Supplementary Information of the Article Entitled "Synthesis and Reactivity of a Ruthenocene-type Complex Bearing an Aromatic π-Ligand with the Heaviest Group 14 Element"

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1. Experimental Section

General procedure: All experiments were performed under argon atmosphere in a glovebox or using a standard Schlenk technique. Diethyl ether, toluene, and benzene-d_6 for NMR measurement were purified potassium mirror before used. ^{1}H NMR (400 or 500 MHz), ^{13}C NMR (101 MHz), ^{7}Li NMR (194 MHz), ^{29}Si NMR (99 MHz) and ^{207}Pb NMR (105 MHz) were recorded on a Bruker DPX-400 Cryo or a AVANCE-500T. The intensity data for X-ray crystallographic analyses were collected at −173 or −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. UV-vis spectra of **6** and **7** were recorded on a Hitachi U-1900 spectrophotometer. Cyclic voltammetry was measured on a Gamry Interface 1000 in THF (1.1 mmol/L) with 0.1 mol/L THF solution of $[Bu_4N]ClO_4$ as an electrolyte.

Preparation of anionic ruthenocene 3. In a glovebox, to a mixture of dilithioplumbole **4**[S1] solvated by two THF molecules (146 mg, 0.18 mmol) and $[Cp^*RuCl]_4$[S2] (50 mg, 0.046 mmol) was added THF (2 mL) at room temperature, and the solution was stirred for 1.5 hours. After removal of the solvent, materials insoluble in hexane (10 mL × 2) were filtered through Celite® to provide a crude product. After recrystallization of the crude product from THF and hexane at −30 °C, anionic ruthenocene **3** was obtained as red crystals (110 mg, 52%). **3**: mp 53 ºC (decomp.). ^{1}H NMR (500 MHz, C_6D_6, 20 °C) δ −0.36 (s, 6H), 0.53 (s, 6H), 1.00 (s, 18H), 1.34-1.36 (m, 16H, thf), 2.13 (s, 15H), 3.52-3.55 (m, 16H, thf), 6.93-6.96 (m, 2H), 7.01-7.04 (m, 4H), 7.46-7.47 (m, 4H); ^{13}C NMR (101 MHz, C_6D_6, 20 °C) δ −1.06 (q), 3.92 (q, J_{PbC} = 90 Hz), 13.93 (q), 17.66 (s), 25.55 (t, thf), 29.16 (q), 68.17 (q, thf), 87.31 (s, Cp*), 121.66 (s, J_{PbC} = 51 Hz, C_β), 125.56 (d), 126.28 (d), 134.67 (d), 145.60 (s, J_{PbC} = 775 Hz, C_α), 150.50 (s, J_{PbC} = 38 Hz, *ipso*); ^{7}Li NMR (194MHz, C_6D_6, 20 °C) δ 1.8; ^{29}Si NMR (99 MHz, C_6D_6, 20 °C) δ 9.0; ^{207}Pb NMR (105 MHz, C_6D_6, 20 °C) δ 1552.5. The elemental analysis failed because the results were not reproducible due to its high sensitivity toward oxygen and moisture.

Reactions of 3 with electrophiles. Anionic ruthenocene **3** (approximately 40 to 60 mg) was dissolved in 3 mL of toluene in a glovebox. To the solution was added a toluene solution of each of the electrophiles examined via syringe under Ar. After the mixture was stirred for 1.5 hours at room temperature, volatile substances were removed in a glovebox. Materials insoluble in hexane (5 mL × 2) were removed by filtration through Celite® to give a crude product. Recrystallization from hexane at −30 °C provided the corresponding plumbole complexes **5**-**8**.

Ethyl-substituted plumbole complex **5** (obtained as red powder): yield 92% (31.7 mg, 0.035 mmol). mp 63 ºC (decomp.). ^{1}H NMR (500 MHz, C_6D_6, 20 °C) δ −0.22 (s, 6H), 0.45 (s, 6H), 1.05 (s, 18H), 1.64 (q, *J* = 8 Hz, 2H), 1.90 (s, 15H), 2.12 (t, *J* = 8 Hz, 3H), 6.78-6.90 (m, 8H), 7.01-7.08 (m, 2H); ^{13}C NMR (101 MHz, C_6D_6, 20 °C) δ −1.05 (q), 0.81 (q), 12.43 (q), 14.00 (q), 18.11 (s), 28.57 (q), 38.68 (t), 89.81 (s, Cp*), 113.18 (s, C_β), 126.04 (d), 126.12 (d), 132.84 (d), 144.13 (s, *ipso*), 151.94 (s, C_α); ^{29}Si NMR (99 MHz, C_6D_6, 20 °C) δ 10.0; ^{207}Pb NMR (105 MHz, C_6D_6, 20 °C) δ −24.5. Anal. Calcd. for $C_{40}H_{60}Si_2RuPb$: C, 53.07; H, 6.68. Found: C, 54.03; H, 6.78.

Isopropyl-substituted plumbole complex **6** (obtained as red crystals): yield 59% (20.6 mg, 0.022 mmol). mp 130 ºC (decomp.). λ / nm (ε / mol cm L^{-1}) = 472 (4700), 568 (650). ^{1}H NMR (500 MHz, C_6D_6, 20 °C) δ −0.35 (s, 6H), 0.52 (s, 6H), 1.08 (s, 18H), 1.95 (s, 15H), 2.10 (d, *J* = 7 Hz, 6H), 3.12 (sept, *J* = 7 Hz, 1H), 6.78-6.86 (m, 10H); ^{13}C NMR (101 MHz, C_6D_6, 20 °C) δ −0.65 (q), 0.38 (q), 12.66 (q), 18.24 (s), 25.03 (q), 28.91 (q), 51.49 (d), 89.60 (s, Cp*), 113.51 (s, C_β), 125.97 (d), 126.02 (d), 133.08 (d), 144.22 (s, *ipso*), 149.76 (s, C_α); ^{29}Si NMR (99 MHz, C_6D_6, 20 °C) δ 10.6; ^{207}Pb NMR (105 MHz, C_6D_6, 20 °C) δ 99.8. Anal. Calcd. for $C_{41}H_{62}Si_2RuPb$: C, 53.65; H, 6.98. Found: C, 53.06; H, 6.71.

Chloro-substituted plumbole complex **7** (obtained as green crystals): yield 44% (21.7 mg, 0.024 mmol). mp 87 ºC (decomp.). λ / nm (ε / mol cm L^{-1}) = 413 (1600), 699 (300). ^{1}H NMR (500 MHz, C_6D_6, 20 °C) δ −0.12 (s, 6H), 0.81 (s, 6H), 0.95 (s, 18H), 1.95 (s, 15H), 6.72-6.80 (m, 10H); ^{13}C NMR (101 MHz, C_6D_6, 20 °C) δ −0.53 (q), 0.84 (q), 11.91 (q), 18.75 (s), 28.93 (q), 92.90 (s, Cp*), 109.09 (s, C_β), 126.29 (d), 126.39 (d), 132.05 (d), 141.23 (s, *ipso*), 176.20 (s, C_α); ^{29}Si NMR (99 MHz, C_6D_6, 20 °C) δ 10.69; ^{207}Pb NMR (105 MHz, C_6D_6, 20 °C) δ −158.7. The elemental analysis failed because the results were not reproducible due to its high sensitivity toward oxygen and moisture.

Iodo-substituted plumbole complex **8** (obtained as green crystals): yield 40% (23.0 mg, 0.021 mmol). mp 83 ºC (decomp.).^{1}H NMR (500 MHz, C_6D_6, 20 °C) δ −0.23 (s, 6H), 0.82 (s, 6H), 0.97 (s, 18H), 2.03 (s, 15H), 6.72-7.02 (m, 10H); ^{13}C NMR (101 MHz, C_6D_6, 20 °C) δ −0.65 (q), 1.80 (q), 18.93 (q), 23.00 (s), 28.72 (q), 92.76 (s, Cp*), 109.48 (s, C_β), 126.28 (d), 126.57 (d), 128.30 (d), 140.87 (s, *ipso*), 170.70 (s, C_α); ^{29}Si NMR (99 MHz, C_6D_6, 20 °C) δ 12.2; ^{207}Pb NMR (105 MHz, C_6D_6, 20 °C) δ 3.6. The elemental analysis failed because the results were not reproducible due to its high sensitivity toward oxygen and moisture.

