Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION – On the ring opening of substituted cyclobutene to benzocyclobutene: analysis of π delocalization, hyperconjugation, and ring strain.†

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Structural parameters

We report here some structural parameters of the computed molecules of Table 1 of the article. Labelling is as in Figure 1 of the article. The details about the benchmarking calculations that have been performed on $C_4H_4R^1_2$ and $C_8H_6R^1_2$ molecules, R^1=H,NH_2,OTMS,CH_3,F,NO_2 follow.

Table 1S: Computed distances (in pm, PBE0/def2-TZVP) of closed forms of molecules in Table 1 of the article. Labels as in Figure 1 of the article.

Molecule	$d_{C_1-C_2}$	$d_{C_2-C_3}$	$d_{C_1-C_4}$	$d_{C_2-R^2}$	$d_{C_3-R^3}$	d_{C-OTMS}
(1c)	151.2	138.3	158.1	138.1	138.1	139.1
(2c)	151.2	136.1	156.4	142.6	142.6	139.5
(3c)	151.1	135.5	156.5	143.7	143.7	139.6
(4c)	151.2	134.7	156.5	144.1	148.1	139.7
(5c)	151.2	134.7	156.5	144.1	147.7	139.7
(6c)	150.9	134.0	156.4	148.3	148.3	140.0
(7c)	150.7	134.0	156.4	148.3	147.8	140.0
(8c)	150.7	133.9	156.5	147.9	147.9	140.0
(9c)	151.0	133.6	156.9	147.8	108.4	139.7
(10c)	150.6	133.3	156.6	108.3	108.3	139.4
(11c)	150.8	133.3	157.0	148.2	148.2	140.1
(12c)	150.5	133.7	158.1	144.7	148.5	139.6

Table 2S: Computed distances (in pm, PBE0/def2-TZVP) of closed forms of molecules in Table 1 in the main text. Labels as in Figure 1 in the main text.

Molecule	$d_{C_1-C_2}$	$d_{C_2-C_3}$	$d_{C_2-R^2}$	$d_{C_3-R^3}$	d_{C-OTMS}	τ
(1o)	135.2	147.0	144.6	144.6	134.7	32.3
(2o)	134.8	148.7	145.2	145.2	134.3	57.2
(3o)	134.6	148.5	146.1	146.1	134.4	57.1
(4o)	134.7	147.6	146.1	150.8	134.4	49.8
(5o)	134.6	148.0	146.1	149.7	134.3	57.6
(6o)	133.9	146.8	150.9	135.6	135.6	45.9
(7o)	133.8	147.2	150.3	149.8	135.5	49.2
(8o)	133.8	147.2	149.8	149.8	135.6	49.1
(9o)	133.8	146.1	149.7	108.8	135.5	44.7
(10o)	133.4	145.4	108.7	108.7	135.0	40.2
(11o)	133.7	146.5	150.8	150.8	135.5	45.6
(12o)	134.4	146.9	145.5	149.9	134.9	38.6

Table 3S:CCSD(T)/def2-TZVP computed ΔE_R and $\Delta E^{\#}$ (kcal/mol) values for model systems $C_4H_4R_2$. Deviations from those values follow for several methods (kcal/mol). Average errors (ae), mean absolute errors (mae) and standard deviations (σ) are also reported. Structures are optimized at each DFT method. SCS-MP2 and CCSD(T) values are from single point calculations on PBE0 structures. The basis set is of def2-TZVP quality.

R	CCSD(T)	SCS-MP2	PBE0	PBE	B3LYP
	ΔE_R				
H	-8.55	0.9	3.7	1.8	-3.1
NH_2	-14.74	0.3	-2.2	-5.6	-8.0
OTMS	-9.37	0.1	-2.2	-5.2	-8.3
CH_3	-9.38	0.7	0.5	-1.8	-6.1
F	-4.57	0.8	1.1	-1.7	-4.4
NO_2	-6.48	0.4	-0.4	-3.3	-7.1
ae		0.5	0.1	-2.6	-6.2
mae		0.5	1.7	3.2	6.2
σ		0.3	1.7	2.1	1.6
	$\Delta E^{\#}$				
H	34.77	1.5	2.1	-2.5	-1.6
NH_2	18.74	-0.1	-2.8	-8.3	-5.6
OTMS	22.30	0.2	-1.8	-7.3	-4.6
CH_3	32.75	0.9	-0.3	-5.5	-4.0
F	27.27	1.0	-0.7	-6.4	-3.3
NO_2	31.01	-0.1	0.1	-5.8	-3.9
ae		0.6	-0.5	-6.0	-3.8
mae		0.6	1.3	6.0	3.8
σ		0.6	1.2	1.4	0.9

Table 4S:SCS-MP2 computed ΔE_R and $\Delta E^{\#}$ (kcal/mol) values for benzocyclobutene derivative systems $C_8H_6R_2$. Deviations from those values follow for several methods (kcal/mol). Average errors (ae), mean absolute errors (mae) and standard deviations (σ) are also reported. Structures are optimized at each DFT method. SCS-MP2 are from single point calculations on PBE0 structures. The basis set is of def2-TZVP quality.

R	SCS-MP2	PBE0	PBE	B3LYP
	ΔE_R			
H	15.71	3.6	0.0	-3.6
NH_2	9.14	-2.3	-8.0	-8.0
OTMS	9.62	0.8	-5.4	-5.2
CH_3	17.97	0.4	-3.8	-6.1
F	18.99	0.9	-3.8	-4.9
NO_2	21.94	-0.8	-6.2	-8.0
ae		0.4	-4.5	-6.0
mae		1.5	4.6	6.0
σ		1.3	2.0	1.4
	$\Delta E^{\#}$			
H	42.86	2.4	-3.9	-2.5
NH_2	23.76	-1.6	-8.8	-5.4
OTMS	26.22	1.4	-7.1	-2.5
CH_3	39.64	0.3	-6.4	-4.2
F	36.72	-0.4	-7.7	-4.1
NO_2	37.41	1.5	-6.3	-3.5
ae		0.6	-6.7	-3.7
mae		1.3	6.7	3.7
σ		1.2	1.2	0.9

List of optimized structures

Molecule (1c) optimized at the PBE0/def2-TZVP level
42
Energy =

C	-4.3888267	-0.1805592	0.7136820
C	-3.1993021	-0.3813376	1.4089203
C	-2.0406578	-0.1985102	0.6796417
C	-0.5330400	-0.3057246	0.7325404
O	0.1130129	0.4131892	1.7326243
Si	1.4819532	0.0488242	2.5926812
C	1.8676140	-1.7780663	2.4736360
C	1.1317073	0.5406953	4.3570740
C	2.9108868	1.0574175	1.9316124
H	-0.1874076	-1.3460314	0.6852574
H	-3.2033536	-0.6728374	2.4532064
H	0.8299281	1.5899507	4.4101570
H	2.0161844	0.4129707	4.9873949
H	2.6837333	2.1258087	1.9797542
H	3.8178587	0.8824591	2.5175364
H	3.1357364	0.8096967	0.8910789
H	2.7373468	-2.0110227	3.0949973
H	2.1035353	-2.0877333	1.4521053
H	1.0354292	-2.3917414	2.8289918
H	-5.3354590	-0.3168502	1.2251737
H	0.3237810	-0.0609274	4.7809605
C	-4.4011142	0.1809632	-0.6350012
C	-3.2248446	0.3800517	-1.3529385
C	-2.0528301	0.1986294	-0.6446788
C	-0.5463351	0.3063315	-0.7250584
O	0.0823070	-0.4119200	-1.7365062
Si	1.4377141	-0.0488044	-2.6180208
C	1.8280820	1.7774203	-2.5029989
C	1.0593492	-0.5378203	-4.3774417
C	2.8754478	-1.0607415	-1.9811046
H	-0.2009979	1.3469838	-0.6840373
H	-3.2486522	0.6696050	-2.3976068
H	0.7549062	-1.5864577	-4.4273935
H	1.9342644	-0.4108185	-5.0211323
H	2.6453321	-2.1286441	-2.0256405
H	3.7729257	-0.8874726	-2.5819569
H	3.1179906	-0.8137215	-0.9443376
H	2.6888172	2.0097043	-3.1369822
H	2.0797760	2.0862445	-1.4850436
H	0.9914491	2.3923216	-2.8455852
H	-5.3571144	0.3165737	-1.1292879
H	0.2462607	0.0661458	-4.7880199

Molecule (1o) optimized at the PBE0/def2-TZVP level
42
Energy =

C	-0.6432481	0.3254482	3.6443068
C	-1.2918333	0.5716327	2.4890992
C	-0.7158250	0.1678004	1.2253364
C	0.7158250	-0.1678004	1.2253364
C	1.2918333	-0.5716327	2.4890992
C	0.6432481	-0.3254482	3.6443068
C	-1.4752004	0.0187992	0.1172536
O	-2.7567034	0.4297104	0.0547451
Si	-3.8812546	-0.0613143	-1.0833514
C	-3.2549614	0.3594489	-2.7931807
C	1.4752004	-0.0187992	0.1172536
O	2.7567034	-0.4297104	0.0547451
Si	3.8812546	0.0613143	-1.0833514
C	5.4137310	-0.9052030	-0.6639986
C	-5.4137310	0.9052030	-0.6639986
C	-4.1529748	-1.9005378	-0.9234821
C	3.2549614	-0.3594489	-2.7931807
C	4.1529748	1.9005378	-0.9234821
H	-1.0638162	-0.4487642	-0.7756206
H	1.0638162	0.4487642	-0.7756206
H	-2.2852529	1.0034227	2.4855205
H	-5.7487799	0.6817686	0.3517693
H	-6.2295655	0.6604016	-1.3494740
H	-4.5125038	-2.1570207	0.0761590
H	-4.8923580	-2.2511610	-1.6490298
H	-3.2273786	-2.4558233	-1.0973936
H	-3.9981624	0.0875586	-3.5482339
H	-2.3334400	-0.1763476	-3.0358571
H	-3.0578889	1.4303878	-2.8871522
H	3.0578889	-1.4303878	-2.8871522
H	2.3334400	0.1763476	-3.0358571
H	3.9981624	-0.0875586	-3.5482339
H	4.8923580	2.2511610	-1.6490298
H	3.2273786	2.4558233	-1.0973936
H	4.5125038	2.1570207	0.0761590
H	5.2283820	-1.9800191	-0.7294353
H	5.7487799	-0.6817686	0.3517693
H	6.2295655	-0.6604016	-1.3494740
H	2.2852529	-1.0034227	2.4855205
H	1.1010456	-0.5876095	4.5916505
H	-1.1010456	0.5876095	4.5916505
H	-5.2283820	1.9800191	-0.7294353

Molecule (2c) optimized at the PBE0/def2-TZVP level

52

Energy =

C	2.9729079	0.4083844	-2.3774881
C	1.6609436	0.1994896	-2.6035188
C	0.6730273	0.1023873	-1.5791345
C	0.7551179	0.2026691	-0.0727709
O	1.6568684	-0.6531633	0.5611747
Si	2.5397649	-0.4428909	1.9464737
C	2.6773116	1.3742575	2.3726652
C	4.2231356	-1.1709009	1.6044914
C	1.7296507	-1.3780488	3.3485571
H	0.8638793	1.2375573	0.2759518
H	4.1335885	-2.2121819	1.2844196
H	4.8529098	-1.1468278	2.4981950
H	1.6124105	-2.4335493	3.0886999
H	2.3364338	-1.3230434	4.2570340
H	0.7400259	-0.9795582	3.5858353
H	3.3093720	1.4977526	3.2570091
H	1.7070815	1.8238246	2.5992833
H	3.1325120	1.9481082	1.5607378
H	4.7410253	-0.6234629	0.8128604
H	1.3211757	0.0915309	-3.6322434
H	3.3228760	0.4985752	-1.3523829
C	3.9594354	0.5091001	-3.4204755
H	3.5973244	0.4114447	-4.4420634
C	5.2625951	0.7108776	-3.2064055
H	5.6587730	0.8120832	-2.2011165
H	5.9686291	0.7798645	-4.0245353
C	-2.9729079	-0.4083844	-2.3774881
C	-1.6609436	-0.1994896	-2.6035188
C	-0.6730273	-0.1023873	-1.5791345
C	-0.7551179	-0.2026691	-0.0727709
O	-1.6568684	0.6531633	0.5611747
Si	-2.5397649	0.4428909	1.9464737
C	-2.6773116	-1.3742575	2.3726652
C	-4.2231356	1.1709009	1.6044914
C	-1.7296507	1.3780488	3.3485571
H	-0.8638793	-1.2375573	0.2759518
H	-4.1335885	2.2121819	1.2844196
H	-4.8529098	1.1468278	2.4981950
H	-1.6124105	2.4335493	3.0886999
H	-2.3364338	1.3230434	4.2570340
H	-0.7400259	0.9795582	3.5858353
H	-3.3093720	-1.4977526	3.2570091
H	-1.7070815	-1.8238246	2.5992833
H	-3.1325120	-1.9481082	1.5607378
H	-4.7410253	0.6234629	0.8128604
H	-1.3211757	-0.0915309	-3.6322434
H	-3.3228760	-0.4985752	-1.3523829
C	-3.9594354	-0.5091001	-3.4204755
H	-3.5973244	-0.4114447	-4.4420634
C	-5.2625951	-0.7108776	-3.2064055
H	-5.6587730	-0.8120832	-2.2011165
H	-5.9686291	-0.7798645	-4.0245353

Molecule (2o) optimized at the PBE0/def2-TZVP level

52

Energy =

C	2.5485119	1.1830811	-2.1536057
C	1.2738634	0.8399646	-1.8851422
C	0.7326608	0.1255563	-0.7426069
C	1.4374778	-0.3349429	0.3105245
O	2.7545031	-0.1379108	0.4832214
Si	3.6815668	-0.7962633	1.7171190
C	2.9672681	-0.2721009	3.3612238
C	5.3765904	-0.0823741	1.4445201
C	3.6765586	-2.6551877	1.5597997
H	0.9228027	-0.9079340	1.0801283
H	5.7655081	-0.3647400	0.4630406
H	6.0784028	-0.4444198	2.2006179
H	4.0703640	-2.9660025	0.5888928
H	4.2959415	-3.1117835	2.3370023
H	2.6676170	-3.0644832	1.6582650
H	3.5809152	-0.6504905	4.1837156
H	1.9539480	-0.6560924	3.5062446
H	2.9306360	0.8171750	3.4431380
H	5.3552542	1.0087657	1.4987882
H	3.3430786	0.9195791	-1.4658277
H	0.5235910	1.1432992	-2.6138885
C	2.9165865	1.9091208	-3.3438129
H	2.1060889	2.1666294	-4.0238380
C	4.1636031	2.2743670	-3.6537766
H	4.9982134	2.0370398	-3.0017734
H	4.3867384	2.8179969	-4.5635213
C	-2.5485119	-1.1830811	-2.1536057
C	-1.2738634	-0.8399646	-1.8851422
C	-0.7326608	-0.1255563	-0.7426069
C	-1.4374778	0.3349429	0.3105245
O	-2.7545031	0.1379108	0.4832214
Si	-3.6815668	0.7962633	1.7171190
C	-2.9672681	0.2721009	3.3612238
C	-5.3765904	0.0823741	1.4445201
C	-3.6765586	2.6551877	1.5597997
H	-0.9228027	0.9079340	1.0801283
H	-5.7655081	0.3647400	0.4630406
H	-6.0784028	0.4444198	2.2006179
H	-4.0703640	2.9660025	0.5888928
H	-4.2959415	3.1117835	2.3370023
H	-2.6676170	3.0644832	1.6582650
H	-3.5809152	0.6504905	4.1837156
H	-1.9539480	0.6560924	3.5062446
H	-2.9306360	-0.8171750	3.4431380
H	-5.3552542	-1.0087657	1.4987882
H	-3.3430786	-0.9195791	-1.4658277
H	-0.5235910	-1.1432992	-2.6138885
C	-2.9165865	-1.9091208	-3.3438129
H	-2.1060889	-2.1666294	-4.0238380
C	-4.1636031	-2.2743670	-3.6537766
H	-4.9982134	-2.0370398	-3.0017734
H	-4.3867384	-2.8179969	-4.5635213

