Supporting Information

for

Expanding the (Cross-)Hyperconjugation of 1,4-Disilacyclohexa-2,5-dienes to Larger Monomers and Oligomers: A Computational Investigation

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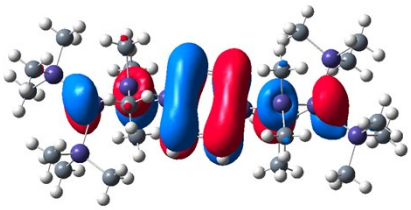
Molecular orbitals



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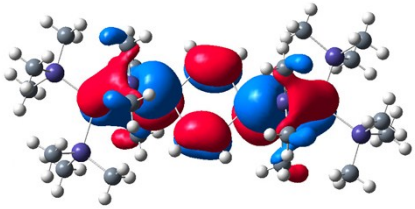

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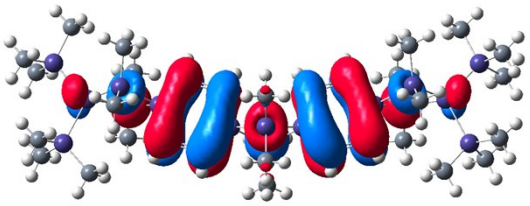

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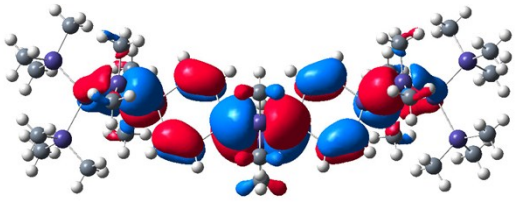

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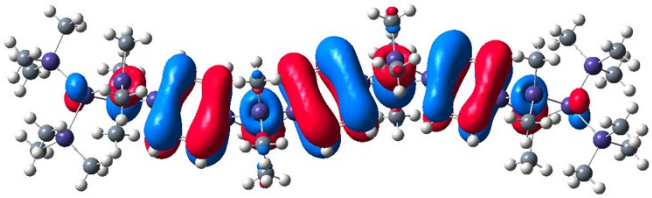

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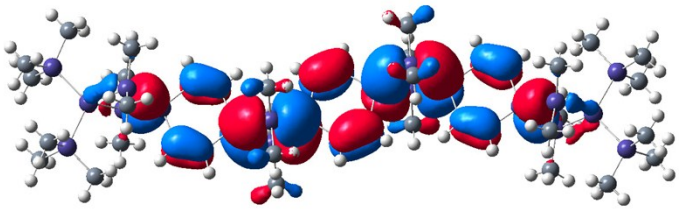

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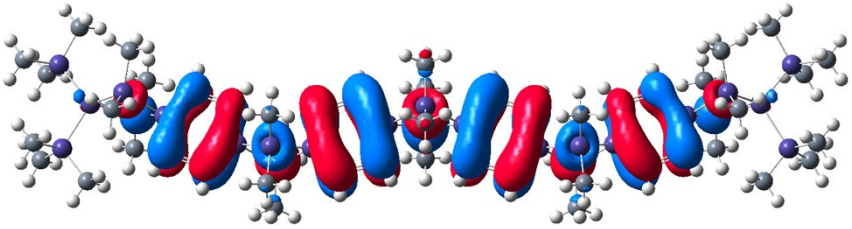

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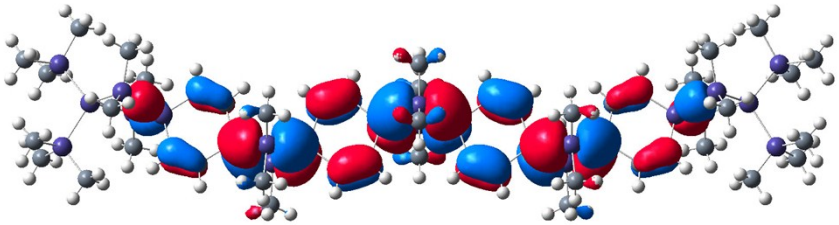

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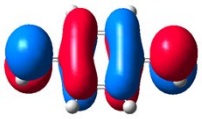

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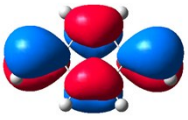

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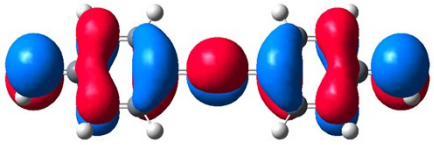

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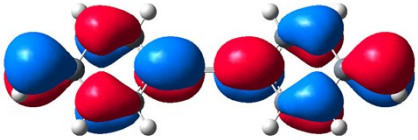

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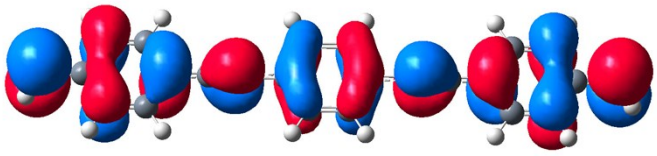

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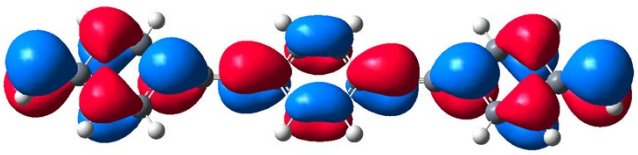

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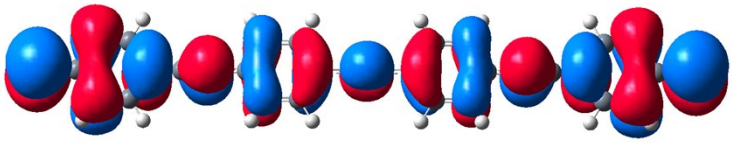

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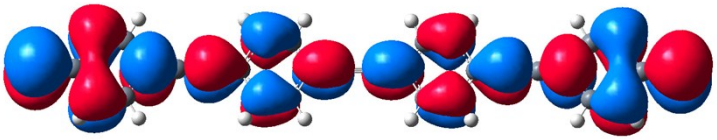

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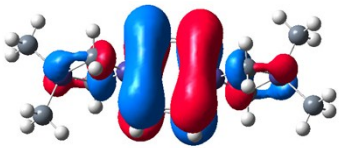

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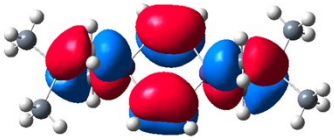

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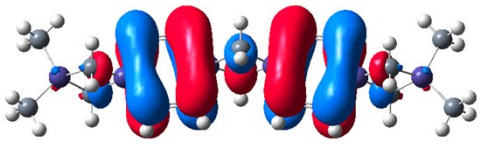

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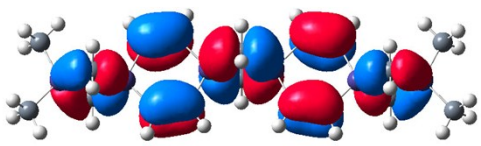

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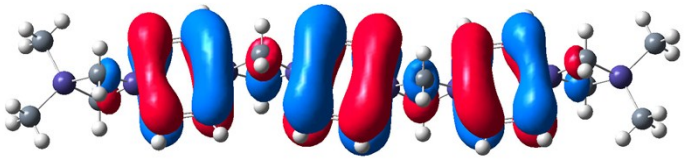

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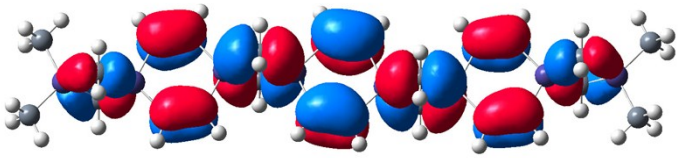

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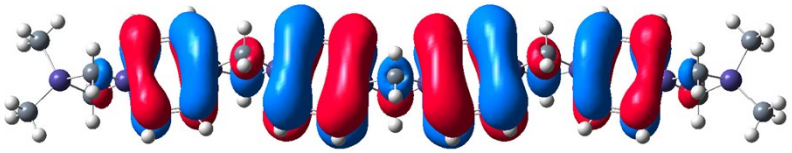

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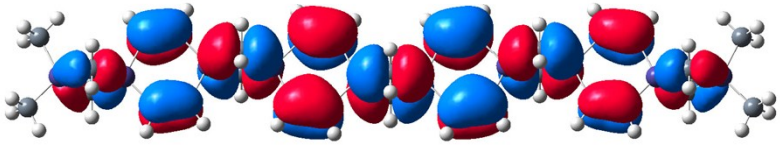

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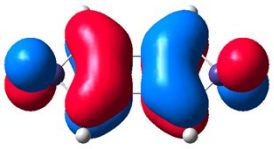

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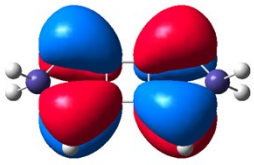

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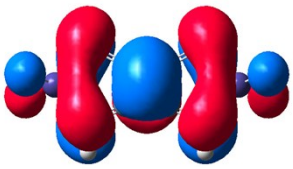

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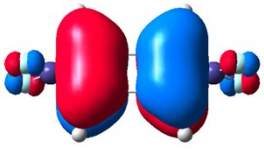

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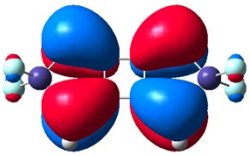

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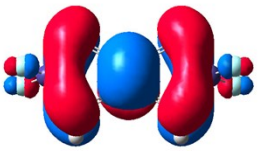

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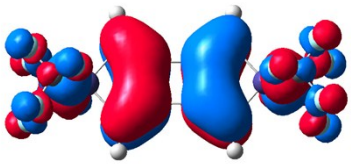

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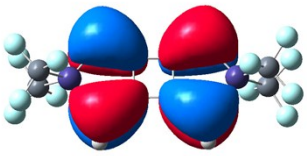

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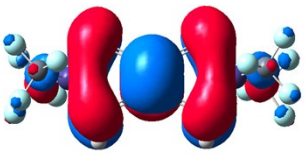

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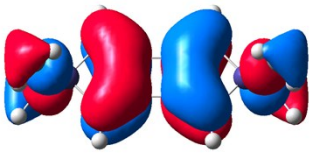

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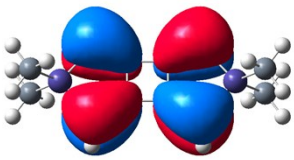

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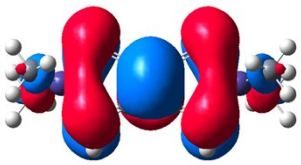

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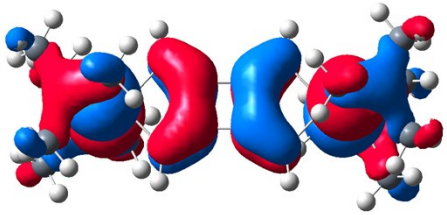

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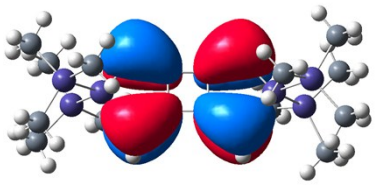

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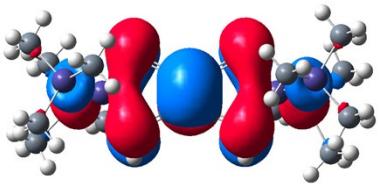

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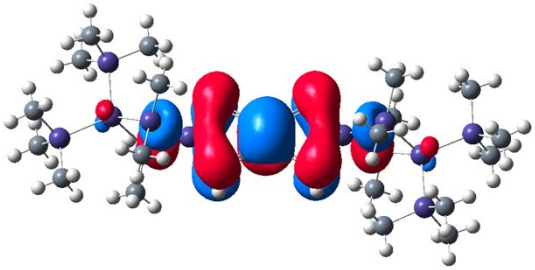

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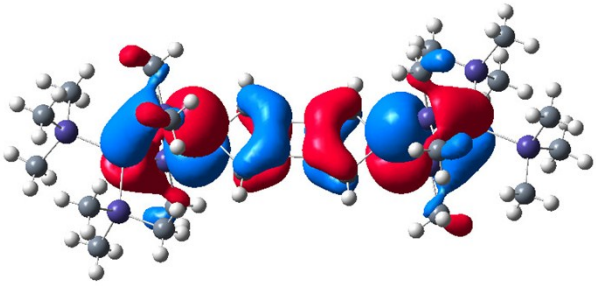

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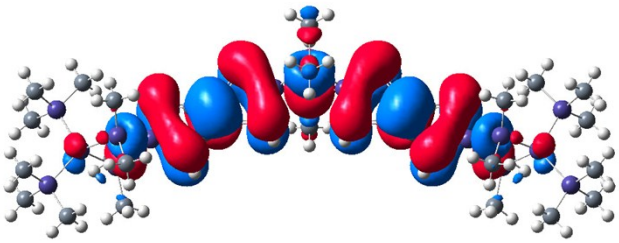

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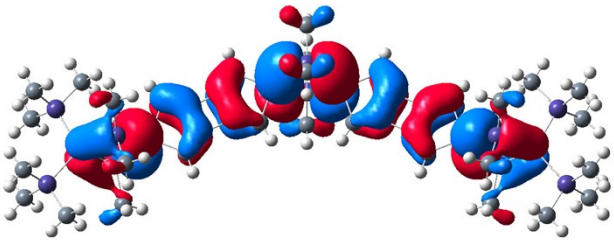

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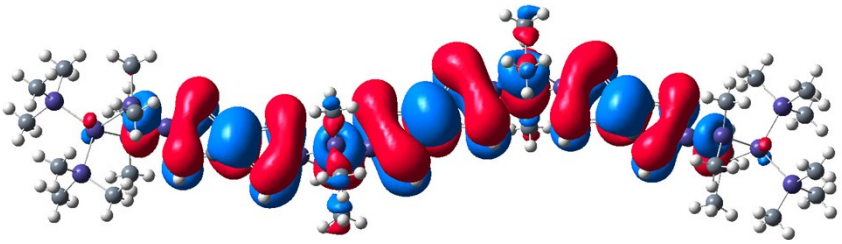

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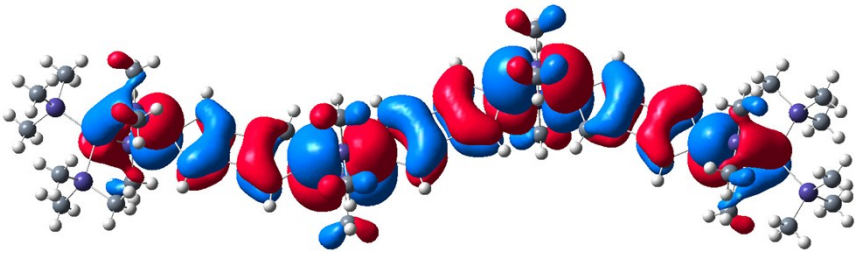

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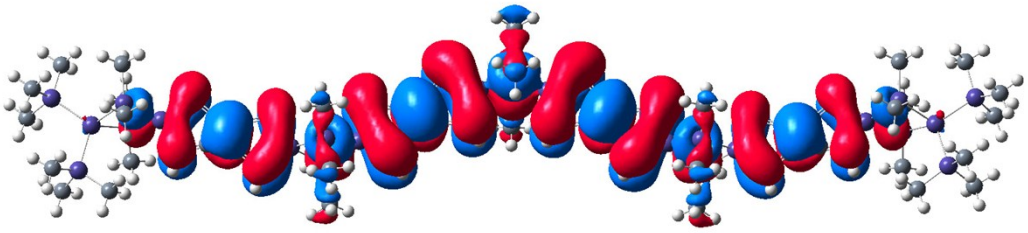

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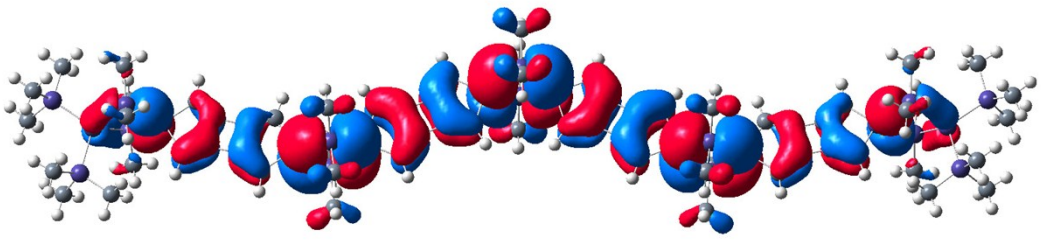

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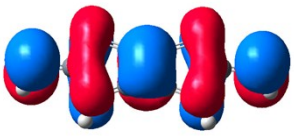

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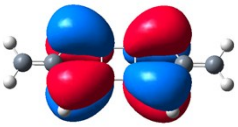

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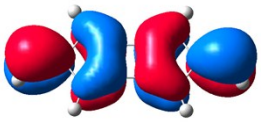

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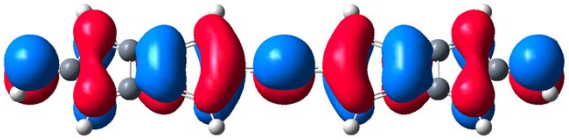

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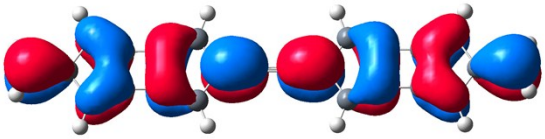

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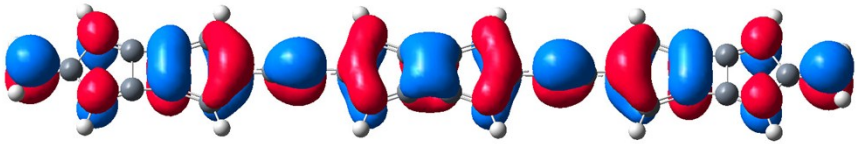

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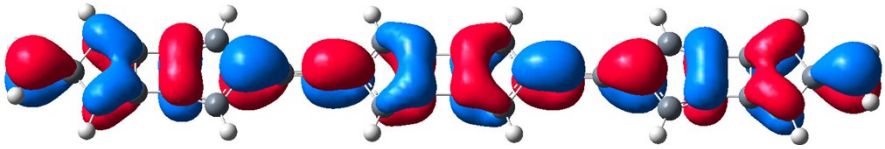

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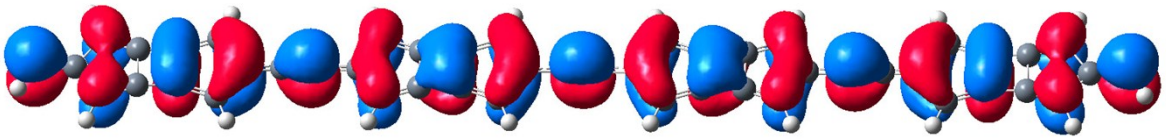

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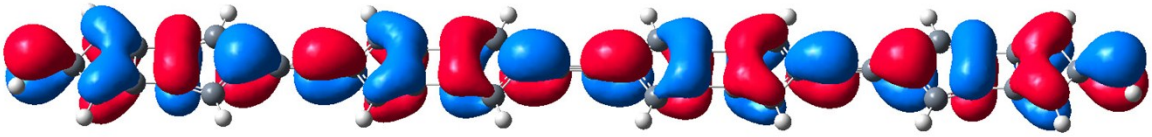
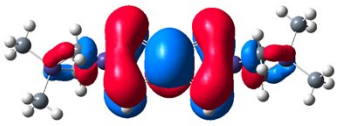
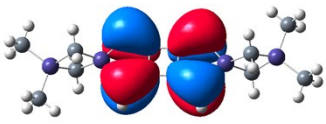


HOMO of **5d**



LUMO of **4a(C)**



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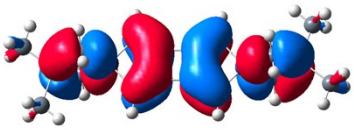
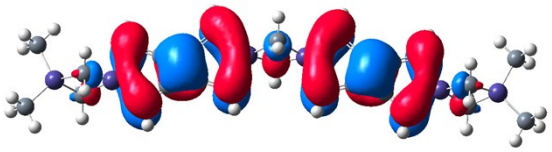


HOMO-2 of **4a(C)**



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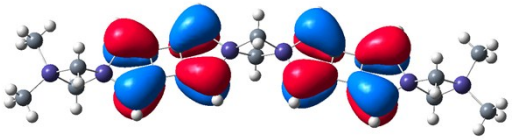
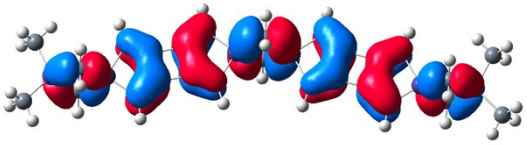
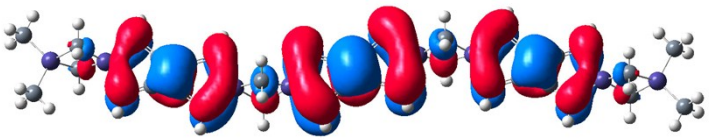


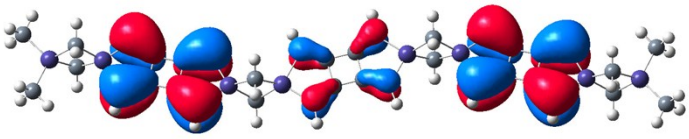
HOMO of **4b(C)**



HOMO-4 of **4b(C)**



LUMO of **4c(C)**



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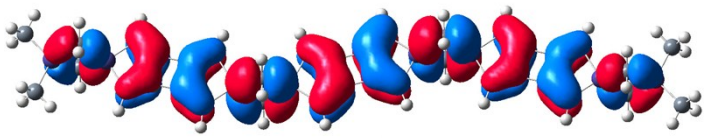
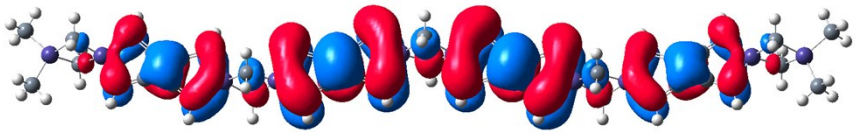
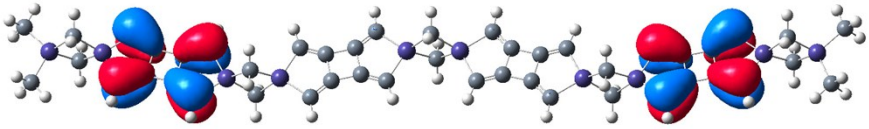


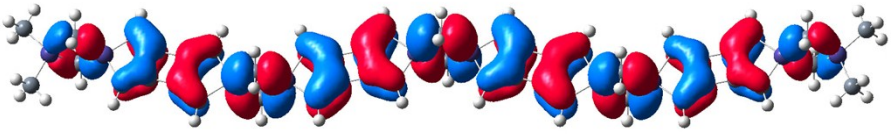
HOMO-5 of **4c(C)**



LUMO of **4d(C)**



HOMO of **4d(C)**



HOMO-7 of **4d(C)**

Orbital energies

Table 1. Orbital energies (in eV) and HOMO-LUMO energy gaps of **1a-d(Si)**. Results from B3LYP/6-311G(2d,p) calculations.