2. X-ray diffraction analyses of compounds 3, 6, 7 and 8

3: Formula, $C_{54}H_{87}LiO_4PbRuSi_2$, FW = 1171.63, crystal dimension 0.15 × 0.12 × 0.10, triclinic, *P*-1, a = 12.7785(7), b = 14.3628(8), c = 15.1226(9) Å, α = 97.8360(10), β = 96.9920(10), γ = 93.2610(10)°, V = 2721.5(3) Å^3, Z = 2, D_{calcd} = 1.430 g cm^{-3}, R_1 = 0.038 ($I > 2\sigma(I)$, 10711 reflections), wR_2 = 0.087 (for all reflections) for 12507 reflections and 568 parameters. GOF=1.005.

6: Formula, $C_{40.55}H_{59.95}Cl_{0.15}PbRuSi_2$, FW = 917.20, crystal dimension 0.20 × 0.20 × 0.03, monoclinic, $P2_1/c$, a = 16.7796(15), b = 11.2019(11), c = 21.597(2) Å, β = 98.9100(10)°, V = 4010.5(6) Å^3, Z = 4, D_{calcd} = 1.519 g cm^{-3}, R_1 = 0.023 ($I > 2\sigma(I)$, 6234 reflections), wR_2 = 0.052 (for all reflections) for 7045 reflections and 432 parameters. GOF=1.025. The crystal contains 85% of **6** and 15% of **7**, and the co-crsytallized **7** may be caused by contaminating LiCl in the starting **3**.

7: Formula, $C_{38}H_{55}ClPbRuSi_2$, FW = 911.72, crystal dimension 0.02 × 0.02 × 0.02, monoclinic, $P2_1/n$, a = 9.7280(12), b = 18.602(2), c = 21.538(3) Å, β = 95.419(2)°, V = 3880.1(8) Å^3, Z = 4, D_{calcd} = 1.561 g cm^{-3}, R_1 = 0.036 ($I > 2\sigma(I)$, 5281 reflections), wR_2 = 0.067 (for all reflections) for 7476 reflections and 403 parameters. GOF=1.023.

8: Formula, $C_{38}H_{55}IPbRuSi_2 \cdot C_6H_{14}$, FW = 1089.33, crystal dimension 0.10 × 0.10 × 0.03, orthorhombic, *Pbca*, a = 10.3930(5), b = 22.3163(10), c = 39.5129(17) Å, V = 9164.4(7) Å^3, Z = 8, D_{calcd} = 1.579 g cm^{-3}, R_1 = 0.047 ($I > 2\sigma(I)$, 8138 reflections), wR_2 = 0.099 (for all reflections) for 10525 reflections and 495 parameters. GOF=1.077.

Crystallographic data for compounds **3**, **6**, **7** and **8** have been deposited with the Cambridge Crystallographic Data Centre as CCDC-1507475, -1511941, -1507473 and -1507474, respectively (www.ccdc.cam.ac.uk/data_request/cif).

3. Theoretical calculations

Optimized structures were obtained by hybrid DFT calculation at the LC-BLYP.[S3] As lead is a heavy element and its relativistic effect may be considerably large, we use the energy-consistent relativistic pseudopotential and correlation consistent basis sets (cc-pVTZ-pp)[S4-S5] for Pb. We use cc-pVTZ-pp also for Ru. The basis functions used are 6-311G(d) for Si, Cl and C in a five-membered ring, 6-31G for H and the other atoms. Electronic excitation energies corresponding to the UV spectra are obtained by TD-DFT, the functional of which is LC-BLYP[S3] using the same basis sets as those for the geometry optimization. All calculations are performed with Gaussion09.[S6]

References

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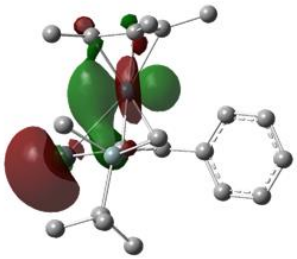
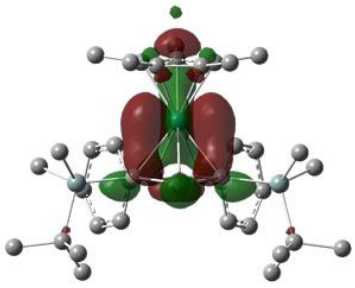
4. Molecular orbitals of 3 having interaction between *d*(Ru) and the plumbole ring

HOMO-2
LP(Sn) and *d*(Ru)–C(α)

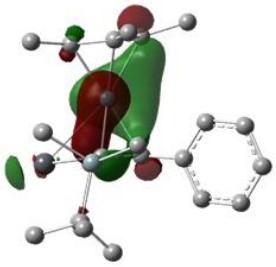


side view

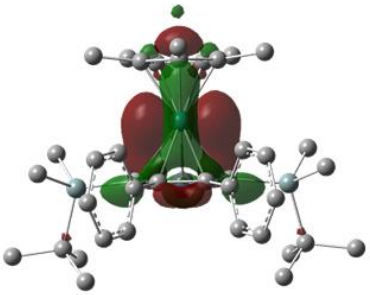
HOMO-3
d(Ru)–C(α) and *d*(Ru)–C(β)



front view

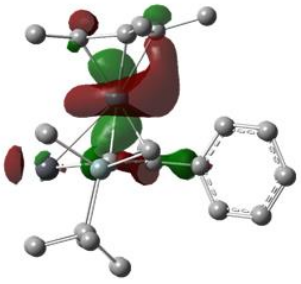


side view



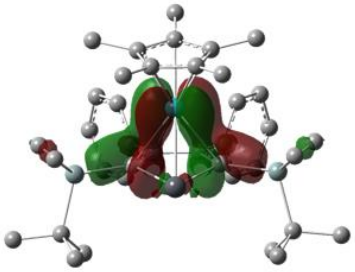
back view

HOMO-5
d(Ru)–C(α)

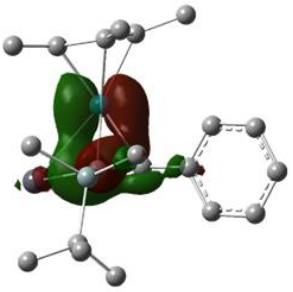


side view

HOMO-6
d(Ru)–{Sn–C(α)} and *d*(Ru)–C(β)



front view



side view

5. Cartesian coordinates for the optimized structure of compound 3

Pb	2.123088	-0.15345	0
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Si	0.691942	-0.45474	-3.18697
Si	0.691942	-0.45474	3.186969
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C	0.378259	-0.32857	-1.37876
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C	-0.84867	-0.58341	-0.71622
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C	-3.02315	-0.02264	1.877187
C	-4.16423	-0.40148	2.563659
C	-4.4091	-1.73951	2.819395
C	-3.50757	-2.6916	2.370389
C	-2.37141	-2.30393	1.681965
C	-2.10331	-0.96072	-1.43593
C	-2.37141	-2.30393	-1.68197
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C	-4.4091	-1.73951	-2.81939
C	-4.16423	-0.40148	-2.56366
C	-3.02315	-0.02264	-1.87719
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C	0.495024	3.270664	0.707644

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C	-0.84583	3.101149	1.1495
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C	1.67455	3.621402	1.556562
C	-1.30018	3.227898	-2.56976
C	-1.30018	3.227898	2.569758
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H	-1.67157	-3.0501	-1.32717
H	-3.69288	-3.74435	-2.55346
H	-5.29984	-2.04093	-3.35907
H	-4.86503	0.354026	-2.90245
H	-2.81446	1.015327	-1.67104
H	-1.32901	0.683613	-4.07221
H	-0.45463	-0.15306	-5.36472
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H	1.145674	-4.26456	-3.22539
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H	0.390672	-2.41237	-5.52655
H	3.530768	-1.46457	-3.65371
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H	-1.50156	-1.0564	4.253975
H	-0.45463	-0.15306	5.364717

