Supporting Information for

(η^4-Butadiene)Sn(0) Complexes: A New Approach for Zero-Valent *p*-Block Elements Utilizing a Butadiene as a 4π-Electron Donor

Takuya Kuwabara,[1] Marisa Nakada,[1] Jumpei Hamada,[1] Jing Dong Guo,[2] Shigeru Nagase,[2] Masaichi Saito[1]*

correspondence to: masaichi@chem.saitama-u.ac.jp

This file includes:

1. Details for the experiments

Reaction of 1 with Cp_2HfCl_2 at room temperature (Run 1, for the isolation of 2): A mixture of compound **1** (49 mg, 0.069 mmol) and Cp_2HfCl_2 (26 mg, 0.068 mmol) was dissolved in THF (1.5 mL) at room temeperature. The solution was stirred for 3.5 h at this temperature and the solvent was evaporated. The resulting solid was extracted with hexane (3 mL × 3) and the mixture was filtered through Celite® to remove insoluble materials in hexane. After evapolation, a crude mixture was obtained as an orange powder and the ^{1}H NMR was measured (**2** : **3** = 6: 1, see Figure S3). After recrystallization of the crude mixture from hexane, compound **2** was isolated as orange crystals (28 mg, 45%). Single crystals of **3** could not be obatained because of its low generation ratio. Single crystals of **2** suitable for X-ray diffraction analysis were obtained from a toluene solution of the crude mixture at –30 °C. **2**: M.p: 102-103 °C (decomp.). ^{1}H NMR (500 MHz, C_6D_6, 293 K) δ –0.07 (s, 6H, Si^{t}Bu*Me*$_2$), 0.06 (s, 6H, Si^{t}Bu*Me*$_2$), 0.80 (s, 18H, Si^t*Bu*Me$_2$), 6.36 (s, 5H, *Cp*), 6.67-6.73 (m, 4H, *Ph*), 6.81-6.87 (m, 2H, *Ph*), 7.13 (d, *J*=8 Hz, 2H, *Ph*), 7.57-7.63 (m, 2H, *Ph*); ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 293 K) δ 0.83 (1°, Si^{t}Bu*Me*$_2$), 3.21 (1°, Si^{t}Bu*Me*$_2$), 19.01 (4°, Si^t*Bu*Me$_2$), 28.46 (1°, Si^t*Bu*Me$_2$), 108.21 (3°, *Cp*), 126.38 (3°, *Ph*), 126.98 (3°, *Ph*), 127.61 (3°, *Ph*), 131.81 (4°, *C*$_\beta$), 132.34 (3°, *Ph*), 133.618 (3°, *Ph*), 140.89 (4°, *Ph*), 141.23 (4°, *C*$_\alpha$); ^{29}Si NMR (99 MHz, C_6D_6, 293 K) δ 2.3; ^{119}Sn NMR (187 MHz, C_6D_6, 293 K) δ –1020.0. Elemental analysis calcd (%) for $C_{40}H_{52}ClHfSi_2Sn$ (**2**•Tol): C 52.13, H 5.69; found: C 51.35, H 5.39.

Reaction of 1 with Cp_2HfCl_2 at low temperature (Run 2, for the preparation of a mixture of 2 and 3): In a glovebox, compound **1** (228 mg, 0.321 mmol) and Cp_2HfCl_2 (121 mg, 0.318 mmol) were put into a J. Young Schlenk® flask. K-mirrored THF (15 mL) was added to the flask by a trap-to-trap distillation. Then, the flask was cooled to –100 °C and slowly warmed to room temperature over 12 hours. After evaporation of the solvent, in a glovebox, materials that were soluble in hexane were extracted and filtered through Celite® to remove insoluble materials in hexane. After evapolation of the filtrate, a crude mixture was obtained and its ^{1}H NMR was measured (**2** : **3** = 5: 2, see Figure S4.). The crude mixture was dissolved in hexane and the solution was cooled down to –30 °C to obtain red-orange crystals (120 mg, mixture of **2** and **3** in the ratio of 2 : 1, estimated by ^{1}H NMR, Figure S6). Recrystallization of the crude products from a mixture of hexane and THF (20 : 1) provided single crystals of **3**, suitable for X-ray diffraction analysis. However, to obtain enough amount of **3** for the NMR measurement failed so far. Partial NMR data for **3**: ^{1}H NMR (500 MHz, C_6D_6, 293 K) δ –0.33 (s, 6H, Si^{t}Bu*Me*$_2$), –0.15 (s, 6H, Si^{t}Bu*Me*$_2$), 1.02 (s, 18H, Si^t*Bu*Me$_2$), 5.81 (s, 5H, *Cp*), 5.87 (s, 5H, *Cp*), signals derived from the Ph groups cannot be assigned because the signals are overlaped with those of **2**. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 293 K) δ 1.09 (1°, Si^{t}Bu*Me*$_2$), 2.36 (1°, Si^{t}Bu*Me*$_2$), 20.55 (4°, Si^t*Bu*Me$_2$), 29.47 (1°, Si^t*Bu*Me$_2$), 104.13 (3°, *Cp*), 104.52 (3°, *Cp*), 128.84 (br), 136.58 (br), 142.63 (4°, *Ph*),

145.00 (4°, C_α), signals derived from the Ph groups and the butadiene moiety cannot be fully assigned because the signals are overlaped with those of **2**. ^{29}Si NMR (99 MHz, C_6D_6, 293 K) δ 2.2; ^{119}Sn NMR (187 MHz, C_6D_6, 293 K) δ –955.6.

Preparation of a sample for VT-NMR measurement: In a glovebox, compound **1** (42 mg, 0.059 mmol) and Cp_2HfCl_2 (22 mg, 0.058 mmol) were put into a J. Young® NMR tube. K-mirrored THF-d_8 (0.6 mL) was added to the NMR tube by a trap-to-trap distillation. After freeze-pump-thaw cycles, the NMR tube was sealed under vacuum and shaken at –20 °C for 5 min. The tube was kept at –30 °C and the NMR was measured at this temperature. ^{119}Sn NMR (187 MHz, THF-d_8, 253 K) δ 984 (br, $\Delta\nu_{1/2}$ = 230 Hz).

2. NMR charts of **2**

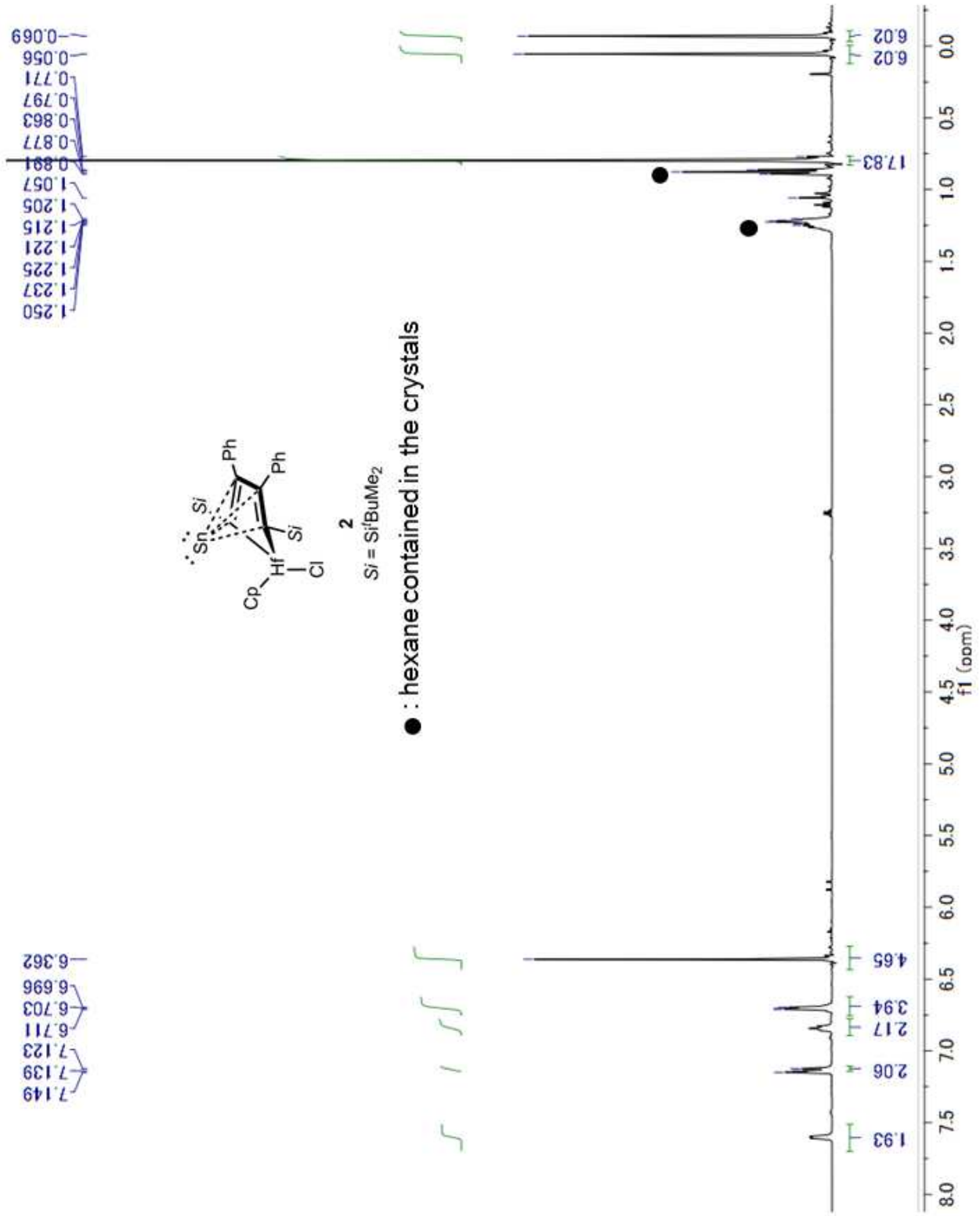

Figure S1. ^{1}H NMR chart of **2**.

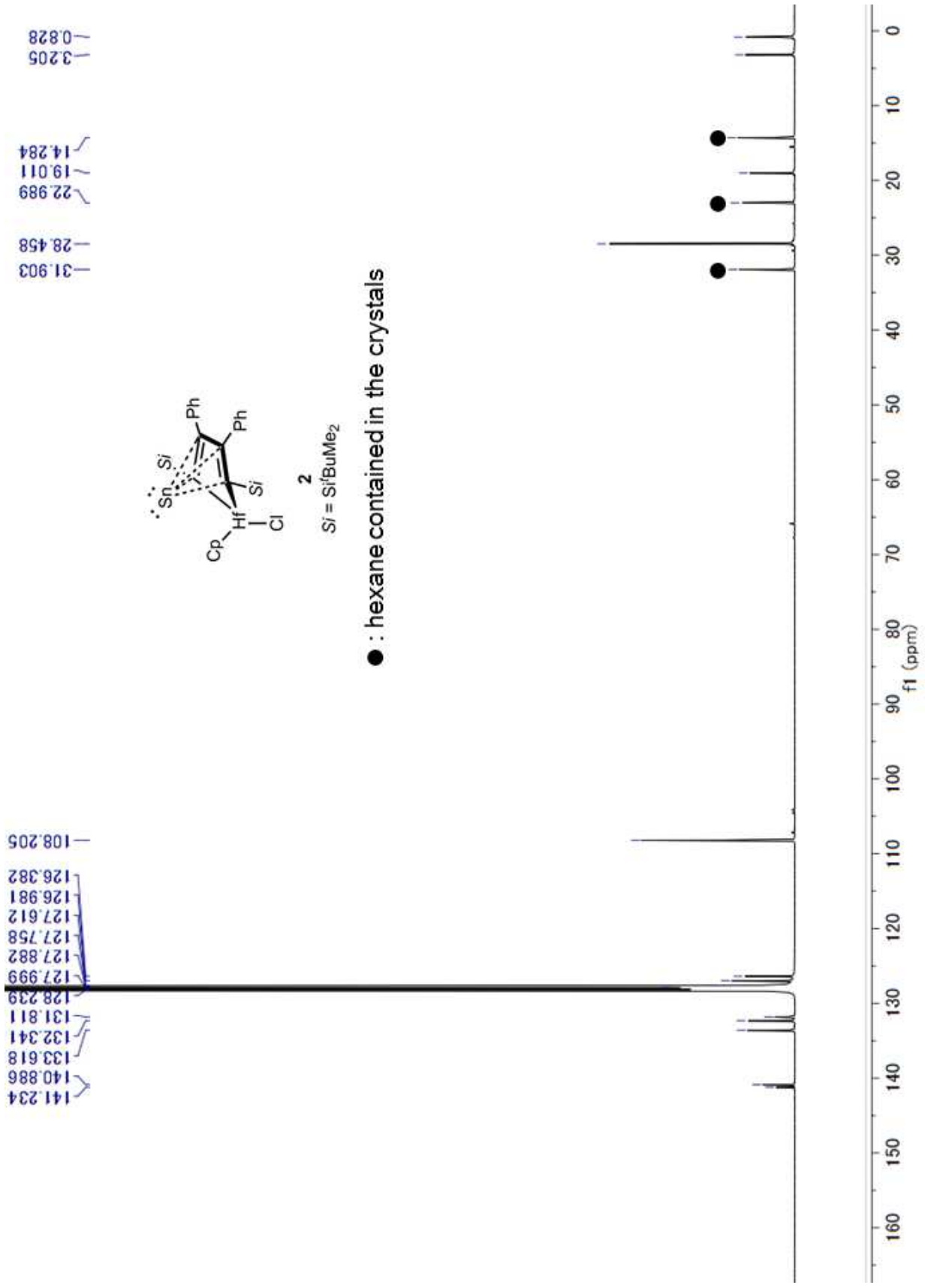

Figure S2. ^{13}C NMR chart of **2**.