	1a(Si)	**1b(Si)**	**1c(Si)**	**1d(Si)**
E_{LUMO+3}	-0.59	-0.69	-0.75	-0.79
E_{LUMO+2}	-0.60	-0.73	-0.79	-0.84
E_{LUMO+1}	-0.75	-0.80	-0.94	-1.05
E_{LUMO}	-1.02	-1.15	-1.21	-1.24
E_{HOMO}	-5.41	-5.24	-5.17	-5.13
E_{HOMO-1}	-6.06	-5.67	-5.45	-5.33
E_{HOMO-2}	-6.23	-6.11	-5.79	-5.60
E_{HOMO-3}	-6.28	-6.15	-6.12	-5.86
$\Delta E_{HOMO-LUMO}$	4.39	4.09	3.96	3.89

Table 2. Orbital energies (in eV) and HOMO-LUMO energy gaps of **2a-d**. Results from B3LYP/6-311G(2d,p) calculations.

	2a	**2b**	**2c**	**2d**
E_{LUMO+3}	1.40	-0.18	-0.25	-0.46
E_{LUMO+2}	1.23	-0.19	-0.37	-1.06
E_{LUMO+1}	-0.02	-0.65	-1.64	-2.05
E_{LUMO}	-1.83	-2.96	-3.46	-3.74
E_{HOMO}	-5.63	-4.84	-4.43	-4.19
E_{HOMO-1}	-7.37	-6.77	-6.11	-5.80
E_{HOMO-2}	-8.41	-7.44	-7.17	-6.62
E_{HOMO-3}	-8.95	-7.44	-7.44	-7.38
$\Delta E_{HOMO-LUMO}$	3.80	1.88	0.97	0.45

Table 3. Orbital energies (in eV) and HOMO-LUMO energy gaps of **1a-d(C)**. Results from B3LYP/6-311G(2d,p) calculations.

	1a(C)	**1b(C)**	**1c(C)**	**1d(C)**
E_{LUMO+3}	0.78	-0.30	-0.40	-0.50
E_{LUMO+2}	0.76	-0.36	-0.57	-0.87
E_{LUMO+1}	-0.29	-0.72	-1.07	-1.26
E_{LUMO}	-1.04	-1.36	-1.49	-1.56
E_{HOMO}	-6.74	-6.60	-6.56	-6.53
E_{HOMO-1}	-6.79	-6.79	-6.80	-6.73
E_{HOMO-2}	-7.05	-6.95	-6.85	-6.81
E_{HOMO-3}	-7.30	-7.07	-6.90	-6.87
$\Delta E_{HOMO-LUMO}$	5.69	5.25	5.07	4.98

Table 4. Orbital energies (in eV) and HOMO-LUMO energy gaps of **3a-e**. Results from B3LYP/6-311G(2d,p) calculations.

	3a	**3b**	**3c**	**3d**	**3e**
E_{LUMO+3}	0.51	0.87	-0.10	1.06	0.24
E_{LUMO+2}	0.33	-0.43	-0.82	0.63	0.16
E_{LUMO+1}	-0.11	-0.68	-1.21	0.26	0.03
E_{LUMO}	-2.77	-3.66	-3.94	-2.39	-2.13
E_{HOMO}	-6.29	-6.93	-7.31	-5.88	-5.79
E_{HOMO-1}	-7.53	-8.24	-8.55	-7.13	-6.01
E_{HOMO-2}	-7.78	-8.90	-8.75	-7.24	-6.60
E_{HOMO-3}	-7.85	-9.07	-8.77	-7.34	-6.76
E_{HOMO-n}	-7.78 $n = 2$	-8.90 $n = 2$	-8.75 $n = 2$	-7.34 $n = 3$	-6.01 $n = 1$
$\Delta E_{HOMO-LUMO}$	3.52	5.69	5.25	5.07	4.98
$\Delta E_{HOMO-n - LUMO}$	5.02	5.24	4.81	4.95	3.88

Table 5. Orbital energies (in eV) and HOMO-LUMO energy gaps of **4a-d(Si)**. Results from B3LYP/6-311G(2d,p) calculations.

	4a(Si)	**4b(Si)**	**4c(Si)**	**4d(Si)**
E_{LUMO+3}	-0.19	-0.79	-0.95	-1.98
E_{LUMO+2}	-0.73	-0.88	-2.02	-2.16
E_{LUMO+1}	-0.79	-2.09	-2.27	-2.39
E_{LUMO}	-2.25	-2.43	-2.51	-2.56
E_{HOMO}	-5.70	-5.60	-5.57	-5.55
E_{HOMO-1}	-5.73	-5.77	-5.76	-5.69
E_{HOMO-2}	-5.92	-5.77	-5.78	-5.79
E_{HOMO-3}	-6.28	-5.93	-5.79	-5.79
$\Delta E_{HOMO-LUMO}$	3.45	3.17	3.05	3.00

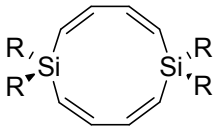
Table 6. Orbital energies (in eV) and HOMO-LUMO energy gaps of **5a-d**. Results from B3LYP/6-311G(2d,p) calculations.

	5a	**5b**	**5c**	**5d**
E_{LUMO+3}	1.44	-0.05	-1.32	-1.78
E_{LUMO+2}	0.15	-1.08	-1.90	-2.70
E_{LUMO+1}	-0.46	-2.13	-3.06	-3.50
E_{LUMO}	-2.80	-3.80	-4.21	-4.45
E_{HOMO}	-5.79	-5.68	-5.42	-5.26
E_{HOMO-1}	-6.24	-5.90	-5.95	-5.97
E_{HOMO-2}	-7.03	-5.91	-5.95	-5.97
E_{HOMO-3}	-8.08	-7.05	-5.95	-5.97
$\Delta E_{HOMO-LUMO}$	2.99	1.87	1.22	0.81

Table 7. Orbital energies (in eV) and HOMO-LUMO energy gaps of **4a-d(C)**. Results from B3LYP/6-311G(2d,p) calculations.

	4a(C)	**4b(C)**	**4c(C)**	**4d(C)**
E_{LUMO+3}	0.77	0.19	0.10	-2.34
E_{LUMO+2}	0.39	0.17	-2.35	-2.50
E_{LUMO+1}	0.26	-2.39	-2.59	-2.72
E_{LUMO}	-2.51	-2.74	-2.85	-2.91
E_{HOMO}	-5.90	-5.95	-5.98	-5.98
E_{HOMO-1}	-6.56	-5.97	-5.98	-5.98
E_{HOMO-2}	-7.01	-6.54	-6.02	-6.03
E_{HOMO-3}	-7.14	-6.85	-6.54	-6.05
E_{HOMO-n}	-7.01 n = 2	-6.96 n = 4	-6.95 n = 5	-6.95 n = 7
$\Delta E_{HOMO-LUMO}$	3.39	3.21	3.13	3.08
$\Delta E_{HOMO-n - LUMO}$	4.50	4.22	4.10	4.05

Characteristics of various 1,6-disilacyclodeca-2,4,7,9-tetraenes and 1,6-disilacyclodecahexanes



6a: R = H
6b: R = F
6c: R = CF_3
6d: R = Me
6e: R = $SiMe_3$

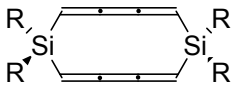
Table 8. The five lowest calculated vertical excitations of **6a-e**. Results from B3LYP/6-311G(2d,p) calculations.[a]

Electronic excitations	**6a**	**6b**	**6c**	**6d**	**6e**
S_1	4.72	4.75	4.70	4.93	4.08
S_2	4.75	4.82	5.09	5.07	4.10
S_3	4.89	5.18	5.13	5.53	4.26
S_4	**5.20**	5.51	5.64	5.58	4.62
S_5	5.90	5.82	5.77	5.64	4.88

[a] Transitions with oscillator strengths above 0.2 are marked in bold and those within 0.05-0.20 are underlined.

Table 9. Orbital energies (in eV) and HOMO-LUMO energy gaps of **6a-e**. Results from B3LYP/6-311G(2d,p) calculations.

	6a	**6b**	**6c**	**6d**	**6e**
E_{LUMO+3}	0.38	-0.28	-1.04	-0.06	0.35
E_{LUMO+2}	0.16	-0.48	-1.74	-0.11	-0.39
E_{LUMO+1}	-1.19	-1.73	-1.74	-0.62	-0.67
E_{LUMO}	-1.31	-1.84	-2.08	-0.67	-1.37
E_{HOMO}	-6.73	-7.27	-7.67	-6.53	-6.05
E_{HOMO-1}	-6.83	-7.72	-8.53	-7.10	-6.24
E_{HOMO-2}	-8.07	-8.62	-8.56	-7.40	-6.27
E_{HOMO-3}	-8.26	-8.77	-8.79	-7.45	-7.18
$\Delta E_{HOMO-LUMO}$	5.42	5.44	5.59	5.86	4.68



7a: R = H
7b: R = F
7c: R = CF_3
7d: R = Me
7e: R = $SiMe_3$

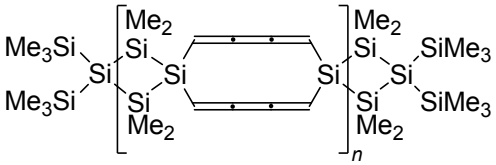
Table 10. The five lowest calculated vertical excitations of **7a-e**. Results from B3LYP/6-311G(2d,p) calculations.[a]

Electronic excitations	**7a**	**7b**	**7c**	**7d**	**7e**
S_1	2.97	2.57	2.80	2.88	2.91
S_2	3.10	3.18	3.07	3.08	2.99
S_3	4.00	3.67	3.83	3.94	3.08
S_4	4.01	3.93	3.86	3.97	3.45
S_5	4.07	4.08	3.90	3.98	3.69

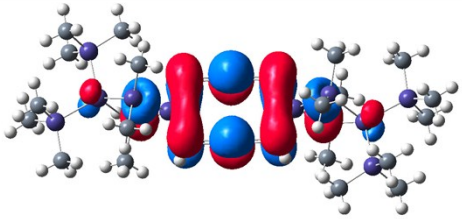
[a] Transitions with oscillator strengths above 0.2 are marked in bold and those within 0.05-0.20 are underlined.

Table 11. Orbital energies (in eV) and HOMO-LUMO energy gaps of **7a-e**. Results from B3LYP/6-311G(2d,p) calculations.

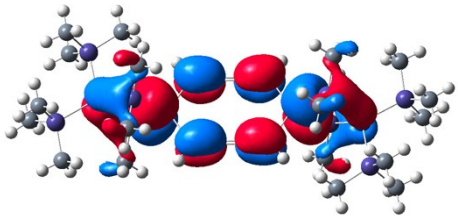
	7a	**7b**	**7c**	**7d**	**7e**
E_{LUMO+3}	0.47	0.37	-0.49	0.95	0.22
E_{LUMO+2}	-0.05	-0.54	-0.79	0.48	0.03
E_{LUMO+1}	-2.09	-2.55	-3.14	-1.69	-1.64
E_{LUMO}	-2.25	-3.26	-3.46	-1.94	-1.85
E_{HOMO}	-6.36	-6.95	-7.39	-5.94	-5.52
E_{HOMO-1}	-6.86	-7.52	-7.95	-6.52	-5.86
E_{HOMO-2}	-6.98	-7.97	-7.96	-6.57	-6.39
E_{HOMO-3}	-7.25	-8.11	-8.18	-6.79	-6.52
E_{HOMO-n} or E_{LUMO+m}	-6.86 n = 1	-7.97 n = 2	-7.95 n = 1	-6.52 n = 1	-1.64 m = 1
$\Delta E_{HOMO-LUMO}$	4.11	3.69	3.93	4.00	3.68
$\Delta E_{HOMO-n - LUMO+m}$	4.61	4.71	4.49	4.58	3.88



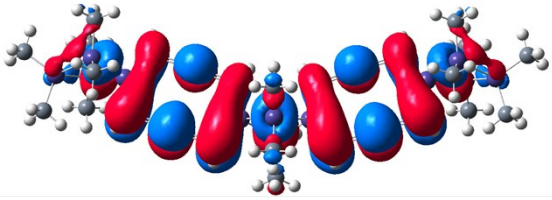
n = 1; 2; 3; 4



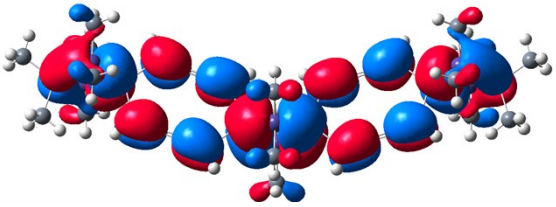
LUMO of monomer



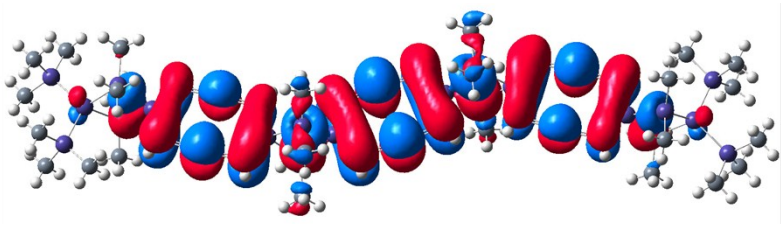
HOMO of monomer



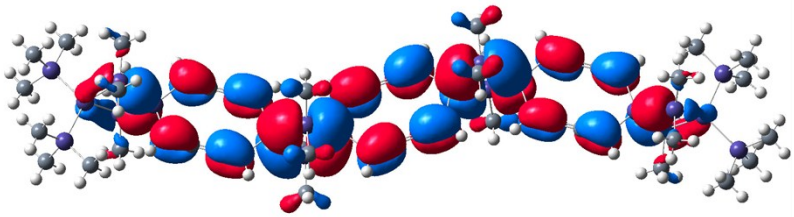
LUMO of dimer



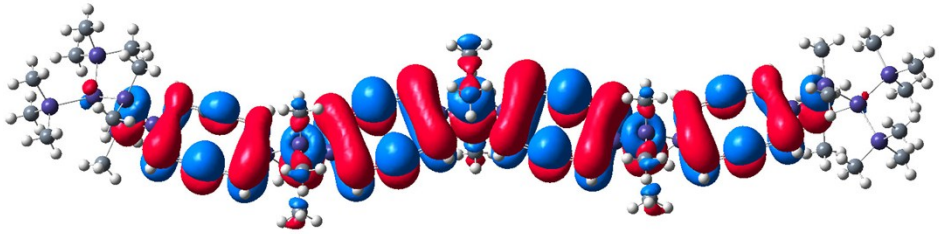
HOMO of dimer



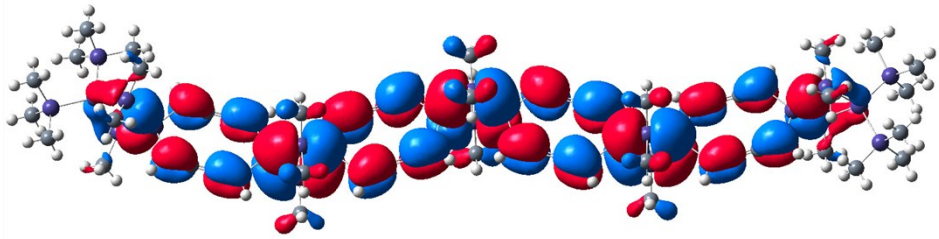
LUMO of trimer



HOMO of trimer



LUMO of tetramer



HOMO of tetramer

Table 12. The five lowest calculated vertical excitations of oligomeric 1,6-disilacyclohexadecaenes. Results from B3LYP/6-311G(2d,p) calculations.[a]

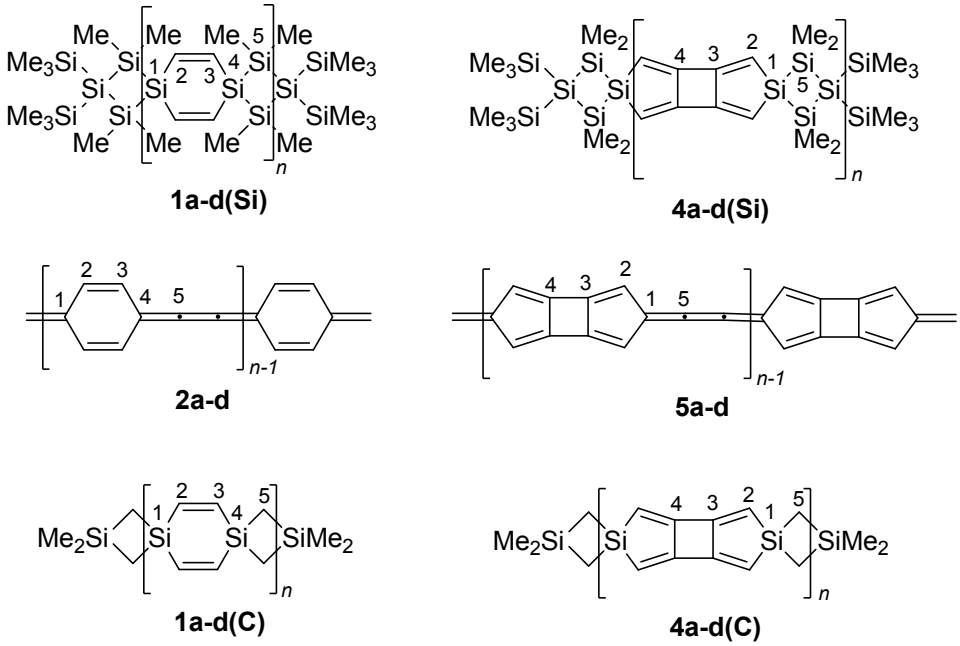
Electronic excitations	monomer	dimer	trimer	tetramer
S_1	2.82	**2.72**	**2.65**	**2.58**
S_2	2.97	<u>2.78</u>	2.71	2.68
S_3	**3.02**	2.81	2.81	2.73
S_4	3.15	2.94	2.82	2.81
S_5	3.58	2.97	2.92	2.81

[a] Transitions with oscillator strengths above 0.2 are marked in bold and those within 0.05-0.20 are underlined.