Molecule (3c) optimized at the PBE0/def2-TZVP level

44

Energy =

C	-2.8941453	0.7506318	3.0081204
C	-1.6270999	0.3942943	3.2294664
C	-0.6535319	0.1780721	2.1946071
C	-0.7290489	0.2839158	0.6888157
O	-1.7211219	-0.4718056	0.0622595
Si	-2.5643169	-0.1820042	-1.3331950
C	-2.5144902	1.6378049	-1.7677526
C	-4.3150311	-0.7359772	-1.0033838
C	-1.8396166	-1.2003686	-2.7244340
H	-0.7267275	1.3231512	0.3365484
H	-4.3324875	-1.7782487	-0.6747309
H	-4.9303485	-0.6569951	-1.9039796
H	-1.8387295	-2.2618580	-2.4625314
H	-2.4243127	-1.0831936	-3.6414373
H	-0.8102260	-0.9097810	-2.9485235
H	-3.1253407	1.8216864	-2.6564402
H	-1.5022108	1.9853672	-1.9894399
H	-2.9138867	2.2575636	-0.9602679
H	-4.7827269	-0.1322519	-0.2215845
H	-1.2883297	0.2521442	4.2533380
H	-3.2733142	0.8845711	2.0017005
H	-3.5870623	0.9069771	3.8257755
C	2.8941453	-0.7506318	3.0081204
C	1.6270999	-0.3942943	3.2294664
C	0.6535319	-0.1780721	2.1946071
C	0.7290489	-0.2839158	0.6888157
O	1.7211219	0.4718056	0.0622595
Si	2.5643169	0.1820042	-1.3331950
C	2.5144902	-1.6378049	-1.7677526
C	4.3150311	0.7359772	-1.0033838
C	1.8396166	1.2003686	-2.7244340
H	0.7267275	-1.3231512	0.3365484
H	4.3324875	1.7782487	-0.6747309
H	4.9303485	0.6569951	-1.9039796
H	1.8387295	2.2618580	-2.4625314
H	2.4243127	1.0831936	-3.6414373
H	0.8102260	0.9097810	-2.9485235
H	3.1253407	-1.8216864	-2.6564402
H	1.5022108	-1.9853672	-1.9894399
H	2.9138867	-2.2575636	-0.9602679
H	4.7827269	0.1322519	-0.2215845
H	1.2883297	-0.2521442	4.2533380
H	3.2733142	-0.8845711	2.0017005
H	3.5870623	-0.9069771	3.8257755

Molecule (3o) optimized at the PBE0/def2-TZVP level

44

Energy =

C	-2.2832536	1.6569869	2.7351278
C	-1.1139336	1.0537563	2.5043369
C	-0.6990012	0.2504811	1.3574898
C	-1.4738364	-0.0792493	0.3078756
O	-2.7361054	0.3484999	0.1335844
Si	-3.7958105	-0.2260745	-1.0318928
C	-3.0418047	0.0243766	-2.7224923
C	-5.3280696	0.8033527	-0.8072082
C	-4.1236429	-2.0359787	-0.7198509
H	-1.0704242	-0.7365683	-0.4609329
H	-5.7363122	0.6796808	0.1988203
H	-6.1020592	0.5118321	-1.5222511
H	-4.5488667	-2.1890971	0.2751729
H	-4.8284367	-2.4365212	-1.4539247
H	-3.2057771	-2.6263312	-0.7852284
H	-3.7350087	-0.3021413	-3.5029279
H	-2.1180599	-0.5468561	-2.8465173
H	-2.8127337	1.0787901	-2.8965751
H	-5.1128805	1.8640694	-0.9571807
H	-3.1114750	1.6075085	2.0431419
H	-2.4213587	2.2301003	3.6447137
H	-0.3358981	1.1754470	3.2551270
C	2.2832536	-1.6569869	2.7351278
C	1.1139336	-1.0537563	2.5043369
C	0.6990012	-0.2504811	1.3574898
C	1.4738364	0.0792493	0.3078756
O	2.7361054	-0.3484999	0.1335844
Si	3.7958105	0.2260745	-1.0318928
C	3.0418047	-0.0243766	-2.7224923
C	5.3280696	-0.8033527	-0.8072082
C	4.1236429	2.0359787	-0.7198509
H	1.0704242	0.7365683	-0.4609329
H	5.7363122	-0.6796808	0.1988203
H	6.1020592	-0.5118321	-1.5222511
H	4.5488667	2.1890971	0.2751729
H	4.8284367	2.4365212	-1.4539247
H	3.2057771	2.6263312	-0.7852284
H	3.7350087	0.3021413	-3.5029279
H	2.1180599	0.5468561	-2.8465173
H	2.8127337	-1.0787901	-2.8965751
H	5.1128805	-1.8640694	-0.9571807
H	3.1114750	-1.6075085	2.0431419
H	2.4213587	-2.2301003	3.6447137
H	0.3358981	-1.1754470	3.2551270

Molecule (4c) optimized at the PBE0/def2-TZVP level

46

Energy =

C	2.8792836	-0.9716458	2.9075639
C	1.6100773	-0.6401476	3.1458862
C	0.6351099	-0.3507030	2.1249291
C	0.7097059	-0.3550205	0.6146654
O	1.6788019	0.4671651	0.0344688
Si	2.5699983	0.2658026	-1.3446408
C	2.5707663	-1.5287716	-1.8771173
C	4.3001851	0.8343786	-0.9384151
C	1.8638647	1.3418169	-2.7020618
H	0.7283651	-1.3657142	0.1890505
H	4.2867924	1.8568619	-0.5524231
H	4.9404514	0.8177835	-1.8247761
H	1.8359287	2.3884302	-2.3872426
H	2.4733447	1.2818095	-3.6083306
H	0.8456846	1.0452182	-2.9667652
H	3.2121203	-1.6527170	-2.7546850
H	1.5729128	-1.8824615	-2.1490201
H	2.9574137	-2.1841110	-1.0918977
H	4.7600687	0.1980764	-0.1780496
C	-2.2838277	1.5306833	3.2853305
C	-1.7137357	0.1172974	3.1919521
C	-0.6681796	-0.0112460	2.1511536
C	-0.7576078	0.1862604	0.6592292
O	-1.7577554	-0.5526551	0.0195771
Si	-2.5907262	-0.2235775	-1.3731148
C	-2.6054306	1.6165143	-1.7147966
C	-4.3212805	-0.8603415	-1.0908073
C	-1.8096408	-1.1361138	-2.8069934
H	-0.7779217	1.2403599	0.3543175
H	-2.5252647	-0.5796850	2.9494518
H	-4.3025163	-1.9199651	-0.8232831
H	-4.9352248	-0.7516157	-1.9890887
H	-1.7702459	-2.2098166	-2.6049045
H	-2.3857663	-0.9901421	-3.7253066
H	-0.7894921	-0.7936354	-2.9981585
H	-3.2149598	1.8235825	-2.5992616
H	-1.6045213	2.0108816	-1.9082276
H	-3.0341807	2.1784660	-0.8805898
H	-3.0783044	1.5814052	4.0329907
H	-4.8116199	-0.3187811	-0.2780108
H	-1.3137899	-0.1943465	4.1611705
H	-1.5087781	2.2484885	3.5626222
H	-2.7052343	1.8482862	2.3286233
H	3.2660342	-1.0297939	1.8965756
H	3.5683765	-1.1843611	3.7156209
H	1.2639343	-0.5766502	4.1754533

Molecule (4o) optimized at the PBE0/def2-TZVP level

46

Energy =

C	2.2858909	-1.2541275	2.9017391
C	1.1206914	-0.6873304	2.5780493
C	0.7045239	-0.0804416	1.3158769
C	1.5048816	0.1231486	0.2512243
O	2.7801048	-0.2945777	0.1724673
Si	3.8600379	0.1300817	-1.0363756
C	3.1618834	-0.3863633	-2.6901402
C	5.4080800	-0.8134881	-0.6222427
C	4.1392785	1.9743373	-0.9881983
H	1.1134199	0.6644894	-0.6083273
H	5.7792422	-0.5374548	0.3678112
H	6.1983368	-0.6042666	-1.3481896
H	4.5291793	2.2839262	-0.0153212
H	4.8590159	2.2789930	-1.7532123
H	3.2122752	2.5253449	-1.1675994
H	3.8678585	-0.1560106	-3.4930829
H	2.2268370	0.1320536	-2.9182529
H	2.9656189	-1.4612995	-2.7137548
H	5.2233968	-1.8904552	-0.6258568
C	-2.3242911	0.5372431	3.1642869
C	-1.2839794	1.2398570	2.2965837
C	-0.6961402	0.3735364	1.2114518
C	-1.4186861	0.0281375	0.1408164
O	-2.6674347	0.5058735	-0.0803523
Si	-3.7970773	-0.1806754	-1.0997610
C	-3.0624675	-0.3875390	-2.8067360
C	-5.2086912	1.0314295	-1.1123886
C	-4.3175706	-1.8380428	-0.4157753
H	-1.0137290	-0.6477287	-0.6103771
H	-1.7521578	2.1112029	1.8268288
H	-5.5934523	1.1895422	-0.1018727
H	-6.0317877	0.6678199	-1.7334021
H	-4.7587906	-1.7311577	0.5785075
H	-5.0585429	-2.3152641	-1.0631856
H	-3.4641785	-2.5161799	-0.3302624
H	-3.8140003	-0.7789898	-3.4983354
H	-2.2217862	-1.0862788	-2.8110405
H	-2.7096637	0.5684705	-3.2021057
H	-2.7211417	1.2155672	3.9242836
H	-4.8899093	1.9995042	-1.5062624
H	-0.4753785	1.6233139	2.9246850
H	-3.1587994	0.1856517	2.5554225
H	-1.9002639	-0.3294409	3.6770957
H	0.3511800	-0.6737107	3.3460356
H	3.1096490	-1.3324242	2.2072075
H	2.4251246	-1.6653396	3.8949470

Molecule (5c) optimized at the PBE0/def2-TZVP level

43

Energy =

C	3.2543449	-0.7155510	2.6116547
C	2.0669797	-0.2820830	3.0355469
C	0.9277320	-0.0551360	2.1830232
C	0.7204434	-0.2226755	0.6945463
O	1.5943827	0.4838403	-0.1354686
Si	2.1856264	0.1130265	-1.6350691
C	2.0511930	-1.7249443	-1.9640832
C	3.9705431	0.6551927	-1.6384799
C	1.2414475	1.0720196	-2.9342712
H	0.6290266	-1.2715978	0.3869742
H	4.0509084	1.7120131	-1.3712055
H	4.4228747	0.5224511	-2.6251762
H	1.2964421	2.1454374	-2.7336960
H	1.6569033	0.8969305	-3.9308223
H	0.1856771	0.7906591	-2.9611059
H	2.5037323	-1.9609453	-2.9315901
H	1.0137066	-2.0675964	-1.9965461
H	2.5749922	-2.3111373	-1.2040044
H	4.5603270	0.0840821	-0.9170470
H	-2.0519539	0.0118056	3.6012882
C	-1.1608462	0.6474356	3.5952039
C	-0.3352008	0.3555672	2.4059942
C	-0.6954505	0.3959262	0.9445416
O	-1.8220605	-0.3505148	0.5864711
Si	-2.8826180	-0.1338048	-0.6663613
C	-2.8957901	1.6547041	-1.2171802
C	-4.5538196	-0.6375367	-0.0094429
C	-2.4097891	-1.2445813	-2.0952037
H	-0.7398209	1.4135075	0.5344838
H	-0.6140730	0.4815777	4.5248952
H	-4.5249291	-1.6599815	0.3759998
H	-5.3160791	-0.5958147	-0.7923558
H	-2.3714299	-2.2891938	-1.7748213
H	-3.1391823	-1.1711888	-2.9070574
H	-1.4308888	-0.9844048	-2.5058275
H	-3.6441171	1.7950590	-2.0026262
H	-1.9319517	1.9710612	-1.6245191
H	-3.1511323	2.3275006	-0.3940497
H	-4.8701692	0.0182270	0.8056191
H	-1.5127613	1.6846384	3.5824541
H	3.4402112	-0.9131895	1.5622056
H	4.0756407	-0.8750231	3.2996072
H	1.9243085	-0.0807477	4.0952912

Molecule (5o) optimized at the PBE0/def2-TZVP level

43

Energy =

C	2.2178109	-1.1580990	2.9820868
C	1.0513586	-0.5920195	2.6608257
C	0.6368829	0.0266560	1.4041574
C	1.4104567	0.1668237	0.3109701
O	2.6640577	-0.3065351	0.2049888
Si	3.7414991	0.0709342	-1.0215959
C	3.0138830	-0.4474197	-2.6618106
C	5.2672828	-0.9094534	-0.6102272
C	4.0704822	1.9075739	-1.0003774
H	1.0117457	0.6941302	-0.5543560
H	5.6647026	-0.6212056	0.3660554
H	6.0504666	-0.7426842	-1.3546511
H	4.4773525	2.2191164	-0.0350721
H	4.7905845	2.1839753	-1.7756668
H	3.1562759	2.4800205	-1.1784491
H	3.7210763	-0.2514688	-3.4728537
H	2.0942489	0.0974654	-2.8910301
H	2.7830856	-1.5156962	-2.6687346
H	5.0494422	-1.9798917	-0.5838799
H	-1.0653288	1.1840888	3.3594007
C	-1.1940233	1.5560970	2.3384051
C	-0.7462996	0.5469304	1.3280150
C	-1.5489814	0.1176442	0.3495231
O	-2.7998396	0.5971214	0.1478209
Si	-4.0025183	-0.1846741	-0.7058640
C	-3.4320171	-0.4854014	-2.4606539
C	-5.4459171	0.9886253	-0.6568961
C	-4.4012983	-1.8052220	0.1311579
H	-1.2036806	-0.6483422	-0.3431163
H	-2.2430515	1.8139554	2.1960023
H	-5.7483408	1.1908484	0.3734973
H	-6.3071626	0.5714655	-1.1856602
H	-4.7260883	-1.6425984	1.1620176
H	-5.2014969	-2.3327403	-0.3956255
H	-3.5294310	-2.4645251	0.1567430
H	-4.2326069	-0.9426306	-3.0491365
H	-2.5718697	-1.1588908	-2.5019898
H	-3.1507703	0.4514483	-2.9484615
H	-5.1902180	1.9417074	-1.1261693
H	-0.5966514	2.4707142	2.2629214
H	0.2760440	-0.5979046	3.4235997
H	3.0473410	-1.2171282	2.2925600
H	2.3525674	-1.5865759	3.9685868

Molecule (6c) optimized at the PBE0/def2-TZVP level

48

Energy =

C	-2.2817227	-1.7628889	-3.1345757
C	-1.6976591	-0.3528703	-3.1379768
C	-0.6513158	-0.1578444	-2.1053800
C	-0.7384347	-0.2571418	-0.6024590
O	-1.7137169	0.5470474	-0.0003206
Si	-2.5860685	0.3072450	1.3841288
C	-2.6503589	-1.5118007	1.8225812
C	-4.2978377	0.9626631	1.0340598
C	-1.8176610	1.2773399	2.7875588
H	-0.7807716	-1.2870020	-0.2271304
H	-2.5029039	0.3687285	-2.9547489
H	-4.2516385	2.0065623	0.7131640
H	-4.9318809	0.9125597	1.9235768
H	-1.7486960	2.3376046	2.5298762
H	-2.4171302	1.1930756	3.6985832
H	-0.8100333	0.9233290	3.0198099
H	-3.2821397	-1.6581196	2.7035748
H	-1.6629739	-1.9176125	2.0575620
H	-3.0753847	-2.1074508	1.0100899
H	-3.0685444	-1.8627088	-3.8855389
H	-4.7829220	0.3898306	0.2397105
H	-1.2886021	-0.1178168	-4.1254007
H	-1.5113362	-2.5071994	-3.3485830
H	-2.7168546	-2.0056400	-2.1620626
C	2.2817227	1.7628889	-3.1345757
C	1.6976591	0.3528703	-3.1379768
C	0.6513158	0.1578444	-2.1053800
C	0.7384347	0.2571418	-0.6024590
O	1.7137169	-0.5470474	-0.0003206
Si	2.5860685	-0.3072450	1.3841288
C	2.6503589	1.5118007	1.8225812
C	4.2978377	-0.9626631	1.0340598
C	1.8176610	-1.2773399	2.7875588
H	0.7807716	1.2870020	-0.2271304
H	2.5029039	-0.3687285	-2.9547489
H	4.2516385	-2.0065623	0.7131640
H	4.9318809	-0.9125597	1.9235768
H	1.7486960	-2.3376046	2.5298762
H	2.4171302	-1.1930756	3.6985832
H	0.8100333	-0.9233290	3.0198099
H	3.2821397	1.6581196	2.7035748
H	1.6629739	1.9176125	2.0575620
H	3.0753847	2.1074508	1.0100899
H	3.0685444	1.8627088	-3.8855389
H	4.7829220	-0.3898306	0.2397105
H	1.2886021	0.1178168	-4.1254007
H	1.5113362	2.5071994	-3.3485830
H	2.7168546	2.0056400	-2.1620626

