067610
H -1.108385 1.160885 -1.413744
H -2.227353 1.189662 -0.067594
H 0.366346 2.130821 0.221408
H -0.496593 1.362080 1.548897
H 2.448698 0.883894 -0.655390
H 1.255578 0.000002 -1.610068
H 2.448697 -0.883894 -0.655391

COMP. 05_E1_M06-2X
C -0.854597 -0.000004 0.555688
C 0.114111 1.192024 0.555854

C 1.241196 0.776496 -0.413385
C 1.241205 -0.776488 -0.413384
C 0.114117 -1.192027 0.555849
C -1.751290 -0.000002 -0.683109
H -1.482752 -0.000006 1.450739
H -0.368011 2.128874 0.266792
H 0.519491 1.327026 1.562967
H 1.042647 1.157808 -1.417153
H 2.204085 1.187280 -0.106756
H 1.042668 -1.157805 -1.417152
H 2.204096 -1.187261 -0.106744
H -0.368000 -2.128877 0.266777
H 0.519495 -1.327036 1.562961
H -2.392716 -0.884459 -0.703002
H -1.156737 0.000003 -1.601515
H -2.392720 0.884453 -0.702996

COMP. 05_E1_MP2
C 0.854509 0.000001 0.555381
C -0.115538 -1.191091 0.559682
C -1.239226 -0.777414 -0.416998
C -1.239229 0.777412 -0.416997
C -0.115539 1.191093 0.559679
C 1.750711 0.000000 -0.685188
H 1.486639 0.000002 1.451541
H 0.365837 -2.133302 0.275983
H -0.526334 -1.317382 1.568668
H -1.034310 -1.161028 -1.421157
H -2.206057 -1.187409 -0.111334
H -1.034321 1.161028 -1.421156
H -2.206061 1.187402 -0.111327
H 0.365836 2.133303 0.275974
H -0.526332 1.317388 1.568665
H 2.392633 0.887188 -0.702142
H 1.155716 0.000001 -1.604921
H 2.392630 -0.887189 -0.702142

COMP. 06_1E_B3LYP
C 0.199134 0.000000 -0.358783
C 1.031112 -1.199885 0.142166
C 2.500474 -0.778846 -0.083861
C 2.500474 0.778846 -0.083861
C 1.031112 1.199885 0.142166
C -1.320896 0.000000 -0.022136
C -1.977058 1.250237 -0.643273
C -1.594775 -0.000001 1.494896
C -1.977059 -1.250236 -0.643274
H 0.264981 0.000000 -1.457656
H 0.848541 -1.356907 1.210465
H 0.786937 -2.134326 -0.367694
H 3.161322 -1.192025 0.681896
H 2.860270 -1.157938 -1.044420
H 3.161322 1.192024 0.681896
H 2.860270 1.157939 -1.044420
H 0.848541 1.356907 1.210465
H 0.786937 2.134325 -0.367694
H -1.791497 1.298801 -1.721318
H -1.597089 2.172100 -0.195347
H -3.061077 1.232092 -0.492721
H -1.180721 0.884488 1.985875
H -1.180721 -0.884490 1.985874
H -2.673469 0.000000 1.679966
H -1.597089 -2.172100 -0.195349
H -1.791497 -1.298799 -1.721319
H -3.061077 -1.232092 -0.492722

COMP. 06_1E_M06-2X
C -0.197945 0.000000 -0.355972
C -1.019715 1.192147 0.156710
C -2.481953 0.776710 -0.090785
C -2.481953 -0.776709 -0.090783
C -1.019714 -1.192147 0.156709
C 1.310838 0.000000 -0.026250
C 1.957535 -1.246602 -0.644193
C 1.587564 -0.000001 1.482669
C 1.957536 1.246603 -0.644192
H -0.276649 0.000001 -1.454204
H -0.845644 1.320342 1.229874
H -0.766863 2.133396 -0.334374
H -3.154020 1.190249 0.662554
H -2.819967 1.153731 -1.058511
H -3.154018 -1.190246 0.662560
H -2.819971 -1.153733 -1.058507
H -0.845642 -1.320345 1.229872
H -0.766864 -2.133396 -0.334377
H 1.755556 -1.299753 -1.718418
H 1.580165 -2.161868 -0.181607
H 3.042201 -1.225008 -0.505419
H 1.176719 -0.885891 1.972236
H 1.176718 0.885888 1.972238
H 2.667195 0.000000 1.658039
H 1.580165 2.161868 -0.181604
H 1.755556 1.299755 -1.718417
H 3.042201 1.225008 -0.505418

COMP. 06_1E_MP2
C -0.199534 0.000000 -0.347739
C -1.023061 1.190445 0.165046
C -2.483105 0.776125 -0.094741
C -2.483105 -0.776125 -0.094742
C -1.023061 -1.190445 0.165046
C 1.310400 0.000000 -0.025807
C 1.955342 -1.244299 -0.648898
C 1.600587 -0.000001 1.479517
C 1.955341 1.244300 -0.648896
H -0.277865 0.000000 -1.450348
H -0.853268 1.318270 1.242066
H -0.768888 2.137884 -0.322052
H -3.164437 1.191914 0.655531
H -2.814717 1.158126 -1.067119
H -3.164438 -1.191916 0.655529
H -2.814715 -1.158125 -1.067121
H -0.853268 -1.318269 1.242067
H -0.768887 -2.137884 -0.322050
H 1.744270 -1.297290 -1.724459
H 1.586724 -2.164130 -0.182436
H 3.044340 -1.217432 -0.519452
H 1.193034 -0.887975 1.974218
H 1.193032 0.887971 1.974220
H 2.684936 0.000000 1.645032
H 1.586723 2.164131 -0.182432
H 1.744268 1.297294 -1.724457
H 3.044340 1.217433 -0.519451

COMP. 06_3T2_B3LYP
C -0.179143 0.046676 -0.458446
C -1.041854 1.212837 0.077154
C -2.481477 0.748390 -0.179018
C -2.450261 -0.738758 0.217217
C -1.028095 -1.231117 -0.163682
C 1.307661 0.004141 0.003458
C 1.450068 -0.147792 1.530696
C 2.011731 1.305877 -0.430546
C 2.012514 -1.182395 -0.685195
H -0.144336 0.164628 -1.549935
H -0.889374 1.346468 1.154161
H -0.810626 2.165209 -0.405634
H -3.226640 1.323058 0.377567
H -2.719543 0.852324 -1.244145
H -2.601094 -0.830314 1.297761
H -3.240124 -1.321487 -0.263020
H -0.598727 -1.825219 0.646002
H -1.055475 -1.881655 -1.041194
H 1.015108 0.699264 2.067372
H 0.974481 -1.060250 1.900136
H 2.508228 -0.198668 1.805393
H 1.922536 1.461063 -1.510738
H 1.589158 2.180838 0.070422
H 3.078157 1.268296 -0.186655
H 1.579506 -2.140586 -0.385824
H 1.935976 -1.105913 -1.774800
H 3.075927 -1.204216 -0.426688

COMP. 06_3T2_M06-2X
C -0.147366 0.069757 -0.614905
C -1.031625 1.241067 -0.114614
C -2.458542 0.684195 -0.087304
C -2.240616 -0.751222 0.395341
C -1.019914 -1.205152 -0.417315
C 1.260520 0.006594 0.026789
C 1.200043 -0.316008 1.525467
C 1.961179 1.357291 -0.167938
C 2.087975 -1.073772 -0.681690
H 0.020939 0.208906 -1.688883
H -0.747138 1.526266 0.902855
H -0.928566 2.131598 -0.737348
H -3.131429 1.262748 0.548432
H -2.879755 0.671995 -1.098370
H -1.996138 -0.740041 1.463394
H -3.109453 -1.397604 0.258684
H -0.480351 -2.020518 0.066733
H -1.349506 -1.580709 -1.389633
H 0.651383 0.444427 2.086149
H 0.726255 -1.282960 1.713203
H 2.212133 -0.359771 1.937693
H 2.000892 1.624240 -1.228525
H 1.443093 2.159196 0.363741
H 2.987401 1.315286 0.208041
H 1.641337 -2.064654 -0.568872
H 2.169023 -0.859576 -1.751486
H 3.099956 -1.115328 -0.268794

COMP. 06_3T2_MP2
C -0.149148 0.069727 -0.601835
C -1.031343 1.239684 -0.094288
C -2.461922 0.687615 -0.104497
C -2.257481 -0.747617 0.389048
C -1.019514 -1.208113 -0.398083
C 1.263192 0.006067 0.025156
C 1.219816 -0.309291 1.525763
C 1.964926 1.354503 -0.182674
C 2.080331 -1.078637 -0.689187
H 0.009394 0.212336 -1.680739
H -0.762352 1.501114 0.936285
H -0.909778 2.141108 -0.702775
H -3.151927 1.271342 0.513316
H -2.853023 0.672231 -1.130125
H -2.034911 -0.731558 1.463725
H -3.125778 -1.396134 0.234831
H -0.480357 -2.011567 0.111565
H -1.329992 -1.602784 -1.372279
H 0.672473 0.454944 2.087188
H 0.751351 -1.279386 1.723103
H 2.239918 -0.346055 1.926112
H 1.987624 1.618455 -1.247046
H 1.457213 2.159658 0.358569
H 2.999545 1.307097 0.177707
H 1.629256 -2.069191 -0.568841
H 2.149546 -0.863793 -1.762316
H 3.098650 -1.121433 -0.284699

COMP. 06_5T1_B3LYP
C 0.105647 -0.023536 -0.799608
C 1.054864 -1.231409 -0.556612
C 2.225069 -0.742152 0.340228
C 2.110554 0.802229 0.410601
C 1.061043 1.189289 -0.650591
C -1.198786 -0.000436 0.066367
C -2.030139 1.250808 -0.285627
C -0.920886 -0.003636 1.581800
C -2.054309 -1.236732 -0.284780
H -0.250928 -0.059147 -1.835276
H 1.447110 -1.568670 -1.520328
H 0.542244 -2.090668 -0.121214
H 3.185538 -1.049280 -0.081344
H 2.171978 -1.181949 1.339308
H 3.068624 1.296009 0.229189
H 1.783969 1.113895 1.405388
H 1.561557 1.348748 -1.611940
H 0.549744 2.123575 -0.411515
H -2.231551 1.301261 -1.360603
H -1.527828 2.176446 0.004933
H -2.994035 1.226754 0.232218
H -0.389822 0.897244 1.898507
H -0.329043 -0.871738 1.885137
H -1.862761 -0.039404 2.138525
H -1.560030 -2.173155 -0.015462
H -2.274708 -1.271078 -1.356588
H -3.008400 -1.205395 0.250401

COMP. 06_5T1_M06-2X
C -0.098813 0.041167 -0.806977
C -1.040521 1.240419 -0.527978
C -2.233232 0.720080 0.314149
C -2.061879 -0.809742 0.419232
C -1.041462 -1.174123 -0.669422
C 1.186331 0.001824 0.064275
C 2.049481 -1.200434 -0.343709
C 0.878349 -0.091313 1.563272
C 2.014922 1.269015 -0.197629
H 0.258791 0.098739 -1.840922
H -1.404699 1.636671 -1.478326
H -0.528064 2.063518 -0.029511
H -3.178070 0.971219 -0.171667
H -2.257856 1.181834 1.303309
H -3.006066 -1.340400 0.283814
H -1.685331 -1.081900 1.406008
H -1.566990 -1.309551 -1.619969
H -0.521583 -2.110492 -0.460732
H 2.285924 -1.165267 -1.411476
H 1.556026 -2.151716 -0.136374
H 2.993055 -1.193217 0.209276
H 0.437743 -1.057434 1.819671
H 0.190807 0.697825 1.883144
H 1.799928 0.014096 2.143103
H 1.524275 2.170437 0.174056
H 2.199075 1.399731 -1.268237
H 2.983980 1.194560 0.303551

COMP. 06_5T1_MP2
C -0.103355 0.037518 -0.797103
C -1.045715 1.237367 -0.525905
C -2.236473 0.720413 0.320098
C -2.068143 -0.809200 0.424250
C -1.052368 -1.172529 -0.666924
C 1.187151 0.000940 0.064197
C 2.026445 -1.225794 -0.317752
C 0.910954 -0.040238 1.570777
C 2.029567 1.246476 -0.248755
H 0.256093 0.094070 -1.835890
H -1.411232 1.626617 -1.483901
H -0.534135 2.070951 -0.035608
H -3.186825 0.974512 -0.162712
H -2.257776 1.186323 1.311627
H -3.018011 -1.339537 0.290447
H -1.689865 -1.089257 1.411660
H -1.580602 -1.299266 -1.622182
H -0.537041 -2.117558 -0.467205
H 2.226555 -1.241812 -1.396455
H 1.531485 -2.164121 -0.049089
H 2.991275 -1.201859 0.203406
H 0.431790 -0.978635 1.867419
H 0.272646 0.791684 1.890639
H 1.855304 0.034922 2.124578
H 1.540244 2.170581 0.074260
H 2.226032 1.324202 -1.325350
H 2.995685 1.188471 0.267050

COMP. 06_E1_B3LYP
C 0.103534 0.000004 -0.809266
C 1.061065 -1.207067 -0.621953
C 2.150922 -0.776291 0.388992
C 2.150935 0.776284 0.388986
C 1.061068 1.207071 -0.621946

C -1.193526 0.000001 0.067494
C -2.039708 1.243967 -0.277016
C -0.904329 -0.000025 1.580720
C -2.039725 -1.243943 -0.277057
H -0.261193 0.000008 -1.842871
H 0.551376 -2.122038 -0.315035
H 1.527945 -1.425582 -1.587762
H 1.928696 -1.158067 1.388328
H 3.126524 -1.183846 0.112620
H 1.928737 1.158074 1.388322
H 3.126539 1.183820 0.112590
H 0.551381 2.122039 -0.315013
H 1.527939 1.425597 -1.587756
H -2.257793 1.288064 -1.348968
H -1.539836 2.174726 0.001255
H -2.995223 1.215052 0.255814
H -0.340427 0.885079 1.886190
H -0.340454 -0.885155 1.886166
H -1.842718 -0.000019 2.144449
H -1.539852 -2.174719 0.001156
H -2.257834 -1.287985 -1.349007
H -2.995228 -1.215049 0.255796

COMP. 06_E1_M06-2X
C -0.095975 0.015210 -0.827461
C -1.060743 1.205358 -0.633648
C -2.117365 0.767417 0.401658
C -2.098281 -0.780532 0.399164
C -1.038481 -1.194194 -0.644586
C 1.174205 0.003527 0.066212
C 2.089556 -1.141888 -0.391299
C 0.856604 -0.184951 1.554048
C 1.949976 1.316204 -0.113226
H 0.279101 0.030154 -1.857017
H -0.559571 2.132499 -0.354001
H -1.555301 1.395012 -1.590625
H -1.878367 1.153179 1.394197
H -3.102412 1.161017 0.145188
H -1.838879 -1.159137 1.389091
H -3.075659 -1.197648 0.150970
H -0.516752 -2.110170 -0.361826
H -1.530611 -1.395367 -1.600220
H 2.376095 -1.015193 -1.439486
H 1.609592 -2.117210 -0.287504
H 3.004503 -1.158840 0.207548
H 0.385953 -1.152922 1.743250
H 0.195992 0.601448 1.927310
H 1.779889 -0.147010 2.139593
H 1.432521 2.164012 0.340012
H 2.104824 1.538293 -1.173523
H 2.932106 1.240968 0.361861

COMP. 06_E1_MP2
C 0.096528 -0.000007 -0.824728
C 1.053279 -1.199401 -0.641361
C 2.107389 -0.775022 0.405535
C 2.107396 0.775026 0.405517
C 1.053279 1.199389 -0.641380
C -1.172739 0.000000 0.066630
C -2.019052 1.239043 -0.262132
C -0.863933 -0.000044 1.568477
C -2.019111 -1.238987 -0.262193
H -0.282206 -0.000013 -1.857066
H 0.542943 -2.126233 -0.365313
H 1.552341 -1.385243 -1.600251
H 1.849583 -1.158797 1.396440
H 3.092408 -1.180884 0.155312
H 1.849604 1.158827 1.396416
H 3.092415 1.180873 0.155273
H 0.542942 2.126224 -0.365341
H 1.552336 1.385220 -1.600274
H -2.234847 1.288397 -1.336202
H -1.517488 2.166897 0.028978
H -2.974294 1.196268 0.274356
H -0.297663 0.889112 1.863573
H -0.297735 -0.889258 1.863535
H -1.801700 -0.000019 2.137472
H -1.517580 -2.166881 0.028848
H -2.234928 -1.288264 -1.336263
H -2.974341 -1.196206 0.274315

COMP. 07_E-T_B3LYP
O -0.062354 -1.228373 -0.192647
C 1.103703 -0.515319 0.213518
C 0.834416 0.931728 -0.198371
C -0.669554 1.074641 0.111982
C -1.200170 -0.377839 0.009829
H 1.244802 -0.595179 1.302700
H 1.961316 -0.972421 -0.282509
H 1.451578 1.653303 0.341163
H 1.023024 1.051517 -1.268531
H -0.817501 1.467031 1.121129
H -1.175386 1.749235 -0.580816
H -1.727116 -0.676677 0.924124
H -1.872254 -0.529086 -0.837834

COMP. 07_E-T_M06-2X
O -0.085320 -1.216766 -0.200949
C 1.080511 -0.535464 0.224024
C 0.850182 0.908096 -0.208656
C -0.640856 1.084507 0.117574
C -1.198715 -0.353881 0.008576
H 1.187182 -0.601138 1.316559
H 1.939523 -1.015235 -0.244423
H 1.489592 1.622014 0.311114
H 1.024889 0.997473 -1.282817
H -0.764214 1.466050 1.132814
H -1.139992 1.774996 -0.561813
H -1.725012 -0.645720 0.923560
H -1.876141 -0.483857 -0.836506

COMP. 07_E-T_MP2
O -0.093278 -1.218893 -0.223973
C 1.069930 -0.542919 0.237449
C 0.860840 0.899419 -0.209483
C -0.631701 1.094372 0.107772
C -1.200058 -0.344120 0.023242
H 1.143014 -0.602620 1.335055
H 1.936691 -1.035332 -0.207354
H 1.506883 1.612851 0.308618
H 1.042206 0.970678 -1.285591
H -0.755288 1.496912 1.117129
H -1.122701 1.775134 -0.591159
H -1.693233 -0.629194 0.961292
H -1.905412 -0.477797 -0.800090

COMP. 07_E_B3LYP
O -0.000018 -1.204699 -0.291314
C 1.136286 -0.469157 0.155649
C 0.776903 1.016049 -0.049797
C -0.776898 1.016056 -0.049720
C -1.136276 -0.469148 0.155752
H 1.323566 -0.682810 1.218776
H 1.998104 -0.803289 -0.422923
H 1.196337 1.645301 0.737816
H 1.163040 1.378170 -1.004330
H -1.196248 1.645307 0.737939
H -1.163126 1.378189 -1.004212
H -1.323464 -0.682803 1.218895
H -1.998148 -0.803270 -0.422746

COMP. 07_E_M06-2X
O -0.001396 -1.192610 -0.302948
C 1.123774 -0.472044 0.162636
C 0.776222 1.010354 -0.053336
C -0.772151 1.014002 -0.048329
C -1.126243 -0.468764 0.158633
H 1.280311 -0.680982 1.230201
H 1.996853 -0.809909 -0.394013
H 1.201126 1.642969 0.726275
H 1.159020 1.356809 -1.013446
H -1.188284 1.641701 0.739953

H -1.159924 1.371476 -1.002341
H -1.290320 -0.681839 1.224165
H -1.997231 -0.800636 -0.404832

COMP. 07_E_MP2TS
O 0.000001 -1.198067 -0.312257
C 1.123090 -0.468786 0.167103
C 0.774885 1.013499 -0.053471
C -0.774885 1.013499 -0.053474
C -1.123091 -0.468786 0.167099
H 1.269110 -0.675933 1.238377
H 2.001672 -0.805780 -0.385357
H 1.195834 1.648708 0.729892
H 1.161208 1.356997 -1.015645
H -1.195837 1.648708 0.729888
H -1.161205 1.356997 -1.015649
H -1.269115 -0.675934 1.238372
H -2.001671 -0.805780 -0.385364

COMP. 07_T_B3LYP
O -0.000012 -1.251665 -0.000006
C -1.169724 -0.428992 -0.130799
C -0.734404 0.995886 0.224887
C 0.734426 0.995870 -0.224890
C 1.169713 -0.429014 0.130807
H -1.534308 -0.486703 -1.164660
H -1.946068 -0.822988 0.530078
H -1.340225 1.756870 -0.271089
H -0.801381 1.158289 1.304930
H 0.801408 1.158263 -1.304935
H 1.340262 1.756844 0.271080
H 1.946062 -0.823026 -0.530055
H 1.534279 -0.486727 1.164675

COMP. 07_T_M06-2X
O -0.000157 -1.242877 -0.000354
C 1.160578 -0.426906 0.136822
C 0.728064 0.989893 -0.236756
C -0.727629 0.990273 0.236506
C -1.160834 -0.426559 -0.136332
H 1.508119 -0.468568 1.175700
H 1.945138 -0.825173 -0.508961
H 1.342211 1.756329 0.236237
H 0.772239 1.127674 -1.320249
H -0.771696 1.128688 1.319922
H -1.341502 1.756704 -0.236848
H -1.944845 -0.824391 0.510401
H -1.509482 -0.468453 -1.174809

COMP. 07_T_MP2TS
O -0.000030 -1.251363 -0.000046
C 1.161848 -0.422594 0.140102
C 0.725630 0.989977 -0.244450
C -0.725548 0.990056 0.244375
C -1.161896 -0.422532 -0.140000
H 1.501724 -0.452807 1.183846
H 1.951105 -0.824904 -0.500624
H 1.345386 1.761733 0.218842
H 0.757503 1.116490 -1.331677
H -0.757400 1.116717 1.331586
H -1.345252 1.761801 -0.219004
H -1.951057 -0.824742 0.500909
H -1.501971 -0.452819 -1.183673

COMP. 08_1E_B3LYP
N -0.000006 -1.172453 -0.346845
C 1.164932 -0.446735 0.168907
C 0.778333 1.028828 -0.056432
C -0.778363 1.028810 -0.056356
C -1.164904 -0.446760 0.169032
H 0.000019 -2.151527 -0.082864
H 1.332048 -0.629015 1.245143
H 2.072267 -0.737756 -0.365702
H 1.196534 1.675114 0.717889
H 1.159393 1.378640 -1.017691
H -1.196504 1.675093 0.718000
H -1.159524 1.378604 -1.017581
H -1.331897 -0.629039 1.245288
H -2.072291 -0.737804 -0.365476

COMP. 08_1E_M06-2X
N -0.000021 -1.164093 -0.359128
C 1.155332 -0.445963 0.176041
C 0.775656 1.024994 -0.058410
C -0.775619 1.025021 -0.058411
C -1.155348 -0.445921 0.176042
H -0.000039 -2.143561 -0.098748
H 1.292434 -0.626354 1.254466
H 2.070777 -0.738634 -0.340099
H 1.194843 1.675343 0.709805
H 1.155105 1.361257 -1.023633
H -1.194783 1.675387 0.709802
H -1.155054 1.361296 -1.023636
H -1.292455 -0.626307 1.254467
H -2.070804 -0.738560 -0.340097

COMP. 08_1E_MP2
N 0.000003 -1.162613 -0.370585
C 1.152826 -0.446294 0.181474
C 0.776506 1.025117 -0.060477
C -0.776513 1.025112 -0.060480
C -1.152823 -0.446301 0.181476
H 0.000006 -2.142390 -0.099486
H 1.272208 -0.625269 1.264554
H 2.076585 -0.741667 -0.323129
H 1.195628 1.678791 0.708762
H 1.158298 1.355600 -1.029373
H -1.195643 1.678787 0.708754
H -1.158303 1.355586 -1.029379
H -1.272200 -0.625274 1.264558
H -2.076581 -0.741681 -0.323123

COMP. 08_3T4_B3LYP
N -0.017165 -1.263179 -0.079691
C 1.197005 -0.433214 0.098741
C 0.745698 1.005633 -0.206367
C -0.717364 1.015366 0.260926
C -1.200990 -0.378899 -0.168591
H -0.114658 -1.934638 0.669020
H 1.582097 -0.498166 1.125413
H 1.995824 -0.761793 -0.572841
H 1.367997 1.752203 0.291622
H 0.794867 1.195601 -1.283431
H -0.763204 1.116296 1.350964
H -1.305570 1.825582 -0.176627
H -2.020297 -0.756730 0.449098
H -1.562996 -0.349416 -1.203640

COMP. 08_3T4_M06-2X
N -0.010800 -1.262297 -0.062316
C 1.195573 -0.422535 0.089365
C 0.729358 1.009632 -0.208746
C -0.721529 0.999765 0.278438
C -1.186417 -0.382172 -0.189401
H -0.113100 -1.887546 0.724291
H 1.594558 -0.481353 1.108450
H 1.982297 -0.745634 -0.595779
H 1.351878 1.760775 0.278555
H 0.754150 1.195000 -1.286294
H -0.749923 1.058186 1.371131
H -1.321487 1.816089 -0.126474
H -2.029176 -0.773209 0.383466
H -1.495506 -0.334372 -1.239077

COMP. 08_3T4_MP2
N -0.029495 -1.258400 -0.102051
C 1.183095 -0.440694 0.123264
C 0.751865 0.985423 -0.234093
C -0.692302 1.020591 0.274176
C -1.203409 -0.357270 -0.162389
H -0.140975 -1.939530 0.638660
H 1.510301 -0.473281 1.172644

H 2.008246 -0.795738 -0.501349
H 1.397673 1.742810 0.218047
H 0.766724 1.120426 -1.321451
H -0.697178 1.100215 1.367770
H -1.282364 1.844293 -0.137429
H -2.018622 -0.730413 0.465612
H -1.572835 -0.308287 -1.193904

COMP. 08_5T1_MP2
N -0.011958 -1.271821 -0.172541
C -1.186262 -0.424447 0.105157
C -0.726051 1.063753 0.032191
C 0.801021 0.976869 -0.180706
C 1.126791 -0.456827 0.266776
H 0.062795 -1.396804 -1.179884
H -1.990154 -0.657762 -0.597750
H -1.546137 -0.657565 1.112592
H -1.218001 1.604641 -0.780721
H -0.960711 1.584852 0.965070
H 1.045611 1.083078 -1.243474
H 1.352115 1.742945 0.372734
H 2.062298 -0.847358 -0.142512
H 1.182898 -0.509369 1.361223

COMP. 08_E1_B3LYP
N 0.000016 -1.269486 -0.190749
C -1.161392 -0.451851 0.189484
C -0.777432 1.030007 -0.070792
C 0.777457 1.029997 -0.070655
C 1.161347 -0.451858 0.189732
H 0.000124 -1.405899 -1.197721
H -2.051851 -0.773002 -0.354426
H -1.354510 -0.609417 1.256395
H -1.163507 1.363009 -1.037798
H -1.193393 1.696703 0.688442
H 1.163705 1.362957 -1.037606
H 1.193295 1.696713 0.688628
H 2.051925 -0.773025 -0.353972
H 1.354223 -0.609408 1.256690

COMP. 08_E1_M06-2X
N 0.002724 -1.262292 -0.205099
C -1.157255 -0.451990 0.176252
C -0.769214 1.032275 -0.047058
C 0.779156 1.016731 -0.096507
C 1.146109 -0.450276 0.215999
H 0.022084 -1.359722 -1.216307
H -2.041870 -0.758707 -0.382408
H -1.356368 -0.631508 1.236972
H -1.183574 1.405109 -0.985491
H -1.150063 1.669964 0.752097
H 1.133039 1.286106 -1.094096
H 1.229589 1.715356 0.610084
H 2.061623 -0.785745 -0.272113
H 1.273696 -0.585252 1.294836

COMP. 08_E1_M06-2X2
N 0.000001 -1.261934 -0.207317
C -1.151375 -0.451752 0.196860
C -0.774843 1.024743 -0.071604
C 0.774846 1.024737 -0.071624
C 1.151370 -0.451751 0.196876
H 0.000010 -1.356170 -1.219060
H -2.053335 -0.773437 -0.324503
H -1.311696 -0.609702 1.267872
H -1.159710 1.345669 -1.041665
H -1.191956 1.694403 0.681930
H 1.159688 1.345620 -1.041710
H 1.191989 1.694423 0.681871
H 2.053343 -0.773447 -0.324457
H 1.311661 -0.609682 1.267896

COMP. 08_E1_MP2
N 0.000005 -1.266079 -0.210771
C -1.151026 -0.451902 0.199217
C -0.775686 1.025647 -0.072089
C 0.775687 1.025641 -0.072120
C 1.151022 -0.451895 0.199242
H 0.000017 -1.338652 -1.226618
H -2.056533 -0.772328 -0.322421
H -1.304636 -0.609961 1.272987
H -1.161328 1.342561 -1.045795
H -1.192182 1.697862 0.683511
H 1.161290 1.342493 -1.045862
H 1.192223 1.697896 0.683422
H 2.056549 -0.772334 -0.322352
H 1.304588 -0.609925 1.273023

COMP. 08_NITROGEN-INVERSION_B3LYP
N 0.000000 -1.199553 -0.000041
C -1.214546 -0.414371 -0.126862
C -0.736189 1.005930 0.224323
C 0.736189 1.005945 -0.224256
C 1.214546 -0.414380 0.126835
H 0.000000 -2.202466 -0.000076
H -1.632277 -0.438944 -1.147038
H -2.003836 -0.753550 0.555307
H -1.331924 1.782516 -0.260025
H -0.796394 1.160258 1.306243
H 0.796395 1.160344 -1.306165
H 1.331925 1.782498 0.260144
H 2.003837 -0.753513 -0.555356
H 1.632275 -0.439021 1.147010

COMP. 08_NITROGEN-INVERSION_M06-2X
N 0.000000 -1.194627 -0.000006
C -1.209530 -0.408982 -0.133656
C -0.728839 0.999343 0.238248
C 0.728840 0.999345 -0.238239
C 1.209530 -0.408984 0.133652
H 0.000000 -2.196661 -0.000010
H -1.608299 -0.418355 -1.158878
H -2.004315 -0.753416 0.535566
H -1.331719 1.785865 -0.216740
H -0.761517 1.123264 1.324225
H 0.761518 1.123276 -1.324215
H 1.331720 1.785863 0.216757
H 2.004315 -0.753412 -0.535573
H 1.608299 -0.418366 1.158875

COMP. 08_NITROGEN-INVERSION_MP2
N 0.000000 1.193916 0.000000
C -1.211039 0.407661 0.136494
C -0.727103 -0.997642 -0.244752
C 0.727103 -0.997642 0.244752
C 1.211039 0.407661 -0.136494
H 0.000000 2.198082 0.000000
H -1.606906 0.407806 1.165316
H -2.009302 0.755545 -0.530637
H -1.334117 -1.789691 0.201910
H -0.749356 -1.111521 -1.334147
H 0.749356 -1.111521 1.334147
H 1.334117 -1.789691 -0.201910
H 2.009302 0.755545 0.530638
H 1.606906 0.407806 -1.165316

COMP. 09_1E_B3LYP
C 0.930678 0.000000 0.016636
C 0.052958 1.239987 0.161033
C -1.395512 0.783549 -0.100115
C -1.395512 -0.783549 -0.100115
C 0.052958 -1.239987 0.161033
O 2.122961 0.000000 -0.171228
H 0.188911 1.606486 1.185561
H 0.407459 2.029570 -0.503523
H -2.081139 1.176647 0.652232
H -1.743785 1.158135 -1.064774
H -2.081139 -1.176647 0.652231
H -1.743785 -1.158135 -1.064775
H 0.188911 -1.606486 1.185561
H 0.407459 -2.029570 -0.503522

COMP. 09_1E_M06-2X
C -0.182623 0.906374 0.000000
C 0.184453 0.094497 1.233226
C 0.184453 -1.374008 0.781109
C 0.184453 -1.374008 -0.781109
C 0.184453 0.094497 -1.233226
O -0.673369 2.002196 0.000000
H 1.184318 0.423664 1.536039
H -0.495011 0.322181 2.053764
H 1.044337 -1.914624 1.175512
H -0.705740 -1.882059 1.153448
H 1.044337 -1.914624 -1.175512
H -0.705740 -1.882059 -1.153448
H 1.184318 0.423664 -1.536039
H -0.495011 0.322181 -2.053764

COMP. 09_1E_MP2
C -0.210886 0.898446 0.000000
C 0.219216 0.108407 1.229716
C 0.219216 -1.364282 0.782288
C 0.219216 -1.364282 -0.782288
C 0.219216 0.108407 -1.229716
O -0.801464 1.960068 0.000000
H 1.232347 0.446329 1.483787
H -0.429424 0.327669 2.080136
H 1.081141 -1.905550 1.179009
H -0.676136 -1.868807 1.155245
H 1.081141 -1.905550 -1.179009
H -0.676136 -1.868807 -1.155245
H 1.232347 0.446329 -1.483787
H -0.429424 0.327669 -2.080136

COMP. 09_3T4_B3LYP
C -0.926256 0.000000 0.000001
C -0.031317 -1.235818 0.121660
C 1.380916 -0.739675 -0.225436
C 1.380919 0.739674 0.225429
C -0.031318 1.235820 -0.121650
O -2.133037 -0.000001 -0.000005
H -0.089040 -1.572184 1.164596
H -0.409097 -2.050582 -0.498478
H 2.170957 -1.324015 0.249712
H 1.540491 -0.796151 -1.307518
H 1.540505 0.796149 1.307509
H 2.170955 1.324013 -0.249728
H -0.409093 2.050571 0.498508
H -0.089053 1.572208 -1.164578

COMP. 09_3T4_M06-2X
C -0.920319 0.000000 -0.000154
C -0.028751 1.232467 -0.127978
C 1.371162 0.732090 0.240043
C 1.371242 -0.732091 -0.239585
C -0.028794 -1.232466 0.127970
O -2.120950 0.000000 -0.000357
H -0.069348 1.546565 -1.177260
H -0.414153 2.053049 0.476810
H 2.170675 1.322733 -0.206949
H 1.502939 0.761316 1.325811
H 1.503380 -0.761318 -1.325309
H 2.170605 -1.322733 0.207675
H -0.413994 -2.053050 -0.476944
H -0.069742 -1.546562 1.177239

COMP. 09_3T4_MP2
C -0.919481 0.000000 0.000000
C -0.024215 -1.232908 0.132303
C 1.372489 -0.729346 -0.248935
C 1.372489 0.729346 0.248934
C -0.024215 1.232908 -0.132302
O -2.134022 0.000000 -0.000001
H -0.052497 -1.541436 1.185923
H -0.411725 -2.059063 -0.468626
H 2.179672 -1.326258 0.183061
H 1.489437 -0.743169 -1.339163
H 1.489440 0.743169 1.339161
H 2.179672 1.326258 -0.183063
H -0.411724 2.059061 0.468630
H -0.052499 1.541438 -1.185920

COMP. 10_1T2_B3LYP
C 0.716568 -0.486974 -0.462052
C -0.057621 0.855960 -0.524939
C -1.520858 0.371930 -0.603004
C -1.596498 -0.864919 0.331908
C -0.132550 -1.361824 0.490081
C 2.198295 -0.409444 -0.094950
C 0.182201 1.778051 0.679199
H 0.644540 -0.925723 -1.466417
H 0.216148 1.404503 -1.433352
H -2.237860 1.151164 -0.330054
H -1.748938 0.074812 -1.631796
H -2.019599 -0.595904 1.303084
H -2.247714 -1.636233 -0.085990
H 0.209607 -1.229253 1.521725
H -0.023810 -2.425306 0.261675
H 2.660423 -1.400640 -0.135478
H 2.343636 -0.022551 0.917901
H 2.748913 0.238606 -0.784381
H 1.222133 2.110320 0.734955
H -0.060231 1.287936 1.627394
H -0.444469 2.671590 0.603283

COMP. 10_1T2_M06-2X
C 0.719851 -0.477339 -0.478897
C -0.063968 0.849502 -0.538125
C -1.512467 0.348557 -0.626386
C -1.574108 -0.839163 0.360004
C -0.117446 -1.357574 0.472280
C 2.186930 -0.366927 -0.084265
C 0.152747 1.728368 0.694794
H 0.664329 -0.916732 -1.482412
H 0.213183 1.419349 -1.430670
H -2.245118 1.126039 -0.397921
H -1.711728 -0.002072 -1.643295
H -1.937533 -0.508328 1.335195
H -2.262641 -1.611196 0.013824
H 0.252234 -1.249656 1.496397
H -0.028563 -2.415380 0.217361
H 2.673930 -1.344470 -0.124437
H 2.291351 0.011441 0.936086
H 2.730136 0.306478 -0.753060
H 1.181863 2.088533 0.756849
H -0.066081 1.182986 1.618116
H -0.504597 2.600463 0.661530

COMP. 10_1T2_MP2
C 0.724981 -0.471277 -0.475757
C -0.068698 0.848721 -0.537344
C -1.511705 0.332917 -0.636741
C -1.568534 -0.847842 0.360880
C -0.106085 -1.354858 0.479477
C 2.194615 -0.353561 -0.085541
C 0.129885 1.731107 0.697703
H 0.668157 -0.915371 -1.480529
H 0.209210 1.423031 -1.430850
H -2.257686 1.105761 -0.421241
H -1.694786 -0.031303 -1.654948
H -1.937281 -0.510058 1.334415
H -2.250372 -1.630780 0.016506
H 0.263218 -1.238528 1.505290
H -0.009143 -2.415371 0.225614
H 2.683215 -1.333257 -0.121991
H 2.299725 0.031759 0.933857
H 2.733623 0.317860 -0.763477
H 1.155187 2.107736 0.763046
H -0.086511 1.183193 1.621611
H -0.543309 2.594086 0.656634

COMP. 10_4E_B3LYP
C 0.316702 0.790241 0.457796
C 0.316710 -0.790238 0.457795

C -1.020469 -1.196463 -0.209423
C -1.954415 -0.000014 0.012200
C -1.020489 1.196453 -0.209409
C 1.526146 1.479339 -0.180924
C 1.526169 -1.479322 -0.180914
H 0.277887 1.111226 1.504895
H 0.277889 -1.111224 1.504893
H -0.864887 -1.340328 -1.286248
H -1.413815 -2.137274 0.185730
H -2.821063 -0.000017 -0.654270
H -2.333149 -0.000023 1.041232
H -0.864914 1.340336 -1.286233
H -1.413849 2.137252 0.185757
H 1.412523 2.566636 -0.126998
H 1.633145 1.214610 -1.237156
H 2.461182 1.223117 0.324895
H 2.461197 -1.223094 0.324916
H 1.633177 -1.214586 -1.237144
H 1.412554 -2.566620 -0.126995

COMP. 10_4E_M06-2X
C -0.310007 -0.785063 0.464571
C -0.310006 0.785056 0.464584
C 1.012757 1.188030 -0.217974
C 1.945962 -0.000002 0.019641
C 1.012754 -1.188027 -0.217996
C -1.519787 -1.457293 -0.179272
C -1.519784 1.457298 -0.179249
H -0.263642 -1.114586 1.507483
H -0.263642 1.114561 1.507501
H 0.844799 1.302839 -1.295800
H 1.402048 2.137734 0.155303
H 2.822465 0.000003 -0.630846
H 2.297610 -0.000012 1.057016
H 0.844796 -1.302816 -1.295824
H 1.402044 -2.137740 0.155264
H -1.408339 -2.544102 -0.141652
H -1.618650 -1.173172 -1.230307
H -2.451921 -1.200468 0.328953
H -2.451919 1.200466 0.328970
H -1.618646 1.173194 -1.230289
H -1.408335 2.544106 -0.141611

