Supporting Information for the Article Entitled "Diverse Coordination Modes in Tin Analogues of Cyclopentadienyl Anion Depending on the Substituents on the Tin Atom"

Takuya Kuwabara,[a] Marisa Nakada,[a] Jing-Dong Guo,[b] Shigeru Nagase,[b] and Masaichi Saito*,[a]

[a]Department of Chemistry, Graduate School of Science and Engineering, Saitama University, Shimo-okubo, Sakura-ku, Saitama-city, Saitama 338-8570, Japan

[b]Fukui Institute for Fundamental Chemistry, Kyoto University, Takano-Nishihiraki-cho, Sakyo-ku, Kyoto 606-8103, Japan

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1. Experimental details

General Procedure. All experiments were performed under argon atmosphere in a glovebox or using a standard Schlenk technique. Compounds **1** was prepared by the literature method.[S1] Toluene, hexane, pentane, diethyl ether, and benzene-d_6 for NMR measurement were purified by potassium mirror before used. CCl_4, MeI, EtBr, and Me_3SiCl were distilled over calcium hydride. ^{1}H NMR (400 or 500 MHz), ^{13}C NMR (101 MHz), ^{7}Li NMR (194 MHz), ^{29}Si NMR (99 MHz) and ^{119}Sn NMR (187 MHz) were recorded on a Bruker DPX-400 Cryo or an AVANCE-500T. The intensity data for X-ray crystallographic analyses were collected at −198 °C on a Bruker SMART APEX equipped with a CCD area detector with graphite-monochromated MoKα radiation (λ = 0.71073 Å) and graphite monochrometer. The structures were solved by direct methods, and refined by full-matrix least-squares method by SHELXL-97 program.[S2] UV-vis spectra were recorded on a Hitachi U-1900 spectrophotometer. Cyclic voltammetry was measured on a Gamry Interface1000 in a glove box.

Synthesis of 2-5 Anionic sandwich complex **1** was put into a Schlenk flask and dissolved in toluene in a glovebox. Stocked solutions of the halides prepared in toluene was injected into the flask via syringe under Ar stream. After from 30 min to 2 hours, the solvent was evaporated in the glovebox. Materials insoluble in hexane were removed by filtration through Celite® to give a crude product. Recrystallization from hexane (**2**), pentane (**3**), Et_2O (**4**, **5**) at –30 °C provided single crystals of the corresponding stannole complexes.

Chloro derivative **2**: green crystals of **2** (34 mg, 56%) was obtained from **1** (80 mg, 0.073 mmol) and CCl_4 (0.20 M in toluene; 0.36 mL, 0.072 mmol). **2**: M.p.: 135 °C (decomp.). ^{1}H NMR (500 MHz, C_6D_6): δ = –0.16 (s, 6H, Si^{t}Bu*Me*$_2$), 0.73 (s, 6H, Si^{t}Bu*Me*$_2$), 1.05 (s, 18H, Si^t*Bu*Me$_2$), 1.85 (s, 15H, *Cp**), 6.71-6.97 (m, 10H, *Ph*). ^{13}C NMR (101 MHz, C_6D_6): δ = –1.34 (1°, $J_{Si–C}$=50 Hz, Si^{t}Bu*Me*$_2$), 0.26 (1°, $J_{Si–C}$=54 Hz, Si^{t}Bu*Me*$_2$), 11.92 (1°, *Cp**), 18.81 (4°, $J_{Si–C}$=56 Hz, Si^t*Bu*Me$_2$), 28.53 (1°, Si^t*Bu*Me$_2$), 92.13 (4°, *Cp**), 108.25 (4°, $^2J_{Sn–C}$=81 Hz, C_β), 126.29 (3°, *Ph*), 126.52 (3°, *Ph*), 132.28 (3°, *Ph*), 140.17 (4°, *Ph*), 140.78 (4°, $J_{Sn–C}$=356, 373 Hz, C_α). ^{29}Si NMR (99 MHz, C_6D_6): δ = 9.8. ^{119}Sn NMR (187 MHz, C_6D_6): δ = –697.5. UV–vis (hexane): λ = 589, 432 nm. elemental analysis calcd (%) for $C_{38}H_{55}Si_2ClRuSn$: C, 55.44; H, 6.73. Found: C, 55.51; H, 6.75.

Me derivative **3**: red crystals of **3** (16 mg, 70%) was obtained from **1** (30 mg, 0.028 mmol) and MeI (0.16 M in toluene; 0.18 mL, 0.029 mmol). **3**: M.p.: 208-209 °C (decomp.). ^{1}H NMR (500 MHz, C_6D_6): δ = –0.28 (s, 6H, Si^{t}Bu*Me*$_2$), 0.29 (s, 6H, Si^{t}Bu*Me*$_2$), 0.75 (s, 3H, Sn*Me*), 1.04 (s, 18H, Si^t*Bu*Me$_2$), 1.88 (s, 15H, *Cp**), 6.79-6.90 (m, 6H, *Ph*), 7.18 (d, *J*=8 Hz, 4H, *Ph*). ^{13}C NMR (101

S1 Kuwabara, T.; Guo, J.-D.; Nagase, S.; Sasamori, T.; Tokitoh, N.; Saito, M. *J. Am. Chem. Soc,* **2014**, *136*, 13059.
S2 Sheldrick, G. M. *Acta Crystallogr. Sect. A*, **2008**, *64*, 112.

MHz, C_6D_6): δ = –6.17 (1°, $J_{Sn–C}$=249 Hz, Sn*Me*), –2.08 (1°, $J_{Si–C}$=52 Hz, Si^{t}Bu*Me$_2$*), 0.17 (1°, $J_{Si–C}$=53 Hz, Si^{t}Bu*Me$_2$*), 12.65 (4°, *Cp**), 18.11 (4°, $J_{Si–C}$=57 Hz, Si^t*Bu*Me$_2$), 28.33 (1°, Si^t*Bu*Me$_2$), 88.44 (4°, *Cp**), 107.24 (4°, $^2J_{Sn–C}$=71 Hz, *C$_\beta$*), 112.18 (4°, $J_{Si–C}$=64 Hz, $J_{Sn–C}$=187 Hz, *C$_\alpha$*), 126.04 (2°, *Ph*), 126.13 (3°, *Ph*), 133.53 (3°, *Ph*), 142.21 (4°, *Ph*). ^{29}Si NMR (99 MHz, C_6D_6): δ = 7.6; ^{119}Sn NMR (187 MHz, C_6D_6): δ = –372.3. UV–vis (hexane): λ = 427 nm. elemental analysis calcd (%) for $C_{39}H_{58}RuSi_2Sn$: C, 58.34; H, 7.28. Found: C, 58.19; H, 7.30.