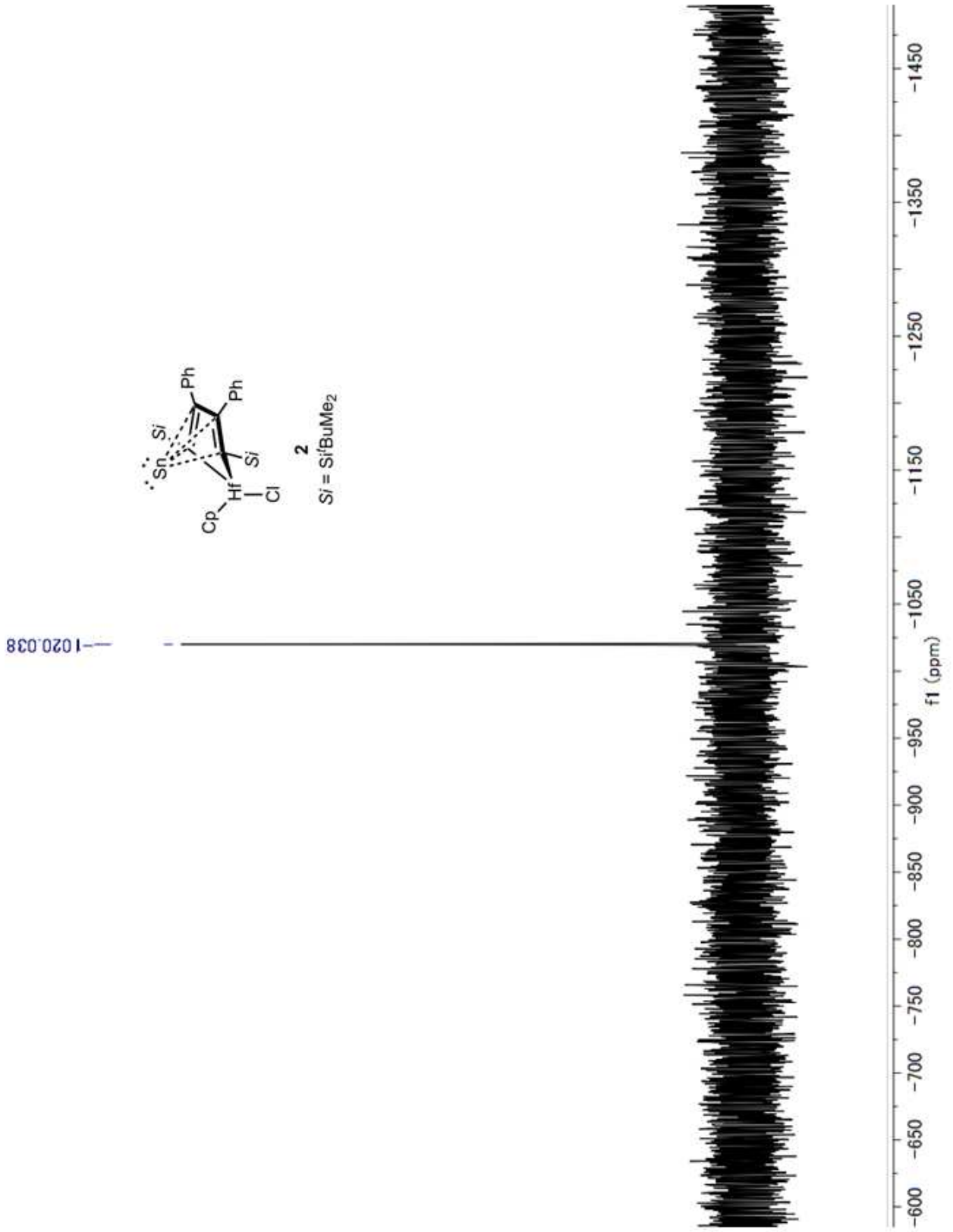

Figure S3. ^{119}Sn NMR chart of **2**.

3. NMR charts of mixtures of **2** and **3**.

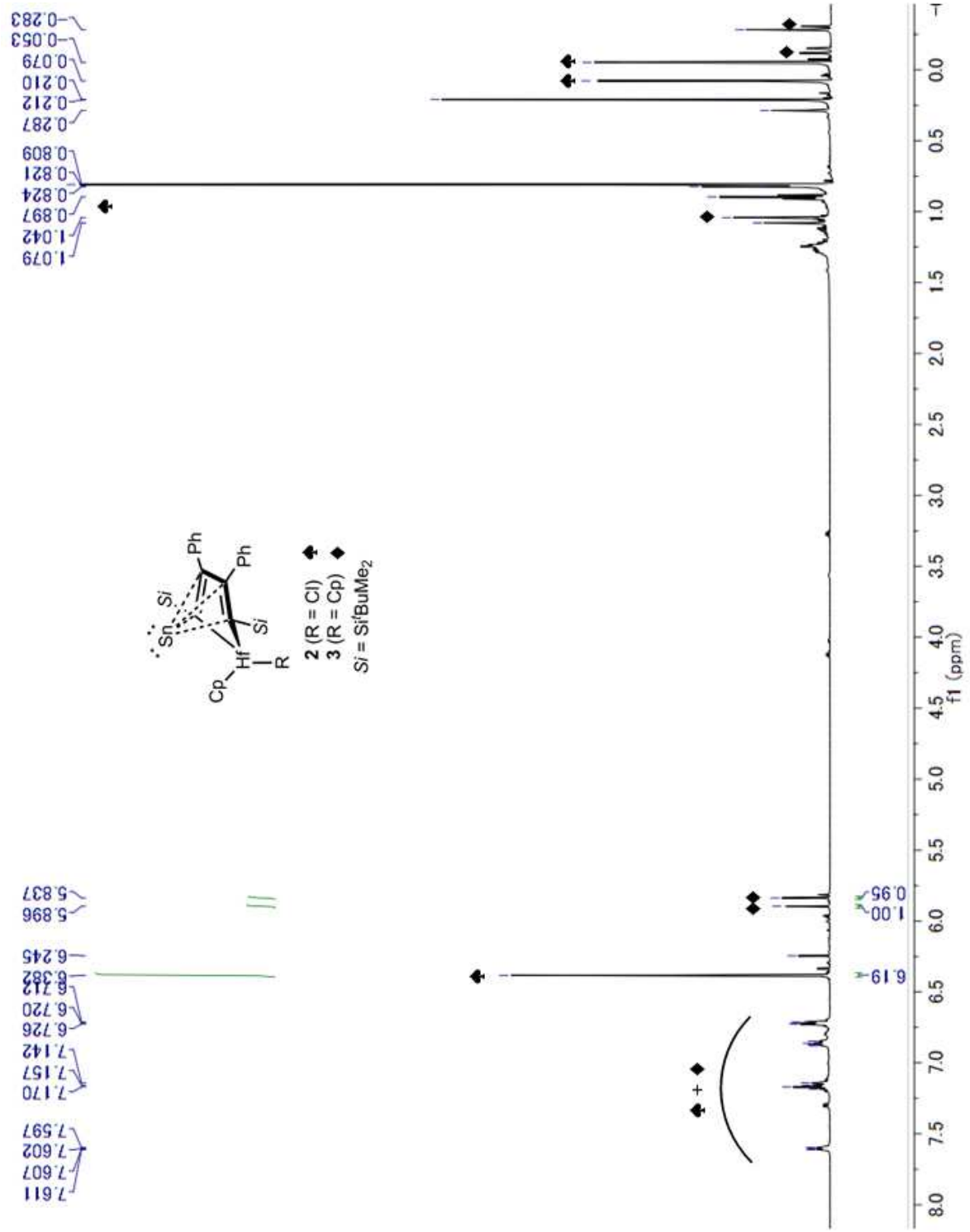

Figure S4. ^{1}H NMR chart of the crude products of run 1.

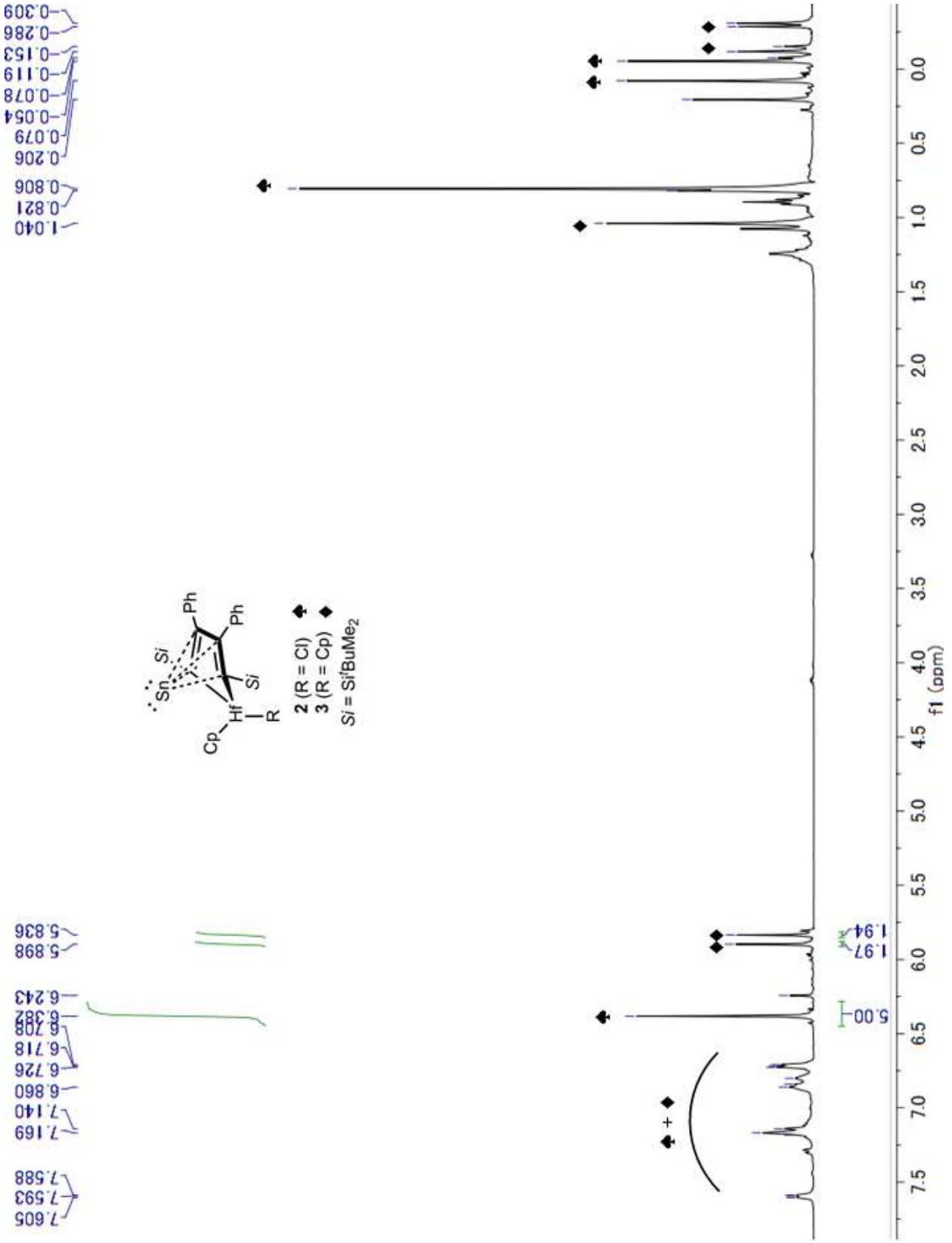

Figure S5. ^{1}H NMR chart of the crude products of run 2.