COMP. 10_4E_MP2
C 0.310291 0.785192 0.463764
C 0.310291 -0.785192 0.463764
C -1.012845 -1.187588 -0.220652
C -1.947110 0.000000 0.024207
C -1.012845 1.187588 -0.220652
C 1.520601 1.462161 -0.179032
C 1.520602 -1.462161 -0.179031
H 0.261791 1.115610 1.509598
H 0.261791 -1.115610 1.509598
H -0.844478 -1.295085 -1.301494
H -1.399646 -2.142435 0.151114
H -2.829464 0.000000 -0.623563
H -2.290287 -0.000001 1.066735
H -0.844479 1.295085 -1.301493
H -1.399647 2.142435 0.151115
H 1.400600 2.550508 -0.141247
H 1.621093 1.176283 -1.231205
H 2.453560 1.209507 0.334546
H 2.453561 -1.209506 0.334547
H 1.621094 -1.176283 -1.231205
H 1.400600 -2.550508 -0.141246

COMP. 10_E4_B3LYP
C -0.353797 -0.790685 0.577580
C -0.353760 0.790700 0.577581
C 1.087023 1.197039 0.157846
C 1.620828 -0.000035 -0.639324
C 1.086964 -1.197092 0.157832
C -1.409377 -1.456897 -0.317024
C -1.409300 1.456963 -0.317033
H -0.540190 -1.133616 1.599922
H -0.540147 1.133639 1.599922
H 1.104654 2.134490 -0.405144
H 1.711004 1.344624 1.046302
H 1.203486 -0.000019 -1.652973
H 2.709584 -0.000061 -0.738660
H 1.104546 -2.134535 -0.405170
H 1.710942 -1.344721 1.046283
H -1.349108 -2.544482 -0.215353
H -1.262525 -1.218200 -1.374679
H -2.426181 -1.160054 -0.047566
H -2.426121 1.160168 -0.047587
H -1.262447 1.218261 -1.374687
H -1.348980 2.544545 -0.215358

COMP. 10_E4_M06-2X
C -0.347984 -0.786105 0.595307
C -0.347938 0.786133 0.595296
C 1.082758 1.187651 0.163733
C 1.573386 -0.000048 -0.665652
C 1.082686 -1.187713 0.163741
C -1.388906 -1.435037 -0.320571
C -1.388812 1.435113 -0.320602
H -0.539289 -1.139941 1.611506
H -0.539231 1.139995 1.611488
H 1.097616 2.135671 -0.379180
H 1.727890 1.299601 1.040754
H 1.090567 -0.000037 -1.649170
H 2.652885 -0.000082 -0.826874
H 1.097485 -2.135736 -0.379168
H 1.727814 -1.299698 1.040760
H -1.334129 -2.522272 -0.228729
H -1.212066 -1.183022 -1.370060
H -2.407400 -1.132675 -0.069966
H -2.407326 1.132805 -0.070013
H -1.211966 1.183082 -1.370086
H -1.333980 2.522346 -0.228767

COMP. 10_E4_MP2
C -0.348528 -0.785943 0.594622
C -0.348525 0.785944 0.594622
C 1.083919 1.186770 0.165283
C 1.570656 -0.000003 -0.670549
C 1.083915 -1.186774 0.165282
C -1.388794 -1.440130 -0.321334
C -1.388788 1.440135 -0.321334
H -0.540928 -1.138545 1.614748
H -0.540925 1.138547 1.614748
H 1.099372 2.141733 -0.371350
H 1.731159 1.288253 1.045429
H 1.082226 -0.000002 -1.653389
H 2.652866 -0.000005 -0.834500
H 1.099363 -2.141737 -0.371351
H 1.731154 -1.288260 1.045428
H -1.329707 -2.529102 -0.222471
H -1.209977 -1.191279 -1.372791
H -2.409037 -1.136660 -0.069394
H -2.409032 1.136669 -0.069395
H -1.209971 1.191284 -1.372792
H -1.329697 2.529107 -0.222471

COMP. 11_1T2_B3LYP
C -0.372103 -0.697886 0.330447
C -0.372100 0.697886 -0.330450
C 1.034565 1.237309 -0.002801
C 1.972136 -0.000001 0.000008
C 1.034563 -1.237310 0.002807
C -1.508077 1.624667 0.100132
C -1.508078 -1.624665 -0.100142
H -0.439972 -0.543761 1.417830
H -0.439963 0.543761 -1.417833
H 1.356522 2.010978 -0.705003
H 1.016008 1.700614 0.990424
H 2.625910 -0.008292 -0.875606
H 2.625900 0.008288 0.875629
H 1.016012 -1.700612 -0.990420
H 1.356514 -2.010982 0.705009
H -1.490887 1.782608 1.184263

H -2.488104 1.216641 -0.163475
H -1.422192 2.604968 -0.378644
H -1.422196 -2.604967 0.378634
H -1.490883 -1.782605 -1.184273
H -2.488106 -1.216640 0.163461

COMP. 11_1T2_M06-2X
C 0.364141 0.690919 0.334262
C 0.364143 -0.690919 -0.334260
C -1.028554 -1.232436 0.015189
C -1.965526 -0.000009 -0.000015
C -1.028565 1.232430 -0.015168
C 1.506104 -1.604960 0.086925
C 1.506089 1.604971 -0.086933
H 0.415057 0.527614 1.420552
H 0.415044 -0.527615 -1.420550
H -1.352711 -2.022599 -0.665140
H -0.991786 -1.667846 1.019697
H -2.616344 -0.005332 -0.875969
H -2.616401 0.005307 0.875897
H -0.991803 1.667884 -1.019657
H -1.352730 2.022561 0.665193
H 1.501520 -1.741579 1.173068
H 2.477754 -1.194757 -0.198556
H 1.413093 -2.591252 -0.374576
H 1.413073 2.591263 0.374569
H 1.501495 1.741590 -1.173076
H 2.477745 1.194777 0.198540

COMP. 11_1T2_MP2
C -0.364051 -0.690582 0.334615
C -0.364051 0.690582 -0.334615
C 1.027672 1.232913 0.021493
C 1.967215 0.000000 0.000001
C 1.027671 -1.232913 -0.021493
C -1.506971 1.608595 0.082587
C -1.506972 -1.608595 -0.082587
H -0.409877 -0.525835 1.423674
H -0.409877 0.525834 -1.423674
H 1.354323 2.029088 -0.655633
H 0.985992 1.660581 1.031780
H 2.618101 0.010717 -0.879342
H 2.618099 -0.010718 0.879345
H 0.985991 -1.660579 -1.031782
H 1.354322 -2.029090 0.655631
H -1.501847 1.744197 1.170866
H -2.480378 1.199066 -0.206337
H -1.407851 2.596000 -0.381125
H -1.407853 -2.596000 0.381125
H -1.501848 -1.744196 -1.170866
H -2.480378 -1.199065 0.206337

COMP. 11_2T1_B3LYP
C 0.652593 -0.649794 0.417833
C -0.652810 -0.649561 -0.417876
C -0.684080 0.768454 -1.036705
C 0.000400 1.702614 0.000011
C 0.684204 0.768117 1.036847
C -1.893963 -0.933725 0.439817
C 1.893671 -0.934133 -0.439911
H 0.600174 -1.411670 1.203533
H -0.600582 -1.411335 -1.203688
H -1.703152 1.085238 -1.274614
H -0.127517 0.777610 -1.977836
H -0.724878 2.358115 0.487931
H 0.726185 2.357473 -0.488018
H 0.127318 0.777353 1.977788
H 1.703308 1.084513 1.275138
H -2.016005 -0.191706 1.235247
H -2.802593 -0.913438 -0.169425
H -1.830738 -1.918737 0.912530
H 1.830202 -1.919062 -0.912763
H 2.015880 -0.192033 -1.235240
H 2.802312 -0.914152 0.169324

COMP. 11_2T1_M06-2X
C 0.640550 -0.665919 0.427813
C -0.640773 -0.665688 -0.427856
C -0.636224 0.736931 -1.063838
C 0.000402 1.668082 0.000020
C 0.636345 0.736604 1.063977
C -1.892936 -0.881730 0.423019
C 1.892645 -0.882138 -0.423116
H 0.592635 -1.447336 1.192906
H -0.593046 -1.447005 -1.193063
H -1.642395 1.054834 -1.346097
H -0.035812 0.736424 -1.976162
H -0.746464 2.321032 0.454814
H 0.747797 2.320359 -0.454875
H 0.035627 0.736194 1.976101
H 1.642536 1.054115 1.346605
H -2.009619 -0.083641 1.162262
H -2.790260 -0.885712 -0.200393
H -1.848385 -1.832696 0.959924
H 1.847873 -1.833038 -0.960119
H 2.009471 -0.084002 -1.162286
H 2.789989 -0.886378 0.200265

COMP. 11_2T1_MP2
C 0.639630 -0.666608 0.428320
C -0.639795 -0.666436 -0.428353
C -0.630503 0.735145 -1.067869
C 0.000302 1.668848 0.000015
C 0.630590 0.734900 1.067973
C -1.895364 -0.879483 0.421106
C 1.895149 -0.879787 -0.421178
H 0.592152 -1.451579 1.194436
H -0.592460 -1.451331 -1.194557
H -1.638114 1.053657 -1.355873
H -0.022240 0.732628 -1.978080
H -0.752410 2.321774 0.451767
H 0.753406 2.321271 -0.451810
H 0.022091 0.732458 1.978027
H 1.638212 1.053122 1.356261
H -2.013989 -0.077109 1.157640
H -2.791727 -0.887089 -0.208191
H -1.848049 -1.831030 0.961890
H 1.847676 -1.831292 -0.962022
H 2.013873 -0.077387 -1.157669
H 2.791527 -0.887568 0.208095

COMP. 11_E1_MP2
C 0.464495 -0.763527 0.375475
C -0.809227 -0.376389 -0.427202
C -0.684491 1.153468 -0.689913
C 0.673202 1.574456 -0.099318
C 0.876694 0.564178 1.034796
C 1.600545 -1.321600 -0.514446
C -2.088811 -0.710801 0.337512
H 0.203555 -1.510780 1.134159
H -0.823794 -0.923729 -1.377210
H -0.777044 1.402236 -1.751717
H -1.491834 1.677987 -0.163420
H 1.465480 1.453288 -0.847173
H 0.688127 2.616928 0.233459
H 1.898073 0.540754 1.429877
H 0.198692 0.802293 1.864869
H 1.925485 -2.307689 -0.168999
H 2.479532 -0.667947 -0.504458
H 1.286646 -1.428377 -1.557716
H -2.094341 -0.207646 1.311720
H -2.178752 -1.788711 0.510105
H -2.974271 -0.377312 -0.214923

COMP. 12_2E_B3LYP
C 1.245365 0.031957 0.402059
C 0.000000 -0.427962 1.196788
C -1.245365 0.031957 0.402059
C -0.778083 1.329617 -0.315185
C 0.778083 1.329617 -0.315185
C 1.792732 -1.024044 -0.569938
C -1.792732 -1.024044 -0.569938

H 2.052361 0.268657 1.103097
H 0.000000 -1.505297 1.390302
H 0.000000 0.068281 2.173489
H -2.052361 0.268657 1.103097
H -1.184066 1.383505 -1.329146
H -1.152919 2.210239 0.213243
H 1.184066 1.383505 -1.329146
H 1.152919 2.210239 0.213243
H 2.696157 -0.657673 -1.067518
H 1.071374 -1.280529 -1.350187
H 2.054931 -1.946989 -0.043364
H -2.054931 -1.946989 -0.043364
H -1.071374 -1.280529 -1.350187
H -2.696157 -0.657673 -1.067518

COMP. 12_2E_M06-2X
C -0.274610 0.297206 1.237245
C -1.165326 0.517763 0.000000
C -0.274610 0.297206 -1.237245
C 1.128823 0.759051 -0.776093
C 1.128823 0.759051 0.776093
C -0.274610 -1.144429 1.751846
C -0.274610 -1.144429 -1.751846
H -0.626597 0.932179 2.054917
H -2.049762 -0.126088 0.000000
H -1.518750 1.553665 0.000000
H -0.626597 0.932179 -2.054917
H 1.904835 0.106253 -1.183087
H 1.339066 1.763739 -1.148532
H 1.904835 0.106253 1.183087
H 1.339066 1.763739 1.148532
H 0.312384 -1.219925 2.670899
H 0.162597 -1.835384 1.028840
H -1.289667 -1.484910 1.971797
H -1.289667 -1.484910 -1.971797
H 0.162597 -1.835384 -1.028840
H 0.312384 -1.219925 -2.670899

COMP. 12_2E_MP2
C -0.275170 0.296799 1.237582
C -1.165066 0.524499 0.000000
C -0.275170 0.296799 -1.237582
C 1.129492 0.759083 -0.777303
C 1.129492 0.759083 0.777303
C -0.275170 -1.148185 1.747317
C -0.275170 -1.148185 -1.747317
H -0.625690 0.931903 2.060111
H -2.056664 -0.114181 0.000000
H -1.508541 1.566931 0.000000
H -0.625690 0.931903 -2.060111
H 1.906930 0.103226 -1.184258
H 1.338877 1.767146 -1.149900
H 1.906930 0.103226 1.184258
H 1.338877 1.767146 1.149900
H 0.314601 -1.225026 2.667383
H 0.161451 -1.835619 1.018138
H -1.293280 -1.487683 1.967163
H -1.293280 -1.487683 -1.967163
H 0.161451 -1.835619 -1.018138
H 0.314601 -1.225026 -2.667383

COMP. 12_E2_B3LYP
C -1.211628 -0.133158 -0.369794
C 0.000001 -1.006432 -0.004982
C 1.211628 -0.133153 -0.369791
C 0.777177 1.286873 0.077663
C -0.777181 1.286877 0.077641
C -2.543251 -0.596193 0.219410
C 2.543255 -0.596190 0.219402
H -1.300962 -0.135051 -1.464337
H 0.000001 -1.207658 1.075786
H 0.000003 -1.973925 -0.516735
H 1.300955 -0.135033 -1.464334
H 1.157344 1.486731 1.085019
H 1.197202 2.058844 -0.572498
H -1.157377 1.486766 1.084980
H -1.197180 2.058833 -0.572554
H -3.359671 0.075804 -0.063308
H -2.497150 -0.620917 1.313678
H -2.806640 -1.600514 -0.126666
H 2.806646 -1.600506 -0.126688
H 2.497158 -0.620929 1.313669
H 3.359671 0.075813 -0.063311

COMP. 12_E2_M06-2X
C -1.202359 -0.134141 -0.374414
C 0.000000 -0.999818 0.011075
C 1.202359 -0.134140 -0.374413
C 0.774902 1.278753 0.078933
C -0.774903 1.278754 0.078927
C -2.531106 -0.591694 0.211559
C 2.531107 -0.591693 0.211557
H -1.277549 -0.139943 -1.468759
H 0.000000 -1.162229 1.098176
H 0.000001 -1.980018 -0.473376
H 1.277547 -0.139938 -1.468759
H 1.154483 1.462823 1.088710
H 1.197758 2.053542 -0.563646
H -1.154492 1.462832 1.088701
H -1.197753 2.053539 -0.563660
H -3.342535 0.084304 -0.070329
H -2.476884 -0.612581 1.304357
H -2.794258 -1.595092 -0.132391
H 2.794260 -1.595090 -0.132397
H 2.476886 -0.612585 1.304355
H 3.342534 0.084306 -0.070329

COMP. 12_E2_MP2
C -1.202103 -0.136239 -0.373517
C 0.000001 -0.999807 0.020110
C 1.202102 -0.136234 -0.373515
C 0.776071 1.278070 0.079253
C -0.776075 1.278074 0.079232
C -2.536687 -0.590027 0.207334
C 2.536691 -0.590024 0.207326
H -1.270213 -0.145001 -1.471112
H 0.000001 -1.152491 1.110789
H 0.000003 -1.985168 -0.460444
H 1.270207 -0.144984 -1.471110
H 1.156682 1.461493 1.091546
H 1.198326 2.054023 -0.567401
H -1.156714 1.461526 1.091510
H -1.198307 2.054012 -0.567454
H -3.346063 0.088298 -0.083916
H -2.485709 -0.604534 1.302379
H -2.798408 -1.596917 -0.135280
H 2.798414 -1.596909 -0.135300
H 2.485716 -0.604544 1.302371
H 3.346062 0.088307 -0.083918

COMP. 13_4T3_M06-2X
C 1.251354 -0.103204 0.480040
C -0.046555 -0.949178 0.485611
C -1.058375 -0.160818 -0.356746
C -0.728278 1.285168 0.025494
C 0.804688 1.311288 0.014745
C 2.324714 -0.690492 -0.434511
C -2.508291 -0.564146 -0.129719
H 1.656012 -0.046926 1.493859
H 0.117453 -1.963281 0.110696
H -0.439350 -1.038760 1.504644
H -0.809355 -0.294928 -1.417893
H -1.177063 2.021678 -0.645109
H -1.108533 1.479367 1.035837
H 1.157320 1.483180 -1.007831
H 1.222802 2.105994 0.635166
H 3.194208 -0.030768 -0.497737
H 1.929916 -0.820639 -1.447382
H 2.663566 -1.665841 -0.076750
H -3.189042 0.040901 -0.733699
H -2.779332 -0.427912 0.921820
H -2.674139 -1.613766 -0.385107

COMP. 13_4T3_MP2
C 1.251028 -0.101375 0.478067
C -0.046450 -0.950912 0.476654
C -1.062433 -0.157625 -0.357925
C -0.730900 1.285531 0.036128
C 0.803258 1.310223 0.004349
C 2.335027 -0.689129 -0.426226
C -2.512573 -0.566758 -0.128618
H 1.647277 -0.038913 1.498364
H 0.121922 -1.963809 0.091891
H -0.439099 -1.048654 1.497838
H -0.816080 -0.283039 -1.423381
H -1.188413 2.031843 -0.622592
H -1.096090 1.466440 1.056960
H 1.140168 1.469425 -1.028371
H 1.234845 2.110506 0.613924
H 3.204907 -0.025201 -0.481574
H 1.946714 -0.820619 -1.443283
H 2.672020 -1.665389 -0.061710
H -3.197404 0.043731 -0.726957
H -2.777191 -0.438992 0.927636
H -2.675320 -1.617062 -0.393326

COMP. 13_4T5_B3LYP
C 1.186355 -0.116738 0.400763
C -0.000006 -1.042141 0.000168
C -1.186336 -0.116834 -0.400725
C -0.761049 1.283635 0.088605
C 0.761052 1.283617 -0.088889
C 2.548755 -0.580627 -0.115094
C -2.548769 -0.580592 0.115164
H 1.233155 -0.079024 1.496215
H 0.278674 -1.697474 -0.831192
H -0.278710 -1.697185 0.831749
H -1.233069 -0.079388 -1.496189
H -1.265310 2.089405 -0.452559
H -1.012016 1.398534 1.151091
H 1.012016 1.398274 -1.151401
H 1.265311 2.089514 0.452087
H 3.345184 0.107449 0.185783
H 2.551761 -0.637292 -1.209168
H 2.805329 -1.572550 0.269692
H -3.345178 0.107409 -0.185936
H -2.551842 -0.636979 1.209253
H -2.805319 -1.572611 -0.269385

COMP. 13_4T5_M06-2X
C -1.177446 -0.113532 -0.404757
C -0.000012 -1.037374 -0.000042
C 1.177485 -0.113636 0.404750
C 0.757451 1.276269 -0.098494
C -0.757442 1.276237 0.098873
C -2.533373 -0.577840 0.112073
C 2.533344 -0.577829 -0.112366
H -1.218503 -0.067066 -1.498859
H -0.286865 -1.690229 0.829535
H 0.286786 -1.690206 -0.829654
H 1.218685 -0.067439 1.498856
H 1.272703 2.086112 0.422943
H 0.990965 1.365794 -1.166646
H -0.990966 1.365460 1.167049
H -1.272698 2.086219 -0.422344
H -3.328335 0.112658 -0.181471
H -2.522826 -0.635525 1.204869
H -2.788044 -1.568402 -0.273188
H 3.328345 0.112603 0.181227
H 2.522651 -0.635268 -1.205174
H 2.788065 -1.568478 0.272638

COMP. 13_4T5_MP2
C 1.178210 -0.111138 0.404279
C -0.000006 -1.035876 0.000052
C -1.178190 -0.111143 -0.404266
C -0.757645 1.277682 0.103580
C 0.757649 1.277685 -0.103570
C 2.534789 -0.581359 -0.111213
C -2.534804 -0.581348 0.111147
H 1.217616 -0.060832 1.501211
H 0.287458 -1.689234 -0.832657
H -0.287497 -1.689130 0.832834
H -1.217524 -0.060856 -1.501202
H -1.278356 2.090396 -0.414443
H -0.983227 1.361356 1.176211
H 0.983227 1.361358 -1.176202
H 1.278358 2.090402 0.414448
H 3.331867 0.112111 0.178592
H 2.519561 -0.645116 -1.205584
H 2.787084 -1.572254 0.281393
H -3.331863 0.112112 -0.178732
H -2.519650 -0.645074 1.205521
H -2.787072 -1.572255 -0.281447

COMP. 13_5T4_B3LYP
C -1.128715 -0.254817 -0.558889
C -0.000001 -1.174810 0.000008
C 1.128720 -0.254818 0.558890
C 0.491402 1.154369 0.590435
C -0.491398 1.154370 -0.590430
C -2.396498 -0.298688 0.305649
C 2.396492 -0.298691 -0.305662
H -1.403332 -0.566474 -1.571344
H -0.395585 -1.830303 0.781395
H 0.395576 -1.830321 -0.781367
H 1.403348 -0.566473 1.571343
H -0.054452 1.298641 1.528837
H 1.236661 1.952658 0.528696
H -1.236657 1.952659 -0.528688
H 0.054456 1.298646 -1.528831
H -3.174255 0.356367 -0.099008
H -2.192005 0.021150 1.332852
H -2.805096 -1.312779 0.352922
H 3.174253 0.356366 0.098984
H 2.191988 0.021144 -1.332864
H 2.805091 -1.312781 -0.352935

COMP. 13_5T4_M06-2X
C 1.112775 -0.260507 0.571494
C 0.000000 -1.180786 -0.000005
C -1.112775 -0.260504 -0.571495
C -0.469269 1.138438 -0.605465
C 0.469268 1.138435 0.605470
C 2.364680 -0.277993 -0.307568
C -2.364679 -0.277995 0.307569
H 1.395824 -0.577525 1.578269
H 0.411268 -1.833380 -0.774654
H -0.411267 -1.833387 0.774639
H -1.395827 -0.577517 -1.578271
H 0.110531 1.266238 -1.524273
H -1.212470 1.938852 -0.574238
H 1.212470 1.938849 0.574247
H -0.110532 1.266231 1.524278
H 3.134676 0.388881 0.088412
H 2.130633 0.044267 -1.326742
H 2.785789 -1.284584 -0.368462
H -3.134676 0.388882 -0.088405
H -2.130630 0.044258 1.326745
H -2.785788 -1.284586 0.368457

COMP. 13_5T4_MP2
C 1.111819 0.260772 -0.573820
C 0.000000 1.182151 0.000001
C -1.111820 0.260772 0.573820
C -0.466230 -1.137928 0.608720
C 0.466230 -1.137928 -0.608720
C 2.363520 0.276220 0.308276
C -2.363520 0.276220 -0.308276
H 1.395437 0.580891 -1.583099
H 0.414017 1.835803 0.776573
H -0.414017 1.835804 -0.776571
H -1.395438 0.580891 1.583099
H 0.120478 -1.263207 1.526325

H -1.212893 -1.939316 0.582234
H 1.212893 -1.939316 -0.582234
H -0.120478 -1.263207 -1.526324
H 3.131732 -0.397654 -0.086355
H 2.123842 -0.041663 1.329247
H 2.787916 1.284308 0.364521
H -3.131731 -0.397654 0.086353
H -2.123841 -0.041662 -1.329248
H -2.787916 1.284308 -0.364521

COMP. 14_1T2I_B3LYP
C 0.694309 -0.539555 -0.465262
C 0.033611 0.859594 -0.522858
C -1.458398 0.479797 -0.604539
C -1.618746 -0.746586 0.337398
C -0.198566 -1.355335 0.481178
O 2.043349 -0.573615 -0.000667
C 0.358344 1.730124 0.696871
H 0.648616 -0.976975 -1.473135
H 0.350630 1.392802 -1.427015
H -2.115726 1.309997 -0.333881
H -1.711030 0.196121 -1.631529
H -2.006358 -0.440812 1.311897
H -2.334014 -1.464527 -0.069683
H 0.186106 -1.241355 1.497877
H -0.163363 -2.420583 0.245349
H 2.615959 -0.204188 -0.680050
H 0.016715 1.270860 1.628745
H 1.433563 1.895185 0.792878
H -0.131214 2.704160 0.607151

COMP. 14_1T2I_M06-2X
C -0.706607 -0.522776 0.471121
C -0.021575 0.854375 0.531149
C 1.452491 0.441433 0.632542
C 1.590400 -0.750143 -0.347191
C 0.166879 -1.341728 -0.484072
O -2.043305 -0.518722 0.004069
C -0.299689 1.690110 -0.716970
H -0.666390 -0.968944 1.474729
H -0.342800 1.410644 1.418146
H 2.133607 1.262330 0.399288
H 1.674157 0.112984 1.652217
H 1.957555 -0.409446 -1.316884
H 2.308321 -1.483864 0.020830
H -0.227616 -1.212351 -1.494415
H 0.121084 -2.406322 -0.253820
H -2.600353 -0.093105 0.660426
H 0.048807 1.182499 -1.620384
H -1.367470 1.876927 -0.840120
H 0.216134 2.650808 -0.652032

COMP. 14_1T2I_MP2
C -0.715519 -0.510338 0.467384
C -0.009406 0.854579 0.529912
C 1.455276 0.411655 0.646308
C 1.577989 -0.771996 -0.347973
C 0.142815 -1.338354 -0.494265
O -2.061429 -0.490926 0.003738
C -0.257742 1.698827 -0.720264
H -0.674286 -0.961342 1.471319
H -0.330003 1.418450 1.416032
H 2.159245 1.221937 0.430574
H 1.655284 0.063580 1.666932
H 1.953989 -0.424203 -1.314439
H 2.282996 -1.524204 0.016350
H -0.247185 -1.194095 -1.506603
H 0.079063 -2.405829 -0.268551
H -2.596258 -0.079270 0.689385
H 0.086519 1.185193 -1.623525
H -1.321866 1.913225 -0.849100
H 0.283456 2.647723 -0.644885

COMP. 14_1T2O_B3LYP
C 0.689845 -0.532644 -0.471405
C 0.028337 0.856567 -0.524923
C -1.465956 0.480397 -0.585573
C -1.621238 -0.762340 0.337400
C -0.192531 -1.349705 0.494907
O 2.060509 -0.432706 -0.085721
C 0.374481 1.732815 0.685704
H 0.630100 -0.973075 -1.477429
H 0.339200 1.382113 -1.433188
H -2.113302 1.308647 -0.287218
H -1.738869 0.217688 -1.612734
H -2.028581 -0.480062 1.310807
H -2.317078 -1.486277 -0.092225
H 0.183116 -1.208443 1.511993
H -0.150263 -2.421126 0.280432
H 2.453662 -1.310299 -0.109671
H 0.046729 1.280783 1.626572
H 1.451236 1.895458 0.754988
H -0.117651 2.705706 0.596780

COMP. 14_1T2O_M06-2X
C 0.709344 -0.505020 -0.480845
C 0.003963 0.853512 -0.534850
C -1.466185 0.423032 -0.615431
C -1.580336 -0.778340 0.355894
C -0.143520 -1.340855 0.489510
O 2.061321 -0.352448 -0.087590
C 0.292748 1.696521 0.706443
H 0.665150 -0.951367 -1.484171
H 0.313147 1.406883 -1.425376
H -2.151255 1.234567 -0.362569
H -1.701523 0.102320 -1.634384
H -1.952810 -0.453602 1.328932
H -2.282729 -1.524530 -0.017060
H 0.245774 -1.194966 1.500125
H -0.086146 -2.408443 0.267252
H 2.476062 -1.217722 -0.061426
H -0.038907 1.191358 1.618112
H 1.361119 1.890842 0.803712
H -0.234534 2.651147 0.643249

COMP. 14_1T2O_MP2
C 0.711905 -0.501138 -0.479548
C 0.000558 0.852748 -0.534133
C -1.465832 0.409294 -0.625585
C -1.576317 -0.784907 0.357636
C -0.134175 -1.338084 0.496462
O 2.072560 -0.339674 -0.091852
C 0.273552 1.699131 0.709898
H 0.662993 -0.951539 -1.483347
H 0.309822 1.411223 -1.425126
H -2.163735 1.217974 -0.386333
H -1.686551 0.073934 -1.646067
H -1.951186 -0.451737 1.329652
H -2.274629 -1.541032 -0.011562
H 0.254488 -1.184965 1.508457
H -0.068890 -2.408425 0.275483
H 2.463581 -1.217410 -0.049002
H -0.044342 1.184047 1.622456
H 1.339041 1.920741 0.804693
H -0.279224 2.642316 0.647133

COMP. 14_1T2TS_MP2
C -0.720795 -0.503352 0.453606
C 0.000660 0.848328 0.537092
C 1.462600 0.397899 0.647087
C 1.580736 -0.790968 -0.343812
C 0.138883 -1.330493 -0.515640
O -2.073678 -0.383035 0.009957
C -0.249687 1.707352 -0.702929
H -0.696829 -0.965532 1.450721
H -0.322535 1.400575 1.427690
H 2.169223 1.203921 0.424636
H 1.667025 0.053236 1.668168
H 1.981566 -0.454706 -1.304391
H 2.264127 -1.555270 0.036512
H -0.237851 -1.158301 -1.528422
H 0.056434 -2.402641 -0.315082

H -2.638078 -0.810199 0.657225
H 0.114234 1.214923 -1.610879
H -1.317336 1.902132 -0.830705
H 0.275069 2.663549 -0.607547

COMP. 14_1T2_B3LYP
C -0.702519 -0.529276 0.453261
C -0.020470 0.854587 0.529272
C 1.467105 0.460145 0.606179
C 1.617635 -0.768412 -0.336342
C 0.189557 -1.352499 -0.496523
O -2.060568 -0.464469 0.002288
C -0.341970 1.740616 -0.680432
H -0.676880 -0.974946 1.455642
H -0.337472 1.378929 1.436989
H 2.131275 1.283979 0.333104
H 1.720782 0.174748 1.632645
H 2.021347 -0.468639 -1.306150
H 2.316526 -1.498090 0.078525
H -0.186117 -1.219964 -1.514123
H 0.137194 -2.421054 -0.275246
H -2.631585 -0.880719 0.651059
H 0.004154 1.295178 -1.617897
H -1.417759 1.901913 -0.769431
H 0.147055 2.713450 -0.575908

COMP. 14_1T2_M06-2X
C -0.718381 -0.507109 0.458540
C -0.002897 0.849893 0.538840
C 1.463125 0.411968 0.636322
C 1.583823 -0.778457 -0.348467
C 0.149735 -1.338730 -0.499204
O -2.059553 -0.397468 0.002974
C -0.271101 1.702632 -0.700063
H -0.701338 -0.961516 1.456754
H -0.322473 1.398907 1.429197
H 2.157470 1.222107 0.404688
H 1.681640 0.076322 1.654575
H 1.965539 -0.441376 -1.313786
H 2.283811 -1.528208 0.022055
H -0.235531 -1.190525 -1.510319
H 0.082230 -2.405750 -0.282151
H -2.651802 -0.789000 0.644831
H 0.085965 1.209035 -1.608427
H -1.339338 1.886462 -0.819641
H 0.244431 2.662113 -0.617373

COMP. 14_1T5I_B3LYPT
C 0.494723 -0.702605 -0.437213
C 0.208582 0.826970 -0.505170
C -1.332940 0.926138 -0.287512
C -1.823514 -0.492295 0.118167
C -0.552438 -1.247729 0.530257
O 1.803882 -1.068577 -0.005669
C 0.994351 1.631320 0.537402
H 0.307681 -1.134971 -1.431277
H 0.476793 1.204480 -1.498019
H -1.547702 1.650164 0.503291
H -1.848753 1.282546 -1.182316
H -2.573467 -0.462817 0.911322
H -2.287678 -0.991809 -0.738256
H -0.253728 -0.996152 1.553442
H -0.648295 -2.333923 0.471735
H 2.435237 -0.847850 -0.697354
H 2.073256 1.546284 0.389510
H 0.777077 1.291842 1.554156
H 0.725945 2.690021 0.473528

COMP. 14_1T5I_M06-2X
C 0.504330 -0.689817 -0.440906
C 0.193251 0.824425 -0.512654
C -1.344822 0.892960 -0.311494
C -1.800011 -0.524281 0.123135
C -0.513049 -1.233289 0.551154
O 1.816839 -1.018240 -0.027135
C 0.942484 1.614754 0.559683
H 0.301651 -1.137027 -1.424893
H 0.473262 1.218243 -1.494449
H -1.580586 1.628850 0.461104
H -1.861602 1.212293 -1.217931
H -2.551901 -0.496722 0.912183
H -2.242244 -1.053911 -0.725029
H -0.210648 -0.937549 1.560349
H -0.579123 -2.321564 0.525085
H 2.438063 -0.733068 -0.701722
H 2.024108 1.551763 0.430455
H 0.709009 1.238849 1.559192
H 0.652208 2.667256 0.519231

COMP. 14_1T5I_M06-2XF
C 0.504330 -0.689817 -0.440906
C 0.193251 0.824425 -0.512654
C -1.344822 0.892960 -0.311494
C -1.800011 -0.524281 0.123135
C -0.513049 -1.233289 0.551154
O 1.816839 -1.018240 -0.027135
C 0.942484 1.614754 0.559683
H 0.301651 -1.137027 -1.424893
H 0.473262 1.218243 -1.494449
H -1.580586 1.628850 0.461104
H -1.861602 1.212293 -1.217931
H -2.551901 -0.496722 0.912183
H -2.242244 -1.053911 -0.725029
H -0.210648 -0.937549 1.560349
H -0.579123 -2.321564 0.525085
H 2.438063 -0.733068 -0.701722
H 2.024108 1.551763 0.430455
H 0.709009 1.238849 1.559192
H 0.652208 2.667256 0.519231

COMP. 14_2EIN_B3LYP
C -0.024858 0.891354 0.457670
C 0.679111 -0.483088 0.459537
C -0.195295 -1.312945 -0.498054
C -1.643451 -0.864072 -0.194322
C -1.519495 0.543607 0.460654
O 0.232988 1.635756 -0.743754
C 2.170839 -0.464928 0.129340
H 0.261889 1.497520 1.326655
H 0.554966 -0.884099 1.475601
H 0.070203 -1.064445 -1.530034
H -0.049041 -2.388860 -0.371430
H -2.254606 -0.839497 -1.098499
H -2.126554 -1.562471 0.494528
H -2.076133 1.313656 -0.075756
H -1.891946 0.528720 1.488396
H 1.168660 1.858921 -0.775336
H 2.732148 0.167114 0.826037
H 2.350156 -0.101144 -0.887409
H 2.595246 -1.471025 0.188320

COMP. 14_2EIN_M06-2X
C -0.056915 0.892937 0.458145
C 0.714305 -0.434153 0.489912
C -0.125654 -1.340503 -0.427274
C -1.586230 -0.840582 -0.289662
C -1.508803 0.446883 0.564236
O 0.082099 1.553064 -0.795484
C 2.183491 -0.336546 0.100968
H 0.241408 1.565955 1.271322
H 0.644536 -0.804820 1.520077
H 0.216436 -1.218819 -1.457988
H -0.012532 -2.394813 -0.168144
H -2.007010 -0.622775 -1.271424
H -2.230317 -1.585558 0.179825
H -2.186461 1.230947 0.225364
H -1.735611 0.231043 1.611534
H 1.001766 1.804103 -0.912749
H 2.727232 0.357628 0.748489
H 2.291405 -0.004664 -0.936067
H 2.671187 -1.310955 0.175676

COMP. 14_2EI_MP2
C -0.064169 0.893800 0.458747
C 0.719963 -0.424630 0.483303
C -0.109672 -1.330767 -0.443723
C -1.578867 -0.858537 -0.282057
C -1.509996 0.430106 0.575254
O 0.051253 1.560149 -0.801978
C 2.194660 -0.322839 0.108803
H 0.233655 1.570635 1.272286
H 0.643466 -0.803707 1.513221
H 0.221468 -1.184580 -1.477129
H 0.022936 -2.389787 -0.200604
H -2.022661 -0.647900 -1.258079
H -2.199097 -1.618525 0.202015
H -2.202250 1.208123 0.242594
H -1.724431 0.207708 1.626521
H 0.981166 1.770227 -0.931832
H 2.732354 0.364562 0.772130
H 2.312886 0.021187 -0.925092
H 2.678965 -1.301931 0.177828

COMP. 14_2T1TS_MP2
C -0.054505 0.883894 0.454910
C 0.721805 -0.436895 0.482614
C -0.116728 -1.331093 -0.449833
C -1.583362 -0.846184 -0.287584
C -1.503524 0.423978 0.595505
O 0.115859 1.505631 -0.829583
C 2.192868 -0.334082 0.102888
H 0.257363 1.568534 1.253683
H 0.637173 -0.823252 1.509226
H 0.219387 -1.180155 -1.481114
H 0.006504 -2.392293 -0.211896
H -2.016357 -0.607364 -1.262221
H -2.217469 -1.608430 0.174302
H -2.206910 1.204246 0.292874
H -1.696056 0.175368 1.645934
H 0.452784 2.392269 -0.687282
H 2.742429 0.305580 0.803087
H 2.291454 0.085428 -0.902102
H 2.663510 -1.322683 0.111182

COMP. 14_2T1_B3LYP
C -0.028500 0.887012 0.450107
C 0.697023 -0.472487 0.467366
C -0.172941 -1.328430 -0.476133
C -1.630152 -0.850078 -0.239643
C -1.511997 0.498143 0.527975
O 0.233019 1.563241 -0.797039
C 2.182113 -0.428749 0.118575
H 0.278980 1.526667 1.284259
H 0.584109 -0.864471 1.488000
H 0.126112 -1.133911 -1.510185
H -0.044653 -2.398774 -0.295988
H -2.158929 -0.723254 -1.186157
H -2.198705 -1.577940 0.344670
H -2.142655 1.285996 0.112472
H -1.794930 0.368801 1.577531
H 0.583189 2.437402 -0.614962
H 2.743700 0.184440 0.831293
H 2.330333 -0.010464 -0.879492
H 2.616019 -1.432891 0.135389

COMP. 14_2T1_M06-2X
C -0.046672 0.883570 0.453330
C 0.714480 -0.447026 0.486004
C -0.130784 -1.329709 -0.448931
C -1.591944 -0.838812 -0.281053
C -1.503718 0.444209 0.580279
O 0.146667 1.502354 -0.821117
C 2.183590 -0.351074 0.104726
H 0.266445 1.560621 1.254562
H 0.626462 -0.831771 1.509785
H 0.202983 -1.170598 -1.477372
H -0.011336 -2.391124 -0.224359
H -2.033498 -0.617996 -1.253152
H -2.222739 -1.589932 0.196699
H -2.187262 1.229139 0.255004
H -1.717933 0.219692 1.629026
H 0.482924 2.390183 -0.700232
H 2.736437 0.287247 0.799752
H 2.282118 0.066711 -0.899127
H 2.652347 -1.337949 0.112212

COMP. 14_3T4I_B3LYPT
C -0.494005 -0.750405 0.536367
C -0.267477 0.804327 0.583048
C 1.255855 0.963866 0.361293
C 1.622472 -0.182542 -0.593235
C 0.798592 -1.362836 -0.052225
O -1.593133 -1.169931 -0.281952
C -1.080335 1.578917 -0.463483
H -0.657772 -1.123948 1.554328
H -0.546605 1.182140 1.572338
H 1.518603 1.953417 -0.022852
H 1.789450 0.833480 1.309885
H 1.315276 0.061484 -1.615019
H 2.695077 -0.389666 -0.618989
H 0.546536 -2.107503 -0.808994
H 1.355487 -1.874638 0.738645
H -2.412671 -0.844304 0.103010
H -2.157714 1.463617 -0.316788
H -0.856592 1.250842 -1.480922
H -0.854615 2.646567 -0.389616