Et derivative **4**: red crystals of **4** (44 mg, 72%) from **1** (82 mg, 0.075 mmol) and EtBr (0.25 M in toluene; 0.30 mL, 0.075 mmol). **4**: M.p: 224-225 °C (decomp.). ^{1}H NMR (500 MHz, C_6D_6): δ = –0.30 (s, 6H, Si^{t}Bu*Me$_2$*), 0.32 (s, 6H, Si^{t}Bu*Me$_2$*), 1.06 (s, 18H, Si^t*Bu*Me$_2$), 1.54-1.66 (m, 5H, -*CH$_2$CH$_3$*), 1.90 (s, 15H, *Cp**), 6.80-6.91 (m, 6H, *Ph*), 7.17 (d, *J*=8 Hz, 4H, *Ph*). ^{13}C NMR (101 MHz, C_6D_6) δ = –2.14 (1°, $J_{Si–C}$=50 Hz, Si^{t}Bu*Me$_2$*), 0.02 (1°, $J_{Si–C}$=52 Hz, Si^{t}Bu*Me$_2$*), 10.34 (2°, $J_{Sn–C}$=161 Hz, -*CH$_2$*CH$_3$), 12.80 (1°, *Cp**), 14.19 (1°, $^2J_{Sn–C}$=50 Hz, -CH$_2$*CH$_3$*), 17.88 (4°, $J_{Si–C}$=57 Hz, Si^t*Bu*Me$_2$), 28.33 (1°, Si^t*Bu*Me$_2$), 88.38 (4°, *Cp**), 107.29 (4°, $^2J_{Sn–C}$=63 Hz, *C$_\beta$*), 109.98 (4°, $J_{Si–C}$=64 Hz, $J_{Sn–C}$=187 Hz, *C$_\alpha$*), 126.01 (3°, *Ph*), 126.10 (3°, *Ph*), 133.62 (3°, *Ph*), 142.18 (4°, *Ph*). ^{29}Si NMR (99 MHz, C_6D_6): δ = 7.5. ^{119}Sn NMR (187 MHz, C_6D_6): δ = –343.3. UV–vis (hexane): λ = 429 nm. elemental analysis calcd (%) for $C_{40}H_{60}RuSi_2Sn$: C, 58.81; H, 7.40. Found: C, 58.84; H, 7.43.

TMS derivative **5**: red crystals of **5** (17 mg, 68%) from **1** (31 mg, 0.029 mmol) and trimethylsilyl chloride (0.23 M in toluene; 0.12 mL, 0.028 mmol). **5**: M.p.: 215-217 °C (decomp.). ^{1}H NMR (500 MHz, C_6D_6): δ = –0.51 (s, 6H, Si^{t}Bu*Me$_2$*), 0.24 (s, 6H, Si^{t}Bu*Me$_2$*), 0.63 (s, 9H, Si*Me$_3$*), 1.04 (s, 18H, Si^t*Bu*Me$_2$), 2.07 (s, 15H, *Cp**), 6.83-7.00 (m, 6H, *Ph*), 7.25-7.41 (m, 4H, *Ph*). ^{13}C NMR (101 MHz, C_6D_6): δ = –2.39 (1°, $J_{Si–C}$=50 Hz, Si^{t}Bu*Me$_2$*), 1.60 (1°, $J_{Si–C}$=52 Hz, Si^{t}Bu*Me$_2$*), 4.58 (1°, $J_{Si–C}$=47 Hz, $^2J_{Sn–C}$=58 Hz, Si*Me$_3$*), 14.04 (1°, *Cp**), 17.92 (4°, $J_{Si–C}$=56 Hz, Si^t*Bu*Me$_2$), 28.60 (1°, Si^t*Bu*Me$_2$), 88.58 (4°, *Cp**), 91.28 (4°, $J_{Sn–C}$=58 Hz *C$_\alpha$*), 109.82 (4°, $J_{Sn–C}$=46 Hz *C$_\beta$*), 125.88 (2°, *Ph*), 126.04 (2°, *Ph*), 134.43 (2°, *Ph*), 142.70 (4°, *Ph*). ^{29}Si NMR (99 MHz, C_6D_6): δ = –2.3 (*Si*Me$_3$), 6.3 (*Si^t*BuMe$_2$). ^{119}Sn NMR (187 MHz, C_6D_6): δ = –170.7. UV–vis (hexane): λ = 418 nm. elemental analysis calcd (%) for $C_{41}H_{64}RuSi_3Sn$: C, 57.19; H, 7.49. Found: C, 56.99; H, 7.61.

2. Crystal data for **2**, **4**, **5**

Crystal Data for **2**: Formula, $C_{38}H_{55}ClRuSi_2Sn$, FW=823.21, Crystal Dimension 0.20 × 0.15 × 0.10, Monoclinic, $P2_1/n$, a= 9.6555(12), b=18.470(2), c=21.490(3) Å, β=95.698(3), V=3813.7(8) Å^3, Z=4, D_{calcd}=1.434 g cm^{-3}. R_1=0.045 ($I > 2\sigma(I)$, 6400 reflections), wR_2=0.101 (for all reflections) for 7894 reflections and 394 parameters. GOF=1.031.

Crystal Data for **4**: Formula, $C_{40}H_{60}RuSi_2Sn$, FW=816.84, Crystal Dimension 0.20 × 0.20 × 0.15, Orthorhombic, *Pnma*, a=17.7751(13), b=21.1737(16), c=10.5846(8) Å, V=3983.7(5) Å^3, Z=4, D_{calcd}=1.362 g cm^{-3}. R_1=0.050 ($I > 2\sigma(I)$, 3959 reflections), wR_2=0.123 (for all reflections) for 4013 reflections and 217 parameters. GOF=1.176.

Crystal Data for **5**: Formula, $C_{41}H_{64}RuSi_3Sn$, FW=860.97, Crystal Dimension 0.10 × 0.10 × 0.10, Monoclinic, $P2_1/n$, a=11.8804(14), b=21.679(3), c=16.7980(18) Å, β=103.113(3), V=4213.6(8) Å^3, Z=4, D_{calcd}=1.357 g cm^{-3}. R_1=0.047 ($I > 2\sigma(I)$, 7789 reflections), wR_2=0.103 (for all reflections) for 9198 reflections and 433 parameters. GOF=1.093.