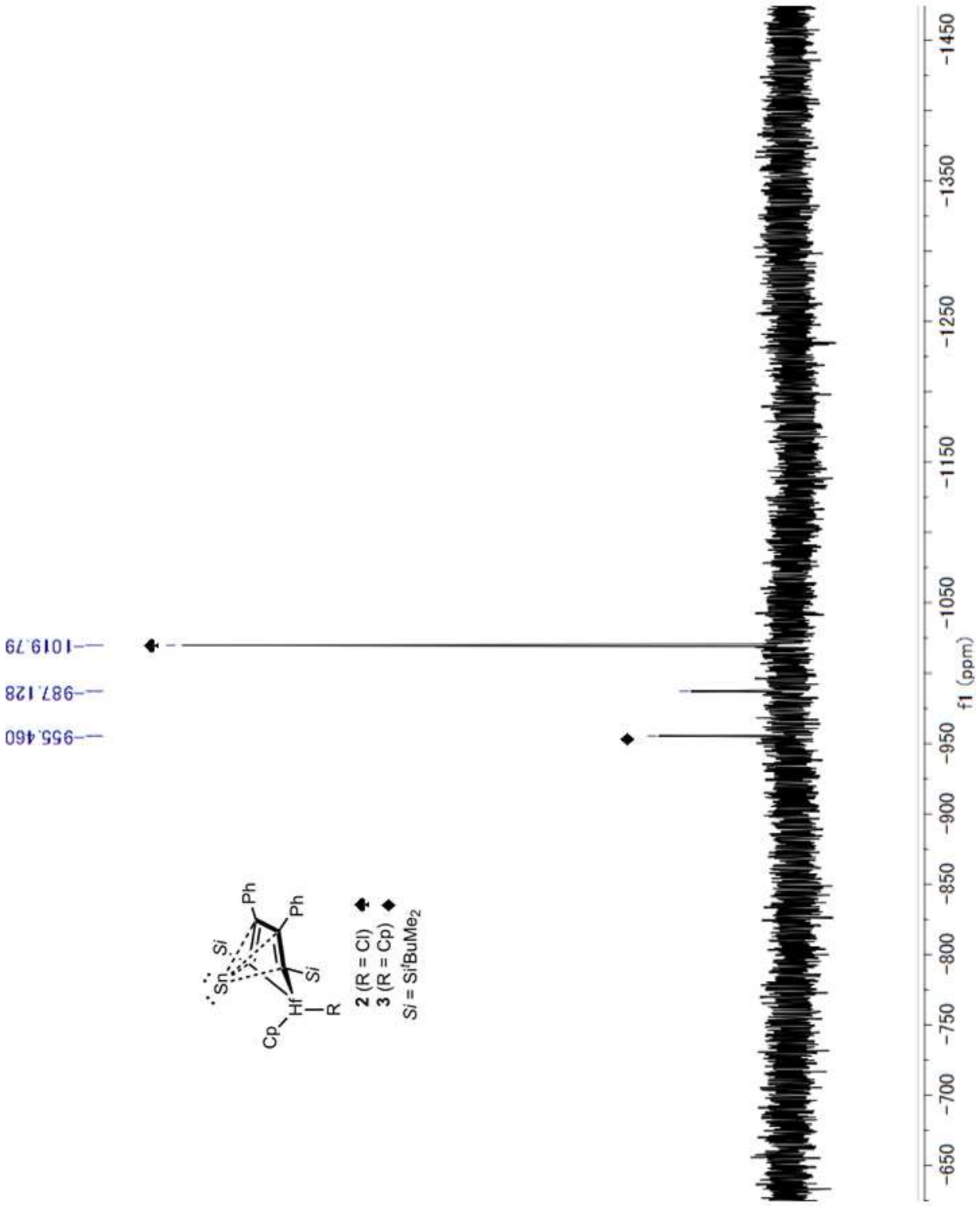

Figure S6. ^{119}Sn NMR chart of the crude products of run 2.

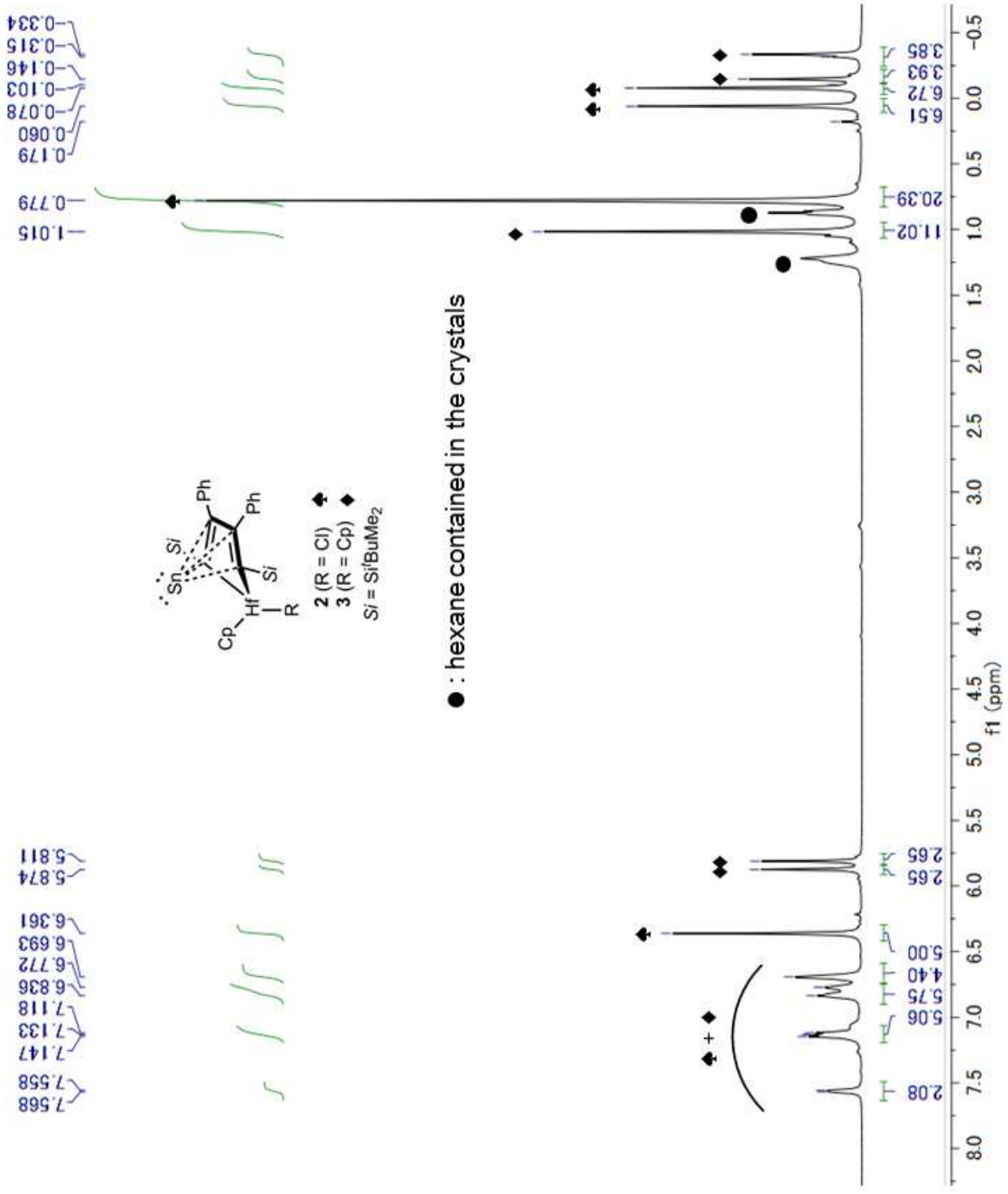

Figure S7. ^{1}H NMR chart of crystals containing **2** and **3** (run 2).

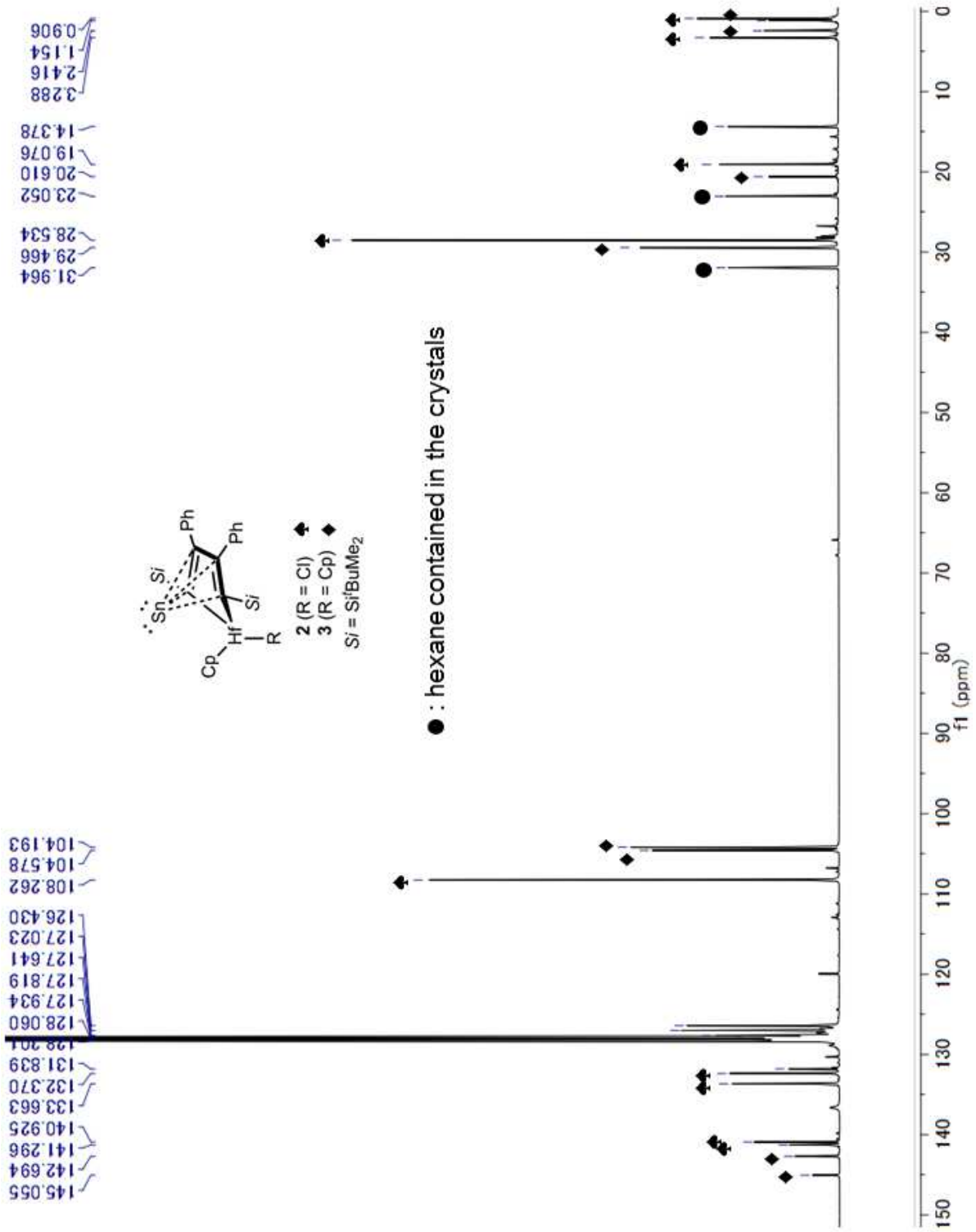

Figure S8. ^{13}C NMR chart of crystals containing **2** and **3** (run 2).

