Supporting Information File

Structures and Electronic Properties of Si-substituted Benzenes and Their Transition-Metal Complexes

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Available Information:

1. Cartesian Coordinates for Ground State Optimized Structures and their Energies in Hartrees.
2. Harmonic Frequencies.
3. Complete Reference 12.

1. H_6C_6:

	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.398803	0.000000
2	6	-1.211399	0.699402	0.000000
3	6	1.211399	0.699402	0.000000
4	1	-2.153099	1.243092	0.000000
5	1	2.153099	1.243092	0.000000
6	6	-1.211399	-0.699402	0.000000
7	6	1.211399	-0.699402	0.000000
8	1	-2.153099	-1.243092	0.000000
9	1	2.153099	-1.243092	0.000000
10	6	0.000000	-1.398803	0.000000
11	1	0.000000	-2.486185	0.000000
12	1	0.000000	2.486185	0.000000

B3LYP/6-31+G(d) = -232.2589322 Hartree

Low frequencies (cm^{-1}): 413.4502 413.4549 620.3197 620.3224 692.8050
712.5618
865.9929 865.9931 983.1435

2. H_6C_5Si:

	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000005	1.247412	1.017910
2	6	0.000000	-0.000005	1.664635
3	6	0.000005	-1.247417	1.017903
4	6	0.000005	-1.449556	-0.369771
5	6	-0.000005	1.449558	-0.369763
6	1	-0.000008	2.129159	1.660199
7	1	0.000000	-0.000008	2.751970
8	1	0.000008	-2.129168	1.660187
9	1	0.000009	-2.471902	-0.739692
10	1	0.000000	0.000008	-2.868406
11	1	-0.000009	2.471906	-0.739678
12	14	0.000000	0.000004	-1.392157

B3LYP/6-31+G(d) = -483.6051409 Hartree

Low frequencies (cm^{-1}): 274.8861 369.1071 427.6451 434.1347 492.0368
584.0740
715.4244 718.5447 765.8282

3. $H_6C_4Si_2$:

	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.583820	0.626983
2	6	0.000000	0.709174	1.711798
3	1	0.000000	2.096550	-2.183944
4	1	0.000000	1.164883	2.702461
5	6	0.000000	-0.709174	1.711798
6	1	0.000000	-2.096550	-2.183944
7	1	0.000000	-1.164883	2.702461
8	6	0.000000	-1.583820	0.626983
9	1	0.000000	-2.646730	0.871542
10	1	0.000000	2.646730	0.871542
11	14	0.000000	1.089945	-1.101625
12	14	0.000000	-1.089945	-1.101625

B3LYP/6-31+G(d) = -734.9692431 Hartree

Low frequencies (cm^{-1}): 75.8642 312.6491 319.8407 321.0863 403.2937 436.8066
541.5052 576.7271 677.1147

4. $H_6C_4Si_2$:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	1.263114	1.168696
6	0.000000	0.000000	1.786498
1	0.000000	2.829511	-1.185813
1	0.000000	0.000000	2.879512
6	0.000000	0.000000	-1.578750
6	0.000000	-1.263114	1.168696
1	0.000000	0.000000	-2.665825
1	0.000000	-2.133405	1.822047
1	0.000000	-2.829511	-1.185813
1	0.000000	2.133405	1.822047
14	0.000000	1.470744	-0.598464
14	0.000000	-1.470744	-0.598464

B3LYP/6-31+G(d) = -734.9707343 Hartree

Low frequencies (cm^{-1}): 253.6025 254.1864 358.0669 362.1902 457.5468 462.1047
481.7770 634.2770 710.9174

5. $H_6C_4Si_2$:

	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.510001	0.700877
2	6	0.000000	1.510001	-0.700877
3	1	0.000000	0.000000	3.135581
4	1	0.000000	2.476235	-1.208534
5	6	0.000000	-1.510001	0.700877
6	1	0.000000	-2.476235	1.208534
7	1	0.000000	0.000000	-3.135581
8	6	0.000000	-1.510001	-0.700877
9	1	0.000000	-2.476235	-1.208534
10	1	0.000000	2.476235	1.208534
11	14	0.000000	0.000000	1.659807
12	14	0.000000	0.000000	-1.659807