Molecule (6o) optimized at the PBE0/def2-TZVP level

48

Energy =

C	2.2228572	-0.1099653	3.1949901
C	1.2594246	-0.9476843	2.3586164
C	0.6982495	-0.2265664	1.1578843
C	1.4655943	0.0020040	0.0848386
O	2.7260107	-0.4848224	-0.0259815
Si	3.8898625	0.0796755	-1.0807492
C	3.2417816	0.0082201	-2.8329271
C	5.3309078	-1.0738969	-0.8456924
C	4.3335719	1.8362958	-0.6284179
H	1.0907770	0.5855333	-0.7538965
H	1.7863916	-1.8410982	2.0086042
H	5.6778380	-1.0572540	0.1903946
H	6.1694471	-0.7886963	-1.4867387
H	4.7090660	1.8942408	0.3964460
H	5.1079756	2.2290948	-1.2933337
H	3.4648620	2.4959717	-0.7030617
H	4.0137165	0.3309301	-3.5375082
H	2.3760594	0.6599205	-2.9770318
H	2.9467403	-1.0092518	-3.1018772
H	2.6100875	-0.6865406	4.0394321
H	5.0522738	-2.1016425	-1.0908802
H	0.4376192	-1.2998152	2.9867400
H	3.0710739	0.2172430	2.5912538
H	1.7349798	0.7819439	3.5949266
C	-2.2228572	0.1099653	3.1949901
C	-1.2594246	0.9476843	2.3586164
C	-0.6982495	0.2265664	1.1578843
C	-1.4655943	-0.0020040	0.0848386
O	-2.7260107	0.4848224	-0.0259815
Si	-3.8898625	-0.0796755	-1.0807492
C	-3.2417816	-0.0082201	-2.8329271
C	-5.3309078	1.0738969	-0.8456924
C	-4.3335719	-1.8362958	-0.6284179
H	-1.0907770	-0.5855333	-0.7538965
H	-1.7863916	1.8410982	2.0086042
H	-5.6778380	1.0572540	0.1903946
H	-6.1694471	0.7886963	-1.4867387
H	-4.7090660	-1.8942408	0.3964460
H	-5.1079756	-2.2290948	-1.2933337
H	-3.4648620	-2.4959717	-0.7030617
H	-4.0137165	-0.3309301	-3.5375082
H	-2.3760594	-0.6599205	-2.9770318
H	-2.9467403	1.0092518	-3.1018772
H	-2.6100875	0.6865406	4.0394321
H	-5.0522738	2.1016425	-1.0908802
H	-0.4376192	1.2998152	2.9867400
H	-3.0710739	-0.2172430	2.5912538
H	-1.7349798	-0.7819439	3.5949266

Molecule (7c) optimized at the PBE0/def2-TZVP level 45
Energy =

C	1.1205498	-0.9417000	3.4918330
C	0.3022132	-0.5604028	2.3199032
C	0.6747061	-0.4866784	0.8616789
O	1.7798118	0.3201678	0.5648153
Si	2.8925965	0.1961574	-0.6524750
C	2.9993311	-1.5652766	-1.2771180
C	4.5193284	0.7352535	0.0849695
C	2.4306384	1.3470954	-2.0536606
H	0.7525352	-1.4674484	0.3751436
H	0.5590368	-0.8577450	4.4242727
H	4.4361038	1.7400063	0.5074546
H	5.3104723	0.7529576	-0.6697263
H	2.3480044	2.3766377	-1.6951116
H	3.1880816	1.3279300	-2.8426317
H	1.4742317	1.0733196	-2.5064302
H	3.7862631	-1.6423329	-2.0330376
H	2.0678337	-1.8992254	-1.7416112
H	3.2458963	-2.2633056	-0.4724530
H	4.8307281	0.0602707	0.8861407
H	1.4825115	-1.9713282	3.4012941
C	-2.6954534	1.4251926	2.9993794
C	-2.1748790	-0.0086501	2.9547458
C	-0.9590463	-0.1553314	2.1187743
C	-0.7529502	0.1164293	0.6490668
O	-1.6300970	-0.5562988	-0.2107004
Si	-2.1890728	-0.1276261	-1.7070740
C	-2.1125351	1.7286435	-1.9379304
C	-3.9527853	-0.7307331	-1.7852607
C	-1.1771881	-0.9807627	-3.0296310
H	-0.6831966	1.1816314	0.3962040
H	-2.9563779	-0.6607502	2.5461239
H	-4.0010390	-1.8041461	-1.5844372
H	-4.3895684	-0.5538751	-2.7720331
H	-1.2052844	-2.0655334	-2.8959613
H	-1.5660612	-0.7567244	-4.0271932
H	-0.1301708	-0.6681169	-3.0045202
H	-2.5472236	1.9998966	-2.9044458
H	-1.0874215	2.1079321	-1.9230483
H	-2.6777235	2.2541116	-1.1633294
H	-3.6074701	1.4919751	3.5966943
H	-4.5749972	-0.2235937	-1.0435626
H	-1.9698111	-0.3671210	3.9682204
H	-1.9538560	2.0990251	3.4344795
H	-2.9268660	1.7904299	1.9958085
H	2.0038353	-0.2997431	3.5645289

Molecule (7o) optimized at the PBE0/def2-TZVP level 45
Energy =

C	1.2183769	-1.6677672	2.2779973
C	0.7116231	-0.6721602	1.2800915
C	1.4946244	-0.1928830	0.3069869
O	2.7616061	-0.6222334	0.0900141
Si	3.8925563	0.1690313	-0.8478221
C	3.2315920	0.3771089	-2.5842146
C	5.3832218	-0.9444650	-0.8213454
C	4.2647881	1.8362867	-0.0934421
H	1.1193978	0.5760829	-0.3660617
H	2.2539727	-1.9333498	2.0691926
H	5.7398705	-1.0936330	0.2007221
H	6.2021187	-0.5153335	-1.4049431
H	4.6505943	1.7271920	0.9233190
H	5.0121700	2.3758635	-0.6819160
H	3.3676073	2.4593371	-0.0443043
H	3.9803456	0.8520865	-3.2246148
H	2.3362306	1.0039053	-2.6090009
H	2.9777391	-0.5900746	-3.0256611
H	5.1460438	-1.9247432	-1.2418065
H	0.6143672	-2.5807598	2.2625090
C	-0.5170494	1.5324435	3.1958743
C	-1.2003850	0.2585301	2.7097694
C	-0.6835064	-0.2124930	1.3797054
C	-1.4552130	-0.2190098	0.2867925
O	-2.7222928	0.2615008	0.2660244
Si	-3.8308670	-0.0061913	-0.9520444
C	-3.1305657	0.5930767	-2.5786154
C	-5.3230216	0.9863970	-0.4512534
C	-4.2208198	-1.8300127	-1.0498851
H	-1.0728085	-0.6214146	-0.6498573
H	-1.0537527	-0.5336629	3.4530658
H	-5.7042384	0.6538672	0.5173617
H	-6.1272638	0.8809068	-1.1843386
H	-4.6283355	-2.1935933	-0.1031644
H	-4.9567571	-2.0312540	-1.8335059
H	-3.3267799	-2.4173757	-1.2757765
H	-3.8674856	0.4769582	-3.3784868
H	-2.2392563	0.0321824	-2.8720722
H	-2.8598849	1.6506103	-2.5230354
H	-0.8939414	1.8312819	4.1772572
H	-5.0768722	2.0478798	-0.3698996
H	-2.2770115	0.4198952	2.6341254
H	0.5645438	1.3969836	3.2758556
H	-0.6940709	2.3561637	2.5000203
H	1.1675773	-1.2711085	3.2968886

Molecule (8c) optimized at the PBE0/def2-TZVP level
42
Energy =

C	-1.6497406	-0.5249993	-3.4790223
C	-0.6304227	-0.2261047	-2.4496756
C	-0.7097278	-0.3289333	-0.9482587
O	-1.7631406	0.3763642	-0.3535426
Si	-2.5900221	0.0689017	1.0456624
C	-2.4929285	-1.7475390	1.4879323
C	-4.3560330	0.5742751	0.7178633
C	-1.8911531	1.1065622	2.4371340
H	-0.6553789	-1.3586342	-0.5723252
H	-1.2857279	-0.3096732	-4.4855186
H	-4.4045239	1.6179209	0.3965366
H	-4.9712402	0.4705504	1.6159666
H	-1.9248807	2.1685625	2.1796092
H	-2.4668259	0.9674260	3.3568479
H	-0.8518335	0.8481492	2.6548837
H	-3.1040719	-1.9463605	2.3732026
H	-1.4728368	-2.0664911	1.7167096
H	-2.8701371	-2.3778193	0.6780535
H	-4.8004476	-0.0394246	-0.0697151
H	-1.9509706	-1.5771947	-3.4413740
H	-2.5516898	0.0700898	-3.3063294
C	1.6497406	0.5249993	-3.4790223
C	0.6304227	0.2261047	-2.4496756
C	0.7097278	0.3289333	-0.9482587
O	1.7631406	-0.3763642	-0.3535426
Si	2.5900221	-0.0689017	1.0456624
C	2.4929285	1.7475390	1.4879323
C	4.3560330	-0.5742751	0.7178633
C	1.8911531	-1.1065622	2.4371340
H	0.6553789	1.3586342	-0.5723252
H	1.2857279	0.3096732	-4.4855186
H	4.4045239	-1.6179209	0.3965366
H	4.9712402	-0.4705504	1.6159666
H	1.9248807	-2.1685625	2.1796092
H	2.4668259	-0.9674260	3.3568479
H	0.8518335	-0.8481492	2.6548837
H	3.1040719	1.9463605	2.3732026
H	1.4728368	2.0664911	1.7167096
H	2.8701371	2.3778193	0.6780535
H	4.8004476	0.0394246	-0.0697151
H	1.9509706	1.5771947	-3.4413740
H	2.5516898	-0.0700898	-3.3063294

Molecule (8o) optimized at the PBE0/def2-TZVP level
42
Energy =

C	-1.1873589	-0.9962138	-2.6904051
C	-0.6921724	-0.2489152	-1.4906616
C	-1.4767236	-0.0165322	-0.4326040
O	-2.7352358	-0.5068322	-0.3176724
Si	-3.9046094	0.0749219	0.7204405
C	-3.2931077	-0.0416956	2.4831555
C	-5.3715885	-1.0350904	0.4403170
C	-4.2926759	1.8495714	0.2877559
H	-1.1109250	0.5841432	0.3985076
H	-2.2064333	-1.3484067	-2.5350643
H	-5.7012448	-0.9900368	-0.6006255
H	-6.2123422	-0.7385775	1.0734049
H	-4.6287488	1.9341917	-0.7489118
H	-5.0826526	2.2466632	0.9316196
H	-3.4141106	2.4894234	0.4069973
H	-4.0706914	0.2844863	3.1799890
H	-2.4162762	0.5882875	2.6544062
H	-3.0243375	-1.0702608	2.7374446
H	-5.1252297	-2.0744796	0.6709657
H	-0.5491192	-1.8591284	-2.9058155
H	-1.1784199	-0.3631247	-3.5830859
C	1.1873589	0.9962138	-2.6904051
C	0.6921724	0.2489152	-1.4906616
C	1.4767236	0.0165322	-0.4326040
O	2.7352358	0.5068322	-0.3176724
Si	3.9046094	-0.0749219	0.7204405
C	3.2931077	0.0416956	2.4831555
C	5.3715885	1.0350904	0.4403170
C	4.2926759	-1.8495714	0.2877559
H	1.1109250	-0.5841432	0.3985076
H	2.2064333	1.3484067	-2.5350643
H	5.7012448	0.9900368	-0.6006255
H	6.2123422	0.7385775	1.0734049
H	4.6287488	-1.9341917	-0.7489118
H	5.0826526	-2.2466632	0.9316196
H	3.4141106	-2.4894234	0.4069973
H	4.0706914	-0.2844863	3.1799890
H	2.4162762	-0.5882875	2.6544062
H	3.0243375	1.0702608	2.7374446
H	5.1252297	2.0744796	0.6709657
H	0.5491192	1.8591284	-2.9058155
H	1.1784199	0.3631247	-3.5830859

Molecule (9c) optimized at the PBE0/def2-TZVP level

39

Energy =

C	-2.0025516	-0.2906621	-3.4812549
C	-0.8574845	-0.0534312	-2.5779196
C	-0.7457433	-0.2373314	-1.0835238
O	-1.7185411	0.4176735	-0.3241733
Si	-2.3684439	0.0134691	1.1442125
C	-2.1945000	-1.8229375	1.4601694
C	-4.1665260	0.5029290	1.0597521
C	-1.5172078	0.9833665	2.4983798
H	-0.6352707	-1.2868307	-0.7833181
H	-1.7646999	-0.0248398	-4.5124961
H	-4.2656729	1.5623672	0.8094018
H	-4.6676932	0.3362230	2.0172292
H	-1.5842174	2.0570426	2.3030381
H	-1.9820495	0.7911515	3.4697239
H	-0.4588131	0.7236044	2.5802952
H	-2.6878288	-2.0842944	2.4009569
H	-1.1500145	-2.1345905	1.5417142
H	-2.6626942	-2.4133632	0.6679759
H	-4.6956077	-0.0724869	0.2960137
H	-2.3101125	-1.3411274	-3.4545992
H	-2.8657825	0.3006725	-3.1611980
C	0.3936115	0.3976155	-2.7051255
C	0.6663127	0.4312769	-1.2266986
O	1.7796193	-0.2931632	-0.7929094
Si	2.7745458	-0.0423814	0.5047204
C	2.6998726	1.7433743	1.0613703
C	4.4929749	-0.4839770	-0.0711007
C	2.2758451	-1.1746717	1.9087498
H	0.6520250	1.4409802	-0.7991083
H	4.5184609	-1.5056980	-0.4586793
H	5.2150942	-0.4168375	0.7473403
H	2.2765728	-2.2174615	1.5800608
H	2.9721190	-1.0887878	2.7480070
H	1.2757300	-0.9426581	2.2834217
H	3.4108675	1.9077442	1.8763085
H	1.7092684	2.0230300	1.4307714
H	2.9634602	2.4277804	0.2505913
H	4.8226426	0.1844433	-0.8699321
H	1.0138098	0.6562209	-3.5561487

Molecule (9o) optimized at the PBE0/def2-TZVP level

39

Energy =

C	-1.1624956	-0.3483913	-2.9070624
C	-0.6650056	0.0795824	-1.5615909
C	-1.4478317	0.0723626	-0.4763219
O	-2.7127462	-0.4124639	-0.4771198
Si	-3.9067543	0.0014087	0.6130026
C	-3.3187663	-0.3434776	2.3541271
C	-5.3467765	-1.0866920	0.1596808
C	-4.3219703	1.8114175	0.4190349
H	-1.0759522	0.4599725	0.4706713
H	-2.2330291	-0.5496268	-2.8896407
H	-5.6615112	-0.9063340	-0.8710498
H	-6.2028825	-0.8948317	0.8120837
H	-4.6594429	2.0279619	-0.5977012
H	-5.1166237	2.1089461	1.1089832
H	-3.4512930	2.4405917	0.6225676
H	-4.1198183	-0.1438709	3.0717250
H	-2.4684205	0.2843999	2.6326241
H	-3.0194747	-1.3884528	2.4685222
H	-5.0818749	-2.1428062	0.2510237
H	-0.6464356	-1.2516670	-3.2480503
H	-0.9637728	0.4286039	-3.6526986
C	0.7224327	0.5251873	-1.4637686
C	1.5588439	0.1598832	-0.4917656
O	2.8129782	0.6508869	-0.3841681
Si	4.0710370	-0.0649178	0.4490780
C	3.5797108	-0.3166176	2.2352447
C	5.4749758	1.1460778	0.2962304
C	4.4830559	-1.7038164	-0.3448142
H	1.2470395	-0.5544940	0.2704152
H	5.7264551	1.3173260	-0.7532324
H	6.3701915	0.7745697	0.8019991
H	4.7552233	-1.5715482	-1.3949949
H	5.3229076	-2.1858530	0.1634612
H	3.6323395	-2.3894966	-0.3044483
H	4.4178046	-0.7272750	2.8057071
H	2.7440284	-1.0138619	2.3372779
H	3.2895928	0.6290286	2.7001795
H	5.2101530	2.1086251	0.7403855
H	1.1049814	1.1786743	-2.2456286