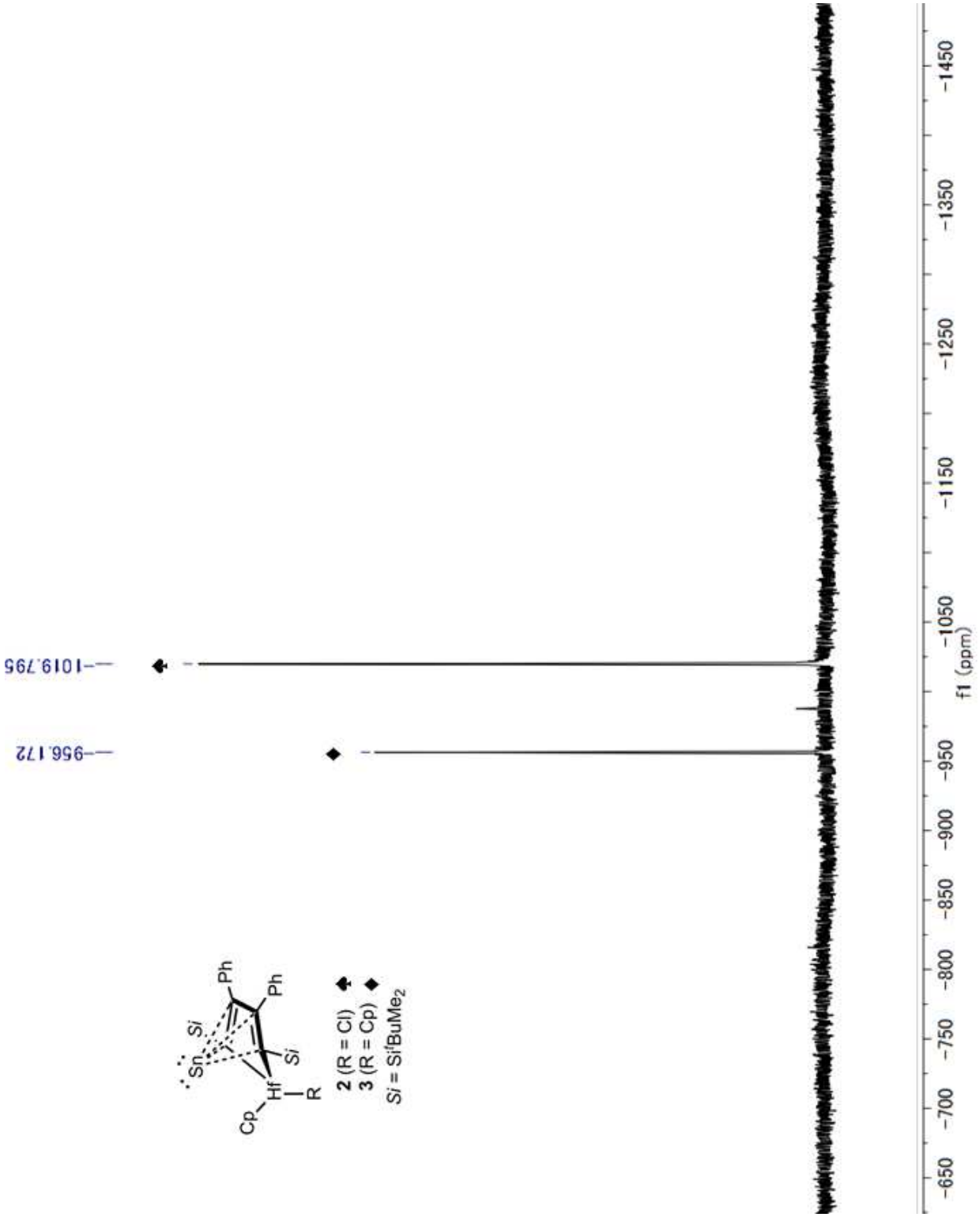

Figure S9. ^{119}Sn NMR chart of crystals containing **2** and **3** (run 2).

4. [119]Sn NMR chart of the reaction intermediate at –30 °C

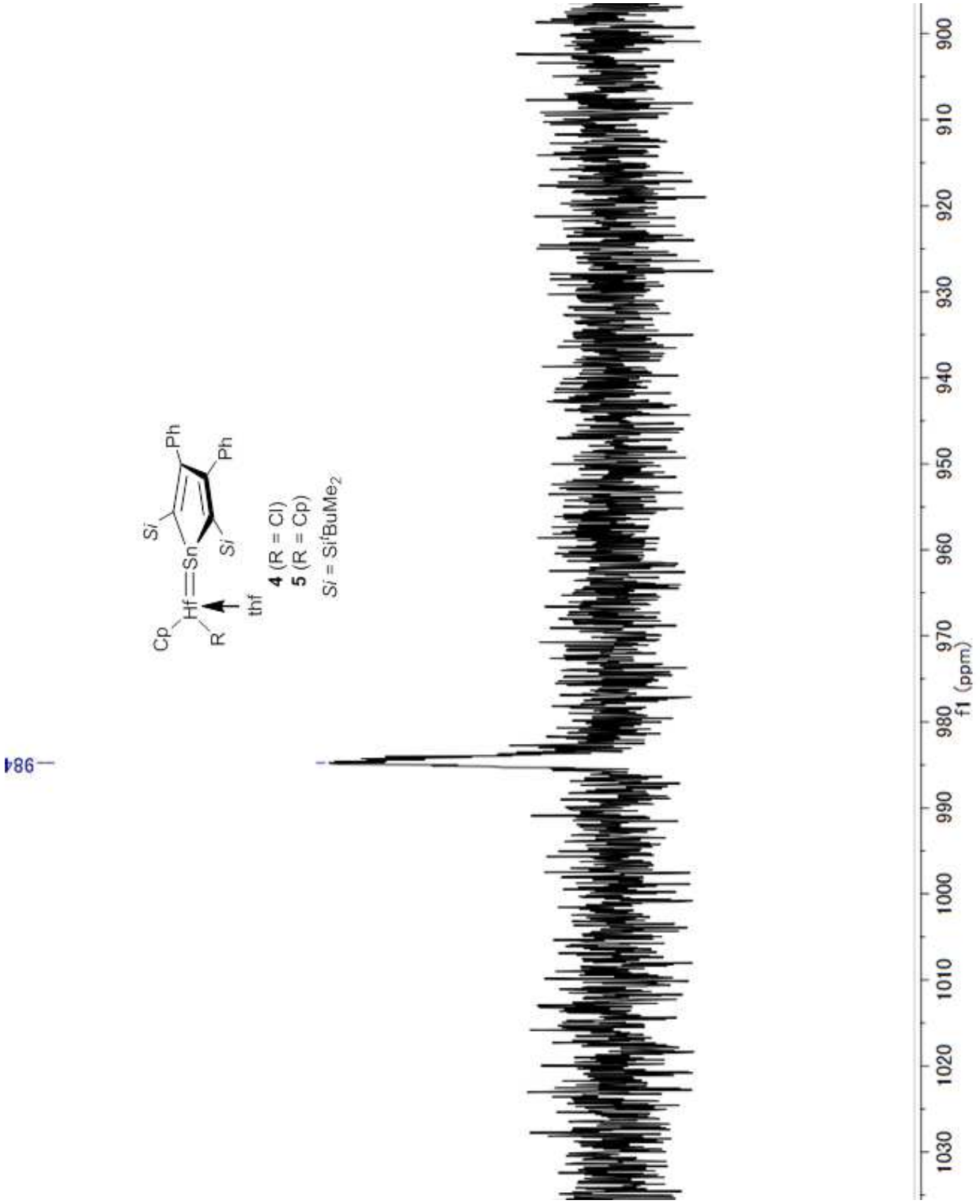

Figure S10. [119]Sn NMR of the green intermediate recorded at –30 °C.

5. X-ray diffraction analyses of compounds **2** and **3**.

5.1 Crystal data of compound **2**

Formula, $C_{40}H_{53}ClHfSi_2Sn$, FW=922.65, Crystal Dimension 0.08 × 0.04 × 0.03, Orthorhombic, *P*nma, *a*=31.894(2), *b*=15.3940(10), *c*=7.9405(5) Å, *V*=3898.6(4) $Å^3$, *Z*=4, D_{calcd}=1.572 g cm^{-3}. R_1=0.039 ($I > 2\sigma(I)$, 4160 reflections), wR_2=0.081 (for all reflections) for 4829 reflections and 214 parameters. GOF=1.099.

5.2 Crystal data of compound **3**

Formula, $C_{42}H_{58}HfOSi_2Sn$, FW=932.26, Crystal Dimension 0.10 × 0.10 × 0.05, Orthorhombic, $P2_12_12_1$, *a*=8.0406(4), *b*=15.0059(7), *c*=33.2314(16) Å, *V*=4009.6(3) $Å^3$, *Z*=4, D_{calcd}=1.544 g cm^{-3}. R_1=0.033 ($I > 2\sigma(I)$, 8142 reflections), wR_2=0.064 (for all reflections) for 8764 reflections and 424 parameters. GOF=1.001.

6. Optimized structure of **2** and its comparison with the experimental data

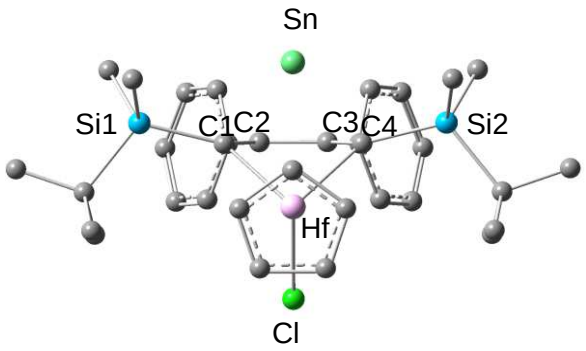

Figure S11. The optimized structure of **2**.

	Calc.	Exp.
Sn–C1/4 (Å)	2.305	2.313(4)
Sn–C2/3 (Å)	2.437	2.451(4)
Hf–C1/4 (Å)	2.155	2.144(4)
Hf–C2/3 (Å)	2.570	2.565(4)
Sn…Hf (Å)	3.181	3.1627(5)
Hf–Cl (Å)	2.430	2.4371(15)
C1–C2, C3–C4 (Å)	1.489	1.485(5)
C1…C4 (Å)	2.948	2.943
C2–C3 (Å)	1.460	1.450(7)

Table S1. Comparison of the optimized structure and the experimental data of **2**.

7. Comparison of the optimized structures of **2** and its protonated derivatives

The distances between Sn and C_β atoms in the protonated species (2.617, 2.627 Å and 2.817, 2.826 Å for singly- and doubly-protonated species, respectively) are much longer than those in **2** (2.437 Å), and the bent angle for SnC_4 cycle becomes smaller upon protonation. These changes are caused by the different roles of the lone pair on the *p* orbital of Sn: the lone pair in **2** is used for the interaction between Sn and $\pi(C_\beta–C_\beta)$ of the butadiene as was found in the HOMO, while the corresponding lone pair in the protonated derivatives is used for the first Sn–H^+ bond. In contrast to the long Sn–C and short Hf–C_α bonds in **2**, the Sn–C_α and the Hf–C_α bonds become shorter and longer, respectively, in the case of doubly protonated species **2•$(H^+)_2$**.

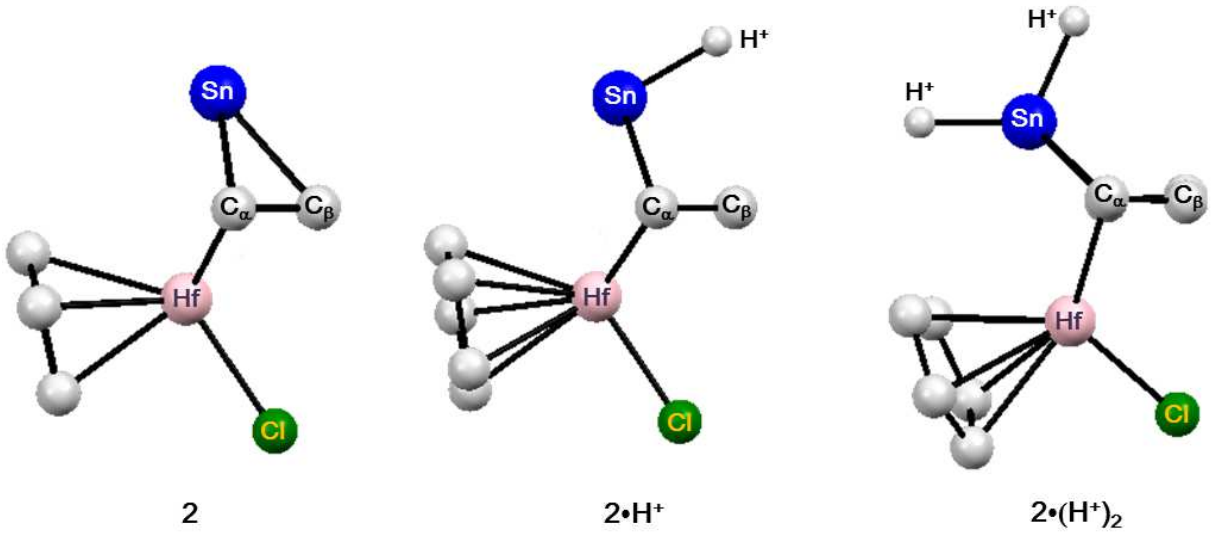

Figure S12. Structural changes upon protonations of **2**. Substituents on the butadiene were omited for clarity. Left: Before protonation, Center: Singly-protonated **2**, Right: Doubly-protonated **2**.