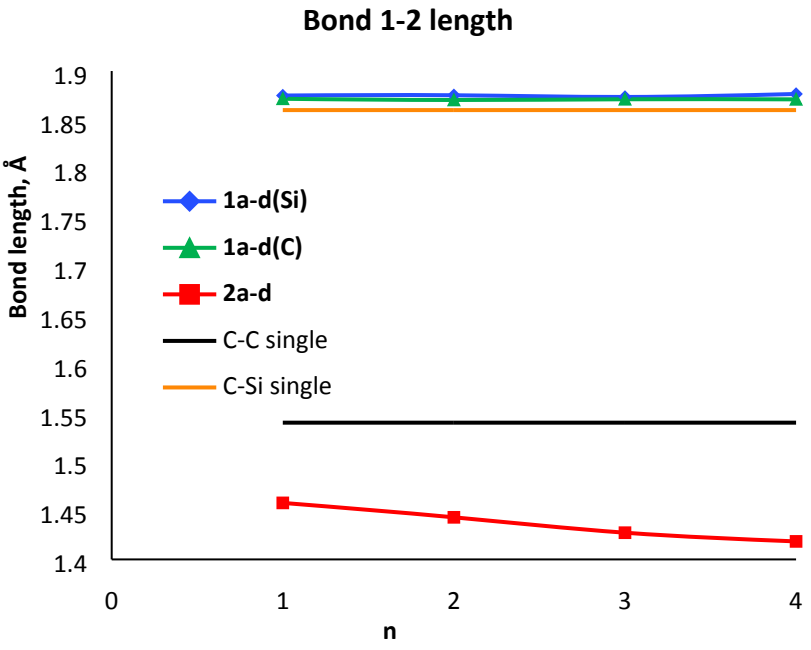
Table 13. Orbital energies (in eV) and HOMO-LUMO energy gaps of oligomeric 1,6-disilacyclohexadecaenes. Results from B3LYP/6-311G(2d,p) calculations.

	monomer	dimer	trimer	tetramer
E_{LUMO+3}	-0.69	-1.61	-1.82	-1.85
E_{LUMO+2}	-0.79	-1.79	-1.84	-1.94
E_{LUMO+1}	-1.74	-1.82	-1.92	-2.00
E_{LUMO}	-1.84	-2.04	-2.13	-2.18
E_{HOMO}	-5.32	-5.20	-5.15	-5.14
E_{HOMO-1}	-5.82	-5.57	-5.40	-5.30
E_{HOMO-2}	-5.89	-5.87	-5.71	-5.54
E_{HOMO-3}	-6.29	-5.89	-5.89	-5.79
$\Delta E_{HOMO-LUMO}$	3.48	3.16	3.03	2.96

Bond lengths

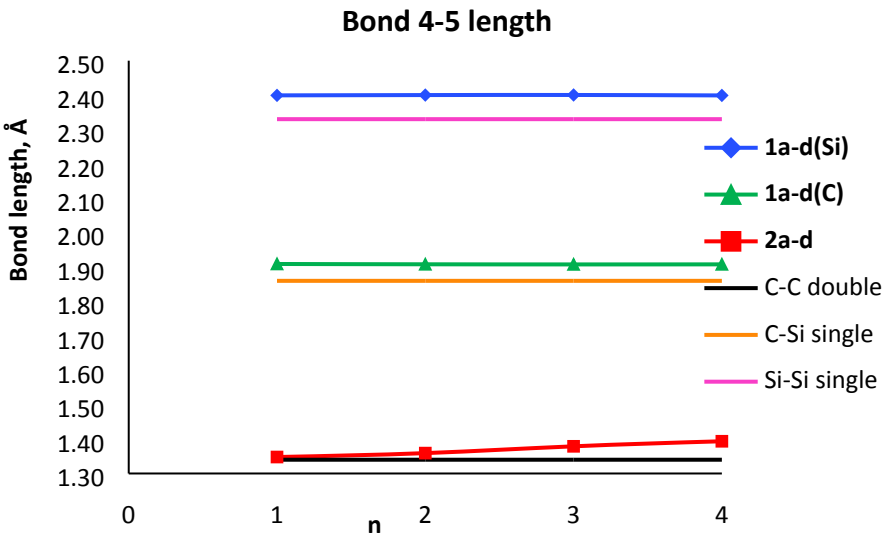


Bond numbering in oligomers from **1a-d(Si)** to **6a-d.**



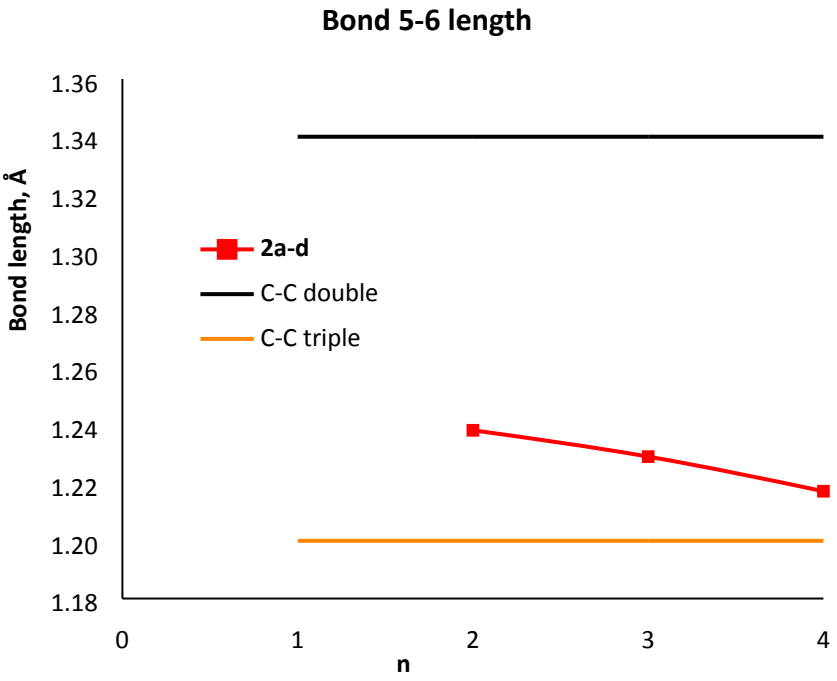
The C1-C2 single bond lengths of **1a-d(Si), 1a-d(C)** and **2a-d**.

Results from B3LYP/6-311G(2d,p) calculations.



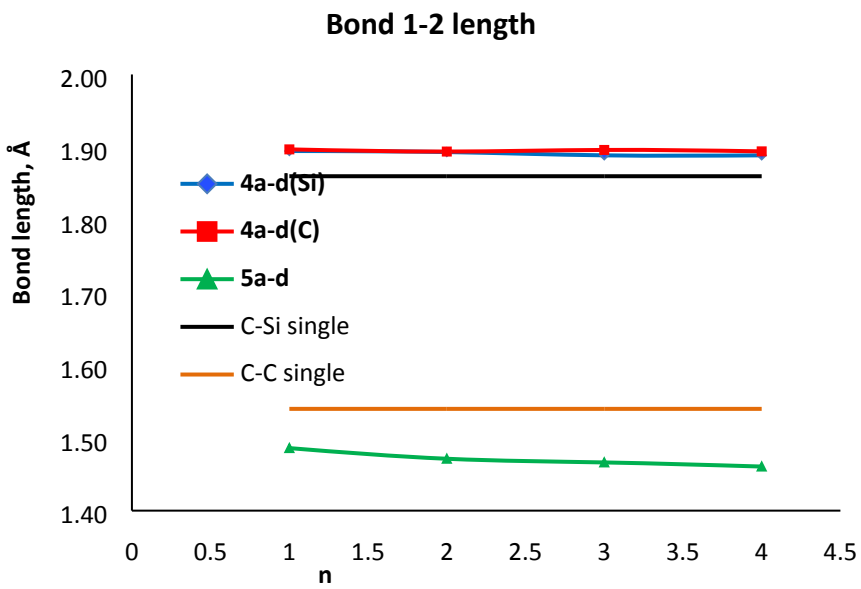
The C4-C5 bond lengths of **1a-d(Si), 1a-d(C)** and **2a-d**.

Results from B3LYP/6-311G(2d,p) calculations.



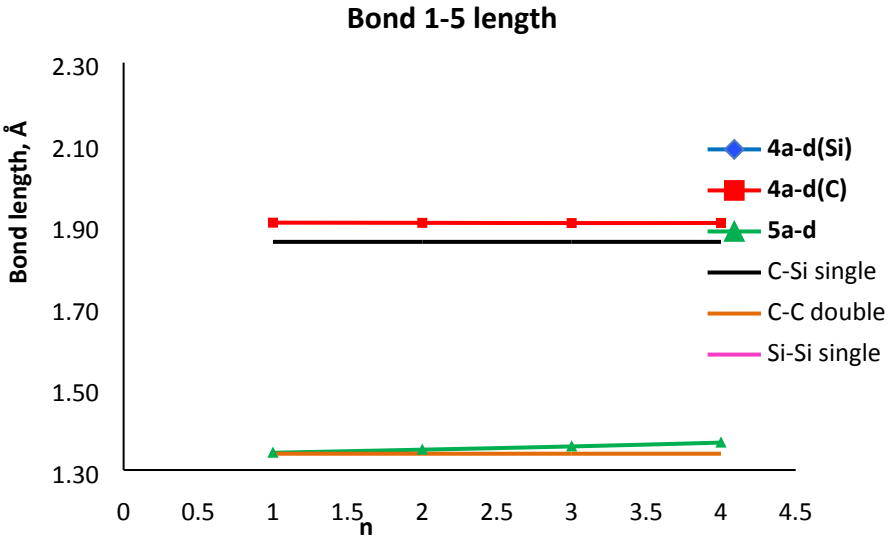
The C5-C6 bond lengths of **2a-d**.

Results from B3LYP/6-311G(2d,p) calculations.



The C1-C2 single bond lengths of **4a-d(Si), 4a-d(C)** and **5a-d**.

Results from B3LYP/6-311G(2d,p) calculations.



The C1-C5 bond lengths of **4a-d(Si), 4a-d(C)** and **5a-d**.

Results from B3LYP/6-311G(2d,p) calculations.

Comparison of few methods of TD-calculations with experimental data for linear oligosilanes

In order to test if the results obtained from B3LYP and CAM-B3LYP calculations are realistic, we have calculated excitation energies of three permethylated linear silanes Si_4Me_{10}, Si_7Me_{16} and $Si_{10}Me_{22}$ and compared the results with experimental data (Table 14). It is obvious that B3LYP shows more realistic results than CAM-B3LYP, especially for longer silane $Si_{10}Me_{22}$, while CAM-B3LYP underestimates experimental results to some extent. Thus, it can be concluded that simpler B3LYP method functions better for longer silanes than long range corrected CAM-B3LYP. Besides that, we also tested LC-ωPBE method, which showed even less realistic results than CAM-B3LYP.

Table 14. The first five excitation energies of Si_4Me_{10}, Si_7Me_{16}, $Si_{10}Me_{22}$ and experimentally observed data.[a,b]

Electronic state	**Si_4Me_{10}**				**Si_7Me_{16}**				**$Si_{10}Me_{22}$**			
	B3LYP	CAM-B3LYP	LC-ωPBE	Exp.	B3LYP	CAM-B3LYP	LC-ωPBE	Exp.	B3LYP	CAM-B3LYP	LC-ωPBE	Exp.
S_1	228.06	**212.49**	**202.71**		**268.76**	**246.78**	**233.77**		**292.02**	**263.33**	**248.12**	
S_2	**226.20**	212.37	200.38	232	249.99	226.51	210.60	273	259.68	233.53	218.62	293
S_3	212.44	187.24	177.09		232.37	212.93	200.39		248.85	224.61	209.80	

[a] Excitation energies (in nm) calculated on TD-B3LYP/6-311G(2d,p)//B3LYP /6-311G(2d,p), TD-CAM-B3LYP/6-311G(2d,p)//B3LYP/6-311G(2d,p) and TD-LC-ωPBE/6-311G(2d,p)//B3LYP/6-311G(2d,p) levels, and experimentally observed.

[b] Transitions with calculated oscillator strengths above 0.2 are marked in bold and those within the range 0.05-0.20 are underlined.

Influence of diffuse functions on TD-calculations and dispersion correction on geometrical optimizations.

For the shortest and longest oligomers among **1a-d(Si)**, **1a-d(C)**, **1a-d(C)** and **2a-d** TD-calculations including diffuse functions were performed aiming to test the influence of diffuse functions on the calculated excitation energies (Table 15). According to calculations adding of diffuse functions gives slightly lower excitation energies, but the difference is not significant for the most of the molecules tested (0.01 – 0.07 eV). The only exception is purely π-conjugated **2a**, which shows slightly more significant difference for the first 3 states (0.09 – 0.14 eV) and a drastic difference for 4^{th} and 5^{th} electronic states. The only allowed excitation among first five excitations for **2a** is the first one and for it the difference is only of 0.14 eV. At the same time, more important for comparison π-conjugated **2d** reveals the difference of only 0.01 – 0.05 eV for all five first excitations. This result confirms that including of diffuse functions to TD-calculations is not strictly necessary for calculations of 1,4-disilacyclohexa-2,5-diene based **1a-d(Si)**, **1a-d(C)** and longest purely π-conjugated oligomers among **2a-d**.

Besides that, the simplest cyclobutadisilole **3a** was tested (Table 15). Calculations demonstrate lower excitation energies again, but the difference between two methods is negligible (0.01 – 0.05 eV). Thus, for cyclobutadisilole based oligomers including of diffuse function is not absolutely required as well.

Table 15. The lowest five vertical excitation energies of **1a(Si)**, **1d(Si)**, **1a(C)**, **1d(C)**, **2a**, **2d** and **3a** calculated with TD-B3LYP including diffuse functions and without them.[a,b]

Method	Electronic state	**1a(Si)**	**1d(Si)**	**1a(C)**	**1d(C)**	**2a**	**2d**	**3a**
TD-B3LYP/ 6-311G+(2d,p)	S_1	3.84	**3.40**	4.87	**4.43**	**4.14**	**1.13**	3.12
	S_2	**3.90**	3.57	5.03	4.51	4.48	1.65	4.05
	S_3	3.98	3.65	**5.12**	4.63	4.74	2.53	<u>4.13</u>
	S_4	3.99	3.66	5.18	4.72	5.12	2.61	**4.48**
	S_5	4.25	3.70	5.49	4.76	5.40	**3.04**	4.92
TD-B3LYP/ 6-311G(2d,p)	S_1	3.88	**3.41**	4.91	**4.46**	**4.28**	**1.14**	3.13
	S_2	**3.93**	3.61	5.07	4.54	4.59	1.66	4.07
	S_3	4.03	3.67	**5.17**	4.66	4.83	2.55	<u>4.14</u>
	S_4	4.04	3.71	5.22	4.76	5.80	2.65	**4.52**
	S_5	4.28	3.75	5.56	4.79	5.98	**3.09**	4.94

[a] Excitation energies (in eV) calculated at TD-B3LYP/6-311G+(2d,p)//B3LYP/6-311G(2d,p) and TD-B3LYP/6-311G+(2d,p)//B3LYP/6-311G(2d,p)level.

[b] Transitions with calculated oscillator strengths above 0.2 are marked in bold and those within the range 0.05-0.20 are underlined.

Adding diffuse functions to CAM-B3LYP shows similar results as B3LYP does: excitation energies are slightly lower with diffuse functions added, the difference between TD-CAM-B3LYP/6-311G+(2d,p) and TD-CAM-B3LYP/6-311G(2d,p) is in the range of 0.02 – 0.07 eV (Table 16). Therefore, for CAM-B3LYP including of diffuse functions is not compulsory either.

Table 16. The lowest five vertical excitation energies of **1d(Si)**, **1d(C)** and **2d** calculated with TD-CAM-B3LYP including diffuse functions and without them.[a,b]

Method	Electronic state	**1d(Si)**	**1d(C)**	**2d**
TD-CAM-B3LYP/ 6-311G+(2d,p)	S_1	4.01	5.24	**1.02**
	S_2	4.08	5.30	1.74
	S_3	**4.09**	**5.31**	2.73
	S_4	**4.12**	5.32	2.89
	S_5	4.31	5.34	**3.40**
TD-CAM-B3LYP/ 6-311G(2d,p)	S_1	4.06	5.27	**1.04**
	S_2	**4.11**	5.34	1.76
	S_3	4.13	**5.35**	2.78
	S_4	4.17	5.35	2.92
	S_5	4.36	5.37	3.47

[a] Excitation energies (in eV) calculated at TD-B3LYP/6-311G+(2d,p)//B3LYP/6-311G(2d,p) and TD-B3LYP/6-311G(2d,p)//B3LYP/6-311G(2d,p) levels.

[b] Transitions with calculated oscillator strengths above 0.2 are marked in bold and those within the range 0.05-0.20 are underlined.

Optimized structures **1d(Si)** and **2d(Si)** with dispersion correction and diffuse functions added to B3LYP calculations were examined (Table 17). Obviously, the only significant difference between B3LYP/6-311G(2d,p) and B3LYP-D3/6-311+G(2d,p) is observed in **2d(Si)** for the dihedral angle in 4-Si ring (~5 °), while all other geometrical characteristics (SiC, C=C bond lengths and plane angle Si-Si-Si) have negligible differences or no differences at all.

Table 17 Geometrical characteristics of **1a(Si)** and **2a (Si)** optimized with dispersion correction and diffuse functions and without them.

Method		**1d(Si)**	**2a(Si)**
B3LYP-D3/ 6-311+G(2d,p)	Si–C bond length, Å	1.873	1.873
	C=C bond length, Å	1.345	1.344
	Si–Si–Si angle, °	87.67	87.51
	Si–Si–Si–Si dihedral angle, °	157.45	146.26
B3LYP/ 6-311G(2d,p)	Si–C bond length, Å	1.875	1.875
	C=C bond length, Å	1.345	1.344
	Si–Si–Si angle, °	87.79	87.51
	Si–Si–Si–Si dihedral angle, °	158.88	151.54

[a] Geometrical characteristics calculated at B3LYP-D3/6-311G+(2d,p) and B3LYP/6-311G(2d,p) levels.

Cartesian coordinates and absolute energies

1a(Si):

B3LYP/6-311G(2d,p): -4427.91988 a.u.

Point group: C_1

Cartesian coordinates:

C	0.88659000	1.41142700	0.20004900
C	-0.44451300	1.60019100	0.22007300
C	-0.88656600	-1.41197500	0.20000500
C	0.44453500	-1.60074000	0.21993200
H	1.52156600	2.29792800	0.22259500
H	-0.80805500	2.62895800	0.25494100
H	-1.52154400	-2.29847500	0.22249600
H	0.80808300	-2.62950900	0.25468300
Si	1.74807100	-0.25436500	0.16221000
Si	-1.74804800	0.25381500	0.16226800
Si	-3.55396800	0.40111700	1.73482000
Si	-3.37447500	0.49533200	-1.58698100
Si	3.37449300	-0.49547900	-1.58708300
Si	3.55403600	-0.40147500	1.73474000
Si	-5.13722900	0.01001500	-0.02992600
Si	-5.82328800	-2.26819700	-0.19946000
Si	-7.03333700	1.45540200	-0.01271000
Si	5.13715500	-0.00992300	-0.03004800
Si	5.82296900	2.26838600	-0.19939900
Si	7.03351600	-1.45501500	-0.01270400
C	7.97225600	-1.27168500	1.62195200
H	8.84903000	-1.92681900	1.62923800
H	8.31888200	-0.24883600	1.78248600
H	7.34542100	-1.54711600	2.47337600
C	6.52469600	-3.26963800	-0.18208100
H	5.84521300	-3.57597300	0.61592100
H	6.03279600	-3.46412900	-1.13683300
H	7.41125200	-3.90913200	-0.12705900
C	8.22313800	-1.05591900	-1.43117400
H	8.64474400	-0.05283800	-1.33742000
H	9.05557900	-1.76646300	-1.43330300
H	7.72834600	-1.12038400	-2.40310000
C	7.10971800	2.69432300	1.12292600
H	6.73239300	2.50412700	2.13021800
H	8.02826600	2.11723200	0.99540400
H	7.37445600	3.75451600	1.06054100
C	4.37221600	3.46860100	0.00889300
H	3.60073800	3.30934900	-0.74737300
H	3.90380200	3.38206800	0.99156400
H	4.72979900	4.49768200	-0.09677500
C	6.58657600	2.59811600	-1.90054500
H	7.45899000	1.96854900	-2.08715100
H	5.86689600	2.41553300	-2.70169400
H	6.90727700	3.64222200	-1.97185300
C	3.18518000	0.64747900	-3.09044400
H	2.29284900	0.37131300	-3.65917600

H	3.08238400	1.69394800	-2.79909600	H	-4.24494100	2.43811700	-2.91297300
H	4.04686500	0.56274300	-3.75802600	H	-3.48068800	3.01411800	-1.42934200
C	3.53441100	0.82896000	3.17799400	H	-2.48221500	2.49128900	-2.78850000
H	2.69289300	0.61944600	3.84392400	C	-6.52431500	3.27004300	-0.18137100
H	4.45399200	0.75386100	3.76476200	H	-5.84510500	3.57609200	0.61697400
H	3.43772200	1.85874800	2.83133000	H	-6.03210100	3.46487900	-1.13588900
C	3.68495700	-2.14775400	2.47643000	H	-7.41089300	3.90951700	-0.12641300
H	4.61674600	-2.26774400	3.03542200	C	-7.97268200	1.27187100	1.62156700
H	2.85577500	-2.32428800	3.16722400	H	-8.84933100	1.92717200	1.62865300
H	3.65061300	-2.92535400	1.71109900	H	-8.31953800	0.24905400	1.78181100
C	3.40216400	-2.28197600	-2.23541800	H	-7.34608400	1.54704500	2.47325000
H	4.24560400	-2.43762400	-2.91346500	C	-8.22244000	1.05678300	-1.43175500
H	3.48144000	-3.01430200	-1.43005100	H	-8.64432800	0.05379300	-1.33831700
H	2.48289100	-2.49143000	-2.78914600	H	-9.05471900	1.76752100	-1.43417300
C	-3.68458300	2.14735700	2.47665600	H	-7.72721300	1.12125600	-2.40345700
H	-4.61632100	2.26739800	3.03572300	C	-4.37254800	-3.46851300	0.00833900
H	-2.85533000	2.32370900	3.16741400	H	-3.60137700	-3.30927700	-0.74824800
H	-3.65019800	2.92503800	1.71140800	H	-3.90371100	-3.38207000	0.99081200
C	-3.53457800	-0.82936900	3.17803500	H	-4.73026000	-4.49755900	-0.09724000
H	-2.69291600	-0.62011200	3.84386700	C	-7.10981200	-2.69415200	1.12308100
H	-4.45406600	-0.75394900	3.76490900	H	-6.73230300	-2.50399900	2.13031100
H	-3.43826900	-1.85919800	2.83139000	H	-8.02834100	-2.11698900	0.99573000
C	-3.18546100	-0.64737600	-3.09056200	H	-7.37464200	-3.75432200	1.06072200
H	-2.29324100	-0.37111100	-3.65942000	C	-6.58718700	-2.59774900	-1.90050400
H	-3.08259800	-1.69389200	-2.79940200	H	-7.45960700	-1.96815300	-2.08697700
H	-4.04727400	-0.56254100	-3.75796500	H	-5.86758800	-2.41513700	-2.70171900
C	-3.40160500	2.28198800	-2.23490800	H	-6.90792000	-3.64184400	-1.97185000

1b(Si):

B3LYP/6-311G(2d,p): -5900.61953 a.u.