B3LYP/6-31+G(d) = -734.9526129 Hartree

Low frequencies (cm^{-1}): 206.9365 251.1908 331.4550 354.2257 362.1066 383.3496 503.2075 599.5605 654.8710

6. $H_6C_3Si_3$:

	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.537976	0.887951	0.000000
2	1	0.000000	3.243745	0.000000
3	1	2.809166	-1.621872	0.000000
4	6	-1.537976	0.887951	0.000000
5	6	0.000000	-1.775901	0.000000
6	1	-2.480605	1.432178	0.000000
7	1	0.000000	-2.864356	0.000000
8	1	-2.809166	-1.621872	0.000000
9	1	2.480605	1.432178	0.000000
10	14	0.000000	1.760495	0.000000
11	14	-1.524634	-0.880248	0.000000
12	14	1.524634	-0.880248	0.000000

B3LYP/6-31+G(d) = -986.3519472 Hartree

Low frequencies (cm^{-1}): 216.3301 216.3324 295.7271 295.7395 314.3256 457.9880 481.9873 514.6421 514.6450

7. $H_6C_3Si_3$:

	Atomic	Coordinates (Angstroms)

	Number	X	Y	Z
1	6	-0.069139	1.431719	1.273747
2	6	-0.092990	2.023798	0.000000
3	1	0.010597	-0.639039	3.138369
4	1	-0.133731	3.115689	0.000000
5	6	-0.069139	1.431719	-1.273747
6	1	0.015094	-3.153844	0.000000
7	1	-0.106123	2.128429	-2.112134
8	1	0.010597	-0.639039	-3.138369
9	1	-0.106123	2.128429	2.112134
10	14	-0.069139	-0.306074	1.695468
11	14	0.259513	-1.692426	0.000000
12	14	-0.069139	-0.306074	-1.695468

B3LYP/6-31+G(d) = -986.3443725 Hartree

Low frequencies (cm^{-1}): 89.6965 231.6217 237.0725 312.3506 325.5892

417.0585438.5486 486.5345 512.1004

8. $H_6C_3Si_3$:

	Atomic	Coordinates (Angstroms)		
	Number	X	Y	Z
1	6	-0.246112	-1.828592	0.196381
2	6	1.106673	-1.523825	0.074433
3	1	-2.994581	-1.174777	0.431354
4	1	1.809652	-2.358475	0.118575
5	1	-1.830934	2.606868	-0.135656
6	1	3.292304	0.203714	-0.246711
7	6	0.805865	1.555972	-0.195420
8	1	1.266318	2.535932	-0.320965
9	1	-0.495210	-2.885411	0.327475
10	14	-1.646345	-0.681918	0.076760
11	14	-0.963467	1.412105	0.001407
12	14	1.820804	0.116300	-0.122912

B3LYP/6-31+G(d) = -986.3336303 Hartree

Low frequencies (cm^{-1}): 81.3573 232.7966 261.6123 283.2628 302.0065 416.7843

426.2498 452.8731 509.3199

9. $H_6C_2Si_4$:

	Atomic	Coordinates (Angstroms)		
	Number	X	Y	Z

1	6	0.030107	-0.693787	1.950121
2	1	0.102847	-1.968722	-2.667739
3	1	0.062921	-1.169746	2.934447
4	6	-0.030107	0.693787	1.950121
5	1	-0.102847	1.968722	-2.667739
6	1	-0.062921	1.169746	2.934447
7	1	-0.047556	3.283713	0.952139
8	1	0.047556	-3.283713	0.952139
9	14	-0.178103	-1.107063	-1.489571
10	14	0.178103	1.107063	-1.489571
11	14	-0.178103	1.857331	0.566744
12	14	0.178103	-1.857331	0.566744

