Supporting Information

for

A computational investigation of the substituent effects on geometric, electronic, and optical properties of siloles and 1,4-disilacyclohexa-2,5-dienes

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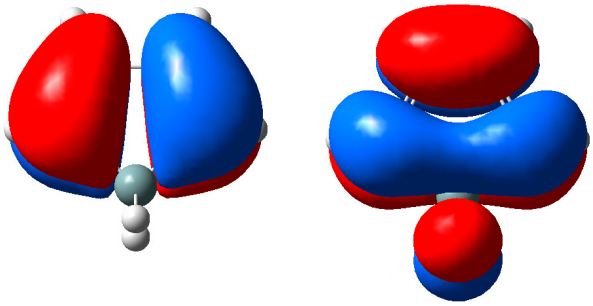
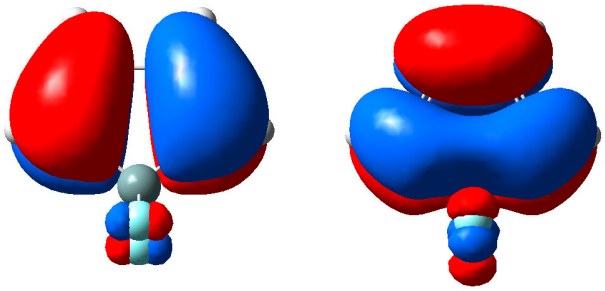
Figure S1: Frontier molecular orbitals of siloles



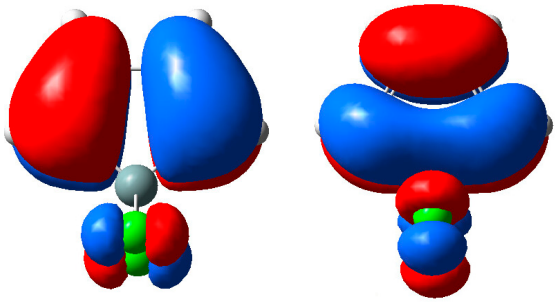
HOMO of **1a**
a_2 symmetry

LUMO of **1a**
b_1 symmetry



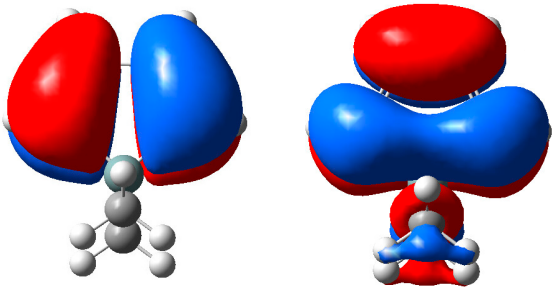
HOMO of **1b**
a_2 symmetry

LUMO of **1b**
b_1 symmetry



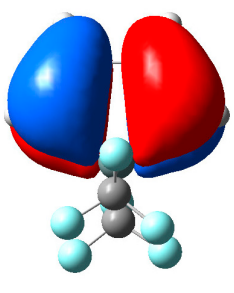
HOMO of **1c**
a_2 symmetry

LUMO of **1c**
b_1 symmetry

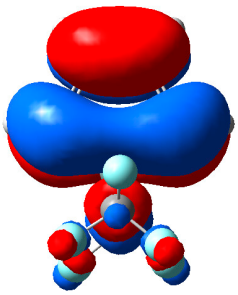


HOMO of **1d**
a_2 symmetry

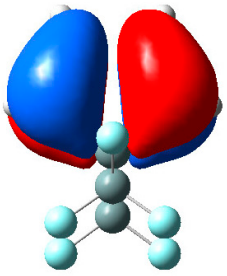
LUMO of **1d**
b_1 symmetry



HOMO of **1e**
a_2 symmetry



LUMO of **1e**
b_1 symmetry



HOMO of **1f**
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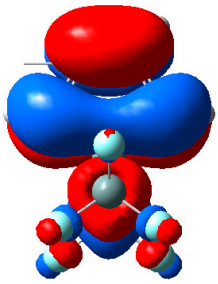

LUMO of **1f**
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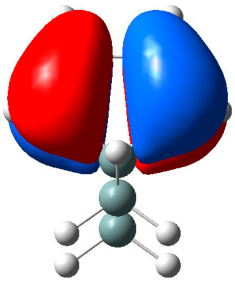

HOMO of **1g**
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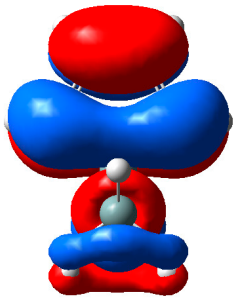
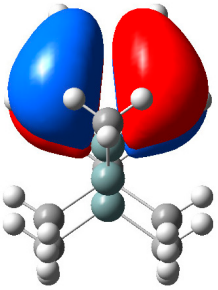


LUMO of **1g**
b_1 symmetry



HOMO of **1h**
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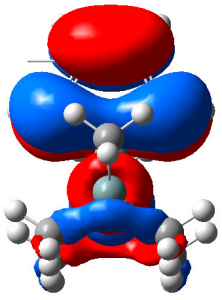
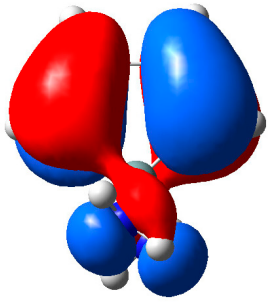
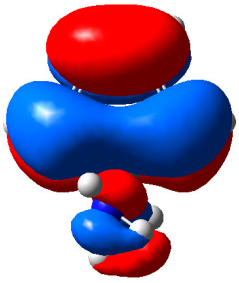


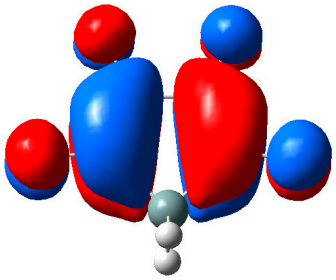
LUMO of **1h**
b_1 symmetry



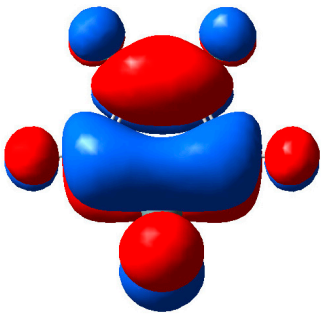
HOMO of **1i**
a_2 symmetry



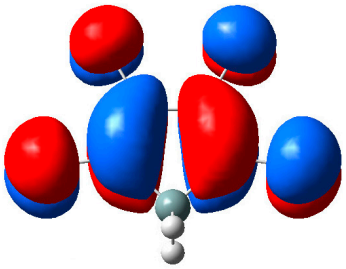
LUMO of **1i**
b_1 symmetry



HOMO of **1j**
a_2 symmetry



LUMO of **1j**
b_1 symmetry



HOMO of **1k**
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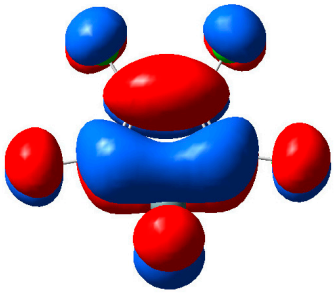

LUMO of **1k**
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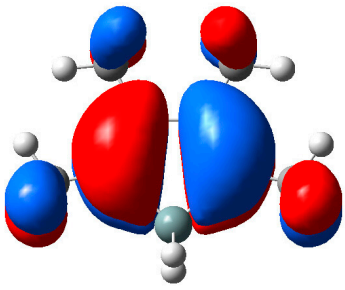

HOMO of **1l**
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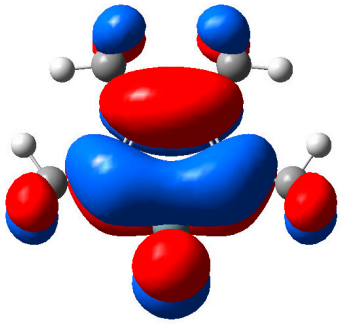

LUMO of **1l**
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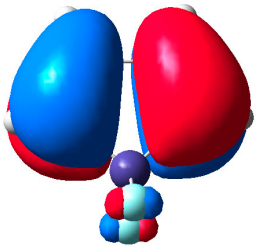

HOMO of **1m**
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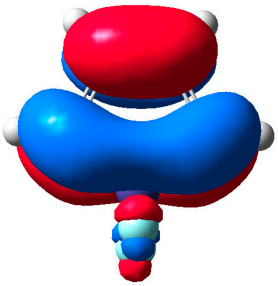

LUMO of **1m**
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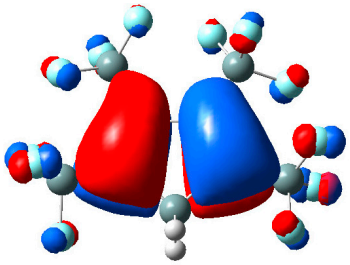
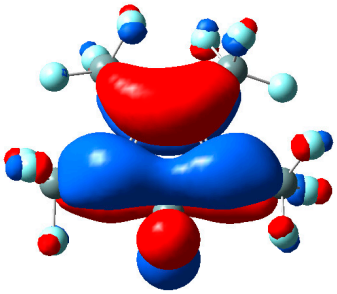
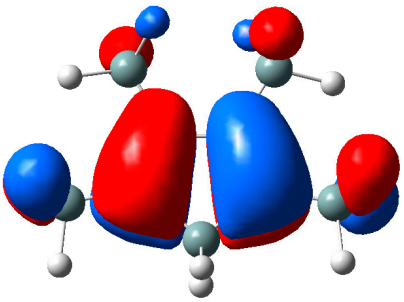


HOMO of **1n**
a_2 symmetry



LUMO of **1n**
b_1 symmetry



HOMO of **1o**
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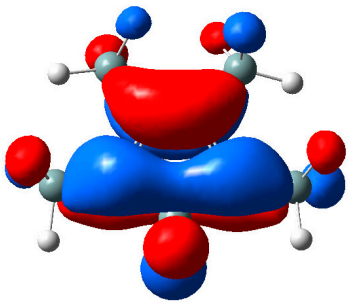
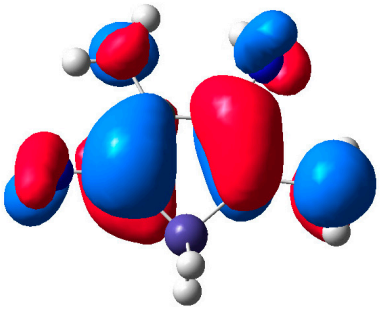
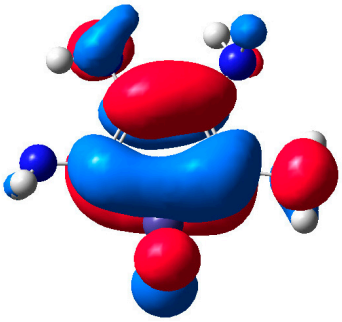