	2	**2•H$^+$**	**2•(H$^+$)$_2$**
Sn–C$_\alpha$	2.305	2.324, 2.343	2.271, 2.184
Sn–C$_\beta$	2.437	2.617, 2.627	2.817, 2.826
Hf–C$_\alpha$	2.155	2.236, 2.251	2.347, 2.544
Hf–C$_\beta$	2.570	2.701, 2.717	2.728, 2.719
C$_\alpha$–C$_\beta$	1.489	1.423, 1.429	1.413, 1.400
C$_\beta$–C$_\beta$	1.460	1.510	1.531
(Sn–C$_\alpha$–C$_\beta$)	97.58	109.13	135.07
(Hf–C$_\alpha$–C$_\beta$)	118.47	123.90	106.61

Table S2. Selected bond lengths (Å) and angles (°) of **2** (calc.) and its protonated derivatives.

8. Optimized structure of the proposed intermediate **4**

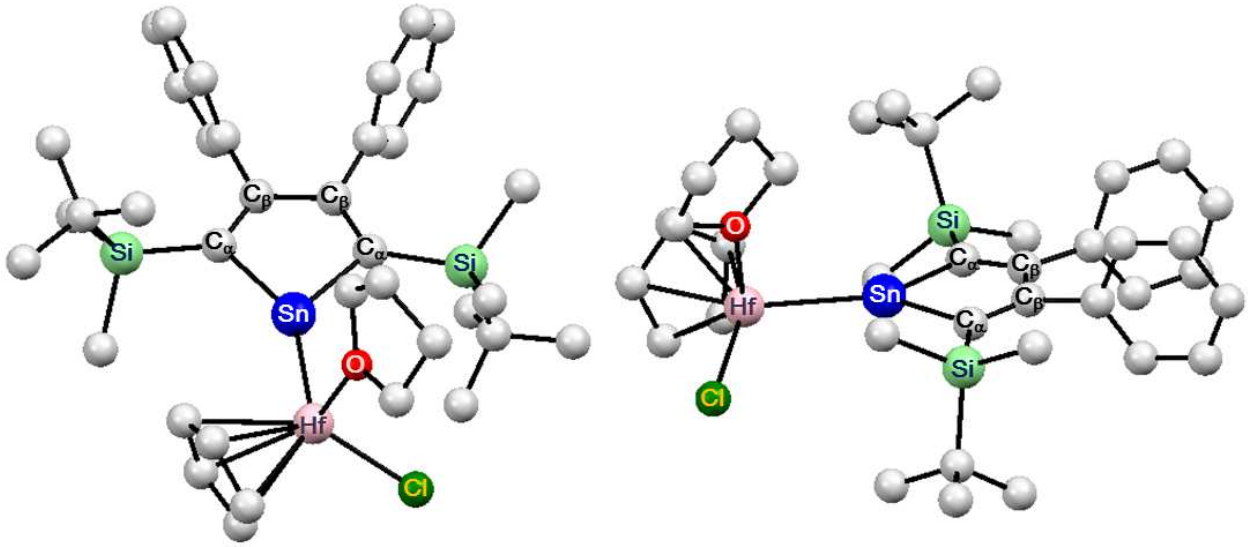

Figure S13. The optimized structure of **4** at B3PW91//Lanl2dz<Hf>/Lanl2dz+d<Sn>/6-31G(d) <C,O,Si,Cl,H>. Front view (left) and side vuew (right).

	4
Sn–C_α	2.173, 2.175
C_α–C_β	1.369, 1.370
C_β–C_β	1.498

Table S3. Selected bond lengths (Å) of **4**.

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

C	-0.708669	-3.501138	-1.719745
C	0.707360	-3.501292	-1.720091
C	1.148186	-3.492489	-0.374278
C	-0.000119	-3.481526	0.461393
C	-1.148841	-3.492241	-0.373713
Hf	-0.000186	-1.275812	-0.758327
C	-0.729825	1.013126	0.153341
C	-1.419802	2.296432	-0.195969
C	-1.720295	3.247931	0.785004
C	-2.356033	4.441474	0.449531
C	-2.692667	4.705559	-0.877213
C	-2.383565	3.770561	-1.863773
C	-1.750856	2.575186	-1.527824
C	1.473995	-0.246578	0.430605
Sn	-0.000044	-0.097068	2.195837
C	-1.474094	-0.246191	0.430566
Si	-3.266307	-0.404479	1.011577
C	-4.571970	-0.677327	-0.389891
C	-4.389775	-2.038255	-1.076116
C	0.730093	1.012923	0.153350
C	1.420451	2.296028	-0.195926
C	1.722156	3.246931	0.785249
C	2.358317	4.440272	0.449847
C	2.694183	4.704736	-0.877014
C	2.383908	3.770319	-1.863757
C	1.750768	2.575151	-1.527887
Si	3.266170	-0.405358	1.011531
C	4.571656	-0.677917	-0.390135
C	4.388981	-2.038450	-1.077010
Cl	-0.000076	-0.396323	-3.023575
C	3.844515	1.058251	2.077523
C	3.331710	-1.884665	2.209485
C	5.976428	-0.634850	0.240150
C	4.480129	0.421759	-1.456638
C	-3.844364	1.059543	2.077133
C	-3.331987	-1.883479	2.209905

C	-5.976674	-0.633552	0.240502
C	-4.480242	0.421795	-1.456940
H	1.456281	3.049754	1.821038
H	2.586488	5.165217	1.227217
H	3.188017	5.636527	-1.140742
H	2.630753	3.970861	-2.903257
H	1.495724	1.856524	-2.300790
H	0.000156	-3.508720	1.544718
H	2.177092	-3.510379	-0.048058
H	1.339384	-3.482619	-2.599569
H	4.756020	0.774711	2.618047
H	3.094275	1.324593	2.833069
H	4.060275	1.960005	1.497154
H	4.369594	-2.119358	2.475865
H	2.875785	-2.800519	1.822832
H	2.817211	-1.632686	3.146859
H	6.112335	-1.398868	1.016037
H	6.197391	0.341399	0.686437
H	6.737995	-0.820052	-0.531955
H	4.590272	1.426252	-1.032313
H	3.523327	0.388997	-1.988503
H	5.277023	0.291447	-2.204801
H	4.473836	-2.873892	-0.370118
H	5.164332	-2.183477	-1.844320
H	3.418177	-2.108831	-1.580976
H	-1.453791	3.051068	1.820690
H	-2.583271	5.166875	1.226748
H	-3.186169	5.637510	-1.140999
H	-2.630986	3.970808	-2.903193
H	-1.496680	1.856121	-2.300605
H	-2.177588	-3.509923	-0.046965
H	-1.341114	-3.482344	-2.598920
H	-4.755898	0.776340	2.617785
H	-3.094039	1.326001	2.832551
H	-4.059987	1.961139	1.496471
H	-4.369894	-2.118176	2.476194
H	-2.875953	-2.799390	1.823498
H	-2.817626	-1.631267	3.147293

H	-6.112698	-1.397096	1.016838
H	-6.197356	0.343002	0.686256
H	-6.738358	-0.819010	-0.531426
H	-4.590101	1.426523	-1.033098
H	-3.523485	0.388515	-1.988861
H	-5.277222	0.291318	-2.204985
H	-4.474520	-2.873318	-0.368764
H	-5.165419	-2.183546	-1.843080
H	-3.419166	-2.109070	-1.580391

10. The Cartesian coordinates of the optimized geometry for **2•H**$^{+}$

C	1.965847	2.538675	-1.435482
C	1.298506	2.423289	-0.207962
C	1.219671	3.541956	0.634277
C	1.818100	4.741263	0.264537
C	2.478384	4.850888	-0.960659
C	2.542496	3.750266	-1.812496
C	0.678713	1.116721	0.142172
Sn	0.043336	-0.296272	2.264091
C	-1.471896	-0.173036	0.506909
Si	-3.340932	-0.492720	0.887278
C	-3.378066	-2.066016	1.945484
Hf	0.012035	-1.362098	-0.697172
C	1.451746	-0.055350	0.407294
Si	3.333178	-0.051271	0.886331
C	3.444942	-1.227262	2.377980
C	-0.335863	-3.650803	-1.654093
C	1.046511	-3.529837	-1.377266
C	1.210668	-3.429825	0.030652
C	-0.079851	-3.502104	0.624006
C	-1.033198	-3.630865	-0.418626
C	-0.829213	1.059744	0.202723
C	-1.550913	2.336084	-0.083447
C	-2.122506	3.104390	0.936432
C	-2.769977	4.301623	0.637569
C	-2.855102	4.741957	-0.682070
C	-2.278839	3.985207	-1.701644
C	-1.619848	2.794701	-1.406740
C	-4.392944	-0.704265	-0.711419
C	-4.258023	0.515582	-1.634804
C	-4.127429	0.821421	1.996628
C	-4.001279	-1.962116	-1.498654
C	-5.867212	-0.838733	-0.279574
C	4.574256	-0.644516	-0.469520
C	4.351942	0.036905	-1.826615
C	3.858264	1.636845	1.549216
C	4.523958	-2.166302	-0.667674

C	5.983674	-0.274411	0.039131
Cl	-0.033143	-0.525878	-2.908089
H	0.708025	3.465504	1.588494
H	1.766160	5.595033	0.934236
H	2.936221	5.792537	-1.250226
H	3.040236	3.830536	-2.774954
H	1.999565	1.690094	-2.110465
H	-0.294368	-3.512392	1.685857
H	2.152768	-3.369011	0.556613
H	1.835744	-3.506820	-2.119226
H	4.793950	1.510024	2.107389
H	3.119539	2.049009	2.245270
H	4.029846	2.383865	0.769064
H	4.494410	-1.459114	2.597843
H	2.922938	-2.180956	2.248235
H	3.044988	-0.745614	3.281203
H	6.210516	-0.718339	1.016401
H	6.126678	0.808565	0.117677
H	6.736809	-0.651944	-0.666259
H	4.409818	1.128447	-1.755783
H	3.380649	-0.226244	-2.264538
H	5.125173	-0.284956	-2.538366
H	4.681273	-2.719305	0.265983
H	5.313932	-2.478796	-1.364675
H	3.572671	-2.487163	-1.103810
H	-2.041537	2.777201	1.968323
H	-3.202249	4.892431	1.440521
H	-3.360907	5.674931	-0.914067
H	-2.335754	4.323010	-2.732581
H	-1.162745	2.216909	-2.204492
H	-2.102489	-3.732333	-0.299227
H	-0.781249	-3.729235	-2.638266
H	-5.059181	0.403857	2.397999
H	-3.495438	1.069590	2.857508
H	-4.371248	1.750795	1.475957
H	-4.414005	-2.403960	2.068856
H	-2.806639	-2.908049	1.548003
H	-2.999959	-1.855360	2.954622

H	-6.036099	-1.689567	0.391732
H	-6.236919	0.064861	0.217299
H	-6.496255	-0.999475	-1.166098
H	-4.497785	1.456126	-1.126696
H	-3.246436	0.606394	-2.045305
H	-4.947537	0.416762	-2.485009
H	-4.135200	-2.878694	-0.911006
H	-4.632319	-2.057967	-2.393189
H	-2.961661	-1.920866	-1.853500
H	0.001618	1.397698	2.783900

11. The Cartesian coordinates of the optimized geometry for **2•(H^+)$_2$**

C	1.690858	2.826257	-1.214581
C	1.776387	2.223723	0.057340
C	2.667672	2.759434	1.008485
C	3.450541	3.865097	0.696244
C	3.388517	4.425365	-0.581643
C	2.513675	3.898562	-1.536058
C	0.936335	1.079635	0.454207
Sn	-0.181267	-0.827593	2.215207
C	-1.363984	0.033905	0.478622
Si	-3.268073	0.038137	0.983020
C	-3.338780	-1.216320	2.416890
Hf	0.118255	-1.131615	-0.919008
C	1.467080	-0.105127	0.978652
Si	3.296864	-0.735818	1.135872
C	3.117852	-2.482513	1.832702
C	-1.331384	-2.891254	-1.857935
C	-0.037122	-3.156971	-2.374620
C	0.795426	-3.539818	-1.291900
C	0.025800	-3.490102	-0.101135
C	-1.296573	-3.094677	-0.452572
C	-0.582030	1.196876	0.297815
C	-1.129489	2.510188	-0.057200
C	-0.770289	3.655748	0.686971
C	-1.360420	4.881735	0.412047
C	-2.266789	5.002919	-0.644520
C	-2.604026	3.883389	-1.410494
C	-2.062020	2.642012	-1.103690
C	-4.637442	-0.460418	-0.290933
C	-4.484887	0.192463	-1.671336
C	-3.633502	1.710434	1.774440
C	-4.749268	-1.984037	-0.466325
C	-5.959947	0.038990	0.336233
C	4.065431	-0.778079	-0.635056
C	4.965594	0.442172	-0.903501
C	4.338098	0.223528	2.376679