3. Side and top views of molecular structures for **2**, **4**, **5**

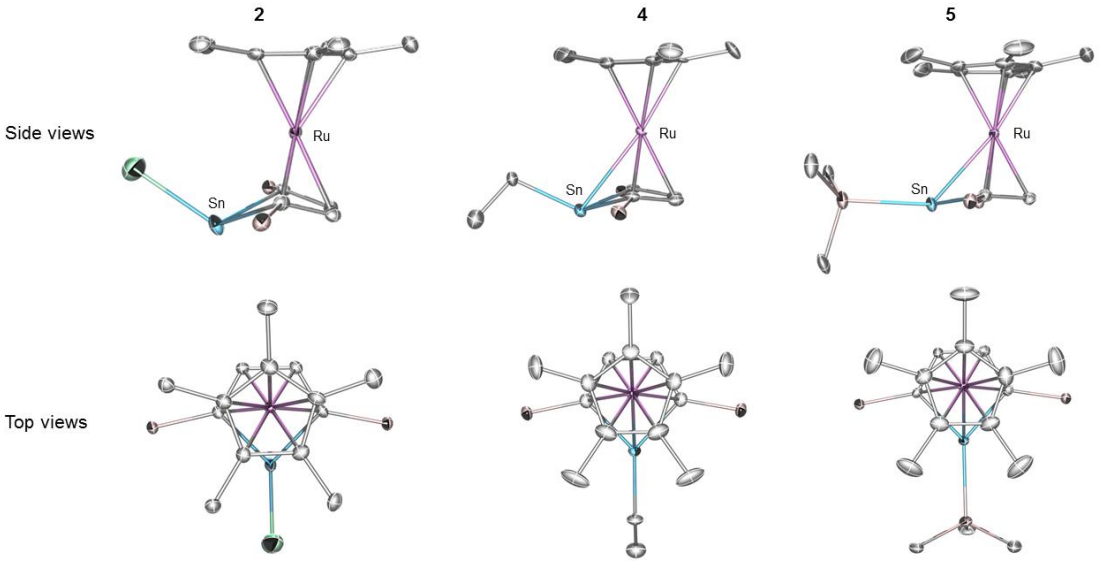


Figure S1. Side and top views of molecular structures for **2**, **4**, **5**.

4. Comparison of the optimized structures and experimental ones for **2**, **4**, **5**

	Cl derivative **2**		Et derivative **4**		TMS derivative **5**	
	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
Sn–C1/C2 (Å)	2.246/ 2.244	2.254/ 2.255	2.167/ 2.168	2.154	2.145/ 2.144	2.123/ 2.124
Sn–Ru/R (Cl,C,Si)(Å)	2.929/ 2.456	2.932/ 2.397	2.794/ 2.203	2.797/ 2.173	2.713/ 2.621	2.690/ 2.578
Ru–C1/C2	2.146/2.151	2.117/2.106	2.242/2.243	2.191	2.314/2.315	2.265/2.260
Ru–C3/C4 (Å)	2.219/2.220	2.207/2.213	2.218	2.188	2.234/2.233	2.204/2.197
C1–C3/ C2–C4 (Å)	1.426	1.419/ 1.411	1.430	1.429	1.431	1.430/ 1.421
C3–C4 (Å)	1.478	1.474	1.465	1.457	1.458	1.453
C1–Si1/ C2–Si2 (Å)	1.901	1.884/ 1.891	1.887/ 1.886	1.874	1.884	1.873/ 1.874

Table S1. Selected bond lengths of optimized structures and experimental ones for **2**, **4**, **5**

5. Relationship between bent angles of the stannole ring and substituents on the tin atom

Judging from the stannole ring in the Cl derivative more bent than the H derivative, electronegativity plays important role for the different coordination modes.

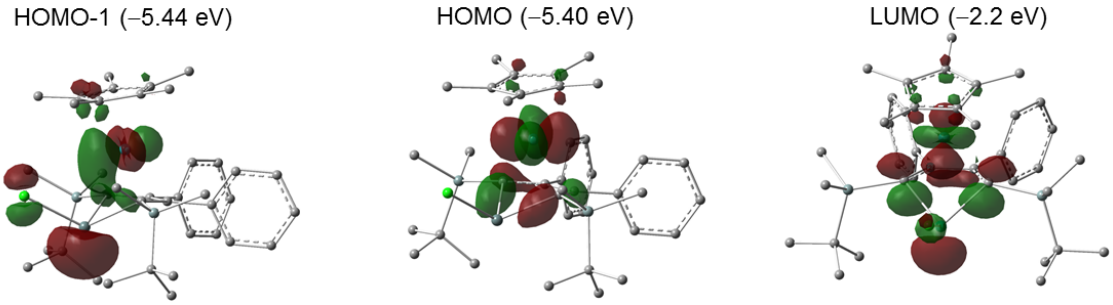
On the other hand, ^{t}Bu derivative has the stannole ring more planar than that of SiH_3 one even though a silyl atom is more positive than a carbon atom.

It is therefore concluded that not only electronegativity but also bulkiness of substituent on the tin atom play important roles for the different coordination modes of the stannole anion ligands.

6. Details for UV-vis absorption spectra

	experimental value (nm)	calculated value (nm)
2 (Cl derivative)	432, 590	430, 586
3 (Me derivative)	427	-
4 (Et derivative)	429	409
5 (trimethylsilyl derivative)	418	402

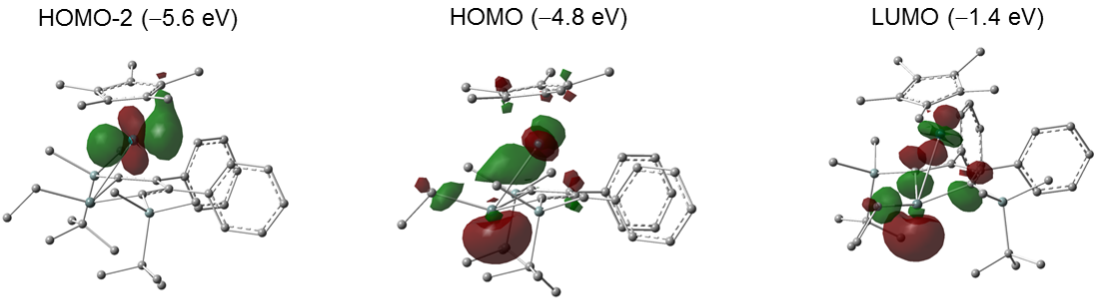
Table S2. Selected bond lengths of optimized structures and experimental ones for **2**, **4**, **5**