LUMO of **1o**
b_1 symmetry

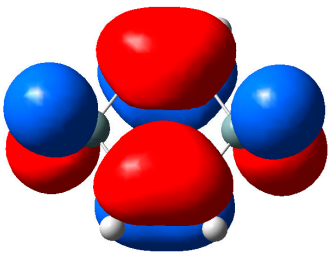


HOMO of **1p**
a_2 symmetry

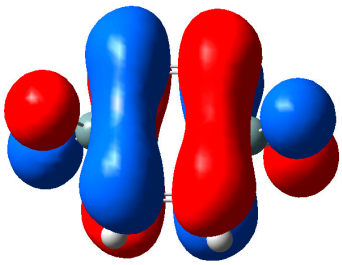


LUMO of **1p**
b_1 symmetry

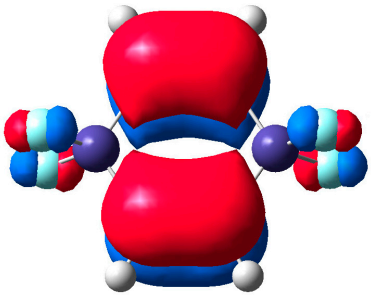
Figure S2: Frontier molecular orbitals of 1,4-disilacyclohexa-2,5-dienes



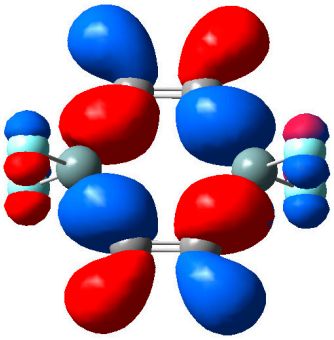
HOMO of **2a**
b_{1u} symmetry



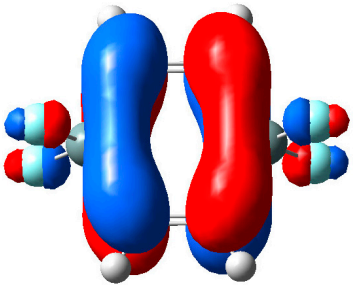
LUMO of **2a**
b_{2g} symmetry



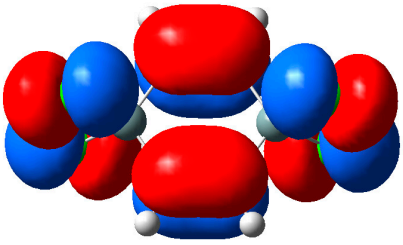
HOMO-2 of **2b**
b_{1u} symmetry



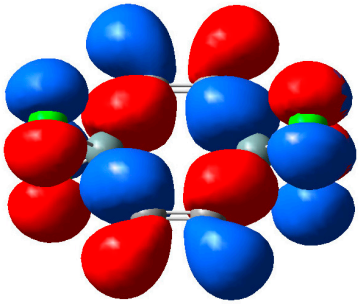
HOMO of **2b**



LUMO of **2b**
b_{2g} symmetry



HOMO-2 of **2c**
b_{1u} symmetry



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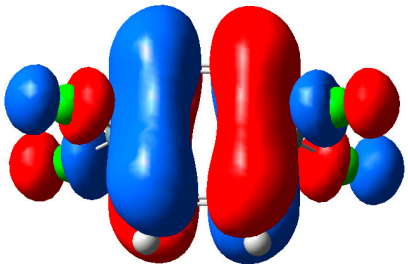
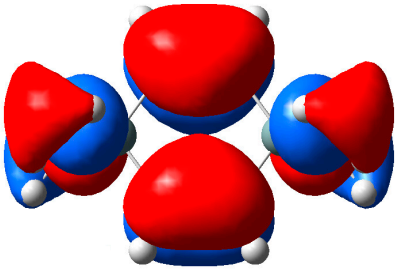
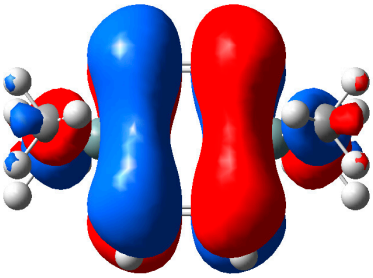


LUMO of **2c**
b_{2g} symmetry



HOMO of **2d**
b_{1u} symmetry



LUMO of **2d**
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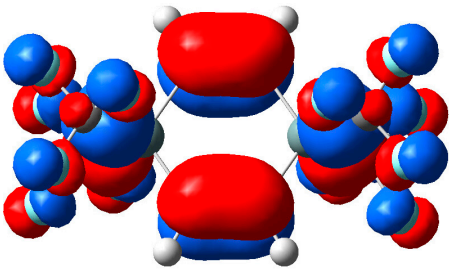
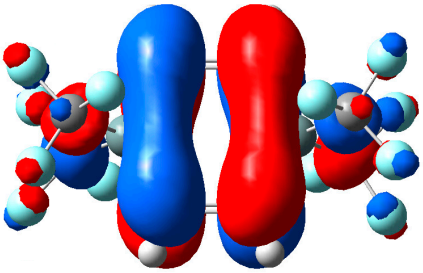


HOMO of **2e**
b_{1u} symmetry



LUMO of **2e**
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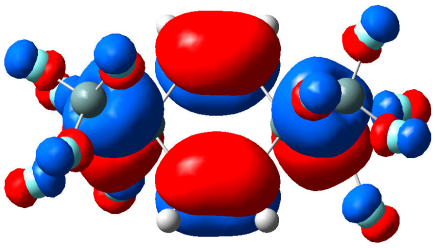
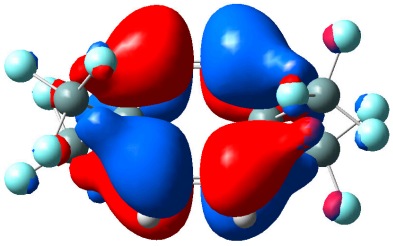
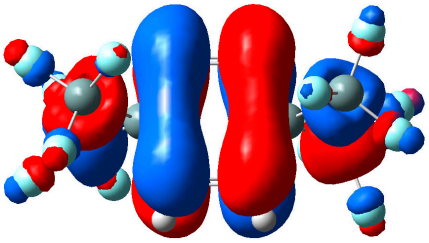