C	2.935178	-0.778422	-1.671499
C	4.906944	-2.058372	-0.798882
Cl	-0.265172	0.072429	-2.882924
H	2.695994	2.341257	2.009457
H	4.106705	4.292986	1.448626
H	4.012181	5.279234	-0.830318
H	2.462912	4.336619	-2.528421
H	0.999275	2.439230	-1.956132
H	0.356213	-3.800998	0.881079
H	1.829291	-3.856200	-1.367164
H	0.255838	-3.087951	-3.415598
H	5.210052	-0.394464	2.626668
H	3.805796	0.411427	3.316293
H	4.706994	1.174928	1.986605
H	4.112050	-2.925290	1.964599
H	2.549966	-3.170911	1.199068
H	2.654960	-2.476769	2.828434
H	4.316725	-2.975828	-0.689967
H	5.721826	-2.103914	-0.067867
H	5.370398	-2.078780	-1.794037
H	5.822497	0.457405	-0.221980
H	4.433603	1.392784	-0.796805
H	5.368602	0.396927	-1.923911
H	2.253625	-1.650654	-1.483448
H	3.282972	-0.963210	-2.697387
H	2.404329	0.181916	-1.696348
H	-0.067341	3.575416	1.509642
H	-1.106868	5.748468	1.014998
H	-2.704400	5.969999	-0.875185
H	-3.289532	3.981955	-2.247143
H	-2.311972	1.777578	-1.707152
H	-2.140790	-3.029257	0.219628
H	-2.190122	-2.588376	-2.444838
H	-4.519121	1.595240	2.410897
H	-2.814722	2.047088	2.419831
H	-3.843998	2.507898	1.056965
H	-4.394753	-1.311339	2.703648
H	-2.997593	-2.235140	2.202918

H	-2.838808	-0.859165	3.328538
H	-6.151138	-0.387894	1.328186
H	-5.998091	1.129623	0.420847
H	-6.797327	-0.266937	-0.304579
H	-4.518962	1.285545	-1.615406
H	-3.555633	-0.101898	-2.176758
H	-5.315559	-0.117173	-2.319347
H	-4.865721	-2.516236	0.484207
H	-5.636302	-2.216974	-1.069841
H	-3.893535	-2.410585	-0.998618
H	-0.400485	0.312035	3.467607
H	-0.326819	-2.455370	2.692224

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

C	2.520120	0.035290	2.902615
O	3.413529	0.240331	1.755852
C	4.701613	0.752875	2.213613
C	4.427782	1.281902	3.609782
C	3.385243	0.288184	4.129607
Hf	3.039094	-0.165036	-0.395180
Sn	0.259712	-0.165738	-0.355172
C	-1.542621	-1.377621	-0.421279
C	-2.583576	-0.532136	-0.140793
C	-2.366694	0.933613	0.078424
C	-3.569630	1.737444	0.479099
C	-4.343265	2.432068	-0.458381
C	-5.449137	3.182697	-0.060102
C	-5.807761	3.244928	1.285508
C	-5.054574	2.545992	2.228334
C	-3.950002	1.798303	1.826557
C	4.050579	-2.414488	0.141401
C	2.860723	-2.663893	-0.581091
C	3.007479	-2.101331	-1.889227
C	4.295814	-1.495292	-1.949821
C	4.937269	-1.687934	-0.690162
Cl	4.012090	1.872722	-1.154946
C	-1.118453	1.484539	-0.029620
Si	-0.616883	3.287071	0.149670
C	-1.765029	4.357374	1.216170
C	1.054275	3.333856	1.057087
C	-0.415705	4.130550	-1.582613
C	-1.717333	4.018081	-2.389019
Si	-1.642781	-3.214044	-0.823093
C	-3.281528	-3.798517	-1.579654
C	-0.391414	-3.551168	-2.213398
C	-1.236192	-4.336938	0.722157
C	-3.997848	-1.019486	-0.042599
C	-4.470436	-1.619932	1.130730
C	-5.782473	-2.084082	1.221439
C	-6.648743	-1.948445	0.137758

C	-6.195232	-1.337761	-1.031406
C	-4.884822	-0.873354	-1.117156
C	0.717531	3.474597	-2.383184
C	-0.083815	5.620397	-1.389704
H	4.235639	-2.701531	1.169832
H	2.008259	-3.217101	-0.214398
H	5.931241	-1.345822	-0.426568
H	2.300988	-2.182172	-2.702643
H	4.723005	-0.985083	-2.804557
H	5.413935	-0.080719	2.217382
H	5.021741	1.509545	1.495074
H	4.008025	2.292331	3.555788
H	5.334544	1.316570	4.220487
H	2.796541	0.681458	4.963166
H	3.869636	-0.637133	4.462480
H	1.702530	0.751234	2.793860
H	2.120283	-0.975798	2.827405
H	-3.800830	-1.715750	1.982044
H	-6.128448	-2.549260	2.141626
H	-7.671592	-2.310630	0.205370
H	-6.864266	-1.224128	-1.881180
H	-4.535004	-0.402249	-2.032215
H	-3.363511	1.257071	2.565337
H	-5.327345	2.583957	3.280544
H	-6.669910	3.829669	1.596754
H	-6.034028	3.716896	-0.805407
H	-4.073980	2.384011	-1.509354
H	1.432853	4.360125	1.142485
H	0.928491	2.946672	2.076400
H	1.828742	2.741843	0.556973
H	-1.297868	5.335787	1.386502
H	-2.748443	4.521491	0.765649
H	-1.930457	3.893982	2.194873
C	-0.397003	-5.547640	0.280331
C	-0.465935	-3.559367	1.799600
C	-2.535969	-4.865584	1.351906
H	-3.179283	-4.849356	-1.883343
H	-4.140580	-3.719955	-0.908722

H	-3.509992	-3.219528	-2.481712
H	0.060286	6.105050	-2.367430
H	-0.888227	6.159120	-0.874970
H	0.840886	5.767871	-0.817905
H	0.813834	3.953224	-3.370240
H	1.685916	3.567766	-1.879703
H	0.535530	2.406190	-2.553335
H	-1.609302	4.525799	-3.360104
H	-1.972609	2.971161	-2.591297
H	-2.566532	4.479535	-1.870310
H	-0.512131	-4.568292	-2.605245
H	-0.575762	-2.852452	-3.039058
H	0.653041	-3.439955	-1.913774
H	-2.308053	-5.460585	2.250035
H	-3.209956	-4.056613	1.654122
H	-3.090237	-5.513739	0.663483
H	-0.224858	-4.217534	2.649406
H	0.477524	-3.143838	1.423854
H	-1.051415	-2.715292	2.182343
H	-0.195901	-6.207936	1.138069
H	-0.913096	-6.150789	-0.477407
H	0.571827	-5.253299	-0.141180

13. Cif file of compound **2**

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cl'   'Cl'     0.1484     0.1585
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 'Sn'   'Sn'   -0.6537     1.4246
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_shelx_space_group_comment
;
The symmetry employed for this shelxl refinement is uniquely defined
by the following loop, which should always be used as a source of
symmetry information in preference to the above space-group names.
They are only intended as comments.
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 '-x, -y, -z'
 'x-1/2, y, -z-1/2'
 'x, -y-1/2, z'
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C1 C 0.39674(11) 0.1544(3) 0.2022(5) 0.0134(8) Uani 1 1 d . . . . .
C2 C 0.36366(11) 0.2029(2) 0.2942(5) 0.0120(8) Uani 1 1 d . . . . .
Si1 Si 0.39465(3) 0.03734(7) 0.13895(14) 0.0143(2) Uani 1 1 d . . . . .
C3 C 0.33976(12) -0.0054(3) 0.1203(6) 0.0228(9) Uani 1 1 d . . . . .
H1 H 0.3406 -0.0654 0.0877 0.034 Uiso 1 1 calc R U . . .
H2 H 0.3248 0.0274 0.0368 0.034 Uiso 1 1 calc R U . . .
H3 H 0.3258 -0.0001 0.2269 0.034 Uiso 1 1 calc R U . . .
C4 C 0.41788(13) 0.0284(3) -0.0773(5) 0.0237(9) Uani 1 1 d . . . . .
H4 H 0.4172 -0.0311 -0.1132 0.036 Uiso 1 1 calc R U . . .
H5 H 0.4464 0.0486 -0.0750 0.036 Uiso 1 1 calc R U . . .
H6 H 0.4019 0.0633 -0.1543 0.036 Uiso 1 1 calc R U . . .
C5 C 0.42367(13) -0.0394(3) 0.2872(6) 0.0199(9) Uani 1 1 d . . . . .
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H7 H 0.4806 -0.0379 0.1638 0.042 Uiso 1 1 calc R U . . .
H8 H 0.4846 -0.0708 0.3499 0.042 Uiso 1 1 calc R U . . .
H9 H 0.4790 0.0286 0.3133 0.042 Uiso 1 1 calc R U . . .
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H10 H 0.4215 -0.1438 0.1239 0.051 Uiso 1 1 calc R U . . .
H11 H 0.3838 -0.1435 0.2507 0.051 Uiso 1 1 calc R U . . .
H12 H 0.4284 -0.1727 0.3111 0.051 Uiso 1 1 calc R U . . .
C8 C 0.41032(15) -0.0252(3) 0.4688(6) 0.0313(11) Uani 1 1 d . . . . .
H13 H 0.3804 -0.0313 0.4777 0.047 Uiso 1 1 calc R U . . .
H14 H 0.4183 0.0321 0.5039 0.047 Uiso 1 1 calc R U . . .
H15 H 0.4237 -0.0674 0.5396 0.047 Uiso 1 1 calc R U . . .
C9 C 0.33039(11) 0.1586(2) 0.3966(5) 0.0136(8) Uani 1 1 d . . . . .
C10 C 0.33940(12) 0.1301(3) 0.5582(5) 0.0178(8) Uani 1 1 d . . . . .
H16 H 0.3658 0.1401 0.6036 0.021 Uiso 1 1 calc R U . . .
C11 C 0.30928(12) 0.0867(3) 0.6533(6) 0.0223(9) Uani 1 1 d . . . . .
H17 H 0.3157 0.0679 0.7615 0.027 Uiso 1 1 calc R U . . .
C12 C 0.26981(13) 0.0715(3) 0.5874(6) 0.0243(10) Uani 1 1 d . . . . .
H18 H 0.2498 0.0415 0.6498 0.029 Uiso 1 1 calc R U . . .
C13 C 0.26046(12) 0.1013(3) 0.4283(6) 0.0228(9) Uani 1 1 d . . . . .
H19 H 0.2337 0.0928 0.3849 0.027 Uiso 1 1 calc R U . . .
C14 C 0.29035(12) 0.1439(3) 0.3315(5) 0.0205(9) Uani 1 1 d . . . . .
H20 H 0.2837 0.1626 0.2234 0.025 Uiso 1 1 calc R U . . .
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Hf1 Hf 0.44078(2) 0.2500 0.28731(3) 0.01221(7) Uani 1 2 d S T P . .
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C15 C 0.48663(18) 0.2500 0.0299(8) 0.0267(15) Uani 1 2 d S T P . .
H21 H 0.4740 0.2500 -0.0757 0.032 Uiso 1 2 calc R U P . .
C16 C 0.49804(12) 0.1764(3) 0.1257(6) 0.0252(10) Uani 1 1 d . . . . .
H22 H 0.4946 0.1188 0.0930 0.030 Uiso 1 1 calc R U . . .
C17 C 0.51525(12) 0.2045(3) 0.2772(6) 0.0272(10) Uani 1 1 d . . . . .
H23 H 0.5251 0.1691 0.3635 0.033 Uiso 1 1 calc R U . . .
C18 C 0.1395(3) 0.2500 0.3029(12) 0.064(3) Uani 1 2 d S T P . .
H24 H 0.1325 0.1912 0.3315 0.096 Uiso 0.5 1 calc R U P . .
H25 H 0.1147 0.2804 0.2681 0.096 Uiso 0.5 1 calc R U P . .
H26 H 0.1514 0.2784 0.3993 0.096 Uiso 0.5 1 calc R U P . .
C19 C 0.1712(2) 0.2500 0.1599(10) 0.0380(18) Uani 1 2 d S T P . .
C20 C 0.18665(16) 0.1728(3) 0.0937(7) 0.0390(13) Uani 1 1 d . . . . .
H27 H 0.1770 0.1201 0.1362 0.047 Uiso 1 1 calc R U . . .
C21 C 0.21617(17) 0.1729(4) -0.0348(7) 0.0436(14) Uani 1 1 d . . . . .
H28 H 0.2263 0.1205 -0.0763 0.052 Uiso 1 1 calc R U . . .
C22 C 0.2306(2) 0.2500 -0.1012(10) 0.0415(19) Uani 1 2 d S T P . .
H29 H 0.2497 0.2500 -0.1895 0.050 Uiso 1 2 calc R U P . .