H	2.7288	0.983245	3.021615
H	1.465231	1.765228	3.9783
H	2.434093	0.478492	4.695004
H	3.530768	-1.46457	3.65371
H	3.340465	-3.21374	3.456197
H	3.007249	-2.12511	2.10094
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H	1.145674	-4.26456	3.225387
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H	1.557389	3.254263	-2.57403
H	2.591532	3.185925	-1.15652
H	1.801351	4.709857	1.60128
H	2.591532	3.185925	1.156521
H	1.557389	3.254263	2.574028
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H	-2.24586	2.712136	2.743129
H	-3.46139	4.184102	0
H	-3.62143	2.664072	0.87847
H	-3.62143	2.664072	-0.87847

6. Cartesian coordinates for the optimized structure of compound 6

Pb	1.766059	-0.84061	0
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Si	0.319608	-0.31989	-3.26588
Si	0.319608	-0.31989	3.265884
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C	0.048147	-0.13625	-1.41262
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C	-1.13404	-0.44059	-0.72829
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C	-3.31015	0.249039	1.78953
C	-4.4926	-0.0583	2.439635
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C	-2.76309	-2.07081	1.670821
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C	-3.94163	-2.38389	-2.32485
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C	-1.21501	0.002612	4.282692
C	1.599377	0.903232	3.86604
C	0.973958	-2.0498	3.750617
C	2.463085	-2.21268	3.437384
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C	0.203906	-3.17935	3.067719
C	3.697143	0.403704	0
C	0.710235	3.224989	-0.71298

C	0.710235	3.224989	0.712981
C	-0.63586	3.224953	-1.14827
C	-0.63586	3.224953	1.148271
C	-1.46677	3.211023	0
C	1.922336	3.473942	-1.55054
C	1.922336	3.473942	1.550542
C	-1.11436	3.396813	-2.55332
C	-1.11436	3.396813	2.553317
C	-2.93854	3.482135	0
C	4.509611	0.069612	1.243356
C	4.509611	0.069612	-1.24336
H	-3.0532	1.274812	1.571201
H	-5.16924	0.735624	2.733828
H	-5.7322	-1.62114	3.227981
H	-4.18704	-3.42024	2.524849
H	-2.09242	-2.86104	1.357297
H	-2.09242	-2.86104	-1.3573
H	-4.18704	-3.42024	-2.52485
H	-5.7322	-1.62114	-3.22798
H	-5.16924	0.735624	-2.73383
H	-3.0532	1.274812	-1.5712
H	-1.70458	0.92984	-3.98215
H	-0.93026	0.100736	-5.33437
H	-1.95562	-0.79606	-4.20424
H	2.389035	1.079256	-3.13593
H	2.065826	0.535721	-4.78456
H	1.142782	1.865751	-4.10315
H	-0.85797	-3.15427	-3.32495
H	0.60092	-4.14912	-3.39132
H	0.295774	-3.1289	-1.9789
H	1.312139	-1.41733	-5.82813
H	1.229638	-3.16323	-5.58771
H	-0.25178	-2.20233	-5.56016
H	3.072672	-1.44236	-3.91731
H	2.66465	-2.18505	-2.36419
H	2.81074	-3.18572	-3.80452

H	-1.70458	0.92984	3.982147
H	-1.95562	-0.79606	4.204239
H	-0.93026	0.100736	5.334366
H	2.389035	1.079256	3.135926
H	1.142782	1.865751	4.103153
H	2.065826	0.535721	4.784565
H	3.072672	-1.44236	3.917306
H	2.81074	-3.18572	3.804519
H	2.66465	-2.18505	2.364188
H	1.312139	-1.41733	5.828133
H	-0.25178	-2.20233	5.560158
H	1.229638	-3.16323	5.587708
H	-0.85797	-3.15427	3.324954
H	0.295774	-3.1289	1.978905
H	0.60092	-4.14912	3.391323
H	2.278941	4.495701	-1.38396
H	1.704972	3.365659	-2.61099
H	2.738668	2.794	-1.30672
H	2.278941	4.495701	1.383957
H	2.738668	2.794	1.306716
H	1.704972	3.365659	2.610994
H	-1.23728	4.460405	-2.78196
H	-2.0762	2.909356	-2.7154
H	-0.41048	2.979262	-3.27138
H	-1.23728	4.460405	2.781958
H	-0.41048	2.979262	3.27138
H	-2.0762	2.909356	2.715401
H	-3.09862	4.565262	0
H	-3.43878	3.080826	0.880229
H	-3.43878	3.080826	-0.88023
H	3.462024	1.468968	0
H	4.002431	0.351638	2.167838
H	4.723041	-1.00363	1.298036
H	5.4759	0.589122	1.221109
H	4.002431	0.351638	-2.16784
H	5.4759	0.589122	-1.22111

H	4.723041	-1.00363	-1.29804

7. Cartesian coordinates for the optimized structure of compound 7.

Pb	1.751325	-1.02037	0
Ru	-0.06361	1.398724	0
Cl	3.831692	0.478876	0
Si	0.449793	-0.30206	-3.26417
Si	0.449793	-0.30206	3.264174
C	0.115673	-0.09119	1.421834
C	0.115673	-0.09119	-1.42183
C	-1.06118	-0.40714	0.732409
C	-1.06118	-0.40714	-0.73241
C	-2.36252	-0.66792	1.417074
C	-3.17967	0.371805	1.82979
C	-4.36922	0.119887	2.490391
C	-4.75735	-1.18383	2.745955
C	-3.95427	-2.23111	2.324558
C	-2.7686	-1.974	1.659053
C	-2.36252	-0.66792	-1.41707
C	-2.7686	-1.974	-1.65905
C	-3.95427	-2.23111	-2.32456
C	-4.75735	-1.18383	-2.74596
C	-4.36922	0.119887	-2.49039
C	-3.17967	0.371805	-1.82979
C	-1.04008	0.108646	-4.31322
C	1.84743	0.813514	-3.78478
C	1.007173	-2.07547	-3.71702
C	0.177324	-3.15869	-3.02974
C	0.826235	-2.23755	-5.23351
C	2.488875	-2.31085	-3.40893
C	-1.04008	0.108646	4.313216
C	1.84743	0.813514	3.784778
C	1.007173	-2.07547	3.717019
C	2.488875	-2.31085	3.40893
C	0.826235	-2.23755	5.233509
C	0.177324	-3.15869	3.02974
C	0.950024	3.189872	-0.71328

C	0.950024	3.189872	0.713281
C	-0.39206	3.253466	-1.14855
C	-0.39206	3.253466	1.148546
C	-1.22488	3.268128	0
C	2.186147	3.376639	-1.52904
C	2.186147	3.376639	1.529039
C	-0.8569	3.444708	-2.55539
C	-0.8569	3.444708	2.555389
C	-2.68708	3.585237	0
H	-2.86529	1.385516	1.629849
H	-4.99454	0.945212	2.810138
H	-5.68594	-1.38479	3.26626
H	-4.25566	-3.25516	2.510249
H	-2.14945	-2.79661	1.323401
H	-2.14945	-2.79661	-1.3234
H	-4.25566	-3.25516	-2.51025
H	-5.68594	-1.38479	-3.26626
H	-4.99454	0.945212	-2.81014
H	-2.86529	1.385516	-1.62985
H	-1.48476	1.061034	-4.02203
H	-0.73551	0.188214	-5.36064
H	-1.82341	-0.64984	-4.24476
H	2.65649	0.833128	-3.05053
H	2.264774	0.466015	-4.73441
H	1.509957	1.83843	-3.94067
H	-0.88209	-3.0743	-3.28372
H	0.518916	-4.14966	-3.35161
H	0.269727	-3.11799	-1.94003
H	1.375288	-1.47846	-5.79932
H	1.209832	-3.21595	-5.54462
H	-0.22472	-2.18559	-5.52666
H	3.133437	-1.59639	-3.92584
H	2.717956	-2.2498	-2.34242
H	2.776016	-3.31586	-3.73966
H	-1.48476	1.061034	4.022027
H	-1.82341	-0.64984	4.244759