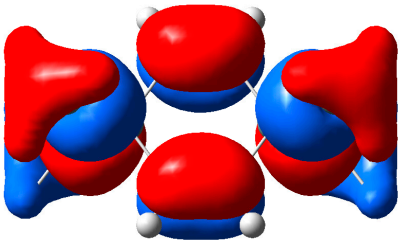
HOMO of **2f**
b_{1u} symmetry



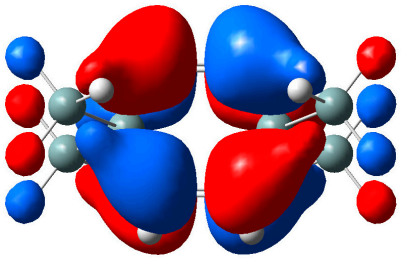
LUMO of **2f**
a_u symmetry



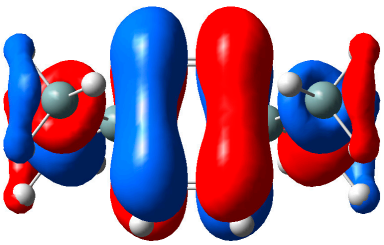
LUMO+1 of **2f**
b_{2g} symmetry



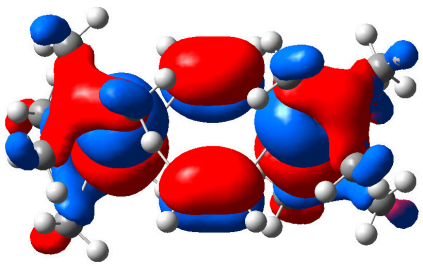
HOMO of **2g**
b_{1u} symmetry



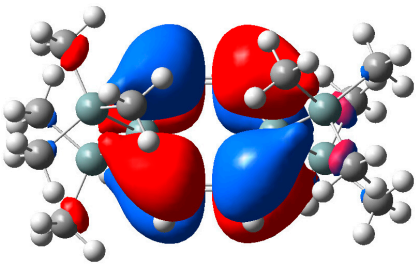
LUMO of **2g**
a_u symmetry



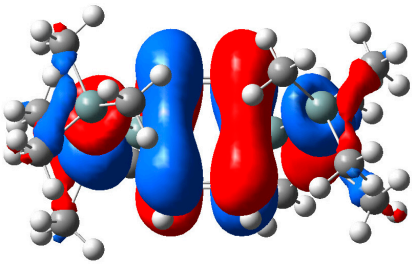
LUMO+1 of **2g**
b_{2g} symmetry



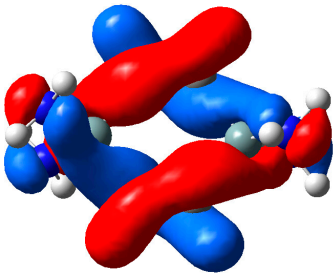
HOMO of **2h**
b_{1u} symmetry



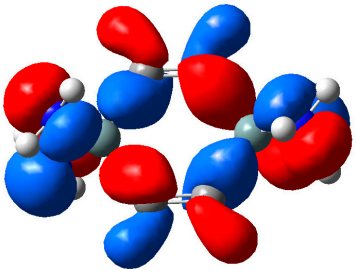
LUMO of **2h**
a_u symmetry



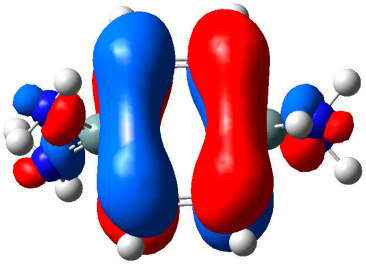
LUMO+1 of **2h**
b_{2g} symmetry



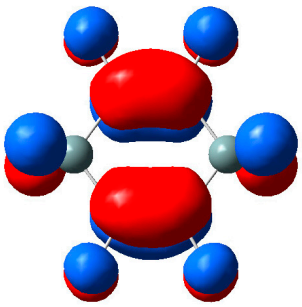
HOMO-4 of **2i**
b_{1u} symmetry



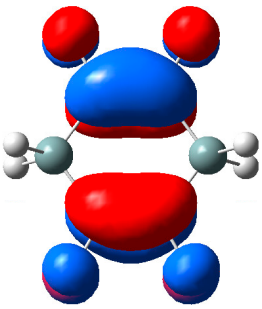
HOMO of **2i**



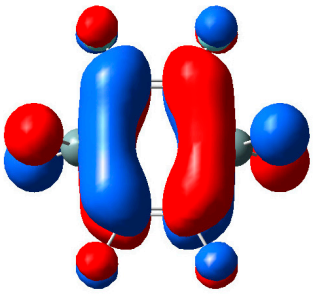
LUMO of **2i**
b_{2g} symmetry



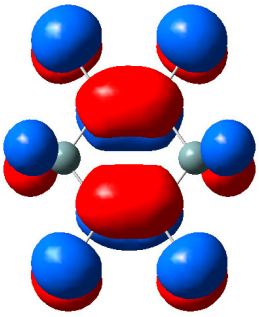
HOMO-1 of **2j**
b_{1u} symmetry



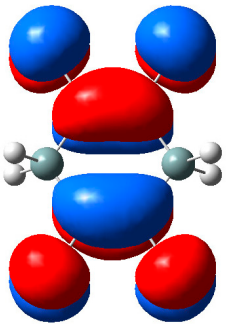
HOMO of **2j**
b_{3g} symmetry



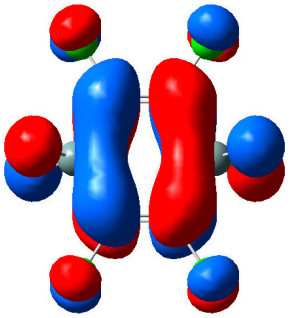
LUMO of **2j**
b_{2g} symmetry



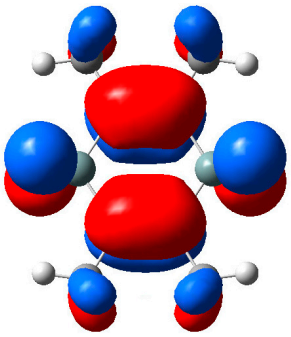
HOMO-1 of **2k**
b_{1u} symmetry



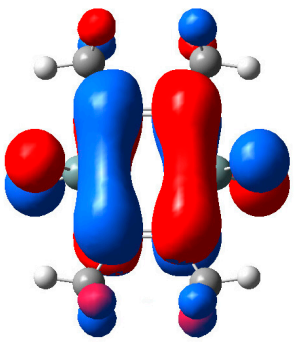
HOMO of **2k**
b_{3g} symmetry



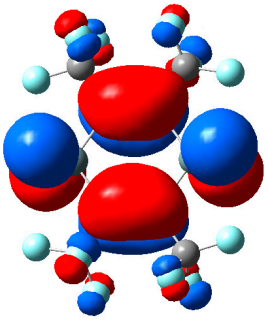
LUMO of **2k**
b_{2g} symmetry



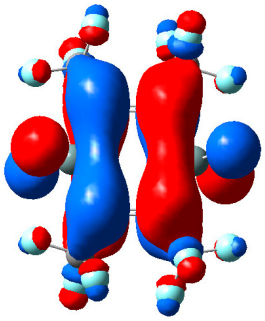
HOMO of **2l**
b_{1u} symmetry



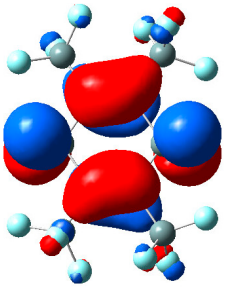
LUMO of **2l**
b_{2g} symmetry



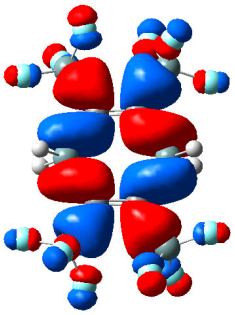
HOMO of **2m**
b_{1u} symmetry



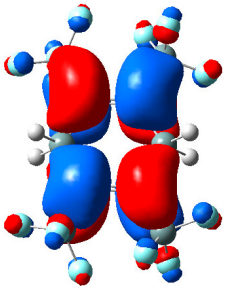
LUMO of **2m**
b_{2g} symmetry



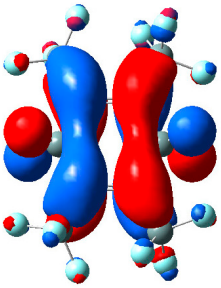
HOMO-1 of **2n**
b_{1u} symmetry



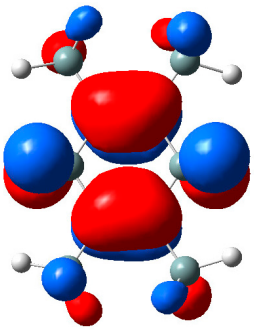
HOMO of **2n**



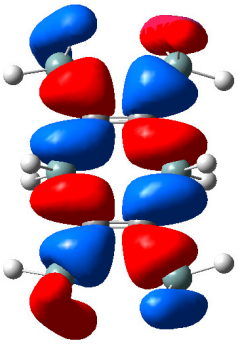
LUMO of **2n**
a_u symmetry



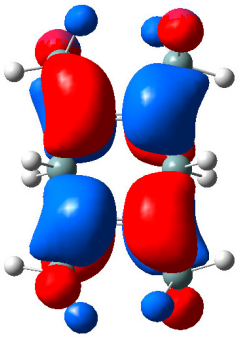
LUMO+1 of **2n**
b_{2g} symmetry



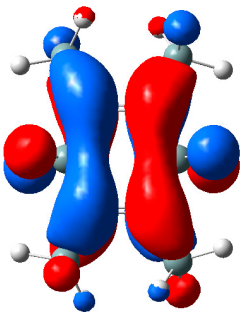
HOMO-1 of **2o**
b_{1u} symmetry



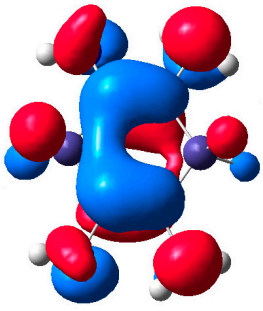
HOMO of **2o**



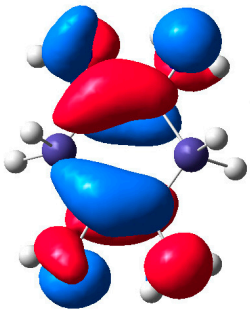
LUMO of **2o**
a_u symmetry



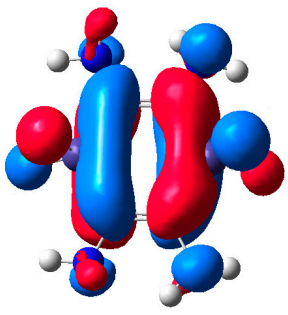
LUMO+1 of **2o**
b_{2g} symmetry



HOMO-1 of **2p**
b_{1u} symmetry



HOMO of **2p**
b_{3g} symmetry



LUMO of **2p**
b_{2g} symmetry

Orbital energies and HOMO-LUMO energy gaps of siloles

Table S1. Orbital energies and HOMO-LUMO energy gaps of siloles **1a – 1i** (in eV, calculated at PBE0/6-31G(d) level).

	1a	**1b**	**1c**	**1d**	**1e**	**1f**	**1g**	**1h**	**1i**
E_{LUMO}	-6.56	-7.06	-7.18	-6.24	-7.29	-7.33	-6.62	-6.14	-6.14
E_{HOMO}	-1.25	-1.92	-2.10	-0.94	-2.11	-2.01	-1.33	-0.79	-0.99
$\Delta E_{HOMO-LUMO}$	5.32	5.14	5.08	5.30	5.18	5.32	5.29	5.35	5.15

Table S2. Orbital energies and HOMO-LUMO energy gaps of siloles **1j – 1p** (in eV, calculated at PBE0/6-31G(d) level).

	1j	**1k**	**1l**	**1m**	**1n**	**1o**	**1p**
E_{LUMO}	-6.58	-6.78	-5.74	-8.44	-8.75	-7.09	-4.58
E_{HOMO}	-1.48	-2.22	-0.65	-3.25	-3.78	-2.31	-0.01
$\Delta E_{HOMO-LUMO}$	5.10	4.57	5.09	5.19	4.98	4.78	4.57

Orbital energies and HOMO – LUMO and HOMO-n – LUMO+m energy gaps of 1,4-disilacyclohexa-2,5-dienes

Table S3. Orbital energies and HOMO-LUMO and HOMO-n – LUMO+m energy gaps of 1,4-disilacyclohexa-2,5-dienes **2a – 2i** (in eV, calculated at PBE0/6-31G(d) level).

	2a	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**	**2i**
E_{LUMO+m}	-	-9.16	-8.85	-	-	-	-	-	-7.01
E_{LUMO}	-7.57	-8.49	-8.59	-7.07	-8.59	-8.06	-6.70	-5.61	-6.40
E_{HOMO}	-0.73	-2.02	-2.24	-0.33	-2.17	-1.96	-1.03	-0.30	-0.52
E_{HOMO-n}	-	-	-	-	-	-1.95	-0.94	-0.12	-
$\Delta E_{HOMO-LUMO}$	6.84	6.47	6.35	6.74	6.42	6.10	5.67	5.32	5.88
$\Delta E_{HOMO-n-LUMO+m}$	-	7.15	6.60	-	-	6.11	5.76	5.49	6.49
	-	n = 2	n = 2	-	-	m = 1	m = 1	m = 1	n = 4

Table S4. Orbital energies and HOMO-LUMO and HOMO-n – LUMO+m energy gaps of 1,4-disilacyclohexa-2,5-dienes **2j – 2p** (in eV, calculated at PBE0/6-31G(d) level).

	2j	**2k**	**2l**	**2m**	**2n**	**2o**	**2p**
E_{LUMO+m}	-7.67	-7.78			-9.13	-7.81	-5.45
E_{LUMO}	-7.54	-7.64	-6.85	-8.89	-8.28	-6.82	-5.12
E_{HOMO}	-1.00	-1.57	-0.33	-2.33	-2.90	-1.60	0.21
E_{HOMO-n}					-2.86	-1.59	
$\Delta E_{HOMO-LUMO}$	6.54	6.07	6.52	6.56	5.38	5.22	5.32
$\Delta E_{HOMO-n-LUMO+m}$	6.67	6.21			6.27	6.22	5.66
	n = 1	n = 1	-	-	m = 1 n = 1	m = 1 n = 1	n = 1

Electronic excitation energies of siloles

Table S5. Electronic excitation energies of siloles **1a – 1i** (in eV, calculated at PBE0/6-31G(d) level).

Electronic state	**1a**	**1b**	**1c**	**1d**	**1e**	**1f**	**1g**	**1h**	**1i**
S_1	**4.40**	**4.12**	**4.06**	**4.35**	**4.18**	**4.35**	**4.34**	**4.41**	**4.13**
S_2	5.68	5.19	4.98	5.44	5.64	5.20	5.18	4.76	4.51
S_3	5.94	6.32	5.77	5.67	5.75	5.27	5.39	5.09	4.90
S_4	5.99	6.33	5.85	5.68	5.97	5.74	5.54	5.46	5.56
S_5	6.10	6.61	6.12	6.03	6.40	5.74	5.57	5.49	5.94

Table S6. Electronic excitation energies of siloles **1j – 1p** (in eV, calculated at PBE0/6-31G(d) level).

Electronic state	**1j**	**1k**	**1l**	**1m**	**1n**	**1o**	**1p**
S_1	**4.20**	**3.71**	**4.14**	**4.36**	**4.19**	**3.95**	**3.60**
S_2	4.87	4.65	5.08	5.21	4.29	4.12	3.77
S_3	5.19	5.05	5.21	5.52	4.33	4.22	3.95
S_4	5.93	5.24	5.57	5.91	5.58	5.43	4.45
S_5	6.37	5.32	5.73	6.79	5.99	5.73	4.90

First allowed excitations are marked in bold.

Electronic excitation energies of 1,4-disilacyclohexa-2,5-dienes

Table S7. Electronic excitation energies of 1,4-disilacyclohexa-2,5-dienes **2a – 2i** (in eV, calculated at PBE0/6-31G(d) level).