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C3 0.019(2) 0.021(2) 0.029(3) -0.0026(19) -0.0044(18) -0.0028(17)
C4 0.027(2) 0.025(2) 0.019(2) -0.0043(19) 0.0005(18) 0.0023(18)
C5 0.021(2) 0.015(2) 0.024(2) -0.0024(18) 0.0002(17) 0.0022(16)
C6 0.024(2) 0.029(2) 0.032(3) -0.005(2) -0.0081(19) 0.0061(19)
C7 0.036(3) 0.016(2) 0.050(3) -0.003(2) -0.006(2) 0.0022(19)
C8 0.037(3) 0.035(3) 0.021(3) 0.010(2) 0.0044(19) 0.015(2)

C9 0.0112(18) 0.0153(19) 0.014(2) -0.0011(16) 0.0017(14) 0.0005(15)
C10 0.014(2) 0.021(2) 0.018(2) 0.0031(17) 0.0006(16) -0.0019(16)
C11 0.021(2) 0.030(2) 0.016(2) 0.0087(19) -0.0009(16) -0.0035(18)
C12 0.022(2) 0.024(2) 0.026(3) -0.0003(19) 0.0077(18) -0.0082(18)
C13 0.013(2) 0.029(2) 0.026(2) -0.002(2) -0.0001(17) -0.0062(17)
C14 0.016(2) 0.031(2) 0.015(2) 0.0006(18) 0.0000(15) -0.0008(17)
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C19 0.028(4) 0.051(5) 0.035(4) 0.000 -0.016(3) 0.000
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C21 0.048(3) 0.038(3) 0.045(4) -0.012(3) -0.019(3) 0.005(3)
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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based

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  on F, with F set to zero for negative F^2^. The threshold expression of
  F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
  not relevant to the choice of reflections for refinement.  R-factors based
  on F^2^ are statistically about twice as large as those based on F, and R-
  factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef    Fsqd
_refine_ls_matrix_type                full
_refine_ls_weighting_scheme           calc
_refine_ls_weighting_details
  'calc w=1/[¥s^2^(Fo^2^)+(0.0025P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary          direct
_atom_sites_solution_secondary        difmap
_atom_sites_solution_hydrogens        geom
_refine_ls_hydrogen_treatment         constr
_refine_ls_extinction_method          none
_refine_ls_extinction_coef            ?
_refine_ls_abs_structure_details
  'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack        0.014(6)
_refine_ls_number_reflns              8764
_refine_ls_number_parameters          424
_refine_ls_number_restraints          0
_refine_ls_R_factor_all               0.0370
_refine_ls_R_factor_gt                0.0331
_refine_ls_wR_factor_ref              0.0637
_refine_ls_wR_factor_gt               0.0623
_refine_ls_goodness_of_fit_ref        1.001
_refine_ls_restrained_S_all           1.001
_refine_ls_shift/su_max               0.002
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C1 C 0.4881(7) 0.4127(3) 0.10269(15) 0.0113(11) Uani 1 1 d . . .
C2 C 0.5702(7) 0.4617(3) 0.13684(13) 0.0083(10) Uani 1 1 d . . .
C3 C 0.5767(7) 0.5565(3) 0.13594(15) 0.0120(11) Uani 1 1 d . . .
C4 C 0.5059(7) 0.6051(3) 0.10139(16) 0.0128(12) Uani 1 1 d . . .
Sn1 Sn 0.28959(4) 0.51729(2) 0.123297(10) 0.01202(8) Uani 1 1 d . . .
Si1 Si 0.39932(16) 0.29797(9) 0.10885(4) 0.0130(3) Uani 1 1 d . . .
C5 C 0.3677(6) 0.2643(3) 0.16314(16) 0.0196(12) Uani 1 1 d . . .
H1 H 0.3223 0.2052 0.1642 0.029 Uiso 1 1 calc R . .
H2 H 0.2922 0.3051 0.1758 0.029 Uiso 1 1 calc R . .
H3 H 0.4725 0.2655 0.1770 0.029 Uiso 1 1 calc R . .
C6 C 0.1804(6) 0.2947(3) 0.08779(16) 0.0191(12) Uani 1 1 d . . .
H4 H 0.1355 0.2358 0.0909 0.029 Uiso 1 1 calc R . .
H5 H 0.1828 0.3101 0.0598 0.029 Uiso 1 1 calc R . .
H6 H 0.1119 0.3365 0.1021 0.029 Uiso 1 1 calc R . .
C7 C 0.5185(6) 0.2033(3) 0.08248(16) 0.0172(12) Uani 1 1 d . . .
C8 C 0.7023(7) 0.1965(3) 0.09580(16) 0.0228(12) Uani 1 1 d . . .
H7 H 0.7586 0.2513 0.0897 0.034 Uiso 1 1 calc R . .
H8 H 0.7552 0.1483 0.0817 0.034 Uiso 1 1 calc R . .
H9 H 0.7074 0.1856 0.1242 0.034 Uiso 1 1 calc R . .
C9 C 0.4366(7) 0.1140(3) 0.09370(16) 0.0259(13) Uani 1 1 d . . .
H10 H 0.4369 0.1071 0.1224 0.039 Uiso 1 1 calc R . .
H11 H 0.4977 0.0659 0.0816 0.039 Uiso 1 1 calc R . .
H12 H 0.3241 0.1132 0.0841 0.039 Uiso 1 1 calc R . .
C10 C 0.5139(7) 0.2131(3) 0.03709(16) 0.0203(13) Uani 1 1 d . . .
H13 H 0.5645 0.2686 0.0296 0.030 Uiso 1 1 calc R . .
H14 H 0.4005 0.2122 0.0281 0.030 Uiso 1 1 calc R . .
H15 H 0.5737 0.1648 0.0249 0.030 Uiso 1 1 calc R . .
C11 C 0.6428(7) 0.4129(3) 0.17268(16) 0.0115(11) Uani 1 1 d . . .
C12 C 0.7740(6) 0.3536(3) 0.16637(15) 0.0148(11) Uani 1 1 d . . .

H16 H 0.8154 0.3447 0.1405 0.018 Uiso 1 1 calc R . .
C13 C 0.8428(7) 0.3080(3) 0.19875(17) 0.0233(13) Uani 1 1 d . . .
H17 H 0.9308 0.2689 0.1945 0.028 Uiso 1 1 calc R . .
C14 C 0.7817(8) 0.3200(3) 0.23724(17) 0.0233(13) Uani 1 1 d . . .
H18 H 0.8267 0.2882 0.2587 0.028 Uiso 1 1 calc R . .
C15 C 0.6539(7) 0.3795(3) 0.24371(17) 0.0239(13) Uani 1 1 d . . .
H19 H 0.6139 0.3890 0.2696 0.029 Uiso 1 1 calc R . .
C16 C 0.5852(6) 0.4250(3) 0.21145(15) 0.0156(11) Uani 1 1 d . . .
H20 H 0.4983 0.4646 0.2160 0.019 Uiso 1 1 calc R . .
C17 C 0.6594(7) 0.6032(3) 0.17028(16) 0.0126(11) Uani 1 1 d . . .
C18 C 0.8282(6) 0.6041(3) 0.17581(16) 0.0160(11) Uani 1 1 d . . .
H21 H 0.8958 0.5759 0.1571 0.019 Uiso 1 1 calc R . .
C19 C 0.9012(7) 0.6461(3) 0.20860(17) 0.0234(13) Uani 1 1 d . . .
H22 H 1.0162 0.6449 0.2117 0.028 Uiso 1 1 calc R . .
C20 C 0.8046(8) 0.6890(3) 0.23628(18) 0.0222(13) Uani 1 1 d . . .
H23 H 0.8538 0.7187 0.2578 0.027 Uiso 1 1 calc R . .
C21 C 0.6319(7) 0.6881(4) 0.23226(16) 0.0232(13) Uani 1 1 d . . .
H24 H 0.5653 0.7159 0.2514 0.028 Uiso 1 1 calc R . .
C22 C 0.5604(7) 0.6455(3) 0.19957(15) 0.0167(10) Uani 1 1 d . . .
H25 H 0.4452 0.6448 0.1969 0.020 Uiso 1 1 calc R . .
Si2 Si 0.50113(17) 0.73029(9) 0.09651(4) 0.0127(3) Uani 1 1 d . . .
C23 C 0.6613(6) 0.7905(3) 0.12783(16) 0.0212(12) Uani 1 1 d . . .
H26 H 0.6510 0.8536 0.1236 0.032 Uiso 1 1 calc R . .
H27 H 0.7706 0.7715 0.1200 0.032 Uiso 1 1 calc R . .
H28 H 0.6438 0.7772 0.1558 0.032 Uiso 1 1 calc R . .
C24 C 0.5619(8) 0.7639(3) 0.04391(15) 0.0215(12) Uani 1 1 d . . .
H29 H 0.5598 0.8277 0.0417 0.032 Uiso 1 1 calc R . .
H30 H 0.4848 0.7386 0.0250 0.032 Uiso 1 1 calc R . .
H31 H 0.6719 0.7426 0.0382 0.032 Uiso 1 1 calc R . .
C25 C 0.2888(6) 0.7848(3) 0.10693(15) 0.0160(11) Uani 1 1 d . . .
C26 C 0.1571(6) 0.7510(3) 0.07757(18) 0.0202(12) Uani 1 1 d . . .
H32 H 0.1932 0.7618 0.0505 0.030 Uiso 1 1 calc R . .
H33 H 0.0542 0.7818 0.0823 0.030 Uiso 1 1 calc R . .
H34 H 0.1410 0.6882 0.0815 0.030 Uiso 1 1 calc R . .
C27 C 0.3039(7) 0.8865(3) 0.10177(17) 0.0228(12) Uani 1 1 d . . .
H35 H 0.3855 0.9091 0.1202 0.034 Uiso 1 1 calc R . .
H36 H 0.1983 0.9138 0.1072 0.034 Uiso 1 1 calc R . .
H37 H 0.3372 0.8998 0.0747 0.034 Uiso 1 1 calc R . .