H	-0.73551	0.188214	5.36064
H	2.65649	0.833128	3.050535
H	1.509957	1.83843	3.940666
H	2.264774	0.466015	4.734406
H	3.133437	-1.59639	3.925843
H	2.776016	-3.31586	3.739656
H	2.717956	-2.2498	2.342416
H	1.375288	-1.47846	5.799319
H	-0.22472	-2.18559	5.526664
H	1.209832	-3.21595	5.544624
H	-0.88209	-3.0743	3.283725
H	0.269727	-3.11799	1.940031
H	0.518916	-4.14966	3.351606
H	2.624584	4.35266	-1.29722
H	1.974288	3.353323	-2.59553
H	2.934554	2.615086	-1.30711
H	2.624584	4.35266	1.297219
H	2.934554	2.615086	1.307114
H	1.974288	3.353323	2.595526
H	-0.92463	4.51304	-2.78408
H	-1.84189	3.007585	-2.72237
H	-0.16954	2.993252	-3.26934
H	-0.92463	4.51304	2.784078
H	-0.16954	2.993252	3.269343
H	-1.84189	3.007585	2.722368
H	-2.81412	4.672544	0
H	-3.19896	3.198484	0.880089
H	-3.19896	3.198484	-0.88009

8. NMR calculations for compounds 4 and 3.

σ^{total} (in ppm) = $\sigma^{dia.} + \sigma^{para.} + \sigma^{so.}$

	^{209}Pb			
	$\sigma^{dia.}$	$\sigma^{para.}$	$\sigma^{so.}$	σ^{total}
Compound **4**	9952.97	−6917.689	2748.333	5783.613
Compound **3**	9948.065	−5551.023	2539.391	6936.433

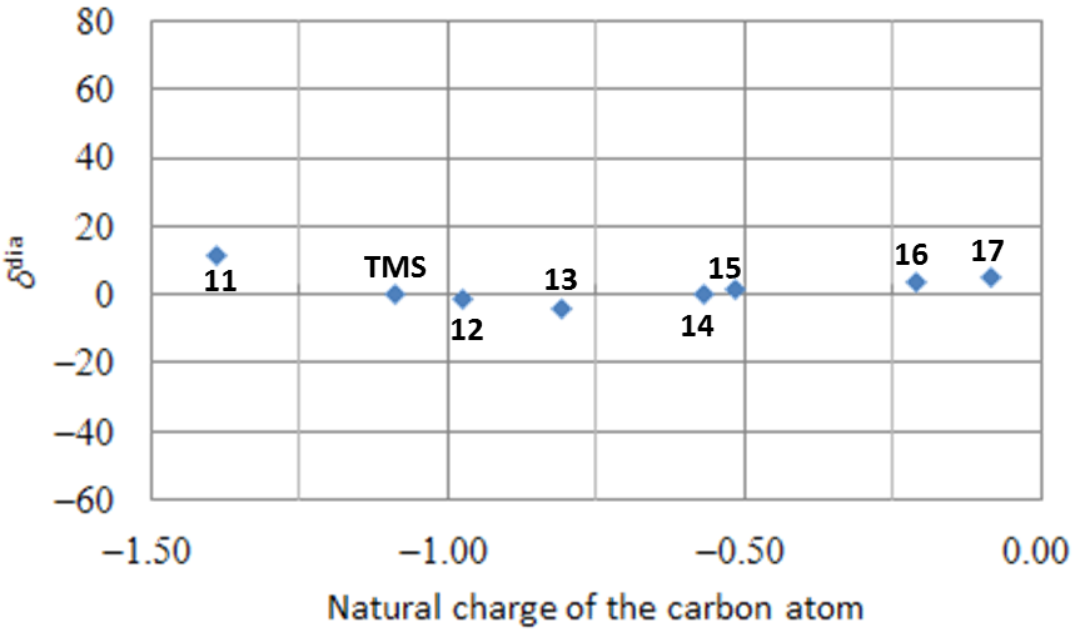
	^{13}C (α)			
	$\sigma^{dia.}$	$\sigma^{para.}$	$\sigma^{so.}$	σ^{total}
Compound **4**	261.682	−270.074	−3.725	−12.117
Compound **3**	257.007	−193.435	−28.542	35.030

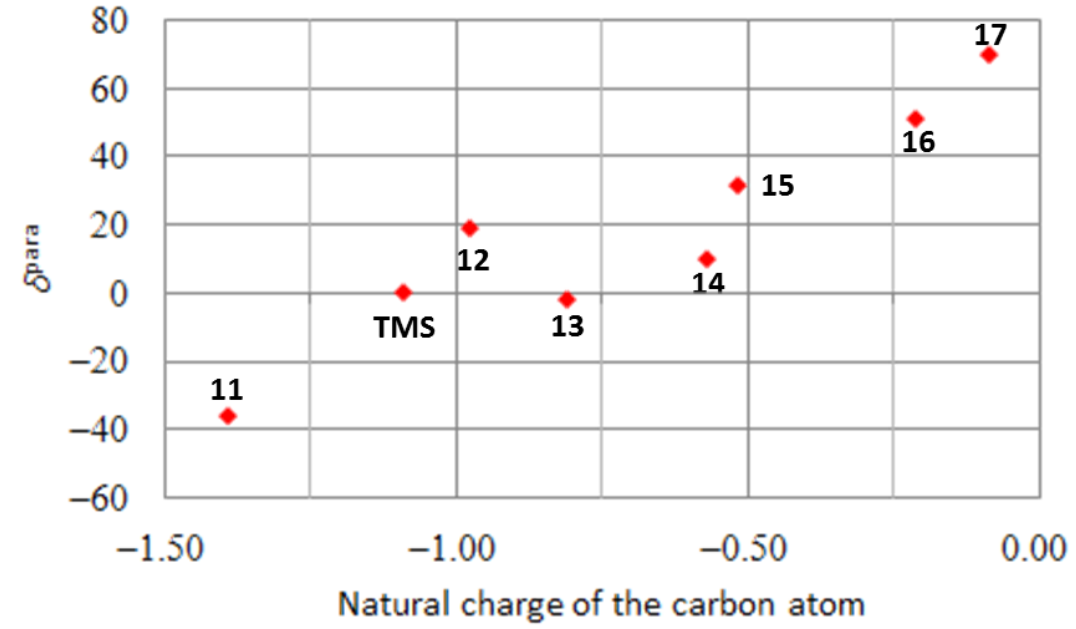
	^{13}C (β)			
	$\sigma^{dia.}$	$\sigma^{para.}$	$\sigma^{so.}$	σ^{total}
Compound **4**	248.646	−233.960	−19.008	−4.322
Compound **3**	252.929	−185.850	−15.271	51.808

The basis sets used are ZORA-TZ2P (Pb and Ru), TZP (C in the plumbole rings), DZP (the other C), and DZ (H) at the B3LYP level of theory.

Cf. The relationship between the diamagnetic and paramagnetic terms (ppm) in the ^{13}C NMR chemical shifts relative to that of Me_4Si and natural charges on the carbon atoms.

Compounds	Natural Charge of Carbon	$\delta^{dia.}$	$\delta^{para.}$	δ^{total}
CH_3-Li (**11**)	−1.3869	11.41	−36.04	−24.63
CH_3-BH_2 (**12**)	−0.9750	−1.28	18.35	17.07
CH_3-H (**13**)	−0.8089	−4.44	−1.88	−6.32
CH_3-CH_3 (**14**)	−0.5686	−0.16	9.43	9.27
CH_3-Cl (**15**)	−0.5164	1.76	31.10	32.86
CH_3-OH (**16**)	−0.2089	3.44	50.85	54.29
CH_3-F (**17**)	−0.0866	4.73	69.74	74.48
Si-Me_4 (**TMS**)	−1.0888	0	0	0



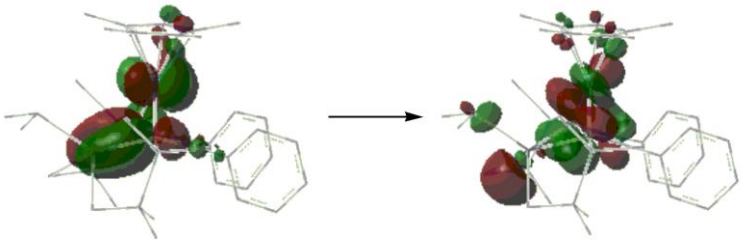


The calculations clearly indicate that the increase of electron density on the carbon atoms causes the decrease of paramagnetic contribution, resulting in upfield shifts in the ^{13}C NMR spectra.