Electronic state	**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**	**2i**
S_1	5.53	4.90	4.92	5.29	5.32	4.86	4.43	4.13	4.55
S_2	5.72	5.57	5.37	5.64	**5.65**	**5.35**	**4.92**	**4.69**	5.00
S_3	5.87	5.97	**5.72**	**5.78**	5.78	5.45	5.32	4.85	5.35
S_4	**5.94**	**6.21**	5.82	5.92	5.79	5.62	5.46	5.08	5.37
S_5	6.24	6.99	6.05	6.13	6.02	5.64	5.48	5.19	5.44
S_6									**5.61**

Table S8. Electronic excitation energies of 1,4-disilacyclohexa-2,5-dienes **2j – 2p** (in eV, calculated at PBE0/6-31G(d) level).

Electronic state	**2j**	**2k**	**2l**	**2m**	**2n**	**2o**	**2p**
S_1	5.59	5.10	5.56	5.37	3.78	3.63	4.27
S_2	5.83	**5.29**	**5.58**	5.44	3.93	3.75	4.34
S_3	**5.83**	5.30	5.61	5.48	4.98	4.97	4.46
S_4	5.84	5.44	5.74	**5.69**	4.99	5.01	**4.78**
S_5	6.27	5.56	5.81	6.04	5.24	5.17	4.79
S_6					**5.43**	**5.31**	

First allowed excitations are marked in bold.

Bond lengths and angles in siloles

Table S9. Bond lengths and angles in siloles **1a – 1i** (optimized at PBE0/6-31G(d) level).

	1a	**1b**	**1c**	**1d**	**1e**	**1f**	**1g**	**1h**	**1i**
Si-C bond length, Å	1.8707	1.8558	1.8571	1.8792	1.8561	1.8632	1.8710	1.8775	1.8821
C=C bond length, Å	1.3475	1.3440	1.3447	1.3476	1.3477	1.3509	1.3517	1.3536	1.3454
C-C bond length, Å	1.4813	1.4948	1.4908	1.4818	1.4856	1.4738	1.4716	1.4680	1.4880
Angle R-Si-R, °	107.7660	105.2960	107.8323	110.2449	106.1945	113.7669	112.1668	117.9339	105.1581

Table S10. Bond lengths and angles in siloles **1j – 1q** (optimized at PBE0/6-31G(d) level).

	1j	**1k**	**1l**	**1m**	**1n**	**1o**	**1p**
Si-C bond length, Å	1.8827	1.8744	1.8673	1.8727	1.8824	1.8741	1.8906
C=C bond length, Å	1.3406	1.3488	1.3555	1.3490	1.3612	1.3646	1.3587
C-C bond length, Å	1.4813	1.4939	1.5071	1.5069	1.5019	1.5074	1.4800
Angle R-Si-R, °	110.6397	110.9590	106.7955	111.6681	110.3776	108.0016	105.9039

Bond lengths and angles in 1,4-disilacyclohexa-2,5-dienes

Table S11. Bond lengths and angles in 1,4-disilacyclohexa-2,5-dienes **2a** – **2i**.

	2a	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**	**2i**
Si-C bond length, Å	1.8713	1.8534	1.8574	1.8762	1.8603	1.8705	1.8764	1.8821	1.8744
C=C bond length, Å	1.3456	1.3457	1.3453	1.3469	1.3460	1.3452	1.3469	1.3485	1.3475
Angle R-Si-R, °	106.1040	105.4189	107.5479	108.6153	105.4290	105.6902	108.1325	110.8760	103.6802

Table S12. Bond lengths and angles in 1,4-disilacyclohexa-2,5-dienes **2j – 2q**.

	2j	**2k**	**2l**	**2m**	**2n**	**2o**	**2p**
Si-C bond length, Å	1.8769	1.8793	1.8715	1.8920	1.8912	1.8821	1.8711
C=C bond length, Å	1.3393	1.3413	1.3526	1.3442	1.3601	1.3606	1.3596
Angle R-Si-R, °	108.8446	109.7295	104.8629	110.9202	108.6589	106.2526	105.4112

Cartesian coordinates and absolute energies

1a:

PBE1PBE/6-31G(d): -445.15015 a.u.

Point group: C_{2v}

Cartesian coordinates:

C	0.00000000	1.35441100	-0.08899000
C	0.00000000	0.74065100	-1.28858500
C	0.00000000	-0.74065100	-1.28858500
C	0.00000000	-1.35441100	-0.08899000
H	0.00000000	2.43427600	0.01363700
H	0.00000000	1.27523400	-2.23839900
H	0.00000000	-1.27523400	-2.23839900
H	0.00000000	-2.43427600	0.01363700
Si	0.00000000	0.00000000	1.20133500
H	-1.20539200	0.00000000	2.08087000
H	1.20539200	0.00000000	2.08087000

1b:

PBE1PBE/6-31G(d): -643.58748 a.u.

Point group: C_{2v}

Cartesian coordinates:

C	0.00000000	1.36818200	-0.65412400
C	0.00000000	0.74740000	-1.84613300
C	0.00000000	-0.74740000	-1.84613300
C	0.00000000	-1.36818200	-0.65412400
H	0.00000000	2.44664600	-0.54850700
H	0.00000000	1.27187100	-2.80044800
H	0.00000000	-1.27187100	-2.80044800
H	0.00000000	-2.44664600	-0.54850700
Si	0.00000000	0.00000000	0.59969700
F	1.27460100	0.00000000	1.57251300
F	-1.27460100	0.00000000	1.57251300

1c:

PBE1PBE/6-31G(d): -1364.13695 a.u.

Point group: C_{2v}

Cartesian coordinates:

C	0.00000000	1.36483800	-1.09635900
C	0.00000000	0.74540800	-2.28985100
C	0.00000000	-0.74540800	-2.28985100
C	0.00000000	-1.36483800	-1.09635900
H	0.00000000	2.44160200	-0.97512800
H	0.00000000	1.27417000	-3.24192000
H	0.00000000	-1.27417000	-3.24192000
H	0.00000000	-2.44160200	-0.97512800
Si	0.00000000	0.00000000	0.16294900
Cl	-1.66462800	0.00000000	1.37609800
Cl	1.66462800	0.00000000	1.37609800

1d:

PBE1PBE/6-31G(d): -523.70931 a.u.

Point group: C_{2v}

Cartesian coordinates:

C	0.00000000	1.35041800	-0.73400900
C	0.00000000	0.74089000	-1.93583500
C	0.00000000	-0.74089000	-1.93583500
C	0.00000000	-1.35041800	-0.73400900
H	0.00000000	2.43239700	-0.63989600
H	0.00000000	1.27451600	-2.88683400
H	0.00000000	-1.27451600	-2.88683400
H	0.00000000	-2.43239700	-0.63989600
Si	0.00000000	0.00000000	0.57280700
C	-1.54716400	0.00000000	1.65122200
H	-1.57555500	-0.88519800	2.29672000
H	-1.57555500	0.88519800	2.29672000
H	-2.45210100	0.00000000	1.03536800
C	1.54716400	0.00000000	1.65122200
H	1.57555500	0.88519800	2.29672000
H	1.57555500	-0.88519800	2.29672000

H 2.45210100 0.00000000 1.03536800

1e:

PBE1PBE/6-31G(d): -1118.59751 a.u.

Point group: C_2

Cartesian coordinates:

C -1.36229200 -0.04530300 1.61761800
C -0.74241200 -0.02418400 2.81408700
C 0.74241200 0.02418400 2.81408700
C 1.36229200 0.04530300 1.61761800
H -2.43980800 -0.07892300 1.50668000
H -1.27324100 -0.04003600 3.76505400
H 1.27324100 0.04003600 3.76505400
H 2.43980800 0.07892300 1.50668000
Si 0.00000000 0.00000000 0.35776000
C -0.06526000 1.54089400 -0.80032800
C 0.06526000 -1.54089400 -0.80032800
F 0.95699500 1.55372800 -1.67662800
F 0.00000000 2.68372400 -0.09294800
F -1.20532600 1.57930800 -1.51534700
F -0.95699500 -1.55372800 -1.67662800
F 0.00000000 -2.68372400 -0.09294800
F 1.20532600 -1.57930800 -1.51534700

1f:

PBE1PBE/6-31G(d): -1621.57674 a.u.

Point group: C_{2v}

Cartesian coordinates:

C 0.00000000 1.35680100 1.81050500
C 0.00000000 0.73689500 3.01075800
C 0.00000000 -0.73689500 3.01075800
C 0.00000000 -1.35680100 1.81050500
H 0.00000000 2.43485100 1.69571700
H 0.00000000 1.27432100 3.95823700
H 0.00000000 -1.27432100 3.95823700
H 0.00000000 -2.43485100 1.69571700
Si 0.00000000 0.00000000 0.53351000
Si -1.93872300 0.00000000 -0.73112700
Si 1.93872300 0.00000000 -0.73112700
F -2.04133500 -1.28389800 -1.67120400
F -2.04133500 1.28389800 -1.67120400
F -3.21554500 0.00000000 0.22237200
F 3.21554500 0.00000000 0.22237200
F 2.04133500 1.28389800 -1.67120400
F 2.04133500 -1.28389800 -1.67120400

1g:

PBE1PBE/6-31G(d): -1026.26938 a.u.

Point group: C_{2v}

Cartesian coordinates:

C 0.00000000 1.35019100 -1.18236000
C 0.00000000 0.73578700 -2.38632600
C 0.00000000 -0.73578700 -2.38632600
C 0.00000000 -1.35019100 -1.18236000
H 0.00000000 2.42955800 -1.07306800
H 0.00000000 1.27425100 -3.33399400
H 0.00000000 -1.27425100 -3.33399400
H 0.00000000 -2.42955800 -1.07306800
Si 0.00000000 0.00000000 0.11286700
Si 1.94444400 0.00000000 1.42029700
H 1.99058500 -1.20673600 2.29662300
H 3.15572600 0.00000000 0.55170400
H 1.99058500 1.20673600 2.29662300
Si -1.94444400 0.00000000 1.42029700
H -1.99058500 -1.20673600 2.29662300
H -1.99058500 1.20673600 2.29662300
H -3.15572600 0.00000000 0.55170400

1h:

PBE1PBE/6-31G(d): -1261.93655 a.u.

Point group: C_{2v}

Cartesian coordinates:

C 0.00000000 1.34355200 1.81700700
C 0.00000000 0.73401300 3.02560900

C 0.00000000 -0.73401300 3.02560900
C 0.00000000 -1.34355200 1.81700700
H 0.00000000 2.42490600 1.71490700
H 0.00000000 1.27403200 3.97311600
H 0.00000000 -1.27403200 3.97311600
H 0.00000000 -2.42490600 1.71490700
Si 0.00000000 0.00000000 0.50556800
Si -2.02050000 0.00000000 -0.71005900
Si 2.02050000 0.00000000 -0.71005900
C 2.13533000 1.54156400 -1.80356500
H 3.09270800 1.55965200 -2.33917300
H 1.33516900 1.56984800 -2.55175300
H 2.06950600 2.45936500 -1.20885300
C 2.13533000 -1.54156400 -1.80356500
H 1.33516900 -1.56984800 -2.55175300
H 3.09270800 -1.55965200 -2.33917300
H 2.06950600 -2.45936500 -1.20885300
C 3.45187000 0.00000000 0.52518100
H 4.41840800 0.00000000 0.00626400
H 3.41209100 0.88326100 1.17156000
H 3.41209100 -0.88326100 1.17156000
C -2.13533000 1.54156400 -1.80356500
H -1.33516900 1.56984800 -2.55175300
H -3.09270800 1.55965200 -2.33917300
H -2.06950600 2.45936500 -1.20885300
C -2.13533000 -1.54156400 -1.80356500
H -3.09270800 -1.55965200 -2.33917300
H -1.33516900 -1.56984800 -2.55175300
H -2.06950600 -2.45936500 -1.20885300
C -3.45187000 0.00000000 0.52518100
H -3.41209100 0.88326100 1.17156000
H -4.41840800 0.00000000 0.00626400
H -3.41209100 -0.88326100 1.17156000

1i:

PBE1PBE/6-31G(d): -555.80032 a.u.