Point group: C_1

Cartesian coordinates:

C	3.19705500	-2.15345800	-0.03402100
C	4.47245800	-1.72795300	-0.01768600
C	3.50948100	1.09810800	0.59117300
C	2.23387100	0.67412500	0.56985700
H	3.01856700	-3.21748100	-0.19976100
H	5.25478500	-2.47289700	-0.16894000
H	3.68955100	2.14935600	0.82339100
H	1.45377000	1.40720800	0.78570900
Si	1.68104500	-1.07780200	0.19371200
Si	5.02347900	0.04628700	0.24270100
Si	-0.02235200	-1.83895100	1.70341900
Si	0.02539000	-1.13916400	-1.53967300
C	-2.22939100	0.68637200	0.51947500
C	-3.19344200	-2.12936000	-0.13572700
C	-3.50399800	1.11373400	0.53812400
H	-1.44840100	1.41709100	0.74020300
C	-4.46709600	-1.69841600	-0.13212600
H	-3.01619000	-3.18834900	-0.33226400
H	-3.68162500	2.16476000	0.77342200
H	-5.24844100	-2.43467000	-0.32497300
Si	-5.01962400	0.06704600	0.18171600
Si	-1.67778500	-1.06664900	0.14597200
Si	-6.83461100	0.21955500	1.74492900
Si	-6.50296000	0.93079800	-1.49512500
Si	6.86191500	0.29038700	1.76215600
Si	6.46591200	0.86204200	-1.49530700
Si	8.37878600	0.51482800	-0.08706300
Si	9.95419900	2.29327700	0.11577800
Si	9.49210000	-1.52658900	-0.62277500
Si	-8.38591700	0.50641800	-0.06931600
Si	-9.94819600	2.29885400	0.13629000
Si	-9.49562100	-1.53630400	-0.60599400
C	10.22478700	-1.44903800	-2.36736000
H	10.95502000	-0.64385500	-2.47104000
H	10.73172500	-2.39044900	-2.60171500
H	9.44847200	-1.29332600	-3.11982600
C	10.89883500	-1.86767000	0.59725800
H	11.67140200	-1.09723700	0.54794100
H	10.53789400	-1.91321900	1.62714700
H	11.37210900	-2.82709600	0.36631100
C	11.03346800	2.03029500	1.64933000
H	11.58815700	1.09106700	1.60232700
H	11.75976100	2.84359600	1.74370900
H	10.43166700	2.01516400	2.56099700
C	9.09536300	3.96972500	0.29957200
H	8.48957200	4.21468900	-0.57490800
H	8.44707800	3.99791500	1.17779500
H	9.84617000	4.75762900	0.41623200
C	11.08377400	2.38716400	-1.40093400

H	11.77156000	3.23327600	-1.30676600	C	0.03103400	-2.81463600	-2.43923900
H	11.68500900	1.48262100	-1.51399200	H	0.92346600	-2.91119200	-3.06315400
H	10.51170600	2.52451200	-2.32150400	H	0.01869500	-3.65677000	-1.74415400
C	8.31513200	-3.00969900	-0.57141600	H	-0.84465700	-2.90488000	-3.08734700
H	7.89161800	-3.16325800	0.42326900	C	-0.02748900	-3.73548200	1.84255700
H	7.48811300	-2.89690000	-1.27559900	H	-0.92086600	-4.07944600	2.37039100
H	8.85759400	-3.92057700	-0.84348300	H	-0.01157800	-4.22050400	0.86442900
C	7.18178900	-1.11845300	2.99183200	H	0.84672300	-4.08162700	2.40026700
H	8.11659700	-0.95251600	3.53441200	C	-0.04455600	-1.09607300	3.44661100
H	6.37315300	-1.17255400	3.72584900	H	0.83373800	-1.41563300	4.01376200
H	7.24782900	-2.08739700	2.49507200	H	-0.04517100	-0.00518900	3.41348500
C	6.67929300	1.89243000	2.77174700	H	-0.93556300	-1.41710700	3.99270900
H	5.85784000	1.79131600	3.48646900	C	-6.46914700	0.08617300	-3.19422800
H	7.58950200	2.10818800	3.33754500	H	-7.27692300	0.45743300	-3.83077100
H	6.46500600	2.75622100	2.13953800	H	-5.52183200	0.29536100	-3.69885700
C	6.11769300	2.69044400	-1.87985600	H	-6.57139000	-0.99708200	-3.11470400
H	6.86257500	3.09176700	-2.57243600	C	-7.09415400	-1.28235200	2.87595000
H	5.13469600	2.79253400	-2.34758800	H	-6.26698600	-1.36359500	3.58654300
H	6.12650400	3.31111200	-0.98221000	H	-8.02025900	-1.18405200	3.44887100
C	6.40718900	-0.08110700	-3.14229400	H	-7.14277300	-2.21641500	2.31424000
H	5.44167600	0.08026100	-3.62990400	C	-6.67462600	1.74720400	2.86474400
H	7.18817000	0.26930000	-3.82253000	H	-7.58482000	1.89776700	3.45150600
H	6.53388500	-1.15645300	-3.00648100	H	-5.84434000	1.61316700	3.56356300
C	0.04544400	0.24685900	-2.83226100	H	-6.48834400	2.65983400	2.29614400
H	0.93331700	0.17221800	-3.46581100	C	-6.19027300	2.78491800	-1.77546500
H	-0.83526700	0.18485300	-3.47710000	H	-5.23003600	2.93048800	-2.27770300
H	0.04924800	1.23131300	-2.36121200	H	-6.96884300	3.22341400	-2.40536900

H -6.16346700 3.34397100 -0.83831900
C -11.31073200 1.87474600 1.38083500
H -10.89704500 1.62587800 2.36083200
H -11.98110400 2.73029000 1.50885600
H -11.91394900 1.02761500 1.04831800
C -10.76107300 2.66909100 -1.53374000
H -11.28482900 1.79933000 -1.93488900
H -11.49058500 3.47784200 -1.42545400
H -10.02430000 2.98463600 -2.27628300
C -9.11087600 3.89029600 0.72740600
H -8.66784100 3.77329300 1.71816700
H -8.32540100 4.21568600 0.04243800
H -9.85183800 4.69381900 0.78733700
C -8.26877000 -2.95476300 -0.87068700
H -7.57413000 -2.75280900 -1.68867100
H -7.68154800 -3.15416300 0.02821100
H -8.81347000 -3.87126500 -1.11830000
C -10.51274700 -1.35539800 -2.19265100
H -11.31232500 -0.62002800 -2.08066200
H -9.89040600 -1.04627400 -3.03551300
H -10.97654300 -2.31196300 -2.45294800
C -10.65731100 -2.05295400 0.79635000
H -10.10907200 -2.21459600 1.72714700
H -11.42507200 -1.30148000 0.98949000
H -11.16324900 -2.98918000 0.54045100

1c(Si):

B3LYP/6-311G(2d,p): -7373.31932 a.u.

Point group: C_1

Cartesian coordinates:

C 0.00593100 1.78439400 0.05145500
C -1.22050500 1.23458400 0.01493300
C 0.02902700 -1.54450100 -0.11535600
C 1.25531200 -0.99529900 -0.06862200
H 0.07444100 2.87214500 0.10942600
H -2.07698700 1.91136100 0.04568500
H -0.03966100 -2.63282500 -0.16155500
H 2.11160400 -1.67285600 -0.07989200
Si 1.62482100 0.84235100 0.01169300
Si -1.58972600 -0.60141800 -0.09953700
Si -3.25933600 -1.30146500 1.47475100
Si 3.26149400 1.35160300 1.68981500
Si 3.25980700 1.48431900 -1.62195100
Si -3.18382100 -1.06199800 -1.83245900
C -6.37092400 -2.07763300 -0.32921500
C -5.59727900 0.85854100 -0.06702200
C -7.67230200 -1.74067500 -0.29593600
H -6.12339400 -3.13398300 -0.44906000
C -6.89837200 1.19401700 -0.02535400
H -4.86554600 1.66753000 -0.01445400
H -8.40396000 -2.54409400 -0.39107500
H -7.14519200 2.25403900 0.05825400
C 5.55128900 -0.69742100 -0.02918400

C	6.45453800	2.21173800	0.05140500	H	-15.19608100	0.52555800	1.46190300
C	6.83554600	-1.09433200	-0.02475100	H	-14.14402200	1.31199700	2.64063900
H	4.78377400	-1.47384000	-0.05679600	C	-14.37794800	2.03824300	-1.32057800
C	7.73936900	1.81443500	0.04318000	H	-14.88622300	1.11305300	-1.59987100
H	6.25643700	3.28484600	0.07826300	H	-15.13846200	2.81920500	-1.22149200
H	7.03352600	-2.16752400	-0.04898200	H	-13.72059300	2.31861900	-2.14697100
H	8.50582000	2.59048200	0.06517000	C	-13.99971800	-2.05163200	-1.45756000
Si	8.33283700	0.03488900	0.01069700	H	-14.83678600	-1.37395000	-1.27504900
Si	-8.34324500	-0.00061000	-0.09373300	H	-13.55578000	-1.78234000	-2.41856000
Si	4.96088700	1.08191200	0.01789100	H	-14.40762900	-3.06309600	-1.55007100
Si	-4.92940300	-0.88902100	-0.19632900	C	-11.43533000	-3.33354400	-0.39526000
Si	-9.94141200	0.20478200	1.68676300	H	-10.90218400	-3.16332800	-1.33287700
Si	-10.10229600	0.56714600	-1.62188600	H	-10.69526000	-3.39983800	0.40538900
Si	9.98435400	-0.45941500	1.67784900	H	-11.92936000	-4.30750000	-0.46821900
Si	9.99953500	-0.42406200	-1.65437500	C	-13.60247100	-2.44190900	1.55994300
Si	11.71979300	-0.35118500	0.02051000	H	-12.90630300	-2.45406300	2.40126600
Si	12.83570800	1.75450600	0.00471100	H	-14.40372400	-1.74061600	1.80099400
Si	13.27360300	-2.15524500	0.08876000	H	-14.04549700	-3.43954200	1.47939900
Si	-11.73850100	0.17654100	0.09292800	C	-10.23838700	-0.44604900	-3.21984800
Si	-13.41366400	1.86053000	0.29994500	H	-9.37558000	-0.25529600	-3.86389900
Si	-12.72691500	-1.98910600	-0.05620000	H	-10.27664300	-1.51823600	-3.02209200
C	-12.65316000	3.54620600	0.70061400	H	-11.13910000	-0.17255400	-3.77620100
H	-12.11724400	3.53192700	1.65123100	C	-9.98469800	2.39935700	-2.11638500
H	-11.95636600	3.87166000	-0.07459300	H	-9.11700900	2.55991700	-2.76204900
H	-13.44350700	4.29984500	0.77384100	H	-10.87581300	2.71366000	-2.66625500
C	-14.64348000	1.44229100	1.67784400	H	-9.87913300	3.05269700	-1.24834000
H	-15.37260300	2.25115900	1.78716100	C	-9.73675400	1.85669000	2.60430900

H	-10.55132800	2.01222100	3.31675700	C	3.33098100	0.49979700	-3.23944600
H	-8.79729100	1.85543600	3.16379500	H	4.20444600	0.79006900	-3.82941700
H	-9.71871300	2.71009800	1.92416700	H	3.39296300	-0.57341500	-3.05114000
C	-9.93051300	-1.17199400	2.99347100	H	2.43872500	0.68464800	-3.84366900
H	-9.01560500	-1.11822400	3.58989400	C	3.35623000	0.21922000	3.20624100
H	-10.78060300	-1.07025300	3.67365100	H	2.44868000	0.30240400	3.80996000
H	-9.97557000	-2.16453100	2.54265400	H	3.47345100	-0.82582500	2.91428700
C	-3.24900700	0.12772100	-3.30579700	H	4.20776300	0.48968400	3.83644500
H	-4.09431200	-0.11083800	-3.95686700	C	3.10808000	3.15323900	2.27635400
H	-3.36085600	1.16196500	-2.97573500	H	3.97089400	3.43434000	2.88579900
H	-2.33397300	0.05959900	-3.90005800	H	3.04620900	3.85491500	1.44217400
C	-3.00449400	-2.83977800	-2.48235600	H	2.20939800	3.28033900	2.88568700
H	-2.08921100	-2.93891600	-3.07186200	C	10.12867800	0.81311000	-3.08841400
H	-2.95904700	-3.57110300	-1.67273000	H	9.22794500	0.76265600	-3.70647000
H	-3.84869400	-3.10418100	-3.12453200	H	10.23371700	1.84088500	-2.73803100
C	-3.38953300	-0.35130600	3.10890600	H	10.98596500	0.58441900	-3.72744100
H	-4.27482300	-0.66415500	3.66887100	C	9.73698600	-2.14382200	-2.42183100
H	-2.51148900	-0.53604900	3.73360800	H	10.57788100	-2.41823500	-3.06456000
H	-3.46071100	0.72440900	2.93906900	H	9.62502200	-2.92266900	-1.66550000
C	-3.10961300	-3.15858700	1.85319600	H	8.83271800	-2.14259100	-3.03669000
H	-3.98269100	-3.50393300	2.41303200	C	10.10233800	0.72766400	3.15387700
H	-3.03884500	-3.75955400	0.94419600	H	9.20045200	0.65448700	3.76787400
H	-2.22058800	-3.35930800	2.45671400	H	10.95903900	0.47893800	3.78633400
C	3.13569800	3.33557100	-2.03802100	H	10.20685900	1.76667200	2.83820300
H	2.23419300	3.53978800	-2.62155800	C	9.72821100	-2.20854600	2.37958100
H	3.10167600	3.95927600	-1.14237400	H	10.57556700	-2.51415100	2.99905600
H	3.99895900	3.65040400	-2.63019500	H	8.83139000	-2.23116800	3.00482700

H 9.60226700 -2.95384100 1.59191400
C 13.84141400 1.96509200 -1.58586900
H 14.60209600 1.18957100 -1.69497200
H 13.20193300 1.93093800 -2.47083500
H 14.35126600 2.93365900 -1.58087900
C 14.01313800 1.91218300 1.47916800
H 14.47116200 2.90617800 1.48850300
H 13.48998600 1.77742000 2.42841200
H 14.82011500 1.17731000 1.43535800
C 11.61222000 3.19840300 0.09121700
H 10.92537000 3.20102700 -0.75778900
H 11.01636500 3.17832300 1.00584000
H 12.15958600 4.14611600 0.07472200
C 14.57919400 -2.00591500 -1.27503800
H 15.20654500 -1.12189300 -1.14160200
H 15.23526500 -2.88195000 -1.26346600
H 14.12373500 -1.94520900 -2.26619400
C 12.40180500 -3.82082800 -0.13181600
H 11.65663300 -3.99474900 0.64701300
H 11.90111700 -3.89103100 -1.09921200
H 13.13553000 -4.63112800 -0.07605700
C 14.16091100 -2.18907600 1.76192200
H 14.85728400 -3.03251300 1.80269900
H 14.73350400 -1.27644400 1.94019300
H 13.45299100 -2.30319200 2.58633400

1d(Si):

B3LYP/6-311G(2d,p): -8846.01910 a.u.

Point group: C_1

Cartesian coordinates:

C 3.57816600 -2.40849600 -0.75095200
C 2.29067800 -2.10929000 -0.50350900
C 3.16793500 0.34022900 1.08636800
C 4.45475000 0.04629400 0.83153600
H 3.78877800 -3.30613000 -1.33514400
H 1.53140300 -2.78472300 -0.90340300
H 2.95858300 1.21884300 1.69901600
H 5.21459700 0.70609700 1.25565400
Si 5.05888300 -1.40621800 -0.19153800
Si 1.68506800 -0.62472700 0.47147000
Si 0.00049600 0.61942100 -0.69880200
Si 6.62912400 -0.69485500 -1.85772300
Si 6.88060000 -2.52358700 0.89635000
Si -0.00138200 -1.20304600 2.07828800
C -3.16919800 0.34035700 1.08249400
C -2.29030700 -2.10900500 -0.50671800
C -4.45574300 0.04642900 0.82630300
H -2.96048100 1.21895900 1.69537900
C -3.57753300 -2.40817500 -0.75558000
H -1.53060700 -2.78431100 -0.90602200
H -5.21602400 0.70623000 1.24964800
H -3.78752700 -3.30564800 -1.34024500
C 8.78415000 0.48522200 0.70638700

C	9.98809300	-1.79917700	-0.91188500	Si	-14.89267600	1.20267600	0.08081900
C	10.01046200	1.01271700	0.86536300	Si	-16.15232400	-0.41852300	-1.13121700
H	7.94648400	1.00319700	1.17817900	Si	-16.28645600	2.99669300	0.80534700
C	11.21463100	-1.27223000	-0.75078100	Si	14.89281300	1.20255000	0.07757600
H	9.90758300	-2.73436500	-1.46920200	Si	16.28721500	2.99790400	0.79782700
H	10.09568400	1.92588000	1.45742000	Si	16.15114900	-0.42002000	-1.13402800
H	12.05644800	-1.81243700	-1.18516300	C	0.00011600	2.44234700	-0.15670300
Si	11.60437300	0.32253300	0.15623000	H	0.88466500	2.95663400	-0.54166000
Si	-5.05884200	-1.40614200	-0.19731200	H	-0.88395000	2.95656900	-0.54285000
Si	8.38864600	-1.06595600	-0.27006600	H	-0.00061600	2.55111000	0.92996700
Si	-1.68570400	-0.62464500	0.46920400	C	-0.00246800	0.01487200	3.53849600
Si	12.92190700	1.86733400	-1.12187200	H	-0.88712100	-0.13530100	4.16282700
Si	13.44761900	0.15941900	1.68766700	H	0.88137400	-0.13513300	4.16401400
Si	-6.88116600	-2.52353500	0.88953700	H	-0.00235400	1.05532200	3.20641600
Si	-6.62814300	-0.69481500	-1.86436100	C	-0.00171200	-2.97305700	2.75501600
C	-9.98798200	-1.79775200	-0.91958900	H	-0.00119000	-3.70855500	1.94867300
C	-8.78331900	0.48577000	0.69940000	H	0.88279300	-3.14991000	3.37268300
C	-11.21448100	-1.27099800	-0.75753100	H	-0.88691300	-3.15002400	3.37165100
H	-9.90762900	-2.73228600	-1.47802500	C	0.00178400	0.54870400	-2.59221400
C	-10.00960500	1.01298900	0.85945200	H	0.00210200	-0.48085600	-2.95394400
H	-7.94535600	1.00391200	1.17047700	H	-0.88254200	1.04787100	-2.99712600
H	-12.05643300	-1.81069600	-1.19228600	H	0.88662200	1.04796600	-2.99588700
H	-10.09451100	1.92611300	1.45161400	C	-6.91578000	-2.51044600	2.78402300
Si	-8.38833000	-1.06533700	-0.27734600	H	-6.09679700	-3.11105600	3.18873500
Si	-13.44443300	0.15684400	1.68628800	H	-6.81675200	-1.49748500	3.17780400
Si	-12.92418700	1.86905000	-1.12163800	H	-7.85594800	-2.92629600	3.15599900
Si	-11.60399900	0.32254200	0.15167500	C	-7.06608600	-4.31779400	0.28727100

H	-6.25458500	-4.93860800	0.67590200	C	17.40421800	-1.28077600	-0.00488000
H	-8.01109100	-4.74236000	0.63615900	H	18.11539700	-0.57486100	0.42846000
H	-7.04978500	-4.39267400	-0.80195000	H	16.90878900	-1.80197000	0.81739800
C	-6.73369900	-1.93042200	-3.30530800	H	17.97432000	-2.02164700	-0.57425100
H	-7.58072700	-1.68960400	-3.95309100	C	17.09586400	0.39051500	-2.56081400
H	-5.82465700	-1.89261800	-3.91120700	H	17.63082100	-0.37000300	-3.13818900
H	-6.86205000	-2.95794100	-2.95932000	H	16.42287200	0.91516400	-3.24258300
C	-6.43220800	1.05226500	-2.57216200	H	17.83311100	1.11025600	-2.19873400
H	-6.36190000	1.79741400	-1.77790200	C	15.04200400	-1.76609000	-1.87229100
H	-5.52819900	1.12329600	-3.18294500	H	14.51848400	-2.33074900	-1.09773300
H	-7.28661100	1.31115800	-3.20324600	H	14.29443100	-1.35401800	-2.55297600
C	6.91436500	-2.51038000	2.79085000	H	15.65163000	-2.47555100	-2.44051000
H	6.81552100	-1.49735500	3.18452000	C	12.92385400	1.65555300	-3.00785100
H	6.09500300	-3.11067500	3.19525800	H	11.93141400	1.87272200	-3.41230200
H	7.85423600	-2.92651800	3.16325000	H	13.63364400	2.34390700	-3.47491400
C	7.06540500	-4.31791500	0.29422400	H	13.19102200	0.64116800	-3.30756800
H	8.01014800	-4.74272400	0.64352500	C	12.38911600	3.65690100	-0.75684900
H	6.25357400	-4.93851900	0.68249900	H	13.09906700	4.37329400	-1.17891600
H	7.04954800	-4.39279800	-0.79500500	H	11.41021500	3.85222500	-1.20343400
C	6.43384900	1.05245100	-2.56514200	H	12.30932600	3.85537900	0.31378100
H	7.28849200	1.31126200	-3.19593600	C	16.82295800	4.03333700	-0.69446100
H	5.53001900	1.12388300	-3.17613900	H	17.45263500	4.86759200	-0.36964900
H	6.36354800	1.79742500	-1.77071600	H	17.39530200	3.44503700	-1.41466400
C	6.73501400	-1.93015100	-3.29891500	H	15.96062400	4.45247700	-1.21809000
H	5.82623900	-1.89201200	-3.90519300	C	15.37489400	4.14384900	1.99623800
H	7.58237700	-1.68940200	-3.94628200	H	14.47093100	4.56118500	1.54809100
H	6.86298300	-2.95777400	-2.95308200	H	15.08813300	3.62703500	2.91405700

H	16.02461600	4.98000800	2.27330400	H	-13.10118200	4.37514500	-1.17401900
C	17.84558300	2.37100300	1.67285600	H	-12.30839900	3.85453200	0.31610800
H	18.48109900	1.78996600	1.00105200	C	-16.82426200	4.03390300	-0.68498000
H	18.43597300	3.21793700	2.03628500	H	-15.96278200	4.45515600	-1.20832400
H	17.60412500	1.74103300	2.53211000	H	-17.39612500	3.44601500	-1.40589900
C	13.14610700	1.22314900	3.23325800	H	-17.45493700	4.86676000	-0.35850900
H	12.34568600	0.78891700	3.83853100	C	-17.84374100	2.36835900	1.68128000
H	14.04546000	1.27233700	3.85294500	H	-17.60134200	1.73667200	2.53900500
H	12.85842200	2.24504500	2.98058600	H	-18.43349600	3.21470000	2.04711800
C	13.92416000	-1.57863000	2.28195700	H	-18.48025400	1.78877500	1.00916500
H	14.86053800	-1.55114800	2.84587300	C	-15.37322400	4.14154600	2.00415200
H	13.14745300	-1.97781900	2.94002800	H	-15.08633200	3.62418600	2.92163500
H	14.04979800	-2.27744800	1.45345800	H	-14.46928600	4.55890900	1.55597300
C	-13.92007100	-1.58205500	2.27883800	H	-16.02263100	4.97773000	2.28189900
H	-13.14219000	-1.98230000	2.93488000	C	-17.09835100	0.39345300	-2.55632000
H	-14.85536300	-1.55521600	2.84459000	H	-17.63341900	-0.36655000	-3.13427200
H	-14.04741800	-2.27969700	1.44961600	H	-17.83560800	1.11250600	-2.19289000
C	-13.13970100	1.21797600	3.23301700	H	-16.42596300	0.91915200	-3.23787600
H	-14.03766900	1.26590100	3.85479500	C	-17.40430400	-1.28061000	-0.00187100
H	-12.33783100	0.78288600	3.83574900	H	-18.11505100	-0.57518900	0.43297500
H	-12.85275400	2.24034300	2.98142500	H	-17.97495800	-2.02079400	-0.57158100
C	-12.93042400	1.66046900	-3.00796400	H	-16.90812600	-1.80279400	0.81933000
H	-13.64098600	2.35000500	-3.47211100	C	-15.04372900	-1.76363200	-1.87204400
H	-11.93883000	1.87788300	-3.41434700	H	-14.29730200	-1.35070700	-2.55347700
H	-13.19882100	0.64675400	-3.30885700	H	-14.51885500	-2.32866900	-1.09869200
C	-12.39041300	3.65794700	-0.75470700	H	-15.65387300	-2.47289000	-2.43995800
H	-11.41242900	3.85398400	-1.20297400				