9. TD-DFT calculations for compounds 6 and 7

Compound **6**

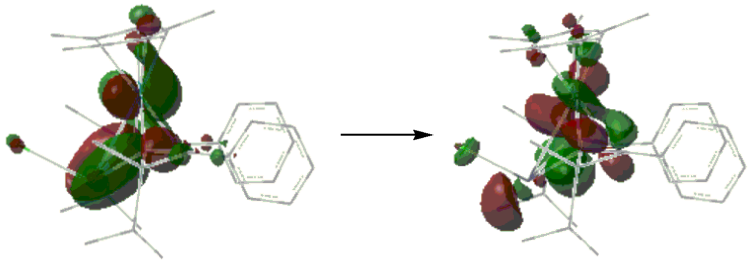
539 nm, *f* = 0.011 HOMO-1 to LUMO



HOMO-1 **LUMO**

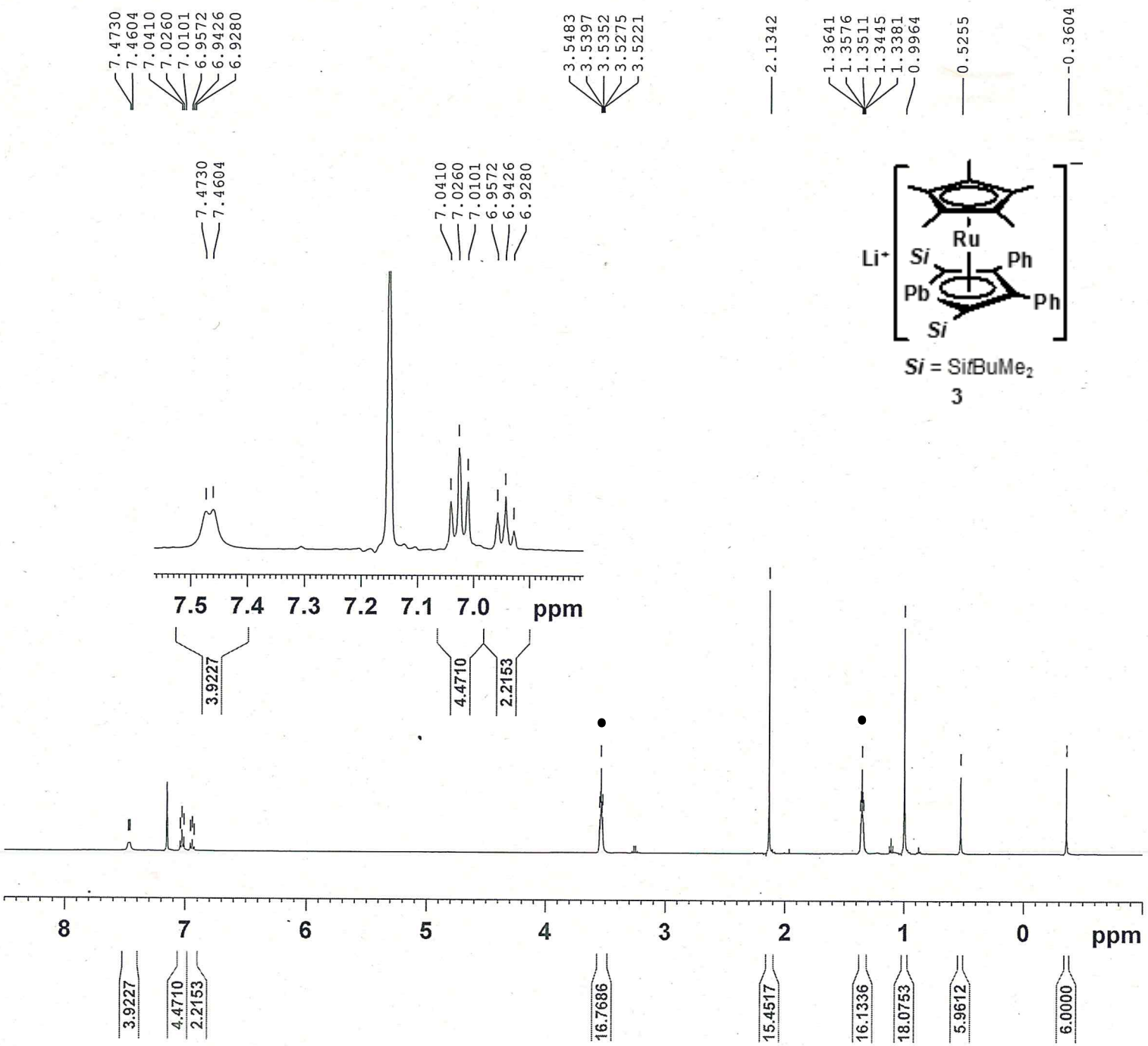
Compound **7**

613 nm, *f* = 0.012 HOMO to LUMO



HOMO **LUMO**

Ex 156 Pb-Ru anion complex 1H in C6D6



Current Data Parameters

NAME	A13MC116BZ
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20130529
Time	15.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	C6D6
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	80.6
DW	48.400 usec
DE	6.50 usec
TE	300.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

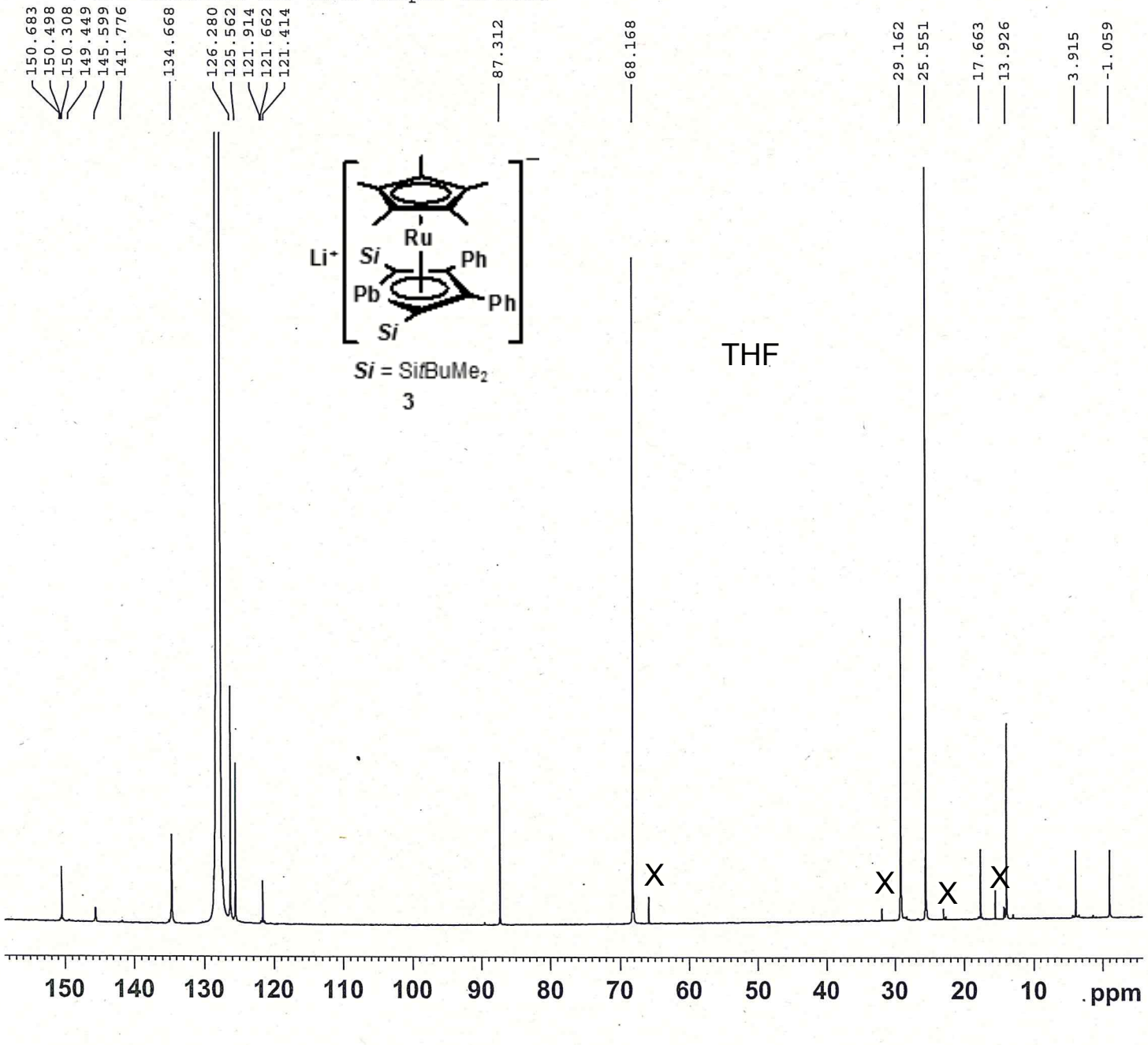
NUC1	1H
P1	12.00 usec
PL1	2.60 dB
PL1W	15.32226563 W
SFO1	500.1330885 MHz