Maximum absorption (λ_{max}) and oscillator strengths (f)

586 nm f = 0.01: HOMO → LUMO (94%)
430 nm, f = 0.09: HOMO-1 → LUMO (54%)

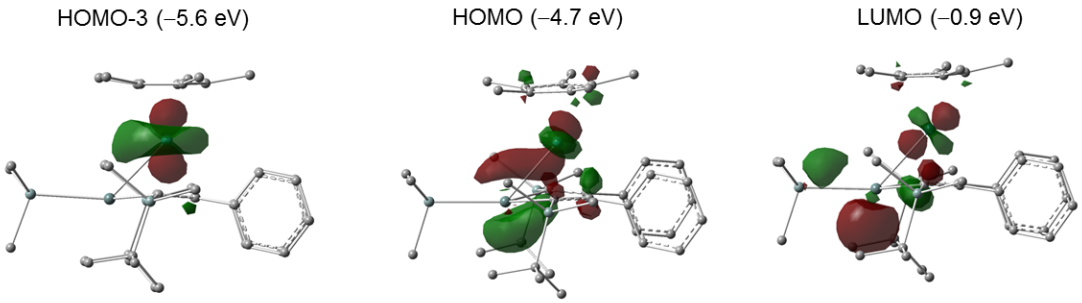
Chart S1. Origin for UV-vis absorptions in chloro derivative **2**.



Maximum absorption (λ_{max}) and oscillator strength (f)

409 nm f = 0.09: HOMO → LUMO (56%)
HOMO-2 → LUMO (13%)

Chart S2. Origin for UV-vis absorptions in ethyl derivative **4**.



Maximum absorption (λ_{max}) and oscillator strength (f)

402 nm f = 0.05: HOMO → LUMO (42%)

HOMO-3 → LUMO (20%)

Chart S3. Origin for UV-vis absorptions in trimethylsilyl derivative **5**.

7. The Cartesian coordinates of the optimized geometry for **2**

Method for optimization: B3PW91//[4333111/433111/43](Sn)/Lanl2dz+f(Ru)/6-31G(d)(C, H, Si, Cl)

Total energy = -8634.790836 au

C	3.301864	-2.323843	-2.904161
C	-3.375569	-2.295677	-2.840637
C	3.006834	0.113254	-3.360449
C	5.214623	-0.762800	-2.602875
C	-3.046895	0.119576	-3.377056
C	-5.256431	-0.691266	-2.561251
C	3.688828	-0.909569	-2.443295
C	-3.731380	-0.861454	-2.417174
C	3.746647	-2.215580	0.337329
C	-3.811518	-2.082947	0.392800
C	-1.691988	2.926229	-1.676845
C	1.664111	2.930433	-1.684875
C	1.430738	-0.252763	-0.260576
C	-1.432678	-0.214328	-0.266350
C	-2.339251	4.157442	-1.761272
C	2.344925	4.142366	-1.780868
C	0.755025	0.999172	-0.361239
C	-0.722369	1.018512	-0.361989
C	4.409320	0.748485	0.085458
C	-4.364746	0.899840	0.072296
C	-1.404938	2.350511	-0.432611
C	1.473663	2.310944	-0.442928
C	-2.702226	4.840822	-0.601141
C	2.838554	4.763670	-0.634117
C	-1.566384	-2.728213	3.028392
C	1.517215	-2.753544	3.026408
C	-1.761560	3.051765	0.721543
C	1.967227	2.947735	0.698109
C	-0.734551	-1.485892	3.024399
C	0.705193	-1.498362	3.024363
C	-2.405679	4.285155	0.641942

C	2.643628	4.162809	0.608074
C	1.159973	-0.166008	3.278564
C	-1.165704	-0.145118	3.278338
C	2.575922	0.238242	3.547562
C	-2.576035	0.291129	3.525541
C	0.004442	0.674148	3.422801
C	0.019163	2.083947	3.930227
H	3.588192	-2.467479	-3.956918
H	-3.688701	-2.468353	-3.881319
H	3.305581	-0.053514	-4.406589
H	5.504450	-0.987657	-3.640122
H	-3.351181	-0.087437	-4.414324
H	2.220234	-2.499745	-2.842495
H	-5.563584	-0.937964	-3.588502
H	-2.295354	-2.485635	-2.799165
H	3.799375	-3.105345	-2.318821
H	-3.869793	-3.050890	-2.219236
H	-1.953771	0.032821	-3.334240
H	1.913560	0.030178	-3.315845
H	5.772106	-1.453927	-1.957438
H	-5.818152	-1.354355	-1.890897
H	3.279729	1.142154	-3.099508
H	5.557372	0.254140	-2.381617
H	-3.315982	1.159192	-3.157878
H	-5.577704	0.337428	-2.362975
H	2.985747	-2.998662	0.252719
H	-1.403579	2.406066	-2.585050
H	-3.073248	-2.889322	0.330881
H	1.275521	2.458828	-2.582443
H	4.682979	-2.612650	-0.073415
H	-4.758052	-2.463552	-0.009891
H	-2.554397	4.585896	-2.737139
H	2.483582	4.605070	-2.754894
H	5.444102	0.384427	0.094366
H	3.919424	-2.028660	1.401510
H	-5.414458	0.582131	0.094679

H	4.373913	1.656728	-0.524579
H	-3.981856	-1.863310	1.451080
H	-4.292090	1.792246	-0.557407
H	-1.313031	-3.387794	2.193305
H	1.254987	-3.406491	2.188880
H	4.148318	1.033023	1.109308
H	-3.205880	5.801860	-0.666565
H	-4.084430	1.194484	1.088238
H	3.366977	5.710632	-0.708698
H	2.587851	-2.548422	2.981839
H	-2.633741	-2.507863	2.981621
H	-1.385947	-3.285915	3.958503
H	1.327634	-3.311471	3.954561
H	1.816895	2.470236	1.659727
H	-1.524235	2.614977	1.684996
H	3.283960	-0.320489	2.930404
H	-3.289487	-0.301855	2.948429
H	-2.676257	4.812653	1.553557
H	3.021136	4.639017	1.509841
H	2.742272	1.302822	3.362181
H	-2.733827	1.340572	3.262474
H	2.832189	0.048077	4.599675
H	-2.832111	0.176368	4.588420
H	0.817702	2.687665	3.491992
H	-0.925639	2.600846	3.743874
H	0.172794	2.080601	5.018694
Si	3.270486	-0.621858	-0.563416
Si	-3.285730	-0.529208	-0.549995
Ru	-0.000032	-0.211712	1.338687
Sn	-0.020815	-1.695750	-1.185898
Cl	-0.057323	-3.932797	-0.171883