C28 C 0.2296(7) 0.7669(3) 0.15004(17) 0.0245(13) Uani 1 1 d . . .
H38 H 0.3118 0.7878 0.1687 0.037 Uiso 1 1 calc R . .
H39 H 0.2133 0.7040 0.1537 0.037 Uiso 1 1 calc R . .
H40 H 0.1265 0.7975 0.1547 0.037 Uiso 1 1 calc R . .
Hf1 Hf 0.56425(2) 0.504508(13) 0.054118(5) 0.01029(5) Uani 1 1 d . . .
C29 C 0.8521(6) 0.5727(3) 0.06612(16) 0.0145(12) Uani 1 1 d . . .
H41 H 0.8587 0.6235 0.0821 0.017 Uiso 1 1 calc R . .
C30 C 0.8319(6) 0.5715(3) 0.02440(16) 0.0163(12) Uani 1 1 d . . .
H42 H 0.8215 0.6211 0.0079 0.020 Uiso 1 1 calc R . .
C31 C 0.8300(5) 0.4821(3) 0.01176(15) 0.0180(12) Uani 1 1 d . . .
H43 H 0.8213 0.4625 -0.0147 0.022 Uiso 1 1 calc R . .
C32 C 0.8436(6) 0.4277(3) 0.04576(16) 0.0156(12) Uani 1 1 d . . .
H44 H 0.8416 0.3658 0.0460 0.019 Uiso 1 1 calc R . .
C33 C 0.8609(5) 0.4840(4) 0.07983(15) 0.0173(11) Uani 1 1 d . . .
H45 H 0.8754 0.4657 0.1063 0.021 Uiso 1 1 calc R . .
C34 C 0.3553(7) 0.4257(4) 0.00898(18) 0.0220(14) Uani 1 1 d . . .
H46 H 0.3377 0.3651 0.0132 0.026 Uiso 1 1 calc R . .
C35 C 0.2662(5) 0.4948(4) 0.02689(13) 0.0197(10) Uani 1 1 d . . .
H47 H 0.1778 0.4889 0.0447 0.024 Uiso 1 1 calc R . .
C36 C 0.3345(7) 0.5750(4) 0.01304(18) 0.0209(13) Uani 1 1 d . . .
H48 H 0.3003 0.6317 0.0207 0.025 Uiso 1 1 calc R . .
C37 C 0.4611(8) 0.5561(4) -0.01379(17) 0.0274(15) Uani 1 1 d . . .
H49 H 0.5253 0.5975 -0.0277 0.033 Uiso 1 1 calc R . .
C38 C 0.4750(7) 0.4626(4) -0.01628(17) 0.0249(14) Uani 1 1 d . . .
H50 H 0.5507 0.4312 -0.0320 0.030 Uiso 1 1 calc R . .
O1 O 0.2432(5) 0.5410(3) 0.25062(14) 0.0404(12) Uani 1 1 d . . .
C39 C 0.2992(9) 0.5582(4) 0.2905(2) 0.0481(19) Uani 1 1 d . . .
H51 H 0.3185 0.6214 0.2942 0.058 Uiso 1 1 calc R . .
H52 H 0.4022 0.5266 0.2957 0.058 Uiso 1 1 calc R . .
C40 C 0.1663(13) 0.5266(6) 0.3180(3) 0.098(4) Uani 1 1 d . . .
H53 H 0.0961 0.5757 0.3265 0.117 Uiso 1 1 calc R . .
H54 H 0.2139 0.4987 0.3417 0.117 Uiso 1 1 calc R . .
C41 C 0.0681(11) 0.4599(5) 0.2937(2) 0.079(3) Uani 1 1 d . . .
H55 H 0.0803 0.4004 0.3047 0.094 Uiso 1 1 calc R . .
H56 H -0.0490 0.4754 0.2933 0.094 Uiso 1 1 calc R . .
C42 C 0.1411(9) 0.4651(4) 0.2522(2) 0.0459(19) Uani 1 1 d . . .
H57 H 0.2059 0.4120 0.2465 0.055 Uiso 1 1 calc R . .
H58 H 0.0532 0.4695 0.2323 0.055 Uiso 1 1 calc R . .

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_atom_site_aniso_U_33
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C1 0.011(3) 0.012(3) 0.010(3) -0.0025(19) -0.002(2) -0.0017(19)
C2 0.008(2) 0.014(2) 0.003(2) -0.0015(16) -0.001(2) 0.001(2)
C3 0.008(2) 0.010(2) 0.018(3) -0.0004(18) 0.004(2) 0.002(2)
C4 0.011(3) 0.014(3) 0.014(3) 0.005(2) -0.002(2) 0.000(2)
Sn1 0.00940(14) 0.01296(19) 0.01369(16) 0.00048(13) 0.00130(13) 0.00016(13)
Si1 0.0130(7) 0.0131(7) 0.0130(7) -0.0004(5) -0.0002(6) -0.0012(5)
C5 0.021(3) 0.017(3) 0.020(3) 0.002(2) 0.003(2) -0.005(2)
C6 0.013(3) 0.021(3) 0.023(3) 0.000(2) 0.000(2) -0.005(2)
C7 0.022(3) 0.013(3) 0.017(3) -0.001(2) -0.002(2) 0.003(2)
C8 0.024(3) 0.020(3) 0.025(3) -0.006(2) -0.005(3) 0.005(3)
C9 0.036(3) 0.016(3) 0.026(3) -0.001(2) 0.001(3) 0.000(3)
C10 0.019(3) 0.018(3) 0.025(3) -0.004(2) -0.001(2) 0.001(2)
C11 0.011(3) 0.011(3) 0.012(3) 0.001(2) -0.003(2) 0.000(2)
C12 0.014(3) 0.016(3) 0.014(3) -0.0008(19) 0.004(2) -0.003(2)
C13 0.019(3) 0.020(3) 0.030(3) -0.001(2) -0.007(3) 0.007(2)
C14 0.029(3) 0.024(3) 0.017(3) 0.007(2) -0.007(3) 0.002(3)
C15 0.032(3) 0.023(3) 0.016(3) 0.004(2) 0.000(3) -0.003(3)
C16 0.018(3) 0.013(3) 0.016(3) 0.0018(19) 0.000(2) 0.003(2)
C17 0.014(3) 0.012(3) 0.012(3) 0.0048(19) 0.000(2) 0.000(2)
C18 0.013(3) 0.019(3) 0.016(3) -0.003(2) 0.002(2) 0.003(2)
C19 0.017(3) 0.027(3) 0.027(3) 0.000(2) -0.002(3) -0.004(2)
C20 0.021(3) 0.025(3) 0.020(3) -0.004(2) -0.004(3) -0.011(3)
C21 0.028(3) 0.029(3) 0.013(3) -0.007(2) 0.001(2) -0.003(2)
C22 0.016(3) 0.018(3) 0.017(3) 0.000(2) -0.001(2) 0.002(2)
Si2 0.0125(7) 0.0113(7) 0.0143(7) 0.0009(5) 0.0007(6) -0.0014(5)
C23 0.024(3) 0.015(3) 0.025(3) 0.003(2) -0.004(3) -0.005(2)
C24 0.027(3) 0.018(3) 0.019(3) 0.0021(19) 0.006(3) 0.000(3)
C25 0.016(3) 0.012(3) 0.020(3) 0.001(2) 0.001(2) 0.003(2)
C26 0.014(3) 0.014(3) 0.032(3) 0.002(2) -0.005(3) 0.001(2)

C27 0.031(3) 0.009(3) 0.028(3) -0.002(2) 0.004(3) 0.002(2)
C28 0.021(3) 0.024(3) 0.028(3) -0.001(2) 0.009(3) 0.004(2)
Hf1 0.00918(8) 0.01200(10) 0.00967(9) 0.00029(9) 0.00042(7) -0.00046(9)
C29 0.006(2) 0.015(3) 0.023(3) -0.005(2) 0.003(2) -0.001(2)
C30 0.016(3) 0.018(3) 0.016(3) 0.006(2) 0.008(2) 0.000(2)
C31 0.007(2) 0.034(3) 0.013(2) -0.005(2) 0.0003(18) 0.003(2)
C32 0.012(3) 0.015(3) 0.020(3) -0.001(2) 0.001(2) 0.0031(19)
C33 0.005(2) 0.031(3) 0.016(2) 0.001(2) -0.0015(19) -0.001(2)
C34 0.023(3) 0.020(3) 0.023(4) 0.000(2) -0.013(3) 0.002(2)
C35 0.010(2) 0.034(3) 0.015(2) 0.004(3) -0.0057(18) -0.002(3)
C36 0.022(3) 0.022(3) 0.019(3) 0.000(2) -0.015(3) 0.007(2)
C37 0.027(4) 0.037(4) 0.019(3) 0.012(2) -0.016(3) -0.020(3)
C38 0.015(3) 0.045(4) 0.015(3) -0.015(2) -0.001(2) 0.001(2)
O1 0.030(2) 0.039(3) 0.052(3) -0.005(2) 0.003(2) -0.0063(19)
C39 0.041(4) 0.040(4) 0.064(5) -0.018(3) -0.012(4) -0.004(3)
C40 0.150(9) 0.091(8) 0.051(6) 0.002(5) -0.014(6) -0.057(7)
C41 0.101(7) 0.088(6) 0.047(5) -0.008(4) 0.014(5) -0.057(6)
C42 0.047(4) 0.047(4) 0.043(4) -0.004(3) 0.007(4) -0.015(3)

_geom_special_details
;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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C1 C2 1.505(7) . ?
C1 Si1 1.875(5) . ?
C1 Hf1 2.209(5) . ?

C1 Sn1 2.341(5) . ?
C2 C3 1.423(6) . ?
C2 C11 1.515(7) . ?
C2 Sn1 2.447(5) . ?
C2 Hf1 2.823(4) . ?
C3 C4 1.475(7) . ?
C3 C17 1.495(7) . ?
C3 Sn1 2.419(6) . ?
C3 Hf1 2.830(5) . ?
C4 Si2 1.886(5) . ?
C4 Hf1 2.229(5) . ?
C4 Sn1 2.300(5) . ?
Sn1 Hf1 3.1936(4) . ?
Si1 C5 1.891(5) . ?
Si1 C6 1.895(5) . ?
Si1 C7 1.925(5) . ?
C5 H1 0.9600 . ?
C5 H2 0.9600 . ?
C5 H3 0.9600 . ?
C6 H4 0.9600 . ?
C6 H5 0.9600 . ?
C6 H6 0.9600 . ?
C7 C10 1.516(7) . ?
C7 C9 1.539(7) . ?
C7 C8 1.546(7) . ?
C8 H7 0.9600 . ?
C8 H8 0.9600 . ?
C8 H9 0.9600 . ?
C9 H10 0.9600 . ?
C9 H11 0.9600 . ?
C9 H12 0.9600 . ?
C10 H13 0.9600 . ?
C10 H14 0.9600 . ?
C10 H15 0.9600 . ?
C11 C16 1.381(7) . ?
C11 C12 1.396(7) . ?
C12 C13 1.390(7) . ?
C12 H16 0.9300 . ?

C13 C14 1.382(8) . ?
C13 H17 0.9300 . ?
C14 C15 1.378(8) . ?
C14 H18 0.9300 . ?
C15 C16 1.386(7) . ?
C15 H19 0.9300 . ?
C16 H20 0.9300 . ?
C17 C18 1.370(7) . ?
C17 C22 1.409(7) . ?
C18 C19 1.388(7) . ?
C18 H21 0.9300 . ?
C19 C20 1.366(8) . ?
C19 H22 0.9300 . ?
C20 C21 1.395(8) . ?
C20 H23 0.9300 . ?
C21 C22 1.385(7) . ?
C21 H24 0.9300 . ?
C22 H25 0.9300 . ?
Si2 C24 1.884(5) . ?
Si2 C23 1.887(5) . ?
Si2 C25 1.925(5) . ?
C23 H26 0.9600 . ?
C23 H27 0.9600 . ?
C23 H28 0.9600 . ?
C24 H29 0.9600 . ?
C24 H30 0.9600 . ?
C24 H31 0.9600 . ?
C25 C26 1.527(7) . ?
C25 C28 1.534(7) . ?
C25 C27 1.539(6) . ?
C26 H32 0.9600 . ?
C26 H33 0.9600 . ?
C26 H34 0.9600 . ?
C27 H35 0.9600 . ?
C27 H36 0.9600 . ?
C27 H37 0.9600 . ?
C28 H38 0.9600 . ?
C28 H39 0.9600 . ?

C28 H40 0.9600 . ?
Hf1 C38 2.527(5) . ?
Hf1 C37 2.526(5) . ?
Hf1 C36 2.529(5) . ?
Hf1 C32 2.539(5) . ?
Hf1 C34 2.544(6) . ?
Hf1 C33 2.552(4) . ?
Hf1 C29 2.562(5) . ?
Hf1 C35 2.566(4) . ?
Hf1 C30 2.572(5) . ?
Hf1 C31 2.581(4) . ?
C29 C30 1.396(7) . ?
C29 C33 1.409(7) . ?
C29 H41 0.9300 . ?
C30 C31 1.406(7) . ?
C30 H42 0.9300 . ?
C31 C32 1.398(7) . ?
C31 H43 0.9300 . ?
C32 C33 1.419(7) . ?
C32 H44 0.9300 . ?
C33 H45 0.9300 . ?
C34 C38 1.392(8) . ?
C34 C35 1.395(7) . ?
C34 H46 0.9300 . ?
C35 C36 1.400(8) . ?
C35 H47 0.9300 . ?
C36 C37 1.382(8) . ?
C36 H48 0.9300 . ?
C37 C38 1.411(7) . ?
C37 H49 0.9300 . ?
C38 H50 0.9300 . ?
O1 C42 1.405(7) . ?
O1 C39 1.423(8) . ?
C39 C40 1.485(11) . ?
C39 H51 0.9700 . ?
C39 H52 0.9700 . ?
C40 C41 1.510(10) . ?
C40 H53 0.9700 . ?

C40 H54 0.9700 . ?
C41 C42 1.501(9) . ?
C41 H55 0.9700 . ?
C41 H56 0.9700 . ?
C42 H57 0.9700 . ?
C42 H58 0.9700 . ?

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