F2 - Processing parameters

SI	32768
SF	500.1300017 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

• THF

Ex 156 Anion sandwich 13C data compl. in C6D6



Current Data Parameters

NAME	A11ds003MNC
EXPNO	1561
PROCNO	1

F2 - Acquisition Parameters

Date_	20130529
Time	20.13
INSTRUM	spect
PROBHD	5 mm CPQNP 1H/
PULPROG	zgpg30
TD	65536
SOLVENT	C6D6
NS	14576
DS	2
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	126.99
DW	16.800 usec
DE	18.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	12.00 usec
PLW1	15.50000000 W
SFO1	100.6248425 MHz

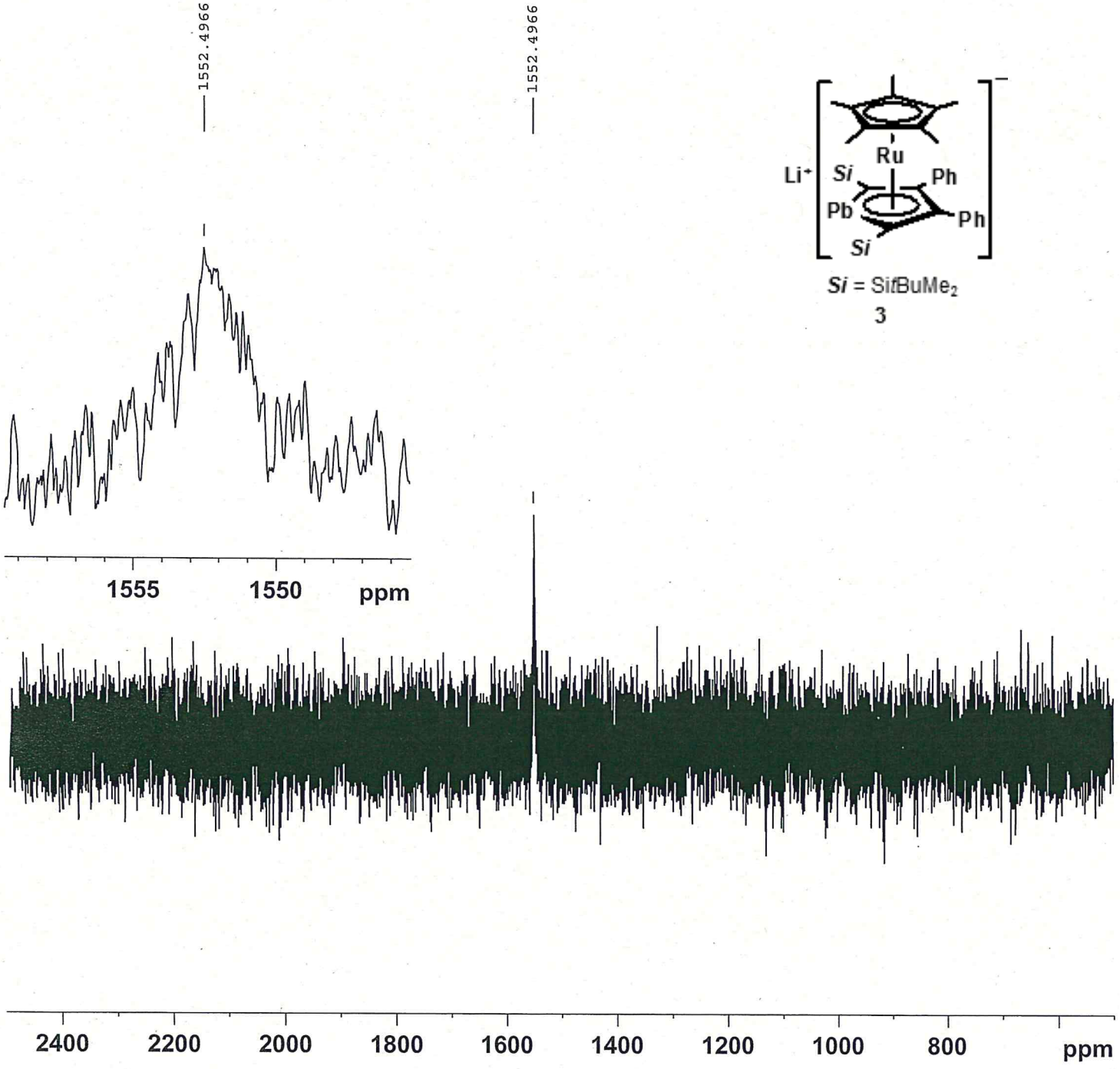
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PLW2	5.19999981 W
PLW12	0.14444000 W
PLW13	0.11700000 W
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127363 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40