8. The Cartesian coordinates of the optimized geometry for **4**

Method for optimization: B3PW91//[4333111/433111/43](Sn)/Lanl2dz+f(Ru)/6-31G(d)(C, H, Si)

Total energy = -8253.783948 au

C	2.544026	4.261131	-0.284268
C	0.231699	3.002517	3.339544
C	2.826974	4.530520	-1.621788
C	-2.557141	4.259888	-0.224550
C	-2.754979	4.595371	-1.562527
C	1.866423	3.094716	0.067774
C	-1.900251	3.076781	0.110049
C	2.416716	3.627987	-2.602739
C	-2.284142	3.740570	-2.558774
C	0.133534	1.512379	3.194092
C	2.680665	0.956186	3.340684
C	-2.456977	1.312590	3.462611
C	1.461635	2.174467	-0.901961
C	1.737209	2.465082	-2.245122
C	1.233579	0.592240	3.219419
C	-1.428950	2.206806	-0.875830
C	-1.082556	0.754194	3.255729
C	-1.624157	2.561585	-2.217575
C	4.397318	0.782955	-0.243594
C	-4.397790	0.843314	-0.154526
C	0.737970	0.909371	-0.551433
C	-0.726896	0.926215	-0.538741
C	0.697774	-0.737570	3.318138
C	-0.733843	-0.635861	3.340889
C	1.420949	-0.320373	-0.292252
C	1.469120	-1.986449	3.608752
C	-1.432122	-0.287689	-0.267297
C	-1.668945	-1.754359	3.675365
C	2.957549	-0.672183	-3.399721
C	3.797546	-2.026499	0.734622
C	-2.992435	-0.495918	-3.369074
C	-3.805159	-2.004540	0.719767

C	5.156091	-1.427812	-2.493233
C	3.632396	-1.461223	-2.270611
C	-5.198018	-1.254341	-2.479446
C	-3.673253	-1.320980	-2.269497
C	3.171938	-2.924656	-2.359074
C	-0.037271	-3.853099	0.554311
C	-3.238335	-2.786556	-2.424759
C	-0.347357	-5.054306	-0.336557
H	2.851221	4.961187	0.489360
H	3.356176	5.438726	-1.899232
H	-2.917002	4.919294	0.561967
H	-0.106532	3.302854	4.341054
H	-3.267140	5.516844	-1.827897
H	1.263206	3.350235	3.235400
H	-0.374557	3.548477	2.611157
H	1.639973	2.882023	1.105929
H	2.922510	1.875360	2.800039
H	-1.749499	2.803398	1.147706
H	-2.541149	2.342742	3.105543
H	2.954199	1.110242	4.394502
H	2.619861	3.831798	-3.651443
H	-2.423954	3.994620	-3.606800
H	-2.707553	1.321302	4.533526
H	3.325639	0.167421	2.946447
H	4.160923	1.285137	0.699608
H	-3.222901	0.721397	2.952988
H	-4.142533	1.322657	0.795895
H	4.323859	1.532639	-1.037730
H	-4.332872	1.611323	-0.931981
H	1.412303	1.773169	-3.016232
H	-1.251989	1.907796	-3.000476
H	5.439251	0.443669	-0.188627
H	-5.440927	0.509436	-0.090651
H	1.543238	-2.142239	4.695056
H	2.485413	-1.942936	3.213423
H	-1.712149	-1.896824	4.765160

H	-2.684323	-1.552324	3.330770
H	3.294743	0.370368	-3.426213
H	-3.305012	0.554314	-3.345741
H	4.010092	-1.577696	1.710575
H	5.542830	-0.403622	-2.542212
H	-4.008341	-1.584483	1.710025
H	-5.568658	-0.223196	-2.485506
H	0.985823	-2.871314	3.184931
H	-1.351698	-2.704970	3.236821
H	1.865642	-0.675131	-3.292374
H	-1.899962	-0.527783	-3.273782
H	4.721800	-2.512474	0.398282
H	5.707180	-1.956771	-1.704940
H	3.196050	-1.120107	-4.376650
H	-4.732068	-2.480243	0.376217
H	-3.250363	-0.894591	-4.362367
H	3.047361	-2.810255	0.883432
H	5.407864	-1.917484	-3.446055
H	-5.751804	-1.805367	-1.708158
H	-3.053328	-2.792333	0.839459
H	-5.463727	-1.702571	-3.448752
H	0.949506	-3.958409	1.018596
H	-0.768171	-3.765045	1.364831
H	2.081819	-3.014775	-2.259785
H	-2.150458	-2.901613	-2.327942
H	3.636104	-3.556883	-1.592578
H	-3.716707	-3.444872	-1.689362
H	3.438227	-3.347340	-3.339842
H	-3.510402	-3.158856	-3.424253
H	-1.339904	-4.977060	-0.794054
H	0.379552	-5.155546	-1.150728
H	-0.324520	-5.988284	0.241279
Si	3.255089	-0.704587	-0.516536
Si	-3.270995	-0.643339	-0.489783
Ru	0.014345	0.130722	1.394925
Sn	-0.025678	-1.920211	-0.502333

9. The Cartesian coordinates of the optimized geometry for **5**

Method for optimization: B3PW91//[4333111/433111/43](Sn)/Lanl2dz+f(Ru)/6-31G(d)(C, H, Si)

Total energy = -8583.775831 au

C	-1.672247	2.440079	3.416786
C	1.519870	3.915471	0.732729
C	1.406681	1.722683	3.669545
C	-1.296550	4.355098	-0.263842
C	0.885434	5.248771	-2.508395
C	-1.084953	1.073961	3.235382
C	0.312851	0.756407	3.341708
C	4.784688	1.664135	0.980200
C	0.972027	3.726642	-2.292875
C	-4.611514	2.397220	-0.254599
C	-3.304994	-0.287901	3.336082
C	-1.817977	-0.157812	3.184393
C	-3.409566	1.780196	0.089010
C	-4.932454	2.606477	-1.594326
C	2.447063	3.312118	-2.398128
C	0.444841	-0.672721	3.328973
C	0.192104	3.028012	-3.414669
C	1.703371	-1.424864	3.631170
C	0.001844	1.440086	-0.352108
C	-0.873607	-1.236708	3.215888
C	-2.504951	1.362033	-0.888998
C	-4.043668	2.186875	-2.583849
C	-1.203377	0.695941	-0.556577
C	-2.845549	1.567777	-2.233078
C	-1.201923	-2.691861	3.342642
C	4.889424	-1.409270	0.854376
C	5.042351	0.238283	-1.727442
C	-1.149924	-0.761193	-0.564409
C	0.106921	-1.418151	-0.370728
C	-3.313489	-1.922903	0.086502
C	-2.403779	-1.515655	-0.891781
C	-4.471522	-2.621772	-0.251374