Molecule (11c) optimized at the PBE0/def2-TZVP level

46

Energy =

C	0.7291178	0.2339876	4.2052408
C	1.5166948	-0.2841995	2.9948716
C	0.6495733	-0.1492572	1.8007666
C	0.7437349	-0.2514140	0.2989000
O	1.6850464	0.5638088	-0.3429871
Si	2.8281221	0.0218185	-1.4152324
C	3.9139703	-1.2663258	-0.5991971
C	3.8160455	1.5334172	-1.8732523
C	2.0050923	-0.7205809	-2.9225375
H	0.7804027	-1.2855860	-0.0696442
H	3.1746606	2.2962244	-2.3216698
H	4.6008813	1.2867468	-2.5936655
H	1.3923615	0.0234134	-3.4382184
H	2.7509947	-1.0920954	-3.6310813
H	1.3576146	-1.5603632	-2.6551813
H	4.6849812	-1.6199204	-1.2898554
H	3.3364679	-2.1383530	-0.2797703
H	4.4154895	-0.8554037	0.2811051
H	4.2919266	1.9703774	-0.9918945
H	2.4514469	0.2735060	2.8729584
H	1.8060602	-1.3336962	3.1392221
H	1.2173874	-0.0765472	5.1331765
H	0.7488697	1.3298152	4.1924484
C	-0.7291178	-0.2339876	4.2052408
C	-1.5166948	0.2841995	2.9948716
C	-0.6495733	0.1492572	1.8007666
C	-0.7437349	0.2514140	0.2989000
O	-1.6850464	-0.5638088	-0.3429871
Si	-2.8281221	-0.0218185	-1.4152324
C	-3.9139703	1.2663258	-0.5991971
C	-3.8160455	-1.5334172	-1.8732523
C	-2.0050923	0.7205809	-2.9225375
H	-0.7804027	1.2855860	-0.0696442
H	-3.1746606	-2.2962244	-2.3216698
H	-4.6008813	-1.2867468	-2.5936655
H	-1.3923615	-0.0234134	-3.4382184
H	-2.7509947	1.0920954	-3.6310813
H	-1.3576146	1.5603632	-2.6551813
H	-4.6849812	1.6199204	-1.2898554
H	-3.3364679	2.1383530	-0.2797703
H	-4.4154895	0.8554037	0.2811051
H	-4.2919266	-1.9703774	-0.9918945
H	-2.4514469	-0.2735060	2.8729584
H	-1.8060602	1.3336962	3.1392221
H	-1.2173874	0.0765472	5.1331765
H	-0.7488697	-1.3298152	4.1924484

Molecule (11o) optimized at the PBE0/def2-TZVP level

46

Energy =

C	-0.3482528	-0.6761445	3.6634121
C	-1.3031099	-0.7711670	2.4764455
C	-0.7155228	-0.1560763	1.2307835
C	-1.4821434	0.1300335	0.1729513
O	-2.7966108	-0.1960471	0.1303635
Si	-3.8219551	0.0574363	-1.1605921
C	-3.8247856	1.8688160	-1.6204429
C	-5.4910793	-0.4922484	-0.5486389
C	-3.2530607	-0.9750238	-2.6108010
H	-1.0740838	0.6560337	-0.6879728
H	-5.4638306	-1.5380276	-0.2331711
H	-6.2469060	-0.3953394	-1.3326410
H	-3.2399100	-2.0368081	-2.3520486
H	-3.9185639	-0.8450200	-3.4688840
H	-2.2451724	-0.6954426	-2.9293458
H	-4.5304954	2.0577814	-2.4344798
H	-2.8399422	2.2053718	-1.9546980
H	-4.1192884	2.4880771	-0.7694032
H	-5.8114848	0.1089763	0.3056103
H	-1.5734966	-1.8159163	2.2836855
H	-2.2429330	-0.2612820	2.7133822
H	-0.8975579	-0.8403462	4.5942959
H	0.4097328	-1.4658747	3.6022168
C	0.3482528	0.6761445	3.6634121
C	1.3031099	0.7711670	2.4764455
C	0.7155228	0.1560763	1.2307835
C	1.4821434	-0.1300335	0.1729513
O	2.7966108	0.1960471	0.1303635
Si	3.8219551	-0.0574363	-1.1605921
C	3.8247856	-1.8688160	-1.6204429
C	5.4910793	0.4922484	-0.5486389
C	3.2530607	0.9750238	-2.6108010
H	1.0740838	-0.6560337	-0.6879728
H	5.4638306	1.5380276	-0.2331711
H	6.2469060	0.3953394	-1.3326410
H	3.2399100	2.0368081	-2.3520486
H	3.9185639	0.8450200	-3.4688840
H	2.2451724	0.6954426	-2.9293458
H	4.5304954	-2.0577814	-2.4344798
H	2.8399422	-2.2053718	-1.9546980
H	4.1192884	-2.4880771	-0.7694032
H	5.8114848	-0.1089763	0.3056103
H	1.5734966	1.8159163	2.2836855
H	2.2429330	0.2612820	2.7133822
H	0.8975579	0.8403462	4.5942959
H	-0.4097328	1.4658747	3.6022168

Molecule (12c) optimized at the PBE0/def2-TZVP level 44
Energy =

C	-0.9777977	-0.5226620	-4.3316327
C	-1.7849548	-0.2986385	-3.0419571
C	-0.8248260	-0.1662050	-1.9168093
C	-0.7383388	-0.2913177	-0.4197269
O	-1.6973312	0.4191327	0.3076010
Si	-2.4371866	0.0528284	1.7417259
C	-2.3929815	-1.7912802	2.0592509
C	-4.1950758	0.6532869	1.5743801
C	-1.5943957	0.9663289	3.1397908
H	-0.6440809	-1.3237240	-0.0592932
H	-4.2162071	1.7180704	1.3278060
H	-4.7528181	0.5127391	2.5044833
H	-1.5792984	2.0418991	2.9433114
H	-2.1219031	0.8074184	4.0848863
H	-0.5611728	0.6375847	3.2780252
H	-2.9462980	-2.0207848	2.9746867
H	-1.3755445	-2.1689910	2.1907617
H	-2.8575586	-2.3513908	1.2432312
H	-4.7195546	0.1163285	0.7798730
H	-2.3794549	0.6230931	-3.1123093
H	-2.5000212	-1.1131528	-2.8985591
C	0.3127371	0.2541868	-4.4248633
C	1.0149683	0.6086681	-3.3416615
C	0.4234445	0.2889676	-2.0609557
C	0.6896963	0.3683849	-0.5816049
O	1.7992365	-0.3395805	-0.1156040
Si	2.7399894	-0.0768514	1.2203592
C	2.6158343	1.7058793	1.7767358
C	4.4861456	-0.4900173	0.7121627
C	2.2049022	-1.2221509	2.5997393
H	0.6694678	1.3909666	-0.1845336
H	4.5456094	-1.5136013	0.3331302
H	5.1749297	-0.4043643	1.5573523
H	2.2604465	-2.2653092	2.2768143
H	2.8499523	-1.1092534	3.4759880
H	1.1777294	-1.0254249	2.9174664
H	3.2922441	1.8781676	2.6190589
H	1.6078016	1.9695341	2.1075562
H	2.9003285	2.3971292	0.9786925
H	0.6996271	0.4573907	-5.4187683
H	4.8344561	0.1795258	-0.0782865
H	-1.6029077	-0.3130435	-5.2034089
H	-0.7149738	-1.5886466	-4.4049146
H	1.9683423	1.1186341	-3.4222237

Molecule (12o) optimized at the PBE0/def2-TZVP level 44
Energy =

C	-0.9121992	-0.0166848	-3.6895166
C	-1.2631302	0.8637465	-2.4892612
C	-0.7138114	0.2690230	-1.2273174
C	-1.4782449	-0.0489818	-0.1791454
O	-2.8015439	0.2354451	-0.1179423
Si	-3.7977228	-0.0684317	1.1852004
C	-3.7638313	-1.8915085	1.5936906
C	-5.4860729	0.4712572	0.6192185
C	-3.2172509	0.9326907	2.6526890
H	-1.0545195	-0.5757007	0.6743765
H	-5.4821562	1.5257743	0.3330185
H	-6.2249842	0.3399867	1.4142878
H	-3.2266742	2.0014483	2.4243018
H	-3.8642394	0.7670041	3.5187696
H	-2.1991817	0.6618347	2.9453740
H	-4.4439358	-2.1136269	2.4209964
H	-2.7655401	-2.2230840	1.8911690
H	-4.0728873	-2.4911032	0.7337843
H	-1.1166845	0.5242842	-4.6196264
H	-5.8132837	-0.1116525	-0.2451251
H	-0.8137373	1.8525361	-2.6432307
H	-2.3416208	1.0012358	-2.4085321
C	0.5173265	-0.4567476	-3.6615152
C	1.2606553	-0.4415049	-2.5504787
C	0.7239555	-0.0304544	-1.2618491
C	1.5024371	0.0941848	-0.1727444
O	2.8091468	-0.2421737	-0.1637984
Si	3.8780924	0.0288971	1.0914454
C	4.0355412	1.8660303	1.3858067
C	5.4791390	-0.7135605	0.5039794
C	3.2522167	-0.8242969	2.6320984
H	1.0884441	0.4804118	0.7571210
H	5.3621711	-1.7803704	0.2988716
H	6.2633814	-0.5979329	1.2569035
H	3.1174385	-1.8949922	2.4589559
H	3.9632232	-0.7034487	3.4543435
H	2.2950893	-0.4137555	2.9645554
H	4.7448618	2.0719194	2.1923909
H	3.0769415	2.3103246	1.6668826
H	4.3893997	2.3766547	0.4866947
H	0.9587673	-0.7987546	-4.5930059
H	5.8190026	-0.2287552	-0.4143572
H	2.3008707	-0.7449383	-2.5826872
H	-1.5663074	-0.8990911	-3.7082208

List of optimized structures, substitution effects on allylic positions

PBE0/def2-TZVP level, c4h4h2 closed
10
Energy = -155.8351364828
C -0.0000494 0.6669881 -0.9222814
H -0.0001535 1.4133060 -1.7086727
C 0.0000549 0.7791942 0.5811297
H -0.8876526 1.2381848 1.0250385
C 0.0000494 -0.6669881 -0.9222814
H 0.0001535 -1.4133060 -1.7086727
C -0.0000549 -0.7791942 0.5811297
H 0.8876526 -1.2381848 1.0250385
H -0.8880220 -1.2379260 1.0247859
H 0.8880220 1.2379260 1.0247859

PBE0/def2-TZVP level, c4h4h2 open
10
Energy = -155.8428712665
C 0.1164163 0.7212970 -0.6090670
H 0.4517732 1.1500578 -1.5510790
C -0.0750105 1.5319361 0.4283410
H -0.4630951 1.1631990 1.3719703
C -0.1164163 -0.7212970 -0.6090670
H -0.4517732 -1.1500578 -1.5510790
C 0.0750105 -1.5319361 0.4283410
H 0.4630951 -1.1631990 1.3719703
H 0.1364269 2.5922681 0.3598348
H -0.1364269 -2.5922681 0.3598348

PBE/def2-TZVP level, c4h4h2 closed
10
Energy = -155.8128586898
C -0.0001120 0.6727977 -0.9280315
H -0.0002563 1.4250486 -1.7191540
C 0.0000743 0.7850516 0.5836924
H -0.8931874 1.2472944 1.0319200
C 0.0001120 -0.6727977 -0.9280315
H 0.0002563 -1.4250486 -1.7191540
C -0.0000743 -0.7850516 0.5836924
H 0.8931874 -1.2472944 1.0319200
H -0.8936630 -1.2469870 1.0315731
H 0.8936630 1.2469870 1.0315731

PBE/def2-TZVP level, c4h4h2 open
10
Energy = -155.8236023863
C 0.1102125 0.7240502 -0.6131900
H 0.4225935 1.1577535 -1.5696066
C -0.0677573 1.5451580 0.4333803
H -0.4376563 1.1770484 1.3928458
C -0.1102125 -0.7240502 -0.6131900
H -0.4225935 -1.1577535 -1.5696066
C 0.0677573 -1.5451580 0.4333803
H 0.4376563 -1.1770484 1.3928458
H 0.1352037 2.6137390 0.3565705
H -0.1352037 -2.6137390 0.3565705

B3LYP/def2-TZVP level, c4h4h2 closed
10
Energy = -155.9238469985
C 0.0000624 0.6676118 -0.9264475
H 0.0000898 1.4119964 -1.7131724
C 0.0000563 0.7848506 0.5844814
H -0.8873243 1.2435529 1.0275551
C -0.0000624 -0.6676118 -0.9264475
H -0.0000898 -1.4119964 -1.7131724
C -0.0000563 -0.7848506 0.5844814
H 0.8873243 -1.2435529 1.0275551
H -0.8874777 -1.2434486 1.0275834

B3LYP/def2-TZVP level, c4h4h2 open
10
Energy = -155.9424176482
C 0.1145732 0.7239933 -0.6053854
H 0.4450379 1.1476014 -1.5504856
C -0.0749625 1.5438461 0.4280783
H -0.4577537 1.1861909 1.3768322
C -0.1145732 -0.7239933 -0.6053854
H -0.4450379 -1.1476014 -1.5504856
C 0.0749625 -1.5438461 0.4280783
H 0.4577537 -1.1861909 1.3768322
H 0.1332975 2.6032478 0.3509606
H -0.1332975 -2.6032478 0.3509606

PBE0/def2-TZVP level, c4h4(nh2)2 closed
14
Energy = -266.4623055774
C -0.2935920 0.5989042 -1.2718795
H -0.5885440 1.2893587 -2.0542201
C -0.3859180 0.6974754 0.2289421
H -1.4055850 0.5581187 0.6067237
C 0.2935920 -0.5989042 -1.2718795
H 0.5885440 -1.2893587 -2.0542201
C 0.3859180 -0.6974754 0.2289421
H 1.4055850 -0.5581187 0.6067237
N 0.1644014 1.8857099 0.8271963
H 0.1409609 1.8403163 1.8381138
H 1.1270226 2.0218809 0.5425330
N -0.1644014 -1.8857099 0.8271963
H -0.1409609 -1.8403163 1.8381138
H -1.1270226 -2.0218809 0.5425330

PBE0/def2-TZVP level, c4h4(nh2)2 open
14
Energy = -266.4893489289
C 0.0651619 0.7231120 -0.7575958
H 0.4098620 1.1910597 -1.6794287
C -0.1951943 1.5096982 0.2955561
H -0.6239615 1.0776108 1.1962210
C -0.0651619 -0.7231120 -0.7575958
H -0.4098620 -1.1910597 -1.6794287
C 0.1951943 -1.5096982 0.2955561
H 0.6239615 -1.0776108 1.1962210
N 0.0985734 2.8608670 0.3994309
H 0.3609278 3.3037007 -0.4683227
H -0.5803431 3.4064067 0.9068077
N -0.0985734 -2.8608670 0.3994309
H -0.3609278 -3.3037007 -0.4683227
H 0.5803431 -3.4064067 0.9068077

PBE/def2-TZVP level, c4h4(nh2)2 closed
14
Energy = -266.4377186289
C -0.2900545 0.6069252 -1.2779444
H -0.5742218 1.3071373 -2.0661581
C -0.3862742 0.7109645 0.2301963
H -1.4131041 0.5708493 0.6106664
C 0.2900545 -0.6069252 -1.2779444
H 0.5742218 -1.3071373 -2.0661581
C 0.3862742 -0.7109645 0.2301963
H 1.4131041 -0.5708493 0.6106664
N 0.1637006 1.9115292 0.8303174
H 0.1374237 1.8629530 1.8506188
H 1.1393132 2.0391147 0.5519775
N -0.1637006 -1.9115292 0.8303174
H -0.1374237 -1.8629530 1.8506188
H -1.1393132 -2.0391147 0.5519775