Ex 156 Pb-Ru anion complex 207Pb in C6D6

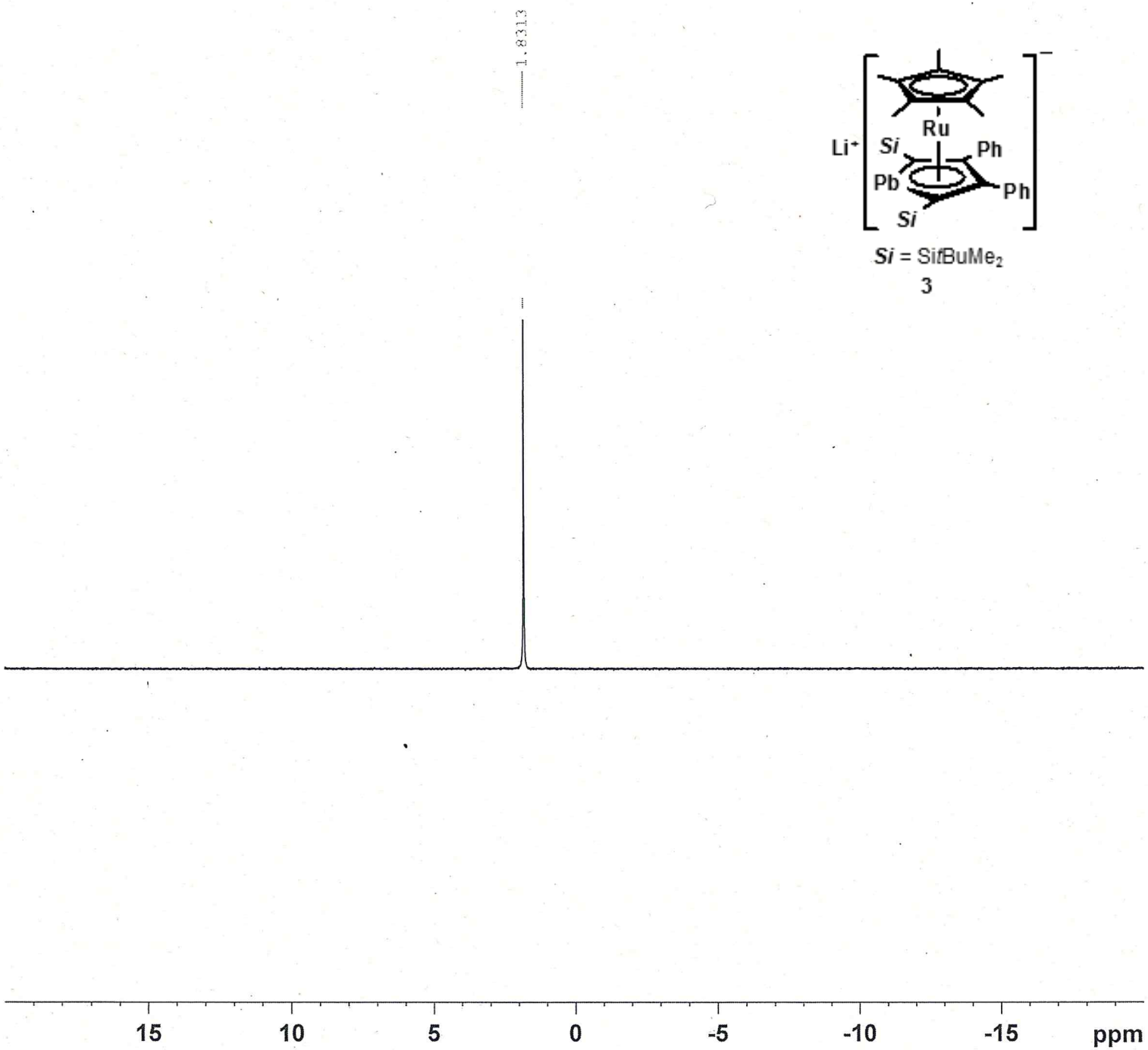


Si = SitBuMe$_2$

3

NAME	A13MC116BO
EXPNO	1
PROCNO	1
Date_	20130529
Time	15.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg
TD	65536
SOLVENT	C6D6
NS	1900
DS	2
SWH	208333.328 Hz
FIDRES	3.178914 Hz
AQ	0.1573364 sec
RG	203
DW	2.400 usec
DE	65.00 usec
TE	300.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	207Pb
P1	12.00 usec
PL1	0.00 dB
SFO1	104.7661849 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.40 dB
PL12	19.02 dB
PL13	22.02 dB
PL2W	15.17711735 W
PL12W	0.33051354 W
PL13W	0.16564916 W
SFO2	500.0320005 MHz
SI	65536
SF	104.6094793 MHz
WDW	EM
SSB	0
LB	10.00 Hz
GB	0
PC	1.40

Ex 156 Pb-Ru anion complex 7Li in C6D6

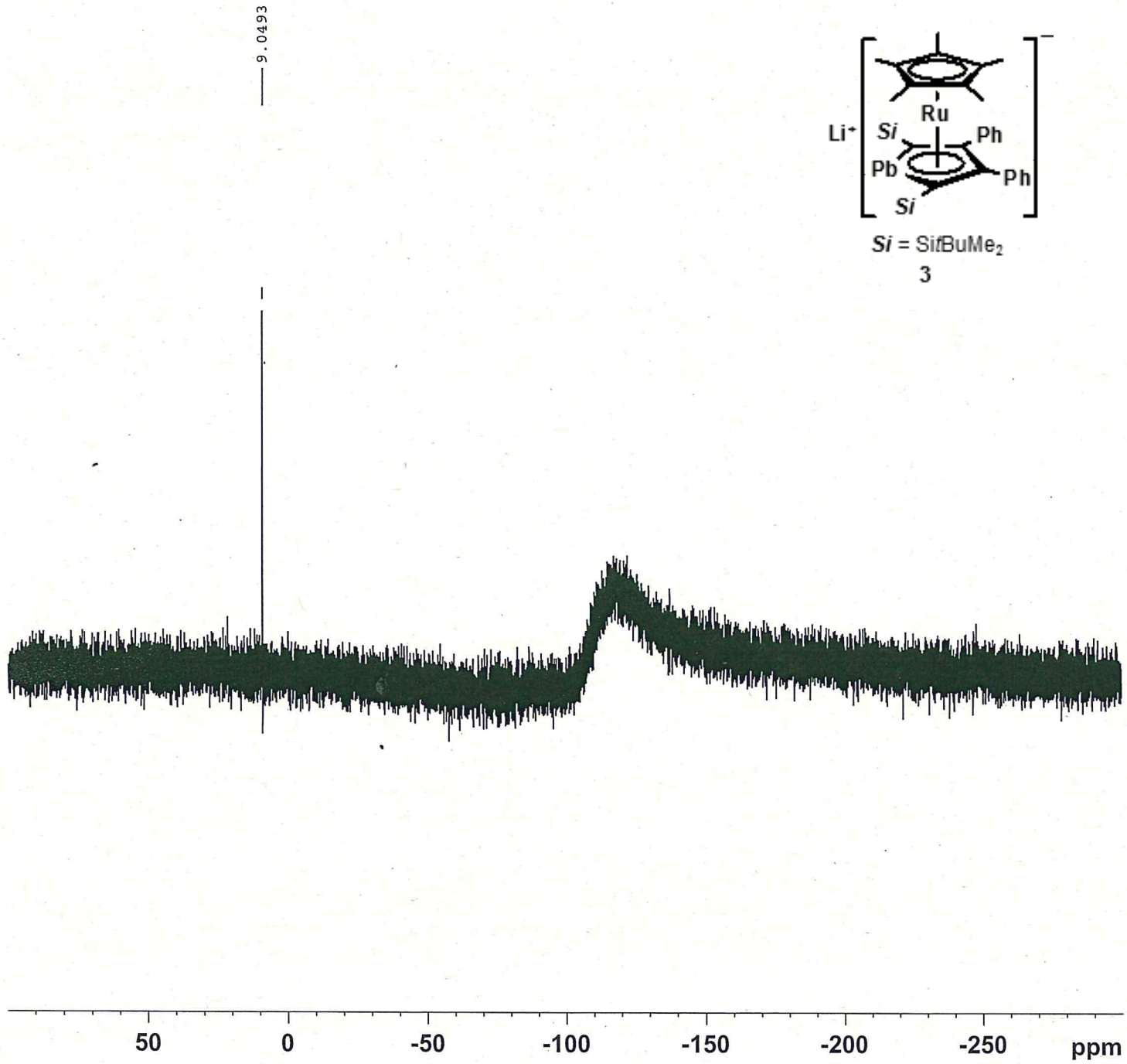


Si = SitBuMe$_2$

3

NAME	A13MC116CA
EXPNO	1
PROCNO	1
Date_	20130529
Time	15.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	262144
SOLVENT	C6D6
NS	16
DS	0
SWH	19531.250 Hz
FIDRES	0.074506 Hz
AQ	6.7109365 sec
RG	203
DW	25.600 usec
DE	6.50 usec
TE	300.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	7Li
P1	20.00 usec
PL1	1.00 dB
SFO1	194.3695082 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.75 dB
PL12	19.50 dB
PL13	19.50 dB
PL2W	18.63472366 W
PL12W	0.31284049 W
PL13W	0.31284049 W
SFO2	500.1330885 MHz
SI	131072
SF	194.3695384 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

Ex 156 Pb-Ru anion complex 29Si in C6D6

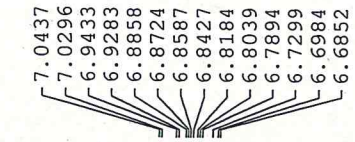


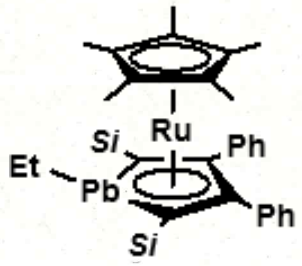
Si = SitBuMe$_2$

3

NAME	A13MC116BM	
EXPNO	1	
PROCNO	1	
Date_	20130529	
Time	15.31	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgig	
TD	65536	
SOLVENT	C6D6	
NS	104	
DS	4	
SWH	39682.539	Hz
FIDRES	0.605507	Hz
AQ	0.8258036	sec
RG	203	
DW	12.600	usec
DE	6.50	usec
TE	300.3	K
D1	5.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	29Si	
P1	15.00	usec
PL1	3.00	dB
PL1W	37.76776123	W
SFO1	99.3319610	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	2.40	dB
PL12	19.02	dB
PL2W	15.17711735	W
PL12W	0.33051354	W
SFO2	500.0320001	MHz
SI	32768	
SF	99.3418950	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