Point group: C_2

Cartesian coordinates:

C 0.00000000 1.35214300 -0.71474800
C -0.00545500 0.74396000 -1.91483700
C 0.00545500 -0.74396000 -1.91483700
C 0.00000000 -1.35214300 -0.71474800
H -0.00790500 2.43414400 -0.61880700
H -0.01586600 1.27360200 -2.86797100
H 0.01586600 -1.27360200 -2.86797100
H 0.00790500 -2.43414400 -0.61880700
Si 0.00000000 0.00000000 0.59448500
N -1.34665600 -0.26261500 1.64427200
H -1.58001600 0.44658400 2.32693000
H -2.17838500 -0.69548100 1.26606500
N 1.34665600 0.26261500 1.64427200
H 2.17838500 0.69548100 1.26606500
H 1.58001600 -0.44658400 2.32693000

1j:

PBE1PBE/6-31G(d): -841.70301 a.u.

Point group: C_{2v}

Cartesian coordinates:

C 0.00000000 1.33852100 0.41179700
C 0.00000000 0.74062400 -0.78813600
C 0.00000000 -0.74062400 -0.78813600
C 0.00000000 -1.33852100 0.41179700
Si 0.00000000 0.00000000 1.73571300
H -1.22040700 0.00000000 2.58013700
H 1.22040700 0.00000000 2.58013700
F 0.00000000 -2.66323600 0.58479600
F 0.00000000 -1.34119300 -1.97058500
F 0.00000000 1.34119300 -1.97058500
F 0.00000000 2.66323600 0.58479600

1k:

PBE1PBE/6-31G(d): -2282.89523 a.u.

Point group: C_{2v}

Cartesian coordinates:

C 0.00000000 1.33810800 0.69318200
C 0.00000000 0.74693400 -0.51916700
C 0.00000000 -0.74693400 -0.51916700
C 0.00000000 -1.33810800 0.69318200
Si 0.00000000 0.00000000 2.00576000
H -1.22256100 0.00000000 2.84664700
H 1.22256100 0.00000000 2.84664700
Cl 0.00000000 -3.03072900 0.95325300
Cl 0.00000000 -1.59684600 -2.00802100
Cl 0.00000000 1.59684600 -2.00802100
Cl 0.00000000 3.03072900 0.95325300

1l:

PBE1PBE/6-31G(d): -602.22836 a.u.

Point group: C_{2v}

Cartesian coordinates:

C 0.00000000 1.36697300 0.45542100
C 0.00000000 0.75357200 -0.75336700
C 0.00000000 -0.75357200 -0.75336700
C 0.00000000 -1.36697300 0.45542100
Si 0.00000000 0.00000000 1.72748700
H -1.20072100 0.00000000 2.61929500
H 1.20072100 0.00000000 2.61929500
C 0.00000000 -2.83715700 0.73189800
H 0.87834300 -3.12735900 1.32363200
H -0.87834300 -3.12735900 1.32363200
H 0.00000000 -3.45073400 -0.17493000
C 0.00000000 -1.46060000 -2.07855000
H 0.87994100 -1.19024500 -2.67569300
H 0.00000000 -2.54647600 -1.96505800
H -0.87994100 -1.19024500 -2.67569300
C 0.00000000 1.46060000 -2.07855000
H -0.87994100 1.19024500 -2.67569300
H 0.00000000 2.54647600 -1.96505800
H 0.87994100 1.19024500 -2.67569300
C 0.00000000 2.83715700 0.73189800
H -0.87834300 3.12735900 1.32363200
H 0.87834300 3.12735900 1.32363200
H 0.00000000 3.45073400 -0.17493000

1m:

PBE1PBE/6-31G(d): -1792.04316 a.u.

Point group: C_2

Cartesian coordinates:

C 0.00438100 1.33218500 0.85851500
C -0.02347400 0.75308700 -0.35957300
C 0.02347400 -0.75308700 -0.35957300
C -0.00438100 -1.33218500 0.85851500
Si 0.00000000 0.00000000 2.17468600
H -1.22619000 0.03471800 3.00727200
H 1.22619000 -0.03471800 3.00727200
C 0.00000000 -2.78845600 1.21938600
C 0.08414800 -1.54379300 -1.65783000
C -0.08414800 1.54379300 -1.65783000
C 0.00000000 2.78845600 1.21938600
F 0.89862300 -0.95278700 -2.53966800
F 0.55908200 -2.77434500 -1.45675000
F -1.12706100 -1.65896300 -2.20889400
F -0.89862300 0.95278700 -2.53966800
F -0.55908200 2.77434500 -1.45675000
F 1.12706100 1.65896300 -2.20889400
F -1.19345500 3.36048700 1.03378400
F 0.92188000 3.50127200 0.56723300
F 0.28181400 2.89674800 2.53839900
F -0.92188000 -3.50127200 0.56723300
F 1.19345500 -3.36048700 1.03378400
F -0.28181400 -2.89674800 2.53839900

1n:

PBE1PBE/6-31G(d): -2797.99971 a.u.

Point group: C_2

Cartesian coordinates:

C 0.00886700 1.35820200 0.97843300
C 0.00000000 0.75093300 -0.23976200

C	0.00000000	-0.75093300	-0.23976200
C	-0.00886700	-1.35820200	0.97843300
Si	0.00000000	0.00000000	2.28180100
H	-1.21946100	-0.00140100	3.12970200
H	1.21946100	0.00140100	3.12970200
Si	-0.00926300	3.14698000	1.40168700
Si	0.01886900	1.75564900	-1.80443900
Si	-0.01886900	-1.75564900	-1.80443900
Si	0.00926300	-3.14698000	1.40168700
F	0.94678200	1.03205900	-2.87246200
F	-1.40943300	2.00453600	-2.43921600
F	0.66069700	3.16697100	-1.45480300
F	1.40312700	3.85535700	1.27483400
F	-1.08785900	3.96012800	0.56700600
F	-0.42892000	3.22082700	2.93621800
F	1.08785900	-3.96012800	0.56700600
F	-1.40312700	-3.85535700	1.27483400
F	0.42892000	-3.22082700	2.93621800
F	1.40943300	-2.00453600	-2.43921600
F	-0.94678200	-1.03205900	-2.87246200
F	-0.66069700	-3.16697100	-1.45480300

1o:

PBE1PBE/6-31G(d): -1607.35242 a.u.

Point group: C_2

Cartesian coordinates:

C	0.00623100	1.37117100	0.71978000
C	0.00110300	0.75370600	-0.49711500
C	-0.00110300	-0.75370600	-0.49711500
C	-0.00623100	-1.37117100	0.71978000
Si	0.00000000	0.00000000	1.99733300
H	-1.20702600	0.00693400	2.87427800
H	1.20702600	-0.00693400	2.87427800
Si	0.00000000	3.20130500	1.09881600
H	-1.09909900	3.92034900	0.39361600
H	-0.20459000	3.36899600	2.56533800
H	1.29352000	3.84803000	0.73646700
Si	-0.00569100	1.73083800	-2.11519200
H	0.44058100	3.12218500	-1.83838100
H	0.92751700	1.11132700	-3.09801300
H	-1.36584600	1.76853500	-2.72136600
Si	0.00569100	-1.73083800	-2.11519200
H	1.36584600	-1.76853500	-2.72136600
H	-0.44058100	-3.12218500	-1.83838100
H	-0.92751700	-1.11132700	-3.09801300
Si	0.00000000	-3.20130500	1.09881600
H	-1.29352000	-3.84803000	0.73646700
H	1.09909900	-3.92034900	0.39361600
H	0.20459000	-3.36899600	2.56533800

1p:

PBE1PBE/6-31G(d): -666.32756 a.u.

Point group: C_1

Cartesian coordinates:

C	-1.37248000	-0.40697700	-0.00726800
C	-0.68915200	0.77834700	-0.00017700
C	0.79021100	0.73592600	-0.00537400
C	1.34224400	-0.50543900	0.01294600
Si	-0.09106000	-1.73829100	0.01130800
H	-0.00584600	-2.64479100	-1.17868000
H	-0.08754900	-2.63363200	1.20977100
N	2.69908900	-0.72351700	0.06555900
H	3.03076800	-1.58358200	-0.34619100
H	3.23752600	0.09190500	-0.21437000
N	1.60541300	1.90256800	-0.05256500
H	1.19404200	2.62517600	-0.63577200
H	1.78625700	2.29769200	0.86702600
N	-1.31738400	2.00150500	-0.05986900
H	-2.31396400	1.90486200	0.11372500
H	-0.87979300	2.73962400	0.47550800
N	-2.80663100	-0.37753600	0.00466600
H	-3.19245200	-0.70398300	-0.87852800
H	-3.18249200	-0.98947400	0.72388800

2a:

PBE1PBE/6-31G(d): -735.62656 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	0.67280800	1.53851300	0.00000000
C	-0.67280800	1.53851300	0.00000000
C	-0.67280800	-1.53851300	0.00000000
C	0.67280800	-1.53851300	0.00000000
H	1.18930500	2.50288400	0.00000000
H	-1.18930500	2.50288400	0.00000000
H	-1.18930500	-2.50288400	0.00000000
H	1.18930500	-2.50288400	0.00000000
Si	1.73805300	0.00000000	0.00000000
H	2.63612100	0.00000000	1.19403000
H	2.63612100	0.00000000	-1.19403000
Si	-1.73805300	0.00000000	0.00000000
H	-2.63612100	0.00000000	-1.19403000
H	-2.63612100	0.00000000	1.19403000

2b:

PBE1PBE/6-31G(d): -1132.59367 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	-0.67284700	1.54804200	0.00000000
C	0.67284700	1.54804200	0.00000000
C	0.67284700	-1.54804200	0.00000000
C	-0.67284700	-1.54804200	0.00000000
H	-1.20135900	2.50444600	0.00000000
H	1.20135900	2.50444600	0.00000000
H	1.20135900	-2.50444600	0.00000000
H	-1.20135900	-2.50444600	0.00000000
Si	-1.69203100	0.00000000	0.00000000
Si	1.69203100	0.00000000	0.00000000
F	-2.66401900	0.00000000	1.27635300
F	-2.66401900	0.00000000	-1.27635300
F	2.66401900	0.00000000	1.27635300
F	2.66401900	0.00000000	-1.27635300

2c:

PBE1PBE/6-31G(d): -2573.68780 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	-0.67263700	0.00000000	1.54554700
C	0.67263700	0.00000000	1.54554700
C	0.67263700	0.00000000	-1.54554700
C	-0.67263700	0.00000000	-1.54554700
H	-1.20334800	0.00000000	2.50039100
H	1.20334800	0.00000000	2.50039100
H	1.20334800	0.00000000	-2.50039100
H	-1.20334800	0.00000000	-2.50039100
Si	-1.70281900	0.00000000	0.00000000
Si	1.70281900	0.00000000	0.00000000
Cl	-2.92026200	1.66183900	0.00000000
Cl	-2.92026200	-1.66183900	0.00000000
Cl	2.92026200	-1.66183900	0.00000000
Cl	2.92026200	1.66183900	0.00000000

2d:

PBE1PBE/6-31G(d): -892.82783 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	-0.67342600	0.00000000	1.52891300
C	0.67342600	0.00000000	1.52891300
C	0.67342600	0.00000000	-1.52891300
C	-0.67342600	0.00000000	-1.52891300
H	-1.18532200	0.00000000	2.49826500
H	1.18532200	0.00000000	2.49826500
H	1.18532200	0.00000000	-2.49826500
H	-1.18532200	0.00000000	-2.49826500
Si	-1.76094000	0.00000000	0.00000000
Si	1.76094000	0.00000000	0.00000000
C	-2.86296200	1.53405900	0.00000000
H	-3.51041300	1.55434600	-0.88453900
H	-3.51041300	1.55434600	0.88453900

H -2.26402300 2.45086100 0.00000000
C -2.86296200 -1.53405900 0.00000000
H -3.51041300 -1.55434600 0.88453900
H -3.51041300 -1.55434600 -0.88453900
H -2.26402300 -2.45086100 0.00000000
C 2.86296200 -1.53405900 0.00000000
H 3.51041300 -1.55434600 -0.88453900
H 3.51041300 -1.55434600 0.88453900
H 2.26402300 -2.45086100 0.00000000
C 2.86296200 1.53405900 0.00000000
H 3.51041300 1.55434600 0.88453900
H 3.51041300 1.55434600 -0.88453900
H 2.26402300 2.45086100 0.00000000

2e:

PBE1PBE/6-31G(d): -2082.60658 a.u.

Point group: C_2

Cartesian coordinates:

C 0.00072000 0.67299700 -1.54836900
C -0.00072000 -0.67299700 -1.54836900
C 0.00071800 -0.67299700 1.54835700
C -0.00071800 0.67299700 1.54835700
H 0.00057000 1.19779200 -2.50661700
H -0.00057000 -1.19779200 -2.50661700
H 0.00056600 -1.19779500 2.50660300
H -0.00056600 1.19779500 2.50660300
Si 0.00000200 1.70419300 -0.00000600
Si -0.00000200 -1.70419300 -0.00000600
C -1.53554900 2.87341700 -0.01602000
C 1.53555100 2.87341900 0.01602200
C 1.53554900 -2.87341700 -0.01602000
C -1.53555100 -2.87341900 0.01602200
F -1.61940100 3.56755600 -1.16607200
F -1.49938600 3.76501300 0.99153500
F -2.67660400 2.17116200 0.11091400
F 1.49938600 3.76503000 -0.99152000
F 1.61940000 3.56754000 1.16608400
F 2.67660900 2.17117000 -0.11092200
F 2.67660400 -2.17116200 0.11091400
F 1.49938600 -3.76501300 0.99153500
F 1.61940100 -3.56755600 -1.16607200
F -1.49938600 -3.76503000 -0.99152000
F -1.61940000 -3.56754000 1.16608400
F -2.67660900 -2.17117000 -0.11092200

2f:

PBE1PBE/6-31G(d): -3088.55474 a.u.

Point group: D_2

Cartesian coordinates:

C -1.54556700 0.00302800 0.67258900
C -1.54556700 -0.00302800 -0.67258900
C 1.54556700 0.00302800 -0.67258900
C 1.54556700 -0.00302800 0.67258900
H -2.50686900 0.00314700 1.19224200
H -2.50686900 -0.00314700 -1.19224200
H 2.50686900 0.00314700 -1.19224200
H 2.50686900 -0.00314700 1.19224200
Si 0.00000000 0.00000000 1.72618800
Si 0.00000000 0.00000000 -1.72618800
F -1.51786300 -2.11096200 3.68323700
F 0.91502100 -1.63211600 4.38448900
F 0.43043000 -3.17717800 2.38453100
F -0.91502100 1.63211600 4.38448900
F 1.51786300 2.11096200 3.68323700
F -0.43043000 3.17717800 2.38453100
F 0.43043000 3.17717800 -2.38453100
F 0.91502100 1.63211600 -4.38448900
F -1.51786300 2.11096200 -3.68323700
F -0.91502100 -1.63211600 -4.38448900
F 1.51786300 -2.11096200 -3.68323700
F -0.43043000 -3.17717800 -2.38453100
Si -0.04569400 -1.85198300 3.13005000
Si 0.04569400 1.85198300 3.13005000
Si -0.04569400 1.85198300 -3.13005000

Si 0.04569400 -1.85198300 -3.13005000

2g:

PBE1PBE/6-31G(d): -1897.93995 a.u.

Point group: D_{2h}

Cartesian coordinates:

C -0.67345800 0.00000000 1.53504900
C 0.67345800 0.00000000 1.53504900
C 0.67345800 0.00000000 -1.53504900
C -0.67345800 0.00000000 -1.53504900
H -1.18835900 0.00000000 2.50043400
H 1.18835900 0.00000000 2.50043400
H 1.18835900 0.00000000 -2.50043400
H -1.18835900 0.00000000 -2.50043400
Si -1.75264800 0.00000000 0.00000000
Si 1.75264800 0.00000000 0.00000000
Si -3.13189300 1.90299100 0.00000000
Si -3.13189300 -1.90299100 0.00000000
Si 3.13189300 -1.90299100 0.00000000
Si 3.13189300 1.90299100 0.00000000
H -4.00968000 1.91265400 1.20728100
H -4.00968000 1.91265400 -1.20728100
H -2.32158100 3.15527300 0.00000000
H 2.32158100 3.15527300 0.00000000
H 4.00968000 1.91265400 -1.20728100
H 4.00968000 1.91265400 1.20728100
H 4.00968000 -1.91265400 1.20728100
H 2.32158100 -3.15527300 0.00000000
H 4.00968000 -1.91265400 -1.20728100
H -2.32158100 -3.15527300 0.00000000
H -4.00968000 -1.91265400 -1.20728100
H -4.00968000 -1.91265400 1.20728100

2h:

PBE1PBE/6-31G(d): -2369.27173 a.u.

Point group: D_2

Cartesian coordinates:

C -1.52780000 0.00196000 0.67426500
C -1.52780000 -0.00196000 -0.67426500
C 1.52780000 0.00196000 -0.67426500
C 1.52780000 -0.00196000 0.67426500
H -2.49747400 0.00411000 1.18437600
H -2.49747400 -0.00411000 -1.18437600
H 2.49747400 0.00411000 -1.18437600
H 2.49747400 -0.00411000 1.18437600
Si 0.00000000 0.00000000 1.77343600
Si 0.00000000 0.00000000 -1.77343600
Si 0.01352700 -1.94807500 3.11545000
Si -0.01352700 1.94807500 3.11545000
Si 0.01352700 1.94807500 -3.11545000
Si -0.01352700 -1.94807500 -3.11545000
C 0.43629700 3.45387600 2.06024000
H 1.42689900 3.33714400 1.60632200
H -0.28525400 3.59605200 1.24798300
H 0.44716400 4.36873000 2.66569400
C 1.23889500 1.79900100 4.53023800
H 1.25159000 2.71690800 5.13108800
H 0.99419600 0.96714400 5.20077300
H 2.25525200 1.63618800 4.15356900
C -1.74132600 2.20883600 3.84885400
H -2.05022600 1.36423700 4.47469500
H -1.76345700 3.11182100 4.47155300
H -2.49113200 2.33164800 3.05902700
C 1.74132600 -2.20883600 3.84885400
H 2.05022600 -1.36423700 4.47469500
H 1.76345700 -3.11182100 4.47155300
H 2.49113200 -2.33164800 3.05902700
C -1.23889500 -1.79900100 4.53023800
H -1.25159000 -2.71690800 5.13108800
H -0.99419600 -0.96714400 5.20077300
H -2.25525200 -1.63618800 4.15356900
C -0.43629700 -3.45387600 2.06024000
H -1.42689900 -3.33714400 1.60632200
H 0.28525400 -3.59605200 1.24798300

H	-0.44716400	-4.36873000	2.66569400
C	-0.43629700	3.45387600	-2.06024000
H	-1.42689900	3.33714400	-1.60632200
H	0.28525400	3.59605200	-1.24798300
H	-0.44716400	4.36873000	-2.66569400
C	1.74132600	2.20883600	-3.84885400
H	2.05022600	1.36423700	-4.47469500
H	1.76345700	3.11182100	-4.47155300
H	2.49113200	2.33164800	-3.05902700
C	-1.23889500	1.79900100	-4.53023800
H	-1.25159000	2.71690800	-5.13108800
H	-0.99419600	0.96714400	-5.20077300
H	-2.25525200	1.63618800	-4.15356900
C	1.23889500	-1.79900100	-4.53023800
H	1.25159000	-2.71690800	-5.13108800
H	0.99419600	-0.96714400	-5.20077300
H	2.25525200	-1.63618800	-4.15356900
C	-1.74132600	-2.20883600	-3.84885400
H	-2.05022600	-1.36423700	-4.47469500
H	-1.76345700	-3.11182100	-4.47155300
H	-2.49113200	-2.33164800	-3.05902700
C	0.43629700	-3.45387600	-2.06024000
H	1.42689900	-3.33714400	-1.60632200
H	-0.28525400	-3.59605200	-1.24798300
H	0.44716400	-4.36873000	-2.66569400

2i:

PBE1PBE/6-31G(d): -957.01293 a.u.