COMP. 14_3T4I_M06-2X
C -0.540339 -0.715608 0.539805
C -0.214718 0.811243 0.594973
C 1.310913 0.865921 0.391349
C 1.584263 -0.265423 -0.604428
C 0.698765 -1.399057 -0.073552
O -1.664353 -1.042691 -0.267394
C -0.945375 1.613797 -0.483262
H -0.713433 -1.090792 1.554635
H -0.488066 1.218004 1.572780
H 1.648473 1.846265 0.047512
H 1.824736 0.649436 1.333906
H 1.267694 0.029567 -1.608319
H 2.638451 -0.541075 -0.659638
H 0.386658 -2.112334 -0.836789
H 1.235449 -1.952003 0.701664
H -2.450659 -0.647532 0.116951
H -2.029108 1.587334 -0.351494
H -0.732835 1.229729 -1.482615
H -0.633585 2.659705 -0.438757

COMP. 14_3T4I_MP2
C -0.556848 -0.702777 0.541212
C -0.196349 0.815074 0.594282
C 1.332150 0.829708 0.402544
C 1.576258 -0.297838 -0.607296
C 0.662296 -1.414157 -0.082705
O -1.698843 -1.013023 -0.261300
C -0.896587 1.639704 -0.490106
H -0.729622 -1.072580 1.560947
H -0.469712 1.228890 1.572800
H 1.699260 1.807873 0.073959
H 1.833829 0.582746 1.347173
H 1.264385 0.015407 -1.609311
H 2.625284 -0.602868 -0.665550
H 0.327660 -2.114206 -0.852613
H 1.188158 -1.986819 0.689181
H -2.451308 -0.547927 0.116710
H -1.982998 1.649963 -0.359755
H -0.691568 1.248987 -1.489988
H -0.548144 2.676432 -0.440736

COMP. 14_3T4O_B3LYPT
C -0.510600 -0.733665 0.536928
C -0.249640 0.806590 0.585687
C 1.274803 0.937683 0.353042
C 1.612313 -0.214041 -0.605895

C 0.778256 -1.377902 -0.046333
O -1.679530 -0.999458 -0.249592
C -1.057415 1.602421 -0.449598
H -0.686045 -1.105610 1.553610
H -0.516658 1.183680 1.577391
H 1.549747 1.921941 -0.035119
H 1.816878 0.798010 1.295703
H 1.289560 0.032429 -1.622155
H 2.681093 -0.437666 -0.649534
H 0.535251 -2.136691 -0.794898
H 1.332027 -1.877564 0.756020
H -1.870676 -1.940527 -0.195820
H -2.129614 1.453795 -0.318185
H -0.812611 1.308561 -1.473221
H -0.839017 2.668799 -0.340040

COMP. 14_3T4O_M06-2X
C -0.577802 -0.677814 0.540574
C -0.170999 0.820744 0.595879
C 1.354575 0.796609 0.388666
C 1.566950 -0.343693 -0.612107
C 0.627704 -1.431064 -0.076328
O -1.769718 -0.814473 -0.223698
C -0.866293 1.661694 -0.476773
H -0.766591 -1.043608 1.556156
H -0.424222 1.236801 1.574008
H 1.738483 1.759002 0.043572
H 1.862711 0.552583 1.327779
H 1.257562 -0.030328 -1.612460
H 2.605345 -0.672604 -0.675538
H 0.297861 -2.136182 -0.842396
H 1.139370 -2.003733 0.702791
H -2.038447 -1.735489 -0.201631
H -1.948860 1.636739 -0.357872
H -0.642877 1.296014 -1.481159
H -0.527403 2.697737 -0.403138

COMP. 14_3T4O_MP2
C -0.563310 -0.691575 0.545306
C -0.187318 0.814922 0.599100
C 1.338102 0.823055 0.380138
C 1.562161 -0.313044 -0.624730
C 0.662130 -1.420338 -0.061241
O -1.753402 -0.850306 -0.232423
C -0.900862 1.651396 -0.468016
H -0.753739 -1.060036 1.562475
H -0.444588 1.222992 1.583008
H 1.696410 1.797435 0.032218
H 1.861458 0.586055 1.315619
H 1.220619 -0.010626 -1.620280
H 2.609762 -0.617602 -0.707300
H 0.352784 -2.158438 -0.808700
H 1.197390 -1.953860 0.733628
H -1.948226 -1.791870 -0.249481
H -1.985129 1.598119 -0.354536
H -0.658583 1.307618 -1.477335
H -0.586365 2.696163 -0.373275

COMP. 14_4T3I_MP2
C -0.357679 -0.780072 0.435090
C -0.313832 0.778006 0.498224
C 1.129271 1.144996 0.058065
C 1.900412 -0.185080 -0.011846
C 0.819126 -1.174525 -0.448459
O -1.556348 -1.340613 -0.090135
C -1.361482 1.449821 -0.389796
H -0.180049 -1.177287 1.446145
H -0.480230 1.096709 1.534704
H 1.093323 1.590251 -0.944180
H 1.596220 1.878288 0.722704
H 2.754392 -0.142533 -0.693762
H 2.278027 -0.463277 0.979811
H 0.542708 -1.002373 -1.496460
H 1.093456 -2.226389 -0.331032
H -2.271771 -1.109435 0.509812
H -2.382877 1.248068 -0.052389
H -1.274846 1.099255 -1.422710
H -1.212460 2.534755 -0.379228

COMP. 14_4T5I_MP2
C 0.437803 -0.742132 -0.432629
C 0.252151 0.792717 -0.516389
C -1.267452 0.993970 -0.250977
C -1.845436 -0.400955 0.092407
C -0.625091 -1.194206 0.564738
O 1.743788 -1.204063 -0.103858
C 1.096768 1.559228 0.506394
H 0.180459 -1.167467 -1.413345
H 0.522370 1.143119 -1.519144
H -1.401451 1.674321 0.597793
H -1.775953 1.447629 -1.106818
H -2.646368 -0.348226 0.834770
H -2.259604 -0.871365 -0.806741
H -0.325468 -0.894869 1.576578
H -0.767799 -2.278246 0.556687
H 2.306313 -0.437868 0.027422
H 2.173536 1.489318 0.307159
H 0.910129 1.201669 1.524457
H 0.841070 2.622760 0.470777

COMP. 14_4T5O_B3LYPT
C -0.313251 -0.799281 0.439516
C -0.361397 0.763175 0.482421
C 1.036958 1.220079 -0.023186
C 1.925129 -0.038084 -0.011624
C 0.939294 -1.154030 -0.378072
O -1.530258 -1.330716 -0.089427
C -1.511031 1.380092 -0.319659
H -0.182817 -1.170666 1.465252
H -0.482657 1.066480 1.527073
H 0.947194 1.589076 -1.050971
H 1.449007 2.037878 0.573046
H 2.771955 0.031145 -0.698533
H 2.334282 -0.211600 0.990366
H 0.688056 -1.103603 -1.443752
H 1.313380 -2.160645 -0.167875
H -1.489171 -2.290613 -0.040703
H -2.482654 1.058777 0.059187
H -1.458121 1.095995 -1.373977
H -1.460599 2.471795 -0.260068

COMP. 14_4T5O_M06-2X
C 0.237743 0.823205 0.450284
C 0.416320 -0.725446 0.471430
C -0.870048 -1.287483 -0.168483
C -1.913591 -0.182055 0.019389
C -1.095469 1.077856 -0.268573
O 1.346902 1.439679 -0.187850
C 1.686610 -1.212497 -0.217627
H 0.173097 1.188162 1.482769
H 0.448025 -1.041795 1.518315
H -0.702491 -1.445574 -1.239846
H -1.165505 -2.245813 0.262512
H -2.781681 -0.289102 -0.632734
H -2.272816 -0.171605 1.053955
H -0.890459 1.143696 -1.342638
H -1.579585 2.005512 0.045666
H 1.212407 2.390192 -0.177208
H 2.580949 -0.814582 0.263182
H 1.704725 -0.893731 -1.261644
H 1.728735 -2.304276 -0.188053

COMP. 14_4T5O_MP2
C 0.231382 0.825390 0.450341
C 0.420659 -0.721778 0.469984
C -0.862024 -1.290486 -0.173599
C -1.914110 -0.192922 0.024763
C -1.102542 1.070965 -0.271242
O 1.344743 1.454293 -0.186347
C 1.695091 -1.210581 -0.215294
H 0.160161 1.188691 1.485522
H 0.450313 -1.038777 1.519803

H -0.693768 -1.436138 -1.248999
H -1.147374 -2.257519 0.252429
H -2.788403 -0.305546 -0.623193
H -2.263363 -0.184923 1.065036
H -0.899199 1.130141 -1.348070
H -1.588387 2.001879 0.040672
H 1.163560 2.399080 -0.189026
H 2.590360 -0.814339 0.270249
H 1.715352 -0.895532 -1.262113
H 1.732068 -2.304886 -0.181246

COMP. 14_E1O_B3LYP
C -0.056673 0.888948 0.461474
C 0.729120 -0.431378 0.472151
C -0.111445 -1.349417 -0.444032
C -1.584511 -0.886894 -0.270365
C -1.517164 0.426922 0.555160
O 0.214683 1.549121 -0.784766
C 2.204527 -0.319147 0.093894
H 0.230981 1.544875 1.293545
H 0.658147 -0.812528 1.499797
H 0.208414 -1.214891 -1.480517
H 0.029048 -2.404500 -0.195996
H -2.052469 -0.716335 -1.241781
H -2.189328 -1.638070 0.243144
H -2.215154 1.192406 0.202287
H -1.760474 0.237649 1.606027
H -0.355996 2.320514 -0.852006
H 2.746203 0.329631 0.789078
H 2.315812 0.096435 -0.909479
H 2.684234 -1.302354 0.114342

COMP. 14_E1O_M06-2X
C -0.063870 0.885798 0.462413
C 0.735559 -0.417748 0.487134
C -0.088307 -1.340876 -0.430042
C -1.559782 -0.873520 -0.289704
C -1.507524 0.400630 0.585180
O 0.169681 1.496911 -0.802981
C 2.196665 -0.273755 0.086421
H 0.230021 1.568460 1.268848
H 0.675658 -0.796000 1.514889
H 0.251822 -1.211552 -1.459945
H 0.046553 -2.391969 -0.168678
H -1.981798 -0.649186 -1.269869
H -2.192599 -1.636958 0.165028
H -2.230230 1.162117 0.279900
H -1.710674 0.161820 1.633097
H -0.421702 2.247353 -0.895228
H 2.733306 0.387039 0.771923
H 2.270110 0.146249 -0.918044
H 2.695630 -1.245837 0.093521

COMP. 14_E1O_MP2
C -0.069794 0.886076 0.464903
C 0.741160 -0.408938 0.485508
C -0.077994 -1.345041 -0.425486
C -1.552520 -0.875193 -0.299322
C -1.506575 0.384744 0.597553
O 0.150269 1.499439 -0.809702
C 2.202991 -0.257982 0.082109
H 0.221795 1.573816 1.271216
H 0.687408 -0.786188 1.517032
H 0.268901 -1.233440 -1.457511
H 0.053884 -2.394052 -0.142375
H -1.957881 -0.630075 -1.284293
H -2.195320 -1.646370 0.134692
H -2.245811 1.142886 0.313866
H -1.690740 0.122890 1.646416
H -0.485237 2.217179 -0.889475
H 2.735663 0.411804 0.765807
H 2.274695 0.154169 -0.927552
H 2.706886 -1.230136 0.098201

COMP. 14_E1TS_MP2
C -0.054515 0.883862 0.454907
C 0.721835 -0.436903 0.482577
C -0.116686 -1.331124 -0.449835
C -1.583357 -0.846422 -0.287411
C -1.503584 0.424074 0.595246
O 0.115949 1.505789 -0.829475
C 2.192904 -0.334095 0.102858
H 0.257254 1.568409 1.253802
H 0.637235 -0.823232 1.509205
H 0.219300 -1.180022 -1.481136
H 0.006694 -2.392337 -0.212037
H -2.016702 -0.608119 -1.262018
H -2.217150 -1.608634 0.174965
H -2.206747 1.204337 0.292073
H -1.696560 0.175931 1.645703
H 0.451994 2.392723 -0.686948
H 2.742360 0.305927 0.802810
H 2.291510 0.085005 -0.902295
H 2.663637 -1.322648 0.111620

COMP. 15_1T2I_B3LYP
C 0.184915 0.784560 0.325162
C 0.552974 -0.559134 -0.330148
C -0.655706 -1.436871 0.036250
C -1.883414 -0.488967 -0.038218
C -1.309099 0.952542 0.028943
O 0.901136 1.914469 -0.172555
C 1.909331 -1.125625 0.082569
H 0.345542 0.700560 1.411956
H 0.551918 -0.385719 -1.414788
H -0.752291 -2.308867 -0.615287
H -0.530731 -1.816802 1.057183
H -2.434757 -0.638304 -0.969478
H -2.585127 -0.687276 0.774942
H -1.400701 1.460584 -0.935169
H -1.805971 1.579635 0.771608
H 1.820223 1.847409 0.104434
H 1.953255 -1.289892 1.165097
H 2.106777 -2.083974 -0.406311
H 2.728779 -0.452137 -0.191084

COMP. 15_1T2I_M06-2X
C 0.191067 0.774541 0.323835
C 0.534393 -0.562553 -0.337881
C -0.673990 -1.419231 0.050259
C -1.885445 -0.456518 -0.026491
C -1.286908 0.971192 -0.001018
O 0.938912 1.879440 -0.147721
C 1.882375 -1.137145 0.070328
H 0.326035 0.667462 1.412216
H 0.520417 -0.386400 -1.421327
H -0.787201 -2.298958 -0.585596
H -0.539335 -1.778522 1.076527
H -2.452437 -0.617492 -0.944554
H -2.573348 -0.623534 0.803302
H -1.342124 1.440736 -0.986569
H -1.781083 1.636196 0.707569
H 1.856072 1.766577 0.113917
H 1.923966 -1.283731 1.154437
H 2.063536 -2.103821 -0.405004
H 2.705253 -0.475756 -0.217341

COMP. 15_1T2I_MP2
C 0.185965 0.774409 0.327754
C 0.538844 -0.559226 -0.335125
C -0.659811 -1.423084 0.067813
C -1.880091 -0.476109 -0.051502
C -1.297692 0.960263 0.013652
O 0.917577 1.897852 -0.150394
C 1.895331 -1.125075 0.063970
H 0.330854 0.667514 1.416676
H 0.513602 -0.386568 -1.421336
H -0.758179 -2.326135 -0.542658
H -0.529226 -1.744736 1.109689
H -2.397593 -0.635336 -1.001929
H -2.606659 -0.660753 0.744540
H -1.365041 1.459475 -0.958726

H -1.797727 1.595952 0.748842
H 1.840638 1.759852 0.083671
H 1.941186 -1.273352 1.149572
H 2.079442 -2.090878 -0.417300
H 2.712812 -0.454920 -0.227261

COMP. 15_1T2O_B3LYP
C 0.196093 0.778002 0.318152
C 0.550701 -0.564185 -0.329508
C -0.677735 -1.431670 0.003414
C -1.894786 -0.461254 0.010097
C -1.292456 0.968383 -0.015037
O 1.053530 1.802982 -0.184803
C 1.892493 -1.146386 0.105778
H 0.330352 0.690771 1.408179
H 0.577085 -0.382286 -1.412427
H -0.801267 -2.256717 -0.701922
H -0.546472 -1.881303 0.994032
H -2.541445 -0.623553 -0.854962
H -2.514143 -0.620541 0.895805
H -1.356594 1.401723 -1.017864
H -1.795744 1.654961 0.671535
H 0.865846 2.623946 0.280231
H 1.903444 -1.337573 1.184720
H 2.096785 -2.093899 -0.401740
H 2.708053 -0.456725 -0.124538

COMP. 15_1T2O_M06-2X
C 0.200416 0.767463 0.317576
C 0.536200 -0.567307 -0.337102
C -0.688239 -1.418796 0.018241
C -1.891847 -0.438264 0.015728
C -1.273602 0.978617 -0.037222
O 1.074975 1.771911 -0.162561
C 1.873207 -1.148403 0.093976
H 0.314981 0.659188 1.408025
H 0.549068 -0.382140 -1.419011
H -0.823242 -2.255915 -0.668371
H -0.548092 -1.843535 1.017733
H -2.544002 -0.607807 -0.841883
H -2.503841 -0.573318 0.908752
H -1.310606 1.382833 -1.052827
H -1.775140 1.688937 0.623741
H 0.867047 2.602166 0.272099
H 1.878865 -1.330863 1.173307
H 2.073445 -2.097773 -0.408308
H 2.684907 -0.456926 -0.139948

COMP. 15_1T2O_MP2
C 0.192579 0.767337 0.318650
C 0.540906 -0.562042 -0.338821
C -0.677733 -1.423701 0.019474
C -1.890143 -0.449831 0.023749
C -1.278113 0.970134 -0.052180
O 1.071263 1.785222 -0.148607
C 1.881785 -1.140937 0.090184
H 0.293806 0.653914 1.411934
H 0.547991 -0.377189 -1.423214
H -0.810738 -2.260475 -0.672691
H -0.530238 -1.850368 1.019586
H -2.555050 -0.632200 -0.824868
H -2.487416 -0.577483 0.931150
H -1.307504 1.353872 -1.078369
H -1.788694 1.692089 0.594069
H 0.791583 2.613645 0.252425
H 1.889012 -1.313559 1.173070
H 2.075642 -2.097387 -0.406505
H 2.695813 -0.452395 -0.154061

COMP. 15_1T2TS_MP2
C 0.229661 0.762064 0.310825
C 0.504795 -0.593992 -0.337432
C -0.741908 -1.390403 0.059148
C -1.911193 -0.371477 -0.012906
C -1.242518 1.025877 -0.015517
O 1.081249 1.790273 -0.197033
C 1.829025 -1.223110 0.069386
H 0.366420 0.662200 1.399242
H 0.496547 -0.422772 -1.424326
H -0.903529 -2.267578 -0.574778
H -0.617834 -1.751435 1.088749
H -2.501604 -0.517722 -0.921824
H -2.592143 -0.494518 0.834043
H -1.273794 1.477156 -1.012997
H -1.706082 1.730140 0.681206
H 1.577775 2.159124 0.536027
H 1.851314 -1.393857 1.152832
H 1.980144 -2.187466 -0.426524
H 2.665612 -0.569204 -0.196416

COMP. 15_1T2_B3LYP
C 0.225408 0.774194 0.312402
C 0.523015 -0.590520 -0.328615
C -0.726662 -1.407224 0.038479
C -1.909748 -0.401455 -0.025352
C -1.265564 1.009993 0.021721
O 1.046428 1.819190 -0.223015
C 1.853231 -1.211030 0.086689
H 0.392363 0.697979 1.396177
H 0.532981 -0.421580 -1.414113
H -0.616428 -1.798411 1.056963
H -0.869661 -2.270229 -0.616324
H -2.483354 -0.530830 -0.946087
H -2.606642 -0.560547 0.800644
H -1.335216 1.509453 -0.948562
H -1.730402 1.671134 0.756734
H 1.558002 2.220094 0.482641
H 1.881186 -1.391324 1.167599
H 2.687871 -0.553009 -0.170751
H 2.019798 -2.169990 -0.412733

COMP. 15_1T2_M06-2X
C 0.231776 0.763227 0.310719
C 0.505068 -0.594544 -0.335952
C -0.741986 -1.390192 0.056000
C -1.908643 -0.372596 -0.020690
C -1.244320 1.025069 -0.000325
O 1.076036 1.782271 -0.204578
C 1.828888 -1.217772 0.074141
H 0.378903 0.665367 1.395932
H 0.500270 -0.423313 -1.420496
H -0.622664 -1.752588 1.083251
H -0.899670 -2.265506 -0.576324
H -2.484298 -0.509595 -0.937305
H -2.602198 -0.506537 0.810536
H -1.285031 1.496439 -0.985533
H -1.704681 1.713090 0.710175
H 1.584548 2.174043 0.505451
H 1.852405 -1.388863 1.155524
H 2.661320 -0.560708 -0.188361
H 1.988119 -2.179150 -0.419592

COMP. 15_2EIN_B3LYP
C -0.638971 -0.692184 -0.402774
C 0.671042 -0.621262 0.409060
C 0.582238 0.774212 1.062019
C -0.060332 1.681134 -0.017555
C -0.820061 0.721136 -0.977198
O -1.770855 -0.945456 0.446197
C 1.908781 -0.784674 -0.483750
H -0.595710 -1.457335 -1.188486
H 0.684702 -1.413765 1.167149
H -0.068553 0.722702 1.937836
H 1.556317 1.140651 1.397213
H -0.727858 2.418869 0.431393
H 0.704106 2.241041 -0.562483
H -1.884897 0.947913 -1.049861
H -0.409190 0.769756 -1.988685
H -1.642324 -1.794507 0.881667
H 2.824533 -0.717796 0.110099
H 1.960065 -0.009269 -1.253967
H 1.909460 -1.754792 -0.990263

COMP. 15_2EIN_M06-2X
C -0.642085 -0.691171 -0.412327
C 0.647115 -0.649073 0.418762
C 0.548259 0.729009 1.090661
C -0.029541 1.652483 -0.006299
C -0.750243 0.714012 -1.009222
O -1.783943 -0.869956 0.420834
C 1.885726 -0.768047 -0.468790
H -0.614765 -1.472419 -1.181734
H 0.653393 -1.460603 1.155042
H -0.145262 0.674172 1.931375
H 1.511982 1.075890 1.469909
H -0.710590 2.389965 0.418256
H 0.767091 2.206693 -0.506770
H -1.801476 0.966936 -1.148342
H -0.271107 0.742546 -1.989794
H -1.690404 -1.700795 0.894093
H 2.795953 -0.730277 0.133356
H 1.933472 0.051661 -1.191172
H 1.887861 -1.707399 -1.027603

COMP. 15_2EI_MP2
C -0.647444 -0.684021 -0.417019
C 0.639328 -0.655591 0.415839
C 0.550959 0.719438 1.095635
C -0.003226 1.654304 -0.005208
C -0.748068 0.726859 -1.003623
O -1.799015 -0.861702 0.416504
C 1.880079 -0.781531 -0.470730
H -0.623041 -1.462317 -1.192824
H 0.638453 -1.473755 1.149233
H -0.155093 0.671405 1.929410
H 1.517745 1.054483 1.486191
H -0.668155 2.412492 0.416029
H 0.810318 2.184490 -0.509872
H -1.802024 0.990587 -1.122931
H -0.283134 0.756549 -1.993818
H -1.671109 -1.682077 0.903852
H 2.790102 -0.746793 0.136488
H 1.932504 0.037010 -1.196258
H 1.875780 -1.725206 -1.026892

COMP. 15_2ETS_B3LYP
C 0.663983 -0.672688 0.378243
C -0.650815 -0.640058 -0.423855
C -0.614687 0.770393 -1.049933
C 0.004413 1.684189 0.040430
C 0.767521 0.731217 1.004360
O 1.763981 -0.878586 -0.533901
C -1.880442 -0.862745 0.467505
H 0.664756 -1.464193 1.135033
H -0.622029 -1.417522 -1.192458
H 0.031289 0.753732 -1.930812
H -1.602885 1.108569 -1.373282
H 0.668871 2.429183 -0.401173
H -0.770367 2.235583 0.579174
H 1.815983 1.004896 1.132417
H 0.307928 0.731334 1.996913
H 2.262512 -1.649537 -0.255487
H -2.797346 -0.821217 -0.127096
H -1.963995 -0.102772 1.250392
H -1.846404 -1.841214 0.957090

COMP. 15_2ETS_M06-2X
C 0.670631 -0.667306 0.389158
C -0.623197 -0.670574 -0.432063
C -0.577178 0.720756 -1.081988
C -0.043646 1.653021 0.031506
C 0.701394 0.727650 1.029209
O 1.778592 -0.798633 -0.506059
C -1.856300 -0.848485 0.453508
H 0.690298 -1.469220 1.134245
H -0.582727 -1.469212 -1.176808
H 0.125102 0.700720 -1.917266
H -1.550835 1.034388 -1.464770
H 0.615522 2.418245 -0.378496
H -0.862928 2.173836 0.531216
H 1.733569 1.032314 1.202486
H 0.194826 0.707271 1.996942
H 2.309353 -1.552711 -0.249171
H -2.765035 -0.846796 -0.152304
H -1.945570 -0.037859 1.182253
H -1.820536 -1.792281 1.004167

COMP. 15_2ETS_MP2
C 0.670857 -0.666322 0.391061
C -0.620162 -0.671800 -0.432551
C -0.576126 0.719005 -1.084718
C -0.048936 1.654090 0.032038
C 0.694970 0.727889 1.032457
O 1.791201 -0.789463 -0.503142
C -1.856849 -0.852053 0.450569
H 0.693451 -1.470712 1.137105
H -0.578688 -1.473272 -1.178508
H 0.130894 0.702047 -1.919300
H -1.552685 1.030476 -1.470314
H 0.613783 2.421065 -0.376729
H -0.874089 2.173278 0.529120
H 1.728011 1.036337 1.210202
H 0.181967 0.703515 1.999619
H 2.277074 -1.579815 -0.258703
H -2.764204 -0.854029 -0.161797
H -1.950701 -0.039996 1.179270
H -1.816939 -1.798048 1.002040

COMP. 15_2T1O_B3LYP
C 0.567358 -0.766924 0.367704
C -0.729221 -0.551808 -0.426857
C -0.536587 0.864457 -1.016698
C 0.274633 1.658015 0.045427
C 0.839171 0.595363 1.028308
O 1.583143 -1.106846 -0.590226
C -1.976376 -0.662893 0.459639
H 0.473234 -1.576278 1.103073
H -0.787743 -1.304507 -1.217881
H 0.033970 0.794753 -1.944639
H -1.491182 1.341201 -1.254846
H 1.074626 2.231544 -0.426434
H -0.354086 2.377152 0.575925
H 1.904056 0.732166 1.239448
H 0.323179 0.640900 1.992123
H 2.434184 -1.124757 -0.141366
H -2.881379 -0.505599 -0.133446
H -1.978081 0.082303 1.261414
H -2.049789 -1.651378 0.923311

COMP. 15_2T1O_M06-2X
C 0.606689 -0.737705 0.382321
C -0.681228 -0.615655 -0.432025
C -0.529062 0.777262 -1.064701
C 0.129945 1.643328 0.036407
C 0.763566 0.641491 1.036129
O 1.650548 -0.989869 -0.553650
C -1.920777 -0.708411 0.456535
H 0.558376 -1.550039 1.117546
H -0.706525 -1.404274 -1.187803
H 0.131167 0.708802 -1.930066
H -1.485775 1.183491 -1.400156
H 0.875627 2.315700 -0.388284
H -0.608919 2.268779 0.540983
H 1.813409 0.859654 1.247751
H 0.238710 0.656806 1.994346
H 2.493412 -0.934153 -0.097324
H -2.828014 -0.630435 -0.146133
H -1.945420 0.100271 1.192936
H -1.955234 -1.657508 0.997405

COMP. 15_2T1O_MP2
C 0.589974 -0.752211 0.382069
C -0.691633 -0.602713 -0.435017
C -0.513362 0.790376 -1.062099

C 0.174943 1.638524 0.038914
C 0.761911 0.617398 1.049452
O 1.637818 -1.007060 -0.560645
C -1.937911 -0.678077 0.448798
H 0.529995 -1.573390 1.110121
H -0.731522 -1.389351 -1.196633
H 0.137762 0.714502 -1.936554
H -1.467646 1.220234 -1.384290
H 0.954690 2.273962 -0.388642
H -0.541535 2.300201 0.534836
H 1.813148 0.812806 1.289273
H 0.210812 0.636758 1.995808
H 2.470504 -0.933648 -0.084175
H -2.841432 -0.590737 -0.162633
H -1.956707 0.133864 1.183928
H -1.984147 -1.628509 0.991420

COMP. 15_3EO_B3LYP
C 0.050899 0.834167 0.349298
C 0.704302 -0.407191 -0.290822
C -0.311371 -1.534565 -0.044390
C -1.668308 -0.843944 -0.253072
C -1.477167 0.545331 0.395827
O 0.408366 1.979909 -0.435025
C 2.127481 -0.684981 0.188006
H 0.438279 0.969940 1.368191
H 0.727812 -0.203064 -1.368966
H -0.155802 -2.391764 -0.704896
H -0.224778 -1.899443 0.987508
H -1.862496 -0.736111 -1.325045
H -2.507173 -1.399250 0.173257
H -2.032327 1.330996 -0.122466
H -1.823841 0.532283 1.433827
H 0.137246 2.774766 0.034362
H 2.559013 -1.547051 -0.329320
H 2.145905 -0.898645 1.262512
H 2.776211 0.175165 0.002159

COMP. 15_3EO_M06-2X
C 0.007155 0.835365 0.353300
C 0.731228 -0.356100 -0.294134
C -0.211520 -1.540484 -0.064203
C -1.595036 -0.919482 -0.278854
C -1.483975 0.428086 0.454383
O 0.240211 1.977704 -0.461704
C 2.157633 -0.547558 0.199718
H 0.419845 1.018719 1.354181
H 0.746081 -0.138025 -1.368721
H -0.000144 -2.381262 -0.728024
H -0.115372 -1.898444 0.968550
H -1.755806 -0.754105 -1.348092
H -2.415142 -1.537547 0.089500
H -2.128132 1.201099 0.030407
H -1.763450 0.302296 1.504010
H -0.106285 2.753694 -0.015136
H 2.650423 -1.372071 -0.320799
H 2.166800 -0.772716 1.270708
H 2.746587 0.357768 0.035791

COMP. 15_3EO_MP2
C 0.124516 0.808984 0.344659
C 0.636679 -0.482611 -0.297412
C -0.468297 -1.492119 0.021055
C -1.748943 -0.688406 -0.243674
C -1.423291 0.715492 0.314113
O 0.663589 1.914212 -0.383264
C 2.038669 -0.873082 0.150973
H 0.479972 0.852219 1.385765
H 0.634351 -0.301441 -1.382295
H -0.396181 -2.404629 -0.579445
H -0.410430 -1.780272 1.080358
H -1.919020 -0.631797 -1.324632
H -2.642035 -1.127502 0.210431
H -1.832715 1.515748 -0.309923
H -1.832266 0.836414 1.323054
H 0.472140 2.711885 0.118707
H 2.381703 -1.777342 -0.362310
H 2.051758 -1.069073 1.229792
H 2.748010 -0.067459 -0.061673

COMP. 15_3T4I_M06-2X
C -0.081965 0.845583 0.366867
C 0.784268 -0.250219 -0.304191
C -0.032076 -1.539976 -0.148449
C -1.476070 -1.052211 -0.289148
C -1.478411 0.228117 0.557504
O -0.211647 2.009254 -0.443140
C 2.208059 -0.329124 0.232313
H 0.352016 1.130746 1.333987
H 0.809324 -0.000933 -1.371817
H 0.250283 -2.304610 -0.875262
H 0.124020 -1.958843 0.853437
H -1.681715 -0.810851 -1.336320
H -2.217769 -1.782109 0.038640
H -2.249053 0.946516 0.276754
H -1.625654 -0.029823 1.609606
H 0.663646 2.374836 -0.596750
H 2.783604 -1.102411 -0.281871
H 2.202335 -0.568468 1.299841
H 2.739302 0.618896 0.105501

COMP. 15_4T3I_B3LYPT
C -0.812335 -0.396126 -0.337054
C 0.538402 -0.675221 0.398108
C 1.032858 0.717924 0.853241
C 0.494803 1.677739 -0.220752
C -0.916263 1.133808 -0.493657
O -1.964950 -0.838459 0.393766
C 1.551661 -1.386650 -0.509268
H -0.806937 -0.889171 -1.317960
H 0.337019 -1.314078 1.263563
H 0.589383 0.972057 1.821561
H 2.119274 0.761317 0.970551
H 0.489432 2.722016 0.100873
H 1.112407 1.623873 -1.124066
H -1.611423 1.489224 0.273100
H -1.320292 1.429093 -1.464327
H -1.967709 -1.800750 0.414030
H 2.484751 -1.585475 0.025636
H 1.797169 -0.784082 -1.389834
H 1.161783 -2.345192 -0.866962

COMP. 15_4T3I_M06-2X
C -0.832267 -0.305838 -0.313193
C 0.495452 -0.679340 0.409831
C 1.152175 0.671366 0.765428
C 0.593349 1.643943 -0.280742
C -0.874604 1.223277 -0.361625
O -1.999464 -0.767647 0.351555
C 1.400229 -1.533919 -0.477655
H -0.812848 -0.712795 -1.333605
H 0.246903 -1.239678 1.315173
H 0.833058 0.995745 1.759905
H 2.243163 0.614549 0.768971
H 0.724561 2.692169 -0.008399
H 1.088088 1.489627 -1.245596
H -1.409478 1.562587 0.531025
H -1.403844 1.601169 -1.237110
H -2.019221 -1.726937 0.312516
H 2.312016 -1.821979 0.050281
H 1.693612 -0.982505 -1.376478
H 0.893698 -2.447710 -0.801377

COMP. 15_4T3I_MP2
C -0.834804 -0.275921 -0.307168
C 0.485401 -0.679556 0.411410
C 1.194561 0.655528 0.732025
C 0.622377 1.640967 -0.297626
C -0.858065 1.253001 -0.321283
O -2.017562 -0.743120 0.342619
C 1.348331 -1.591150 -0.463481
H -0.813526 -0.655762 -1.340492

H 0.222168 -1.209385 1.334183
H 0.922164 0.995345 1.738086
H 2.285518 0.564692 0.694043
H 0.788869 2.688518 -0.029993
H 1.076812 1.471421 -1.282026
H -1.344165 1.585236 0.604126
H -1.419927 1.655580 -1.168583
H -2.032599 -1.701436 0.259055
H 2.252028 -1.906736 0.067807
H 1.657556 -1.068874 -1.376392
H 0.798801 -2.490850 -0.764020

COMP. 15_4T3O_B3LYPT
C -0.782609 -0.476403 -0.357120
C 0.560382 -0.680073 0.387824
C 0.908130 0.721168 0.936001
C 0.415876 1.683131 -0.157442
C -0.911887 1.050249 -0.622866
O -1.831620 -0.977251 0.487274
C 1.652330 -1.237538 -0.535880
H -0.787397 -1.043883 -1.296167
H 0.391055 -1.392370 1.198802
H 0.353334 0.901875 1.862395
H 1.971871 0.834137 1.162968
H 0.289624 2.708524 0.198492
H 1.133839 1.719091 -0.983043
H -1.738069 1.429846 -0.013414
H -1.144702 1.274816 -1.667199
H -2.676293 -0.824535 0.051426
H 2.594201 -1.359044 0.006643
H 1.845093 -0.577870 -1.388185
H 1.367068 -2.215782 -0.934015

COMP. 15_4T3O_M06-2X
C -0.804954 -0.412003 -0.340159
C 0.525396 -0.686578 0.398622
C 0.993423 0.696945 0.884752
C 0.512431 1.649404 -0.215359
C -0.896125 1.120992 -0.514045
O -1.869078 -0.937112 0.446316
C 1.555397 -1.341915 -0.522041
H -0.798804 -0.915513 -1.315159
H 0.313801 -1.356107 1.234585
H 0.493661 0.950679 1.824440
H 2.071461 0.737996 1.056042
H 0.514683 2.697577 0.087796
H 1.151222 1.563298 -1.099348
H -1.589401 1.496986 0.245104
H -1.274300 1.417372 -1.494548
H -2.701636 -0.727477 0.015453
H 2.491710 -1.524635 0.009955
H 1.779336 -0.706112 -1.384052
H 1.187476 -2.298241 -0.901416

COMP. 15_4T3O_MP2
C -0.804917 -0.413468 -0.347856
C 0.517886 -0.694650 0.397976
C 0.975146 0.684235 0.906730
C 0.527939 1.642582 -0.204325
C -0.877554 1.120134 -0.538430
O -1.878961 -0.921080 0.452257
C 1.557072 -1.333251 -0.527073
H -0.805651 -0.930437 -1.318199
H 0.302143 -1.380056 1.223913
H 0.445210 0.933796 1.833876
H 2.050715 0.719071 1.110094
H 0.524446 2.692903 0.102399
H 1.189702 1.554601 -1.073412
H -1.589889 1.511044 0.198262
H -1.225985 1.406724 -1.535996
H -2.699113 -0.681219 0.009311
H 2.496291 -1.508533 0.007528
H 1.773689 -0.689404 -1.386892
H 1.196696 -2.293344 -0.911074

COMP. 15_5EIN_M06-2X
C 0.350568 -0.862540 0.330239
C -0.846136 -0.257082 -0.432585
C -0.440330 1.219109 -0.705330
C 0.940919 1.416745 -0.047963
C 0.987549 0.330427 1.032020
O 1.338527 -1.374553 -0.558704
C -2.137902 -0.359208 0.377808
H 0.033158 -1.647423 1.027553
H -0.979491 -0.802270 -1.372684
H -1.176024 1.886162 -0.245961
H -0.421652 1.451191 -1.770935
H 1.735788 1.231979 -0.772310
H 1.074935 2.422714 0.352007
H 1.993018 0.096853 1.384107
H 0.375442 0.615656 1.893382
H 0.934709 -2.046856 -1.112692
H -2.023131 0.130871 1.349515
H -2.420435 -1.399864 0.555455
H -2.962546 0.132706 -0.142933

COMP. 15_5T1I_B3LYPT
C 0.435674 -0.842490 0.348650
C -0.814462 -0.388009 -0.435080
C -0.465887 1.056448 -0.894659
C 0.690162 1.549570 0.024468
C 0.911431 0.423707 1.058309
O 1.496287 -1.244136 -0.532879
C -2.084917 -0.446152 0.424501
H 0.210090 -1.658518 1.047377
H -0.960699 -1.046030 -1.299935
H -0.149620 1.063549 -1.939495
H -1.344500 1.703762 -0.826696
H 1.598278 1.698836 -0.562055
H 0.458550 2.502440 0.505791
H 1.950128 0.329537 1.380604
H 0.301404 0.585983 1.952039
H 1.181084 -1.969934 -1.080889
H -2.009082 0.205701 1.300279
H -2.282990 -1.462102 0.780215
H -2.954939 -0.118581 -0.151332

COMP. 15_5T1I_M06-2X
C 0.375708 -0.863653 0.331306
C -0.834250 -0.313052 -0.444191
C -0.436979 1.147070 -0.796196
C 0.854329 1.454343 -0.000422
C 0.924503 0.352661 1.065666
O 1.407778 -1.294598 -0.550402
C -2.111835 -0.377674 0.392893
H 0.093393 -1.680128 1.007144
H -0.983115 -0.908479 -1.351202
H -0.278333 1.274669 -1.867646
H -1.244002 1.827067 -0.510420
H 1.724496 1.373129 -0.652916
H 0.851496 2.456460 0.430138
H 1.932262 0.170521 1.440861
H 0.278243 0.587566 1.916179
H 1.055150 -1.978005 -1.125416
H -1.999106 0.191063 1.320526
H -2.367845 -1.407063 0.656202
H -2.953720 0.051817 -0.154562