2a:

B3LYP/6-311G(2d,p): -309.70512 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	0.00000000	0.00000000	2.79002300
H	0.00000000	0.92473100	3.35352000
H	0.00000000	-0.92473100	3.35352000
C	0.00000000	1.23735600	0.67125800
H	0.00000000	2.17305000	1.21969800
C	0.00000000	-1.23735600	0.67125800
H	0.00000000	-2.17305000	1.21969800
C	0.00000000	-1.23735600	-0.67125800
H	0.00000000	-2.17305000	-1.21969800
C	0.00000000	1.23735600	-0.67125800
H	0.00000000	2.17305000	-1.21969800
C	0.00000000	0.00000000	-2.79002300
H	0.00000000	0.92473100	-3.35352000
H	0.00000000	-0.92473100	-3.35352000
C	0.00000000	0.00000000	-1.44216900
C	0.00000000	0.00000000	1.44216900

2b:

B3LYP/6-311G(2d,p): -616.97162 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	0.00000000	0.00000000	6.20144400
H	0.00000000	0.92469800	6.76446400
H	0.00000000	-0.92469800	6.76446400
C	0.00000000	1.23206200	4.07955600
H	0.00000000	2.17013600	4.62324400
C	0.00000000	-1.23206200	4.07955600
H	0.00000000	-2.17013600	4.62324400
C	0.00000000	-1.23240900	2.72914300
H	0.00000000	-2.16444700	2.17751300
C	0.00000000	1.23240900	2.72914300
H	0.00000000	2.16444700	2.17751300
C	0.00000000	0.00000000	0.61914700
C	0.00000000	0.00000000	-0.61914700
C	0.00000000	1.23240900	-2.72914300
H	0.00000000	2.16444700	-2.17751300
C	0.00000000	-1.23240900	-2.72914300
H	0.00000000	-2.16444700	-2.17751300
C	0.00000000	-1.23206200	-4.07955600
H	0.00000000	-2.17013600	-4.62324400
C	0.00000000	1.23206200	-4.07955600
H	0.00000000	2.17013600	-4.62324400
C	0.00000000	0.00000000	-6.20144400
H	0.00000000	-0.92469800	-6.76446400
H	0.00000000	0.92469800	-6.76446400
C	0.00000000	0.00000000	-4.84645700
C	0.00000000	0.00000000	-1.97834400
C	0.00000000	0.00000000	1.97834400
C	0.00000000	0.00000000	4.84645700

2c:

B3LYP/6-311G(2d,p): -924.24653 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	0.00000000	0.00000000	9.62463400
H	0.00000000	0.92481500	10.18714200
H	0.00000000	-0.92481500	10.18714200
C	0.00000000	1.22928500	7.50064500
H	0.00000000	2.16828400	8.04254200
C	0.00000000	-1.22928500	7.50064500
H	0.00000000	-2.16828400	8.04254200
C	0.00000000	-1.22789600	6.14595900
H	0.00000000	-2.16041100	5.59512200
C	0.00000000	1.22789600	6.14595900
H	0.00000000	2.16041100	5.59512200
C	0.00000000	0.00000000	4.02900500
C	0.00000000	0.00000000	2.79983700
C	0.00000000	1.22124300	0.68201900
H	0.00000000	2.15629200	1.22787600
C	0.00000000	-1.22124300	0.68201900
H	0.00000000	-2.15629200	1.22787600
C	0.00000000	-1.22124300	-0.68201900
H	0.00000000	-2.15629200	-1.22787600
C	0.00000000	1.22124300	-0.68201900
H	0.00000000	2.15629200	-1.22787600
C	0.00000000	0.00000000	-2.79983700
C	0.00000000	0.00000000	-4.02900500
C	0.00000000	-1.22789600	-6.14595900
H	0.00000000	-2.16041100	-5.59512200
C	0.00000000	1.22789600	-6.14595900
H	0.00000000	2.16041100	-5.59512200
C	0.00000000	1.22928500	-7.50064500
H	0.00000000	2.16828400	-8.04254200
C	0.00000000	-1.22928500	-7.50064500
H	0.00000000	-2.16828400	-8.04254200
C	0.00000000	0.00000000	-9.62463400
H	0.00000000	-0.92481500	-10.18714200
H	0.00000000	0.92481500	-10.18714200
C	0.00000000	0.00000000	-1.42086700
C	0.00000000	0.00000000	-5.40171000
C	0.00000000	0.00000000	-8.26498300
C	0.00000000	0.00000000	1.42086700
C	0.00000000	0.00000000	5.40171000
C	0.00000000	0.00000000	8.26498300

2d:

B3LYP/6-311G(2d,p): -1231.52872 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	0.00000000	0.00000000	13.06579700
H	0.00000000	0.92498300	13.62772300
H	0.00000000	-0.92498300	13.62772300
C	0.00000000	1.22683100	10.93920700
H	0.00000000	2.16650800	11.47970100

C 0.00000000 -1.22683100 10.93920700
H 0.00000000 -2.16650800 11.47970100
C 0.00000000 -1.22400600 9.58076800
H 0.00000000 -2.15671900 9.03033200
C 0.00000000 1.22400600 9.58076800
H 0.00000000 2.15671900 9.03033200
C 0.00000000 0.00000000 7.45709100
C 0.00000000 0.00000000 6.23425200
C 0.00000000 1.21535500 4.10924700
H 0.00000000 2.15138400 4.65317400
C 0.00000000 -1.21535500 4.10924700
H 0.00000000 -2.15138400 4.65317400
C 0.00000000 -1.21430500 2.73742500
H 0.00000000 -2.15002700 2.19283900
C 0.00000000 1.21430500 2.73742500
H 0.00000000 2.15002700 2.19283900
C 0.00000000 0.00000000 0.60858800
C 0.00000000 0.00000000 -0.60858800
C 0.00000000 -1.21430500 -2.73742500
H 0.00000000 -2.15002700 -2.19283900
C 0.00000000 1.21430500 -2.73742500
H 0.00000000 2.15002700 -2.19283900
C 0.00000000 1.21535500 -4.10924700
H 0.00000000 2.15138400 -4.65317400
C 0.00000000 -1.21535500 -4.10924700
H 0.00000000 -2.15138400 -4.65317400
C 0.00000000 0.00000000 -6.23425200
C 0.00000000 0.00000000 -7.45709100
C 0.00000000 -1.22400600 -9.58076800
H 0.00000000 -2.15671900 -9.03033200
C 0.00000000 1.22400600 -9.58076800
H 0.00000000 2.15671900 -9.03033200
C 0.00000000 1.22683100 -10.93920700
C 0.00000000 -1.22683100 -10.93920700
H 0.00000000 -2.16650800 -11.47970100
C 0.00000000 0.00000000 -13.06579700
H 0.00000000 0.92498300 -13.62772300
H 0.00000000 -0.92498300 -13.62772300
H 0.00000000 2.16650800 -11.47970100
C 0.00000000 0.00000000 -11.70143500
C 0.00000000 0.00000000 -8.84189400
C 0.00000000 0.00000000 -4.84059900
C 0.00000000 0.00000000 -2.00860600
C 0.00000000 0.00000000 2.00860600
C 0.00000000 0.00000000 4.84059900
C 0.00000000 0.00000000 8.84189400
C 0.00000000 0.00000000 11.70143500

1a(C):

B3LYP/6-311G(2d,p): -1630.02667 a.u.

Point group: C_1

Cartesian coordinates:

C 0.54238100 -1.57624100 0.00021200
C -0.79464100 -1.46674900 0.00018900

C	-0.54237300	1.57619500	-0.00010700
C	0.79464600	1.46670400	0.00004100
H	0.97411400	-2.58000800	0.00024500
H	-1.38183900	-2.38823500	0.00021000
H	-0.97413700	2.57995000	-0.00007100
H	1.38187800	2.38817300	0.00019000
Si	1.74728700	-0.14427100	0.00007800
Si	-1.74728300	0.14421900	-0.00001200
Si	4.40413300	-0.00018900	-0.00004300
Si	-4.40414300	0.00039500	-0.00004900
C	-3.08594600	0.21946700	1.35897000
H	-3.03326600	-0.53975900	2.13971500
H	-3.12705900	1.19808400	1.84479100
C	-3.08584000	0.21882100	-1.35902600
H	-3.12687600	1.19725700	-1.84523200
H	-3.03305700	-0.54067400	-2.13949900
C	3.08586600	-0.21877700	-1.35901400
H	3.12733200	-1.19700500	-1.84558000
H	3.03278500	0.54096300	-2.13923500
C	3.08589600	-0.21850500	1.35908500
H	3.03282400	0.54137100	2.13917200
H	3.12739800	-1.19664800	1.84582000
C	-5.76269500	1.30347900	-0.00007000
H	-6.39832900	1.20595000	0.88430500
H	-5.34411100	2.31293600	-0.00057500
H	-6.39925400	1.20539500	-0.88370400
C	-5.16016600	-1.72433300	0.00002600
H	-4.38905000	-2.49881000	-0.00024100
H	-5.78532100	-1.87831500	0.88371300
H	-5.78534300	-1.87788900	-0.88375700
C	5.16119600	1.72404900	-0.00025900
H	4.39048300	2.49894100	-0.00039900
H	5.78639500	1.87759500	0.88348700
H	5.78647400	1.87736300	-0.88399000
C	5.76169800	-1.30430800	0.00007100
H	6.39785000	-1.20723000	-0.88397000
H	6.39789800	-1.20698900	0.88405100
H	5.34218000	-2.31339000	0.00022000

1b(C):

B3LYP/6-311G(2d,p): -2442.59168 a.u.

Point group: C_1

Cartesian coordinates:

C	3.50987500	-1.53421200	-0.00055300
C	2.18221600	-1.34112300	-0.00077800
C	2.62679600	1.67969900	-0.00025800
C	3.95427800	1.48627500	-0.00013900
H	3.87754900	-2.56313200	-0.00085300
H	1.53845800	-2.22398100	-0.00124800
H	2.25875500	2.70852800	-0.00018500
H	4.59825300	2.36887800	0.00002400
Si	4.80352300	-0.18167200	-0.00007600
Si	1.33510800	0.32699600	-0.00045300
C	-2.62698700	1.67955800	-0.00033500

C	-2.18216000	-1.34122800	-0.00035600
C	-3.95442400	1.48582400	-0.00024700
H	-2.25915500	2.70845700	-0.00047700
C	-3.50977500	-1.53462900	-0.00023900
H	-1.53822300	-2.22396000	-0.00050100
H	-4.59860200	2.36828700	-0.00031900
H	-3.87720200	-2.56363100	-0.00029200
Si	-4.80353700	-0.18222300	-0.00003500
Si	7.46332700	-0.17272700	0.00043700
Si	-1.33519200	0.32697300	-0.00034300
Si	-7.46334000	-0.17254500	0.00037900
C	-8.29341900	1.51759900	0.00036900
H	-8.92491000	1.64378000	-0.88323500
H	-8.92461100	1.64393700	0.88416600
H	-7.55722500	2.32532100	0.00017000
C	-8.76283800	-1.53449100	0.00077200
H	-9.40249600	-1.46549600	0.88492700
H	-9.40290300	-1.46570600	-0.88310300
H	-8.29925900	-2.52412500	0.00078700
C	8.76287300	-1.53465100	0.00045800
H	9.40267000	-1.46550500	-0.88359400
H	9.40279700	-1.46575000	0.88442600
H	8.29949800	-2.52437400	0.00034200
C	8.29380800	1.51718200	0.00079600
H	8.92549000	1.64331500	-0.88268400
H	7.55796700	2.32522200	0.00071600
H	8.92493900	1.64298600	0.88471900
C	6.13535700	-0.33516300	1.35826500
H	6.12921900	-1.32086700	1.83163400
H	6.11911200	0.41560500	2.14858200
C	6.13577500	-0.33517100	-1.35783200
H	6.11981000	0.41574400	-2.14802300
H	6.12976000	-1.32078600	-1.83136200
C	-0.00003100	0.48612600	1.35348500
H	-0.00003100	-0.25771500	2.15004800
H	-0.00000900	1.47507800	1.82055900
C	-0.00005400	0.48627500	-1.35422800
H	-0.00013700	1.47526000	-1.82123000
H	-0.00001200	-0.25750800	-2.15084500
C	-6.13541300	-0.33513300	1.35826800
H	-6.11885800	0.41600800	2.14822900
H	-6.12968700	-1.32061800	1.83207700
C	-6.13581900	-0.33529500	-1.35788900
H	-6.13020400	-1.32085400	-1.83155000
H	-6.11953300	0.41572200	-2.14797000

1c(C):

B3LYP/6-311G(2d,p): -3255.15668 a.u.

Point group: C_1

Cartesian coordinates:

C	0.39587700	-1.61885000	-0.00017300
C	-0.92579600	-1.38833800	-0.00014400
C	-0.39587100	1.61854300	-0.00002000
C	0.92579900	1.38803300	-0.00004100

H	0.73470800	-2.65761500	-0.00026700	H	3.04225300	-1.48892300	1.80826500
H	-1.59411800	-2.25268000	-0.00021700	H	3.06795900	0.23996500	2.15791100
H	-0.73474100	2.65729700	-0.00000200	C	3.05700400	-0.49435300	-1.35312800
H	1.59414700	2.25235700	-0.00003900	H	3.06787700	0.24020600	-2.15802600
Si	1.72581900	-0.30339400	-0.00009500	H	3.04217500	-1.48872200	-1.80858200
Si	-1.72581100	0.30307200	-0.00005300	C	-3.05700100	0.49431900	1.35295100
C	-5.67760600	1.70622500	-0.00003100	H	-3.06800800	-0.24000100	2.15806300
C	-5.25167200	-1.31732200	-0.00010000	H	-3.04201100	1.48882400	1.80810000
C	-7.00623000	1.52069800	-0.00001000	C	-3.05703000	0.49441000	-1.35304800
H	-5.30335900	2.73278700	-0.00005400	H	-3.04205500	1.48895100	-1.80811900
C	-6.58047600	-1.50231500	-0.00006200	H	-3.06803900	-0.23984600	-2.15821900
H	-4.61350800	-2.20422500	-0.00017200	C	-9.19854100	-0.28792300	1.35823600
H	-7.64480700	2.40721500	-0.00001400	H	-9.17911900	0.46392200	2.14746600
H	-6.95424200	-2.52901900	-0.00010400	H	-9.19677600	-1.27291600	1.83306800
Si	-7.86594600	-0.14194700	0.00002000	C	-9.19864900	-0.28791600	-1.35811300
Si	4.39448900	-0.34568500	-0.00008600	H	-9.19691300	-1.27290200	-1.83295800
Si	-4.39446900	0.34555900	-0.00005000	H	-9.17928200	0.46394000	-2.14733500
Si	-10.52574200	-0.12068500	0.00010800	C	5.67762000	-1.70632800	-0.00010700
C	-11.35003100	1.57225900	0.00012900	H	5.30350100	-2.73293000	-0.00022700
H	-11.98095300	1.70060500	-0.88356300	C	5.25163000	1.31723400	-0.00000800
H	-11.98094900	1.70059200	0.88382600	H	4.61332300	2.20403600	-0.00001700
H	-10.61117600	2.37754800	0.00013400	C	7.00621400	-1.52060100	0.00000200
C	-11.82997200	-1.47805900	0.00017000	H	7.64491400	-2.40701900	-0.00003800
H	-12.46951500	-1.40679300	0.88422300	Si	7.86589300	0.14207500	0.00006800
H	-12.46964700	-1.40676200	-0.88378500	C	6.58040600	1.50242100	0.00008200
H	-11.37007900	-2.46940100	0.00011900	H	6.95405300	2.52916300	0.00012500
C	3.05705800	-0.49450100	1.35292900	C	9.19855200	0.28779800	-1.35810700

H 9.19685900 1.27261000 -1.83332100
H 9.17913200 -0.46432200 -2.14708200
C 9.19849300 0.28797400 1.35824300
Si 10.52568900 0.12088800 0.00013700
H 9.17917100 -0.46409400 2.14727500
H 9.19669400 1.27280800 1.83340200
C 11.35047900 -1.57178800 0.00032500
H 11.98185400 -1.69961900 0.88377000
H 10.61189200 -2.37732900 0.00094700
H 11.98101900 -1.70021400 -0.88362600
C 11.82976700 1.47841000 -0.00012900
H 12.46954400 1.40724200 0.88376700
H 12.46923600 1.40694000 -0.88422600
H 11.36993400 2.46977200 -0.00022700

1d(C):

B3LYP/6-311G(2d,p): -4067.72167 a.u.

Point group: C_1

Cartesian coordinates:

C -3.46973500 1.60929400 -0.00010500
C -2.14636200 1.38882400 -0.00011700
C -2.65377900 -1.62202100 -0.00011100
C -3.97714800 -1.40134900 -0.00010700
H -3.81628800 2.64549900 -0.00010700
H -1.48476000 2.25830200 -0.00012700
H -2.30713500 -2.65818700 -0.00011600
H -4.63894300 -2.27069500 -0.00011000
Si -4.78996500 0.28400600 -0.00009500
Si -1.33391200 -0.29656800 -0.00011300
C 2.65369500 -1.62210700 -0.00012400
C 2.14639700 1.38875900 -0.00015400
C 3.97707200 -1.40148400 -0.00010500
H 2.30701000 -2.65825900 -0.00013500
C 3.46977900 1.60918100 -0.00014400
H 1.48483000 2.25826300 -0.00018700
H 4.63883700 -2.27085200 -0.00010300
H 3.81636700 2.64537300 -0.00016900
Si 4.78995600 0.28384100 -0.00009200
Si -7.45904300 0.31565600 -0.00007100
Si 1.33388100 -0.29660100 -0.00012800
Si 7.45903600 0.31554500 -0.00002500
C -6.12196200 0.46670200 1.35320300
H -6.11085800 1.45956900 1.81193000
H -6.13015100 -0.27047000 2.15578400
C -6.12198800 0.46671600 -1.35337600
H -6.13019800 -0.27045300 -2.15596000
H -6.11088600 1.45958600 -1.81209600
C -0.00001200 -0.47616400 1.35212400
H -0.00000600 0.25007200 2.16447800
H -0.00001300 -1.47554200 1.79696100
C -0.00002400 -0.47617800 -1.35236500
H -0.00003300 -1.47556400 -1.79718500
H -0.00002200 0.25004500 -2.16473200
C 6.12193000 0.46650800 1.35324100

H 6.13013100 -0.27075800 2.15573700
H 6.11078900 1.45931900 1.81208500
C 6.12199600 0.46647500 -1.35336000
H 6.11087500 1.45926900 -1.81224000
H 6.13023900 -0.27082100 -2.15583000
C -8.74366200 1.67485500 -0.00005100
H -8.37069400 2.70187900 -0.00005800
C -8.31411800 -1.34827000 -0.00008900
H -7.67480200 -2.23434800 -0.00011700
C -10.07204400 1.48764400 -0.00001600
H -10.71173100 2.37336000 -0.00000600
Si -10.92981700 -0.17603000 0.00003100
C -9.64269700 -1.53488200 -0.00005600
H -10.01521300 -2.56203500 -0.00007100
C -12.26236700 -0.32332300 -1.35803900
H -12.25983000 -1.30832500 -1.83284200
H -12.24366700 0.42851900 -2.14729600
C -12.26216700 -0.32333400 1.35830400
Si -13.58959000 -0.15714300 0.00023100
H -12.24337500 0.42852300 2.14754600
H -12.25954300 -1.30831600 1.83314700
C -14.41509600 1.53520100 0.00031600
H -15.04616500 1.66301900 0.88397900
H -13.67681300 2.34101700 0.00044600
H -15.04604200 1.66317700 -0.88341000
C -14.89276900 -1.51550400 0.00021100
H -15.53248900 -1.44471600 0.88417300
H -15.53237700 -1.44464700 -0.88383100
H -14.43215900 -2.50651000 0.00019600
C 8.31420200 -1.34833600 0.00001800
H 7.67491700 -2.23443800 0.00003600
C 8.74357300 1.67482000 -0.00001900
H 8.37056500 2.70182800 -0.00005800
C 10.07196400 1.48766400 0.00002800
C 9.64278800 -1.53489000 0.00004200
H 10.01535800 -2.56202400 0.00007200
Si 10.92982700 -0.17596000 0.00006800
H 10.71161400 2.37340900 0.00001500
C 12.26221400 -0.32325000 1.35830300
C 12.26234000 -0.32319800 -1.35804500
H 12.25981900 -1.30820100 -1.83284500
H 12.24360000 0.42864100 -2.14730300
Si 13.58960600 -0.15704000 0.00019000
H 12.25961600 -1.30822000 1.83316700
H 12.24344000 0.42862500 2.14753000
C 14.41524700 1.53522800 0.00026100
H 13.67706900 2.34113800 0.00006900
H 15.04611700 1.66310400 0.88405800
H 15.04642700 1.66297500 -0.88333300
C 14.89272900 -1.51545800 0.00011400
H 15.53236100 -1.44457100 -0.88390900
H 15.53243700 -1.44474500 0.88409300
H 14.43209100 -2.50645100 0.00003600

3a:

B3LYP/6-311G(2d,p): -888.63325435 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	-0.63169900	1.64681100	0.00000000
C	0.63169900	1.64681100	0.00000000
C	1.94531700	1.57913800	0.00000000
H	2.51015500	2.51282000	0.00000000
C	-1.94531700	1.57913800	0.00000000
H	-2.51015500	2.51282000	0.00000000
Si	-2.95044500	0.00000000	0.00000000
H	-3.83860900	0.00000000	1.19061900
H	-3.83860900	0.00000000	-1.19061900
Si	2.95044500	0.00000000	0.00000000
H	3.83860900	0.00000000	-1.19061900
H	3.83860900	0.00000000	1.19061900
C	-1.94531700	-1.57913800	0.00000000
H	-2.51015500	-2.51282000	0.00000000
C	1.94531700	-1.57913800	0.00000000
H	2.51015500	-2.51282000	0.00000000
C	-0.63169900	-1.64681100	0.00000000
C	0.63169900	-1.64681100	0.00000000

3b:

B3LYP/6-311G(2d,p): -1286.03941 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	-1.90829100	1.41279600	0.00000000
C	-0.74503700	0.75805400	0.00000000
C	-0.74503700	-0.75805400	0.00000000
C	-1.90829100	-1.41279600	0.00000000
H	-2.04074800	2.48519100	0.00000000
H	-2.04074800	-2.48519100	0.00000000
Si	-3.14455100	0.00000000	0.00000000
C	0.74503700	0.75805400	0.00000000
C	0.74503700	-0.75805400	0.00000000
C	1.90829100	1.41279600	0.00000000
H	2.04074800	2.48519100	0.00000000
C	1.90829100	-1.41279600	0.00000000
H	2.04074800	-2.48519100	0.00000000
Si	3.14455100	0.00000000	0.00000000
F	-4.11345700	0.00000000	-1.26644100
F	-4.11345700	0.00000000	1.26644100
F	4.11345700	0.00000000	-1.26644100
F	4.11345700	0.00000000	1.26644100

3c:

B3LYP/6-311G(2d,p): -2237.24020 a.u.