Point group: D_2

Cartesian coordinates:

C	-0.01062000	1.52545600	-0.67365700
C	0.01062000	1.52545600	0.67365700
C	-0.01062000	-1.52545600	0.67365700
C	0.01062000	-1.52545600	-0.67365700
H	-0.02007900	2.49245300	-1.19011300
H	0.02007900	2.49245300	1.19011300
H	-0.02007900	-2.49245300	1.19011300
H	0.02007900	-2.49245300	-1.19011300
Si	0.00000000	0.00000000	-1.76274400
Si	0.00000000	0.00000000	1.76274400
N	-1.34701800	0.20820400	-2.83378600
H	-2.21681600	0.55915900	-2.45518600
H	-1.51851900	-0.50378400	-3.53233400
N	1.34701800	-0.20820400	-2.83378600
H	2.21681600	-0.55915900	-2.45518600
H	1.51851900	0.50378400	-3.53233400
N	1.34701800	0.20820400	2.83378600
H	1.51851900	-0.50378400	3.53233400
H	2.21681600	0.55915900	2.45518600
N	-1.34701800	-0.20820400	2.83378600
H	-2.21681600	-0.55915900	2.45518600
H	-1.51851900	0.50378400	3.53233400

2j:

PBE1PBE/6-31G(d): -1132.27222 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	-1.51781600	0.66967000	0.00000000
C	-1.51781600	-0.66967000	0.00000000
C	1.51781600	-0.66967000	0.00000000
C	1.51781600	0.66967000	0.00000000
Si	0.00000000	1.77376600	0.00000000
Si	0.00000000	-1.77376600	0.00000000
H	0.00000000	-2.63789500	1.20799500
H	0.00000000	-2.63789500	-1.20799500
H	0.00000000	2.63789500	-1.20799500
H	0.00000000	2.63789500	1.20799500
F	2.69342600	-1.33152500	0.00000000
F	2.69342600	1.33152500	0.00000000
F	-2.69342600	1.33152500	0.00000000
F	-2.69342600	-1.33152500	0.00000000

2k:

PBE1PBE/6-31G(d): -2573.46601 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	-1.54105000	0.67066200	0.00000000
C	-1.54105000	-0.67066200	0.00000000
C	1.54105000	-0.67066200	0.00000000
C	1.54105000	0.67066200	0.00000000
Si	0.00000000	1.74630200	0.00000000
Si	0.00000000	-1.74630200	0.00000000
H	0.00000000	-2.60030300	1.21353200
H	0.00000000	-2.60030300	-1.21353200
H	0.00000000	2.60030300	-1.21353200
H	0.00000000	2.60030300	1.21353200
Cl	3.00748100	-1.60651300	0.00000000
Cl	3.00748100	1.60651300	0.00000000
Cl	-3.00748100	1.60651300	0.00000000
Cl	-3.00748100	-1.60651300	0.00000000

2l:

PBE1PBE/6-31G(d): -892.78180 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	-1.57418500	0.67629900	0.00000000
C	-1.57418500	-0.67629900	0.00000000
C	1.57418500	-0.67629900	0.00000000
C	1.57418500	0.67629900	0.00000000
Si	0.00000000	1.68842200	0.00000000
Si	0.00000000	-1.68842200	0.00000000
H	0.00000000	-2.60154000	1.18705500
H	0.00000000	-2.60154000	-1.18705500
H	0.00000000	2.60154000	-1.18705500
H	0.00000000	2.60154000	1.18705500
C	2.86803700	-1.45934900	0.00000000
H	3.47705800	-1.21990900	-0.88179900
H	3.47705800	-1.21990900	0.88179900
H	2.70567700	-2.54243400	0.00000000
C	2.86803700	1.45934900	0.00000000
H	3.47705800	1.21990900	0.88179900
H	3.47705800	1.21990900	-0.88179900
H	2.70567700	2.54243400	0.00000000
C	-2.86803700	1.45934900	0.00000000
H	-3.47705800	1.21990900	-0.88179900
H	-3.47705800	1.21990900	0.88179900
H	-2.70567700	2.54243400	0.00000000
C	-2.86803700	-1.45934900	0.00000000
H	-3.47705800	-1.21990900	0.88179900
H	-3.47705800	-1.21990900	-0.88179900
H	-2.70567700	-2.54243400	0.00000000

2m:

PBE1PBE/6-31G(d): -2082.60716 a.u.

Point group: C_2

Cartesian coordinates:

C	-0.01714500	0.67189600	-1.55494700
C	0.01714500	-0.67189600	-1.55494700
C	0.01712800	-0.67189400	1.55492700
C	-0.01712800	0.67189400	1.55492700
Si	0.01712800	1.74924500	-0.00000800
Si	-0.01712800	-1.74924500	-0.00000800
H	-1.27987400	-2.52389000	-0.00003000
H	1.15827700	-2.65287200	0.00001200
H	1.27987400	2.52389000	-0.00003000
H	-1.15827700	2.65287200	0.00001200
C	0.08024900	-1.50469100	2.82335000
C	-0.08024900	1.50469100	2.82335000
C	-0.08022400	1.50472600	-2.82335300
C	0.08022400	-1.50472600	-2.82335300
F	-0.24873600	-2.78294700	2.53139100
F	1.31826700	-1.52918500	3.32690200
F	-0.75799400	-1.09900800	3.77824600
F	-1.31826700	1.52918500	3.32690200
F	0.75799400	1.09900800	3.77824600
F	0.24873600	2.78294700	2.53139100
F	0.24841700	2.78304100	-2.53127300
F	-1.31816100	1.52897000	-3.32711800

F 0.75829300 1.09930300 -3.77811900
F -0.75829300 -1.09930300 -3.77811900
F 1.31816100 -1.52897000 -3.32711800
F -0.24841700 -2.78304100 -2.53127300

2n:

PBE1PBE/6-31G(d): -3088.55133 a.u.

Point group: D_2

Cartesian coordinates:

C 1.57179000 0.02077900 0.67974700
C 1.57179000 -0.02077900 -0.67974700
C -1.57179000 0.02077900 -0.67974700
C -1.57179000 -0.02077900 0.67974700
Si 0.00000000 0.00000000 1.73117100
Si 0.00000000 0.00000000 -1.73117100
H -0.00186000 1.20712300 -2.59763800
H 0.00186000 -1.20712300 -2.59763800
H -0.00186000 -1.20712300 2.59763800
H 0.00186000 1.20712300 2.59763800
Si -3.12876700 -0.07079700 1.69704200
Si -3.12876700 0.07079700 -1.69704200
Si 3.12876700 -0.07079700 -1.69704200
Si 3.12876700 0.07079700 1.69704200
F -2.76656900 0.47387100 3.14789800
F -3.72418000 -1.52902600 1.88059600
F -4.24649000 0.87414800 1.07596700
F -4.24649000 -0.87414800 -1.07596700
F -3.72418000 1.52902600 -1.88059600
F -2.76656900 -0.47387100 -3.14789800
F 2.76656900 0.47387100 -3.14789800
F 3.72418000 -1.52902600 -1.88059600
F 4.24649000 0.87414800 -1.07596700
F 4.24649000 -0.87414800 1.07596700
F 3.72418000 1.52902600 1.88059600
F 2.76656900 -0.47387100 3.14789800

2o:

PBE1PBE/6-31G(d): -1897.90629 a.u.

Point group: D_2

Cartesian coordinates:

C 1.58089200 0.00687100 0.68027300
C 1.58089200 -0.00687100 -0.68027300
C -1.58089200 0.00687100 -0.68027300
C -1.58089200 -0.00687100 0.68027300
Si 0.00000000 0.00000000 1.70152300
Si 0.00000000 0.00000000 -1.70152300
H -0.00180900 1.19493400 -2.59784800
H 0.00180900 -1.19493400 -2.59784800
H -0.00180900 -1.19493400 2.59784800
H 0.00180900 1.19493400 2.59784800
Si -3.16818900 -0.03601700 1.71215400
Si -3.16818900 0.03601700 -1.71215400
Si 3.16818900 -0.03601700 -1.71215400
Si 3.16818900 0.03601700 1.71215400
H -2.84886300 0.40272500 3.09971200
H -3.73602500 -1.41253400 1.77526500
H -4.19500700 0.88286800 1.14394000
H -4.19500700 -0.88286800 -1.14394000
H -3.73602500 1.41253400 -1.77526500
H -2.84886300 -0.40272500 -3.09971200
H 2.84886300 0.40272500 -3.09971200
H 3.73602500 -1.41253400 -1.77526500
H 4.19500700 -0.88286800 1.14394000
H 2.84886300 -0.40272500 3.09971200
H 3.73602500 1.41253400 1.77526500
H 4.19500700 0.88286800 -1.14394000

2p:

PBE1PBE/6-31G(d): -956.88898 a.u.

Point group: C_s

Cartesian coordinates:

C 0.68363800 -0.03399200 1.54979300
C -0.67587700 -0.04245400 1.54598200
C -0.67587700 -0.04245400 -1.54598200

C	0.68363800	-0.03399200	-1.54979300
Si	1.69496400	0.24253600	0.00000000
Si	-1.68748400	0.17318400	0.00000000
N	-1.32829500	-0.19770200	2.80572500
H	-1.18190800	0.60770900	3.41030100
H	-2.32532600	-0.35759300	2.72198700
N	1.37420000	-0.13196000	-2.76071300
H	2.29422600	-0.54832400	-2.68850400
H	0.81150500	-0.60184800	-3.46768600
N	1.37420000	-0.13196000	2.76071300
H	0.81150500	-0.60184800	3.46768600
H	2.29422600	-0.54832400	2.68850400
N	-1.32829500	-0.19770200	-2.80572500
H	-2.32532600	-0.35759300	-2.72198700
H	-1.18190800	0.60770900	-3.41030100
H	-2.79535900	-0.84027300	0.00000000
H	-2.40644000	1.49063900	0.00000000
H	2.32902500	1.59477200	0.00000000
H	2.83525100	-0.73249600	0.00000000

3a:

PBE1PBE/6-31G(d): -887.88012 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	-1.91875300	1.40178600	0.00000000
C	-0.74518400	0.74806700	0.00000000
C	-0.74518400	-0.74806700	0.00000000
C	-1.91875300	-1.40178600	0.00000000
H	-2.04610500	2.47940000	0.00000000
H	-2.04610500	-2.47940000	0.00000000
Si	-3.18535900	0.00000000	0.00000000
C	0.74518400	0.74806700	0.00000000
C	0.74518400	-0.74806700	0.00000000
C	1.91875300	1.40178600	0.00000000
H	2.04610500	2.47940000	0.00000000
C	1.91875300	-1.40178600	0.00000000
H	2.04610500	-2.47940000	0.00000000
Si	3.18535900	0.00000000	0.00000000
H	4.07041200	0.00000000	1.20279800
H	4.07041200	0.00000000	-1.20279800
H	-4.07041200	0.00000000	-1.20279800
H	-4.07041200	0.00000000	1.20279800

3b:

PBE1PBE/6-31G(d): -1284.75765 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	1.90752500	1.41674600	0.00000000
C	0.74244400	0.75580200	0.00000000
C	0.74244400	-0.75580200	0.00000000
C	1.90752500	-1.41674600	0.00000000
H	2.04051400	2.49269500	0.00000000
H	2.04051400	-2.49269500	0.00000000
Si	3.13868900	0.00000000	0.00000000
C	-0.74244400	0.75580200	0.00000000
C	-0.74244400	-0.75580200	0.00000000
C	-1.90752500	1.41674600	0.00000000
H	-2.04051400	2.49269500	0.00000000
C	-1.90752500	-1.41674600	0.00000000
H	-2.04051400	-2.49269500	0.00000000
Si	-3.13868900	0.00000000	0.00000000
F	4.10664800	0.00000000	1.27567700
F	4.10664800	0.00000000	-1.27567700
F	-4.10664800	0.00000000	1.27567700
F	-4.10664800	0.00000000	-1.27567700

3h:

PBE1PBE/6-31G(d): -2521.45264 a.u.