B3LYP/6-31+G(d) = -1237.7178633 Hartree

Low frequencies (cm^{-1}): 105.4045 146.8174 188.7185 236.7439 321.2806 357.4862

373.8083 380.2395 434.0659

10. $H_6C_2Si_4$:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
1	6	0.000000	0.000000	1.932696
2	1	0.000000	2.827380	1.907276
3	1	0.000000	-2.827380	1.907276
4	1	0.000000	2.827380	-1.907276
5	1	0.000000	-2.827380	-1.907276
6	6	0.000000	0.000000	-1.932696
7	1	0.000000	0.000000	-3.024732
8	1	0.000000	0.000000	3.024732
9	14	0.000000	1.579017	1.110204
10	14	0.000000	1.579017	-1.110204
11	14	0.000000	-1.579017	1.110204
12	14	0.000000	-1.579017	-1.110204

B3LYP/6-31+G(d) = -1237.7094307 Hartree

Low frequencies (cm^{-1}): 92.6779 96.5143 219.4706 221.9674 250.9033 304.5814

403.5295 410.8711 415.0709

11. $H_6C_2Si_4$:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
1	6	0.090401	1.167062	1.567507
2	1	0.183073	3.472306	0.000000

3	1	0.073847	-1.108931	3.149848
4	6	0.090401	1.167062	-1.567507
5	1	0.146550	1.785152	-2.464163
6	1	0.172444	-3.265033	0.000000
7	1	0.073847	-1.108931	-3.149848
8	1	0.146550	1.785152	2.464163
9	14	0.126476	1.990660	0.000000
10	14	0.090401	-0.597168	-1.751769
11	14	-0.441644	-1.908071	0.000000
12	14	0.090401	-0.597168	1.751769

B3LYP/6-31+G(d) = -1237.72449135 Hartree

Low frequencies (cm^{-1}): 123.5088 189.0899 193.1785 242.1422 280.4304

336.1504

390.8952 450.2868 456.2813

12. $H_6C_1Si_5$:

Atomic		Coordinates (Angstroms)		
Number		X	Y	Z
1	6	0	-0.003175	-2.096100	-0.294018
2	1	0	0.007995	-2.619634	2.423952
3	1	0	0.007995	-1.851648	-3.051135
4	1	0	-0.221967	0.960877	3.353256
5	1	0	-0.221967	1.846360	-2.959487
6	1	0	-0.230802	3.418406	0.479497
7	1	0	-0.030522	-3.177585	-0.445717
8	14	0	-0.080185	-1.548447	1.396417
9	14	0	0.243073	0.592960	1.988297
10	14	0	-0.275171	1.942716	0.272503
11	14	0	0.243073	1.117107	-1.748427
12	14	0	-0.080185	-1.104501	-1.768544

B3LYP/6-31+G(d) = -1489.1042174 Hartree

Low frequencies (cm^{-1}): 109.5813 109.7184 163.4449 178.2905 236.1815 292.5505

317.8130 377.0508 427.2493

13. H_6Si_6:

Atomic		Coordinates (Angstroms)		
Number		X	Y	Z
1	1	0	0.000000	3.668626	0.057918
2	1	0	-3.177123	-1.834313	0.057918

3	1	0	3.177123	1.834313	-0.057918
4	1	0	0.000000	-3.668626	-0.057918
5	1	0	3.177123	-1.834313	0.057918
6	1	0	-3.177123	1.834313	-0.057918
7	14	0	0.000000	2.204312	-0.217620
8	14	0	1.908990	-1.102156	-0.217620
9	14	0	0.000000	-2.204312	0.217620
10	14	0	-1.908990	-1.102156	-0.217620
11	14	0	-1.908990	1.102156	0.217620
12	14	0	1.908990	1.102156	0.217620

B3LYP/6-31+G(d) = -1740.4943622 Hartree

Low frequencies (cm^{-1}): 105.2759 105.2759 149.1546 149.1546 150.2375 192.2548

351.2242 373.0539 373.0539

Complete Reference 15:

Gaussian 03, Revision C.01,
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