PBE/def2-TZVP level, c4h4(nh2)2 open
14
Energy = -266.4700948754
C 0.0496993 0.7247612 -0.7615921
H 0.3571168 1.2013664 -1.7012325
C -0.1937013 1.5228429 0.3047540
H -0.5966157 1.0930021 1.2271657
C -0.0496993 -0.7247612 -0.7615921
H -0.3571168 -1.2013664 -1.7012325
C 0.1937013 -1.5228429 0.3047540
H 0.5966157 -1.0930021 1.2271657
N 0.1031970 2.8834793 0.3952229
H 0.3432691 3.3243348 -0.4907220
H -0.5722924 3.4375151 0.9165547
N -0.1031970 -2.8834793 0.3952229
H -0.3432691 -3.3243348 -0.4907220
H 0.5722924 -3.4375151 0.9165547

B3LYP/def2-TZVP level, c4h4(nh2)2 closed
14
Energy = -266.6116799199
C -0.2947068 0.5990660 -1.2765415
H -0.5905883 1.2864725 -2.0596402
C -0.3890246 0.7041222 0.2307219
H -1.4063609 0.5698950 0.6123570
C 0.2947068 -0.5990660 -1.2765415
H 0.5905883 -1.2864725 -2.0596402
C 0.3890246 -0.7041222 0.2307219
H 1.4063609 -0.5698950 0.6123570
N 0.1658445 1.9004766 0.8288284
H 0.1298255 1.8690046 1.8411018
H 1.1312276 2.0391216 0.5509967
N -0.1658445 -1.9004766 0.8288284
H -0.1298255 -1.8690046 1.8411018
H -1.1312276 -2.0391216 0.5509967

B3LYP/def2-TZVP level, c4h4(nh2)2 open
14
Energy = -266.6479309728
C 0.0632504 0.7257569 -0.7483611
H 0.4008045 1.1881949 -1.6747311
C -0.1943301 1.5233356 0.3000137
H -0.6158427 1.1057719 1.2091546
C -0.0632504 -0.7257569 -0.7483611
H -0.4008045 -1.1881949 -1.6747311
C 0.1943301 -1.5233356 0.3000137
H 0.6158427 -1.1057719 1.2091546
N 0.0992373 2.8835674 0.3882923
H 0.3573388 3.3216765 -0.4846435
H -0.5758592 3.4350519 0.8971170
N -0.0992373 -2.8835674 0.3882923
H -0.3573388 -3.3216765 -0.4846435
H 0.5758592 -3.4350519 0.8971170

PBE/def2-TZVP level, c4h4(otms)2 closed
36
Energy = -1123.054294826
C -0.1601058 0.4766212 -2.7649477
H -0.2896683 1.0503629 -3.6836756
C -0.3394365 0.8613446 -1.3113999
H -1.4015167 0.8849159 -1.0050350
O 0.3617792 2.0039701 -0.8717728
Si 0.0143842 2.8291375 0.5515735
C 0.2586069 1.6981647 2.0363048
H 0.0254177 2.2220429 2.9759614
H -0.3957199 0.8156179 1.9702288
H 1.2984157 1.3435142 2.0963386
C 1.2331885 4.2531985 0.5701593
H 1.0938142 4.9029424 -0.3060208
H 1.1067256 4.8689228 1.4733563
H 2.2684692 3.8826003 0.5548762
C -1.7610656 3.4577573 0.5206422
H -1.9747695 4.0517777 1.4226046
H -1.9388438 4.0998742 -0.3546620
H -2.4903735 2.6345294 0.4918512
C 0.2086972 -0.7872972 -2.4937594
H 0.4003092 -1.6670073 -3.1101698
C 0.2601032 -0.5689674 -0.9905728
H 1.2896536 -0.4606479 -0.6037806
O -0.5274529 -1.3894592 -0.1499191
Si -0.0083732 -2.8272057 0.5460176
C -1.4675085 -3.3981120 1.5748539
H -1.2460435 -4.3500589 2.0803293
H -1.7199582 -2.6556883 2.3457841
H -2.3565857 -3.5472709 0.9450874
C 0.4145049 -4.0917942 -0.7845906
H 1.2708017 -3.7673298 -1.3948793
H 0.6809622 -5.0594868 -0.3321950
H -0.4393469 -4.2588667 -1.4576991
C 1.5047656 -2.5223223 1.6255345
H 1.8177994 -3.4541729 2.1212662
H 2.3632369 -2.1600695 1.0402060
H 1.2911743 -1.7796020 2.4084123

PBE/def2-TZVP level, c4h4(otms)2 open
36
Energy = -1123.077535645
C 0.1664957 0.7084142 -1.7917023
H 0.5728614 1.1406862 -2.7119029
C -0.0020902 1.5353159 -0.7407386
H -0.4844316 1.1851615 0.1812915
O 0.4124509 2.8349634 -0.7604911
Si -0.0190459 4.0087002 0.3773994
C 0.4963498 3.4413927 2.0952224
H 0.2752266 4.2202242 2.8411072
H -0.0359061 2.5298947 2.4054517
H 1.5756879 3.2333852 2.1344798
C 0.9357260 5.5269568 -0.1575071
H 0.6570184 5.8257632 -1.1783666
H 0.7325292 6.3761440 0.5120151
H 2.0184596 5.3355147 -0.1445649
C -1.8751370 4.2932119 0.3113028
H -2.1798893 5.0735028 1.0253638
H -2.1887580 4.6119582 -0.6935309
H -2.4310810 3.3772294 0.5613371
C -0.1664957 -0.7084142 -1.7917023
H -0.5728614 -1.1406862 -2.7119029
C 0.0020902 -1.5353159 -0.7407386
H 0.4844316 -1.1851615 0.1812915
O -0.4124509 -2.8349634 -0.7604911
Si 0.0190459 -4.0087002 0.3773994
C -0.4963498 -3.4413927 2.0952224
H -0.2752266 -4.2202242 2.8411072
H 0.0359061 -2.5298947 2.4054517
H -1.5756879 -3.2333852 2.1344798
C -0.9357260 -5.5269568 -0.1575071
H -0.6570184 -5.8257632 -1.1783666
H -0.7325292 -6.3761440 0.5120151
H -2.0184596 -5.3355147 -0.1445649
C 1.8751370 -4.2932119 0.3113028
H 2.1798893 -5.0735028 1.0253638
H 2.1887580 -4.6119582 -0.6935309
H 2.4310810 -3.3772294 0.5613371

B3LYP/def2-TZVP level, c4h4(otms)2 closed
36
Energy = -1123.660605227
C -0.1839536 0.4821863 -2.7113082
H -0.3518661 1.0687519 -3.6053132
C -0.3368233 0.8264887 -1.2461197
H -1.3804949 0.8391620 -0.9137341
O 0.3687819 1.9542735 -0.7939630
Si 0.0146783 2.8934558 0.5350797
C 0.1626060 1.8836235 2.1116660
H -0.0886692 2.4869821 2.9884770
H -0.5116960 1.0233167 2.0980205
H 1.1799086 1.5077886 2.2471137
C 1.2833776 4.2670643 0.4979104
H 1.1988298 4.8544240 -0.4193732
H 1.1555554 4.9463549 1.3449471
H 2.2974358 3.8630459 0.5428858
C -1.7275961 3.5842688 0.3934018
H -1.9487883 4.2439000 1.2372555
H -1.8489081 4.1659675 -0.5237944
H -2.4845201 2.7959175 0.3920901
C 0.2217098 -0.7682693 -2.4845604
H 0.4323243 -1.6144955 -3.1258510
C 0.2870798 -0.5964368 -0.9774471
H 1.3079155 -0.4940699 -0.5942205
O -0.4815271 -1.4529859 -0.1672526
Si -0.0119379 -2.8853018 0.5370261
C -1.4974437 -3.4380671 1.5299054
H -1.3020405 -4.3861372 2.0379615
H -1.7587438 -2.6980602 2.2898935
H -2.3687132 -3.5764308 0.8854496
C 0.4214937 -4.1554629 -0.7787016
H 1.2864122 -3.8458694 -1.3714244
H 0.6678764 -5.1186115 -0.3229232
H -0.4144707 -4.3163954 -1.4638863
C 1.4765477 -2.6101904 1.6506760
H 1.7581827 -3.5406767 2.1515473
H 2.3505893 -2.2669525 1.0911706
H 1.2621054 -1.8684519 2.4239667

B3LYP/def2-TZVP level, c4h4(otms)2 open
36
Energy = -1123.688709930
C 0.1704996 0.7091766 -1.7288539
H 0.5940671 1.1279545 -2.6373414
C -0.0130396 1.5353200 -0.6947137
H -0.5019796 1.1956832 0.2160515
O 0.3943497 2.8320793 -0.7152153
Si -0.0164249 4.0498678 0.3578280
C 0.4790740 3.5502583 2.0979646
H 0.2679390 4.3566900 2.8056154
H -0.0637168 2.6662287 2.4420180
H 1.5478312 3.3295889 2.1537700
C 0.9592195 5.5314362 -0.2262587
H 0.6908765 5.7961693 -1.2515080
H 0.7695116 6.4029828 0.4057297
H 2.0321823 5.3273982 -0.2035409
C -1.8633703 4.3627674 0.2735083
H -2.1552175 5.1743259 0.9456994
H -2.1687235 4.6396427 -0.7383731
H -2.4343516 3.4761185 0.5608304
C -0.1704996 -0.7091766 -1.7288539

```
H    -0.5940671   -1.1279545   -2.6373414
C     0.0130396   -1.5353200   -0.6947137
H     0.5019796   -1.1956832    0.2160515
O    -0.3943497   -2.8320793   -0.7152153
Si    0.0164249   -4.0498678    0.3578280
C    -0.4790740   -3.5502583    2.0979646
H    -0.2679390   -4.3566900    2.8056154
H     0.0637168   -2.6662287    2.4420180
H    -1.5478312   -3.3295889    2.1537700
C    -0.9592195   -5.5314362   -0.2262587
H    -0.6908765   -5.7961693   -1.2515080
H    -0.7695116   -6.4029828    0.4057297
H    -2.0321823   -5.3273982   -0.2035409
C     1.8633703   -4.3627674    0.2735083
H     2.1552175   -5.1743259    0.9456994
H     2.1687235   -4.6396427   -0.7383731
H     2.4343516   -3.4761185    0.5608304
```

PBE0/def2-TZVP level, c4h4(ch3)2 closed

```
16
Energy = -234.3963994584
C    -0.3424553    0.5715004   -1.2730376
H    -0.7176163    1.2184139   -2.0592059
C    -0.4089329    0.6686028    0.2337934
H    -1.4202486    0.5150206    0.6292215
C     0.3424553   -0.5715004   -1.2730376
H     0.7176163   -1.2184139   -2.0592059
C     0.4089329   -0.6686028    0.2337934
H     1.4202486   -0.5150206    0.6292215
C     0.2296873    1.8736483    0.8920090
H     1.2476559    2.0247563    0.5219858
H     0.2769046    1.7529409    1.9779439
H    -0.3389377    2.7844328    0.6845366
C    -0.2296873   -1.8736483    0.8920090
H    -1.2476559   -2.0247563    0.5219858
H    -0.2769046   -1.7529409    1.9779439
H     0.3389377   -2.7844328    0.6845366
```

PBE0/def2-TZVP level, c4h4(ch3)2 open

```
16
Energy = -234.4105042776
C     0.0744296    0.7258122   -0.7013809
H     0.3772524    1.1746904   -1.6467951
C    -0.1500248    1.5351392    0.3341830
H    -0.5115723    1.1012159    1.2649004
C    -0.0744296   -0.7258122   -0.7013809
H    -0.3772524   -1.1746904   -1.6467951
C     0.1500248   -1.5351392    0.3341830
H     0.5115723   -1.1012159    1.2649004
C     0.0413723    3.0111509    0.3178011
H     0.3784254    3.3602744   -0.6602397
H     0.7828516    3.3211026    1.0621734
H    -0.8868582    3.5351508    0.5685817
C    -0.0413723   -3.0111509    0.3178011
H    -0.3784254   -3.3602744   -0.6602397
H    -0.7828516   -3.3211026    1.0621734
H     0.8868582   -3.5351508    0.5685817
```

PBE/def2-TZVP level, c4h4(ch3)2 closed

```
16
Energy = -234.3580131107
C    -0.3429390    0.5777786   -1.2816945
H    -0.7165001    1.2325325   -2.0725238
C    -0.4099993    0.6761498    0.2337441
H    -1.4289488    0.5219707    0.6308917
C     0.3429390   -0.5777786   -1.2816945
H     0.7165001   -1.2325325   -2.0725238
C     0.4099993   -0.6761498    0.2337441
H     1.4289488   -0.5219707    0.6308917
C     0.2311048    1.8875129    0.8992851
H     1.2566837    2.0415151    0.5302647
H     0.2754058    1.7656672    1.9924869
H    -0.3409922    2.8044949    0.6904023
C    -0.2311048   -1.8875129    0.8992851
H    -1.2566837   -2.0415151    0.5302647
H    -0.2754058   -1.7656672    1.9924869
H     0.3409922   -2.8044949    0.6904023
```

PBE/def2-TZVP level, c4h4(ch3)2 open

```
16
Energy = -234.3758999081
C     0.0668459    0.7278948   -0.7032052
H     0.3391672    1.1818323   -1.6643134
C    -0.1397008    1.5501085    0.3421099
H    -0.4754830    1.1170789    1.2917074
C    -0.0668459   -0.7278948   -0.7032052
H    -0.3391672   -1.1818323   -1.6643134
C     0.1397008   -1.5501085    0.3421099
H     0.4754830   -1.1170789    1.2917074
```

```
C     0.0393964    3.0337557    0.3127832
H     0.3510098    3.3843798   -0.6812888
H     0.8009089    3.3584523    1.0419300
H    -0.8913783    3.5574108    0.5876609
C    -0.0393964   -3.0337557    0.3127832
H    -0.3510098   -3.3843798   -0.6812888
H    -0.8009089   -3.3584523    1.0419300
H     0.8913783   -3.5574108    0.5876609
```

B3LYP/def2-TZVP level, c4h4(ch3)2 closed

```
16
Energy = -234.5262797880
C    -0.3407001    0.5732489   -1.2799855
H    -0.7124183    1.2196524   -2.0666656
C    -0.4098704    0.6751603    0.2342292
H    -1.4214027    0.5261342    0.6278330
C     0.3407001   -0.5732489   -1.2799855
H     0.7124183   -1.2196524   -2.0666656
C     0.4098704   -0.6751603    0.2342292
H     1.4214027   -0.5261342    0.6278330
C     0.2296636    1.8869550    0.8975746
H     1.2485109    2.0411413    0.5329770
H     0.2720169    1.7662709    1.9834021
H    -0.3402098    2.7962168    0.6882144
C    -0.2296636   -1.8869550    0.8975746
H    -1.2485109   -2.0411413    0.5329770
H    -0.2720169   -1.7662709    1.9834021
H     0.3402098   -2.7962168    0.6882144
```

B3LYP/def2-TZVP level, c4h4(ch3)2 open

```
16
Energy = -234.5509406532
C     0.0741069    0.7285003   -0.6966566
H     0.3762935    1.1708220   -1.6443261
C    -0.1503180    1.5460890    0.3351614
H    -0.5111408    1.1217900    1.2691816
C    -0.0741069   -0.7285003   -0.6966566
H    -0.3762935   -1.1708220   -1.6443261
C     0.1503180   -1.5460890    0.3351614
H     0.5111408   -1.1217900    1.2691816
C     0.0419105    3.0292284    0.3130423
H     0.3795172    3.3760979   -0.6651800
H     0.7825651    3.3419056    1.0567589
H    -0.8865052    3.5538433    0.5609398
C    -0.0419105   -3.0292284    0.3130423
H    -0.3795172   -3.3760979   -0.6651800
H    -0.7825651   -3.3419056    1.0567589
H     0.8865052   -3.5538433    0.5609398
```

PBE0/def2-TZVP level, c4h4f2 closed

```
10
Energy = -354.2208054573
C    -0.2630822    0.6133915   -1.3237824
H    -0.5207790    1.3256743   -2.0970104
C    -0.3941495    0.6666919    0.1700789
H    -1.4085058    0.5553136    0.5613893
F     0.2004417    1.7275922    0.8108665
C     0.2630822   -0.6133915   -1.3237824
H     0.5207790   -1.3256743   -2.0970104
C     0.3941495   -0.6666919    0.1700789
H     1.4085058   -0.5553136    0.5613893
F    -0.2004417   -1.7275922    0.8108665
```