COMP. 15_5T1I_MP2
C 0.354438 -0.865133 0.331275
C -0.841729 -0.275565 -0.438696
C -0.435154 1.196652 -0.737448
C 0.920848 1.422805 -0.029886
C 0.956542 0.335112 1.051694
O 1.370701 -1.345728 -0.555893
C -2.132465 -0.362146 0.379589
H 0.042720 -1.667803 1.014339
H -0.982028 -0.840810 -1.369471
H -0.371236 1.395854 -1.810956
H -1.196479 1.872610 -0.330418
H 1.743875 1.257454 -0.729486
H 1.016568 2.434115 0.375638

H 1.959369 0.117429 1.429533
H 0.316978 0.608713 1.899363
H 0.955503 -1.989885 -1.137617
H -2.014162 0.150739 1.340686
H -2.412586 -1.402022 0.579259
H -2.959013 0.119085 -0.152897

COMP. 15_5T4I_B3LYP
C 0.298909 -0.847132 0.355833
C -0.865292 -0.093629 -0.362705
C -0.399762 1.386374 -0.464625
C 1.112813 1.361629 -0.188486
C 1.245917 0.246412 0.859243
O 1.056881 -1.666418 -0.549631
C -2.218462 -0.252626 0.337249
H -0.077082 -1.473442 1.174683
H -0.944956 -0.511787 -1.372332
H -0.903474 1.979193 0.308369
H -0.654378 1.836413 -1.427429
H 1.664048 1.085326 -1.092009
H 1.499133 2.324365 0.155344
H 2.260014 -0.137451 0.984626
H 0.898061 0.606866 1.834031
H 0.466703 -2.315636 -0.945454
H -2.171121 0.107221 1.370609
H -2.541091 -1.298315 0.362607
H -2.995636 0.322428 -0.175051

COMP. 15_5T4I_MP2
C 0.574940 -0.746668 0.388186
C -0.704596 -0.573229 -0.429246
C -0.537775 0.832410 -1.043469
C 0.226721 1.662027 0.021562
C 0.813248 0.627759 1.022941
O 1.707278 -1.010963 -0.455173
C -1.939989 -0.681883 0.467317
H 0.480256 -1.540906 1.139080
H -0.770965 -1.348056 -1.204276
H -1.489330 1.272620 -1.352258
H 0.087123 0.778791 -1.935198
H 0.992882 2.319000 -0.395768
H -0.470405 2.332849 0.526602
H 1.880606 0.762345 1.209524
H 0.319944 0.703620 1.999680
H 1.502933 -1.781549 -0.994522
H -2.034080 0.179182 1.137786
H -1.903355 -1.583551 1.086363
H -2.849126 -0.729136 -0.139383

COMP. 15_E1O_B3LYP
C 0.485987 -0.823694 0.340711
C -0.785908 -0.455622 -0.438087
C -0.499014 0.983951 -0.940582
C 0.526679 1.603491 0.054589
C 0.875719 0.476227 1.056862
O 1.469729 -1.205910 -0.634699
C -2.043940 -0.539560 0.436201
H 0.318483 -1.654771 1.037773
H -0.893344 -1.148931 -1.276599
H -0.072411 0.949682 -1.944436
H -1.418995 1.571400 -1.002264
H 1.419452 1.934009 -0.479522
H 0.124412 2.479490 0.568475
H 1.927542 0.479907 1.359532
H 0.285662 0.570912 1.974048
H 2.314296 -1.323806 -0.188464
H -1.997224 0.146687 1.287834
H -2.191593 -1.550304 0.828828
H -2.931241 -0.275751 -0.145769

COMP. 15_E1O_M06-2X
C 0.406573 -0.862976 0.310900
C -0.821761 -0.361338 -0.453030
C -0.462498 1.099555 -0.831475
C 0.751460 1.498844 0.046634
C 0.887521 0.368000 1.078306
O 1.362692 -1.255205 -0.670079
C -2.087242 -0.440215 0.400186
H 0.167869 -1.710821 0.964152
H -0.948249 -0.981519 -1.343055
H -0.212961 1.180072 -1.889685
H -1.317442 1.756036 -0.651179
H 1.652874 1.543177 -0.565974
H 0.625886 2.474885 0.516834
H 1.905035 0.250561 1.461400
H 0.233516 0.537903 1.938570
H 2.192162 -1.455146 -0.228871
H -1.993093 0.165699 1.306357
H -2.304468 -1.468357 0.700117
H -2.946981 -0.062075 -0.157161

COMP. 15_E1O_MP2
C 0.418331 -0.859970 0.316236
C -0.813101 -0.383921 -0.455324
C -0.464126 1.071727 -0.860352
C 0.710921 1.514112 0.054661
C 0.868670 0.381091 1.084995
O 1.392130 -1.234347 -0.665295
C -2.077711 -0.451640 0.403720
H 0.192548 -1.713991 0.969798
H -0.939125 -1.023142 -1.335763
H -0.170845 1.123076 -1.912093
H -1.338602 1.719311 -0.733329
H 1.625744 1.605996 -0.536212
H 0.526578 2.481027 0.531316
H 1.890727 0.287363 1.470407
H 0.207559 0.534678 1.945696
H 2.222848 -1.376909 -0.200460
H -1.990523 0.189218 1.288137
H -2.277956 -1.474553 0.740281
H -2.943904 -0.105686 -0.169039

COMP. 15_E4I_B3LYP
C -0.248557 0.845690 0.364245
C 0.856533 -0.012406 -0.333748
C 0.306675 -1.460722 -0.344892
C -1.217031 -1.301310 -0.240023
C -1.362267 -0.137655 0.752714
O -0.827457 1.817525 -0.522278
C 2.241717 0.116369 0.304635
H 0.152940 1.364658 1.243881
H 0.912746 0.339991 -1.370073
H 0.627220 -2.019865 -1.227895
H 0.680633 -2.002509 0.532999
H -1.638484 -1.019027 -1.209994
H -1.723207 -2.212484 0.088486
H -2.337313 0.352381 0.735063
H -1.187192 -0.499442 1.771963
H -0.134595 2.416892 -0.817988
H 2.973235 -0.514552 -0.209234
H 2.220315 -0.192496 1.355178
H 2.610938 1.146449 0.268258

COMP. 15_E4I_MP2
C -0.049370 0.841719 0.368396
C 0.765848 -0.290647 -0.300842
C -0.099632 -1.544513 -0.118230
C -1.520973 -0.999830 -0.294599
C -1.482060 0.298587 0.527237
O -0.102560 2.029321 -0.429461
C 2.194982 -0.412304 0.217771
H 0.383915 1.087995 1.349001
H 0.783796 -0.055214 -1.374414
H 0.162639 -2.341049 -0.822472
H 0.026146 -1.939062 0.900078
H -1.696441 -0.772238 -1.352559
H -2.301753 -1.690402 0.037737
H -2.207633 1.051134 0.207606
H -1.673195 0.069902 1.581578
H 0.803739 2.329507 -0.552927
H 2.737728 -1.210225 -0.299492
H 2.193297 -0.641886 1.289444

H 2.755469 0.518900 0.073711

COMP. 15_E4O_B3LYP
C -0.243558 0.839993 0.358275
C 0.850831 -0.029418 -0.320801
C 0.304690 -1.476305 -0.294940
C -1.221152 -1.310031 -0.249458
C -1.392735 -0.127212 0.715982
O -0.640956 1.839930 -0.595652
C 2.243873 0.126412 0.290997
H 0.146782 1.340263 1.253384
H 0.885213 0.310578 -1.360767
H 0.646547 -1.988571 0.613533
H 0.652959 -2.065339 -1.147321
H -1.602064 -1.043281 -1.240585
H -1.746366 -2.211449 0.076068
H -2.370683 0.359026 0.656627
H -1.263431 -0.474725 1.747895
H -1.285605 2.421243 -0.179443
H 2.247274 -0.166245 1.346765
H 2.591854 1.161371 0.226343
H 2.973476 -0.502942 -0.227619

COMP. 15_E4O_M06-2X
C 0.343097 -0.853557 0.320006
C -0.852409 -0.214177 -0.412285
C -0.475463 1.282837 -0.583829
C 0.976421 1.412388 -0.095582
C 1.067194 0.323228 0.976809
O 1.162338 -1.464985 -0.673942
C -2.160246 -0.395798 0.354672
H 0.016011 -1.608330 1.044945
H -0.931968 -0.705755 -1.384213
H -1.129185 1.894124 0.047445
H -0.604885 1.627503 -1.610576
H 1.671246 1.181372 -0.905860
H 1.210928 2.409432 0.280047
H 2.088002 0.073001 1.278364
H 0.518833 0.629652 1.874669
H 1.956015 -1.802843 -0.250988
H -2.073528 0.011267 1.367461
H -2.434131 -1.450375 0.434524
H -2.977602 0.131308 -0.143023

COMP. 15_E4O_MP2
C 0.334388 -0.851740 0.327023
C -0.853698 -0.199990 -0.405730
C -0.469158 1.296497 -0.563562
C 0.997240 1.403509 -0.111555
C 1.087449 0.317111 0.965472
O 1.136551 -1.491699 -0.674360
C -2.170226 -0.383238 0.349356
H -0.001025 -1.594706 1.063749
H -0.927392 -0.683924 -1.385310
H -1.099761 1.903221 0.099456
H -0.626101 1.657034 -1.584337
H 1.668806 1.154834 -0.938689
H 1.256418 2.401185 0.255062
H 2.110671 0.048652 1.252818
H 0.556061 0.638749 1.871213
H 1.931529 -1.813364 -0.236692
H -2.087964 0.016694 1.367149
H -2.447586 -1.440216 0.417838
H -2.982035 0.152539 -0.153399

COMP. 15_E4_B3LYP
C 0.225409 0.774193 0.312400
C 0.523014 -0.590520 -0.328617
C -0.726667 -1.407223 0.038470
C -1.909750 -0.401448 -0.025337
C -1.265560 1.009996 0.021709
O 1.046436 1.819186 -0.223010
C 1.853227 -1.211036 0.086691
H 0.392355 0.697977 1.396177
H 0.532985 -0.421578 -1.414114
H -0.616429 -1.798428 1.056947
H -0.869672 -2.270217 -0.616347
H -2.483386 -0.530827 -0.946053
H -2.606620 -0.560531 0.800681
H -1.335203 1.509436 -0.948586
H -1.730398 1.671156 0.756705
H 1.558007 2.220088 0.482650
H 1.881177 -1.391330 1.167601
H 2.687870 -0.553018 -0.170746
H 2.019791 -2.169996 -0.412730

COMP. 15_E4_M06-2X
C 0.372571 -0.839764 0.314073
C -0.844407 -0.243066 -0.427811
C -0.502604 1.260786 -0.619293
C 0.926453 1.440962 -0.077755
C 1.020634 0.360066 1.002861
O 1.301323 -1.373991 -0.634086
C -2.142180 -0.442676 0.353394
H 0.068761 -1.619661 1.019611
H -0.920960 -0.748646 -1.392558
H -1.198798 1.867882 -0.031209
H -0.597999 1.577645 -1.658658
H 1.659084 1.227451 -0.859395
H 1.113850 2.447568 0.298712
H 2.037270 0.138943 1.330298
H 0.425324 0.647628 1.876790
H 1.446254 -2.302289 -0.450769
H -2.057562 -0.015854 1.358069
H -2.391855 -1.501901 0.454740
H -2.976752 0.055319 -0.145756

COMP. 16_1T2A_B3LYP
C -0.493922 -0.476331 0.398402
C 0.762517 0.384014 0.638121
C 1.876131 -0.669669 0.625888
C 1.423452 -1.754645 -0.396280
C -0.058640 -1.437766 -0.722511
O -1.631484 0.322511 0.124807
O 1.016828 1.294175 -0.426324
C -2.850849 -0.396765 0.088086
C 0.375706 2.558827 -0.316484
H -0.677223 -1.050303 1.323439
H 0.703803 0.934440 1.586094
H 2.827367 -0.205320 0.364349
H 1.981831 -1.100195 1.625725
H 2.033585 -1.727491 -1.300414
H 1.531991 -2.755306 0.028948
H -0.141758 -0.908010 -1.674712
H -0.676773 -2.336065 -0.778137
H -0.710176 2.472990 -0.395936
H 0.630736 3.042763 0.636956
H 0.758654 3.170849 -1.134465
H -3.649466 0.335158 -0.037588
H -2.885294 -1.105349 -0.748495
H -3.016400 -0.947638 1.025036

COMP. 16_1T2A_M06-2X
C -0.509221 -0.453555 0.453291
C 0.772517 0.359688 0.663297
C 1.831902 -0.736083 0.652360
C 1.383641 -1.686893 -0.483891
C -0.131043 -1.423390 -0.678616
O -1.610135 0.380670 0.184690
O 1.035430 1.210740 -0.433377
C -2.817179 -0.328440 0.034230
C 0.453358 2.495900 -0.338597
H -0.703961 -1.018420 1.380227
H 0.748484 0.939456 1.594322
H 2.824446 -0.315314 0.494730
H 1.827959 -1.252702 1.615735
H 1.924909 -1.459087 -1.401967
H 1.589988 -2.728381 -0.234507
H -0.316144 -0.916040 -1.628243
H -0.722050 -2.340095 -0.659452
H -0.636607 2.445208 -0.336997
H 0.794631 3.005609 0.571435

H 0.796066 3.059021 -1.206217
H -3.614041 0.406178 -0.073998
H -2.799705 -0.969606 -0.853981
H -3.020175 -0.950464 0.915972

COMP. 16_1T2A_MP2
C -0.508189 -0.464279 0.436198
C 0.762886 0.352655 0.675077
C 1.827347 -0.736215 0.670751
C 1.401749 -1.677418 -0.481741
C -0.109400 -1.413116 -0.703080
O -1.619117 0.381253 0.164963
O 1.053887 1.214519 -0.424421
C -2.839984 -0.344484 0.048643
C 0.443124 2.505890 -0.337751
H -0.717889 -1.040223 1.357789
H 0.721657 0.932485 1.610115
H 2.823544 -0.306091 0.533666
H 1.815494 -1.262460 1.633639
H 1.964206 -1.445916 -1.390534
H 1.602366 -2.725514 -0.235973
H -0.284296 -0.891432 -1.650117
H -0.699406 -2.335594 -0.709557
H -0.646035 2.440059 -0.388328
H 0.741073 3.007627 0.593476
H 0.826687 3.071891 -1.188598
H -3.631907 0.398308 -0.058111
H -2.835776 -1.000456 -0.830036
H -3.023071 -0.947056 0.949653

COMP. 16_1T2T_MP2
C 0.736703 0.211140 0.426486
C -0.734730 -0.130242 0.624853
C -1.375419 1.252023 0.692109
C -0.623179 2.059183 -0.397193
C 0.693437 1.285122 -0.669578
O 1.479653 -0.959569 0.131191
O -1.196906 -0.807077 -0.547356
C 2.874860 -0.701581 0.012143
C -1.989944 -1.952411 -0.259430
H 1.115426 0.649066 1.369825
H -0.899508 -0.750127 1.516669
H -2.454839 1.198078 0.518532
H -1.217548 1.688345 1.687193
H -1.221613 2.122359 -1.310331
H -0.431365 3.085410 -0.066598
H 0.657288 0.773753 -1.637533
H 1.572168 1.938416 -0.660414
H 3.357990 -1.671848 -0.111876
H 3.094603 -0.073174 -0.859573
H 3.264374 -0.213050 0.917277
H -1.407823 -2.703479 0.289561
H -2.883720 -1.686509 0.322509
H -2.297772 -2.363472 -1.222273

COMP. 16_1T2_B3LYP
C 0.741473 0.200190 0.388099
C -0.744403 -0.123437 0.598430
C -1.373969 1.275121 0.668020
C -0.559580 2.134462 -0.345075
C 0.712471 1.309030 -0.682356
O 1.476239 -0.964050 0.073867
O -1.235442 -0.829178 -0.539826
C 2.878200 -0.775102 0.057286
C -2.030079 -1.959372 -0.240810
H 1.121613 0.619818 1.335675
H -0.902712 -0.716765 1.505162
H -2.439054 1.234960 0.434055
H -1.274821 1.674381 1.682448
H -1.139116 2.332004 -1.248160
H -0.305905 3.105203 0.087172
H 0.618388 0.832702 -1.661152
H 1.617490 1.919783 -0.686515
H 3.329112 -1.753446 -0.112607
H 3.193189 -0.097196 -0.746035
H 3.241308 -0.377235 1.016488
H -1.466428 -2.705973 0.333428
H -2.936434 -1.688496 0.319769
H -2.327684 -2.399272 -1.193622

COMP. 16_1T2_M06-2X
C 0.736262 0.201349 0.436876
C -0.742187 -0.129373 0.620585
C -1.373704 1.259723 0.678500
C -0.601839 2.062866 -0.400868
C 0.711064 1.278393 -0.659456
O 1.471560 -0.957602 0.148679
O -1.195793 -0.807366 -0.536999
C 2.849148 -0.715022 0.000977
C -1.987668 -1.937458 -0.267867
H 1.103433 0.642000 1.379128
H -0.916787 -0.737223 1.514389
H -2.446988 1.213261 0.490755
H -1.222052 1.693258 1.670850
H -1.186566 2.129315 -1.318099
H -0.407239 3.082729 -0.066651
H 0.672881 0.768195 -1.624652
H 1.592490 1.920706 -0.642224
H 3.335804 -1.680641 -0.129715
H 3.057279 -0.090534 -0.875251
H 3.263089 -0.222913 0.891635
H -1.421235 -2.691728 0.290473
H -2.888745 -1.672480 0.300774
H -2.287953 -2.357077 -1.227338

COMP. 16_2T1A_B3LYP
C -0.341531 0.361616 0.565690
C 0.665279 -0.758401 0.214590
C -0.138363 -1.712301 -0.676821
C -1.597572 -1.623635 -0.159192
C -1.617858 -0.445738 0.855067
O -0.471215 1.209386 -0.568571
O 1.852334 -0.368323 -0.437620
C -1.146811 2.424526 -0.313874
C 2.715952 0.434013 0.343881
H -0.023658 0.959211 1.431711
H 0.921067 -1.256305 1.166129
H -0.060944 -1.350655 -1.703970
H 0.266265 -2.725541 -0.649248
H -2.286910 -1.438818 -0.984824
H -1.918081 -2.552378 0.318212
H -2.517300 0.168550 0.779475
H -1.577560 -0.819126 1.883562
H -0.647204 3.000086 0.478895
H -2.194560 2.269917 -0.024018
H -1.122287 3.001614 -1.238904
H 3.631507 0.569716 -0.232766
H 2.964700 -0.054772 1.297426
H 2.281442 1.419524 0.551808

COMP. 16_2T1A_M06-2X
C -0.272093 0.375047 0.580445
C 0.572296 -0.864361 0.244892
C -0.343606 -1.695361 -0.655382
C -1.784472 -1.359467 -0.200620
C -1.637323 -0.252324 0.869227
O -0.288765 1.195870 -0.568300
O 1.790503 -0.620269 -0.402770
C -0.803058 2.483265 -0.334680
C 2.646971 0.234116 0.314405
H 0.121644 0.942244 1.435259
H 0.760170 -1.388269 1.197254
H -0.169080 -1.368412 -1.681375
H -0.110114 -2.758290 -0.594782
H -2.370225 -0.995124 -1.044859
H -2.304929 -2.229299 0.201830
H -2.446677 0.478758 0.845360
H -1.621435 -0.683087 1.874552
H -0.221689 3.003810 0.438069
H -1.854289 2.459432 -0.024875
H -0.725386 3.036153 -1.269886
H 3.602846 0.245138 -0.207595

H 2.803780 -0.128092 1.339610
H 2.249187 1.254748 0.350269

COMP. 16_2T1A_MP2
C -0.292394 0.361597 0.586321
C 0.614095 -0.826920 0.240731
C -0.259207 -1.699043 -0.661323
C -1.713503 -1.440368 -0.198931
C -1.615970 -0.341885 0.883971
O -0.361974 1.182178 -0.577223
O 1.824273 -0.520749 -0.426639
C -0.963269 2.447850 -0.328818
C 2.668992 0.342049 0.326375
H 0.075071 0.957708 1.437759
H 0.844894 -1.346811 1.190259
H -0.100143 -1.362963 -1.690348
H 0.030585 -2.752824 -0.604316
H -2.323776 -1.094755 -1.038430
H -2.190634 -2.344381 0.193722
H -2.469028 0.344319 0.881034
H -1.564842 -0.783191 1.888357
H -0.415364 2.991220 0.454469
H -2.014763 2.354243 -0.029195
H -0.905616 3.004106 -1.265559
H 3.614705 0.395225 -0.215162
H 2.848545 -0.061068 1.333910
H 2.239523 1.348070 0.404441

COMP. 16_2T1S_B3LYP
C 0.683566 -0.191024 0.614674
C -0.790690 0.157764 0.376865
C -0.727813 1.263795 -0.694634
C 0.542345 2.076340 -0.326630
C 1.335170 1.200411 0.689512
O 1.154349 -0.930831 -0.506031
O -1.548389 -0.988954 0.058874
C 2.346270 -1.649392 -0.264253
C -2.945429 -0.768191 0.037567
H 0.816772 -0.783043 1.529285
H -1.171486 0.590070 1.318592
H -0.617656 0.786238 -1.671014
H -1.626528 1.883352 -0.718006
H 1.137403 2.285595 -1.216994
H 0.286061 3.041967 0.115488
H 2.402600 1.154797 0.466210
H 1.238459 1.596936 1.705117
H 2.214965 -2.374480 0.551107
H 3.189898 -0.990685 -0.014781
H 2.584401 -2.188630 -1.181798
H -3.417396 -1.736892 -0.129997
H -3.243524 -0.086377 -0.769022
H -3.302157 -0.358788 0.994460

COMP. 16_2T1S_M06-2X
C 0.676984 -0.203585 0.640831
C -0.789899 0.154140 0.424944
C -0.728129 1.229653 -0.671126
C 0.586600 1.997191 -0.381697
C 1.326996 1.180368 0.708806
O 1.117152 -0.913622 -0.498312
O -1.550752 -0.984605 0.129571
C 2.324443 -1.603565 -0.296286
C -2.920560 -0.706366 -0.025214
H 0.823813 -0.810591 1.542710
H -1.158850 0.606725 1.361030
H -0.677666 0.719817 -1.635795
H -1.601607 1.882941 -0.670398
H 1.190531 2.065230 -1.286416
H 0.396184 3.016877 -0.044466
H 2.404552 1.136112 0.546368
H 1.163672 1.611184 1.700380
H 2.221209 -2.349535 0.501556
H 3.149531 -0.927114 -0.040656
H 2.564839 -2.112678 -1.228703
H -3.431112 -1.659692 -0.154590
H -3.109238 -0.080009 -0.904593
H -3.325670 -0.200459 0.861956

COMP. 16_2T1S_MP2
C 0.674125 -0.195894 0.640447
C -0.787306 0.166313 0.413474
C -0.713741 1.238824 -0.681783
C 0.599128 2.004136 -0.376522
C 1.328497 1.182906 0.717603
O 1.119712 -0.904641 -0.515108
O -1.548637 -0.989135 0.111167
C 2.317010 -1.636369 -0.282021
C -2.938631 -0.705328 -0.007368
H 0.813241 -0.814940 1.539918
H -1.169216 0.613504 1.351238
H -0.660421 0.728020 -1.649079
H -1.588524 1.897384 -0.690567
H 1.213927 2.079263 -1.277909
H 0.403809 3.026510 -0.036106
H 2.410853 1.133319 0.562236
H 1.163709 1.613654 1.713897
H 2.159626 -2.400743 0.491188
H 3.145694 -0.982728 0.021930
H 2.570259 -2.121101 -1.226042
H -3.439107 -1.666689 -0.131561
H -3.147896 -0.072707 -0.878757
H -3.319044 -0.210068 0.898166

COMP. 16_2T1T_MP2
C 0.540783 -0.268974 0.591721
C -0.806556 0.324654 0.187017
C -0.410954 1.428012 -0.794520
C 0.901091 2.002012 -0.210218
C 1.365976 0.987476 0.871386
O 1.045926 -0.971989 -0.541945
O -1.696724 -0.633139 -0.370494
C 2.072273 -1.895948 -0.202672
C -2.948737 -0.700104 0.303912
H 0.457476 -0.953288 1.450930
H -1.254695 0.767204 1.092543
H -0.244264 0.956493 -1.767669
H -1.199108 2.179586 -0.911845
H 1.656995 2.113235 -0.992896
H 0.747760 2.993686 0.228899
H 2.441238 0.786182 0.831880
H 1.144229 1.357351 1.881196
H 1.688848 -2.668858 0.477633
H 2.933015 -1.399911 0.265814
H 2.390553 -2.360102 -1.137311
H -3.541738 -1.449804 -0.222300
H -3.473679 0.264427 0.271694
H -2.823490 -1.007947 1.351188

COMP. 16_2T1_B3LYP
C 0.559662 -0.265073 0.578657
C -0.811465 0.316192 0.189030
C -0.450926 1.456907 -0.775009
C 0.857106 2.053556 -0.196350
C 1.387640 1.006650 0.831545
O 1.054647 -1.007101 -0.528871
O -1.701171 -0.635932 -0.364691
C 2.103528 -1.896927 -0.208139
C -2.943356 -0.751385 0.302049
H 0.492819 -0.918951 1.458850
H -1.245824 0.737822 1.106972
H -0.282797 1.018703 -1.760723
H -1.254858 2.190575 -0.865471
H 1.585819 2.234179 -0.988217
H 0.678137 3.013943 0.293055
H 2.457507 0.816553 0.727464
H 1.224991 1.352015 1.857560
H 1.783758 -2.635927 0.540180
H 2.993592 -1.376749 0.172394
H 2.370898 -2.418511 -1.127846
H -3.520315 -1.507893 -0.231380
H -3.504713 0.193306 0.289647
H -2.819956 -1.074323 1.345313

COMP. 16_2T1_M06-2X
C 0.536585 -0.279978 0.587600
C -0.812628 0.320471 0.185896
C -0.413835 1.430493 -0.789542
C 0.900141 1.999070 -0.205757
C 1.367427 0.975663 0.867187
O 1.035338 -0.985820 -0.528882
O -1.702130 -0.617282 -0.367522
C 2.081172 -1.869104 -0.213321
C -2.938276 -0.706064 0.297738
H 0.451212 -0.954779 1.449538
H -1.248491 0.764451 1.092605
H -0.242994 0.961944 -1.759927
H -1.197281 2.180826 -0.903398
H 1.650553 2.113397 -0.987816
H 0.750191 2.983040 0.241193
H 2.438126 0.773384 0.819700
H 1.150546 1.340310 1.874915
H 1.746783 -2.635963 0.496787
H 2.947016 -1.348593 0.214514
H 2.385840 -2.353055 -1.140348
H -3.534245 -1.450815 -0.228422
H -3.473204 0.251920 0.282709
H -2.813243 -1.024557 1.340365

COMP. 16_4EA_B3LYP
C -0.143575 0.597553 0.440135
C -0.072875 -0.976629 0.321004
C -1.409537 -1.400393 -0.300355
C -2.392508 -0.295920 0.105396
C -1.558235 0.985398 -0.050055
O 0.906121 1.192241 -0.304386
O 0.985096 -1.483695 -0.461233
C 1.045345 2.582322 -0.079761
C 2.248365 -1.498602 0.183493
H -0.023911 0.879614 1.497423
H 0.010437 -1.385348 1.339717
H -1.281340 -1.413338 -1.387508
H -1.712451 -2.401788 0.011832
H -3.298977 -0.285664 -0.503828
H -2.706097 -0.425053 1.147907
H -1.484813 1.249395 -1.110701
H -1.980221 1.841877 0.480997
H 1.207169 2.800929 0.986117
H 0.168572 3.146325 -0.422920
H 1.917090 2.910899 -0.646787
H 2.205899 -2.079162 1.116761
H 2.602540 -0.486325 0.399032
H 2.944496 -1.983101 -0.502221

COMP. 16_4EA_M06-2X
C -0.153014 0.583559 0.444983
C -0.048329 -0.979888 0.337778
C -1.386171 -1.434986 -0.250352
C -2.366664 -0.317670 0.108410
C -1.532376 0.942824 -0.132955
O 0.924511 1.190417 -0.226497
O 0.993104 -1.443002 -0.478382
C 0.943566 2.589091 -0.076373
C 2.257539 -1.436285 0.147343
H -0.115880 0.871646 1.507005
H 0.080122 -1.389212 1.350210
H -1.260021 -1.485979 -1.335853
H -1.682048 -2.422634 0.104072
H -3.281262 -0.343484 -0.484878
H -2.654775 -0.384260 1.162990
H -1.413217 1.104565 -1.209931
H -1.965364 1.843508 0.305662
H 0.965382 2.872800 0.984512
H 0.072499 3.059025 -0.547371
H 1.847154 2.954120 -0.562914
H 2.251843 -2.081853 1.035633
H 2.556560 -0.424461 0.431040
H 2.970780 -1.832974 -0.574150

COMP. 16_4EA_MP2
C -0.162214 0.581965 0.447045
C -0.046912 -0.978082 0.333335
C -1.369366 -1.439515 -0.278014
C -2.367650 -0.349950 0.113501
C -1.556667 0.931451 -0.098112
O 0.905636 1.195612 -0.264660
O 1.014267 -1.446543 -0.479704
C 0.928632 2.607234 -0.078314
C 2.283861 -1.411958 0.172522
H -0.090111 0.876622 1.509484
H 0.070611 -1.397010 1.347688
H -1.238621 -1.459475 -1.367286
H -1.647360 -2.447066 0.047072
H -3.287060 -0.374814 -0.480728
H -2.657865 -0.451381 1.168148
H -1.456456 1.132567 -1.173241
H -1.999762 1.814565 0.374982
H 0.989726 2.860932 0.990139
H 0.042463 3.088072 -0.510812
H 1.820376 2.970799 -0.591067
H 2.261232 -2.021488 1.087525
H 2.579166 -0.386712 0.412755
H 2.996342 -1.845037 -0.531521

COMP. 16_4ES_B3LYP
C 0.786036 0.021319 0.428359
C -0.786037 0.021319 0.428357
C -1.202034 1.366398 -0.209321
C 0.000000 2.291352 0.026502
C 1.202034 1.366398 -0.209319
O 1.292860 -1.116134 -0.236891
H 1.124280 -0.006841 1.475764
O -1.292860 -1.116134 -0.236893
H -1.124282 -0.006841 1.475763
H -1.339542 1.202194 -1.283756
H -2.136752 1.762580 0.193870
H 0.000000 3.164492 -0.629857
H -0.000001 2.663696 1.057603
H 1.339544 1.202194 -1.283754
H 2.136751 1.762580 0.193873
C 2.675134 -1.324953 -0.027546
H 2.909613 -1.403319 1.044462
H 3.288675 -0.524169 -0.461875
H 2.930673 -2.266104 -0.515643
C -2.675134 -1.324953 -0.027550
H -3.288674 -0.524169 -0.461879
H -2.909614 -1.403319 1.044458
H -2.930672 -2.266104 -0.515647

COMP. 16_4ES_M06-2X
C -0.455149 0.001593 0.780869
C -0.455149 0.001593 -0.780869
C 0.200271 1.332015 -1.194011
C -0.052923 2.254465 0.000000
C 0.200271 1.332015 1.194011
O 0.200271 -1.134633 1.276849
H -1.499652 -0.012947 1.127994
O 0.200271 -1.134633 -1.276849
H -1.499652 -0.012947 -1.127994
H 1.275896 1.155337 -1.302862
H -0.181157 1.726473 -2.137209
H 0.584448 3.139393 0.000000
H -1.093106 2.597297 0.000000
H 1.275896 1.155337 1.302862
H -0.181157 1.726473 2.137209
C 0.091006 -1.254062 2.672901
H -0.961465 -1.267394 2.987643
H 0.602329 -0.436052 3.194921
H 0.558221 -2.197363 2.952464
C 0.091006 -1.254062 -2.672901
H 0.602329 -0.436052 -3.194921
H -0.961465 -1.267394 -2.987643
H 0.558221 -2.197363 -2.952464

COMP. 16_4ES_MP2

C 0.780241 0.017768 0.448652
C -0.780241 0.017768 0.448652
C -1.193740 1.338853 -0.220537
C 0.000000 2.264125 0.023484
C 1.193740 1.338853 -0.220537
O 1.273633 -1.139949 -0.204769
H 1.132533 0.005862 1.495477
O -1.273633 -1.139949 -0.204769
H -1.132534 0.005862 1.495477
H -1.306857 1.150625 -1.296666
H -2.141016 1.737668 0.157978
H 0.000000 3.144807 -0.627356
H 0.000000 2.625544 1.060885
H 1.306857 1.150625 -1.296665
H 2.141016 1.737668 0.157979
C 2.682565 -1.270705 -0.052950
H 2.963299 -1.277439 1.010571
H 3.226249 -0.464088 -0.561646
H 2.951400 -2.226085 -0.505772
C -2.682565 -1.270704 -0.052950
H -3.226249 -0.464088 -0.561646
H -2.963299 -1.277438 1.010571
H -2.951400 -2.226085 -0.505772

COMP. 16_E4A_B3LYP
C -0.344941 -0.525866 0.578569
C 0.744292 0.619586 0.522743
C 2.052691 -0.088671 0.124322
C 1.610076 -1.350150 -0.628540
C 0.407813 -1.823408 0.199690
O -1.395278 -0.222486 -0.330746
O 0.479881 1.624622 -0.437724
C -0.457956 2.607078 -0.032424
C -2.582643 -0.954375 -0.097305
H -0.767501 -0.594498 1.590815
H 0.830171 1.090961 1.511908
H 2.682855 0.585438 -0.457310
H 2.605631 -0.372643 1.026683
H 1.291036 -1.089999 -1.641984
H 2.398089 -2.102989 -0.707200
H -0.241202 -2.526723 -0.326857
H 0.759088 -2.323309 1.110000
H -0.138317 3.090505 0.902728
H -1.457678 2.183706 0.099185
H -0.488082 3.356570 -0.824429
H -2.973763 -0.769223 0.913867
H -2.438228 -2.035594 -0.221300
H -3.314915 -0.614452 -0.830677

COMP. 16_E4A_M06-2X
C -0.364721 -0.509589 0.583306
C 0.766266 0.582989 0.542979
C 2.040101 -0.182093 0.167471
C 1.531221 -1.364317 -0.658436
C 0.325702 -1.823428 0.164895
O -1.389710 -0.149800 -0.319678
O 0.550522 1.564167 -0.440520
C -0.348729 2.577394 -0.051766
C -2.598187 -0.828482 -0.082599
H -0.790561 -0.582111 1.593037
H 0.857078 1.071097 1.522441
H 2.732226 0.476159 -0.357188
H 2.530834 -0.552073 1.073358
H 1.200040 -1.012774 -1.639176
H 2.277344 -2.146764 -0.803620
H -0.357945 -2.477650 -0.378739
H 0.670683 -2.362733 1.053055
H 0.025766 3.104795 0.835903
H -1.343179 2.174211 0.154265
H -0.412611 3.281025 -0.881042
H -2.987470 -0.602146 0.918912
H -2.486003 -1.915226 -0.174626
H -3.312620 -0.485593 -0.830099

COMP. 16_E4A_MP2
C -0.331656 -0.531349 0.587203
C 0.737025 0.618406 0.544615
C 2.047000 -0.073294 0.154728
C 1.599987 -1.289499 -0.656962
C 0.427860 -1.806644 0.179013
O -1.374907 -0.223229 -0.336569
O 0.470875 1.602105 -0.445321
C -0.498691 2.566267 -0.039585
C -2.559567 -0.970418 -0.083214
H -0.766835 -0.616407 1.596872
H 0.806149 1.112875 1.527662
H 2.695831 0.625642 -0.381208
H 2.575583 -0.409034 1.057543
H 1.249731 -0.973901 -1.646457
H 2.391650 -2.034159 -0.794597
H -0.224133 -2.509921 -0.349708
H 0.811020 -2.318340 1.073222
H -0.163304 3.085778 0.870046
H -1.474927 2.104293 0.132355
H -0.571357 3.283840 -0.858702
H -2.952702 -0.750341 0.919869
H -2.390951 -2.051515 -0.169745
H -3.285248 -0.660627 -0.836822

COMP. 16_E4S_B3LYP
C 0.786924 0.008029 0.563903
C -0.786924 0.008028 0.563903
C -1.195917 1.444423 0.155441
C -0.000001 1.975125 -0.645801
C 1.195917 1.444423 0.155440
O 1.274178 -0.971301 -0.335907
O -1.274178 -0.971300 -0.335908
C -2.615385 -1.344649 -0.097401
C 2.615386 -1.344648 -0.097400
H 1.148776 -0.232085 1.573450
H -1.148776 -0.232086 1.573450
H -2.136009 1.448645 -0.400154
H -1.342752 2.057953 1.052150
H -0.000001 1.541560 -1.650214
H -0.000001 3.062896 -0.749319
H 2.136008 1.448645 -0.400157
H 1.342753 2.057953 1.052149
H -3.316048 -0.509136 -0.233627
H -2.743471 -1.743780 0.919488
H -2.859377 -2.125620 -0.818530
H 2.743472 -1.743779 0.919488
H 3.316048 -0.509134 -0.233626
H 2.859378 -2.125618 -0.818530

COMP. 16_E4S_M06-2X
C 0.782833 0.004022 0.578229
C -0.782833 0.004022 0.578229
C -1.187077 1.432020 0.160975
C 0.000000 1.918285 -0.671755
C 1.187077 1.432020 0.160975
O 1.257764 -0.959581 -0.330674
O -1.257764 -0.959581 -0.330674
C -2.597792 -1.314935 -0.104551
C 2.597792 -1.314935 -0.104551
H 1.153338 -0.240920 1.582585
H -1.153338 -0.240920 1.582585
H -2.136639 1.435795 -0.376314
H -1.299627 2.064867 1.047465
H 0.000000 1.414081 -1.641980
H 0.000000 2.996051 -0.840502
H 2.136639 1.435795 -0.376314
H 1.299627 2.064867 1.047465
H -3.278625 -0.460997 -0.209539
H -2.727761 -1.742665 0.898316
H -2.860293 -2.065990 -0.848535
H 2.727761 -1.742665 0.898316
H 3.278625 -0.460997 -0.209539
H 2.860293 -2.065990 -0.848535

COMP. 16_E4S_MP2
C 0.781853 0.011835 0.578591
C -0.781853 0.011834 0.578591

C -1.186422 1.437076 0.160437
C 0.000000 1.925845 -0.671183
C 1.186421 1.437076 0.160437
O 1.254505 -0.962484 -0.343763
O -1.254505 -0.962484 -0.343763
C -2.606576 -1.326248 -0.094306
C 2.606576 -1.326248 -0.094306
H 1.155106 -0.242511 1.584286
H -1.155106 -0.242511 1.584286
H -2.141430 1.440443 -0.374863
H -1.301173 2.074588 1.048633
H 0.000000 1.434293 -1.651082
H 0.000000 3.009732 -0.830792
H 2.141430 1.440443 -0.374864
H 1.301173 2.074588 1.048633
H -3.292693 -0.475273 -0.201377
H -2.715931 -1.747535 0.915300
H -2.860156 -2.085363 -0.835718
H 2.715931 -1.747535 0.915300
H 3.292693 -0.475273 -0.201377
H 2.860156 -2.085363 -0.835718

COMP. 17_1T2A_B3LYPT
C 0.466197 -0.218634 0.410584
C -0.850230 0.295833 -0.276280
C -0.750131 1.823399 -0.219901
C 0.763810 2.005891 -0.383415
C 1.240221 1.073089 0.742872
O 1.129633 -1.037309 -0.558497
O -2.063123 -0.156699 0.293205
C 2.257965 -1.733702 -0.064332
C -2.345590 -1.518625 0.020865
H 0.259649 -0.819343 1.305622
H -0.775115 -0.037067 -1.321232
H -1.398005 2.339091 -0.929962
H -1.039298 2.139332 0.788657
H 1.063503 1.558264 -1.339918
H 1.143804 3.028318 -0.368921
H 2.316244 0.961339 0.888562
H 0.828515 1.448474 1.687710
H 2.587186 -2.405783 -0.857512
H 3.085304 -1.060672 0.193449
H 2.001182 -2.328170 0.824394
H -2.580644 -1.669220 -1.041642
H -1.506083 -2.173460 0.286860
H -3.211768 -1.792544 0.623911