C	1.789596	-3.782281	0.718588
C	-2.698546	-1.809883	-2.230258
C	-4.743841	-2.923847	-1.584119
C	-3.853033	-2.510369	-2.574457
C	2.689641	-3.136333	-2.395532
C	-0.995772	-4.410078	-0.276219
C	1.243049	-3.643375	-2.301321
C	0.431607	-3.003374	-3.435132
C	1.255272	-5.168766	-2.507944
H	-1.700463	2.706333	4.483577
H	-1.006991	5.411611	-0.199949
H	-1.087326	3.208191	2.903160
H	1.020224	4.158606	1.677178
H	2.009377	4.833541	0.384389
H	1.516882	1.819315	4.759830
H	1.205068	2.717274	3.268632
H	1.403010	5.813798	-1.722286
H	-2.698050	2.500027	3.042878
H	-0.151728	5.600609	-2.544645
H	-1.790400	4.087880	0.675762
H	1.356022	5.522026	-3.465134
H	2.300645	3.180860	0.952629
H	2.369494	1.394587	3.268148
H	-2.039049	4.251746	-1.061067
H	4.358457	1.678339	1.988302
H	-5.297641	2.716805	0.526544
H	4.509177	2.598822	0.481730
H	-3.606248	0.036405	4.342134
H	5.878577	1.650171	1.079156
H	-3.868895	0.312809	2.616903
H	3.070477	3.795873	-1.635852
H	-3.148794	1.620653	1.128328
H	-5.868863	3.087213	-1.866349
H	1.817767	-1.560586	4.716892
H	-0.865180	3.317329	-3.420199
H	2.854162	3.592785	-3.381825

H	-3.633036	-1.325322	3.226236
H	2.585770	-0.887933	3.270566
H	0.611276	3.293780	-4.397500
H	2.568618	2.225744	-2.298712
H	-1.335342	-2.968349	4.398590
H	0.243523	1.936706	-3.316767
H	4.466270	-1.541171	1.854921
H	-4.286090	2.334786	-3.633587
H	1.709726	-2.415299	3.172158
H	4.760192	1.154055	-2.257172
H	5.979511	-1.324230	0.959871
H	6.135693	0.233461	-1.623623
H	-2.121688	-2.957172	2.814095
H	-2.164247	1.234050	-3.009992
H	-0.401998	-3.316715	2.938463
H	-3.098170	-1.679270	1.119912
H	4.682441	-2.314481	0.274931
H	4.762015	-0.614356	-2.355042
H	2.541902	-3.008701	0.899410
H	-5.163062	-2.930358	0.529455
H	1.317804	-4.017422	1.678894
H	2.742250	-2.044564	-2.294078
H	-2.016798	-1.480511	-3.008412
H	-1.501145	-4.172454	0.664956
H	2.312108	-4.688789	0.388637
H	3.336975	-3.581187	-1.629683
H	0.403019	-1.910880	-3.339848
H	-5.645469	-3.469797	-1.850622
H	-1.746485	-4.355480	-1.070596
H	-4.060007	-2.727137	-3.619868
H	3.120583	-3.389649	-3.376414
H	-0.640775	-5.446420	-0.211102
H	-0.601289	-3.369722	-3.453696
H	0.881928	-3.240397	-4.411507
H	1.804762	-5.694107	-1.716178
H	0.242776	-5.586517	-2.545713

H	1.746383	-5.417664	-3.461014
Si	0.251731	3.297737	-0.538151
Si	4.246074	0.145172	-0.012068
Si	0.481406	-3.255130	-0.552878
Ru	-0.396790	-0.016152	1.401058
Sn	1.651156	0.068747	-0.375658

10. The Cartesian coordinates of the optimized geometry for H derivative

Method for optimization: B3PW91//[4333111/433111/43](Sn)/Lanl2dz+f(Ru)/6-31G(d)(C, H, Si)

Total energy = -8175.1833377 au

C	-2.380590	3.756790	-2.202622
C	-1.741805	2.537411	-1.985317
C	-1.387507	2.132048	-0.692090
C	-1.664870	2.994082	0.371217
C	-2.302982	4.215099	0.159562
C	-2.669548	4.598894	-1.129113
C	-0.710170	0.812322	-0.480223
Ru	0.005764	-0.179606	1.376881
Sn	-0.041971	-2.041696	-0.740721
H	-0.083455	-3.413374	0.353978
C	0.759329	0.780029	-0.478175
C	1.498727	2.063687	-0.701137
C	2.074135	2.773388	0.355472
C	2.764234	3.963785	0.134203
C	2.891008	4.467559	-1.158950
C	2.318622	3.772350	-2.223767
C	1.625835	2.584923	-1.995606
C	1.420657	-0.470524	-0.287828
Si	3.241829	-0.891538	-0.575386
C	3.591157	-1.365937	-2.430453
C	2.889813	-0.412171	-3.406260
C	5.111462	-1.277602	-2.665098
C	3.147890	-2.804142	-2.740742
C	-1.429738	-0.406307	-0.299098
Si	-3.280715	-0.724089	-0.534900
C	-3.709747	-1.323095	-2.338356
C	-5.233963	-1.194249	-2.526465
C	-3.329361	-2.797403	-2.548256
C	-3.017616	-0.481663	-3.417828
C	3.707475	-2.407606	0.465100
C	4.444184	0.487786	-0.079788
C	-3.840970	-2.127863	0.609665