PBE0/def2-TZVP level, c4h4f2 open

```
10
Energy = -354.2262393357
C     0.1080620    0.7201897   -0.7290180
H     0.5243522    1.1853617   -1.6179546
C    -0.2002983    1.4959709    0.2997762
H    -0.6860014    1.1690194    1.2123788
F     0.0533742    2.8067362    0.2928929
C    -0.1080620   -0.7201897   -0.7290180
H    -0.5243522   -1.1853617   -1.6179546
C     0.2002983   -1.4959709    0.2997762
H     0.6860014   -1.1690194    1.2123788
F    -0.0533742   -2.8067362    0.2928929
```

PBE/def2-TZVP level, c4h4f2 closed

```
10
Energy = -354.2208054573
C    -0.2630822    0.6133915   -1.3237824
H    -0.5207790    1.3256743   -2.0970104
C    -0.3941495    0.6666919    0.1700789
H    -1.4085058    0.5553136    0.5613893
F     0.2004417    1.7275922    0.8108665
C     0.2630822   -0.6133915   -1.3237824
H     0.5207790   -1.3256743   -2.0970104
C     0.3941495   -0.6666919    0.1700789
H     1.4085058   -0.5553136    0.5613893
F    -0.2004417   -1.7275922    0.8108665
```

PBE/def2-TZVP level, c4h4f2 open

```
10
Energy = -354.2178314484
C     0.0981246    0.7229352   -0.7320644
H     0.4801374    1.1963056   -1.6410714
C    -0.1926914    1.5083045    0.3108339
H    -0.6532944    1.1867666    1.2470881
F     0.0526942    2.8382262    0.2872129
C    -0.0981246   -0.7229352   -0.7320644
H    -0.4801374   -1.1963056   -1.6410714
C     0.1926914   -1.5083045    0.3108339
H     0.6532944   -1.1867666    1.2470881
F    -0.0526942   -2.8382262    0.2872129
```

B3LYP/def2-TZVP level, c4h4f2 closed

```
10
Energy = -354.4265777016
C    -0.2757935    0.6086569   -1.3255145
H    -0.5492085    1.3134911   -2.0984982
C    -0.4020188    0.6666549    0.1746343
H    -1.4091569    0.5624219    0.5810493
F     0.2041123    1.7435897    0.8081174
C     0.2757935   -0.6086569   -1.3255145
H     0.5492085   -1.3134911   -2.0984982
C     0.4020188   -0.6666549    0.1746343
H     1.4091569   -0.5624219    0.5810493
F    -0.2041123   -1.7435897    0.8081174
```

B3LYP/def2-TZVP level, c4h4f2 open

```
10
Energy = -354.4408231834
C     0.1032120    0.7235152   -0.7171862
H     0.5063440    1.1839629   -1.6135904
C    -0.1974701    1.5093777    0.3081732
H    -0.6698996    1.2010438    1.2318915
F     0.0537034    2.8323523    0.2788370
C    -0.1032120   -0.7235152   -0.7171862
H    -0.5063440   -1.1839629   -1.6135904
C     0.1974701   -1.5093777    0.3081732
H     0.6698996   -1.2010438    1.2318915
F    -0.0537034   -2.8323523    0.2788370
```

PBE0/def2-TZVP level, c4h4(no2)2 closed

```
14
Energy = -564.6005785415
C    -0.3597968    0.5605892   -1.7271506
H    -0.7543584    1.2185725   -2.4887875
C    -0.4611098    0.6136111   -0.2241710
H    -1.4480666    0.4593504    0.2094392
C     0.3597968   -0.5605892   -1.7271506
H     0.7543584   -1.2185725   -2.4887875
C     0.4611098   -0.6136111   -0.2241710
H     1.4480666   -0.4593504    0.2094392
N     0.0780313    1.8642083    0.4062813
O    -0.5667409    2.8628217    0.1931563
O     1.0915984    1.7944140    1.0596701
N    -0.0780313   -1.8642083    0.4062813
O     0.5667409   -2.8628217    0.1931563
O    -1.0915984   -1.7944140    1.0596701
```

PBE0/def2-TZVP level, c4h4(no2)2 open

```
14
Energy = -564.6114982508
C     0.0621753    0.7224427   -0.7965002
H     0.3467172    1.2117760   -1.7232294
C    -0.1878730    1.4954885    0.2536315
H    -0.5375264    1.1812975    1.2262578
C    -0.0621753   -0.7224427   -0.7965002
H    -0.3467172   -1.2117760   -1.7232294
C     0.1878730   -1.4954885    0.2536315
H     0.5375264   -1.1812975    1.2262578
N    -0.0202286    2.9371373    0.1636650
O     0.3185795    3.4226663   -0.8927010
O    -0.2388174    3.5493157    1.1882748
N     0.0202286   -2.9371373    0.1636650
O    -0.3185795   -3.4226663   -0.8927010
O     0.2388174   -3.5493157    1.1882748
```

PBE/def2-TZVP level, c4h4(no2)2 closed

```
14
Energy = -564.6332958385
C    -0.3653264    0.5638666   -1.7370924
H    -0.7632181    1.2263569   -2.5036632
C    -0.4651359    0.6182874   -0.2255857
H    -1.4575767    0.4644877    0.2146407
C     0.3653264   -0.5638666   -1.7370924
H     0.7632181   -1.2263569   -2.5036632
C     0.4651359   -0.6182874   -0.2255857
H     1.4575767   -0.4644877    0.2146407
N     0.0802559    1.8921351    0.4099103
O    -0.6110046    2.8914703    0.2405606
O     1.1450390    1.8391733    1.0182238
N    -0.0802559   -1.8921351    0.4099103
O     0.6110046   -2.8914703    0.2405606
O    -1.1450390   -1.8391733    1.0182238
```

PBE/def2-TZVP level, c4h4(no2)2 open

```
14
Energy = -564.6488571320
C     0.0530610    0.7253392   -0.7179946
H     0.2915808    1.2262861   -1.6685199
C    -0.1712543    1.5199160    0.3512087
H    -0.4853127    1.2082354    1.3524224
C    -0.0530610   -0.7253392   -0.7179946
H    -0.2915808   -1.2262861   -1.6685199
C     0.1712543   -1.5199160    0.3512087
H     0.4853127   -1.2082354    1.3524224
N    -0.0177488    2.9729581    0.2425815
O     0.2993228    3.4656382   -0.8489524
O    -0.2244476    3.6098416    1.2892544
N     0.0177488   -2.9729581    0.2425815
O    -0.2993228   -3.4656382   -0.8489524
O     0.2244476   -3.6098416    1.2892544
```

B3LYP/def2-TZVP level, c4h4(no2)2 closed
14
Energy = -564.9301588937
C -0.3596945 0.5614718 -1.7383023
H -0.7527019 1.2177781 -2.5003725
C -0.4643056 0.6175922 -0.2289168
H -1.4500818 0.4677819 0.2042892
C 0.3596945 -0.5614718 -1.7383023
H 0.7527019 -1.2177781 -2.5003725
C 0.4643056 -0.6175922 -0.2289168
H 1.4500818 -0.4677819 0.2042892
N 0.0778183 1.8805459 0.4087230
O -0.5739556 2.8857901 0.1984361
O 1.1000878 1.8140098 1.0652417
N -0.0778183 -1.8805459 0.4087230
O 0.5739556 -2.8857901 0.1984361
O -1.1000878 -1.8140098 1.0652417

B3LYP/def2-TZVP level, c4h4(no2)2 open
14
Energy = -564.9517753959
C 0.0592350 0.7249471 -0.7934658
H 0.3329156 1.2067668 -1.7256858
C -0.1826127 1.5056979 0.2562031
H -0.5205479 1.1969641 1.2330448
C -0.0592350 -0.7249471 -0.7934658
H -0.3329156 -1.2067668 -1.7256858
C 0.1826127 -1.5056979 0.2562031
H 0.5205479 -1.1969641 1.2330448
N -0.0196835 2.9556636 0.1626441
O 0.3123299 3.4479319 -0.9033481
O -0.2343927 3.5744952 1.1953342
N 0.0196835 -2.9556636 0.1626441
O -0.3123299 -3.4479319 -0.9033481
O 0.2343927 -3.5744952 1.1953342

PBE0/def2-TZVP level, c8h6h2 closed
16
Energy = -309.3635554853
C -0.6968145 0.0000845 -1.8773023
C -1.4316623 -0.0000263 -0.6914268
C -0.6937017 -0.0000158 0.4743299
C -0.7838893 -0.0000103 1.9834618
H -1.2394909 0.8873747 2.4290835
H -1.2394629 -0.8874027 2.4290954
H -2.5161416 -0.0002043 -0.7085837
H -1.2194544 0.0004082 -2.8276442
C 0.6968145 -0.0000845 -1.8773023
C 1.4316623 0.0000263 -0.6914268
C 0.6937017 0.0000158 0.4743299
C 0.7838893 0.0000103 1.9834618
H 1.2394909 -0.8873747 2.4290835
H 1.2394629 0.8874027 2.4290954
H 2.5161416 0.0002043 -0.7085837
H 1.2194544 -0.0004082 -2.8276442

PBE0/def2-TZVP level, c8h6h2 open
16
Energy = -309.3328118523
C -0.7136507 0.1103928 -1.8051892
C -1.3972100 0.1730939 -0.6506348
C -0.7418254 -0.0016201 0.6339936
C -1.4751070 -0.2195693 1.7388636
H -2.5574967 -0.1840968 1.6978835
H -1.0236560 -0.4580694 2.6936202
H -2.4746227 0.2997770 -0.6505510
H -1.2328322 0.2036281 -2.7523070
C 0.7136507 -0.1103928 -1.8051892
C 1.3972100 -0.1730939 -0.6506348
C 0.7418254 0.0016201 0.6339936
C 1.4751070 0.2195693 1.7388636
H 2.5574967 0.1840968 1.6978835
H 1.0236560 0.4580694 2.6936202
H 2.4746227 -0.2997770 -0.6505510
H 1.2328322 -0.2036281 -2.7523070

PBE/def2-TZVP level, c8h6h2 closed
16
Energy = -309.3277867020
C -0.7016163 0.0001918 -1.8902608
C -1.4416562 -0.0000983 -0.6958181
C -0.6994636 -0.0000141 0.4782844
C -0.7897046 -0.0000178 1.9960135
H -1.2481490 0.8929938 2.4460023
H -1.2484050 -0.8927760 2.4462635
H -2.5336654 0.0000782 -0.7134569
H -1.2282190 0.0001045 -2.8468055
C 0.7016163 -0.0001918 -1.8902608
C 1.4416562 0.0000983 -0.6958181
C 0.6994636 0.0000141 0.4782844
C 0.7897046 0.0000178 1.9960135
H 1.2481490 -0.8929938 2.4460023
H 1.2484050 0.8927760 2.4462635
H 2.5336654 -0.0000782 -0.7134569
H 1.2282190 -0.0001045 -2.8468055

PBE/def2-TZVP level, c8h6h2 open
16
Energy = -309.3026679060
C -0.7152194 0.1055407 -1.8202788
C -1.4039203 0.1669578 -0.6523234
C -0.7461538 0.0005718 0.6357107
C -1.4886252 -0.2108099 1.7528911
H -2.5778795 -0.1700603 1.7103654
H -1.0378701 -0.4493928 2.7161079
H -2.4899946 0.2845113 -0.6524058
H -1.2405753 0.1920089 -2.7731036

```
C     0.7152194   -0.1055407   -1.8202788
C     1.4039203   -0.1669578   -0.6523234
C     0.7461538   -0.0005718    0.6357107
C     1.4886252    0.2108099    1.7528911
H     2.5778795    0.1700603    1.7103654
H     1.0378701    0.4493928    2.7161079
H     2.4899946   -0.2845113   -0.6524058
H     1.2405753   -0.1920089   -2.7731036
```

B3LYP/def2-TZVP level, c8h6h2 closed

```
16
Energy = -309.5369648812
C    -0.6985385    0.0000211   -1.8847430
C    -1.4335402    0.0000004   -0.6939775
C    -0.6952296   -0.0000104    0.4750930
C    -0.7895665   -0.0000142    1.9918904
H    -1.2444797    0.8867215    2.4377218
H    -1.2444502   -0.8867648    2.4377215
H    -2.5170788    0.0000168   -0.7104423
H    -1.2218100    0.0000193   -2.8335225
C     0.6985385   -0.0000211   -1.8847430
C     1.4335402   -0.0000004   -0.6939775
C     0.6952296    0.0000104    0.4750930
C     0.7895665    0.0000142    1.9918904
H     1.2444797   -0.8867215    2.4377218
H     1.2444502    0.8867648    2.4377215
H     2.5170788   -0.0000168   -0.7104423
H     1.2218100   -0.0000193   -2.8335225
```

B3LYP/def2-TZVP level, c8h6h2 open

```
16
Energy = -309.5176585504
C    -0.7161279    0.1055605   -1.8103094
C    -1.4022750    0.1655809   -0.6539944
C    -0.7457621   -0.0015558    0.6370144
C    -1.4840830   -0.2093331    1.7441501
H    -2.5652780   -0.1756554    1.7002928
H    -1.0398769   -0.4353763    2.7037568
H    -2.4791555    0.2868103   -0.6557597
H    -1.2337525    0.1949137   -2.7575858
C     0.7161279   -0.1055605   -1.8103094
C     1.4022750   -0.1655809   -0.6539944
C     0.7457621    0.0015558    0.6370144
C     1.4840830    0.2093331    1.7441501
H     2.5652780    0.1756554    1.7002928
H     1.0398769    0.4353763    2.7037568
H     2.4791555   -0.2868103   -0.6557597
H     1.2337525   -0.1949137   -2.7575858
```

PBE0/def2-TZVP level, c8h6(nh2)2 closed

```
20
Energy = -419.9893859831
C    -0.6754154   -0.1751304   -2.4724163
C    -1.3839615   -0.3688026   -1.2879986
C    -0.6650993   -0.1925717   -0.1217023
C    -0.7530147   -0.2747643    1.3851447
H    -0.7610967   -1.3107625    1.7447287
H    -2.4307348   -0.6508620   -1.2997005
H    -1.1803058   -0.3066172   -3.4234186
C     0.6754154    0.1751304   -2.4724163
C     1.3839615    0.3688026   -1.2879986
C     0.6650993    0.1925717   -0.1217023
C     0.7530147    0.2747643    1.3851447
H     0.7610967    1.3107625    1.7447287
H     2.4307348    0.6508620   -1.2997005
H     1.1803058    0.3066172   -3.4234186
N    -1.8338885    0.4359076    2.0137821
H    -1.7624987    0.4071966    3.0230864
H    -1.8469138    1.4070661    1.7262584
N     1.8338885   -0.4359076    2.0137821
H     1.7624987   -0.4071966    3.0230864
H     1.8469138   -1.4070661    1.7262584
```

PBE0/def2-TZVP level, c8h6(nh2)2 open

```
20
Energy = -419.9785123420
C     0.0242916    0.7362365    0.1823447
C    -0.2635676    1.4403188    1.3078306
H    -0.6586422    0.9101555    2.1689258
C    -0.0242916   -0.7362365    0.1823447
C     0.2635676   -1.4403188    1.3078306
H     0.6586422   -0.9101555    2.1689258
N    -0.0496926    2.7854038    1.5247345
H     0.1754287    3.3410553    0.7162064
H    -0.7170208    3.2397892    2.1266395
N     0.0496926   -2.7854038    1.5247345
H    -0.1754287   -3.3410553    0.7162064
H     0.7170208   -3.2397892    2.1266395
C     0.3137413    1.3692786   -1.0831480
H     0.5684781    2.4239559   -1.1152486
C    -0.3137413   -1.3692786   -1.0831480
H    -0.5684781   -2.4239559   -1.1152486
C     0.1976687    0.6912071   -2.2444191
H     0.3731778    1.1924874   -3.1894682
C    -0.1976687   -0.6912071   -2.2444191
H    -0.3731778   -1.1924874   -3.1894682
```