COMP. 17_1T2A_M06-2X
C 0.472137 -0.279792 -0.245508
C -0.867660 0.254814 0.260557
C -1.850549 -0.864535 -0.078203
C -1.035219 -2.178775 -0.013118
C 0.439110 -1.753332 0.173077
O 1.538441 0.459703 0.308040
O -1.304787 1.451267 -0.333161
C 2.801169 0.064226 -0.174070
C -0.628838 2.610622 0.110711
H 0.487258 -0.184963 -1.343826
H -0.775374 0.390429 1.350124
H -2.713440 -0.858393 0.587195
H -2.217810 -0.677341 -1.089948
H -1.360617 -2.820168 0.806334
H -1.161671 -2.752973 -0.931914
H 0.729815 -1.802610 1.227459
H 1.131186 -2.378940 -0.391971
H 3.535996 0.756191 0.235353
H 3.054960 -0.952964 0.145030
H 2.836405 0.110282 -1.270188
H -0.657723 2.682698 1.204827
H 0.415328 2.618573 -0.209865
H -1.154450 3.463046 -0.318326

COMP. 17_1T2A_MP2
C 0.409711 -0.339772 0.366667
C -0.824429 0.189405 -0.423794
C -0.633856 1.713661 -0.500993
C 0.852272 1.867528 -0.168563
C 0.898602 0.932592 1.041798
O 1.314443 -0.841737 -0.633827
O -2.069257 -0.068951 0.230469
C 2.432760 -1.529278 -0.081036
C -2.479871 -1.426332 0.098277
H 0.190358 -1.163725 1.061677
H -0.826574 -0.284410 -1.417090
H -0.959105 2.145088 -1.452723
H -1.252174 2.151526 0.292743
H 1.464756 1.450876 -0.978044
H 1.197859 2.892956 -0.003006
H 1.811452 0.875155 1.643922
H 0.103564 1.237142 1.739862
H 3.054836 -1.831012 -0.924974
H 3.019910 -0.889608 0.587975
H 2.105327 -2.422530 0.469815
H -2.643246 -1.682282 -0.957300
H -1.742375 -2.120863 0.521519
H -3.417219 -1.519632 0.648345

COMP. 17_1T2S_M06-2X
C 0.000000 0.759755 -0.041213
C 0.000000 -0.759755 -0.041213
C 0.519540 -1.123443 1.355546
C 0.000000 0.000000 2.285813
C -0.519540 1.123443 1.355546
O -0.791950 1.237576 -1.099070
O 0.791950 -1.237576 -1.099070
C -0.694067 2.629095 -1.280272
C 0.694067 -2.629095 -1.280272
H 1.040719 1.096112 -0.174172
H -1.040719 -1.096112 -0.174172
H 0.204765 -2.115069 1.682348
H 1.612715 -1.119888 1.311290
H -0.798024 -0.358869 2.936573
H 0.798024 0.358869 2.936573
H -1.612715 1.119888 1.311290
H -0.204765 2.115069 1.682348
H -1.283416 2.883275 -2.160181
H -1.088049 3.179596 -0.417345
H 0.347510 2.931707 -1.447758
H 1.088049 -3.179596 -0.417345
H -0.347510 -2.931707 -1.447758
H 1.283416 -2.883275 -2.160181

COMP. 17_1T2S_MP2
C 0.724224 -0.022198 0.226316
C -0.724224 -0.022198 -0.226316
C -1.225988 1.371666 0.165962
C 0.000000 2.303195 0.000001
C 1.225988 1.371666 -0.165963
O 1.412926 -1.094907 -0.400396
O -1.412926 -1.094906 0.400396
C 2.704504 -1.315967 0.156810
C -2.704504 -1.315967 -0.156809
H 0.739808 -0.163738 1.321710
H -0.739808 -0.163738 -1.321710
H -2.086060 1.701009 -0.425604
H -1.547599 1.321468 1.213792
H -0.109722 2.957818 -0.870417
H 0.109722 2.957816 0.870420
H 1.547597 1.321468 -1.213793
H 2.086061 1.701009 0.425602
H 3.110991 -2.194751 -0.345747
H 3.371556 -0.460895 -0.012978
H 2.634472 -1.512247 1.235679
H -3.371556 -0.460895 0.012978
H -2.634472 -1.512248 -1.235678
H -3.110992 -2.194751 0.345748

COMP. 17_1TS_B3LYPT
C -0.731775 -0.011201 -0.218794
C 0.731774 -0.011199 0.218799
C 1.232860 1.398071 -0.150056
C 0.000000 2.330578 -0.000032

C -1.232855 1.398075 0.150043
O -1.425525 -1.067956 0.420624
O 1.425522 -1.067965 -0.420605
C -2.678428 -1.376286 -0.160111
C 2.678426 -1.376285 0.160132
H -0.756767 -0.163922 -1.308945
H 0.756765 -0.163907 1.308951
H 2.076959 1.720223 0.462663
H 1.575727 1.369943 -1.188824
H 0.095346 2.984051 0.869646
H -0.095350 2.984000 -0.869748
H -1.575696 1.369968 1.188820
H -2.076970 1.720214 -0.462662
H -3.074083 -2.239646 0.375921
H -3.392482 -0.546821 -0.069120
H -2.571301 -1.635401 -1.222622
H 3.392481 -0.546822 0.069126
H 2.571302 -1.635383 1.222648
H 3.074080 -2.239654 -0.375887

COMP. 17_2EA_B3LYP
C 0.519180 -0.334973 0.271360
C -0.728936 -0.096618 -0.603250
C -0.609982 1.375526 -0.990252
C -0.100217 2.071438 0.290120
C 0.687953 0.979833 1.069790
O -1.924136 -0.259944 0.161299
O 1.601631 -0.581160 -0.628274
C 2.758795 -1.115970 -0.016008
C -2.360558 -1.600705 0.286630
H 0.394848 -1.206363 0.927202
H -0.737341 -0.772912 -1.466203
H 0.126866 1.459942 -1.793244
H -1.560601 1.771463 -1.352122
H -0.943479 2.423373 0.887502
H 0.518307 2.941383 0.060009
H 1.747375 1.227123 1.166965
H 0.293319 0.861441 2.081370
H 2.538960 -2.070244 0.483756
H 3.196264 -0.429177 0.720336
H 3.487916 -1.289519 -0.808248
H -1.638077 -2.228764 0.824367
H -2.548679 -2.050212 -0.698110
H -3.293045 -1.579891 0.851879

COMP. 17_2EA_MP2
C -0.547953 -0.254497 -0.252847
C 0.726684 -0.107938 0.592681
C 0.755682 1.365252 0.963984
C 0.340001 2.049306 -0.341784
C -0.777312 1.137493 -0.890719
O 1.884644 -0.361419 -0.213447
O -1.596321 -0.626621 0.650294
C -2.782818 -1.025843 -0.027772
C 2.192247 -1.748779 -0.314883
H -0.430986 -1.046695 -1.008555
H 0.707047 -0.788568 1.456178
H 0.011154 1.546042 1.749727
H 1.739875 1.669233 1.334105
H 1.190658 2.071249 -1.030137
H 0.000517 3.080809 -0.198189
H -1.759598 1.504761 -0.571754
H -0.779831 1.097735 -1.985399
H -2.582699 -1.883475 -0.685473
H -3.206231 -0.208643 -0.625369
H -3.497815 -1.316197 0.743322
H 1.372210 -2.319025 -0.770148
H 2.413374 -2.170606 0.674634
H 3.076558 -1.822256 -0.949672

COMP. 17_2T1A_B3LYP
C 0.486369 -0.205280 0.347561
C -0.841471 0.241546 -0.332941
C -0.838373 1.776504 -0.314462
C 0.646254 2.156616 -0.228854
C 1.209101 1.101645 0.738133
O 1.214908 -0.982297 -0.607635
O -2.012724 -0.232200 0.318315
C 2.284740 -1.727469 -0.058307
C -2.293844 -1.599979 0.079404
H 0.270778 -0.829328 1.224857
H -0.815942 -0.139145 -1.362950
H -1.356514 2.201011 -1.176513
H -1.367454 2.104413 0.586434
H 1.123702 2.058747 -1.209272
H 0.806055 3.181640 0.113436
H 2.296172 1.003866 0.699386
H 0.942164 1.365888 1.767220
H 1.929425 -2.418142 0.719938
H 3.062724 -1.085547 0.374669
H 2.722396 -2.305128 -0.873307
H -2.418060 -1.798260 -0.993848
H -3.226099 -1.827812 0.597383
H -1.503482 -2.257731 0.463917

COMP. 17_2T1S_B3LYP
C 0.665127 -0.391534 0.381436
C -0.665132 -0.391528 -0.381439
C -0.712717 1.009198 -1.014585
C 0.000011 1.944867 0.000002
C 0.712723 1.009187 1.014589
O 1.688612 -0.589804 -0.595807
O -1.688617 -0.589798 0.595804
C 2.953771 -0.916140 -0.054075
C -2.953777 -0.916135 0.054075
H 0.694716 -1.200204 1.121533
H -0.694726 -1.200193 -1.121541
H -0.166573 0.981343 -1.960386
H -1.734709 1.322966 -1.237624
H 0.712423 2.594808 -0.511817
H -0.712388 2.594822 0.511821
H 1.734717 1.322945 1.237637
H 0.166572 0.981330 1.960386
H 2.903677 -1.834552 0.547531
H 3.360518 -0.110530 0.570772
H 3.627779 -1.079169 -0.895822
H -3.627784 -1.079163 0.895824
H -2.903684 -1.834547 -0.547530
H -3.360527 -0.110525 -0.570772

COMP. 17_2T1S_M06-2X
C -0.660327 -0.422508 -0.382194
C 0.660309 -0.422532 0.382194
C 0.670371 0.961467 1.038444
C 0.000056 1.895035 -0.000002
C -0.670366 0.961506 -1.038417
O -1.680121 -0.561858 0.591824
O 1.680098 -0.561880 -0.591830
C -2.944204 -0.851995 0.047482
C 2.944185 -0.852019 -0.047497
H -0.705729 -1.248272 -1.102126
H 0.705695 -1.248313 1.102108
H 0.075787 0.914094 1.952215
H 1.677390 1.280966 1.310530
H -0.732688 2.541686 0.483590
H 0.732884 2.541573 -0.483620
H -1.677392 1.281049 -1.310426
H -0.075849 0.914129 -1.952231
H -2.918822 -1.786332 -0.527220
H -3.305957 -0.048794 -0.604394
H -3.636025 -0.965202 0.881152
H 3.635994 -0.965246 -0.881174
H 2.918801 -1.786346 0.527219
H 3.305953 -0.048811 0.604361

COMP. 17_2T1S_MP2
C 0.656439 -0.413605 0.386193
C -0.656440 -0.413604 -0.386193
C -0.667129 0.967732 -1.041210
C 0.000003 1.899623 0.000000
C 0.667130 0.967729 1.041211
O 1.685030 -0.546501 -0.602696

O -1.685031 -0.546500 0.602696
C 2.950888 -0.877420 -0.040586
C -2.950889 -0.877418 0.040585
H 0.708410 -1.247809 1.101480
H -0.708412 -1.247807 -1.101481
H -0.075543 0.924413 -1.961963
H -1.679028 1.286932 -1.312191
H 0.737343 2.549264 -0.481558
H -0.737332 2.549271 0.481556
H 1.679028 1.286927 1.312196
H 0.075540 0.924411 1.961962
H 2.897669 -1.831058 0.502012
H 3.311594 -0.096806 0.640601
H 3.644026 -0.972049 -0.877730
H -3.644028 -0.972046 0.877728
H -2.897670 -1.831057 -0.502011
H -3.311594 -0.096805 -0.640603

COMP. 17_2T1TS_MP2
C 0.563801 -0.399846 0.347758
C -0.727039 -0.183392 -0.457240
C -0.570294 1.239336 -1.010196
C 0.211438 2.020987 0.081409
C 0.754879 0.947494 1.065054
O 1.595172 -0.672122 -0.603462
O -1.833843 -0.245482 0.451378
C 2.792741 -1.170120 -0.038963
C -2.824295 -1.198238 0.114543
H 0.465911 -1.245176 1.040723
H -0.832228 -0.938832 -1.241163
H 0.008398 1.195417 -1.935773
H -1.543659 1.677428 -1.239015
H 1.022327 2.600026 -0.364828
H -0.435414 2.727615 0.604729
H 1.795237 1.117012 1.350556
H 0.162532 0.937063 1.983118
H 2.613269 -2.101729 0.516150
H 3.268018 -0.446955 0.636192
H 3.473470 -1.375294 -0.865989
H -3.596254 -1.140973 0.883214
H -2.419008 -2.219228 0.095864
H -3.280614 -0.982867 -0.861287

COMP. 17_2T1_B3LYP
C 0.563801 -0.399846 0.347758
C -0.727039 -0.183392 -0.457240
C -0.570294 1.239336 -1.010196
C 0.211438 2.020987 0.081409
C 0.754879 0.947494 1.065054
O 1.595172 -0.672122 -0.603462
O -1.833843 -0.245482 0.451378
C 2.792741 -1.170120 -0.038963
C -2.824295 -1.198238 0.114543
H 0.465911 -1.245176 1.040723
H -0.832228 -0.938832 -1.241163
H 0.008398 1.195417 -1.935773
H -1.543659 1.677428 -1.239015
H 1.022327 2.600026 -0.364828
H -0.435414 2.727615 0.604729
H 1.795237 1.117012 1.350556
H 0.162532 0.937063 1.983118
H 2.613269 -2.101729 0.516150
H 3.268018 -0.446955 0.636192
H 3.473470 -1.375294 -0.865989
H -3.596254 -1.140973 0.883214
H -2.419008 -2.219228 0.095864
H -3.280614 -0.982867 -0.861287

COMP. 17_2T3A_B3LYPT
C 0.455871 -0.257202 0.359694
C -0.839650 0.208614 -0.368934
C -0.773234 1.745112 -0.425879
C 0.703513 2.092556 -0.182039
C 1.129533 1.037663 0.851005
O -2.036890 -0.175219 0.298150
O 1.247908 -0.953553 -0.606649
C 2.371980 -1.657611 -0.093310
C -2.395643 -1.531923 0.106144
H 0.208864 -0.934333 1.186802
H -0.823489 -0.231633 -1.374005
H -1.170763 2.141985 -1.361940
H -1.392937 2.133327 0.388625
H 0.847268 3.118305 0.165213
H 1.284747 1.970018 -1.101270
H 2.211463 0.931273 0.959949
H 0.723912 1.299253 1.834947
H 2.492725 -1.510819 0.984812
H 3.282405 -1.313097 -0.593178
H 2.249260 -2.728652 -0.287008
H -1.641325 -2.220983 0.508240
H -2.538964 -1.757404 -0.959403
H -3.335526 -1.690320 0.636125

COMP. 17_3ETS_B3LYP
C 0.651055 -0.110277 0.339085
C -0.786127 0.179151 -0.137302
C -0.965791 1.691575 0.035877
C 0.409538 2.247628 -0.357947
C 1.403531 1.247640 0.277476
O 1.201737 -1.124288 -0.499281
O -1.747107 -0.583855 0.583211
C 2.359154 -1.742846 0.030180
C -2.584269 -1.405899 -0.211913
H 0.602214 -0.490628 1.367576
H -0.826754 -0.080139 -1.202576
H -1.791178 2.087953 -0.559959
H -1.183980 1.900460 1.089046
H 0.514606 2.242370 -1.448035
H 0.570328 3.275055 -0.024135
H 2.331420 1.159174 -0.291827
H 1.671305 1.573882 1.286600
H 2.150004 -2.210620 1.002370
H 3.187625 -1.032577 0.154247
H 2.662679 -2.514340 -0.678456
H -3.183555 -0.814452 -0.917615
H -3.259540 -1.923129 0.471104
H -2.004756 -2.149703 -0.772512

COMP. 17_3ETS_MP2
C 0.648438 -0.103208 0.340358
C -0.780227 0.183546 -0.125198
C -0.959836 1.684937 0.071543
C 0.398337 2.232557 -0.373402
C 1.403099 1.243079 0.250604
O 1.180287 -1.127167 -0.505489
O -1.728069 -0.599238 0.599358
C 2.346652 -1.732005 0.043730
C -2.567732 -1.392537 -0.236579
H 0.605422 -0.482645 1.373310
H -0.830251 -0.064669 -1.196682
H -1.810877 2.085609 -0.489555
H -1.134815 1.881784 1.137617
H 0.468732 2.205220 -1.468232
H 0.574000 3.267667 -0.062341
H 2.320660 1.140755 -0.338594
H 1.692559 1.584473 1.251826
H 2.122519 -2.194558 1.014642
H 3.158295 -1.003765 0.171695
H 2.661249 -2.500640 -0.663758
H -3.162052 -0.764640 -0.913856
H -3.238953 -1.935912 0.430528
H -1.976621 -2.105652 -0.823887

COMP. 17_3T4A_M06-2X
C 0.506459 -0.083079 0.326733
C -0.884079 0.196522 -0.285214
C -1.113156 1.693423 -0.117876
C 0.294068 2.269877 -0.284065
C 1.153638 1.302013 0.543703
O 1.227320 -0.901377 -0.579340
O -1.928639 -0.534713 0.311043
C 2.352305 -1.514468 0.001046

C -1.860323 -1.913943 0.028877
H 0.382653 -0.621674 1.276634
H -0.814458 -0.059552 -1.353357
H -1.845184 2.082004 -0.826163
H -1.485656 1.875910 0.895341
H 0.591337 2.226533 -1.336269
H 0.379867 3.306184 0.044484
H 2.206067 1.303102 0.254803
H 1.097694 1.575177 1.600905
H 2.055774 -2.171939 0.829113
H 3.070391 -0.778076 0.380878
H 2.834423 -2.109977 -0.773100
H -1.899043 -2.095233 -1.052200
H -2.718395 -2.383972 0.507429
H -0.938387 -2.361833 0.418663

COMP. 17_4EA_B3LYP
C -0.560945 0.008514 -0.195063
C 0.829027 -0.076376 0.499033
C 1.320784 1.373741 0.633354
C 0.527269 2.164118 -0.420142
C -0.863357 1.514552 -0.356958
O -1.514535 -0.710514 0.579264
O 1.781530 -0.800988 -0.278365
C -2.774954 -0.857669 -0.048339
C 1.573327 -2.201956 -0.282855
H -0.476946 -0.459929 -1.187194
H 0.709252 -0.569077 1.472037
H 1.077488 1.746310 1.633513
H 2.403426 1.426614 0.510197
H 0.503663 3.239046 -0.226128
H 0.969851 2.019409 -1.411114
H -1.397667 1.858621 0.536227
H -1.485122 1.737407 -1.227277
H -2.677549 -1.349905 -1.026814
H -3.280868 0.105828 -0.189719
H -3.385467 -1.482833 0.604113
H 0.615011 -2.478736 -0.740902
H 1.598354 -2.608986 0.737334
H 2.383706 -2.641298 -0.865649

COMP. 17_4EA_B3LYPF
C -0.560945 0.008514 -0.195063
C 0.829027 -0.076376 0.499033
C 1.320784 1.373741 0.633354
C 0.527269 2.164118 -0.420142
C -0.863357 1.514552 -0.356958
O -1.514535 -0.710514 0.579264
O 1.781530 -0.800988 -0.278365
C -2.774954 -0.857669 -0.048339
C 1.573327 -2.201956 -0.282855
H -0.476946 -0.459929 -1.187194
H 0.709252 -0.569077 1.472037
H 1.077488 1.746310 1.633513
H 2.403426 1.426614 0.510197
H 0.503663 3.239046 -0.226128
H 0.969851 2.019409 -1.411114
H -1.397667 1.858621 0.536227
H -1.485122 1.737407 -1.227277
H -2.677549 -1.349905 -1.026814
H -3.280868 0.105828 -0.189719
H -3.385467 -1.482833 0.604113
H 0.615011 -2.478736 -0.740902
H 1.598354 -2.608986 0.737334
H 2.383706 -2.641298 -0.865649

COMP. 17_4EA_M06-2X
C -0.539123 0.038140 -0.181100
C 0.844841 -0.103061 0.495456
C 1.413129 1.317989 0.583448
C 0.606260 2.125603 -0.440670
C -0.802633 1.548083 -0.279529
O -1.498537 -0.689898 0.554361
O 1.730552 -0.897623 -0.270627
C -2.767849 -0.701320 -0.053454
C 1.369514 -2.259306 -0.277541
H -0.462440 -0.380428 -1.197325
H 0.707138 -0.562902 1.482517
H 1.237318 1.719955 1.584785
H 2.487815 1.309798 0.402102
H 0.650777 3.202732 -0.275181
H 0.978254 1.925197 -1.450059
H -1.243820 1.887134 0.664764
H -1.479970 1.816300 -1.092240
H -2.710402 -1.097000 -1.076310
H -3.208640 0.301568 -0.088838
H -3.408290 -1.348606 0.544113
H 0.374811 -2.416458 -0.711442
H 1.366729 -2.666963 0.741061
H 2.109761 -2.786920 -0.877488

COMP. 17_4EA_MP2
C -0.541331 0.039327 -0.185557
C 0.834370 -0.099406 0.502622
C 1.396824 1.321447 0.602439
C 0.611856 2.123528 -0.441721
C -0.800259 1.547593 -0.301747
O -1.509333 -0.683437 0.574627
O 1.744450 -0.881439 -0.277517
C -2.783827 -0.717197 -0.061540
C 1.395732 -2.264226 -0.280130
H -0.472422 -0.401638 -1.195707
H 0.698683 -0.577405 1.485456
H 1.195012 1.726283 1.602277
H 2.480569 1.315157 0.451738
H 0.652824 3.205739 -0.277998
H 1.005377 1.924486 -1.446505
H -1.261931 1.896908 0.632367
H -1.466329 1.810306 -1.130814
H -2.701888 -1.134081 -1.075631
H -3.233386 0.281699 -0.118875
H -3.417084 -1.363480 0.547919
H 0.407913 -2.435684 -0.725762
H 1.394297 -2.664209 0.742850
H 2.157228 -2.771469 -0.874386

COMP. 17_4ES_B3LYP
C -0.731011 -0.096444 -0.229942
C 0.694384 -0.181374 0.362936
C 1.134549 1.277913 0.618037
C 0.238221 2.121351 -0.304269
C -1.114619 1.398901 -0.218247
O -1.596361 -0.937808 0.522951
O 1.517753 -0.852658 -0.593538
C -2.861886 -1.143426 -0.076654
C 2.730288 -1.350942 -0.061772
H -0.675189 -0.467082 -1.262677
H 0.663592 -0.772010 1.285967
H 0.937207 1.539179 1.663366
H 2.202553 1.422091 0.441730
H 0.182203 3.171840 -0.009182
H 0.619737 2.088967 -1.330178
H -1.602920 1.627076 0.736217
H -1.802268 1.671513 -1.021941
H -2.759083 -1.562981 -1.087336
H -3.445749 -0.215750 -0.138460
H -3.399779 -1.855337 0.550402
H 2.542428 -2.063187 0.753708
H 3.380563 -0.550353 0.315547
H 3.246019 -1.866118 -0.873009

COMP. 17_4ES_M06-2X
C -0.667601 -0.412919 -0.381919
C 0.652993 -0.432014 0.382318
C 0.673225 0.946088 1.048763
C 0.045964 1.894345 -0.001373
C -0.668632 0.977536 -1.026780
O -1.689570 -0.553786 0.589702
O 1.670328 -0.571412 -0.594145
C -2.952288 -0.841722 0.041121
C 2.936256 -0.861314 -0.053914
H -0.719118 -1.231440 -1.109628

H 0.691747 -1.264352 1.095063
H 0.052579 0.901454 1.945352
H 1.677149 1.247991 1.350671
H -0.651718 2.586056 0.471480
H 0.810820 2.493655 -0.496227
H -1.678336 1.314601 -1.265825
H -0.102938 0.929627 -1.958529
H -2.927771 -1.778682 -0.529315
H -3.307914 -0.040150 -0.616233
H -3.648380 -0.948475 0.872077
H 2.910750 -1.790688 0.528793
H 3.304471 -0.053864 0.588914
H 3.623095 -0.984149 -0.890343

COMP. 17_4ES_MP2
C 0.656439 -0.413608 0.386193
C -0.656441 -0.413605 -0.386191
C -0.667134 0.967731 -1.041204
C 0.000008 1.899625 -0.000003
C 0.667136 0.967728 1.041206
O 1.685025 -0.546530 -0.602702
O -1.685031 -0.546519 0.602704
C 2.950898 -0.877400 -0.040584
C -2.950899 -0.877400 0.040580
H 0.708397 -1.247802 1.101490
H -0.708404 -1.247801 -1.101484
H -0.075552 0.924408 -1.961959
H -1.679033 1.286934 -1.312179
H 0.737345 2.549261 -0.481568
H -0.737321 2.549273 0.481560
H 1.679032 1.286926 1.312195
H 0.075543 0.924407 1.961954
H 2.897704 -1.831031 0.502027
H 3.311579 -0.096764 0.640587
H 3.644035 -0.972022 -0.877728
H -2.897700 -1.831042 -0.502011
H -3.311572 -0.096776 -0.640609
H -3.644044 -0.972005 0.877720

COMP. 17_4E_B3LYP
C 0.560529 -0.402992 0.348600
C -0.730506 -0.179169 -0.454402
C -0.570801 1.245155 -1.003578
C 0.235554 2.018672 0.076537
C 0.758038 0.942607 1.067094
O 1.588377 -0.681031 -0.604568
O -1.836870 -0.241744 0.454142
C 2.788708 -1.174588 -0.042022
C -2.829582 -1.189938 0.111096
H 0.458966 -1.248263 1.041209
H -0.839301 -0.931748 -1.240860
H -0.010465 1.201967 -1.940293
H -1.545188 1.690946 -1.212372
H 1.058741 2.570696 -0.381420
H -0.388586 2.748483 0.595594
H 1.796014 1.103755 1.366154
H 0.154617 0.937150 1.978026
H 2.611077 -2.098807 0.525892
H 3.270336 -0.444118 0.620576
H 3.463167 -1.391689 -0.871143
H -2.426754 -2.211804 0.086700
H -3.284254 -0.967716 -0.863975
H -3.602076 -1.135135 0.879377

COMP. 17_5T1A_M06-2X
C 0.382132 -0.476228 0.278821
C -0.794350 0.050726 -0.554878
C -0.444292 1.525472 -0.820963
C 0.674627 1.899377 0.182095
C 0.718046 0.722141 1.166010
O 1.403509 -0.776185 -0.655405
O -1.998662 0.006565 0.190904
C 2.581984 -1.286648 -0.081141
C -2.620246 -1.256973 0.189452
H 0.128732 -1.377822 0.851764
H -0.900799 -0.534466 -1.475668
H -0.116558 1.663243 -1.851257
H -1.347034 2.118850 -0.670746
H 1.631403 1.979767 -0.337273
H 0.486975 2.850361 0.681062
H 1.665243 0.625272 1.698737
H -0.077928 0.815793 1.909527
H 2.361774 -2.127898 0.588649
H 3.130085 -0.522553 0.480811
H 3.210930 -1.638302 -0.898179
H -2.867343 -1.569495 -0.832549
H -3.539557 -1.163890 0.766338
H -1.992101 -2.029101 0.648413

COMP. 17_5T1A_MP2
C 0.434728 -0.447654 0.257981
C -0.747235 -0.030895 -0.621400
C -0.452645 1.433950 -0.932166
C 0.326159 1.974718 0.293476
C 0.593478 0.748844 1.193315
O 1.539360 -0.590804 -0.642055
O -1.970936 -0.075548 0.121001
C 2.677277 -1.199807 -0.040424
C -2.515851 -1.387847 0.231889
H 0.269798 -1.398036 0.788806
H -0.827176 -0.661855 -1.519473
H 0.159346 1.491264 -1.837702
H -1.390253 1.966932 -1.118251
H 1.266835 2.434859 -0.024210
H -0.243930 2.739308 0.830287
H 1.573835 0.778628 1.680554
H -0.164159 0.673922 1.981493
H 2.422054 -2.191381 0.358481
H 3.092442 -0.584137 0.766634
H 3.422136 -1.306068 -0.830473
H -2.675173 -1.827019 -0.762190
H -3.475585 -1.278265 0.739204
H -1.873024 -2.055190 0.819241

COMP. 17_5T4A_M06-2X
C 0.419107 -0.338995 0.331873
C -0.826412 0.163453 -0.433990
C -0.653499 1.687224 -0.569695
C 0.767593 1.991247 -0.074070
C 0.981523 0.919239 0.997990
O 1.302139 -0.872923 -0.640998
O -2.024786 -0.091886 0.274173
C 2.407469 -1.554168 -0.099563
C -2.480963 -1.416745 0.137338
H 0.154832 -1.120594 1.055916
H -0.855122 -0.341310 -1.407217
H -0.843393 2.037195 -1.584295
H -1.390661 2.151297 0.090568
H 1.493001 1.851305 -0.879123
H 0.873223 3.008462 0.304920
H 2.016732 0.811706 1.325208
H 0.371871 1.145160 1.878783
H 2.946386 -2.004957 -0.932035
H 3.087039 -0.882620 0.436297
H 2.081634 -2.346062 0.587257
H -2.707365 -1.645699 -0.911213
H -1.745420 -2.144565 0.500589
H -3.390485 -1.508372 0.729646

COMP. 17_5T4A_MP2
C 0.415691 -0.342013 0.335667
C -0.818164 0.155252 -0.444329
C -0.642847 1.676533 -0.590876
C 0.763279 1.990284 -0.058377
C 0.964665 0.913974 1.011237
O 1.313825 -0.865435 -0.652316
O -2.033736 -0.080242 0.274778
C 2.432667 -1.546594 -0.093241
C -2.499514 -1.420501 0.139872
H 0.153892 -1.138828 1.049226
H -0.857304 -0.363324 -1.413982
H -0.802917 2.012496 -1.620230

H -1.405600 2.151380 0.037595
H 1.513405 1.872048 -0.847975
H 0.846627 3.009975 0.332913
H 1.999768 0.808325 1.351999
H 0.345489 1.135317 1.891261
H 2.970249 -1.991952 -0.931745
H 3.104209 -0.866186 0.443700
H 2.100909 -2.339052 0.592223
H -2.705484 -1.654532 -0.913093
H -1.775884 -2.147160 0.531040
H -3.422734 -1.484707 0.717662

COMP. 17_E1S_MP2
C -0.656446 -0.413600 -0.386190
C 0.656438 -0.413610 0.386190
C 0.667136 0.967722 1.041210
C 0.000025 1.899625 -0.000001
C -0.667132 0.967738 -1.041199
O -1.685035 -0.546515 0.602702
O 1.685024 -0.546527 -0.602704
C -2.950904 -0.877399 0.040578
C 2.950895 -0.877409 -0.040584
H -0.708408 -1.247791 -1.101490
H 0.708392 -1.247808 1.101483
H 0.075532 0.924398 1.961952
H 1.679030 1.286913 1.312212
H -0.737290 2.549293 0.481557
H 0.737376 2.549244 -0.481570
H -1.679030 1.286949 -1.312168
H -0.075557 0.924412 -1.961959
H -2.897700 -1.831037 -0.502017
H -3.311579 -0.096773 -0.640608
H -3.644047 -0.972010 0.877718
H 3.644033 -0.972032 -0.877728
H 2.897692 -1.831042 0.502021
H 3.311578 -0.096777 0.640590

COMP. 17_E1TS_MP2
C 0.546942 -0.424043 0.343240
C -0.719565 -0.192146 -0.474420
C -0.525790 1.217116 -1.025858
C 0.222657 1.978961 0.096076
C 0.702621 0.898088 1.096111
O 1.595136 -0.630713 -0.611639
O -1.828678 -0.204076 0.439736
C 2.789010 -1.138014 -0.024148
C -2.818332 -1.172544 0.106818
H 0.457279 -1.301988 1.001718
H -0.848274 -0.955793 -1.252293
H 0.085780 1.164315 -1.932869
H -1.489749 1.667001 -1.285130
H 1.066882 2.540369 -0.315896
H -0.434129 2.699158 0.593460
H 1.728846 1.060260 1.442147
H 0.055237 0.873704 1.979475
H 2.599434 -2.099138 0.473218
H 3.216837 -0.436490 0.702511
H 3.496428 -1.284019 -0.841785
H -3.251438 -0.973296 -0.882446
H -3.598165 -1.091541 0.865834
H -2.401894 -2.188743 0.120357

COMP. 17_E3A_B3LYPT
C -0.539183 -0.299326 -0.256129
C 0.720953 -0.117114 0.604529
C 0.668157 1.352880 0.991947
C 0.278527 2.035729 -0.325072
C -0.722557 1.056267 -0.982447
O 1.885518 -0.314638 -0.178756
O -1.603174 -0.583495 0.634963
C -2.766900 -1.035932 -0.011955
C 2.257258 -1.665972 -0.307046
H -0.423270 -1.134764 -0.958502
H 0.711774 -0.801921 1.460207
H -0.116079 1.484981 1.741982
H 1.617760 1.697204 1.402640
H 1.165339 2.141370 -0.951669
H -0.147798 3.028210 -0.175765
H -1.750666 1.395116 -0.836699
H -0.555120 0.967447 -2.056548
H -2.571881 -1.964918 -0.563219
H -3.163131 -0.291312 -0.712507
H -3.513333 -1.227272 0.757829
H 1.473915 -2.267028 -0.783800
H 2.485276 -2.103846 0.672460
H 3.150930 -1.697393 -0.929041

COMP. 17_E3A_M06-2X
C -0.539183 -0.299326 -0.256129
C 0.720953 -0.117114 0.604529
C 0.668157 1.352880 0.991947
C 0.278527 2.035729 -0.325072
C -0.722557 1.056267 -0.982447
O 1.885518 -0.314639 -0.178756
O -1.603174 -0.583495 0.634963
C -2.766900 -1.035932 -0.011955
C 2.257258 -1.665973 -0.307046
H -0.423270 -1.134764 -0.958502
H 0.711774 -0.801921 1.460207
H -0.116079 1.484981 1.741982
H 1.617760 1.697204 1.402640
H 1.165339 2.141370 -0.951669
H -0.147797 3.028210 -0.175765
H -1.750666 1.395116 -0.836699
H -0.555120 0.967447 -2.056548
H -2.571881 -1.964918 -0.563219
H -3.163131 -0.291312 -0.712507
H -3.513333 -1.227271 0.757829
H 1.473915 -2.267028 -0.783800
H 2.485276 -2.103847 0.672460
H 3.150930 -1.697394 -0.929041

COMP. 17_E3S_B3LYP
C -0.720274 -0.257386 -0.340228
C 0.635377 -0.377599 0.380086
C 0.856677 1.013164 0.989731
C 0.361299 1.965418 -0.111157
C -0.866941 1.243965 -0.719000
H 0.232174 1.100170 1.884991
H 1.891118 1.193169 1.291044
H 0.601299 -1.181045 1.124910
O 1.603444 -0.691088 -0.624654
O -1.721869 -0.693917 0.579760
H -0.722589 -0.913305 -1.218678
H -1.793128 1.625849 -0.281418
H -0.932640 1.389310 -1.799271
H 1.139162 2.085987 -0.868961
H 0.116948 2.960119 0.268332
C -2.987636 -0.912505 -0.012454
H -2.927692 -1.668382 -0.808242
H -3.413446 0.007034 -0.435571
H -3.650072 -1.275010 0.774392
C 2.857500 -1.104730 -0.116748
H 2.750655 -1.980701 0.538336
H 3.365987 -0.309153 0.442757
H 3.473605 -1.375969 -0.974852

COMP. 17_E3S_MP2
C -0.720184 -0.185115 -0.280920
C 0.664303 -0.277205 0.384429
C 0.991719 1.150515 0.828630
C 0.334434 2.003245 -0.260232
C -1.028660 1.319971 -0.419354
H 0.513873 1.347732 1.798379
H 2.066690 1.321609 0.945862
H 0.637306 -1.006570 1.207096
O 1.572870 -0.731511 -0.630315
O -1.654097 -0.880999 0.550403
H -0.665188 -0.686034 -1.259848
H -1.679749 1.607994 0.417133
H -1.543847 1.574839 -1.351779
H 0.915010 1.931469 -1.187230

H 0.249921 3.063545 0.002351
C -2.937836 -0.981011 -0.058316
H -2.866428 -1.486367 -1.031617
H -3.398821 0.004927 -0.198564
H -3.555127 -1.574893 0.617203
C 2.798931 -1.219740 -0.094629
H 2.614497 -2.060734 0.587525
H 3.354834 -0.439636 0.440165
H 3.390603 -1.561756 -0.945044

COMP. 17_E4A_B3LYP
C 0.486371 -0.205276 0.347561
C -0.841470 0.241548 -0.332939
C -0.838379 1.776505 -0.314453
C 0.646248 2.156620 -0.228858
C 1.209105 1.101650 0.738124
O 1.214905 -0.982301 -0.607631
O -2.012723 -0.232206 0.318318
C 2.284740 -1.727468 -0.058306
C -2.293837 -1.599984 0.079401
H 0.270779 -0.829318 1.224861
H -0.815944 -0.139140 -1.362948
H -1.356530 2.201014 -1.176497
H -1.367453 2.104409 0.586450
H 1.123687 2.058750 -1.209281
H 0.806050 3.181644 0.113429
H 2.296177 1.003872 0.699364
H 0.942181 1.365894 1.767214
H 1.929431 -2.418128 0.719954
H 3.062731 -1.085543 0.374653
H 2.722386 -2.305141 -0.873302
H -2.418028 -1.798268 -0.993854
H -3.226104 -1.827816 0.597358
H -1.503486 -2.257738 0.463934

COMP. 17_E4A_MP2
C 0.488145 -0.159574 0.344582
C -0.849066 0.261832 -0.305002
C -0.900629 1.783189 -0.212783
C 0.574023 2.186223 -0.274007
C 1.233963 1.152249 0.647014
O 1.173769 -0.987249 -0.605523
O -1.995149 -0.296389 0.331099
C 2.246051 -1.721323 -0.022896
C -2.145565 -1.685446 0.043822
H 0.295688 -0.746876 1.256848
H -0.817691 -0.064337 -1.358160
H -1.524354 2.224418 -0.996460
H -1.333863 2.055319 0.758610
H 0.956120 2.079174 -1.297076
H 0.753680 3.219620 0.041092
H 2.314812 1.054137 0.501627
H 1.065885 1.436216 1.694332
H 1.876882 -2.373974 0.780889
H 3.022268 -1.060443 0.382753
H 2.673586 -2.330233 -0.820825
H -2.252941 -1.848751 -1.036787
H -3.051334 -2.009599 0.558423
H -1.289234 -2.268473 0.405749

COMP. 17_E5TS_MP2
C 0.662280 -0.055101 0.213535
C -0.783534 0.144979 -0.232754
C -1.036025 1.667103 -0.143566
C 0.332358 2.303459 0.193639
C 1.362013 1.238155 -0.206053
O 1.159635 -1.240014 -0.360849
O -1.665888 -0.609082 0.573894
C 2.419697 -1.617668 0.139592
C -2.511972 -1.479279 -0.141550
H 0.667113 -0.144264 1.311589
H -0.847180 -0.201621 -1.271366
H -1.424040 2.050223 -1.089062
H -1.784840 1.863073 0.624488
H 0.493605 3.256619 -0.310335
H 0.403060 2.489034 1.268670
H 1.506543 1.219958 -1.292101
H 2.334086 1.386330 0.266866
H 2.393250 -1.724939 1.231315
H 3.195222 -0.889788 -0.126102
H 2.670869 -2.579169 -0.306303
H -1.931603 -2.211374 -0.713887
H -3.169152 -0.927802 -0.825417
H -3.125809 -2.003402 0.590216