Point group: C_1

Cartesian coordinates:

C	1.93073900	-0.11295900	-1.38749000
C	0.74750100	-0.13508200	-0.74034100
C	0.74466300	-0.13471400	0.74344900
C	1.92515700	-0.11094800	1.39563400

H	2.05755400	-0.10084700	-2.46620900
H	2.04733100	-0.10009400	2.47489900
Si	3.21326200	-0.06193500	0.00685100
C	-0.74466500	-0.13473200	-0.74344300
C	-0.74750400	-0.13506300	0.74034600
C	-1.92515900	-0.11098100	-1.39562900
H	-2.04733300	-0.10015600	-2.47489400
C	-1.93074200	-0.11292300	1.38749500
H	-2.05755700	-0.10078300	2.46621400
Si	-3.21326500	-0.06193300	-0.00684800
Si	-4.61754600	-1.96074400	-0.03294000
Si	4.32679700	2.02126500	-0.03211700
Si	4.61755100	-1.96074000	0.03296200
Si	-4.32680200	2.02126600	0.03209300
C	-3.55551500	-3.51028200	0.17886400
H	-4.17464200	-4.41574600	0.15937100
H	-2.81338400	-3.58963400	-0.62293200
H	-3.01277800	-3.48987100	1.12997100
C	-5.53791400	-2.05210300	-1.68530700
H	-4.83853800	-2.11539600	-2.52636600
H	-6.17962700	-2.94140600	-1.71784100
H	-6.17455800	-1.17474300	-1.84518700
C	-3.05202700	3.38729100	-0.25347700
H	-2.58878000	3.29490400	-1.24154600
H	-3.51828600	4.37804300	-0.18647900
H	-2.25081600	3.33745300	0.49189000
C	-5.65403000	2.10830900	-1.31727700
H	-6.12015500	3.10150400	-1.33073900
H	-5.23074300	1.92662200	-2.31151700
H	-6.44873400	1.37186300	-1.15160600
C	3.05202100	3.38729300	0.25343300
H	2.58876400	3.29491000	1.24149900
H	3.51828100	4.37804400	0.18643600
H	2.25081600	3.33745200	-0.49194000
C	5.65401800	2.10831800	1.31726000
H	6.12013100	3.10151900	1.33073200
H	5.23072800	1.92662000	2.31149700
H	6.44873100	1.37188300	1.15158800
C	5.53793200	-2.05208700	1.68532200
H	4.83856400	-2.11538300	2.52638700
H	6.17965200	-2.94138600	1.71785300
H	6.17457200	-1.17472300	1.84519300
C	3.55552700	-3.51028500	-0.17882600
H	4.17466100	-4.41574500	-0.15934600
H	2.81341100	-3.58964500	0.62298300
H	3.01277300	-3.48987700	-1.12992400
C	-5.14679300	2.27314200	1.72033500
H	-5.88619200	1.49372300	1.93532900
H	-4.40441600	2.26101300	2.52602300
H	-5.66196700	3.24120700	1.75574500
C	-5.88157400	-1.86438600	1.37413300
H	-5.39206000	-1.78097600	2.35086100
H	-6.54719200	-1.00145600	1.25788900
H	-6.50637500	-2.76611900	1.39111500
C	5.88156700	-1.86438000	-1.37412100
H	5.39204600	-1.78094600	-2.35084400
H	6.54719700	-1.00146000	-1.25786900
H	6.50635700	-2.76612000	-1.39112300
C	5.14679900	2.27313000	-1.72035600
H	5.88619400	1.49370500	-1.93534300
H	4.40442700	2.26100500	-2.52604800
H	5.66198100	3.24119100	-1.75576400

Silole with $SiF(SiMe_3)$ moiety:

PBE1PBE/6-31G(d): -952.75657 a.u.

Point group: C_s

Cartesian coordinates:

C	-1.12415100	1.34325000	1.35411300
C	-1.12415100	2.54422200	0.74156800
C	-1.12415100	2.54422200	-0.74156800
C	-1.12415100	1.34325000	-1.35411300
H	-1.10843400	1.24128100	2.43454100
H	-1.12017100	3.49608100	1.27285600
H	-1.12017100	3.49608100	-1.27285600

H	-1.10843400	1.24128100	-2.43454100
Si	-0.94985200	0.06298700	0.00000000
Si	1.16003000	-0.97076700	0.00000000
C	1.34731800	-2.04514000	1.54523700
H	0.57475800	-2.82058100	1.59007700
H	2.32372800	-2.54497400	1.54851600
H	1.27650800	-1.44713500	2.46054500
C	1.34731800	-2.04514000	-1.54523700
H	2.32372800	-2.54497400	-1.54851600
H	0.57475800	-2.82058100	-1.59007700
H	1.27650800	-1.44713500	-2.46054500
C	2.47266800	0.38904400	0.00000000
H	2.38081200	1.02901600	0.88418700
H	3.48034300	-0.04383000	0.00000000
H	2.38081200	1.02901600	-0.88418700
F	-2.12238100	-1.06632100	0.00000000

1,4-Disilacyclohexa-2,5-diene with $SiF(SiMe_3)$ moiety (Z-isomer):

PBE1PBE/6-31G(d): -1750.92456 a.u.

Point group: C_2

Cartesian coordinates:

C	-1.30185800	1.04765600	-1.17695300
C	-1.64916800	-0.25390000	-1.17139300
C	1.30185800	-1.04765600	-1.17695300
C	1.64916800	0.25390000	-1.17139300
H	-2.09618300	1.79683900	-1.25710900
H	-2.71133800	-0.50834400	-1.24683600
H	2.09618300	-1.79683900	-1.25710900
H	2.71133800	0.50834400	-1.24683600
Si	0.45119000	1.68464800	-1.03528700
Si	-0.45119000	-1.68464800	-1.03528700
Si	0.78647100	2.97221400	0.90219200
Si	-0.78647100	-2.97221400	0.90219200
C	2.62224000	3.40138900	1.06190000
H	2.98048200	3.95706100	0.18824000
H	2.79515700	4.02490700	1.94760000
H	3.23880600	2.50133000	1.16451400
C	-0.22687500	4.56376100	0.75979800
H	-0.04768000	5.21395500	1.62484200
H	0.03966500	5.12417600	-0.14287900
H	-1.30196900	4.35500500	0.71927300
C	0.22687500	2.00300500	2.42592900
H	-0.83184200	1.72861600	2.35661000
H	0.80393000	1.08056900	2.55321000
H	0.35677000	2.60576400	3.33295400
C	0.22687500	-4.56376100	0.75979800
H	0.04768000	-5.21395500	1.62484200
H	-0.03966500	-5.12417600	-0.14287900
H	1.30196900	-4.35500500	0.71927300
C	-2.62224000	-3.40138900	1.06190000
H	-2.98048200	-3.95706100	0.18824000
H	-2.79515700	-4.02490700	1.94760000
H	-3.23880600	-2.50133000	1.16451400
C	-0.22687500	-2.00300500	2.42592900
H	0.83184200	-1.72861600	2.35661000
H	-0.80393000	-1.08056900	2.55321000
H	-0.35677000	-2.60576400	3.33295400
F	-0.72569600	-2.67302900	-2.30808700
F	0.72569600	2.67302900	-2.30808700

1,4-Disilacyclohexa-2,5-diene with $SiF(SiMe_3)$ moiety (E-isomer):

PBE1PBE/6-31G(d): -1750.92508 a.u.

Point group: C_2

Cartesian coordinates:

C	0.33021700	0.58765100	-1.53016400
C	-0.33021700	-0.58765100	-1.53016400
C	-0.33016500	-0.58767700	1.53103700
C	0.33016500	0.58767700	1.53103700
H	0.58171000	1.03984400	-2.49540000
H	-0.58171000	-1.03984400	-2.49540000
H	-0.58161800	-1.03990300	2.49626600
H	0.58161800	1.03990300	2.49626600

Si	0.76206900	1.57044300	0.00043700
Si	-0.76206900	-1.57044300	0.00043700
Si	-0.33016500	3.65006900	-0.00016900
Si	0.33016500	-3.65006900	-0.00016900
C	0.14848100	4.62842600	1.54701500
H	1.22928000	4.80083200	1.59475300
H	-0.34732100	5.60685400	1.55046000
H	-0.14944300	4.10376500	2.46185500
C	0.14959600	4.62745500	-1.54764400
H	-0.34616500	5.60590100	-1.55203400
H	1.23043100	4.79978900	-1.59480300
H	-0.14776800	4.10221100	-2.46233200
C	-2.19349200	3.33018200	-0.00093700
H	-2.50066100	2.75985500	-0.88466200
H	-2.50174900	2.76096600	0.88311900
H	-2.74984300	4.27541800	-0.00188900
C	2.19349200	-3.33018200	-0.00093700
H	2.50066100	-2.75985500	-0.88466200
H	2.50174900	-2.76096600	0.88311900
H	2.74984300	-4.27541800	-0.00188900
C	-0.14848100	-4.62842600	1.54701500
H	-1.22928000	-4.80083200	1.59475300
H	0.34732100	-5.60685400	1.55046000
H	0.14944300	-4.10376500	2.46185500
C	-0.14959600	-4.62745500	-1.54764400
H	0.34616500	-5.60590100	-1.55203400
H	-1.23043100	-4.79978900	-1.59480300
H	0.14776800	-4.10221100	-2.46233200
F	-2.37702700	-1.82553600	0.00056400
F	2.37702700	1.82553600	0.00056400

1,4-Disilacyclohexa-2,5-diene with one SiF_2 and one $Si(SiMe_3)_2$ moiety:

PBE1PBE/6-31G(d): -1750.93752 a.u.

Point group: C_2

Cartesian coordinates:

C	1.28320600	-0.83415900	0.75581100
C	1.29277900	-0.83662500	2.10466700
C	-1.29277900	0.83662500	2.10466700
C	-1.28320600	0.83415900	0.75581100
H	2.09383600	-1.35932800	0.23954700
H	2.10061700	-1.35825600	2.62572900
H	-2.10061700	1.35825600	2.62572900
H	-2.09383600	1.35932800	0.23954700
Si	0.00000000	0.00000000	-0.34229500
Si	0.00000000	0.00000000	3.12004500
Si	-1.11276900	-1.64174200	-1.62681400
Si	1.11276900	1.64174200	-1.62681400
C	1.57220100	3.08587200	-0.49759700
H	0.67968600	3.54705700	-0.06086900
H	2.20985100	2.75470300	0.32967200
H	2.11594800	3.85966000	-1.05328200
C	0.00000000	2.25842400	-3.02907100
H	0.50769200	3.04348100	-3.60315900
H	-0.25266100	1.45064200	-3.72562100
H	-0.93773800	2.68026100	-2.65006500
C	2.68360700	0.89020000	-2.36903100
H	2.45950200	0.03754300	-3.01992500
H	3.21615300	1.63735500	-2.97044200
H	3.36893700	0.54503800	-1.58678800
C	-2.68360700	-0.89020000	-2.36903100
H	-2.45950200	-0.03754300	-3.01992500
H	-3.21615300	-1.63735500	-2.97044200
H	-3.36893700	-0.54503800	-1.58678800
C	0.00000000	-2.25842400	-3.02907100
H	-0.50769200	-3.04348100	-3.60315900
H	0.25266100	-1.45064200	-3.72562100
H	0.93773800	-2.68026100	-2.65006500
C	-1.57220100	-3.08587200	-0.49759700
H	-0.67968600	-3.54705700	-0.06086900
H	-2.20985100	-2.75470300	0.32967200
H	-2.11594800	-3.85966000	-1.05328200
F	-0.68847900	-1.06491400	4.11307400
F	0.68847900	1.06491400	4.11307400