Point group: C_2

Cartesian coordinates:

C	0.00119900	1.40851100	1.91302000
C	0.00000000	0.75208000	0.74637100
C	0.00000000	-0.75208000	0.74637100
C	-0.00119900	-1.40851100	1.91302000

H -0.00011400 2.48039000 2.04837100
H 0.00011400 -2.48039000 2.04837100
Si 0.00000000 0.00000000 3.15254800
C -0.00057400 0.75208300 -0.74630900
C 0.00057400 -0.75208300 -0.74630900
C -0.00223200 1.40850500 -1.91296000
H -0.00173300 2.48038400 -2.04832300
C 0.00223200 -1.40850500 -1.91296000
H 0.00173300 -2.48038400 -2.04832300
Si 0.00000000 0.00000000 -3.15250900
C 1.53973500 -0.01995800 4.32448400
C -1.53973500 0.01995800 4.32448400
C -1.53970100 -0.02149900 -4.32448700
C 1.53970100 0.02149900 -4.32448700
F -2.69122300 0.08396800 -3.62404300
F -1.60953900 -1.17110700 -5.03275100
F -1.51969600 0.99645700 -5.21388900
F 1.51969600 -0.99645700 -5.21388900
F 1.60953900 1.17110700 -5.03275100
F 2.69122300 -0.08396800 -3.62404300
F 2.69117200 0.08484000 3.62379000
F 1.51958000 0.99918300 5.21257000
F 1.60981900 -1.16862200 5.03420800
F -1.51958000 -0.99918300 5.21257000
F -1.60981900 1.16862200 5.03420800
F -2.69117200 -0.08484000 3.62379000

3d:

B3LYP/6-311G(2d,p): -1046.02566 a.u.

Point group: D_{2h}

Cartesian coordinates:

C 1.92075200 0.00000000 1.39679100
C 0.74837100 0.00000000 0.75012700
C 0.74837100 0.00000000 -0.75012700
C 1.92075200 0.00000000 -1.39679100
H 2.03653000 0.00000000 2.47353100
H 2.03653000 0.00000000 -2.47353100
Si 3.21020000 0.00000000 0.00000000
C -0.74837100 0.00000000 0.75012700
C -0.74837100 0.00000000 -0.75012700
C -1.92075200 0.00000000 1.39679100
H -2.03653000 0.00000000 2.47353100
C -1.92075200 0.00000000 -1.39679100
H -2.03653000 0.00000000 -2.47353100
Si -3.21020000 0.00000000 0.00000000
C 4.29712700 1.53876200 0.00000000
H 3.69222200 2.44737400 0.00000000
H 4.94143300 1.55958600 0.88298700
H 4.94143300 1.55958600 -0.88298700
C 4.29712700 -1.53876200 0.00000000
H 4.94143300 -1.55958600 -0.88298700
H 4.94143300 -1.55958600 0.88298700
H 3.69222200 -2.44737400 0.00000000
C -4.29712700 -1.53876200 0.00000000

H	-4.94143300	-1.55958600	-0.88298700
H	-3.69222200	-2.44737400	0.00000000
H	-4.94143300	-1.55958600	0.88298700
C	-4.29712700	1.53876200	0.00000000
H	-4.94143300	1.55958600	-0.88298700
H	-4.94143300	1.55958600	0.88298700
H	-3.69222200	2.44737400	0.00000000

3e:

B3LYP/6-311G(2d,p): -2523.64177 a.u.

Point group: C_1

Cartesian coordinates:

C	-1.92959400	-0.11306700	1.38651800
C	-0.75018900	-0.14033300	0.74221100
C	-0.74750300	-0.14012700	-0.74509300
C	-1.92435100	-0.11163700	-1.39411700
H	-2.05300400	-0.10017000	2.46214900
H	-2.04328400	-0.09874800	-2.47025400
Si	-3.21900400	-0.05905600	-0.00642500
C	0.74749600	-0.14021200	0.74511900
C	0.75018000	-0.14023000	-0.74218800
C	1.92434500	-0.11180200	1.39414400
H	2.04329000	-0.09906400	2.47028300
C	1.92958500	-0.11290300	-1.38649200
H	2.05299800	-0.09988000	-2.46212200
Si	3.21899500	-0.05905600	0.00645800
Si	4.63090900	-1.98019800	0.02807300
Si	-4.34593300	2.04237800	0.02838800
Si	-4.63092000	-1.98020100	-0.02809900
Si	4.34594900	2.04237400	-0.02835400
C	3.56851600	-3.53082000	-0.15812400
H	4.19288100	-4.42938700	-0.14197200
H	2.84126100	-3.61099700	0.65275500
H	3.01544500	-3.52057100	-1.09975400
C	5.57532800	-2.07068200	1.66504500
H	4.89174800	-2.12480900	2.51560000
H	6.20753100	-2.96352200	1.68933700
H	6.22137300	-1.20187200	1.81024400
C	3.07994600	3.42013300	0.22830400
H	2.60177600	3.34088700	1.20684700
H	3.56214600	4.40043900	0.16533200
H	2.29379100	3.38119300	-0.52876100
C	5.65077000	2.14316000	1.33952000
H	6.11196900	3.13552700	1.34862300
H	5.21372200	1.97214700	2.32621400
H	6.44791200	1.41005600	1.19479000
C	-3.07989300	3.42012600	-0.22816100
H	-2.60163600	3.34086400	-1.20666000
H	-3.56210600	4.40042900	-0.16525200
H	-2.29380500	3.38120900	0.52897500
C	-5.65058500	2.14318900	-1.33964900
H	-6.11169300	3.13559900	-1.34884900
H	-5.21341200	1.97211700	-2.32627700
H	-6.44780600	1.41015800	-1.19500800

C	-5.57537200	-2.07067400	-1.66505300
H	-4.89180400	-2.12479100	-2.51561900
H	-6.20755900	-2.96352600	-1.68934300
H	-6.22143200	-1.20187400	-1.81023500
C	-3.56855200	-3.53084600	0.15805400
H	-4.19295900	-4.42938500	0.14195100
H	-2.84135100	-3.61106500	-0.65286900
H	-3.01542500	-3.52061100	1.09965100
C	5.19350700	2.28896500	-1.70202500
H	5.93592000	1.51316500	-1.90208900
H	4.46769000	2.27552100	-2.51846000
H	5.70665500	3.25513500	-1.72878300
C	5.87628100	-1.90845300	-1.39476800
H	5.37679500	-1.83584600	-2.36374800
H	6.54777200	-1.05209300	-1.29891000
H	6.49204200	-2.81299200	-1.40587000
C	-5.87625900	-1.90846600	1.39477300
H	-5.37674800	-1.83575900	2.36373200
H	-6.54782300	-1.05216900	1.29888000
H	-6.49193700	-2.81306000	1.40595500
C	-5.19366300	2.28904700	1.70195800
H	-5.93610900	1.51327600	1.90200400
H	-4.46792100	2.27565000	2.51846100
H	-5.70679000	3.25523200	1.72860500

4a(Si):

B3LYP/6-311G(2d,p): -4580.29719 a.u.

Point group: C_1

Cartesian coordinates:

C	-2.10254100	-1.10637200	0.03556500
C	-0.84563700	-0.63086500	0.04281800
C	-0.63459900	0.84388000	0.04535700
C	-1.70921100	1.65140700	0.04724100
H	-2.37748300	-2.15238100	0.03391400
H	-1.68359300	2.73326100	0.04827900
Si	-3.17508700	0.45549100	0.03438800
C	0.63450300	-0.84289500	0.04553200
C	0.84554600	0.63185100	0.04291700
C	1.70911000	-1.65042600	0.04764800
H	1.68348000	-2.73228100	0.04876000
C	2.10245400	1.10735200	0.03582500
H	2.37740900	2.15335900	0.03413300
Si	3.17499400	-0.45451800	0.03484500
Si	4.87548600	-0.61040500	-1.64904200
Si	-4.92046400	0.57608200	1.67095900
Si	-4.87583000	0.61080000	-1.64927800
Si	4.92054600	-0.57547700	1.67121500
Si	-6.52283700	-0.00864700	-0.01539000
Si	6.52293700	0.00845900	-0.01539600
Si	8.56157400	-1.22630500	0.04386000
Si	6.92861200	2.35592700	-0.09443800
Si	-8.56204400	1.22516900	0.04411800

Si	-6.92773900	-2.35624400	-0.09428900	H	3.80899000	0.19719900	-3.75277100
C	5.32194000	3.34941200	0.03191500	H	4.52016000	1.55553400	-2.87904300
H	4.64065200	3.12820100	-0.79244600	C	5.04228800	-2.39442800	-2.27954700
H	4.79218900	3.15251300	0.96592000	H	4.15521500	-2.67021900	-2.85594500
H	5.54634500	4.42008700	-0.00262000	H	5.91155100	-2.49203100	-2.93553800
C	8.05141900	2.88745000	1.33442400	H	5.15213500	-3.11489700	-1.46723500
H	9.03465200	2.41561100	1.27403800	C	4.76154800	0.54768500	3.19006300
H	8.20186500	3.97127500	1.31237700	H	3.92696300	0.21948500	3.81537200
H	7.61642100	2.63060300	2.30307900	H	5.67113800	0.50970700	3.79590600
C	7.76556100	2.82862100	-1.72486200	H	4.58186000	1.58731800	2.91299400
H	7.95282100	3.90661600	-1.75254000	C	5.12888700	-2.35968200	2.29256800
H	8.72315100	2.32043200	-1.85312800	H	6.03091500	-2.45733400	2.90289800
H	7.13758500	2.57766700	-2.58267900	H	4.27387800	-2.64419600	2.91159100
C	9.40750800	-1.01503200	1.72510100	H	5.19977700	-3.07556300	1.47152700
H	10.33778700	-1.59117100	1.75323500	C	-4.76083000	-0.54678900	3.18995800
H	9.65698400	0.02800100	1.93106700	H	-3.92608600	-0.21835000	3.81493200
H	8.77207100	-1.37211800	2.53902300	H	-5.67022600	-0.50878300	3.79609400
C	9.76185600	-0.64916800	-1.30212300	H	-4.58110600	-1.58646200	2.91306700
H	10.09077100	0.37920300	-1.13734400	C	-5.12948000	2.36027000	2.29213900
H	10.65307300	-1.28448700	-1.30634100	H	-6.03151600	2.45763000	2.90250100
H	9.31192000	-0.70054800	-2.29623400	H	-4.27455700	2.64517300	2.91110200
C	8.24744100	-3.07444100	-0.21422100	H	-5.20068000	3.07604700	1.47103300
H	7.57939100	-3.48146400	0.54754900	C	-5.04343300	2.39469500	-2.27991500
H	7.80609900	-3.27879400	-1.19147300	H	-4.15649200	2.67087000	-2.85632700
H	9.19300400	-3.62250500	-0.15397300	H	-5.91273800	2.49182600	-2.93592400
C	4.67327900	0.51344100	-3.16263600	H	-5.15363900	3.11516900	-1.46765800
H	5.55642700	0.46165400	-3.80542500	C	-4.67343300	-0.51312300	-3.16278500

H	-5.55674400	-0.46178800	-3.80538800
H	-3.80940700	-0.19660700	-3.75316000
H	-4.51982400	-1.55512200	-2.87909800
C	-7.76466500	-2.82931400	-1.72459900
H	-7.13668200	-2.57842800	-2.58243300
H	-7.95182700	-3.90732700	-1.75211700
H	-8.72228400	-2.32121000	-1.85296600
C	-8.05022600	-2.88798600	1.33474500
H	-8.19987400	-3.97192900	1.31315400
H	-7.61549400	-2.63040000	2.30332300
H	-9.03379900	-2.41689200	1.27406500
C	-5.32076800	-3.34924300	0.03189200
H	-4.63973500	-3.12793200	-0.79265900
H	-4.79083000	-3.15211600	0.96573700
H	-5.54488600	-4.41998500	-0.00250800
C	-9.40762100	1.01334200	1.72546500
H	-10.33868900	1.58820600	1.75350200
H	-9.65562200	-0.02996500	1.93182000
H	-8.77259400	1.37157400	2.53920700
C	-9.76218700	0.64750200	-1.30178200
H	-10.09065000	-0.38101900	-1.13705200
H	-10.65368100	1.28243300	-1.30589200
H	-9.31235600	0.69914100	-2.29593000
C	-8.24900000	3.07349500	-0.21399900
H	-7.58137500	3.48101000	0.54787800
H	-7.80761000	3.27808000	-1.19118500
H	-9.19493800	3.62094100	-0.15398300

4b(Si):

B3LYP/6-311G(2d,p): -6205.37332 a.u.

Point group: C_1

Cartesian coordinates:

C	6.89257500	-1.37206600	-0.00487700
C	5.55245500	-1.27091100	0.01626000
C	4.93455000	0.08368200	0.06775500
C	5.73724600	1.16142100	0.08746400
H	7.45232400	-2.29682400	-0.04242100
H	5.40720700	2.19139800	0.12261700
Si	7.48020800	0.42845900	0.03707800
C	4.19142400	-1.89124000	0.01048500
C	3.57473300	-0.53601800	0.06512600
C	3.38773700	-2.96890800	-0.02384600
H	3.71497000	-3.99930700	-0.06656400
C	2.23478600	-0.43371200	0.08317300
H	1.67749900	0.49317500	0.12082000
Si	1.64878600	-2.23269700	0.01530500
Si	0.00004200	-2.81582200	1.65227600
Si	9.04831900	1.12117200	-1.64001600
Si	9.11203000	1.04388800	1.68035400
Si	-0.00002700	-2.64914000	-1.67586400
C	-2.23481500	-0.43374900	0.08326400
C	-3.38772400	-2.96896300	-0.02373400
H	-1.67754400	0.49314800	0.12090000
C	-3.57476200	-0.53607700	0.06527200
H	-3.71494300	-3.99936700	-0.06644700

C	-4.19142900	-1.89131100	0.01064700	H	-14.03714300	1.92555800	1.61576600
Si	10.81207500	1.03753200	-0.01322700	H	-12.80984300	2.85064000	2.48195300
Si	-1.64878600	-2.23272500	0.01536100	C	-13.08748100	-1.26739700	1.39361900
C	-4.93459100	0.08359600	0.06796600	H	-13.89697900	-0.53443700	1.37898300
C	-5.55247200	-1.27101000	0.01650200	H	-13.54165800	-2.26307500	1.38219000
C	-5.73731100	1.16131800	0.08765800	H	-12.55308500	-1.15533000	2.33946300
H	-5.40729100	2.19130300	0.12277400	C	-12.95514800	-1.23092900	-1.67266800
C	-6.89259000	-1.37219300	-0.00458600	H	-13.45516800	-2.20433400	-1.69414900
H	-7.45232400	-2.29695800	-0.04214600	H	-13.72609400	-0.46060200	-1.74059600
Si	-7.48026100	0.42831800	0.03733200	H	-12.33168300	-1.15791500	-2.56660900
Si	-9.11213600	1.04400000	1.68049500	C	-10.69475700	-2.50207200	-0.05693400
Si	-9.04826400	1.12098600	-1.63988800	H	-10.01598700	-2.47574100	-0.91174600
Si	-10.81208700	1.03759200	-0.01319300	H	-10.08830400	-2.50066700	0.85093700
Si	-12.33714000	2.86795800	0.01704700	H	-11.23483300	-3.45338300	-0.09279900
Si	-11.92936300	-1.06613600	-0.09007200	C	-9.32011500	-0.11160200	3.16961700
Si	11.92942000	-1.06613300	-0.09039600	H	-8.42002900	-0.08625100	3.78984400
Si	12.33716000	2.86786900	0.01761300	H	-10.16382500	0.20340900	3.79005200
C	-11.41374500	4.51951300	0.00632800	H	-9.48823900	-1.14673000	2.86938500
H	-10.76067400	4.62463700	0.87479100	C	-8.73654300	2.78047600	2.35534400
H	-10.80233100	4.63636500	-0.89045400	H	-8.56824400	3.50573600	1.55717700
H	-12.13277200	5.34440700	0.02902100	H	-9.56107700	3.14554100	2.97384700
C	-13.47461300	2.83621100	-1.49688200	H	-7.83804400	2.75286500	2.97755200
H	-14.10794900	1.94678800	-1.51403000	C	-9.21010600	0.01705100	-3.17249200
H	-14.13227000	3.71113600	-1.48807400	H	-10.02777200	0.36148800	-3.81175900
H	-12.90597800	2.85836500	-2.42954300	H	-8.28816200	0.05016500	-3.75914000
C	-13.41559500	2.82236400	1.57317200	H	-9.40136800	-1.02408500	-2.90938200
H	-14.08260100	3.69001100	1.59147500	C	-8.64279500	2.87733200	-2.23972500

H	-7.71900300	2.86585700	-2.82427500	C	9.31981900	-0.11176800	3.16946000
H	-9.43985700	3.26462500	-2.88023300	H	10.16344900	0.20323600	3.79000800
H	-8.50655600	3.57634500	-1.41270800	H	8.41965600	-0.08645400	3.78957600
C	-0.00003000	-4.45943600	-2.24509100	H	9.48799600	-1.14688100	2.86920300
H	-0.88459000	-4.66594000	-2.85308800	C	10.69484300	-2.50209900	-0.05714600
H	0.88449200	-4.66592200	-2.85314900	H	10.08864400	-2.50079100	0.85090000
H	0.00000600	-5.15757800	-1.40626500	H	10.01582700	-2.47567800	-0.91175700
C	-0.00004800	-1.51633800	-3.18940700	H	11.23491400	-3.45340200	-0.09327000
H	-0.88522000	-1.69649100	-3.80505200	C	8.73655600	2.78038600	2.35522900
H	-0.00006100	-0.46576400	-2.89554200	H	7.83803800	2.75281900	2.97741400
H	0.88511900	-1.69646600	-3.80506700	H	9.56109600	3.14537100	2.97377000
C	0.00003500	-4.67993300	2.01348700	H	8.56832300	3.50568500	1.55708400
H	0.88417600	-4.95326300	2.59527600	C	12.95491000	-1.23080600	-1.67319400
H	-0.88418600	-4.95329700	2.59513400	H	13.45553200	-2.20390400	-1.69448200
H	0.00012700	-5.28102900	1.10241000	H	12.33107000	-1.15854000	-2.56693900
C	0.00003600	-1.86930700	3.28937200	H	13.72532900	-0.46001100	-1.74170500
H	-0.88489800	-2.12368600	3.87867400	C	13.08775000	-1.26748000	1.39311500
H	0.88495300	-2.12369300	3.87869700	H	13.54170700	-2.26326000	1.38169100
H	0.00004300	-0.79062300	3.12671900	H	13.89740800	-0.53470200	1.37823200
C	9.21013400	0.01723700	-3.17262500	H	12.55357000	-1.15520000	2.33905200
H	8.28821100	0.05043300	-3.75930300	C	13.41499500	2.82202600	1.57416300
H	10.02784500	0.36162700	-3.81186100	H	14.03644100	1.92515300	1.61687200
H	9.40130400	-1.02391900	-2.90953400	H	14.08208100	3.68960000	1.59286700
C	8.64301200	2.87754900	-2.23986100	H	12.80887900	2.85021800	2.48270300
H	9.44012300	3.26477400	-2.88034900	C	13.47523200	2.83625700	-1.49586800
H	7.71923400	2.86615000	-2.82443600	H	14.13281200	3.71123900	-1.48673400
H	8.50681500	3.57657600	-1.41284900	H	14.10865000	1.94689200	-1.51283800

H 12.90696100 2.85844800 -2.42875100
C 11.41384600 4.51946500 0.00664600
H 10.80273600 4.63638900 -0.89033200
H 10.76048700 4.62456300 0.87489700
H 12.13289600 5.34433000 0.02963600

4c(Si):

B3LYP/6-311G(2d,p): -7830.44949 a.u.