COMP. 17_E5_M06-2X
C 0.662280 -0.055101 0.213535
C -0.783534 0.144979 -0.232754
C -1.036025 1.667103 -0.143566
C 0.332358 2.303459 0.193639
C 1.362013 1.238155 -0.206053
O 1.159635 -1.240014 -0.360849
O -1.665888 -0.609082 0.573894
C 2.419697 -1.617668 0.139592
C -2.511972 -1.479279 -0.141550
H 0.667113 -0.144264 1.311589
H -0.847180 -0.201621 -1.271366
H -1.424040 2.050223 -1.089062
H -1.784840 1.863073 0.624488
H 0.493605 3.256619 -0.310335
H 0.403060 2.489034 1.268670
H 1.506543 1.219958 -1.292101
H 2.334086 1.386330 0.266866
H 2.393250 -1.724939 1.231315
H 3.195222 -0.889788 -0.126102
H 2.670869 -2.579169 -0.306303
H -1.931603 -2.211374 -0.713887
H -3.169152 -0.927802 -0.825417
H -3.125809 -2.003402 0.590216

COMP. 17_TDI1T2AS
C 0.508452 -0.352944 0.271777
C -0.731768 -0.088448 -0.605640
C -0.583307 1.383048 -0.986573
C -0.033934 2.068467 0.285690
C 0.670448 0.942938 1.097178
O 1.595974 -0.579611 -0.626844
O -1.932453 -0.233640 0.153674
C 2.747798 -1.134537 -0.022407
C -2.389871 -1.567613 0.277746
H 0.378722 -1.238527 0.907473
H -0.750157 -0.759688 -1.472573
H 0.139624 1.453677 -1.802988
H -1.531356 1.800647 -1.330195
H 0.648795 2.883833 0.038296
H -0.850331 2.498005 0.869290
H 1.726927 1.155886 1.274210
H 0.200918 0.819549 2.075740
H 3.480507 -1.289811 -0.815149
H 3.183766 -0.468882 0.733768
H 2.522191 -2.100929 0.450731
H -2.577089 -2.016108 -0.707656
H -1.681174 -2.205286 0.822300
H -3.326428 -1.531814 0.835485

COMP. 18_2EI_B3LYP
C 1.229675 0.498442 0.380538
C 0.000000 0.065647 1.202494
C -1.229675 0.498442 0.380538
C -0.775839 1.781282 -0.341632
C 0.775839 1.781282 -0.341632
O 1.614659 -0.451982 -0.612113
O -1.614659 -0.451982 -0.612113
C 2.287845 -1.585744 -0.107499
C -2.287846 -1.585744 -0.107499
H 2.095796 0.682947 1.032524
H 0.000000 -0.996164 1.455851
H 0.000000 0.617529 2.149939
H -2.095796 0.682947 1.032524
H -1.194958 1.788205 -1.348420
H -1.165114 2.658833 0.180796
H 1.194958 1.788205 -1.348420

H 1.165114 2.658832 0.180797
H 1.648386 -2.203818 0.536938
H 3.183283 -1.298380 0.463674
H 2.592432 -2.183430 -0.967427
H -3.183283 -1.298379 0.463674
H -1.648387 -2.203818 0.536938
H -2.592432 -2.183430 -0.967427

COMP. 18_2EI_M06-2X
C 1.214114 0.520987 0.368737
C 0.000000 0.161475 1.234924
C -1.214114 0.520987 0.368737
C -0.774338 1.794453 -0.365750
C 0.774338 1.794453 -0.365750
O 1.514320 -0.455470 -0.611017
O -1.514320 -0.455469 -0.611017
C 2.031361 -1.652424 -0.092041
C -2.031361 -1.652424 -0.092041
H 2.110225 0.685507 0.983335
H 0.000000 -0.866315 1.599669
H 0.000000 0.814574 2.114094
H -2.110225 0.685508 0.983335
H -1.195364 1.786505 -1.370742
H -1.161932 2.673776 0.152293
H 1.195364 1.786505 -1.370742
H 1.161933 2.673776 0.152293
H 1.278743 -2.224806 0.463075
H 2.886301 -1.462106 0.571180
H 2.365162 -2.251768 -0.938337
H -2.886301 -1.462106 0.571180
H -1.278744 -2.224805 0.463075
H -2.365163 -2.251767 -0.938337

COMP. 18_2EI_MP2
C 1.215105 0.519109 0.376138
C 0.000000 0.144796 1.231633
C -1.215105 0.519109 0.376138
C -0.773493 1.788042 -0.362271
C 0.773492 1.788042 -0.362271
O 1.530499 -0.457355 -0.619804
O -1.530499 -0.457355 -0.619804
C 2.113058 -1.639493 -0.090027
C -2.113058 -1.639493 -0.090027
H 2.113394 0.687082 0.994477
H 0.000000 -0.894805 1.572213
H 0.000000 0.776359 2.132332
H -2.113394 0.687081 0.994477
H -1.197096 1.777990 -1.370517
H -1.163905 2.673306 0.152935
H 1.197096 1.777990 -1.370517
H 1.163905 2.673306 0.152935
H 1.399814 -2.220942 0.508352
H 2.989812 -1.402402 0.530522
H 2.425852 -2.237311 -0.947558
H -2.989812 -1.402402 0.530522
H -1.399814 -2.220942 0.508352
H -2.425852 -2.237311 -0.947558

COMP. 18_2EN_B3LYP
C 1.110912 0.250534 0.657305
C -0.278435 0.170141 1.294556
C -1.271898 0.634216 0.210389
C -0.484176 1.672683 -0.614182
C 1.020612 1.470653 -0.290961
O 1.359116 -0.978957 -0.022655
O -1.681977 -0.400069 -0.681669
C 2.702462 -1.160356 -0.419719
C -2.568258 -1.346328 -0.121400
H 1.895593 0.390103 1.414939
H -0.485875 -0.825528 1.688955
H -0.324660 0.875082 2.132228
H -2.172816 1.071220 0.665518
H -0.709316 1.519520 -1.670212
H -0.804731 2.684813 -0.355731
H 1.618682 1.313364 -1.190333
H 1.430467 2.352501 0.210211
H 3.383916 -1.113411 0.442820
H 3.026175 -0.415727 -1.159221
H 2.769940 -2.150306 -0.872292
H -3.456831 -0.857989 0.306306
H -2.093111 -1.955694 0.657651
H -2.881854 -2.004999 -0.932163

COMP. 18_2EN_M06-2X
C 1.081267 0.239277 0.691512
C -0.315569 0.263209 1.298617
C -1.241931 0.686049 0.146652
C -0.382159 1.636070 -0.708218
C 1.079844 1.468818 -0.232496
O 1.223935 -0.982020 -0.009183
O -1.643003 -0.378380 -0.695111
C 2.540905 -1.247687 -0.419699
C -2.442188 -1.349096 -0.069590
H 1.868070 0.304936 1.455872
H -0.580242 -0.687534 1.761181
H -0.350596 1.038308 2.070623
H -2.145374 1.177276 0.534168
H -0.509559 1.349367 -1.751939
H -0.715099 2.669737 -0.603850
H 1.780532 1.359109 -1.060936
H 1.398906 2.340748 0.344622
H 3.225721 -1.266089 0.438766
H 2.907357 -0.509831 -1.142838
H 2.538765 -2.228021 -0.894425
H -3.256857 -0.885662 0.503814
H -1.858376 -1.992739 0.596851
H -2.871725 -1.966246 -0.858229

COMP. 18_2EN_M06-2XF
C 1.081267 0.239277 0.691512
C -0.315569 0.263209 1.298617
C -1.241931 0.686049 0.146652
C -0.382159 1.636070 -0.708218
C 1.079844 1.468818 -0.232496
O 1.223935 -0.982020 -0.009183
O -1.643003 -0.378380 -0.695111
C 2.540905 -1.247687 -0.419699
C -2.442188 -1.349096 -0.069590
H 1.868070 0.304936 1.455872
H -0.580242 -0.687534 1.761181
H -0.350596 1.038308 2.070623
H -2.145374 1.177276 0.534168
H -0.509559 1.349367 -1.751939
H -0.715099 2.669737 -0.603850
H 1.780532 1.359109 -1.060936
H 1.398906 2.340748 0.344622
H 3.225721 -1.266089 0.438766
H 2.907357 -0.509831 -1.142838
H 2.538765 -2.228021 -0.894425
H -3.256857 -0.885662 0.503814
H -1.858376 -1.992739 0.596851
H -2.871725 -1.966246 -0.858229

COMP. 18_2EN_MP2
C 1.082462 0.259230 0.683304
C -0.307745 0.270854 1.302856
C -1.248519 0.682350 0.162261
C -0.412425 1.647551 -0.694496
C 1.061272 1.472113 -0.260043
O 1.228739 -0.985671 -0.005030
O -1.628923 -0.392871 -0.699477
C 2.566946 -1.241405 -0.412522
C -2.441743 -1.374832 -0.071396
H 1.880437 0.339559 1.440792
H -0.555202 -0.684811 1.773303
H -0.343806 1.047870 2.079729
H -2.167691 1.152299 0.552009
H -0.570625 1.388980 -1.745304
H -0.744718 2.682172 -0.554392
H 1.736312 1.339635 -1.110989
H 1.411069 2.355372 0.289632
H 3.246995 -1.237608 0.451768

H 2.921011 -0.507860 -1.147967
H 2.564543 -2.231949 -0.869627
H -3.285214 -0.908356 0.459015
H -1.868453 -1.992018 0.630163
H -2.824671 -2.010102 -0.871866

COMP. 18_2EO_B3LYP
C 1.228116 0.446739 0.491515
C 0.000000 0.392396 1.406162
C -1.228117 0.446738 0.491516
C -0.776531 1.314194 -0.711292
C 0.776528 1.314191 -0.711295
O 1.576340 -0.885685 0.122075
O -1.576338 -0.885685 0.122073
C 2.853621 -1.005369 -0.467875
C -2.853619 -1.005372 -0.467876
H 2.089541 0.897059 1.005462
H 0.000001 -0.494338 2.040804
H 0.000000 1.279264 2.048594
H -2.089542 0.897055 1.005465
H -1.187394 0.919007 -1.642112
H -1.161179 2.332307 -0.603932
H 1.187385 0.918996 -1.642116
H 1.161180 2.332303 -0.603944
H 3.640944 -0.630534 0.203213
H 2.928092 -0.468294 -1.423472
H 3.020770 -2.067067 -0.653010
H -2.928092 -0.468295 -1.423470
H -3.640943 -0.630541 0.203215
H -3.020765 -2.067069 -0.653013

COMP. 18_2EO_M06-2X
C 1.215410 0.472021 0.474068
C 0.000000 0.503807 1.396706
C -1.215410 0.472021 0.474068
C -0.774531 1.288762 -0.759735
C 0.774531 1.288762 -0.759735
O 1.501309 -0.877101 0.160037
O -1.501309 -0.877101 0.160037
C 2.760927 -1.056325 -0.433694
C -2.760927 -1.056326 -0.433694
H 2.098810 0.914667 0.954571
H 0.000000 -0.324431 2.105100
H 0.000000 1.449015 1.947929
H -2.098810 0.914666 0.954572
H -1.184348 0.852580 -1.671495
H -1.159069 2.308746 -0.690707
H 1.184347 0.852580 -1.671495
H 1.159069 2.308745 -0.690708
H 3.563399 -0.703256 0.228113
H 2.847169 -0.532200 -1.393528
H 2.886869 -2.124184 -0.607718
H -2.847169 -0.532200 -1.393528
H -3.563399 -0.703256 0.228113
H -2.886869 -2.124184 -0.607718

COMP. 18_2EO_MP2
C 1.214120 0.480905 0.472447
C 0.000000 0.512912 1.394147
C -1.214120 0.480905 0.472447
C -0.774238 1.293848 -0.761329
C 0.774238 1.293848 -0.761329
O 1.492144 -0.885828 0.159098
O -1.492144 -0.885828 0.159098
C 2.772808 -1.063694 -0.431181
C -2.772808 -1.063694 -0.431181
H 2.106302 0.916462 0.952930
H 0.000000 -0.314630 2.109469
H 0.000000 1.461851 1.948311
H -2.106302 0.916462 0.952930
H -1.187312 0.857418 -1.675654
H -1.160337 2.318291 -0.693268
H 1.187312 0.857418 -1.675654
H 1.160337 2.318291 -0.693268
H 3.566916 -0.703280 0.239061
H 2.859329 -0.544698 -1.395116
H 2.891039 -2.136271 -0.591696
H -2.859330 -0.544698 -1.395116
H -3.566916 -0.703280 0.239061
H -2.891039 -2.136271 -0.591696

COMP. 18_3T2I_B3LYPT
C 1.208083 0.217640 0.377622
C 0.000467 -0.641178 -0.047912
C -1.204863 0.260485 0.269810
C -0.738082 1.650908 -0.176422
C 0.777207 1.684557 0.127095
O 2.405416 -0.042924 -0.344600
O -2.409051 -0.077072 -0.399774
C 3.013224 -1.282619 -0.033994
C -3.053330 -1.234142 0.099884
H 1.411602 0.059062 1.447814
H 0.039277 -0.802448 -1.131165
H -0.035122 -1.613298 0.448395
H -1.391459 0.254446 1.356685
H -0.925143 1.730845 -1.250832
H -1.297805 2.450133 0.312613
H 1.352357 2.076851 -0.713130
H 1.009066 2.306978 0.994081
H 2.391266 -2.135183 -0.336213
H 3.224174 -1.364938 1.042050
H 3.954270 -1.322641 -0.583534
H -3.263957 -1.141229 1.174915
H -2.458768 -2.141932 -0.065022
H -3.996903 -1.330589 -0.438161

COMP. 18_3T2I_M06-2X
C 1.191251 0.246206 0.334636
C 0.000188 -0.608165 -0.113561
C -1.190973 0.258341 0.307605
C -0.766112 1.680901 -0.072037
C 0.776141 1.689922 0.008853
O 2.409922 -0.043557 -0.310689
O -2.411185 -0.049516 -0.324186
C 2.927624 -1.311089 0.012973
C -2.937584 -1.299865 0.048985
H 1.329588 0.124474 1.420813
H 0.010036 -0.693130 -1.206740
H -0.008080 -1.608108 0.324136
H -1.324856 0.177848 1.398719
H -1.108056 1.857780 -1.093846
H -1.238868 2.427411 0.566104
H 1.223188 1.951777 -0.951588
H 1.161260 2.390363 0.750078
H 2.288490 -2.117967 -0.364043
H 3.038983 -1.426868 1.099142
H 3.907827 -1.389429 -0.455275
H -3.046754 -1.373383 1.138981
H -2.306046 -2.125450 -0.298996
H -3.919805 -1.388237 -0.413208

COMP. 18_3T2I_MP2
C 1.189824 0.247399 0.322841
C 0.000000 -0.609018 -0.116750
C -1.189824 0.247382 0.322877
C -0.772653 1.681720 -0.024200
C 0.772639 1.681708 -0.024309
O 2.420950 -0.041673 -0.333479
O -2.420949 -0.041664 -0.333460
C 2.962984 -1.305216 0.038503
C -2.962970 -1.305232 0.038454
H 1.341121 0.136440 1.411940
H -0.000013 -0.688217 -1.213026
H 0.000010 -1.616526 0.311486
H -1.341126 0.136368 1.411969
H -1.173055 1.906719 -1.018442
H -1.205002 2.407055 0.671695
H 1.172900 1.906593 -1.018635
H 1.205107 2.407105 0.671447
H 2.335025 -2.133425 -0.312450
H 3.078944 -1.376191 1.129277
H 3.943301 -1.371007 -0.435436

H -3.078930 -1.376267 1.129224
H -2.335003 -2.133415 -0.312544
H -3.943287 -1.371007 -0.435489

COMP. 18_3T2N_M06-2X
C 1.110517 -0.203885 0.356031
C -0.235764 -0.810204 -0.033308
C -1.238305 0.303304 0.281479
C -0.523430 1.555378 -0.217705
C 0.952970 1.331059 0.155659
O 2.124549 -0.782103 -0.438198
O -2.486119 0.182936 -0.357627
C 3.419826 -0.468948 0.012557
C -3.245283 -0.912156 0.095364
H 1.330406 -0.419866 1.411782
H -0.238182 -0.984390 -1.114576
H -0.426540 -1.755708 0.475551
H -1.395435 0.363335 1.371644
H -0.651539 1.585974 -1.302820
H -0.946238 2.471331 0.195266
H 1.623313 1.669170 -0.636791
H 1.220578 1.872708 1.065255
H 3.606354 0.611758 -0.004319
H 4.124676 -0.959153 -0.657505
H 3.580106 -0.836138 1.034647
H -3.377815 -0.877248 1.184695
H -2.778802 -1.866751 -0.173308
H -4.221509 -0.848974 -0.383390

COMP. 18_3T2N_MP2
C 1.095788 0.192108 0.530731
C -0.227543 -0.269571 1.170155
C -1.347370 0.501632 0.451489
C -0.639379 1.736714 -0.094861
C 0.696015 1.170500 -0.586349
O 1.803339 -0.963517 0.077695
O -1.843984 -0.210850 -0.688635
C 3.092538 -0.642611 -0.433826
C -2.726074 -1.272611 -0.344272
H 1.727631 0.710383 1.273611
H -0.325514 -1.352285 1.047754
H -0.241180 -0.057905 2.246134
H -2.193646 0.744772 1.114140
H -1.231509 2.228202 -0.872927
H -0.475644 2.457441 0.718416
H 0.540593 0.602721 -1.510889
H 1.450770 1.942247 -0.772564
H 3.026708 -0.035469 -1.345281
H 3.577116 -1.591744 -0.667242
H 3.687869 -0.102372 0.316506
H -3.590147 -0.893439 0.219550
H -2.224705 -2.048611 0.247430
H -3.067029 -1.705970 -1.285524

COMP. 18_3T2O_M06-2X
C 1.200735 -0.194212 0.349335
C -0.000108 -1.060903 -0.005841
C -1.190357 -0.171142 0.314572
C -0.759327 1.199707 -0.232917
C 0.760717 1.262398 0.030856
O 2.326197 -0.622294 -0.385481
O -2.357678 -0.697368 -0.269362
C 3.520702 -0.010890 0.036239
C -3.517182 0.033249 0.049908
H 1.427333 -0.287287 1.422111
H 0.010268 -1.251807 -1.083482
H -0.015450 -2.015954 0.518593
H -1.331524 -0.106861 1.406582
H -0.967418 1.200222 -1.307008
H -1.299350 2.035353 0.214475
H 1.299847 1.613878 -0.851400
H 1.000575 1.939690 0.852544
H 3.725254 -0.232748 1.091818
H 3.487570 1.077898 -0.092800
H 4.326349 -0.414260 -0.575575
H -3.489859 1.043386 -0.374924
H -3.647812 0.110814 1.137333
H -4.365006 -0.504277 -0.372437

COMP. 18_3T2O_MP2
C 1.189252 -0.185637 0.320909
C -0.000281 -1.048008 -0.067403
C -1.184871 -0.172541 0.304260
C -0.770939 1.223549 -0.193737
C 0.771533 1.255465 -0.062336
O 2.354609 -0.652322 -0.352288
O -2.367531 -0.687048 -0.296254
C 3.537161 -0.004326 0.102913
C -3.536561 0.016342 0.110337
H 1.366093 -0.255442 1.409113
H 0.003946 -1.198508 -1.154528
H -0.006298 -2.026424 0.420841
H -1.321847 -0.163437 1.401438
H -1.075456 1.297859 -1.244785
H -1.258534 2.039603 0.349282
H 1.241444 1.508325 -1.019587
H 1.111188 1.992780 0.672621
H 3.672601 -0.152129 1.183771
H 3.517933 1.071674 -0.112784
H 4.368362 -0.463957 -0.433426
H -3.528122 1.054695 -0.243828
H -3.636627 0.009284 1.205056
H -4.383073 -0.508433 -0.334511

COMP. 18_4T5I_B3LYP
C 1.197237 0.378082 0.226792
C 0.041838 -0.599549 0.569436
C -1.262021 0.249749 0.559297
C -0.803803 1.692316 0.277957
C 0.512359 1.540885 -0.491948
O 2.213304 -0.174676 -0.596100
O -2.155082 -0.130486 -0.489070
C 3.057215 -1.097814 0.065371
C -2.834325 -1.348148 -0.255977
H 1.660304 0.743462 1.157843
H -0.013815 -1.355719 -0.218595
H 0.194786 -1.116012 1.519899
H -1.802268 0.175874 1.513025
H -1.574992 2.243163 -0.261863
H -0.627488 2.207452 1.228807
H 0.322022 1.246723 -1.528278
H 1.125042 2.444459 -0.502097
H 2.513854 -1.994819 0.390762
H 3.538638 -0.641520 0.942410
H 3.827724 -1.394017 -0.647218
H -3.416130 -1.306743 0.676399
H -2.148812 -2.204536 -0.201441
H -3.515632 -1.499610 -1.093858

COMP. 18_4T5I_M06-2X
C 1.188330 0.402871 0.215523
C 0.057162 -0.587087 0.574492
C -1.250517 0.246420 0.568982
C -0.805739 1.688534 0.297564
C 0.475916 1.531075 -0.518441
O 2.200542 -0.148235 -0.593955
O -2.115218 -0.133917 -0.488039
C 2.980296 -1.109748 0.073752
C -2.758391 -1.363346 -0.263402
H 1.644822 0.795886 1.138331
H 0.005987 -1.337689 -0.220000
H 0.225922 -1.103277 1.521284
H -1.798801 0.158065 1.515791
H -1.595250 2.244632 -0.207090
H -0.585675 2.186468 1.247166
H 0.244231 1.191057 -1.531670
H 1.080182 2.436273 -0.582207
H 2.385252 -1.984596 0.362530
H 3.442965 -0.686145 0.974996
H 3.763869 -1.426928 -0.612985
H -3.365802 -1.326829 0.650509
H -2.044274 -2.191190 -0.174552

H -3.408364 -1.550827 -1.116973

COMP. 18_E2I_B3LYP
C 1.200855 0.231629 0.310743
C 0.000000 -0.627266 -0.121726
C -1.200855 0.231627 0.310746
C -0.774775 1.676217 -0.014080
C 0.774775 1.676216 -0.014091
O 2.423793 -0.056309 -0.350573
O -2.423792 -0.056308 -0.350571
C 3.034370 -1.268623 0.050483
C -3.034370 -1.268624 0.050478
H 1.355657 0.116830 1.395813
H -0.000001 -0.719197 -1.213827
H 0.000001 -1.628612 0.314157
H -1.355657 0.116822 1.395816
H -1.170663 1.925756 -1.001047
H -1.203430 2.387624 0.694128
H 1.170648 1.925743 -1.001067
H 1.203442 2.387630 0.694103
H 2.434115 -2.144874 -0.226454
H 3.207085 -1.288701 1.136096
H 3.995351 -1.325781 -0.461753
H -3.207085 -1.288708 1.136091
H -2.434114 -2.144873 -0.226463
H -3.995351 -1.325780 -0.461758

COMP. 18_E2I_M06-2X
C 1.190696 0.251738 0.320442
C 0.000001 -0.607094 -0.118447
C -1.190694 0.251830 0.320242
C -0.772301 1.685956 -0.031222
C 0.772374 1.686024 -0.030616
O 2.411579 -0.046327 -0.315711
O -2.411590 -0.046371 -0.315808
C 2.932600 -1.306218 0.031845
C -2.932672 -1.306137 0.032112
H 1.324020 0.148274 1.409424
H 0.000074 -0.687307 -1.212032
H -0.000061 -1.608859 0.315146
H -1.323983 0.148674 1.409262
H -1.167268 1.905552 -1.024896
H -1.204166 2.409776 0.659937
H 1.168128 1.906259 -1.023831
H 1.203583 2.409497 0.661317
H 2.298168 -2.121839 -0.334020
H 3.039963 -1.402954 1.120238
H 3.915056 -1.388819 -0.430916
H -3.040008 -1.402567 1.120534
H -2.298298 -2.121895 -0.333549
H -3.915147 -1.388809 -0.430596

COMP. 18_E2N_B3LYP
C 1.118867 -0.177002 0.297054
C -0.209669 -0.804286 -0.121416
C -1.239456 0.255140 0.299558
C -0.574754 1.589353 -0.080854
C 0.954809 1.337208 -0.012391
O 2.187615 -0.810625 -0.390353
O -2.504584 0.165455 -0.336943
C 3.471469 -0.458147 0.090739
C -3.304355 -0.917040 0.102338
H 1.269557 -0.318202 1.379425
H -0.225993 -0.910044 -1.211627
H -0.364000 -1.788509 0.324619
H -1.391632 0.202339 1.390172
H -0.886798 1.831827 -1.099456
H -0.908254 2.406841 0.560723
H 1.428629 1.547825 -0.974690
H 1.446590 1.962874 0.735551
H 3.573779 -0.689802 1.160734
H 3.690839 0.606747 -0.060575
H 4.195924 -1.049040 -0.470542
H -3.460526 -0.882424 1.190056
H -2.864519 -1.887786 -0.159411
H -4.269296 -0.822644 -0.396782

COMP. 18_E2OT_MP2
C 1.188535 -0.177163 0.315530
C 0.000000 -1.046363 -0.059116
C -1.188535 -0.177163 0.315531
C -0.774391 1.243155 -0.124732
C 0.774391 1.243154 -0.124736
O 2.359578 -0.670574 -0.328298
O -2.359578 -0.670572 -0.328300
C 3.539680 0.001549 0.101304
C -3.539680 0.001548 0.101303
H 1.351394 -0.207803 1.408199
H 0.000000 -1.202842 -1.145456
H 0.000000 -2.022119 0.434571
H -1.351395 -0.207806 1.408199
H -1.165717 1.407130 -1.135702
H -1.192741 2.023226 0.519863
H 1.165711 1.407123 -1.135709
H 1.192745 2.023228 0.519853
H 3.660174 -0.078022 1.191048
H 3.528169 1.061314 -0.183179
H 4.375384 -0.494926 -0.393638
H -3.528169 1.061315 -0.183175
H -3.660175 -0.078027 1.191047
H -4.375384 -0.494925 -0.393641

COMP. 18_E2O_B3LYP
C 1.200360 -0.160939 0.311544
C 0.000000 -1.034751 -0.041357
C -1.200360 -0.160941 0.311547
C -0.776437 1.269900 -0.115439
C 0.776436 1.269896 -0.115456
O 2.361420 -0.651917 -0.341269
O -2.361418 -0.651913 -0.341274
C 3.566854 -0.052374 0.095343
C -3.566853 -0.052377 0.095341
H 1.373746 -0.187299 1.399573
H -0.000001 -1.222478 -1.119998
H 0.000001 -1.996459 0.473731
H -1.373751 -0.187311 1.399575
H -1.163706 1.454029 -1.121173
H -1.192394 2.038330 0.539646
H 1.163682 1.454002 -1.121204
H 1.192413 2.038337 0.539603
H 3.706379 -0.180038 1.178507
H 3.604267 1.019349 -0.139672
H 4.380868 -0.554802 -0.428106
H -3.604266 1.019350 -0.139660
H -3.706383 -0.180054 1.178503
H -4.380866 -0.554798 -0.428118

COMP. 18_E2O_M06-2X
C 1.189163 -0.190842 0.312985
C 0.000000 -1.056980 -0.069510
C -1.189163 -0.190843 0.312987
C -0.773991 1.233391 -0.121205
C 0.773991 1.233388 -0.121216
O 2.357309 -0.667109 -0.313108
O -2.357308 -0.667106 -0.313112
C 3.517490 0.018131 0.091890
C -3.517490 0.018129 0.091891
H 1.334701 -0.218904 1.404941
H -0.000001 -1.198708 -1.155016
H 0.000001 -2.033866 0.413342
H -1.334705 -0.218912 1.404941
H -1.161503 1.400765 -1.129594
H -1.192275 2.005836 0.525736
H 1.161489 1.400747 -1.129614
H 1.192288 2.005840 0.525708
H 3.652741 -0.044356 1.179733
H 3.486294 1.075038 -0.198531
H 4.364283 -0.458344 -0.400012
H -3.486294 1.075040 -0.198517
H -3.652744 -0.044371 1.179733
H -4.364281 -0.458339 -0.400020

COMP. 18_E2O_MP2
C 1.188534 -0.177164 0.315529
C 0.000000 -1.046364 -0.059119
C -1.188535 -0.177166 0.315533
C -0.774391 1.243155 -0.124719
C 0.774391 1.243148 -0.124749
O 2.359580 -0.670580 -0.328286
O -2.359577 -0.670572 -0.328299
C 3.539679 0.001557 0.101301
C -3.539679 0.001553 0.101299
H 1.351383 -0.207797 1.408200
H -0.000001 -1.202839 -1.145460
H 0.000002 -2.022121 0.434565
H -1.351393 -0.207818 1.408202
H -1.165733 1.407148 -1.135680
H -1.192726 2.023221 0.519895
H 1.165695 1.407101 -1.135731
H 1.192759 2.023231 0.519823
H 3.660171 -0.077985 1.191047
H 3.528167 1.061316 -0.183209
H 4.375385 -0.494929 -0.393627
H -3.528166 1.061319 -0.183182
H -3.660179 -0.078020 1.191042
H -4.375382 -0.494920 -0.393648

COMP. 18_E3IT_MP2
C 0.978518 0.557372 0.352748
C -0.174076 0.125165 1.272212
C -1.437243 0.361287 0.442603
C -1.126673 1.687250 -0.240145
C 0.340411 1.522454 -0.675414
O 1.531173 -0.592048 -0.312448
O -1.603271 -0.579478 -0.620018
C 2.929664 -0.750699 -0.101669
C -1.735935 -1.930502 -0.191745
H 1.777816 1.045801 0.927632
H -0.035668 -0.898329 1.631651
H -0.224640 0.781639 2.152390
H -2.351486 0.380959 1.059099
H -1.807104 1.875802 -1.076281
H -1.237894 2.505090 0.483810
H 0.394396 1.039082 -1.654904
H 0.871007 2.479295 -0.736778
H 3.161793 -0.896570 0.962575
H 3.492000 0.115205 -0.476826
H 3.226776 -1.640499 -0.659459
H -2.467389 -2.015402 0.625007
H -0.773834 -2.345344 0.127658
H -2.096979 -2.488490 -1.057390

COMP. 18_E4ITS_B3LYP
C 1.210082 0.108664 0.574860
C -0.161551 -0.586667 0.766779
C -1.237996 0.406029 0.235540
C -0.447783 1.492477 -0.501777
C 0.861393 1.580465 0.289756
O 1.888571 -0.445402 -0.561816
O -2.189915 -0.171923 -0.646139
C 3.152194 -1.015399 -0.283603
C -3.135750 -1.006868 -0.007076
H 1.849954 0.003650 1.457130
H -0.180376 -1.507496 0.180349
H -0.331766 -0.847578 1.814436
H -1.778285 0.852773 1.085236
H -0.251745 1.142749 -1.519255
H -0.993390 2.436030 -0.564070
H 1.668434 2.087844 -0.241449
H 0.697477 2.106525 1.238308
H 3.075701 -1.859189 0.416520
H 3.852367 -0.276674 0.131335
H 3.551624 -1.381886 -1.230249
H -3.690364 -0.460780 0.769960
H -2.666425 -1.887521 0.451484
H -3.835992 -1.342059 -0.772966

COMP. 18_E4ITS_M06-2X
C 1.194980 0.103644 0.592237
C -0.181430 -0.564199 0.795052
C -1.225713 0.426977 0.215065
C -0.403081 1.472410 -0.534201
C 0.867366 1.573662 0.308908
O 1.832494 -0.447699 -0.554944
O -2.159304 -0.165202 -0.658977
C 3.086726 -1.029144 -0.298175
C -3.075988 -1.002390 0.000906
H 1.846997 -0.017850 1.463091
H -0.207585 -1.501894 0.235961
H -0.368670 -0.784033 1.848073
H -1.773047 0.909901 1.039725
H -0.163050 1.070774 -1.522210
H -0.937424 2.414581 -0.657603
H 1.695711 2.078422 -0.189009
H 0.657709 2.092462 1.250926
H 3.005448 -1.866884 0.405919
H 3.795135 -0.295330 0.106895
H 3.470329 -1.402319 -1.247124
H -3.643352 -0.446307 0.759075
H -2.575351 -1.847842 0.488645
H -3.765521 -1.386235 -0.749746

COMP. 18_E4IT_MP2
C 1.210082 0.108664 0.574860
C -0.161551 -0.586667 0.766779
C -1.237996 0.406029 0.235540
C -0.447783 1.492477 -0.501777
C 0.861393 1.580465 0.289756
O 1.888571 -0.445402 -0.561816
O -2.189915 -0.171923 -0.646139
C 3.152194 -1.015399 -0.283603
C -3.135750 -1.006868 -0.007076
H 1.849954 0.003650 1.457130
H -0.180376 -1.507496 0.180349
H -0.331766 -0.847578 1.814436
H -1.778285 0.852773 1.085236
H -0.251745 1.142749 -1.519255
H -0.993390 2.436030 -0.564070
H 1.668434 2.087844 -0.241449
H 0.697477 2.106525 1.238308
H 3.075701 -1.859189 0.416520
H 3.852367 -0.276674 0.131335
H 3.551624 -1.381886 -1.230249
H -3.690364 -0.460780 0.769960
H -2.666425 -1.887521 0.451484
H -3.835992 -1.342059 -0.772966

COMP. 18_E4N_B3LYP
C 1.158891 -0.172147 0.576688
C -0.250738 -0.799004 0.485165
C -1.238325 0.369492 0.245669
C -0.375043 1.461115 -0.387550
C 0.943276 1.350781 0.385903
O 1.955071 -0.751176 -0.460973
O -2.329643 0.057178 -0.605852
C 3.345428 -0.536962 -0.314640
C -3.296885 -0.793771 -0.020394
H 1.643053 -0.385718 1.539050
H -0.268173 -1.461662 -0.383878
H -0.493373 -1.392973 1.368464
H -1.636178 0.727484 1.209578
H -0.226463 1.213424 -1.442957
H -0.838229 2.448242 -0.332768
H 1.786018 1.825652 -0.119998
H 0.845807 1.828144 1.367950
H 3.613418 0.526629 -0.365485
H 3.835849 -1.059276 -1.136786
H 3.712559 -0.944407 0.638339
H -2.891053 -1.789678 0.200078
H -3.697439 -0.363276 0.908886
H -4.108838 -0.897615 -0.740923

COMP. 18_E4N_M06-2X
C 1.144406 -0.172178 0.624963

C -0.282406 -0.753504 0.607195
C -1.222545 0.413922 0.230354
C -0.304756 1.433061 -0.432662
C 0.957892 1.343450 0.422157
O 1.855500 -0.760592 -0.453804
O -2.265945 0.055335 -0.645034
C 3.247007 -0.570363 -0.383641
C -3.217335 -0.792562 -0.049851
H 1.675869 -0.397816 1.558095
H -0.326224 -1.514000 -0.176490
H -0.545574 -1.222353 1.556406
H -1.659249 0.851460 1.142622
H -0.098011 1.092631 -1.451184
H -0.745529 2.429163 -0.478401
H 1.831000 1.814031 -0.031229
H 0.790148 1.821524 1.393192
H 3.524573 0.488974 -0.431921
H 3.685695 -1.085299 -1.237317
H 3.655318 -0.997325 0.541526
H -2.778014 -1.755423 0.237315
H -3.658085 -0.326851 0.841674
H -4.001930 -0.967621 -0.784672

COMP. 18_E4N_MP2
C 1.147462 -0.151462 0.659840
C -0.282863 -0.717017 0.692334
C -1.212962 0.426024 0.228669
C -0.286087 1.423954 -0.453384
C 0.970275 1.355042 0.412553
O 1.817127 -0.793181 -0.435672
O -2.228634 0.018528 -0.683574
C 3.226192 -0.590528 -0.425970
C -3.225820 -0.784283 -0.060745
H 1.709750 -0.364037 1.583184
H -0.340547 -1.547926 -0.019768
H -0.544960 -1.098763 1.685190
H -1.697637 0.903250 1.099689
H -0.075918 1.062372 -1.466526
H -0.727074 2.423105 -0.525551
H 1.851298 1.813872 -0.046550
H 0.798957 1.864418 1.371785
H 3.493791 0.464246 -0.565179
H 3.624687 -1.172675 -1.258041
H 3.663904 -0.949761 0.516037
H -2.810947 -1.732486 0.304496
H -3.691990 -0.248321 0.778439
H -3.978442 -0.990458 -0.823013

COMP. 18_E4OTS_B3LYP
C 1.210795 -0.183807 0.522284
C -0.112096 -0.949632 0.320587
C -1.220200 0.114618 0.218615
C -0.496577 1.322782 -0.389089
C 0.851045 1.319704 0.343379
O 2.140920 -0.656094 -0.454557
O -2.313507 -0.329031 -0.579636
C 3.484909 -0.301616 -0.193801
C -3.567379 -0.360251 0.074840
H 1.639994 -0.363191 1.517344
H -0.057542 -1.474833 -0.636106
H -0.298896 -1.691374 1.099608
H -1.587700 0.377337 1.220357
H -0.359834 1.135289 -1.458580
H -1.054714 2.255491 -0.278944
H 1.633933 1.862207 -0.190046
H 0.746867 1.789490 1.327943
H 3.818583 -0.693234 0.777958
H 3.640273 0.785503 -0.203402
H 4.090850 -0.747269 -0.983415
H -3.871302 0.636172 0.424218
H -3.565263 -1.049085 0.930792
H -4.297535 -0.712284 -0.655076

COMP. 18_E4OTS_M06-2X
C 1.208588 -0.193121 0.558563
C -0.122596 -0.949507 0.404133
C -1.207529 0.121539 0.218075
C -0.447699 1.285385 -0.415254
C 0.848204 1.302185 0.394013
O 2.080359 -0.644764 -0.465913
O -2.271378 -0.340034 -0.590007
C 3.424874 -0.291712 -0.255312
C -3.532321 -0.322160 0.033382
H 1.684847 -0.382817 1.528885
H -0.070799 -1.536747 -0.515368
H -0.328542 -1.628980 1.231860
H -1.599586 0.437996 1.194762
H -0.245873 1.029254 -1.459490
H -1.003156 2.224138 -0.387935
H 1.652960 1.866167 -0.079062
H 0.668289 1.745353 1.379016
H 3.801399 -0.720982 0.682195
H 3.567945 0.794939 -0.223579
H 3.999052 -0.695721 -1.088064
H -3.820759 0.694405 0.328368
H -3.551761 -0.967099 0.920624
H -4.254984 -0.697173 -0.690442

COMP. 18_E4OT_MP2
C 1.202025 -0.189841 0.544592
C -0.118350 -0.950327 0.346233
C -1.207431 0.119159 0.213572
C -0.466265 1.295867 -0.413665
C 0.845933 1.305486 0.370638
O 2.108619 -0.655254 -0.464969
O -2.294852 -0.335148 -0.595190
C 3.459306 -0.286057 -0.209045
C -3.550214 -0.333285 0.076178
H 1.654867 -0.385064 1.529790
H -0.061334 -1.491217 -0.605241
H -0.320201 -1.679656 1.137658
H -1.589914 0.412536 1.204728
H -0.290631 1.063993 -1.471231
H -1.026561 2.235353 -0.356518
H 1.649485 1.860705 -0.123283
H 0.690354 1.765547 1.356592
H 3.798473 -0.695026 0.753028
H 3.594191 0.803099 -0.201410
H 4.053554 -0.714662 -1.017227
H -3.830306 0.678993 0.397433
H -3.537526 -0.999176 0.949527
H -4.284610 -0.698215 -0.643589