C	-4.360710	0.778310	-0.123646
C	1.170358	0.126256	3.275123
C	0.699957	-1.225593	3.201512
C	-0.737487	-1.197017	3.202612
C	-1.153275	0.174376	3.271670
C	0.025878	0.992288	3.314541
C	2.591477	0.540086	3.502124
C	1.521352	-2.465754	3.361829
C	0.062520	2.458800	3.624160
C	-1.598129	-2.409226	3.373990
C	-2.560236	0.654211	3.451084
H	2.836660	0.483710	4.572647
H	5.466891	0.091170	-0.060840
H	3.294889	-0.106763	2.970871
H	3.952702	-2.116265	1.491828
H	4.598692	-2.895816	0.051543
H	1.532341	-2.775866	4.416954
H	2.556300	-2.311024	3.053600
H	5.677875	-1.924820	-1.982725
H	2.778835	1.569148	3.182646
H	5.487775	-0.255316	-2.546746
H	4.217066	0.869041	0.920666
H	5.352378	-1.600077	-3.689175
H	2.909675	-3.157269	0.511146
H	1.120914	-3.297025	2.774861
H	4.423649	1.340620	-0.765470
H	3.205151	4.497268	0.973125
H	0.359152	2.609715	4.671691
H	0.770549	3.011428	3.000950
H	3.644286	-3.540669	-2.097895
H	1.975771	2.367888	1.355924
H	3.428078	5.395956	-1.336106
H	-1.558145	-2.749637	4.418889
H	3.203530	0.627791	-3.258924
H	3.394595	-3.058625	-3.782730
H	-0.918894	2.924808	3.501181

H	-1.265060	-3.237387	2.742075
H	3.127754	-0.684298	-4.446019
H	2.063867	-2.936336	-2.628597
H	-2.807480	0.735826	4.519260
H	1.799413	-0.455001	-3.294309
H	2.404880	4.158133	-3.236646
H	-2.642649	-2.207549	3.134830
H	-2.722573	1.637337	2.999738
H	1.175933	2.055795	-2.830326
H	-3.279299	-0.033528	2.999101
H	-1.364939	2.689438	1.367438
H	-3.106686	-2.937106	0.683416
H	-2.512136	4.868659	1.003300
H	-4.035203	-1.754843	1.620230
H	-2.247140	-2.961650	-2.460145
H	-1.511222	1.892579	-2.827618
H	-4.079390	1.206543	0.843595
H	-4.779822	-2.562306	0.245149
H	-3.830009	-3.464278	-1.836588
H	-1.925009	-0.534074	-3.332555
H	-3.168472	5.549925	-1.297570
H	-4.282277	1.577779	-0.867191
H	-2.647919	4.051510	-3.214646
H	-3.618688	-3.121096	-3.559643
H	-5.412204	0.472109	-0.060344
H	-3.315813	0.571420	-3.362515
H	-3.288730	-0.847006	-4.420172
H	-5.798495	-1.767164	-1.779486
H	-5.568471	-0.152132	-2.471748
H	-5.524247	-1.581026	-3.514867

11. The Cartesian coordinates of the optimized geometry for ^{t}Bu derivative

Method for optimization: B3PW91//[4333111/433111/43](Sn)/Lanl2dz+f(Ru)/6-31G(d)(C, H, Si)

Total energy = -8332.3689431 au

C	2.546419	1.394928	3.391538
C	3.918948	-1.754515	0.782942
C	1.631224	-1.618592	3.696747
C	4.386799	1.022002	-0.242895
C	5.264532	-1.178026	-2.461653
C	1.143539	0.899056	3.219608
C	0.734075	-0.473195	3.350987
C	1.182992	-4.464640	0.681314
C	3.740448	-1.246911	-2.256015
C	2.579622	4.356575	-0.274320
C	-0.070252	3.204030	3.316220
C	-0.036539	1.711423	3.167630
C	1.915676	3.181020	0.072272
C	2.811949	4.658509	-1.614683
C	3.310887	-2.717220	-2.347977
C	-0.699434	-0.509321	3.349707
C	3.058265	-0.471921	-3.391181
C	-1.535802	-1.701627	3.692096
C	1.440901	-0.221270	-0.344213
C	-1.174990	0.841601	3.215665
C	1.472309	2.285034	-0.901959
C	2.366665	3.778565	-2.601013
C	0.750525	1.015995	-0.559508
C	1.699724	2.607278	-2.246886
C	-2.603493	1.267131	3.356280
C	-1.322061	-4.431283	0.661416
C	-0.058005	-4.702696	-1.468037
C	-0.707912	1.040332	-0.562867
C	-1.438162	-0.175619	-0.355667
C	-1.725602	3.281504	0.068341
C	-1.385564	2.335292	-0.900771
C	-2.349961	4.478292	-0.279927

C	-3.948412	-1.642305	0.782480
C	-1.667027	2.633216	-2.241117
C	-2.642450	4.753564	-1.614164
C	-2.293324	3.826379	-2.595884
C	-3.409288	-2.617003	-2.348403
C	-4.333012	1.161283	-0.233919
C	-3.791912	-1.134055	-2.249686
C	-3.108291	-0.382453	-3.399353
C	-5.316946	-1.017578	-2.428792
H	2.811807	1.429043	4.458462
H	5.433817	0.701377	-0.168211
H	3.272854	0.745865	2.894801
H	4.161280	-1.231693	1.715347
H	4.843285	-2.236976	0.440735
H	1.775159	-1.676579	4.785842
H	2.616161	-1.519211	3.237684
H	5.819193	-1.689649	-1.664484
H	2.679211	2.405102	2.994477
H	5.626633	-0.145007	-2.510705
H	4.127991	1.528471	0.691910
H	5.539353	-1.665116	-3.409612
H	3.201433	-2.543051	1.023884
H	1.209127	-2.573389	3.371921
H	4.312456	1.761563	-1.045704
H	1.243772	-4.011858	1.676131
H	2.918189	5.036350	0.504373
H	2.108118	-4.235396	0.142570
H	0.244787	3.480325	4.332422
H	1.151084	-5.557603	0.818619
H	0.588244	3.727974	2.617989
H	3.790018	-3.340116	-1.582544
H	1.736634	2.931669	1.110975
H	3.330054	5.573810	-1.889842
H	-1.707408	-1.749686	4.777672
H	3.361623	0.581155	-3.406807
H	3.580846	-3.136955	-3.329261