PBE/def2-TZVP level, c8h6(nh2)2 closed

```
20
Energy = -419.9514472698
C    -0.6807910   -0.1729384   -2.4886406
C    -1.3945995   -0.3656409   -1.2951837
C    -0.6710803   -0.1927514   -0.1202985
C    -0.7645253   -0.2774125    1.3944406
H    -0.7684493   -1.3200993    1.7587158
H    -2.4496117   -0.6460010   -1.3071475
H    -1.1899178   -0.3042078   -3.4458404
C     0.6807910    0.1729384   -2.4886406
C     1.3945995    0.3656409   -1.2951837
C     0.6710803    0.1927514   -0.1202985
C     0.7645253    0.2774125    1.3944406
H     0.7684493    1.3200993    1.7587158
H     2.4496117    0.6460010   -1.3071475
H     1.1899178    0.3042078   -3.4458404
N    -1.8613651    0.4309932    2.0235339
H    -1.7851884    0.4032685    3.0422240
H    -1.8675454    1.4131236    1.7389437
N     1.8613651   -0.4309932    2.0235339
H     1.7851884   -0.4032685    3.0422240
H     1.8675454   -1.4131236    1.7389437
```

H -0.3724242 -1.1939072 -3.1931385

PBE/def2-TZVP level, c8h6(nh2)2 open
20
Energy = -419.9495772400
C 0.0149356 0.7400209 0.1728086
C -0.2661363 1.4428261 1.3219153
H -0.6688981 0.9062748 2.1849712
C -0.0149356 -0.7400209 0.1728086
C 0.2661363 -1.4428261 1.3219153
H 0.6688981 -0.9062748 2.1849712
N -0.0219753 2.7879676 1.5537818
H 0.2515240 3.3450014 0.7497622
H -0.6946344 3.2669874 2.1458936
N 0.0219753 -2.7879676 1.5537818
H -0.2515240 -3.3450014 0.7497622
H 0.6946344 -3.2669874 2.1458936
C 0.2673636 1.3849815 -1.0957529
H 0.4645871 2.4597583 -1.1301755
C -0.2673636 -1.3849815 -1.0957529
H -0.4645871 -2.4597583 -1.1301755
C 0.1676716 0.6991484 -2.2720140
H 0.3101161 1.2169170 -3.2222107
C -0.1676716 -0.6991484 -2.2720140
H -0.3101161 -1.2169170 -3.2222107

B3LYP/def2-TZVP level, c8h6(nh2)2 closed
20
Energy = -420.2234209704
C -0.6760874 -0.1793259 -2.4811109
C -1.3836635 -0.3773830 -1.2918958
C -0.6657062 -0.1959588 -0.1221054
C -0.7599357 -0.2770323 1.3914775
H -0.7732132 -1.3086471 1.7586714
H -2.4279233 -0.6647224 -1.3033273
H -1.1802270 -0.3153570 -3.4306547
C 0.6760874 0.1793259 -2.4811109
C 1.3836635 0.3773830 -1.2918958
C 0.6657062 0.1959588 -0.1221054
C 0.7599357 0.2770323 1.3914775
H 0.7732132 1.3086471 1.7586714
H 2.4279233 0.6647224 -1.3033273
H 1.1802270 0.3153570 -3.4306547
N -1.8475749 0.4424412 2.0183889
H -1.7884201 0.4101310 3.0296971
H -1.8623289 1.4151461 1.7319400
N 1.8475749 -0.4424412 2.0183889
H 1.7884201 -0.4101310 3.0296971
H 1.8623289 -1.4151461 1.7319400

B3LYP/def2-TZVP level, c8h6(nh2)2 open
20
Energy = -420.2215888393
C 0.0258480 0.7405922 0.1876957
C -0.2584957 1.4527971 1.3122243
H -0.6427691 0.9331814 2.1823163
C -0.0258480 -0.7405922 0.1876957
C 0.2584957 -1.4527971 1.3122243
H 0.6427691 -0.9331814 2.1823163
N -0.0499065 2.8082022 1.5210838
H 0.1559121 3.3673803 0.7086087
H -0.7084654 3.2595821 2.1368518
N 0.0499065 -2.8082022 1.5210838
H -0.1559121 -3.3673803 0.7086087
H 0.7084654 -3.2595821 2.1368518
C 0.3133406 1.3725076 -1.0851098
H 0.5687512 2.4257168 -1.1174087
C -0.3133406 -1.3725076 -1.0851098
H -0.5687512 -2.4257168 -1.1174087
C 0.1972636 0.6932332 -2.2487985
H 0.3724242 1.1939072 -3.1931385
C -0.1972636 -0.6932332 -2.2487985

PBE/def2-TZVP level, c8h6(otms)2 closed
42
Energy = -1276.564259549
C -0.7014369 -0.1707242 -4.4349117
C -1.4099961 -0.3630624 -3.2394394
C -0.6790127 -0.1935840 -2.0689394
C -0.7417214 -0.3063237 -0.5533794
O -1.7575634 0.4204323 0.0936115
Si -2.6058570 0.0451307 1.4908593
C -2.4753189 -1.7920240 1.8821381
C -4.3849138 0.5361732 1.1507370
C -1.9280074 1.0674423 2.9181840
H -0.6985195 -1.3552947 -0.2081525
H -2.4658818 -0.6409319 -3.2490329
H -4.4445563 1.5928253 0.8508829
H -5.0133771 0.4029989 2.0444022
H -1.9712934 2.1409869 2.6809012
H -2.5131451 0.9029735 3.8361279
H -0.8809493 0.8139706 3.1405864
H -3.0867343 -2.0263510 2.7673182
H -1.4433514 -2.1006938 2.1057359
H -2.8439004 -2.4133698 1.0522247
H -1.2149023 -0.2995883 -5.3900629
H -4.8148134 -0.0681688 0.3386262
C 0.6618967 0.1718058 -4.4409024
C 1.3812305 0.3630048 -3.2517736
C 0.6609813 0.1925423 -2.0747821
C 0.7366776 0.3051477 -0.5595736
O 1.7575354 -0.4217316 0.0792394
Si 2.6189576 -0.0449680 1.4679671
C 2.4949776 1.7930141 1.8572211
C 4.3940267 -0.5396059 1.1125996
C 1.9525297 -1.0630524 2.9037420
H 0.6961546 1.3541461 -0.2141825
H 2.4369724 0.6405400 -3.2708751
H 4.4492859 -1.5969461 0.8144283
H 5.0306935 -0.4055663 2.0003357
H 1.9908399 -2.1371393 2.6682324
H 2.5470289 -0.8982491 3.8156301
H 0.9083230 -0.8066231 3.1359481
H 3.1130619 2.0272637 2.7377393
H 1.4652895 2.1040073 2.0878221
H 2.8588759 2.4121948 1.0236983
H 1.1665952 0.3017533 -5.4005452
H 4.8175646 0.0623704 0.2954532

PBE/def2-TZVP level, c8h6(otms)2 open
42
Energy = -1276.557606997
C -0.6541953 0.3032822 3.7014928
C -1.3130735 0.5359437 2.5318305
C -0.7218660 0.1586583 1.2646268
C 0.7218660 -0.1586583 1.2646268
C 1.3130735 -0.5359437 2.5318305
C 0.6541953 -0.3032822 3.7014928
C -1.4824562 0.0080841 0.1370469
O -2.7763394 0.4231374 0.0714925
Si -3.8906123 -0.0599602 -1.1099834
C -3.2354803 0.4027415 -2.8108629
C 1.4824562 -0.0080841 0.1370469
O 2.7763394 -0.4231374 0.0714925
Si 3.8906123 0.0599602 -1.1099834
C 5.4393652 -0.9004659 -0.6857779
C -5.4393652 0.9004659 -0.6857779
C -4.1574177 -1.9144569 -0.9861646
C 3.2354803 -0.4027415 -2.8108629
C 4.1574177 1.9144569 -0.9861646
H -1.0639671 -0.4591858 -0.7617492
H 1.0639671 0.4591858 -0.7617492
H -2.3289450 0.9329188 2.5293468
H -5.7897113 0.6528652 0.3267105
H -6.2511798 0.6679782 -1.3911704
H -4.5212713 -2.1934709 0.0134823
H -4.8984042 -2.2559367 -1.7249632
H -3.2237391 -2.4667730 -1.1693479
H -3.9715432 0.1479509 -3.5886992
H -2.3045767 -0.1308887 -3.0536486
H -3.0352482 1.4822260 -2.8766390
H 3.0352482 -1.4822260 -2.8766390
H 2.3045767 0.1308887 -3.0536486
H 3.9715432 -0.1479509 -3.5886992
H 4.8984042 2.2559367 -1.7249632
H 3.2237391 2.4667730 -1.1693479
H 4.5212713 2.1934709 0.0134823
H 5.2550271 -1.9837377 -0.7256135
H 5.7897113 -0.6528652 0.3267105
H 6.2511798 -0.6679782 -1.3911704
H 2.3289450 -0.9329188 2.5293468
H 1.1293667 -0.5463122 4.6539163
H -1.1293667 0.5463122 4.6539163
H -5.2550271 1.9837377 -0.7256135

B3LYP/def2-TZVP level, c8h6(otms)2 closed
42
Energy = -1277.270749754
C -0.8997398 -0.1408787 -4.1265620
C -1.5408193 -0.2986209 -2.8953913
C -0.7409906 -0.1591836 -1.7741284
C -0.7143648 -0.2637550 -0.2542652
O -1.5941620 0.5387566 0.4888163
Si -2.8828348 0.0372707 1.4155297
C -4.1518422 -0.8450761 0.3469144
C -3.5927908 1.6112004 2.1326976
C -2.2943895 -1.1193595 2.7738713
H -0.7130616 -1.3024787 0.0948798
H -2.5983491 -0.5277803 -2.8441603
H -2.8577012 2.1259048 2.7557189
H -4.4696996 1.4029248 2.7513647
H -1.5494456 -0.6335395 3.4088624
H -3.1287451 -1.4233662 3.4121720
H -1.8448931 -2.0305853 2.3708685
H -5.0168880 -1.1517399 0.9415932
H -3.7378506 -1.7461691 -0.1136364
H -4.5133908 -0.1952729 -0.4539969
H -1.4699919 -0.2471100 -5.0417706
H -3.8971139 2.2980566 1.3395215
C 0.4686006 0.1386714 -4.2131293
C 1.2594393 0.2957685 -3.0723861
C 0.6065526 0.1560502 -1.8600373
C 0.7765513 0.2562588 -0.3511343
O 1.7575357 -0.5433126 0.2550375
Si 2.9957808 -0.0351209 1.2454431
C 4.0752742 1.2119360 0.3450821
C 3.9552117 -1.5900085 1.6419415
C 2.3015707 0.7453861 2.8065295
H 0.8174575 1.2946826 -0.0031202
H 2.3154557 0.5233065 -3.1533665
H 3.3223431 -2.3214599 2.1499315
H 4.8069148 -1.3744040 2.2925399
H 1.6633308 0.0418823 3.3467929
H 3.1068280 1.0505093 3.4806624
H 1.7053618 1.6348885 2.5871009
H 4.9036535 1.5382173 0.9801831
H 3.5146226 2.1055697 0.0582629
H 4.5035067 0.7806849 -0.5632619
H 0.9189865 0.2448046 -5.1928802
H 4.3379571 -2.0559136 0.7309664

B3LYP/def2-TZVP level, c8h6(otms)2 open
42
Energy = -1277.263753242
C -0.6524595 0.3105462 3.6361388

```
C    -1.3062762    0.5454887    2.4785008
C    -0.7223723    0.1590091    1.2067238
C     0.7223723   -0.1590091    1.2067238
C     1.3062762   -0.5454887    2.4785008
C     0.6524595   -0.3105462    3.6361388
C    -1.4833628    0.0096406    0.0965059
O    -2.7801227    0.4033873    0.0423192
Si   -3.9434019   -0.0574654   -1.0740409
C    -3.3456112    0.3475666   -2.8062685
C     1.4833628   -0.0096406    0.0965059
O     2.7801227   -0.4033873    0.0423192
Si    3.9434019    0.0574654   -1.0740409
C     5.4460146   -0.9545239   -0.6212357
C    -5.4460146    0.9545239   -0.6212357
C    -4.2697057   -1.8952990   -0.9084489
C     3.3456112   -0.3475666   -2.8062685
C     4.2697057    1.8952990   -0.9084489
H    -1.0746025   -0.4371183   -0.8050414
H     1.0746025    0.4371183   -0.8050414
H    -2.3071053    0.9559499    2.4773692
H    -5.7705659    0.7390295    0.3993281
H    -6.2819575    0.7371294   -1.2912523
H    -4.6088672   -2.1448087    0.0996955
H    -5.0406770   -2.2215364   -1.6118955
H    -3.3696701   -2.4816757   -1.1100019
H    -4.1160713    0.1060528   -3.5437051
H    -2.4505210   -0.2179461   -3.0770311
H    -3.1131879    1.4108274   -2.9038365
H     3.1131879   -1.4108274   -2.9038365
H     2.4505210    0.2179461   -3.0770311
H     4.1160713   -0.1060528   -3.5437051
H     5.0406770    2.2215364   -1.6118955
H     3.3696701    2.4816757   -1.1100019
H     4.6088672    2.1448087    0.0996955
H     5.2334607   -2.0240539   -0.6860119
H     5.7705659   -0.7390295    0.3993281
H     6.2819575   -0.7371294   -1.2912523
H     2.3071053   -0.9559499    2.4773692
H     1.1159394   -0.5602308    4.5829899
H    -1.1159394    0.5602308    4.5829899
H    -5.2334607    2.0240539   -0.6860119
```

PBE0/def2-TZVP level, c8h6(ch3)2 closed
22
Energy = -387.9245226635

```
C    -0.6596956   -0.2243035   -2.4542982
C    -1.3537827   -0.4636875   -1.2678769
C    -0.6538605   -0.2288906   -0.1015929
C    -0.7398138   -0.2722982    1.4109620
H    -0.7802787   -1.2960386    1.8005588
H    -2.3791748   -0.8173350   -1.2861002
H    -1.1544025   -0.3928252   -3.4047596
C     0.6596956    0.2243035   -2.4542982
C     1.3537827    0.4636875   -1.2678769
C     0.6538605    0.2288906   -0.1015929
C     0.7398138    0.2722982    1.4109620
H     0.7802787    1.2960386    1.8005588
H     2.3791748    0.8173350   -1.2861002
H     1.1544025    0.3928252   -3.4047596
C    -1.7901200    0.5841523    2.0862511
H    -1.7560079    1.6104157    1.7108711
H    -1.6376820    0.6118387    3.1687294
H    -2.7949988    0.1953486    1.9019868
C     1.7901200   -0.5841523    2.0862511
H     1.7560079   -1.6104157    1.7108711
H     1.6376820   -0.6118387    3.1687294
H     2.7949988   -0.1953486    1.9019868
```

PBE0/def2-TZVP level, c8h6(ch3)2 open
22
Energy = -387.8952847843

```
C    -0.6908494    0.2042977   -2.2172593
C    -1.3690196    0.3336847   -1.0623835
C    -0.7410394    0.0430007    0.2128854
C    -1.4554505   -0.2278467    1.3267799
H    -0.9054937   -0.5938859    2.1899650
H    -2.4209210    0.5902640   -1.0833906
H    -1.1897914    0.3776540   -3.1641836
C     0.6908494   -0.2042977   -2.2172593
C     1.3690196   -0.3336847   -1.0623835
C     0.7410394   -0.0430007    0.2128854
C     1.4554505    0.2278467    1.3267799
H     0.9054937    0.5938859    2.1899650
H     2.4209210   -0.5902640   -1.0833906
H     1.1897914   -0.3776540   -3.1641836
C    -2.9261691   -0.1120827    1.5136016
H    -3.1500889    0.4604370    2.4198296
H    -3.3823326   -1.0988962    1.6546836
H    -3.4337976    0.3729329    0.6806310
C     2.9261691    0.1120827    1.5136016
H     3.1500889   -0.4604370    2.4198296
H     3.3823326    1.0988962    1.6546836
H     3.4337976   -0.3729329    0.6806310
```