COMP. 18_E4O_B3LYP
C 1.255817 -0.159553 0.566223
C -0.019576 -1.027283 0.536723
C -1.208909 -0.064183 0.397147
C -0.603268 1.173051 -0.290253
C 0.759747 1.300613 0.401983
O 2.092801 -0.581471 -0.514120
O -2.254124 -0.712398 -0.311034
C 3.428222 -0.124680 -0.426169
C -3.478290 -0.002476 -0.320185
H 1.816756 -0.282412 1.502279
H 0.016805 -1.660982 -0.352209
H -0.110032 -1.678397 1.407656
H -1.585907 0.226732 1.391773
H -0.474862 0.952663 -1.355067
H -1.215718 2.072803 -0.197345
H 1.471329 1.918531 -0.149191
H 0.637043 1.755471 1.391730
H 3.905893 -0.467998 0.502760
H 3.500830 0.970193 -0.471276
H 3.964959 -0.544537 -1.277594
H -3.402747 0.944657 -0.869640
H -3.824662 0.209919 0.701581
H -4.211551 -0.638622 -0.817039

COMP. 18_E4O_M06-2X
C 1.262341 -0.172862 0.619800
C -0.019957 -1.017987 0.709642
C -1.196255 -0.063451 0.458063

C -0.559493 1.146790 -0.237178
C 0.766284 1.280749 0.512069
O 1.956471 -0.572604 -0.552563
O -2.186402 -0.734134 -0.287189
C 3.285396 -0.116574 -0.605356
C -3.342506 0.038850 -0.497555
H 1.922218 -0.317970 1.484314
H -0.001375 -1.763347 -0.087367
H -0.110893 -1.539670 1.662412
H -1.635344 0.266534 1.413577
H -0.375874 0.888058 -1.284917
H -1.170921 2.049694 -0.196626
H 1.486202 1.935899 0.019983
H 0.589198 1.678596 1.517101
H 3.861632 -0.485876 0.252851
H 3.349313 0.977724 -0.624014
H 3.723795 -0.507315 -1.522725
H -3.139272 0.906089 -1.136446
H -3.760572 0.392265 0.454465
H -4.073512 -0.599857 -0.991511

COMP. 18_E4O_MP2
C 1.265205 -0.143115 0.655350
C -0.023947 -0.960140 0.824999
C -1.190032 -0.022220 0.477973
C -0.538300 1.155997 -0.255274
C 0.785878 1.307239 0.493611
O 1.905390 -0.621532 -0.536934
O -2.150011 -0.754131 -0.280417
C 3.244880 -0.160457 -0.675773
C -3.324975 0.003249 -0.550803
H 1.962845 -0.266245 1.499021
H -0.015426 -1.794725 0.116560
H -0.120151 -1.373322 1.834296
H -1.681841 0.348332 1.395945
H -0.356745 0.863241 -1.296806
H -1.145626 2.067425 -0.247634
H 1.514695 1.943215 -0.018526
H 0.610184 1.745572 1.486593
H 3.848433 -0.451565 0.195418
H 3.297797 0.928541 -0.799178
H 3.642746 -0.640702 -1.570865
H -3.116122 0.849690 -1.216714
H -3.772246 0.378866 0.380748
H -4.023831 -0.676329 -1.040546

COMP. 18_E5ITS_B3LYP
C 1.164337 0.132213 0.209260
C -0.097185 -0.740354 0.358887
C -1.281725 0.249026 0.524813
C -0.689256 1.652721 0.256638
C 0.641278 1.405638 -0.465663
O 2.176022 -0.520671 -0.552189
O -2.329499 0.025356 -0.418954
C 3.405722 -0.719168 0.119114
C -3.082218 -1.146588 -0.173934
H 1.565163 0.385181 1.200596
H -0.223301 -1.294354 -0.575673
H -0.014349 -1.465724 1.171447
H -1.714442 0.190234 1.533330
H -1.396032 2.256822 -0.313483
H -0.513149 2.161533 1.210158
H 0.476924 1.190098 -1.525868
H 1.340695 2.241966 -0.396105
H 3.289024 -1.354982 1.007552
H 3.863284 0.232184 0.423346
H 4.073717 -1.219366 -0.583305
H -3.530162 -1.128690 0.830435
H -2.476238 -2.057209 -0.270112
H -3.879035 -1.176102 -0.917859

COMP. 18_E5ITS_M06-2X
C 1.149514 0.137327 0.201717
C -0.099989 -0.732238 0.405031
C -1.280900 0.258652 0.542751
C -0.680649 1.650230 0.271811
C 0.604035 1.374254 -0.508739
O 2.141062 -0.535160 -0.547917
O -2.289155 0.027638 -0.425785
C 3.372155 -0.692161 0.114934
C -3.015553 -1.153087 -0.191592
H 1.563458 0.434984 1.175316
H -0.232433 -1.314299 -0.511450
H -0.003360 -1.427652 1.240485
H -1.741115 0.208531 1.538453
H -1.401398 2.274151 -0.255967
H -0.441759 2.135892 1.222704
H 0.378521 1.101369 -1.543753
H 1.308627 2.207291 -0.514785
H 3.262340 -1.283091 1.032715
H 3.817972 0.277282 0.369379
H 4.039896 -1.219113 -0.565653
H -3.501629 -1.125583 0.792730
H -2.376949 -2.043387 -0.241033
H -3.779113 -1.224054 -0.965003

COMP. 18_E5IT_MP2
C 1.164337 0.132213 0.209260
C -0.097185 -0.740354 0.358887
C -1.281725 0.249026 0.524813
C -0.689256 1.652721 0.256638
C 0.641278 1.405638 -0.465663
O 2.176022 -0.520671 -0.552189
O -2.329499 0.025356 -0.418954
C 3.405722 -0.719168 0.119114
C -3.082218 -1.146588 -0.173934
H 1.565163 0.385181 1.200596
H -0.223301 -1.294354 -0.575673
H -0.014349 -1.465724 1.171447
H -1.714442 0.190234 1.533330
H -1.396032 2.256822 -0.313483
H -0.513149 2.161533 1.210158
H 0.476924 1.190098 -1.525868
H 1.340695 2.241966 -0.396105
H 3.289024 -1.354982 1.007552
H 3.863284 0.232184 0.423346
H 4.073717 -1.219366 -0.583305
H -3.530162 -1.128690 0.830435
H -2.476238 -2.057209 -0.270112
H -3.879035 -1.176102 -0.917859

COMP. 18_E5I_MP2
C 1.075988 0.621777 0.227062
C 0.032876 -0.041485 1.155945
C -1.328536 0.313545 0.548317
C -1.094344 1.713619 -0.003786
C 0.284120 1.593301 -0.664411
O 1.744054 -0.311385 -0.628004
O -1.659372 -0.499737 -0.580420
C 2.767356 -1.036159 0.043010
C -1.993286 -1.840261 -0.244324
H 1.841263 1.151228 0.818583
H 0.200200 -1.118369 1.253350
H 0.089243 0.386526 2.166266
H -2.147784 0.261399 1.284657
H -1.886991 2.011493 -0.696945
H -1.074847 2.432317 0.826507
H 0.190446 1.129502 -1.651000
H 0.794164 2.554483 -0.785812
H 2.366167 -1.650041 0.860757
H 3.527824 -0.354668 0.450263
H 3.224650 -1.687987 -0.702918
H -2.781668 -1.867736 0.521600
H -1.122903 -2.403839 0.112870
H -2.362270 -2.301352 -1.161665

COMP. 18_E5N_B3LYP
C 1.134126 0.003888 0.421603
C -0.200337 -0.709394 0.707560
C -1.317684 0.352876 0.517582
C -0.578047 1.658120 0.170971
C 0.743893 1.203654 -0.460364

O 2.039786 -0.921767 -0.161245
O -2.185837 0.048636 -0.576002
C 3.365920 -0.441479 -0.279857
C -3.084961 -1.012171 -0.319968
H 1.572529 0.378256 1.361340
H -0.318494 -1.504455 -0.032727
H -0.211858 -1.172661 1.696264
H -1.931708 0.464875 1.421625
H -1.187977 2.288254 -0.477721
H -0.381179 2.217863 1.092008
H 0.579142 0.852051 -1.483885
H 1.499445 1.992200 -0.484806
H 3.764537 -0.124689 0.694712
H 3.439011 0.400413 -0.980043
H 3.970706 -1.266284 -0.658213
H -3.717137 -0.795224 0.553450
H -2.567023 -1.965007 -0.147815
H -3.719042 -1.113506 -1.201372

COMP. 18_E5N_M06-2X
C 1.118415 0.016612 0.463984
C -0.215111 -0.659279 0.817145
C -1.320382 0.381929 0.517849
C -0.565290 1.664707 0.157040
C 0.727758 1.158454 -0.482520
O 1.994066 -0.946055 -0.077473
O -2.094134 0.022892 -0.615203
C 3.274170 -0.435948 -0.361205
C -2.996223 -1.025099 -0.361973
H 1.580049 0.446883 1.367517
H -0.330447 -1.521105 0.155767
H -0.231596 -1.020268 1.846194
H -1.996048 0.527745 1.370403
H -1.168128 2.301351 -0.490151
H -0.335000 2.220537 1.071620
H 0.521909 0.739681 -1.472664
H 1.492913 1.930801 -0.576158
H 3.721459 0.026512 0.528681
H 3.244361 0.306505 -1.166881
H 3.894281 -1.274230 -0.675920
H -3.704839 -0.749385 0.430080
H -2.482683 -1.947475 -0.065121
H -3.545710 -1.210501 -1.283878

COMP. 18_E5N_MP2
C 0.995975 0.413370 0.577589
C -0.324690 0.191247 1.323959
C -1.415464 0.534431 0.308072
C -0.820547 1.742049 -0.403178
C 0.643189 1.324235 -0.625995
O 1.489134 -0.872528 0.183558
O -1.580570 -0.458562 -0.706609
C 2.794711 -0.800892 -0.377597
C -1.994014 -1.730113 -0.217404
H 1.752017 0.881120 1.230400
H -0.373855 -0.819830 1.737205
H -0.408144 0.894230 2.163607
H -2.389710 0.733164 0.784959
H -1.352869 1.967137 -1.332627
H -0.885999 2.620628 0.251892
H 0.715820 0.728840 -1.541542
H 1.317175 2.182900 -0.722004
H 3.500830 -0.348969 0.334239
H 2.806145 -0.221403 -1.309517
H 3.098305 -1.827231 -0.589010
H -2.841243 -1.628623 0.476121
H -1.171453 -2.256438 0.278868
H -2.310496 -2.302758 -1.090854

COMP. 18_E5OTS_B3LYP
C 1.193926 0.001930 0.444743
C -0.079505 -0.798992 0.787647
C -1.282936 0.143615 0.535228
C -0.650776 1.521223 0.253044
C 0.691631 1.184170 -0.407280
O 2.127364 -0.858560 -0.192305
O -2.017036 -0.289661 -0.619647
C 3.409334 -0.288767 -0.376813
C -3.374130 -0.607098 -0.381125
H 1.654996 0.395330 1.365516
H -0.147508 -1.654326 0.113294
H -0.054004 -1.178638 1.811288
H -1.962402 0.181215 1.392723
H -1.305353 2.142667 -0.360332
H -0.480369 2.045144 1.201424
H 0.531846 0.836587 -1.433017
H 1.382963 2.029531 -0.432298
H 3.836348 0.051845 0.577677
H 3.388464 0.558407 -1.074294
H 4.048136 -1.069206 -0.791713
H -3.936175 0.257038 0.000533
H -3.481214 -1.438214 0.329818
H -3.803621 -0.908101 -1.337665

COMP. 18_E5OTS_M06-2X
C 1.176551 0.118688 0.515733
C -0.088434 -0.511901 1.133897
C -1.284696 0.259550 0.549841
C -0.674262 1.578864 0.068876
C 0.658312 1.123393 -0.528999
O 1.994934 -0.903087 -0.011052
O -1.803491 -0.434949 -0.579411
C 3.210815 -0.422751 -0.528800
C -3.166662 -0.764637 -0.480493
H 1.747618 0.659976 1.286199
H -0.144165 -1.564256 0.853874
H -0.068503 -0.444899 2.223023
H -2.082262 0.408869 1.284600
H -1.326222 2.093190 -0.638193
H -0.500222 2.237940 0.926598
H 0.474088 0.583737 -1.462966
H 1.350103 1.944443 -0.723629
H 3.766823 0.144203 0.230149
H 3.053638 0.220471 -1.402543
H 3.799895 -1.288362 -0.828910
H -3.790900 0.131797 -0.373641
H -3.358371 -1.431563 0.369452
H -3.442808 -1.278486 -1.400630

COMP. 18_E5OT_MP2
C 1.193926 0.001930 0.444743
C -0.079505 -0.798992 0.787647
C -1.282936 0.143615 0.535228
C -0.650776 1.521223 0.253044
C 0.691631 1.184170 -0.407280
O 2.127364 -0.858560 -0.192305
O -2.017036 -0.289661 -0.619647
C 3.409334 -0.288767 -0.376813
C -3.374130 -0.607098 -0.381125
H 1.654996 0.395330 1.365516
H -0.147508 -1.654326 0.113294
H -0.054004 -1.178638 1.811288
H -1.962402 0.181215 1.392723
H -1.305353 2.142667 -0.360332
H -0.480369 2.045144 1.201424
H 0.531846 0.836587 -1.433017
H 1.382963 2.029531 -0.432298
H 3.836348 0.051845 0.577677
H 3.388464 0.558407 -1.074294
H 4.048136 -1.069206 -0.791713
H -3.936175 0.257038 0.000533
H -3.481214 -1.438214 0.329818
H -3.803621 -0.908101 -1.337665

COMP. 19_1T5IT_B3LYP
C -1.036875 0.050645 -0.088847
C 0.099610 -0.471633 0.800670
C 1.326002 0.379819 0.414488
C 0.746168 1.693026 -0.177807
C -0.787571 1.564611 -0.109909
O -2.322214 -0.280012 0.430761
O 2.126664 -0.231794 -0.602648

C -3.146470 -1.037389 -0.435205
C 2.991122 -1.246700 -0.129954
H -0.932563 -0.358773 -1.101498
H -0.179833 -0.282021 1.842716
H 0.276900 -1.543866 0.695801
H 1.966234 0.572195 1.285178
H 1.115003 2.575579 0.348336
H 1.093834 1.762283 -1.210983
H -1.180799 1.977913 0.824474
H -1.297805 2.069042 -0.933410
H -2.696429 -2.008629 -0.682376
H -3.360192 -0.500019 -1.369168
H -4.085812 -1.210787 0.091615
H 2.443798 -2.098255 0.295452
H 3.679907 -0.858301 0.633847
H 3.570235 -1.596182 -0.985509

COMP. 19_1T5I_B3LYP
C -1.101823 0.209080 -0.245797
C -0.025068 -0.534461 0.569130
C 1.258900 0.320035 0.420664
C 0.785464 1.701103 -0.097244
C -0.749622 1.680935 -0.030380
O -2.437639 -0.036679 0.167418
O 2.182571 -0.208919 -0.532999
C -2.938179 -1.306767 -0.206765
C 2.965092 -1.283315 -0.049329
H -1.003353 -0.045978 -1.312401
H -0.349361 -0.553203 1.615408
H 0.137435 -1.565923 0.250629
H 1.776028 0.407557 1.385310
H 1.226181 2.526921 0.464107
H 1.127729 1.791178 -1.131408
H -1.110414 1.973563 0.961363
H -1.222916 2.338473 -0.761987
H -2.398584 -2.125441 0.287130
H -2.880892 -1.453950 -1.294581
H -3.984043 -1.340697 0.100352
H 2.355193 -2.156575 0.218343
H 3.550812 -0.983979 0.831542
H 3.648141 -1.566822 -0.850829

COMP. 19_1T5I_M06-2X
C 1.077099 0.056640 0.608938
C -0.000003 -0.874637 0.000015
C -1.077093 0.056638 -0.608932
C -0.423760 1.435982 -0.637070
C 0.423766 1.435983 0.637072
O 2.216923 0.150667 -0.233963
O -2.216932 0.150673 0.233948
C 3.076369 -0.956798 -0.137578
C -3.076370 -0.956796 0.137570
H 1.399948 -0.276108 1.603203
H 0.448028 -1.518830 -0.759286
H -0.448040 -1.518812 0.759327
H -1.399926 -0.276120 -1.603200
H 0.227392 1.515176 -1.511055
H -1.175880 2.223743 -0.677063
H 1.175887 2.223744 0.677064
H -0.227383 1.515179 1.511059
H 2.581318 -1.891565 -0.428608
H 3.458091 -1.069599 0.885435
H 3.912855 -0.779223 -0.812382
H -2.581328 -1.891554 0.428648
H -3.458058 -1.069632 -0.885452
H -3.912880 -0.779203 0.812340

COMP. 19_1T5I_MP2
C -1.006553 0.036274 -0.526360
C -0.051341 -0.793862 0.368444
C 1.139802 0.127620 0.666795
C 0.538391 1.524346 0.595385
C -0.375477 1.429621 -0.628891
O -2.295765 0.196577 0.085173
O 2.131167 0.056610 -0.369039
C -3.068006 -0.997570 0.045594
C 2.989665 -1.070691 -0.241501
H -1.148962 -0.424251 -1.516437
H -0.569778 -1.038015 1.304323
H 0.263939 -1.736462 -0.091437
H 1.617565 -0.094030 1.634432
H -0.051744 1.714300 1.500796
H 1.314177 2.291800 0.514396
H -1.157319 2.194125 -0.666277
H 0.225408 1.499768 -1.541550
H -2.597243 -1.809981 0.614918
H -3.217792 -1.329588 -0.991593
H -4.033241 -0.757942 0.494114
H 2.440593 -2.017762 -0.322565
H 3.522457 -1.048065 0.719298
H 3.709835 -1.003824 -1.058280

COMP. 19_1T5N_B3LYP
C -1.014244 -0.168761 -0.134449
C 0.193154 -0.697319 0.642744
C 1.308201 0.351041 0.429568
C 0.582637 1.642013 -0.028959
C -0.925645 1.353507 0.075838
O -2.198201 -0.782304 0.353009
O 2.232346 -0.011569 -0.599701
C -3.348564 -0.534086 -0.433929
C 3.202117 -0.961142 -0.200980
H -0.904794 -0.399822 -1.205543
H -0.087796 -0.746520 1.700017
H 0.493065 -1.699942 0.333701
H 1.874443 0.511951 1.356300
H 0.886550 2.516238 0.549811
H 0.874031 1.822487 -1.066602
H -1.303703 1.579853 1.079064
H -1.512059 1.932337 -0.641026
H -3.195568 -0.850529 -1.475442
H -3.633027 0.525988 -0.426879
H -4.162008 -1.118411 -0.002432
H 2.753660 -1.923097 0.080250
H 3.795486 -0.591349 0.647493
H 3.862632 -1.119723 -1.054177

COMP. 19_1T5N_M06-2X
C -0.847822 -0.258911 -0.025814
C 0.212134 -0.402479 1.065025
C 1.353510 0.469947 0.544299
C 0.611546 1.725217 0.104237
C -0.660662 1.180133 -0.585108
O -2.124807 -0.497734 0.530470
O 1.956297 -0.075888 -0.618722
C -3.131570 -0.603810 -0.445977
C 2.718385 -1.235011 -0.384924
H -0.668111 -0.994109 -0.821030
H -0.179962 0.032714 1.989311
H 0.479244 -1.439304 1.270667
H 2.128554 0.664371 1.297283
H 0.347896 2.301685 0.994281
H 1.229353 2.353629 -0.536531
H -1.537547 1.784442 -0.343861
H -0.554125 1.170155 -1.670193
H -2.925739 -1.433387 -1.134855
H -3.228264 0.319379 -1.030585
H -4.070576 -0.794288 0.072150
H 2.091353 -2.101598 -0.146628
H 3.271464 -1.445814 -1.299760
H 3.431420 -1.079417 0.435334

COMP. 19_1T5N_MP2
C -0.969711 -0.359552 -0.360273
C 0.199192 -0.958671 0.446307
C 1.208744 0.179998 0.645120
C 0.354414 1.437489 0.559246
C -0.598700 1.115225 -0.594092
O -2.141042 -0.497518 0.461934
O 2.145429 0.250320 -0.441617
C -3.352021 -0.290929 -0.256909
C 3.201463 -0.695782 -0.325091

H -1.145236 -0.896437 -1.305334
H -0.199300 -1.298355 1.409791
H 0.649484 -1.824103 -0.050007
H 1.766009 0.095882 1.591384
H -0.207104 1.560383 1.493879
H 0.967266 2.329378 0.396506
H -1.484064 1.758381 -0.623895
H -0.071022 1.220594 -1.548702
H -3.437733 -1.006130 -1.086898
H -3.425795 0.728614 -0.655675
H -4.163446 -0.457524 0.453138
H 2.831965 -1.729306 -0.342392
H 3.767584 -0.534988 0.602932
H 3.856010 -0.535477 -1.183107

COMP. 19_1T5OT_B3LYP
C 1.274570 -0.049014 0.621151
C -0.018441 -0.826220 0.864331
C -1.031067 -0.196906 -0.092796
C -0.713231 1.310423 -0.001473
C 0.817873 1.385240 0.215501
O 1.982488 -0.707803 -0.434335
O -2.348144 -0.550453 0.304920
C 3.322225 -0.282703 -0.585032
C -3.349005 -0.211397 -0.636627
H 1.916795 -0.035900 1.511616
H 0.118181 -1.897686 0.714772
H -0.370851 -0.662526 1.888349
H -0.854818 -0.561087 -1.115594
H -1.038321 1.875229 -0.877698
H -1.248039 1.709898 0.866362
H 1.335498 1.680776 -0.699926
H 1.077692 2.121818 0.979527
H 3.894479 -0.437053 0.341174
H 3.396538 0.776195 -0.867580
H 3.762299 -0.886782 -1.379219
H -3.148141 -0.670108 -1.615184
H -3.440141 0.874547 -0.769836
H -4.293467 -0.597805 -0.251772

COMP. 19_2T1I_B3LYPT
C 1.275672 0.300850 0.587746
C -0.053184 -0.438791 0.797599
C -0.969263 0.125421 -0.308485
C -0.530051 1.595967 -0.479619
C 0.840792 1.730055 0.229740
O 2.010815 -0.219004 -0.525706
O -2.358263 0.085741 0.002768
C 2.711261 -1.418004 -0.257861
C -2.930526 -1.206502 -0.063112
H 1.917340 0.270338 1.478912
H 0.052664 -1.525308 0.774461
H -0.470646 -0.163066 1.772957
H -0.802822 -0.431836 -1.240064
H -0.473412 1.865547 -1.535285
H -1.287204 2.235111 -0.020749
H 1.601610 2.210357 -0.387021
H 0.744449 2.313906 1.149159
H 2.039206 -2.255578 -0.029159
H 3.409632 -1.291328 0.581730
H 3.278665 -1.662754 -1.156536
H -2.521083 -1.880589 0.700985
H -2.775870 -1.661795 -1.051786
H -4.001161 -1.090874 0.109854

COMP. 19_4EN_B3LYPT
C 1.153649 -0.102456 0.445477
C -0.227900 -0.791066 0.364423
C -1.190936 0.234780 -0.278465
C -0.554903 1.590472 0.032559
C 0.946942 1.324262 -0.127451
O 2.100700 -0.881254 -0.281810
O -2.517224 0.198318 0.227502
C 3.440911 -0.458531 -0.115306
C -3.269757 -0.920203 -0.204854
H 1.490338 -0.042864 1.490466
H -0.139139 -1.720315 -0.200151
H -0.597006 -1.036123 1.364304
H -1.223673 0.084020 -1.368745
H -0.928435 2.389792 -0.610726
H -0.799924 1.854686 1.067024
H 1.215161 1.305543 -1.189563
H 1.568230 2.079383 0.358759
H 3.730062 -0.460973 0.945637
H 3.612485 0.546373 -0.522606
H 4.068803 -1.167757 -0.655629
H -2.849551 -1.866133 0.160938
H -3.326976 -0.962436 -1.301867
H -4.276231 -0.803253 0.198322

COMP. 19_4EN_MP2
C 1.110879 -0.139372 0.350226
C -0.225882 -0.843332 0.065953
C -1.228045 0.269144 -0.316498
C -0.535251 1.573856 0.066415
C 0.940043 1.282098 -0.205170
O 2.158809 -0.895174 -0.256998
O -2.475780 0.188972 0.370648
C 3.451768 -0.388127 0.059972
C -3.287921 -0.879431 -0.106699
H 1.302871 -0.088191 1.436050
H -0.070623 -1.570830 -0.737965
H -0.590961 -1.384681 0.945645
H -1.425924 0.253165 -1.401909
H -0.929220 2.436570 -0.479834
H -0.707247 1.747293 1.136760
H 1.140214 1.258299 -1.285414
H 1.615465 2.014846 0.248675
H 3.595276 -0.336018 1.148516
H 3.613717 0.606986 -0.372499
H 4.170633 -1.088188 -0.367951
H -2.810650 -1.854145 0.057473
H -3.500151 -0.759528 -1.178315
H -4.221175 -0.834979 0.456366

COMP. 19_4T5I_B3LYPT
C 1.206970 0.258250 0.298659
C 0.000001 -0.675946 -0.000010
C -1.206973 0.258252 -0.298662
C -0.752614 1.655209 0.140586
C 0.752614 1.655209 -0.140584
O 2.401792 -0.087743 -0.389473
O -2.401788 -0.087746 0.389480
C 3.062989 -1.222504 0.137569
C -3.062991 -1.222503 -0.137564
H 1.414589 0.260072 1.379015
H 0.238171 -1.318673 -0.851315
H -0.238167 -1.318691 0.851282
H -1.414602 0.260079 -1.379015
H -1.296578 2.451446 -0.370933
H -0.948858 1.755850 1.213386
H 0.948858 1.755854 -1.213384
H 1.296578 2.451443 0.370938
H 2.453630 -2.132095 0.051759
H 3.325960 -1.075476 1.194853
H 3.977979 -1.357069 -0.440250
H -2.453631 -2.132095 -0.051768
H -3.325973 -1.075467 -1.194845
H -3.977974 -1.357072 0.440264

COMP. 19_4T5I_M06-2X
C -1.199971 0.275379 -0.294083
C 0.000004 -0.659423 -0.000049
C 1.199961 0.275373 0.294071
C 0.745557 1.659651 -0.163425
C -0.745557 1.659650 0.163429
O -2.385656 -0.083764 0.379222
O 2.385681 -0.083747 -0.379183
C -2.982096 -1.246933 -0.140945
C 2.982084 -1.246944 0.140965
H -1.398361 0.293610 -1.375914
H -0.239957 -1.300036 0.852221

H 0.239982 -1.299943 -0.852384
H 1.398294 0.293578 1.375912
H 1.307574 2.462743 0.313410
H 0.905191 1.727722 -1.244296
H -0.905187 1.727705 1.244302
H -1.307573 2.462751 -0.313391
H -2.321221 -2.117488 -0.047717
H -3.242329 -1.116425 -1.199344
H -3.891192 -1.430345 0.430068
H 2.321217 -2.117493 0.047641
H 3.242239 -1.116492 1.199390
H 3.891222 -1.430324 -0.429991

COMP. 19_4T5I_MP2
C -1.198137 -0.271349 0.296920
C 0.000000 0.661557 -0.000001
C 1.198137 -0.271349 -0.296920
C 0.746982 -1.656152 0.158740
C -0.746982 -1.656152 -0.158740
O -2.394241 0.082333 -0.395130
O 2.394241 0.082334 0.395131
C -3.011499 1.244621 0.149363
C 3.011500 1.244621 -0.149362
H -1.411941 -0.285923 1.379262
H -0.245341 1.305198 -0.852869
H 0.245341 1.305200 0.852866
H 1.411942 -0.285923 -1.379262
H 1.308582 -2.459849 -0.327234
H 0.918344 -1.732351 1.240383
H -0.918344 -1.732351 -1.240383
H -1.308583 -2.459849 0.327235
H -2.364232 2.126550 0.057606
H -3.263792 1.093060 1.208191
H -3.925830 1.407254 -0.422933
H 2.364232 2.126550 -0.057607
H 3.263794 1.093059 -1.208190
H 3.925830 1.407254 0.422934

COMP. 19_4T5O_B3LYPT
C -1.195844 -0.154737 -0.327427
C -0.000001 -1.072087 0.000012
C 1.195848 -0.154736 0.327435
C 0.756328 1.254398 -0.126230
C -0.756328 1.254398 0.126240
O -2.358470 -0.652164 0.324088
O 2.358465 -0.652165 -0.324092
C -3.560601 -0.020768 -0.074660
C 3.560601 -0.020769 0.074639
H -1.382889 -0.144599 -1.411947
H -0.262826 -1.715691 0.841190
H 0.262821 -1.715709 -0.841153
H 1.382906 -0.144597 1.411953
H 1.275616 2.063606 0.392253
H 0.966115 1.353406 -1.197578
H -0.966116 1.353404 1.197588
H -1.275617 2.063605 -0.392244
H -3.707719 -0.093575 -1.161821
H -3.587503 1.038373 0.212765
H -4.376100 -0.541287 0.428589
H 3.707733 -0.093572 1.161798
H 3.587500 1.038372 -0.212789
H 4.376094 -0.541289 -0.428619

COMP. 19_4T5O_M06-2X
C 1.184605 -0.180126 0.341888
C -0.000001 -1.097636 0.000009
C -1.184600 -0.180121 -0.341879
C -0.752817 1.218041 0.131093
C 0.752818 1.218044 -0.131058
O 2.350290 -0.671722 -0.283706
O -2.350296 -0.671725 0.283687
C 3.508119 0.051357 0.055996
C -3.508119 0.051358 -0.056026
H 1.351221 -0.156460 1.429331
H 0.279320 -1.737890 -0.837411
H -0.279328 -1.737876 0.837438
H -1.351195 -0.156439 -1.429325
H -1.276609 2.033174 -0.370800
H -0.953150 1.291676 1.206193
H 0.953149 1.291698 -1.206157
H 1.276610 2.033169 0.370848
H 3.651138 0.079003 1.144272
H 3.469160 1.080619 -0.319802
H 4.354676 -0.459108 -0.401186
H -3.651118 0.079020 -1.144304
H -3.469168 1.080615 0.319787
H -4.354684 -0.459113 0.401133

COMP. 19_4T5O_MP2
C 1.183783 0.168280 -0.341410
C 0.000000 1.085257 0.000000
C -1.183783 0.168280 0.341411
C -0.753069 -1.227784 -0.131897
C 0.753069 -1.227784 0.131897
O 2.352906 0.676261 0.301308
O -2.352906 0.676261 -0.301308
C 3.530655 -0.036050 -0.064598
C -3.530655 -0.036050 0.064598
H 1.365908 0.149098 -1.429969
H 0.280502 1.729752 0.839036
H -0.280502 1.729753 -0.839035
H -1.365909 0.149098 1.429969
H -1.279034 -2.046729 0.370228
H -0.956627 -1.303681 -1.209154
H 0.956627 -1.303681 1.209155
H 1.279034 -2.046729 -0.370227
H 3.662474 -0.039482 -1.155887
H 3.507682 -1.071241 0.298311
H 4.365779 0.489750 0.400276
H -3.662474 -0.039482 1.155886
H -3.507682 -1.071241 -0.298312
H -4.365778 0.489750 -0.400277

COMP. 19_5T4IT_B3LYP
C 1.102711 -0.105901 0.535713
C -0.131357 -0.923425 0.092767
C -1.126367 0.088249 -0.548738
C -0.399356 1.442079 -0.521819
C 0.577375 1.330507 0.657937
O 2.111626 -0.156239 -0.486522
O -2.327576 0.223344 0.218628
C 3.356882 -0.679154 -0.068974
C -3.227825 -0.856386 0.073093
H 1.524445 -0.478701 1.474889
H 0.171644 -1.716903 -0.592820
H -0.607226 -1.389365 0.959853
H -1.401344 -0.204303 -1.570340
H 0.162624 1.569088 -1.450843
H -1.112817 2.262731 -0.434956
H 1.388524 2.060651 0.631473
H 0.039535 1.444855 1.604804
H 3.270109 -1.720422 0.272160
H 3.801520 -0.080984 0.738697
H 4.022299 -0.648801 -0.932995
H -2.807740 -1.803688 0.438151
H -3.522851 -0.989391 -0.977884
H -4.113497 -0.617424 0.663087

COMP. 19_5T4IT_M06-2X
C 1.089017 -0.121238 0.551034
C -0.143593 -0.932691 0.117967
C -1.106014 0.082323 -0.555684
C -0.358671 1.418950 -0.534710
C 0.559116 1.305911 0.685595
O 2.066305 -0.151115 -0.486074
O -2.298496 0.246925 0.198481
C 3.316128 -0.657627 -0.088405
C -3.189013 -0.831933 0.065337
H 1.528315 -0.501922 1.478632
H 0.154993 -1.750821 -0.538751
H -0.639348 -1.355801 0.995354
H -1.375637 -0.220045 -1.574975

H 0.251358 1.508278 -1.436163
H -1.061083 2.251183 -0.495068
H 1.368400 2.036983 0.702683
H -0.025949 1.397343 1.605366
H 3.238537 -1.697674 0.253053
H 3.756561 -0.054561 0.715615
H 3.972801 -0.619968 -0.957023
H -2.750561 -1.774284 0.417027
H -3.495472 -0.960778 -0.980973
H -4.067209 -0.606580 0.669170

COMP. 19_5T4I_B3LYP
C 1.093966 0.066720 0.597542
C -0.000098 -0.861807 0.000784
C -1.093693 0.066524 -0.597237
C -0.457558 1.460422 -0.616115
C 0.457885 1.460622 0.616064
O 2.253446 0.135891 -0.239940
O -2.253772 0.136170 0.239373
C 3.111648 -0.981924 -0.135443
C -3.111818 -0.981776 0.134972
H 1.407493 -0.259422 1.597994
H 0.434390 -1.510447 -0.763588
H -0.435011 -1.508932 0.766204
H -1.406534 -0.260121 -1.597737
H 0.141584 1.574366 -1.523972
H -1.221134 2.239661 -0.605053
H 1.221449 2.239872 0.604751
H -0.141231 1.574816 1.523913
H 2.628799 -1.913571 -0.460925
H 3.465981 -1.116394 0.896787
H 3.968292 -0.789699 -0.782545
H -2.629138 -1.913174 0.461418
H -3.465375 -1.116946 -0.897432
H -3.968955 -0.789192 0.781315

COMP. 19_5T4I_M06-2X
C -1.077096 0.056637 -0.608930
C -0.000001 -0.874637 0.000006
C 1.077098 0.056639 0.608933
C 0.423768 1.435985 0.637068
C -0.423765 1.435983 -0.637068
O -2.216927 0.150668 0.233959
O 2.216925 0.150666 -0.233963
C -3.076375 -0.956795 0.137569
C 3.076373 -0.956797 -0.137573
H -1.399935 -0.276116 -1.603197
H -0.448036 -1.518816 0.759317
H 0.448031 -1.518828 -0.759297
H 1.399943 -0.276110 1.603199
H -0.227376 1.515185 1.511058
H 1.175890 2.223745 0.677055
H -1.175887 2.223743 -0.677058
H 0.227379 1.515181 -1.511059
H -2.581334 -1.891560 0.428623
H -3.458078 -1.069607 -0.885450
H -3.912874 -0.779208 0.812354
H 2.581332 -1.891563 -0.428619
H 3.458082 -1.069602 0.885445
H 3.912869 -0.779212 -0.812363

COMP. 19_5T4I_MP2
C 1.071718 0.054408 0.613043
C -0.000116 -0.875949 0.000804
C -1.071433 0.054215 -0.612734
C -0.423869 1.434975 -0.636429
C 0.424213 1.435175 0.636413
O 2.221378 0.157179 -0.242326
O -2.221744 0.157490 0.241701
C 3.091615 -0.962500 -0.132712
C -3.091761 -0.962374 0.132235
H 1.403860 -0.279953 1.608390
H 0.453339 -1.525044 -0.756790
H -0.454029 -1.523473 0.759474
H -1.402853 -0.280646 -1.608151
H 0.224373 1.526203 -1.515826
H -1.184085 2.220946 -0.674078
H 1.184410 2.221177 0.673813
H -0.224004 1.526628 1.515813
H 2.599842 -1.897252 -0.433072
H 3.460557 -1.069367 0.897013
H 3.931131 -0.768954 -0.802065
H -2.600108 -1.896845 0.433666
H -3.459882 -1.070045 -0.897701
H -3.931825 -0.768438 0.800787

COMP. 19_5T4N_B3LYP
C -1.010492 -0.348761 -0.408055
C 0.204821 -0.989145 0.304164
C 1.198092 0.154317 0.618892
C 0.342804 1.421782 0.551454
C -0.632327 1.135553 -0.599482
O -2.142370 -0.519326 0.454399
O 2.218705 0.276801 -0.378839
C -3.389781 -0.283051 -0.168299
C 3.260630 -0.670883 -0.263233
H -1.231418 -0.837054 -1.366059
H -0.152113 -1.465178 1.220277
H 0.673506 -1.762748 -0.306978
H 1.679081 0.024076 1.597276
H -0.206690 1.534619 1.490951
H 0.958006 2.310565 0.401976
H -1.507535 1.788548 -0.603391
H -0.119756 1.260165 -1.557592
H -3.534266 -0.946152 -1.033370
H -3.501042 0.756351 -0.503941
H -4.161099 -0.494230 0.573383
H 2.906968 -1.702117 -0.397596
H 3.757795 -0.598640 0.714841
H 3.985399 -0.446871 -1.046895

COMP. 19_5T4N_M06-2X
C -1.022419 -0.376104 -0.489676
C 0.233827 -1.036395 0.106317
C 1.142275 0.114264 0.600908
C 0.250950 1.353153 0.559361
C -0.634595 1.098197 -0.662345
O -2.067079 -0.535055 0.461433
O 2.221770 0.347450 -0.293566
C -3.343611 -0.223455 -0.039170
C 3.264159 -0.586109 -0.164969
H -1.331693 -0.842959 -1.433160
H -0.071293 -1.704881 0.912577
H 0.758135 -1.627726 -0.646484
H 1.548088 -0.077316 1.601755
H -0.366815 1.386421 1.460125
H 0.847512 2.263341 0.499936
H -1.499463 1.759647 -0.727675
H -0.045337 1.213442 -1.576011
H -3.579551 -0.834584 -0.919978
H -3.436678 0.833809 -0.312105
H -4.061685 -0.445011 0.749510
H 2.931404 -1.609789 -0.376566
H 3.690443 -0.561602 0.846325
H 4.035878 -0.313263 -0.883745

COMP. 19_5T4N_MP2
C -0.969715 -0.359553 -0.360284
C 0.199194 -0.958682 0.446283
C 1.208739 0.179990 0.645119
C 0.354406 1.437480 0.559252
C -0.598699 1.115224 -0.594095
O -2.141038 -0.497518 0.461933
O 2.145432 0.250327 -0.441610
C -3.352024 -0.290922 -0.256897
C 3.201472 -0.695768 -0.325081
H -1.145251 -0.896432 -1.305346
H -0.199295 -1.298394 1.409759
H 0.649493 -1.824097 -0.050053
H 1.765996 0.095865 1.591387
H -0.207119 1.560364 1.493881
H 0.967258 2.329371 0.396525

H -1.484061 1.758382 -0.623903
H -0.071013 1.220594 -1.548700
H -3.437745 -1.006118 -1.086889
H -3.425801 0.728624 -0.655656
H -4.163442 -0.457519 0.453158
H 2.831980 -1.729294 -0.342383
H 3.767589 -0.534972 0.602944
H 3.856021 -0.535461 -1.183095