Point group: C_1

Cartesian coordinates:

C -2.23080600 0.95594600 -0.12655000
C -0.88743800 0.91356000 -0.10038000
C -0.21184100 -0.41308800 -0.04325700
C -0.96650600 -1.52536700 -0.01832500
H -2.82958700 1.85647500 -0.16659400
H -0.59350300 -2.54009400 0.02431200
Si -2.73628900 -0.86792300 -0.06692900
C 0.44521300 1.59217400 -0.09519400
C 1.11961600 0.26499300 -0.03851000
C 1.20135300 2.70403900 -0.11434100
H 0.83028100 3.71957100 -0.15386300
C 2.46253400 0.22085400 -0.00809600
H 3.05941700 -0.68088700 0.03413300
Si 2.97017000 2.04421800 -0.05681700
Si 4.56470400 2.67348800 1.61802000
Si -4.32713500 -1.58168900 -1.71480400
Si -4.34517500 -1.43361300 1.61870200
Si 4.62785300 2.55905500 -1.71037200
C -6.97236900 0.37197200 -0.15039800
C -7.60390900 -2.33917700 -0.01077600
H -6.60808600 1.38962300 -0.20400100
C -8.26626900 0.00784000 -0.13135900
H -7.72196800 -3.41308100 0.04842800
C -8.60377200 -1.44126600 -0.05047900
C 6.88161300 0.38056300 0.05202700
C 7.98228600 2.94073700 0.00387300
H 6.34345500 -0.55819900 0.06542000
C 8.21914900 0.51105600 0.05678100
H 8.28855900 3.97821500 -0.01797200
C 8.80789900 1.87956500 0.03327200
Si -6.04377300 -1.27588700 -0.06661300
Si 6.25895000 2.16777600 0.00257400
C 9.59127900 -0.08025100 0.06876700
C 10.18157200 1.28744100 0.04816200
C 10.41552800 -1.14166500 0.08047300
H 10.10602500 -2.17851900 0.09316700
C 11.51953400 1.41615300 0.04586100
H 12.06102900 2.35243300 0.03041800
Si 12.14336800 -0.37265900 0.06332400
Si 13.77247200 -0.98439800 1.71097200
Si 13.73918900 -0.99928400 -1.61266900
Si 15.48640600 -0.92207600 0.03180900
C -9.72276600 0.34621500 -0.14299200
C -10.05953300 -1.10204500 -0.05352600

C	-10.72398600	1.24198400	-0.18780000	H	13.26826300	-3.45417000	1.55899800
C	-11.35241700	-1.46612600	-0.00793200	C	13.95189700	0.15755000	3.21405200
Si	-12.28686700	0.17989900	-0.09024700	H	14.10980500	1.19760500	2.92571900
H	-10.60600600	2.31580800	-0.25088100	H	13.04717100	0.11438200	3.82643400
H	-11.71603300	-2.48243100	0.06195600	H	14.79448000	-0.15349300	3.83800300
Si	-14.04835000	0.33404400	-1.71125600	C	17.70544400	1.39646600	1.50942100
Si	-13.93240800	0.58824700	1.60360500	H	18.52117500	0.67039900	1.50249600
Si	-15.66061000	0.01472100	0.04234700	H	18.15135400	2.39595300	1.51356700
Si	17.03260800	-2.73444000	0.03121100	H	17.15644000	1.27261200	2.44543400
Si	16.57466700	1.19814300	0.00429800	C	15.31922600	2.61599100	0.03670400
Si	-16.29312600	-2.27706900	0.22931100	H	14.65571500	2.59337000	-0.83006300
Si	-17.56766000	1.44750100	0.06149100	H	14.69742000	2.59265800	0.93377500
C	18.15721100	-2.67188800	-1.49142800	H	15.84648400	3.57505100	0.02446400
H	18.78135500	-1.77588500	-1.50313800	C	17.62367600	1.39964500	-1.55875500
H	18.82363400	-3.54015000	-1.49929300	H	18.09612300	2.38691200	-1.56698200
H	17.58055500	-2.68817900	-2.41928600	H	18.41761200	0.65207000	-1.61516400
C	16.12552500	-4.39481100	0.00691700	H	17.01901900	1.31280800	-2.46431300
H	15.47964800	-4.51654600	0.87856000	C	13.89324100	0.14265500	-3.11841700
H	15.50878000	-4.50592900	-0.88691100	H	14.72041500	-0.17330400	-3.76021100
H	16.85229600	-5.21314500	0.01408300	H	12.97562000	0.10741500	-3.71174100
C	18.12289300	-2.69732500	1.57932800	H	14.06523400	1.18078500	-2.83120000
H	18.79982500	-3.55745800	1.58035700	C	13.37426700	-2.74840700	-2.25879100
H	18.73474500	-1.79422500	1.62910500	H	12.46013400	-2.73980200	-2.85841900
H	17.52523000	-2.74492100	2.49267300	H	14.18840100	-3.10674700	-2.89472700
C	13.42187300	-2.73409200	2.36477700	H	13.23707700	-3.46867800	-1.45033200
H	14.24959500	-3.09215500	2.98314000	C	4.70460300	1.46638200	-3.25113500
H	12.52056200	-2.72687600	2.98351000	H	3.81250700	1.60568800	-3.86728700

H	5.57898200	1.71897800	-3.85677400	H	-3.58257200	-0.33878200	3.72643000
H	4.77169400	0.41081100	-2.98418300	H	-4.63475400	0.74851800	2.81126000
C	4.56020600	4.38127500	-2.23669300	H	-5.33637100	-0.58018000	3.74215600
H	5.44719300	4.64038900	-2.82053200	C	-14.01464600	-0.93788500	-3.11565700
H	3.68047900	4.56418600	-2.85912400	H	-14.91248100	-0.85477900	-3.73430800
H	4.51217100	5.05854700	-1.38230500	H	-13.14673400	-0.76700200	-3.75805200
C	4.49015400	4.53132600	2.00186800	H	-13.95552600	-1.96007300	-2.73939600
H	3.58814700	4.76519900	2.57328800	C	-14.11625600	2.06065600	-2.49797700
H	5.35511300	4.82829200	2.60067400	H	-13.26937600	2.19766100	-3.17565700
H	4.48252400	5.14400400	1.09867100	H	-15.03467700	2.18381300	-3.07825000
C	4.57006200	1.70677500	3.24314800	H	-14.08114700	2.85674200	-1.75261500
H	4.60659600	0.63077300	3.06738200	C	-13.94608800	2.42984800	2.07223900
H	5.43756800	1.98150800	3.84898500	H	-14.81357500	2.66713600	2.69393900
H	3.66888900	1.92551100	3.82208100	H	-13.04622500	2.67618500	2.64206600
C	-4.09996500	-3.41696400	-2.14320900	H	-13.97381700	3.07933600	1.19536500
H	-4.94937100	-3.77695100	-2.72947100	C	-17.29446500	-2.82559300	-1.28070000
H	-3.19297100	-3.56208300	-2.73565500	H	-16.71729500	-2.72126700	-2.20210700
H	-4.02063600	-4.04163100	-1.25144000	H	-17.57327100	-3.87928800	-1.18041500
C	-4.45399700	-0.57238400	-3.30839600	H	-18.21376100	-2.24820700	-1.39700400
H	-4.59342400	0.48809200	-3.09354600	C	-17.34726000	-2.55256200	1.77757000
H	-3.54566400	-0.68114200	-3.90672400	H	-18.28978200	-2.00281400	1.72773300
H	-5.30120100	-0.91070500	-3.91064200	H	-17.58924600	-3.61457900	1.88429200
C	-4.12411300	-3.22252000	2.21462000	H	-16.82390000	-2.23704500	2.68294100
H	-3.22543600	-3.30895400	2.83087100	C	-18.85146500	0.89254000	-1.21418100
H	-4.98060300	-3.53087400	2.81969100	H	-19.25659500	-0.09328700	-0.97616500
H	-4.02958600	-3.92592000	1.38514700	H	-19.68779100	1.59802700	-1.23838100
C	-4.48849900	-0.28848900	3.11679700	H	-18.42644100	0.84491600	-2.21947300

C	-18.37705400	1.42847200	1.77308400
H	-19.26698200	2.06558600	1.77652900
H	-18.68507100	0.42337400	2.06778400
H	-17.69650600	1.80559100	2.54014300
C	-17.09481500	3.23713800	-0.33122900
H	-16.35922400	3.62684800	0.37540300
H	-16.68192100	3.33831800	-1.33667500
H	-17.98321500	3.87363100	-0.27047600
C	-14.78063600	-3.41075000	0.34363100
H	-14.14215600	-3.32092300	-0.53775700
H	-14.16913800	-3.19780800	1.22272800
H	-15.10625000	-4.45348900	0.41146200
C	-13.79831700	-0.41211600	3.20748500
H	-12.90161200	-0.11927800	3.76009300
H	-14.66399500	-0.23069600	3.85066100
H	-13.73723900	-1.48417000	3.01592900

4d(Si):

B3LYP/6-311G(2d,p): -9455.52569 a.u.

Point group: C_1

Cartesian coordinates:

C	-6.87775400	0.98513100	0.16905200
C	-5.53638900	0.90010200	0.14143500
C	-4.90291000	-0.44804900	0.11254900
C	-5.69207500	-1.53632400	0.11208300
H	-7.44807300	1.90459800	0.18931900
H	-5.35079900	-2.56281900	0.08986000
Si	-7.44036900	-0.82282200	0.14776200
C	-4.18297400	1.53617000	0.11562100
C	-3.55094100	0.18732500	0.08863200
C	-3.39209300	2.62370500	0.10213000
H	-3.73089200	3.65110900	0.11690900
C	-2.21029500	0.10000000	0.05390300
H	-1.64252200	-0.82096300	0.03059300
Si	-1.64541500	1.90700800	0.04961100
Si	0.04832300	2.41822200	1.66571800
Si	-9.06093000	-1.38051400	-1.53054900
Si	-9.04851200	-1.46542900	1.80798300
Si	-0.04966100	2.42428100	-1.66193900
C	-11.68834400	0.46967200	0.19671200
C	-12.32040200	-2.24355400	0.11110100
H	-11.32345300	1.48798700	0.22947600
C	-12.98237400	0.10579700	0.17825900
H	-12.43872500	-3.31840400	0.07347600
C	-13.31998500	-1.34469500	0.12742500
C	2.20982100	0.10152400	-0.05702300
C	3.39091000	2.62568100	-0.09800700
H	1.64231700	-0.81966400	-0.03618100
C	3.55045800	0.18932200	-0.09075400
H	3.72942800	3.65321300	-0.10995000
C	4.18210600	1.53841100	-0.11414700
Si	-10.76003300	-1.17993100	0.15076100
Si	1.64441400	1.90836600	-0.04788800
C	4.90262200	-0.44560000	-0.11521400

C	5.53572400 0.90279600 -0.14082600	H	8.28010000 -0.31443300 3.64568100
C	5.69211000 -1.53363800 -0.11635900	H	10.03687300 -0.53383800 3.66151100
H	5.35111600 -2.56027500 -0.09641300	C	9.16781700 -0.40241100 -3.37361800
C	6.87707600 0.98827200 -0.16760900	H	10.01576200 -0.71928600 -3.98644600
H	7.44714900 1.90794000 -0.18554000	H	8.25916100 -0.49842500 -3.97358700
Si	7.44021600 -0.81955400 -0.14957700	H	9.30300900 0.65213800 -3.12890000
Si	9.06005100 -1.37982700 1.52859300	C	8.85020500 -3.28389700 -2.29437900
Si	9.04914400 -1.45921900 -1.81018600	H	7.95007100 -3.42289200 -2.89867900
Si	10.75998000 -1.17708900 -0.15166900	H	9.70915300 -3.61499800 -2.88375000
C	-14.43907200 0.44463000 0.17188600	H	8.77169700 -3.93605000 -1.42242700
C	-14.77536900 -1.00525700 0.11328200	C	-0.09840600 1.40473800 -3.25340900
C	-15.44066100 1.34109400 0.18833500	H	-0.99794800 1.63739500 -3.82942200
C	-16.06784800 -1.37043800 0.06688600	H	0.77123100 1.62672700 -3.87753100
Si	-17.00293100 0.27702800 0.10006400	H	-0.09917300 0.33454400 -3.04200100
H	-15.32330500 2.41615000 0.22676800	C	-0.05881400 4.27005500 -2.10591000
H	-16.43065900 -2.38844200 0.02172200	H	0.81262000 4.51686400 -2.71787700
Si	-18.62256300 0.63020600 -1.63352000	H	-0.95540900 4.51743000 -2.68017800
Si	-18.79089300 0.46347500 1.68531300	H	-0.03981700 4.91089100 -1.22270600
Si	-20.37142000 0.08493000 -0.08227600	C	0.05577800 4.26216300 2.11710200
Si	-20.99184700 -2.20971600 -0.28148800	H	-0.81593800 4.50581100 2.72992900
Si	-22.29440800 1.49436800 -0.03729200	H	0.95213100 4.50811900 2.69235000
C	8.86659800 -3.17792800 2.10560500	H	0.03625800 4.90633300 1.23634600
H	9.72784100 -3.47889800 2.70762100	C	0.09822100 1.39187900 3.25273700
H	7.96906000 -3.28506300 2.72023800	H	0.10080500 0.32266000 3.03646200
H	8.78365200 -3.87390100 1.26862900	H	0.99726600 1.62336800 3.82999800
C	9.18606600 -0.24725500 3.03777800	H	-0.77192500 1.60962700 3.87763700
H	9.31979600 0.79425800 2.74190300	C	-8.86752200 -3.17779400 -2.11012100

H	-9.72889900	-3.47810300	-2.71227200	C	-21.76864700	-2.53620400	-1.97667500
H	-7.97015900	-3.28392500	-2.72518600	H	-21.06674900	-2.31863800	-2.78479400
H	-8.78417200	-3.87488800	-1.27411900	H	-22.05755100	-3.58859600	-2.06038700
C	-9.18740700	-0.24586000	-3.03813000	H	-22.66285700	-1.93152300	-2.14079700
H	-9.32080200	0.79528500	-2.74081500	C	-22.24844800	-2.68568000	1.05219700
H	-8.28168300	-0.31241300	-3.64646300	H	-23.17980200	-2.12448100	0.94801900
H	-10.03850400	-0.53143000	-3.66193200	H	-22.49313100	-3.74968500	0.97546300
C	-8.85005700	-3.29128200	2.28796400	H	-21.86002500	-2.50486400	2.05690500
H	-7.94949800	-3.43219900	2.89117700	C	-23.48029400	1.08862000	-1.45649400
H	-9.70870600	-3.62324200	2.87729000	H	-23.87980700	0.07556300	-1.37333300
H	-8.77268200	-3.94147300	1.41444400	H	-24.32783500	1.78097200	-1.44641600
C	-9.16589300	-0.41193900	3.37372400	H	-22.99136200	1.17575100	-2.42960400
H	-8.25710000	-0.50990300	3.97317300	C	-23.22225200	1.27245400	1.59846400
H	-9.30033400	0.64323500	3.13128900	H	-24.10550700	1.91843800	1.62182600
H	-10.01386100	-0.72946600	3.98617700	H	-23.55851700	0.24361900	1.74244900
C	-18.44441800	-0.44602200	-3.18360100	H	-22.59407100	1.53897700	2.45175300
H	-19.30269500	-0.31792600	-3.84892800	C	-21.81376800	3.31814700	-0.18537700
H	-17.54491500	-0.16118000	-3.73593600	H	-21.13930600	3.62554400	0.61654000
H	-18.36128100	-1.50491000	-2.93530900	H	-21.32383100	3.53142000	-1.13712700
C	-18.62992200	2.44568600	-2.19038200	H	-22.71000600	3.94331500	-0.12375900
H	-17.71151400	2.66887800	-2.73978900	C	-19.49756300	-3.36056600	-0.11055100
H	-19.47577000	2.64362800	-2.85420600	H	-18.75109400	-3.17293500	-0.88540600
H	-18.69442300	3.13832900	-1.34960000	H	-19.00679700	-3.25823900	0.85951900
C	-18.88673600	2.22408300	2.39355400	H	-19.82210700	-4.40114800	-0.20940200
H	-19.81706000	2.37026800	2.94900300	C	-18.77692100	-0.74819300	3.14117900
H	-18.05493100	2.39765600	3.08149600	H	-17.92239000	-0.54820300	3.79294600
H	-18.83810500	2.98552100	1.61297000	H	-19.68734600	-0.64577200	3.73819800

H	-18.70613500	-1.78326400	2.80468100	C	21.81515600	3.31616500	0.18668800
C	11.68897100	0.47218300	-0.19536900	H	21.14029600	3.62402500	-0.61471500
H	11.32449100	1.49067700	-0.22715000	H	21.32575500	3.52903400	1.13880200
C	12.31992300	-2.24138500	-0.11278900	H	22.71143800	3.94124900	0.12488300
H	12.43780000	-3.31632700	-0.07640000	C	22.24843100	-2.68702000	-1.05316200
C	13.31987400	-1.34291500	-0.12775600	H	21.86012600	-2.50596000	-2.05787200
C	12.98284700	0.10776400	-0.17710400	H	23.17975700	-2.12582500	-0.94872100
C	14.43967100	0.44600300	-0.17038300	H	22.49313400	-3.75103900	-0.97667500
C	14.77539500	-1.00406800	-0.11311600	C	19.49700300	-3.36168000	0.10837800
C	15.44160800	1.34208600	-0.18619900	H	18.74999900	-3.17380600	0.88265000
C	16.06773300	-1.36978500	-0.06701900	H	19.00706800	-3.25895200	-0.86207000
H	16.43016400	-2.38796800	-0.02281700	H	19.82094000	-4.40244200	0.20730700
Si	17.00346800	0.27734800	-0.09898800	C	21.76790800	-2.53903400	1.97565900
H	15.32466500	2.41722100	-0.22369500	H	21.06585000	-2.32181500	2.78373100
Si	18.62371800	0.62887800	1.63433500	H	22.05664000	-3.59151500	2.05883100
Si	18.79111400	0.46359500	-1.68466300	H	22.66216000	-1.93456600	2.14032300
Si	20.37189800	0.08349700	0.08238500	C	18.88764200	2.22432800	-2.39249100
Si	20.99162500	-2.21144700	0.28046300	H	18.05558900	2.39851200	-3.07997900
Si	22.29533800	1.49235900	0.03753300	H	18.83977000	2.98557500	-1.61167600
C	23.48157800	1.08565300	1.45617600	H	19.81776500	2.37019300	-2.94836000
H	23.88074200	0.07249900	1.37253500	C	18.77598200	-0.74775200	-3.14078700
H	24.32933900	1.77773800	1.44602700	H	19.68668700	-0.64646800	-3.73756500
H	22.99302400	1.17262200	2.42949300	H	18.70369800	-1.78277700	-2.80446400
C	23.22272100	1.27094200	-1.59855200	H	17.92186800	-0.54651900	-3.79272000
H	24.10629200	1.91650200	-1.62170900	C	18.44541600	-0.44794800	3.18399400
H	23.55847000	0.24201900	-1.74313000	H	19.30429800	-0.32124500	3.84880100
H	22.59453300	1.53821700	-2.45159700	H	17.54664000	-0.16231500	3.73710800

H 18.36081700 -1.50660000 2.93518400
C 18.63199200 2.44411100 2.19201800
H 19.47776100 2.64120300 2.85619800
H 18.69716500 3.13715900 1.35162200
H 17.71355700 2.66756900 2.74127100

5a:

B3LYP/6-311G(2d,p): -462.03168 a.u.

Point group: D_{2h}

Cartesian coordinates:

C 0.00000000 1.20817000 2.00287400
C 0.00000000 -1.20817000 2.00287400
C 0.00000000 -0.74154800 0.73917200
C 0.00000000 0.74154800 0.73917200
C 0.00000000 0.74154800 -0.73917200
C 0.00000000 -0.74154800 -0.73917200
C 0.00000000 1.20817000 -2.00287400
C 0.00000000 -1.20817000 -2.00287400
H 0.00000000 2.22038000 -2.37961100
H 0.00000000 -2.22038000 -2.37961100
H 0.00000000 -2.22038000 2.37961100
H 0.00000000 2.22038000 2.37961100
C 0.00000000 0.00000000 -4.21037800
H 0.00000000 -0.92458400 -4.77473200
H 0.00000000 0.92458400 -4.77473200
C 0.00000000 0.00000000 4.21037800
H 0.00000000 -0.92458400 4.77473200
H 0.00000000 0.92458400 4.77473200
C 0.00000000 0.00000000 2.86806500
C 0.00000000 0.00000000 -2.86806500

5b:

B3LYP/6-311G(2d,p): -921.62336 a.u.

Point group: D_{2h}

Cartesian coordinates:

C 0.00000000 1.20785800 6.82362600
C 0.00000000 -1.20785800 6.82362600
C 0.00000000 -0.74199400 5.55736700
C 0.00000000 0.74199400 5.55736700
C 0.00000000 0.74162900 4.08600500
C 0.00000000 -0.74162900 4.08600500
C 0.00000000 -1.20732300 2.81539800
C 0.00000000 1.20732300 2.81539800
C 0.00000000 0.00000000 0.62088600
C 0.00000000 0.00000000 -0.62088600
C 0.00000000 1.20732300 -2.81539800
C 0.00000000 -1.20732300 -2.81539800
C 0.00000000 -0.74162900 -4.08600500
C 0.00000000 0.74162900 -4.08600500
C 0.00000000 -0.74199400 -5.55736700
C 0.00000000 0.74199400 -5.55736700
C 0.00000000 -1.20785800 -6.82362600
C 0.00000000 1.20785800 -6.82362600
C 0.00000000 0.00000000 -9.03010000

H	0.00000000	0.92464900	-9.59412400
H	0.00000000	-0.92464900	-9.59412400
H	0.00000000	2.21967700	7.20101100
H	0.00000000	-2.21967700	7.20101100
H	0.00000000	-2.21389600	2.42749700
H	0.00000000	2.21389600	2.42749700
H	0.00000000	2.21389600	-2.42749700
H	0.00000000	-2.21389600	-2.42749700
H	0.00000000	-2.21967700	-7.20101100
H	0.00000000	2.21967700	-7.20101100
C	0.00000000	0.00000000	9.03010000
H	0.00000000	0.92464900	9.59412400
H	0.00000000	-0.92464900	9.59412400
C	0.00000000	0.00000000	1.97081700
C	0.00000000	0.00000000	7.68503700
C	0.00000000	0.00000000	-1.97081700
C	0.00000000	0.00000000	-7.68503700

5c:

B3LYP/6-311G(2d,p): -1381.21807 a.u.