PBE/def2-TZVP level, c8h6(ch3)2 closed
22
Energy = -387.8726427333

```
C    -0.6648636   -0.2238994   -2.4721009
C    -1.3641422   -0.4634270   -1.2768851
C    -0.6597249   -0.2292125   -0.1021677
C    -0.7468629   -0.2733711    1.4194532
H    -0.7861459   -1.3049400    1.8103875
H    -2.3975705   -0.8169692   -1.2957618
H    -1.1638928   -0.3927700   -3.4286174
C     0.6648636    0.2238994   -2.4721009
C     1.3641422    0.4634270   -1.2768851
C     0.6597249    0.2292125   -0.1021677
C     0.7468629    0.2733711    1.4194532
H     0.7861459    1.3049400    1.8103875
H     2.3975705    0.8169692   -1.2957618
H     1.1638928    0.3927700   -3.4286174
C    -1.8043662    0.5844736    2.1024400
H    -1.7714695    1.6197419    1.7307261
```

```
H    -1.6530817    0.6066206    3.1924972
H    -2.8155595    0.1934603    1.9142944
C     1.8043662   -0.5844736    2.1024400
H     1.7714695   -1.6197419    1.7307261
H     1.6530817   -0.6066206    3.1924972
H     2.8155595   -0.1934603    1.9142944

PBE/def2-TZVP level, c8h6(ch3)2 open
22
Energy = -387.8501228917
C    -0.6933904    0.1980695   -2.2369603
C    -1.3775107    0.3246193   -1.0682525
C    -0.7451537    0.0418727    0.2091262
C    -1.4657740   -0.2294714    1.3372842
H    -0.9110329   -0.6036987    2.2034295
H    -2.4412182    0.5650931   -1.0892460
H    -1.2002706    0.3633277   -3.1895778
C     0.6933904   -0.1980695   -2.2369603
C     1.3775107   -0.3246193   -1.0682525
C     0.7451537   -0.0418727    0.2091262
C     1.4657740    0.2294714    1.3372842
H     0.9110329    0.6036987    2.2034295
H     2.4412182   -0.5650931   -1.0892460
H     1.2002706   -0.3633277   -3.1895778
C    -2.9410855   -0.1051472    1.5292872
H    -3.1628214    0.4699014    2.4437327
H    -3.4086733   -1.0949435    1.6734076
H    -3.4529151    0.3871147    0.6931971
C     2.9410855    0.1051472    1.5292872
H     3.1628214   -0.4699014    2.4437327
H     3.4086733    1.0949435    1.6734076
H     3.4529151   -0.3871147    0.6931971

B3LYP/def2-TZVP level, c8h6(ch3)2 closed
22
Energy = -388.1390395593
C    -0.6610272   -0.2256255   -2.4649494
C    -1.3549522   -0.4653759   -1.2735000
C    -0.6553052   -0.2293594   -0.1037100
C    -0.7458319   -0.2737519    1.4165183
H    -0.7882330   -1.2963043    1.8057985
H    -2.3790531   -0.8197934   -1.2912457
H    -1.1564308   -0.3954180   -3.4136069
C     0.6610272    0.2256255   -2.4649494
C     1.3549522    0.4653759   -1.2735000
C     0.6553052    0.2293594   -0.1037100
C     0.7458319    0.2737519    1.4165183
H     0.7882330    1.2963043    1.8057985
H     2.3790531    0.8197934   -1.2912457
H     1.1564308    0.3954180   -3.4136069
C    -1.8036972    0.5836278    2.0968693
H    -1.7719308    1.6117853    1.7281449
H    -1.6537974    0.6055443    3.1795264
H    -2.8070883    0.1934569    1.9090868
C     1.8036972   -0.5836278    2.0968693
H     1.7719308   -1.6117853    1.7281449
H     1.6537974   -0.6055443    3.1795264
H     2.8070883   -0.1934569    1.9090868

B3LYP/def2-TZVP level, c8h6(ch3)2 open
22
Energy = -388.1200710289
C    -0.6920169    0.2068581   -2.2235399
C    -1.3711924    0.3379747   -1.0662904
C    -0.7454615    0.0436832    0.2155902
C    -1.4650621   -0.2270059    1.3294516
H    -0.9217107   -0.5901269    2.1959949
H    -2.4208306    0.5980994   -1.0886502
H    -1.1886828    0.3830884   -3.1699825
C     0.6920169   -0.2068581   -2.2235399
C     1.3711924   -0.3379747   -1.0662904
C     0.7454615   -0.0436832    0.2155902
C     1.4650621    0.2270059    1.3294516
H     0.9217107    0.5901269    2.1959949
H     2.4208306   -0.5980994   -1.0886502
H     1.1886828   -0.3830884   -3.1699825
C    -2.9436054   -0.1139232    1.5176708
H    -3.1679082    0.4585112    2.4234910
H    -3.3971949   -1.1014954    1.6597462
H    -3.4537572    0.3686101    0.6857764
C     2.9436054    0.1139232    1.5176708
H     3.1679082   -0.4585112    2.4234910
H     3.3971949    1.1014954    1.6597462
H     3.4537572   -0.3686101    0.6857764
```

PBE0/def2-TZVP level, c8h6f2 closed
16
Energy = -507.7453883835
C -0.6799974 -0.1615276 -2.5490272
C -1.3942752 -0.3436156 -1.3692513
C -0.6680450 -0.1802195 -0.2050693
C -0.7199059 -0.2962712 1.2960636
F -1.6726412 0.4375760 1.9573375
H -0.7452419 -1.3195534 1.6814595
H -2.4454857 -0.6062263 -1.3824574
H -1.1851219 -0.2828202 -3.5008312
C 0.6799974 0.1615276 -2.5490272
C 1.3942752 0.3436156 -1.3692513
C 0.6680450 0.1802195 -0.2050693
C 0.7199059 0.2962712 1.2960636
F 1.6726412 -0.4375760 1.9573375
H 0.7452419 1.3195534 1.6814595
H 2.4454857 0.6062263 -1.3824574
H 1.1851219 0.2828202 -3.5008312

PBE0/def2-TZVP level, c8h6f2 open
16
Energy = -507.7137083322
C -0.6935420 0.2006654 -2.2460903
C -1.3793946 0.3282031 -1.0964167
C -0.7353403 0.0423392 0.1701022
C -1.4424376 -0.2311015 1.2759589
F -2.7699173 -0.0892263 1.3094331
H -1.0374489 -0.6028369 2.2085275
H -2.4343115 0.5715203 -1.0959494
H -1.1898324 0.3703437 -3.1946224
C 0.6935420 -0.2006654 -2.2460903
C 1.3793946 -0.3282031 -1.0964167
C 0.7353403 -0.0423392 0.1701022
C 1.4424376 0.2311015 1.2759589
F 2.7699173 0.0892263 1.3094331
H 1.0374489 0.6028369 2.2085275
H 2.4343115 -0.5715203 -1.0959494
H 1.1898324 -0.3703437 -3.1946224

PBE/def2-TZVP level, c8h6f2 closed
16
Energy = -507.7192249877
C -0.6842686 -0.1633292 -2.5676014
C -1.4034065 -0.3477323 -1.3788112
C -0.6733117 -0.1842055 -0.2064888
C -0.7253272 -0.3013726 1.3027024
F -1.6965279 0.4403084 1.9728709
H -0.7512284 -1.3300342 1.6962984
H -2.4616684 -0.6129827 -1.3922610
H -1.1931334 -0.2863675 -3.5255828
C 0.6842686 0.1633292 -2.5676014
C 1.4034065 0.3477323 -1.3788112
C 0.6733117 0.1842055 -0.2064888
C 0.7253272 0.3013726 1.3027024
F 1.6965279 -0.4403084 1.9728709
H 0.7512284 1.3300342 1.6962984
H 2.4616684 0.6129827 -1.3922610
H 1.1931334 0.2863675 -3.5255828

PBE/def2-TZVP level, c8h6f2 open
16
Energy = -507.6950956561
C -0.6960211 0.1930389 -2.2679254
C -1.3885640 0.3168152 -1.1045643
C -0.7393551 0.0403968 0.1639766
C -1.4494126 -0.2342024 1.2865958
F -2.7928565 -0.0811468 1.3265652
H -1.0445970 -0.6145320 2.2244873
H -2.4547772 0.5433710 -1.1044036
H -1.2015212 0.3542099 -3.2215143
C 0.6960211 -0.1930389 -2.2679254
C 1.3885640 -0.3168152 -1.1045643
C 0.7393551 -0.0403968 0.1639766
C 1.4494126 0.2342024 1.2865958
F 2.7928565 0.0811468 1.3265652
H 1.0445970 0.6145320 2.2244873
H 2.4547772 -0.5433710 -1.1044036
H 1.2015212 -0.3542099 -3.2215143

B3LYP/def2-TZVP level, c8h6f2 closed
16
Energy = -508.0360788447
C -0.6784370 -0.1753095 -2.5554064
C -1.3896735 -0.3704672 -1.3710050
C -0.6665605 -0.1916085 -0.2035456
C -0.7234700 -0.2988781 1.3040561
F -1.6843392 0.4599073 1.9552852
H -0.7635600 -1.3117194 1.7096589
H -2.4351166 -0.6512079 -1.3837002
H -1.1816882 -0.3068546 -3.5055881
C 0.6784370 0.1753095 -2.5554064
C 1.3896735 0.3704672 -1.3710050
C 0.6665605 0.1916085 -0.2035456
C 0.7234700 0.2988781 1.3040561
F 1.6843392 -0.4599073 1.9552852
H 0.7635600 1.3117194 1.7096589
H 2.4351166 0.6512079 -1.3837002
H 1.1816882 0.3068546 -3.5055881

B3LYP/def2-TZVP level, c8h6f2 open
16
Energy = -508.0136392808
C -0.6970083 0.1952808 -2.2507325
C -1.3846109 0.3197363 -1.0987480
C -0.7396805 0.0404648 0.1750427
C -1.4513175 -0.2246916 1.2825186
F -2.7917111 -0.0861709 1.3061914
H -1.0598222 -0.5840233 2.2233722
H -2.4398553 0.5555150 -1.0994569
H -1.1936328 0.3599261 -3.1988000
C 0.6970083 -0.1952808 -2.2507325
C 1.3846109 -0.3197363 -1.0987480
C 0.7396805 -0.0404648 0.1750427
C 1.4513175 0.2246916 1.2825186
F 2.7917111 0.0861709 1.3061914
H 1.0598222 0.5840233 2.2233722
H 2.4398553 -0.5555150 -1.0994569
H 1.1936328 -0.3599261 -3.1988000

PBE0/def2-TZVP level, c8h6(no2)2 closed
20
Energy = -718.1282222559
C -0.6209251 -0.3189560 -3.1653089
C -1.2770705 -0.6661440 -1.9858932
C -0.6090261 -0.3280637 -0.8294037
C -0.6504812 -0.4151543 0.6767677
H -0.5606108 -1.4085420 1.1163436
H -2.2382006 -1.1648021 -1.9919510
H -1.0828373 -0.5564823 -4.1167948
C 0.6209251 0.3189560 -3.1653089
C 1.2770705 0.6661440 -1.9858932
C 0.6090261 0.3280637 -0.8294037
C 0.6504812 0.4151543 0.6767677
H 0.5606108 1.4085420 1.1163436
H 2.2382006 1.1648021 -1.9919510
H 1.0828373 0.5564823 -4.1167948
N -1.8453290 0.2119457 1.3320410
O -2.9035000 -0.3112374 1.0779722
O -1.6747871 1.1662951 2.0521382
N 1.8453290 -0.2119457 1.3320410
O 2.9035000 0.3112374 1.0779722
O 1.6747871 -1.1662951 2.0521382

PBE0/def2-TZVP level, c8h6(no2)2 open
20
Energy = -718.0946043722
C 0.0788609 0.7394876 -0.3656891
C -0.2149411 1.3879422 0.7854690
H -0.6396913 0.8925983 1.6446536
C -0.0788609 -0.7394876 -0.3656891
C 0.2149411 -1.3879422 0.7854690
H 0.6396913 -0.8925983 1.6446536
N -0.0965890 2.8014227 1.0325794
O 0.4258134 3.5292300 0.2109894
O -0.5456580 3.1716678 2.1013837
N 0.0965890 -2.8014227 1.0325794
O -0.4258134 -3.5292300 0.2109894
O 0.5456580 -3.1716678 2.1013837
C 0.4104699 1.3655482 -1.6240311
H 0.7029104 2.4033515 -1.6244223
C -0.4104699 -1.3655482 -1.6240311
H -0.7029104 -2.4033515 -1.6244223
C 0.2399798 0.6773328 -2.7696880
H 0.4313006 1.1644708 -3.7187857
C -0.2399798 -0.6773328 -2.7696880
H -0.4313006 -1.1644708 -3.7187857

PBE/def2-TZVP level, c8h6(no2)2 closed
20
Energy = -718.1479774214
C -0.6237220 -0.3233877 -3.1891402
C -1.2832045 -0.6748161 -2.0003718
C -0.6129250 -0.3337310 -0.8354279
C -0.6548019 -0.4189246 0.6791397
H -0.5649118 -1.4169983 1.1275474
H -2.2490204 -1.1806080 -2.0069403
H -1.0889248 -0.5649273 -4.1463271
C 0.6237220 0.3233877 -3.1891402
C 1.2832045 0.6748161 -2.0003718
C 0.6129250 0.3337310 -0.8354279
C 0.6548019 0.4189246 0.6791397
H 0.5649118 1.4169983 1.1275474
H 2.2490204 1.1806080 -2.0069403
H 1.0889248 0.5649273 -4.1463271
N -1.8709295 0.2149470 1.3428206
O -2.9408478 -0.3326865 1.0975462
O -1.7043827 1.1991296 2.0567282
N 1.8709295 -0.2149470 1.3428206
O 2.9408478 0.3326865 1.0975462
O 1.7043827 -1.1991296 2.0567282

PBE/def2-TZVP level, c8h6(no2)2 open
20
Energy = -718.1229750651
C 0.0742671 0.7434373 -0.3757431
C -0.2051605 1.4041598 0.7926291
H -0.6199093 0.9035061 1.6633883
C -0.0742671 -0.7434373 -0.3757431
C 0.2051605 -1.4041598 0.7926291
H 0.6199093 -0.9035061 1.6633883
N -0.0899008 2.8249566 1.0422190
O 0.4297253 3.5725350 0.2038274
O -0.5386750 3.1980807 2.1369352
N 0.0899008 -2.8249566 1.0422190
O -0.4297253 -3.5725350 0.2038274
O 0.5386750 -3.1980807 2.1369352
C 0.3707481 1.3812742 -1.6381036
H 0.6260743 2.4370541 -1.6350689
C -0.3707481 -1.3812742 -1.6381036
H -0.6260743 -2.4370541 -1.6350689
C 0.2150513 0.6855710 -2.7995553
H 0.3833339 1.1883875 -3.7533694
C -0.2150513 -0.6855710 -2.7995553
H -0.3833339 -1.1883875 -3.7533694

B3LYP/def2-TZVP level, c8h6(no2)2 closed
20
Energy = -718.5424725307
C -0.6208065 -0.3229770 -3.1787107
C -1.2756899 -0.6722020 -1.9944737
C -0.6091487 -0.3309955 -0.8341555
C -0.6541493 -0.4191864 0.6788878
H -0.5684596 -1.4099987 1.1200625
H -2.2332855 -1.1752131 -2.0009719
H -1.0824367 -0.5634394 -4.1282955
C 0.6208065 0.3229770 -3.1787107
C 1.2756899 0.6722020 -1.9944737
C 0.6091487 0.3309955 -0.8341555
C 0.6541493 0.4191864 0.6788878
H 0.5684596 1.4099987 1.1200625
H 2.2332855 1.1752131 -2.0009719
H 1.0824367 0.5634394 -4.1282955
N -1.8627141 0.2132353 1.3381007
O -2.9242715 -0.3328068 1.1056818
O -1.7006050 1.1944401 2.0386606
N 1.8627141 -0.2132353 1.3381007
O 2.9242715 0.3328068 1.1056818
O 1.7006050 -1.1944401 2.0386606

B3LYP/def2-TZVP level, c8h6(no2)2 open
20
Energy = -718.5202243058
C 0.0773530 0.7440081 -0.3649284
C -0.2093986 1.3996936 0.7881695
H -0.6225888 0.9091705 1.6533567
C -0.0773530 -0.7440081 -0.3649284
C 0.2093986 -1.3996936 0.7881695
H 0.6225888 -0.9091705 1.6533567
N -0.0942522 2.8205540 1.0347995
O 0.4204546 3.5596376 0.2040414
O -0.5380304 3.1936875 2.1162516
N 0.0942522 -2.8205540 1.0347995
O -0.4204546 -3.5596376 0.2040414
O 0.5380304 -3.1936875 2.1162516
C 0.4005478 1.3706423 -1.6303226
H 0.6852157 2.4089386 -1.6330898
C -0.4005478 -1.3706423 -1.6303226
H -0.6852157 -2.4089386 -1.6330898
C 0.2341212 0.6809522 -2.7792873
H 0.4211004 1.1695191 -3.7272694
C -0.2341212 -0.6809522 -2.7792873

H -0.4211004 -1.1695191 -3.7272694