COMP. 19_5T4OT_B3LYP
C -1.075648 -0.312473 -0.409682
C 0.083386 -1.097967 0.249062
C 1.197619 -0.078409 0.554343
C 0.452875 1.259502 0.651277
C -0.591353 1.155441 -0.470604
O -2.229658 -0.479458 0.423341
O 2.127270 -0.024034 -0.540915
C -3.447917 -0.107480 -0.190463
C 3.468427 -0.310260 -0.197873
H -1.314985 -0.695762 -1.409725
H -0.298988 -1.540585 1.172048
H 0.459756 -1.902715 -0.384019
H 1.738086 -0.325535 1.473779
H -0.043309 1.329254 1.625011
H 1.128570 2.110746 0.547467
H -1.414370 1.865655 -0.367852
H -0.111118 1.338741 -1.435860
H -3.623543 -0.685982 -1.108814
H -3.482081 0.961168 -0.440539
H -4.243808 -0.324161 0.523188
H 3.580806 -1.328911 0.199266
H 3.862041 0.400488 0.542324
H 4.057700 -0.224580 -1.112042

COMP. 19_5T4OT_M06-2X
C -1.073346 -0.331503 -0.446938
C 0.091617 -1.133231 0.169811
C 1.172517 -0.107568 0.547014
C 0.401606 1.206119 0.673317
C -0.569216 1.121064 -0.507664
O -2.185165 -0.466486 0.429699
O 2.110244 0.014935 -0.520402
C -3.404663 -0.058948 -0.138753
C 3.440895 -0.253472 -0.154499
H -1.359536 -0.708105 -1.436334
H -0.290860 -1.646593 1.054033
H 0.500627 -1.875970 -0.515390
H 1.698962 -0.381372 1.466595
H -0.155612 1.215308 1.614627
H 1.066091 2.070510 0.642367
H -1.382857 1.846160 -0.462604
H -0.020144 1.276791 -1.439583
H -3.631106 -0.641565 -1.041067
H -3.405135 1.005244 -0.401658
H -4.182210 -0.236121 0.603416
H 3.559367 -1.283496 0.204947
H 3.789540 0.434373 0.626237
H 4.055772 -0.117523 -1.043686

COMP. 19_5T4O_B3LYP
C -1.137694 -0.321782 -0.502493
C 0.000000 -1.234688 0.000002
C 1.137695 -0.321782 0.502495
C 0.506458 1.081568 0.576768
C -0.506458 1.081568 -0.576764
O -2.196471 -0.387984 0.461826
O 2.196469 -0.387980 -0.461829
C -3.427532 0.144264 0.014032
C 3.427533 0.144262 -0.014036
H -1.532098 -0.648925 -1.473296
H -0.386956 -1.874798 0.794489
H 0.386955 -1.874802 -0.794482
H 1.532104 -0.648925 1.473295
H -0.015551 1.190520 1.532431
H 1.246613 1.881782 0.510528
H -1.246612 1.881783 -0.510525
H 0.015553 1.190520 -1.532426
H -3.773057 -0.365256 -0.896948
H -3.370478 1.221581 -0.189868
H -4.154552 -0.021274 0.810094
H 3.773058 -0.365263 0.896941
H 3.370483 1.221578 0.189869
H 4.154550 -0.021275 -0.810100

COMP. 19_5T4O_M06-2X
C -1.125441 -0.343120 -0.510278
C -0.000001 -1.258715 0.000002
C 1.125442 -0.343123 0.510280
C 0.476864 1.044830 0.598473
C -0.476860 1.044832 -0.598467
O -2.163900 -0.372068 0.460922
O 2.163898 -0.372071 -0.460923
C -3.372990 0.190388 0.015450
C 3.372988 0.190389 -0.015457
H -1.532724 -0.678234 -1.472001
H -0.398927 -1.894688 0.790852
H 0.398923 -1.894691 -0.790848
H 1.532727 -0.678238 1.472001
H -0.096243 1.116040 1.526820
H 1.205245 1.856662 0.583217
H -1.205238 1.856666 -0.583210
H 0.096248 1.116043 -1.526814
H -3.734774 -0.320557 -0.886192
H -3.278452 1.260166 -0.203482
H -4.102524 0.060716 0.814040
H 3.734771 -0.320544 0.886192
H 3.278450 1.260170 0.203461
H 4.102523 0.060707 -0.814045

COMP. 19_5T4O_MP2
C -1.119061 -0.343245 -0.519069
C 0.000000 -1.258067 0.000002
C 1.119062 -0.343247 0.519071
C 0.476571 1.045791 0.598210
C -0.476569 1.045792 -0.598205
O -2.167290 -0.385182 0.464335
O 2.167288 -0.385182 -0.464337
C -3.383596 0.200464 0.013347
C 3.383596 0.200464 -0.013352
H -1.530151 -0.680919 -1.483309
H -0.406664 -1.898762 0.789224
H 0.406662 -1.898765 -0.789218
H 1.530155 -0.680922 1.483309
H -0.094357 1.130933 1.531005
H 1.212090 1.856264 0.577945
H -1.212088 1.856266 -0.577938
H 0.094359 1.130937 -1.531000
H -3.729893 -0.285373 -0.909628
H -3.282768 1.277931 -0.166551
H -4.115048 0.037525 0.806370
H 3.729895 -0.285372 0.909621
H 3.282768 1.277931 0.166544
H 4.115045 0.037525 -0.806378

COMP. 19_E2N_B3LYPT
C -0.918883 -0.206379 -0.066003
C 0.193791 -0.499841 0.942078
C 1.341651 0.418089 0.504940
C 0.635962 1.714613 0.062458
C -0.815526 1.319497 -0.320771
O -2.164945 -0.633449 0.469395
O 2.042399 -0.098158 -0.633018
C -3.226032 -0.627978 -0.467098
C 2.958709 -1.134093 -0.335794
H -0.726832 -0.754280 -0.998927
H -0.155304 -0.205935 1.938318
H 0.464079 -1.556314 0.984563
H 2.065802 0.594184 1.311502
H 0.637645 2.433486 0.885398
H 1.189101 2.162840 -0.764001
H -1.541787 1.824631 0.322477
H -1.052045 1.582867 -1.353319

H -2.993777 -1.258976 -1.336864
H -3.458456 0.384976 -0.821138
H -4.102691 -1.032249 0.040333
H 2.463612 -2.036288 0.046001
H 3.704082 -0.805340 0.402517
H 3.468900 -1.384190 -1.266741

COMP. 19_E2N_M06-2X
C -0.918535 -0.199025 -0.060550
C 0.209581 -0.509346 0.913980
C 1.329223 0.430019 0.460393
C 0.599299 1.699404 -0.033580
C -0.897729 1.334960 -0.121937
O -2.124991 -0.755579 0.409192
O 2.041720 -0.105040 -0.647237
C -3.198947 -0.603025 -0.487327
C 2.991864 -1.079771 -0.293086
H -0.679957 -0.618409 -1.049158
H -0.128186 -0.238279 1.919837
H 0.494737 -1.561664 0.922504
H 2.042810 0.646250 1.264775
H 0.767710 2.542969 0.636575
H 1.017625 1.963135 -1.005403
H -1.443448 1.700928 0.753808
H -1.376817 1.744659 -1.011865
H -2.950182 -1.013448 -1.474532
H -3.483515 0.448980 -0.604644
H -4.044349 -1.153275 -0.076172
H 2.530389 -1.965922 0.157183
H 3.727882 -0.671833 0.411621
H 3.502933 -1.378430 -1.207526

COMP. 19_E3O_B3LYP
C 1.271806 -0.069031 0.597582
C -0.018955 -0.875898 0.779177
C -1.052799 -0.187983 -0.114341
C -0.731790 1.308566 0.071345
C 0.808116 1.365550 0.190739
O 2.045124 -0.702077 -0.431774
O -2.364904 -0.573430 0.285980
C 3.384097 -0.233938 -0.536686
C -3.399792 -0.178652 -0.606955
H 1.871940 -0.055310 1.518008
H 0.132372 -1.929158 0.542347
H -0.369071 -0.802045 1.814089
H -0.897198 -0.480696 -1.164584
H -1.109833 1.939538 -0.735844
H -1.207443 1.637866 1.001436
H 1.263256 1.618677 -0.769979
H 1.130882 2.123569 0.908187
H 3.929628 -0.371292 0.409872
H 3.437015 0.828099 -0.816639
H 3.872588 -0.823447 -1.315748
H -3.221760 -0.564856 -1.621873
H -3.506412 0.913622 -0.661308
H -4.331821 -0.602198 -0.226774

COMP. 19_E4IT_MP2
C 1.118023 -0.066305 0.608014
C -0.168533 -0.856829 0.368208
C -1.058408 0.067859 -0.498953
C -0.344221 1.428240 -0.527631
C 0.642380 1.382712 0.644041
O 1.987503 -0.233362 -0.527922
O -2.351874 0.269905 0.089793
C 3.273410 -0.736807 -0.185188
C -3.172920 -0.888651 -0.000358
H 1.641607 -0.379493 1.521984
H 0.043167 -1.828665 -0.089464
H -0.677405 -1.025654 1.326251
H -1.199798 -0.337406 -1.512823
H 0.209265 1.534566 -1.466339
H -1.077412 2.237929 -0.463369
H 1.474039 2.088210 0.547161
H 0.125958 1.578597 1.592973
H 3.202656 -1.730543 0.277938
H 3.798452 -0.056871 0.499523
H 3.835289 -0.813177 -1.117528
H -2.752000 -1.733519 0.560591
H -3.308133 -1.189083 -1.049124
H -4.139100 -0.618545 0.428457

COMP. 19_E4I_MP2
C -1.030171 0.037259 -0.560821
C -0.033706 -0.841992 0.236640
C 1.114700 0.094788 0.651498
C 0.489134 1.482973 0.620517
C -0.386565 1.423095 -0.632533
O -2.272434 0.190155 0.143930
O 2.165581 0.099436 -0.327194
C -3.088790 -0.972408 0.070336
C 3.042888 -1.013561 -0.204276
H -1.245846 -0.375233 -1.558788
H -0.538059 -1.239216 1.125847
H 0.337702 -1.695380 -0.340910
H 1.543739 -0.167492 1.631555
H -0.133863 1.625796 1.512165
H 1.255056 2.264040 0.596284
H -1.157219 2.198077 -0.683001
H 0.243776 1.494875 -1.525544
H -2.609502 -1.841897 0.539532
H -3.324053 -1.216739 -0.975213
H -4.010139 -0.738895 0.605926
H 2.521903 -1.967580 -0.358510
H 3.521876 -1.024745 0.784691
H 3.804517 -0.893264 -0.976100

COMP. 19_E4OT_MP2
C -1.037115 -0.318837 -0.369424
C 0.074846 -1.084836 0.372408
C 1.203084 -0.077026 0.592073
C 0.472957 1.259411 0.687567
C -0.557494 1.145172 -0.440272
O -2.230386 -0.464012 0.418645
O 2.046853 -0.050994 -0.575879
C -3.409418 -0.099564 -0.290374
C 3.416009 -0.310239 -0.288830
H -1.230303 -0.733335 -1.370611
H -0.337871 -1.415042 1.333514
H 0.428910 -1.964990 -0.172791
H 1.809133 -0.308781 1.478591
H -0.029958 1.336919 1.660470
H 1.156239 2.107872 0.577297
H -1.389639 1.850164 -0.344500
H -0.066562 1.328560 -1.402693
H -3.528051 -0.718167 -1.190877
H -3.402971 0.958164 -0.582826
H -4.244873 -0.278935 0.388023
H 3.550232 -1.309977 0.146374
H 3.828723 0.440301 0.399171
H 3.948040 -0.257192 -1.240154

COMP. 19_E4O_MP2
C -1.074549 -0.297326 -0.456207
C -0.023183 -1.252607 0.137913
C 1.163167 -0.387834 0.565561
C 0.548105 0.999672 0.762550
C -0.428590 1.096676 -0.411253
O -2.228077 -0.377709 0.398864
O 2.094564 -0.407848 -0.527866
C -3.393630 0.194992 -0.183470
C 3.341640 0.205024 -0.219156
H -1.376049 -0.585417 -1.474979
H -0.473613 -1.754875 1.001250
H 0.308353 -2.016649 -0.571850
H 1.667999 -0.771230 1.466634
H 0.000254 1.016623 1.713484
H 1.288608 1.805416 0.789287
H -1.171828 1.892619 -0.299480
H 0.124283 1.277886 -1.340366
H -3.638242 -0.302546 -1.132295
H -3.278545 1.271143 -0.364456

H -4.203501 0.036729 0.530283
H 3.781086 -0.240861 0.684180
H 3.246076 1.287957 -0.073312
H 3.995461 0.016084 -1.071998

COMP. 19_E5N_M06-2X
C -1.084648 -0.166268 -0.283546
C 0.220819 -0.848009 0.145027
C 1.254924 0.288267 0.343385
C 0.528161 1.574416 -0.060990
C -0.943713 1.276774 0.220312
O -2.178109 -0.880651 0.247378
O 2.415454 0.149967 -0.449446
C -3.425071 -0.383729 -0.174892
C 3.283303 -0.854919 0.015433
H -1.166133 -0.152414 -1.381386
H 0.027215 -1.391454 1.072331
H 0.569885 -1.564332 -0.600628
H 1.556127 0.341108 1.399125
H 0.911622 2.454525 0.455337
H 0.687605 1.717436 -1.134248
H -1.147226 1.288076 1.297212
H -1.621592 1.980431 -0.265393
H -3.488862 -0.356462 -1.270535
H -3.612761 0.623780 0.214062
H -4.189166 -1.058235 0.209113
H 2.800966 -1.839985 0.016736
H 3.630907 -0.634466 1.032999
H 4.140006 -0.881728 -0.656563

COMP. 20_1E_B3LYP
O -0.065120 -1.120170 -0.134229
C -0.768441 0.013251 0.366861
C 0.067191 1.217377 -0.057218
C 1.512622 0.679558 -0.036373
C 1.336432 -0.862294 -0.007770
O -2.044035 0.067896 -0.198228
H -0.840076 -0.072167 1.464663
H -0.246275 1.491814 -1.066672
H -0.085377 2.077359 0.596317
H 2.073453 1.006397 -0.912993
H 2.057763 1.021883 0.845764
H 1.834939 -1.372189 -0.833314
H 1.709948 -1.285642 0.933235
H -2.517967 -0.736622 0.039655

COMP. 20_1E_M06-2X
O -0.071419 -1.105345 -0.161753
C -0.756201 0.016424 0.359727
C 0.071115 1.211415 -0.085297
C 1.508928 0.673016 -0.015180
C 1.319332 -0.865252 -0.000886
O -2.038245 0.072236 -0.167418
H -0.789172 -0.068837 1.458821
H -0.224396 1.439062 -1.110924
H -0.098433 2.090953 0.534466
H 2.103752 1.001377 -0.866534
H 2.016639 1.005441 0.891055
H 1.834952 -1.372803 -0.815295
H 1.662761 -1.292756 0.947873
H -2.487840 -0.751182 0.043718

COMP. 20_1E_MP2
O -0.061267 -1.106749 -0.208370
C -0.757718 -0.006643 0.359647
C 0.071764 1.221239 -0.003033
C 1.508969 0.666644 -0.108487
C 1.313532 -0.855677 0.067956
O -2.034731 0.081843 -0.188440
H -0.808240 -0.155020 1.452549
H -0.290672 1.583469 -0.967834
H -0.035332 2.018061 0.735777
H 1.944010 0.894727 -1.083536
H 2.171005 1.071749 0.660621
H 1.902955 -1.460158 -0.622561
H 1.549234 -1.159485 1.098091
H -2.484251 -0.747465 0.004882

COMP. 20_2E_B3LYP
O 0.009593 -1.153703 0.421811
C -0.841935 -0.027413 0.479130
C 0.077952 1.187173 0.479990
C 1.210197 0.722129 -0.451729
C 1.275607 -0.789304 -0.176630
O -1.677426 0.056842 -0.666231
H -1.450928 -0.142174 1.381015
H -0.434020 2.085261 0.135422
H 0.447210 1.357819 1.494853
H 0.939721 0.913217 -1.491459
H 2.159633 1.219930 -0.247750
H 1.423982 -1.379755 -1.083777
H 2.061008 -1.048336 0.539713
H -2.134870 -0.786587 -0.757224

COMP. 20_2E_M06-2X
O -0.009070 -1.142655 -0.447928
C 0.840087 -0.025718 -0.481813
C -0.079962 1.182692 -0.497045
C -1.181096 0.719417 0.463662
C -1.249239 -0.788762 0.182361
O 1.627594 0.054360 0.684203
H 1.473165 -0.135424 -1.365948
H 0.433263 2.087722 -0.176861
H -0.470890 1.323447 -1.506981
H -0.872607 0.903951 1.492756
H -2.135985 1.214532 0.290245
H -1.372306 -1.380071 1.091296
H -2.053052 -1.042041 -0.513039
H 2.071478 -0.791527 0.795350

COMP. 20_2E_MP2
O -0.010522 -1.145718 -0.475880
C 0.841659 -0.024721 -0.483012
C -0.079238 1.181199 -0.508925
C -1.176707 0.723362 0.460754
C -1.236547 -0.791734 0.202243
O 1.609910 0.058631 0.704077
H 1.490416 -0.135302 -1.357379
H 0.430823 2.095243 -0.201148
H -0.474338 1.303520 -1.521663
H -0.870527 0.927059 1.488517
H -2.137213 1.208927 0.274834
H -1.316174 -1.370936 1.126134
H -2.060374 -1.066395 -0.463149
H 2.047279 -0.794059 0.801917

COMP. 20_E4_B3LYP
O -0.055353 -1.069361 0.538642
C -0.815328 0.122399 0.467710
C 0.166320 1.258774 0.123358
C 1.506525 0.535768 -0.141634
C 1.072384 -0.919085 -0.338501
O -1.788338 0.062140 -0.563554
H -1.305757 0.226753 1.439879
H -0.201280 1.782308 -0.760086
H 0.241049 1.979581 0.938568
H 2.037937 0.934983 -1.007542
H 2.165798 0.613364 0.726241
H 0.770396 -1.113350 -1.374542
H 1.818307 -1.656208 -0.040979
H -2.356335 -0.696802 -0.387845

COMP. 20_E4_M06-2X
O -0.067141 -1.045800 0.576297
C -0.811255 0.141390 0.472025
C 0.186542 1.259977 0.132508
C 1.498826 0.506841 -0.162943
C 1.020371 -0.933923 -0.338181
O -1.740789 0.066447 -0.584052
H -1.327382 0.268034 1.426650
H -0.183584 1.803168 -0.736664
H 0.293287 1.961649 0.958866

H 2.016392 0.886406 -1.043604
H 2.177277 0.567986 0.689438
H 0.668429 -1.114600 -1.359596
H 1.758286 -1.688545 -0.070842
H -2.306170 -0.694993 -0.422656

COMP. 20_E4_MP2
O -0.057941 -1.063616 0.551594
C -0.805367 0.133050 0.472245
C 0.179527 1.255650 0.105258
C 1.510236 0.513757 -0.120709
C 1.036035 -0.916558 -0.361816
O -1.774362 0.071485 -0.557534
H -1.288345 0.251448 1.447033
H -0.174403 1.739112 -0.808070
H 0.246672 2.006685 0.894917
H 2.086415 0.917895 -0.956544
H 2.127553 0.543645 0.781140
H 0.688482 -1.052500 -1.393536
H 1.770606 -1.685263 -0.117832
H -2.321128 -0.699366 -0.369455

COMP. 20_OE_B3LYP
O 0.059235 -1.058766 -0.611718
C 0.838969 0.107994 -0.472203
C -0.154981 1.256383 -0.288089
C -1.409555 0.571859 0.312296
C -1.071514 -0.933595 0.270024
O 1.665754 0.055723 0.681925
H 1.451429 0.176964 -1.375691
H 0.264900 2.028468 0.356111
H -0.378419 1.702661 -1.258660
H -1.603055 0.901893 1.333804
H -2.297420 0.794128 -0.282045
H -0.806592 -1.310757 1.262719
H -1.867467 -1.554256 -0.142087
H 2.219200 -0.730597 0.612041

COMP. 20_OE_M06-2X
O 0.073507 -1.031890 -0.638560
C 0.829464 0.137221 -0.473307
C -0.180399 1.261933 -0.246864
C -1.431107 0.527198 0.287393
C -1.011371 -0.951956 0.284434
O 1.644501 0.059850 0.674246
H 1.438888 0.245825 -1.373443
H 0.223977 1.989916 0.454479
H -0.392394 1.765882 -1.189554
H -1.710438 0.859282 1.286585
H -2.283822 0.687771 -0.372454
H -0.674190 -1.267288 1.275996
H -1.787260 -1.631843 -0.063618
H 2.201649 -0.719609 0.586580

COMP. 20_OE_MP2
O 0.070417 -1.041688 -0.641519
C 0.830248 0.131849 -0.474869
C -0.176258 1.260185 -0.257524
C -1.428136 0.534703 0.289990
C -1.015744 -0.947113 0.291663
O 1.646338 0.065168 0.680691
H 1.440863 0.231297 -1.377294
H 0.231229 1.998738 0.434429
H -0.390666 1.749270 -1.210168
H -1.695451 0.874442 1.292741
H -2.285905 0.696559 -0.366626
H -0.677981 -1.260351 1.285159
H -1.797169 -1.623687 -0.056902
H 2.180379 -0.731844 0.589731

COMP. 21_1E_B3LYP
O -0.046265 -0.920023 0.302808
C -1.187690 -0.070184 0.341102
C -0.736095 1.229248 -0.313893
C 0.740529 1.333041 0.101872
C 1.149151 -0.128532 0.446041
O -2.237479 -0.650438 -0.377485
C 2.231388 -0.719871 -0.442733
H -1.486010 0.078939 1.392428
H -0.844415 1.104703 -1.393839
H -1.338564 2.084402 -0.004118
H 1.361933 1.745521 -0.695323
H 0.861914 1.978011 0.975440
H 1.472411 -0.185973 1.493748
H -2.453738 -1.496618 0.029354
H 1.944615 -0.649095 -1.495450
H 2.392789 -1.772781 -0.200339
H 3.175324 -0.185633 -0.298813

COMP. 21_1E_M06-2X
O -0.044240 -0.922665 0.218973
C -1.172017 -0.079508 0.336546
C -0.740470 1.226729 -0.307853
C 0.734751 1.324658 0.101751
C 1.127530 -0.138560 0.442360
O -2.249866 -0.636591 -0.338432
C 2.247735 -0.700758 -0.408357
H -1.409120 0.051979 1.405264
H -0.852063 1.101264 -1.386583
H -1.345243 2.073959 0.013304
H 1.355933 1.724795 -0.700739
H 0.864270 1.968960 0.972781
H 1.396454 -0.212285 1.503552
H -2.417435 -1.509430 0.028604
H 1.987447 -0.614150 -1.465769
H 2.412759 -1.753892 -0.176019
H 3.174674 -0.152516 -0.225408

COMP. 21_1E_MP2
O -0.046090 -0.933499 0.200836
C -1.169529 -0.074487 0.333044
C -0.731638 1.221358 -0.324555
C 0.734710 1.324187 0.118795
C 1.127523 -0.143147 0.445131
O -2.265079 -0.627246 -0.327279
C 2.251816 -0.696342 -0.408477
H -1.388388 0.066157 1.406072
H -0.815940 1.074341 -1.404774
H -1.344233 2.075667 -0.028769
H 1.372938 1.742944 -0.663948
H 0.835595 1.954669 1.006889
H 1.390006 -0.230156 1.509258
H -2.427782 -1.489493 0.069133
H 2.000396 -0.584899 -1.467367
H 2.407915 -1.757035 -0.194618
H 3.181553 -0.155656 -0.203965

COMP. 21_2E_B3LYP
O -0.073431 -0.719762 -0.836325
C 1.203542 -0.280479 -0.418006
C 1.053279 1.202792 -0.098690
C -0.376990 1.254910 0.457165
C -1.109031 0.195873 -0.382014
O 1.618333 -0.944127 0.767753
C -2.200306 -0.572467 0.344213
H 1.900234 -0.504141 -1.232175
H 1.815035 1.544446 0.601776
H 1.137664 1.783171 -1.021765
H -0.380829 0.970537 1.512404
H -0.838145 2.240078 0.365669
H -1.527841 0.656475 -1.285631
H 1.542789 -1.892313 0.612488
H -1.799756 -1.051008 1.241584
H -2.623779 -1.344735 -0.302100
H -3.007549 0.104824 0.640323

COMP. 21_2E_M06-2X
O 0.076865 -0.643166 0.924550
C -1.185145 -0.311477 0.408988
C -1.108102 1.165632 0.060965
C 0.321056 1.255277 -0.480525
C 1.079994 0.247625 0.395750

O -1.449823 -1.015687 -0.784271
C 2.140247 -0.546451 -0.341868
H -1.922326 -0.567585 1.174366
H -1.874502 1.453529 -0.656690
H -1.222462 1.757125 0.971965
H 0.343368 0.933893 -1.524053
H 0.746508 2.256552 -0.414303
H 1.526144 0.753656 1.258557
H -1.309620 -1.950442 -0.606480
H 1.685877 -1.074942 -1.183055
H 2.606228 -1.276297 0.321889
H 2.916147 0.121692 -0.724301

COMP. 21_2E_MP2
O 0.082297 -0.658703 0.922121
C -1.185648 -0.313278 0.412604
C -1.105066 1.166175 0.079791
C 0.315561 1.246875 -0.487706
C 1.082286 0.247466 0.389158
O -1.466562 -0.999986 -0.795273
C 2.153126 -0.540370 -0.341752
H -1.917059 -0.578168 1.182793
H -1.885688 1.471435 -0.619006
H -1.191328 1.746847 1.003386
H 0.320520 0.914309 -1.529608
H 0.746215 2.249779 -0.432998
H 1.519945 0.761334 1.254895
H -1.335607 -1.935846 -0.607971
H 1.706739 -1.074004 -1.185788
H 2.623585 -1.265548 0.327543
H 2.925238 0.138160 -0.720604

COMP. 21_E4_B3LYP
O -0.086929 -0.459383 1.079215
C -1.176191 0.084961 0.354927
C -0.625716 1.250976 -0.484342
C 0.863276 1.329013 -0.095411
C 1.160374 -0.073809 0.458784
O -1.754096 -0.861724 -0.530495
C 1.612528 -1.087462 -0.590614
H -1.917693 0.384770 1.102568
H -0.763119 1.010498 -1.539639
H -1.159293 2.180253 -0.280970
H 1.506975 1.591587 -0.937266
H 1.016285 2.073649 0.689680
H 1.891078 -0.041931 1.270481
H -2.046215 -1.616008 -0.006386
H 0.913964 -1.135691 -1.428818
H 1.678769 -2.083407 -0.146367
H 2.601824 -0.816930 -0.973109

COMP. 21_E4_M06-2X
O -0.102785 -0.405482 1.109141
C -1.156037 0.135741 0.348194
C -0.556758 1.251455 -0.521147
C 0.919971 1.293788 -0.099512
C 1.143517 -0.111110 0.467711
O -1.726787 -0.825457 -0.509354
C 1.486455 -1.146147 -0.595825
H -1.905176 0.484241 1.064641
H -0.675179 0.967513 -1.567398
H -1.064802 2.202499 -0.367330
H 1.591774 1.522368 -0.927677
H 1.073805 2.035915 0.686023
H 1.897184 -0.123149 1.256916
H -2.024253 -1.562292 0.032536
H 0.757404 -1.127355 -1.408466
H 1.482848 -2.145965 -0.158528
H 2.480087 -0.948623 -1.005527

COMP. 21_E4_MP2
O -0.103927 -0.412765 1.114925
C -1.155808 0.142920 0.347147
C -0.544593 1.242929 -0.532934
C 0.924996 1.292354 -0.086688
C 1.146880 -0.117615 0.465804
O -1.751697 -0.813336 -0.509114
C 1.492193 -1.146315 -0.604172
H -1.893875 0.507662 1.069695
H -0.641409 0.939436 -1.578043
H -1.057890 2.197862 -0.402985
H 1.610785 1.538095 -0.901855
H 1.058206 2.022906 0.716470
H 1.900304 -0.137377 1.258596
H -2.060008 -1.530280 0.055663
H 0.765638 -1.125357 -1.420213
H 1.492137 -2.149965 -0.170310
H 2.489101 -0.939806 -1.008452

COMP. 21_OE_B3LYP
O -0.036616 -0.435259 1.102028
C -1.188426 -0.080457 0.369576
C -0.869585 1.235899 -0.351800
C 0.667061 1.383922 -0.240033
C 1.142540 0.082536 0.442822
O -1.520560 -1.052516 -0.614696
C 1.754766 -0.940216 -0.511780
H -2.000258 -0.005552 1.099359
H -1.216865 1.178428 -1.383342
H -1.384798 2.067593 0.131004
H 1.139765 1.517186 -1.214751
H 0.926726 2.249603 0.372300
H 1.850656 0.289951 1.248645
H -1.639363 -1.896527 -0.164340
H 1.084551 -1.151793 -1.347532
H 1.956731 -1.875892 0.015393
H 2.702127 -0.560901 -0.908099

COMP. 21_OE_M06-2X
O -0.034659 -0.396622 1.123492
C -1.177186 -0.110623 0.364756
C -0.906017 1.213459 -0.351944
C 0.625775 1.387315 -0.268748
C 1.121386 0.116953 0.448957
O -1.415153 -1.095645 -0.618186
C 1.725467 -0.912860 -0.496824
H -2.013351 -0.075486 1.067794
H -1.275318 1.155345 -1.374746
H -1.423003 2.028284 0.154164
H 1.083580 1.483949 -1.253698
H 0.880841 2.277204 0.307059
H 1.838085 0.352135 1.237784
H -1.468203 -1.945979 -0.171298
H 1.047665 -1.119125 -1.326901
H 1.920294 -1.844848 0.037058
H 2.671364 -0.538805 -0.896855

COMP. 21_OE_MP2
O -0.033679 -0.403669 1.130072
C -1.179808 -0.112367 0.366284
C -0.909535 1.212787 -0.347596
C 0.623985 1.386607 -0.270438
C 1.123756 0.117435 0.446277
O -1.426622 -1.093948 -0.627317
C 1.737855 -0.908622 -0.498648
H -2.012427 -0.077907 1.076200
H -1.281607 1.159097 -1.372061
H -1.424004 2.027108 0.167131
H 1.077863 1.483167 -1.259934
H 0.880731 2.277428 0.307961
H 1.838236 0.357828 1.238981
H -1.462830 -1.939416 -0.166305
H 1.064891 -1.118252 -1.333368
H 1.939747 -1.840748 0.036877
H 2.684291 -0.522411 -0.892791

COMP. 22_1E_B3LYP
O -0.073280 -0.928649 0.479253
C 1.172730 -0.273854 0.497746
C 0.853271 1.216900 0.422398
C -0.455928 1.259830 -0.397762
C -0.964404 -0.205205 -0.405306

O 1.967732 -0.610644 -0.631356
C -2.388079 -0.405364 0.082696
H 1.672240 -0.586154 1.419593
H 0.695779 1.598452 1.433301
H 1.671127 1.775032 -0.032848
H -1.189936 1.928608 0.057164
H -0.277094 1.608521 -1.415818
H -0.856757 -0.628563 -1.409957
H 2.067912 -1.569321 -0.644737
H -2.512901 0.010231 1.086459
H -2.639094 -1.468141 0.115595
H -3.092443 0.091835 -0.590565

COMP. 22_1E_M06-2X
O -0.081860 -0.868337 0.564556
C 1.178917 -0.264141 0.489656
C 0.911479 1.230523 0.336829
C -0.470769 1.275052 -0.347544
C -0.935234 -0.196187 -0.370709
O 1.885942 -0.690500 -0.653519
C -2.372820 -0.421431 0.043200
H 1.715694 -0.540287 1.400478
H 0.876857 1.696183 1.321865
H 1.701771 1.701955 -0.244981
H -1.172316 1.885715 0.224227
H -0.416759 1.682334 -1.356820
H -0.756459 -0.621983 -1.363838
H 1.946143 -1.650091 -0.620442
H -2.538784 -0.020452 1.045591
H -2.609832 -1.486376 0.049813
H -3.048406 0.080803 -0.652784

COMP. 22_1E_MP2
O -0.084717 -0.869475 0.575075
C 1.181321 -0.262134 0.488263
C 0.917511 1.232339 0.324445
C -0.479587 1.280462 -0.333244
C -0.935302 -0.191621 -0.370360
O 1.893605 -0.695885 -0.656906
C -2.375116 -0.427419 0.034602
H 1.716067 -0.533785 1.403718
H 0.904000 1.707589 1.307979
H 1.699815 1.694495 -0.279731
H -1.173847 1.876386 0.266684
H -0.447279 1.705401 -1.339109
H -0.746355 -0.610863 -1.366429
H 1.927196 -1.657662 -0.606332
H -2.548814 -0.028512 1.038286
H -2.606859 -1.495796 0.034285
H -3.047998 0.075859 -0.666927

COMP. 22_1T2_B3LYP
O -0.049448 -1.018537 0.304088
C 1.138690 -0.291314 0.515828
C 0.718154 1.172001 0.553509
C -0.410823 1.210362 -0.492529
C -0.988232 -0.226497 -0.473831
O 2.060192 -0.455916 -0.553563
C -2.363274 -0.358530 0.162791
H 1.571286 -0.667795 1.447751
H 0.342617 1.408801 1.552025
H 1.547960 1.840539 0.325058
H -1.173142 1.955177 -0.255824
H -0.004959 1.445031 -1.477544
H -1.012668 -0.641763 -1.486269
H 2.208588 -1.401185 -0.669313
H -2.371631 0.080435 1.164630
H -2.645646 -1.410465 0.247765
H -3.115449 0.150708 -0.447083

COMP. 22_1T2_M06-2X
O -0.039529 -1.042028 0.253776
C 1.115651 -0.296551 0.527099
C 0.652797 1.147970 0.597337
C -0.379062 1.176872 -0.536181
C -0.974279 -0.244700 -0.500283
O 2.051679 -0.393477 -0.522543
C -2.324458 -0.326663 0.188007
H 1.536725 -0.692201 1.454907
H 0.183678 1.326680 1.567076
H 1.476241 1.846836 0.460799
H -1.146665 1.938406 -0.394198
H 0.122406 1.359648 -1.486550
H -1.040371 -0.666757 -1.506509
H 2.208388 -1.327679 -0.688661
H -2.271591 0.136360 1.176912
H -2.624144 -1.368410 0.311737
H -3.085754 0.189589 -0.401255

COMP. 22_1T2_MP2
O -0.054828 -1.037485 0.305182
C 1.124003 -0.301440 0.525952
C 0.679563 1.147671 0.599108
C -0.367085 1.183485 -0.522890
C -0.966571 -0.238245 -0.490553
O 2.026406 -0.411025 -0.560499
C -2.335279 -0.318457 0.161794
H 1.570205 -0.699687 1.442683
H 0.221064 1.328042 1.575688
H 1.508513 1.841936 0.451911
H -1.133839 1.946127 -0.362804
H 0.122307 1.372855 -1.480442
H -1.002053 -0.669775 -1.496954
H 2.159359 -1.353973 -0.706269
H -2.307156 0.149275 1.151068
H -2.638752 -1.362059 0.280281
H -3.080064 0.197256 -0.453092

COMP. 22_4E_B3LYP
O -0.063009 -0.856588 0.514034
C 1.190708 -0.205770 0.466637
C 0.916101 1.270560 0.120019
C -0.604210 1.319662 -0.135748
C -0.971943 -0.152309 -0.360429
O 2.024127 -0.743290 -0.549288
C -2.393557 -0.547498 -0.012867
H 1.651591 -0.360882 1.446737
H 1.222514 1.933872 0.930004
H 1.492580 1.532872 -0.768189
H -1.135685 1.696419 0.743297
H -0.870852 1.948766 -0.987418
H -0.747191 -0.437302 -1.397096
H 2.135615 -1.684031 -0.370546
H -2.616975 -0.296944 1.027582
H -2.541674 -1.621135 -0.149129
H -3.101461 -0.020480 -0.658880

COMP. 22_4E_M06-2X
O -0.068452 -0.831709 0.556967
C 1.187246 -0.210069 0.469857
C 0.928075 1.265935 0.124431
C -0.584206 1.314964 -0.154839
C -0.945718 -0.158206 -0.351678
O 1.958244 -0.762708 -0.572352
C -2.372702 -0.530856 -0.020510
H 1.680228 -0.369261 1.432053
H 1.219203 1.924223 0.942144
H 1.519848 1.524374 -0.753560
H -1.127354 1.702002 0.711304
H -0.839057 1.924837 -1.021867
H -0.695271 -0.468313 -1.374243
H 2.037571 -1.707172 -0.407702
H -2.596888 -0.259310 1.013308
H -2.529299 -1.603756 -0.140449
H -3.063486 -0.002901 -0.681472

COMP. 22_4E_MP2
O -0.070873 -0.837458 0.554011
C 1.187603 -0.202409 0.467470
C 0.924827 1.266915 0.095944
C -0.597444 1.318098 -0.119984
C -0.949950 -0.149597 -0.353082

O 1.982991 -0.762480 -0.561118
C -2.375358 -0.543442 -0.033822
H 1.665946 -0.345899 1.441487
H 1.261018 1.947599 0.880923
H 1.472789 1.494340 -0.821341
H -1.108711 1.663090 0.784899
H -0.889715 1.958908 -0.956064
H -0.692223 -0.435630 -1.383011
H 2.050634 -1.704151 -0.368118
H -2.605616 -0.291658 1.005457
H -2.521277 -1.617303 -0.176420
H -3.067863 -0.007175 -0.690113

COMP. 22_OE_B3LYP
O 0.082863 -0.907514 -0.458023
C 1.021721 -0.247226 0.382859
C 0.704818 1.249160 0.294922
C -0.733806 1.321604 -0.262346
C -1.138626 -0.152425 -0.520360
O 2.323116 -0.489894 -0.080037
C -2.167610 -0.689840 0.472932
H 0.916795 -0.637562 1.406503
H 0.810370 1.735336 1.265948
H 1.425428 1.702389 -0.387537
H -1.424116 1.798274 0.436925
H -0.762289 1.896918 -1.188955
H -1.517912 -0.288460 -1.536253
H 2.477425 -1.441002 -0.065397
H -1.832650 -0.554691 1.506068
H -2.339449 -1.755328 0.304226
H -3.120421 -0.164246 0.354919

COMP. 22_OE_M06-2X
O 0.099970 -0.857173 -0.553075
C 0.986967 -0.242782 0.359961
C 0.685151 1.251959 0.286803
C -0.762967 1.323043 -0.234050
C -1.136254 -0.148753 -0.529961
O 2.300675 -0.489522 -0.026411
C -2.081782 -0.738183 0.509562
H 0.806494 -0.652749 1.364788
H 0.822052 1.738923 1.251723
H 1.388541 1.689880 -0.422227
H -1.447071 1.754587 0.498362
H -0.821266 1.929368 -1.137509
H -1.569077 -0.265081 -1.524874
H 2.430463 -1.441776 -0.060283
H -1.683249 -0.605865 1.519417
H -2.225232 -1.804721 0.329966
H -3.053496 -0.240714 0.462630

COMP. 22_OE_MP2
O 0.105669 -0.859431 -0.575172
C 0.982419 -0.245210 0.358825
C 0.672539 1.248973 0.301286
C -0.767355 1.321008 -0.247826
C -1.139797 -0.152584 -0.531489
O 2.306888 -0.474945 -0.022350
C -2.069798 -0.739618 0.524985
H 0.796917 -0.669872 1.357605
H 0.785617 1.721657 1.279288
H 1.386718 1.702755 -0.389644
H -1.464945 1.767900 0.465944
H -0.802612 1.912173 -1.165613
H -1.584998 -0.274892 -1.522792
H 2.431539 -1.429545 -0.045351
H -1.664112 -0.589298 1.530952
H -2.204593 -1.811624 0.357991
H -3.048034 -0.249663 0.477115