H	-1.079074	3.602523	3.177840
H	-1.042159	-2.632490	3.399144
H	3.325491	-0.906143	-4.367009
H	2.223797	-2.821811	-2.242684
H	-2.859547	1.418053	4.415089
H	1.965482	-0.508224	-3.300451
H	-1.390072	-3.973822	1.653239
H	2.531501	4.007640	-3.651218
H	-2.512486	-1.674585	3.204790
H	0.836203	-4.468833	-2.054955
H	-1.319009	-5.524288	0.801963
H	-0.077089	-5.794954	-1.325193
H	-2.811442	2.203850	2.832067
H	1.343897	1.934914	-3.021812
H	-3.285662	0.511924	2.958680
H	-1.490800	3.063187	1.103220
H	-2.231226	-4.181846	0.104935
H	-0.935610	-4.439323	-2.067671
H	-3.254267	-2.457961	1.000035
H	-2.608031	5.197718	0.493961
H	-4.158374	-1.126129	1.725885
H	-2.323769	-2.755684	-2.267933
H	-1.386635	1.922240	-3.012294
H	-4.032762	1.667831	0.688055
H	-4.893521	-2.089832	0.449782
H	-3.890423	-3.224253	-1.571851
H	-2.015461	-0.451478	-3.329958
H	-3.130243	5.685592	-1.888659
H	-4.248304	1.887577	-1.047693
H	-2.501849	4.034850	-3.642648
H	-3.714141	-3.029045	-3.322702
H	-5.389281	0.881663	-0.132138
H	-3.380802	0.678919	-3.412477
H	-3.406998	-0.810798	-4.368590
H	-5.873375	-1.518108	-1.625891
H	-5.648043	0.026423	-2.463429

H	-5.622616	-1.488899	-3.375278
Si	3.301546	-0.508494	-0.511578
C	-0.057831	-4.021421	-0.093369
Si	-3.306983	-0.407210	-0.511349
Ru	0.002099	0.258463	1.396432
Sn	-0.023612	-1.789949	-0.419454

12. The Cartesian coordinates of the optimized geometry for SiH_3 derivative

Method for optimization: B3PW91//[4333111/433111/43](Sn)/Lanl2dz+f(Ru)/6-31G(d)(C, H, Si)

Total energy = -8465.8432786 au

C	-2.295747	3.976128	-2.179733
C	-1.677956	2.745307	-1.966801
C	-1.349940	2.319122	-0.673041
C	-1.633651	3.171906	0.395428
C	-2.250579	4.404742	0.188723
C	-2.590109	4.809604	-1.100806
C	-0.690652	0.987702	-0.475834
Ru	0.008477	-0.028762	1.377081
Sn	-0.065344	-1.856600	-0.708672
Si	-0.183738	-4.291786	0.165910
H	-0.105001	-5.227890	-0.991404
C	0.772845	0.933805	-0.474623
C	1.534491	2.208018	-0.679324
C	2.088094	2.920529	0.386422
C	2.800094	4.099829	0.174536
C	2.970990	4.589713	-1.118777
C	2.419853	3.892099	-2.193349
C	1.705724	2.715685	-1.974290
C	1.423845	-0.332779	-0.349715
Si	3.242831	-0.755332	-0.625300
C	3.579487	-1.262740	-2.472164
C	2.936716	-0.277955	-3.457562
C	5.102698	-1.263344	-2.702801
C	3.053478	-2.674570	-2.773066
C	-1.435685	-0.226606	-0.356295
Si	-3.290817	-0.499849	-0.589537
C	-3.714156	-1.084626	-2.397446
C	-5.235688	-0.949831	-2.599269
C	-3.333774	-2.557685	-2.614016
C	-3.007580	-0.235824	-3.461979
C	3.711342	-2.252187	0.441889
C	4.449900	0.629421	-0.160688

H	0.932524	-4.638437	1.091723
H	-1.470326	-4.559882	0.869825
C	-3.892181	-1.886882	0.555537
C	-4.344995	1.021487	-0.183953
C	1.169456	0.322012	3.266235
C	0.705333	-1.035165	3.224281
C	-0.730570	-1.013032	3.219690
C	-1.151820	0.359990	3.256478
C	0.022514	1.183212	3.301857
C	2.590431	0.737350	3.494149
C	1.550404	-2.252891	3.425431
C	0.052117	2.650515	3.610441
C	-1.606703	-2.210491	3.412358
C	-2.562812	0.829917	3.431515
H	2.844776	0.651527	4.560637
H	5.472488	0.232154	-0.146796
H	3.292975	0.109239	2.939293
H	3.978040	-1.935350	1.455973
H	4.587867	-2.765188	0.027094
H	1.640330	-2.477094	4.498488
H	2.559152	-2.117960	3.031366
H	5.630343	-1.934936	-2.013229
H	2.770350	1.775803	3.202626
H	5.536425	-0.262972	-2.593275
H	4.232451	1.023197	0.837176
H	5.327806	-1.607957	-3.723305
H	2.904588	-2.988295	0.525977
H	1.122658	-3.134009	2.940431
H	4.422332	1.474037	-0.856335
H	3.224010	4.635204	1.021064
H	0.371558	2.802508	4.651084
H	0.739145	3.212986	2.972640
H	3.489913	-3.432238	-2.111009
H	1.956337	2.525294	1.386677
H	3.525586	5.509153	-1.288697
H	-1.734990	-2.415541	4.485309

H	3.307383	0.743843	-3.314677
H	3.301447	-2.960401	-3.806731
H	-0.937014	3.106157	3.512722
H	-1.176793	-3.106846	2.957103
H	3.163141	-0.569051	-4.494763
H	1.960872	-2.734430	-2.681132
H	-2.815381	0.905596	4.499008
H	1.845280	-0.259497	-3.349742
H	2.539809	4.267578	-3.206707
H	-2.598981	-2.067737	2.982244
H	-2.731219	1.813202	2.982877
H	1.273043	2.184238	-2.816610
H	-3.274586	0.137646	2.974915
H	-1.356304	2.850155	1.392188
H	-3.183163	-2.717262	0.636678
H	-2.464551	5.050655	1.037204
H	-4.077381	-1.503190	1.564365
H	-2.251620	-2.721927	-2.521757
H	-1.442645	2.106920	-2.812766
H	-4.064838	1.439908	0.787921
H	-4.842517	-2.296911	0.192387
H	-3.838260	-3.227821	-1.907811
H	-1.916218	-0.295605	-3.365872
H	-3.072397	5.769842	-1.265626
H	-4.244820	1.822411	-0.923071
H	-2.542328	4.286831	-3.192249
H	-3.617067	-2.877515	-3.628355
H	-5.402260	0.733496	-0.131712
H	-3.298855	0.818759	-3.397360
H	-3.271405	-0.587957	-4.470999
H	-5.809170	-1.529718	-1.864635
H	-5.567305	0.092703	-2.534887
H	-5.518118	-1.323226	-3.595102