Point group: D_{2h}

Cartesian coordinates:

C	0.00000000	1.20631200	7.63228300
C	0.00000000	-1.20631200	7.63228300
C	0.00000000	-0.74203300	8.90496300
C	0.00000000	0.74203300	8.90496300
C	0.00000000	0.74232700	10.37430100
C	0.00000000	-0.74232700	10.37430100
C	0.00000000	1.20785400	11.64163900
C	0.00000000	-1.20785400	11.64163900
C	0.00000000	0.00000000	5.43689100
C	0.00000000	0.00000000	4.19928900
C	0.00000000	-1.20525700	2.00633300
C	0.00000000	1.20525700	2.00633300
C	0.00000000	0.74253100	0.72987700
C	0.00000000	-0.74253100	0.72987700
C	0.00000000	-0.74253100	-0.72987700
C	0.00000000	0.74253100	-0.72987700
C	0.00000000	1.20525700	-2.00633300
C	0.00000000	-1.20525700	-2.00633300
C	0.00000000	0.00000000	-4.19928900
C	0.00000000	0.00000000	-5.43689100
C	0.00000000	-1.20631200	-7.63228300
C	0.00000000	1.20631200	-7.63228300
C	0.00000000	0.74203300	-8.90496300
C	0.00000000	-0.74203300	-8.90496300
C	0.00000000	0.74232700	-10.37430100
C	0.00000000	-0.74232700	-10.37430100
C	0.00000000	1.20785400	-11.64163900
C	0.00000000	-1.20785400	-11.64163900
C	0.00000000	0.00000000	-13.84755000
H	0.00000000	-0.92462300	-14.41154100
H	0.00000000	0.92462300	-14.41154100
H	0.00000000	2.21952900	12.01935000

H	0.00000000	-2.21952900	12.01935000
H	0.00000000	-2.21246200	7.24336700
H	0.00000000	2.21246200	7.24336700
H	0.00000000	-2.21097800	2.39613600
H	0.00000000	2.21097800	2.39613600
H	0.00000000	2.21097800	-2.39613600
H	0.00000000	-2.21097800	-2.39613600
H	0.00000000	-2.21246200	-7.24336700
H	0.00000000	2.21246200	-7.24336700
H	0.00000000	2.21952900	-12.01935000
H	0.00000000	-2.21952900	-12.01935000
C	0.00000000	0.00000000	13.84755000
H	0.00000000	-0.92462300	14.41154100
H	0.00000000	0.92462300	14.41154100
C	0.00000000	0.00000000	-12.50165800
C	0.00000000	0.00000000	-6.79198600
C	0.00000000	0.00000000	-2.84143200
C	0.00000000	0.00000000	2.84143200
C	0.00000000	0.00000000	6.79198600
C	0.00000000	0.00000000	12.50165800

5d:

B3LYP/6-311G(2d,p): -1840.81438 a.u.

Point group: C_1

Cartesian coordinates:

C	2.81071700	-1.20341700	-0.00099700
C	2.81073500	1.20344400	-0.00089700
C	4.09112500	0.74310100	-0.00085700
C	4.09111400	-0.74309300	-0.00089700
C	5.54607500	-0.74305300	-0.00076500
C	5.54609000	0.74303500	-0.00069400
C	6.82542500	-1.20428600	-0.00059000
C	6.82544800	1.20424200	-0.00051000
C	0.61568800	0.00002200	-0.00094200
C	9.01842700	-0.00004600	-0.00021400
C	10.25365200	-0.00004200	0.00001000
C	-0.61568800	0.00003400	-0.00091700
C	-2.81072300	1.20347900	-0.00090500
C	-2.81072800	-1.20338100	-0.00080500
C	12.44995400	1.20564100	0.00042500
C	12.44996900	-1.20569600	0.00038500
C	-4.09112100	-0.74304600	-0.00074400
C	-4.09111700	0.74314900	-0.00078300
C	13.72390700	0.74218000	0.00063600
C	13.72391600	-0.74221800	0.00061800
C	-5.54608200	0.74309700	-0.00063100
C	-5.54608100	-0.74299100	-0.00056100
C	15.19194100	-0.74248600	0.00079900
C	15.19193400	0.74246300	0.00082800
C	-6.82543700	-1.20420900	-0.00036500
C	-6.82543500	1.20431800	-0.00044200
C	16.45986900	1.20779700	0.00093100
C	16.45988100	-1.20780700	0.00089800
C	-9.01842700	0.00004700	-0.00004800

C -10.25365200 0.00003600 0.00012100
C 18.66562700 0.00000800 0.00110000
H 19.22956700 -0.92461500 0.00113300
H 19.22955500 0.92463900 0.00114300
C -12.44998200 1.20567800 0.00042200
C -12.44994200 -1.20566000 0.00046200
C -13.72390000 -0.74221200 0.00063300
C -13.72392500 0.74218600 0.00061400
C -15.19192500 -0.74251400 0.00077800
C -15.19195100 0.74243500 0.00074800
C -16.45985400 -1.20786300 0.00083900
C -16.45989600 1.20774200 0.00080600
C -18.66562700 -0.00009500 0.00093700
H -19.22957400 0.92452400 0.00095900
H -19.22954900 -0.92473000 0.00098200
H 16.83775400 -2.21939500 0.00090100
H 16.83773200 2.21938900 0.00097500
H 12.06054200 2.21156100 0.00036900
H 12.06057200 -2.21162200 0.00030200
H 7.21618500 -2.20957600 -0.00057600
H 7.21623000 2.20952400 -0.00040300
H 2.41942800 2.20850700 -0.00088300
H 2.41939600 -2.20847500 -0.00104400
H -2.41940700 2.20854000 -0.00096100
H -2.41941500 -2.20844300 -0.00080000
H -7.21621000 -2.20949500 -0.00025900
H -7.21620400 2.20960500 -0.00042800
H -12.06059600 2.21160800 0.00035100
H -12.06051900 -2.21157600 0.00042200
H -16.83770500 -2.21945900 0.00087100
H -16.83778200 2.21932500 0.00079600
C -17.31899900 -0.00007600 0.00088100
C -11.61232100 0.00002500 0.00031400
C -7.65578200 0.00005600 -0.00024800
C -1.98293800 0.00004900 -0.00087400
C 1.98293900 0.00002100 -0.00096200
C 7.65578200 -0.00003000 -0.00042900
C 11.61232000 -0.00003300 0.00024900
C 17.31899900 -0.00000100 0.00100000

4a(C):

B3LYP/6-311G(2d,p): -1782.39449 a.u.

Point group: C_1

Cartesian coordinates:

C 2.00634800 -1.27022800 0.00002200
C 0.79486100 -0.70013300 0.00001200
C 0.69727800 0.79813800 -0.00001400
C 1.82449000 1.52073100 -0.00005700
H 2.19601300 -2.33607700 0.00000800
H 1.87739500 2.60190300 -0.00003500
Si 3.19369600 0.20916200 -0.00003800
C -0.69715600 -0.79733800 0.00009000
C -0.79473600 0.70093400 0.00002700
C -1.82437200 -1.51992800 0.00019800

H -1.87727300 -2.60110000 0.00022400
C -2.00621900 1.27103400 -0.00000200
H -2.19588800 2.33688400 -0.00003600
Si -3.19357400 -0.20834900 0.00010100
Si 5.83832200 -0.03448000 -0.00003000
Si -5.83837900 0.03378100 -0.00008000
C -4.53063600 -0.24903500 -1.35916800
H -4.60589000 -1.23315500 -1.82901200
H -4.44724000 0.49627300 -2.14986000
C -4.53088000 -0.24874700 1.35921600
H -4.44771600 0.49645900 2.15001500
H -4.60613400 -1.23295300 1.82891500
C 4.53094200 0.24953200 -1.35916700
H 4.60678400 1.23404100 -1.82814500
H 4.44729700 -0.49503800 -2.15051100
C 4.53092900 0.24960600 1.35909600
H 4.44731500 -0.49490800 2.15049200
H 4.60675800 1.23416500 1.82797100
C 6.49749300 -1.79719600 0.00013900
H 7.11285900 -1.98595200 0.88389800
H 5.68298700 -2.52589800 0.00016200
H 7.11308900 -1.98624300 -0.88339100
C 7.25945800 1.19853600 -0.00010800
H 7.89014200 1.06934500 0.88371200
H 7.88979900 1.06965900 -0.88421500
H 6.89068000 2.22717300 0.00015000
C -6.49960500 1.79572500 0.00004700
H -5.68594700 2.52537500 0.00037400
H -7.11523300 1.98418400 -0.88358000
H -7.11535000 1.98359000 0.88373800
C -7.25811900 -1.20084900 -0.00022900
H -7.88917200 -1.07216600 0.88340000
H -7.88836300 -1.07275400 -0.88452400
H -6.88826600 -2.22909400 0.00027200

4b(C):

B3LYP/6-311G(2d,p): -2747.32722 a.u.

Point group: C_1

Cartesian coordinates:

C 6.62526400 1.15193100 0.00002900
C 5.33914600 0.78011200 -0.00000900
C 5.00665100 -0.68390200 -0.00005000
C 6.00576100 -1.57532300 -0.00006700
H 6.98069200 2.17450100 0.00005300
H 5.88778300 -2.65129200 -0.00008700
Si 7.56518300 -0.49631200 -0.00000200
C 3.88176000 1.11207300 -0.00002500
C 3.54867500 -0.35269300 -0.00004700
C 2.88309400 2.00397000 -0.00002900
H 3.00032000 3.07995300 -0.00002800
C 2.26231000 -0.72403400 -0.00007300
H 1.90540300 -1.74592900 -0.00010500
Si 1.32677200 0.92464500 -0.00002300
C -2.26234100 -0.72398600 -0.00000100

C	-2.88309300	2.00402600	0.00000600
H	-1.90544100	-1.74588500	0.00000600
C	-3.54870600	-0.35263600	-0.00001500
H	-3.00031300	3.08000900	0.00002400
C	-3.88176100	1.11213500	-0.00000600
Si	10.21562200	-0.55951900	0.00003600
Si	-1.32678200	0.92468700	0.00002400
C	-5.00669200	-0.68382200	-0.00003100
C	-5.33914700	0.78019800	-0.00000100
C	-6.00585600	-1.57519200	-0.00008300
H	-5.88793800	-2.65117000	-0.00007800
C	-6.62524300	1.15207900	0.00001700
H	-6.98063800	2.17465800	0.00003800
Si	-7.56522900	-0.49608900	-0.00003500
Si	-10.21562900	-0.55976400	0.00002000
C	0.00000900	1.15730300	-1.34943900
H	-0.00002200	0.47672400	-2.19885000
H	0.00004800	2.18191800	-1.73240900
C	-0.00001300	1.15726500	1.34942800
H	-0.00001800	0.47666800	2.19882400
H	0.00000100	2.18187100	1.73242400
C	8.88454500	-0.72709600	-1.35588200
H	8.88303000	-0.01031400	-2.17630000
H	8.84985700	-1.73287800	-1.78372000
C	11.02307100	1.14046100	0.00001700
H	10.27524500	1.93737700	-0.00022800
H	11.65247900	1.27534400	0.88374700
H	11.65287300	1.27518200	-0.88345900
C	11.52729300	-1.90831300	0.00007900
H	12.16633500	-1.83264800	-0.88395300
H	12.16656100	-1.83233700	0.88392100
H	11.07351900	-2.90235700	0.00031000
C	8.88445800	-0.72710000	1.35591100
H	8.84980700	-1.73284500	1.78382700
H	8.88287900	-0.01024100	2.17626500
C	-8.88451400	-0.72714700	-1.35591200
H	-8.84938600	-1.73279800	-1.78400600
H	-8.88325900	-0.01016900	-2.17617500
C	-8.88453000	-0.72721100	1.35587600
H	-8.88322000	-0.01033600	2.17622500
H	-8.84942300	-1.73292700	1.78381900
C	-11.02254500	1.14044100	0.00009300
H	-11.65184100	1.27550400	0.88388900
H	-10.27449800	1.93714200	-0.00023400
H	-11.65244900	1.27539900	-0.88328700
C	-11.52759600	-1.90824600	0.00005200
H	-12.16689700	-1.83205100	0.88385300
H	-12.16656500	-1.83251300	-0.88402400
H	-11.07401800	-2.90237600	0.00040200

4c(C):

B3LYP/6-311G(2d,p): -3712.25982 a.u.

Point group: C_1

Cartesian coordinates:

C	-2.22050400	-0.84099100	-0.00020500	Si	5.73356100	-0.93135000	-0.00002200
C	-0.91931100	-0.52595900	-0.00017000	C	9.44607900	0.59875800	0.00004400
C	-0.52236700	0.92258900	-0.00011200	C	9.74770000	-0.87191200	0.00003500
C	-1.48092200	1.85747300	-0.00008200	C	10.46363100	1.46901500	0.00011400
H	-2.62134600	-1.84643400	-0.00023200	H	10.36821900	2.54722100	0.00010900
H	-1.31673600	2.92725900	-0.00001300	C	11.02571800	-1.27072800	0.00004200
Si	-3.08354600	0.84738300	-0.00013300	H	11.35960800	-2.30054800	0.00008400
C	0.52218300	-0.92137100	-0.00015000	Si	12.00011000	0.35747600	0.00008800
C	0.91912000	0.52717800	-0.00010300	Si	14.65154900	0.37838100	0.00009300
C	1.48075600	-1.85624000	-0.00012100	C	-9.44581200	-0.59896900	-0.00003100
H	1.31660000	-2.92603200	-0.00010800	C	-9.74786100	0.87161300	0.00007100
C	2.22030800	0.84223300	-0.00004700	C	-10.46312500	-1.46950400	-0.00002200
H	2.62112600	1.84768500	0.00002000	C	-11.02599200	1.27007400	0.00015900
Si	3.08336400	-0.84612600	-0.00006500	Si	-11.99992100	-0.35839900	0.00010200
C	-6.70307800	-0.69639900	-0.00013200	H	-10.36743300	-2.54768500	-0.00009800
C	-7.26676200	2.04412600	0.00002000	H	-11.36016100	2.29980200	0.00026200
H	-6.36751200	-1.72549900	-0.00020100	Si	-14.65133900	-0.37996000	0.00011700
C	-7.98136000	-0.29829600	-0.00006700	C	4.40009700	-1.13148800	1.34834200
H	-7.36133500	3.12231400	0.00008300	H	4.36702000	-2.15985100	1.71996400
C	-8.28383000	1.17321500	0.00002800	H	4.42139200	-0.46027600	2.20479100
C	6.70338400	0.69701600	0.00004000	C	4.40012100	-1.13142100	-1.34844000
C	7.26623600	-2.04368000	-0.00001400	H	4.42139300	-0.46016400	-2.20485400
H	6.36814300	1.72622100	0.00006300	H	4.36710300	-2.15977200	-1.72010200
C	7.98154400	0.29851700	0.00002400	C	-4.40033200	1.13286500	-1.34843200
H	7.36046200	-3.12189900	-0.00000300	H	-4.42152000	0.46209900	-2.20522500
C	8.28357600	-1.17308300	0.00000800	H	-4.36742900	2.16144400	-1.71950400
Si	-5.73374400	0.93226500	-0.00008300	C	-4.40029900	1.13274800	1.34823800

H -4.36733300 2.16129100 1.71940600
H -4.42150200 0.46191000 2.20497500
C -13.32282800 -0.56450300 -1.35622200
H -13.30320100 -1.56862400 -1.78874500
H -13.31085000 0.15592300 -2.17341200
C -13.32288300 -0.56460800 1.35642400
H -13.31085200 0.15575800 2.17366600
H -13.30334900 -1.56875500 1.78889000
C -15.98077100 -1.71113500 0.00004000
H -16.61894500 -1.62652900 0.88387300
H -16.61868900 -1.62654500 -0.88398400
H -15.54058500 -2.71126000 0.00010600
C -15.43643900 1.33040300 0.00013500
H -14.67828800 2.11750600 0.00011000
H -16.06427800 1.47337400 -0.88344300
H -16.06422000 1.47339000 0.88375700
C 13.32309800 0.56319700 -1.35624000
H 13.30387600 1.56721100 -1.78900600
H 13.31085200 -0.15742200 -2.17326400
C 13.32307300 0.56294100 1.35646400
H 13.31076600 -0.15781300 2.17336600
H 13.30389400 1.56687900 1.78941800
C 15.98066500 1.70987900 0.00003200
H 16.61904600 1.62536400 0.88372200
H 16.61843800 1.62551100 -0.88412700
H 15.54023100 2.70989000 0.00024200
C 15.43693400 -1.33185300 0.00001300
H 16.06506400 -1.47461000 0.88340900
H 14.67889500 -2.11906600 0.00035100
H 16.06444700 -1.47484700 -0.88380200

4d(C):

B3LYP/6-311G(2d,p): -4677.19242 a.u.

Point group: C_1

Cartesian coordinates:

C 6.62681000 0.83107000 0.00001800
C 5.33553800 0.47745300 0.00001200
C 4.98195900 -0.98222600 0.00007100
C 5.96787000 -1.88815700 0.00012700
H 6.99768200 1.84795000 -0.00003500
H 5.83549800 -2.96234800 0.00019100
Si 7.53988500 -0.83083000 0.00011900
C 3.88287200 0.82970800 -0.00006300
C 3.52936500 -0.63011800 -0.00001000
C 2.89682100 1.73555500 -0.00016700
H 3.02888100 2.80976800 -0.00019600
C 2.23815800 -0.98386600 -0.00007000
H 1.86746000 -2.00080300 -0.00005500
Si 1.32543000 0.67784400 -0.00018700
C 11.13362900 0.79199000 0.00009900
C 11.74389300 -1.93856500 0.00020800
H 10.78065400 1.81524300 0.00008500
C 12.41853500 0.41568000 0.00014100
H 11.85686800 -3.01498100 0.00023000

C	12.74596100	-1.05046300	0.00019400	C	-11.74389200	-1.93856100	-0.00008100
C	-2.23815700	-0.98385900	-0.00023900	H	-11.85686600	-3.01497800	-0.00001900
C	-2.89682200	1.73556300	-0.00042200	C	-12.74596100	-1.05046100	-0.00006100
H	-1.86745900	-2.00079600	-0.00015600	C	-12.41853500	0.41568300	-0.00013800
C	-3.52936400	-0.63011200	-0.00031100	C	-13.87775700	0.74117000	-0.00008600
H	-3.02888300	2.80977500	-0.00050300	C	-14.20458800	-0.72406400	0.00002000
C	-3.88287200	0.82971500	-0.00040000	C	-14.88024400	1.62876300	-0.00005300
Si	10.19224800	-0.85306900	0.00014800	C	-15.48924500	-1.10088500	0.00017500
Si	-1.32543000	0.67785300	-0.00030300	H	-15.84073900	-2.12481300	0.00025300
C	-4.98195800	-0.98221900	-0.00033100	Si	-16.43564600	0.54376800	0.00015800
C	-5.33553900	0.47745900	-0.00038300	H	-14.76640500	2.70517600	-0.00009000
C	-5.96786900	-1.88815100	-0.00029400	Si	-19.08625200	0.60054300	0.00043900
H	-5.83549700	-2.96234200	-0.00027500	C	0.00006100	0.92289200	-1.34844100
C	-6.62681000	0.83107600	-0.00037100	H	0.00011100	0.25353300	-2.20655100
H	-6.99768300	1.84795600	-0.00039200	H	0.00005500	1.95281700	-1.71727400
Si	-7.53988500	-0.83082500	-0.00029500	C	-0.00006000	0.92293300	1.34795200
Si	-10.19224800	-0.85306400	-0.00018400	C	-8.86329900	-1.07887900	1.34879800
C	13.87775600	0.74116900	0.00015500	C	-8.86340700	-1.07898600	-1.34926900
C	14.20458900	-0.72406500	0.00019400	C	-17.75555200	0.77016200	-1.35576400
C	14.88024200	1.62876200	0.00011400	C	-17.75526800	0.77033300	1.35632900
C	15.48924600	-1.10088500	0.00016300	C	-19.89050800	-1.10084700	0.00062400
Si	16.43564500	0.54376900	0.00012200	C	-20.40000900	1.94723200	0.00054200
H	14.76640200	2.70517500	0.00005100	C	8.86333700	-1.07888700	1.34917700
H	15.84074100	-2.12481300	0.00019800	C	8.86336900	-1.07898800	-1.34889100
Si	19.08625000	0.60054900	0.00006500	C	17.75543800	0.77027700	1.35613600
C	-11.13363000	0.79199400	-0.00020900	C	17.75537800	0.77022200	-1.35595500
H	-10.78065600	1.81524700	-0.00029200	C	19.89051400	-1.10084700	0.00009200

C 20.40000900 1.94724500 -0.00003500
H 20.52010300 -1.23671500 0.88353500
H 20.51957600 -1.23699000 -0.88368200
H 19.14112400 -1.89629700 0.00045000
H 21.03877600 1.87072100 0.88410800
H 21.03928300 1.86995000 -0.88375100
H 19.94787800 2.94202700 -0.00060800
H 17.75239900 0.05234800 2.17556500
H 17.72300500 1.77548500 1.78543300
H 17.72293300 1.77537600 -1.78536200
H 17.75228200 0.05218900 -2.17529500
H 8.85470400 -2.10531400 1.72727600
H 8.86882800 -0.40220700 2.20161300
H 8.85480200 -2.10543700 -1.72692900
H 8.86884500 -0.40235500 -2.20136300
H -0.00011700 0.25334800 2.20589300
H -0.00004300 1.95275200 1.71704600
H -8.85470700 -2.10529800 1.72691500
H -8.86893800 -0.40237400 -2.20175800
H -8.86873400 -0.40218000 2.20121900
H -8.85479800 -2.10544300 -1.72728700
H -17.75210000 0.05236800 2.17572900
H -17.72279200 1.77552200 1.78565000
H -17.75258100 0.05216300 -2.17513200
H -17.72315400 1.77533300 -1.78514800
H -20.51948900 -1.23691900 0.88446600
H -19.14111400 -1.89629400 0.00026500
H -20.52017500 -1.23678800 -0.88275100
H -19.94788000 2.94201400 0.00099700
H -21.03920800 1.87000600 0.88431900
H -21.03885100 1.87063500 -0.88354100