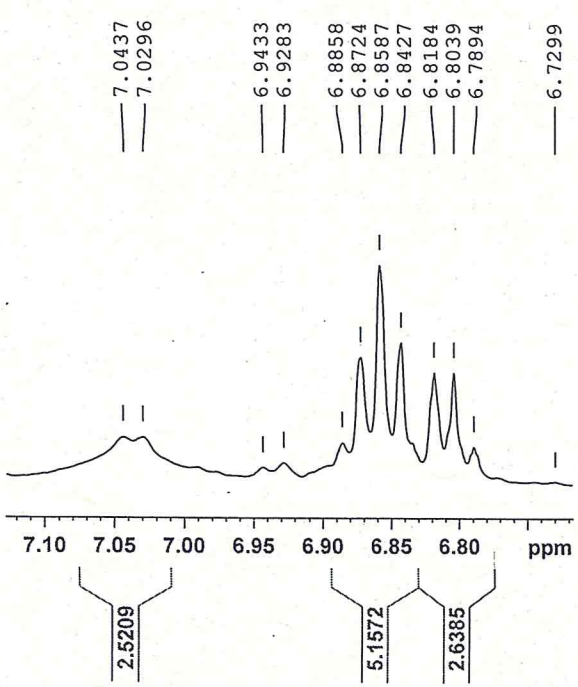
Et ruthenocene comp. 1H in C6D6

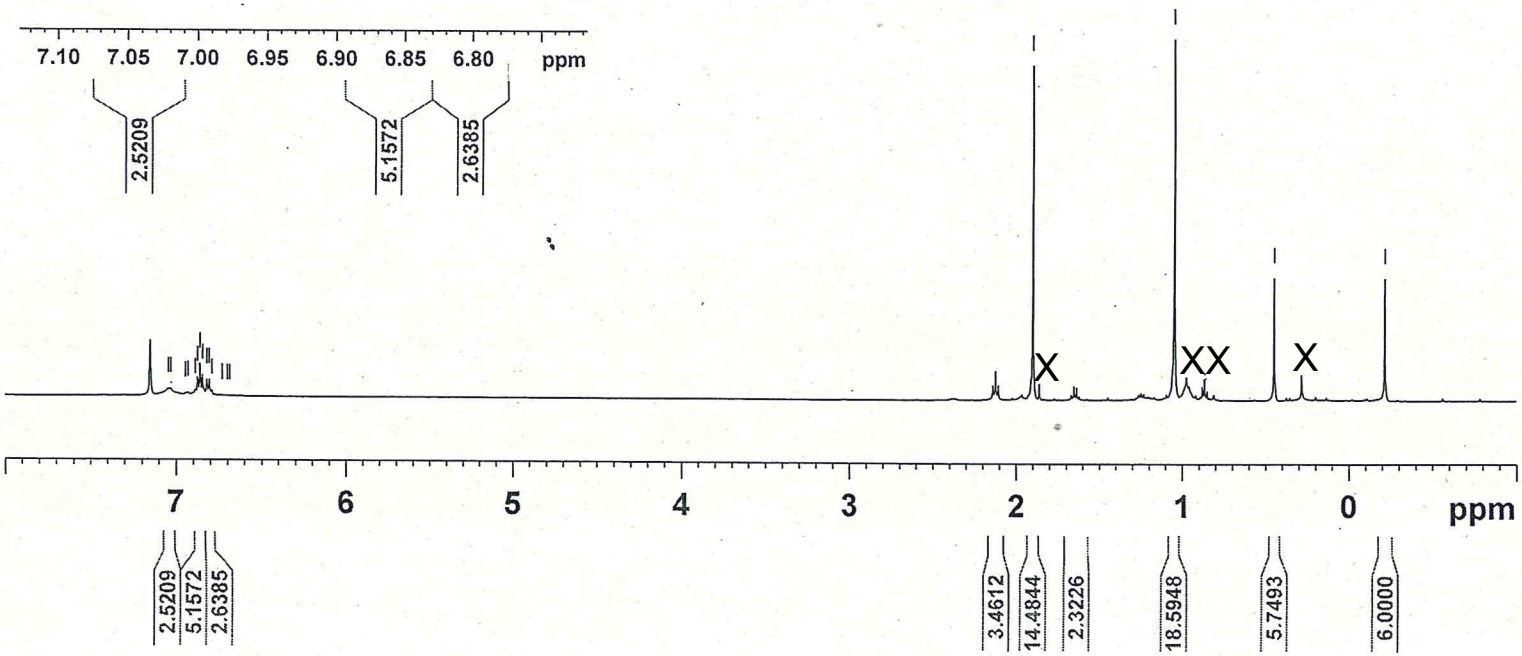




Si = Si*t*BuMe$_2$

5



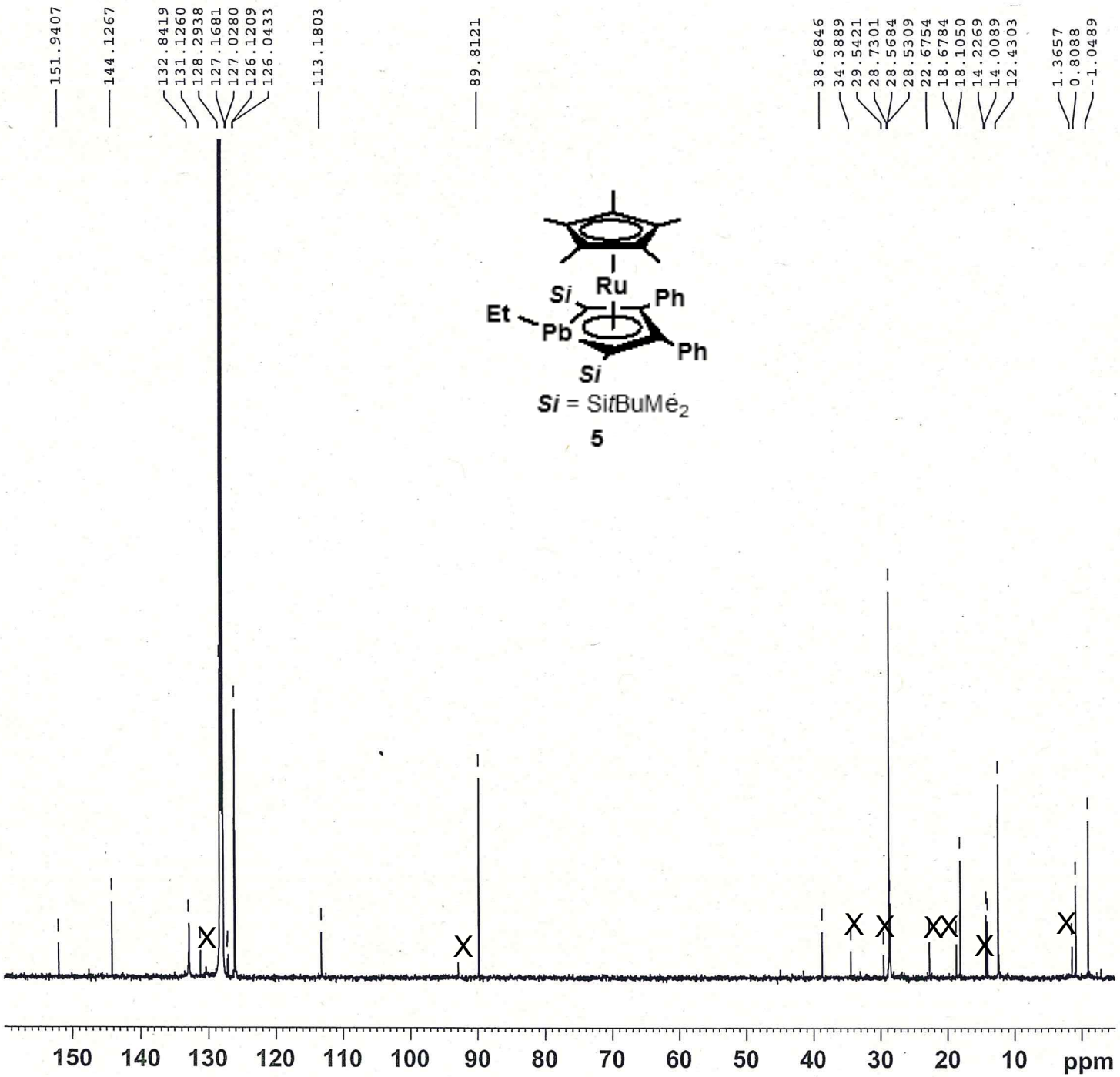


BRUKER

NAME	A13MC116EA
EXPNO	1
PROCNO	1
Date_	20140224
Time	10.44
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	C6D6
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	40.3
DW	48.400 usec
DE	6.50 usec
TE	299.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 usec
PL1	2.60 dB
PL1W	15.32226563 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300035 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

X hexane, pentane and impurities

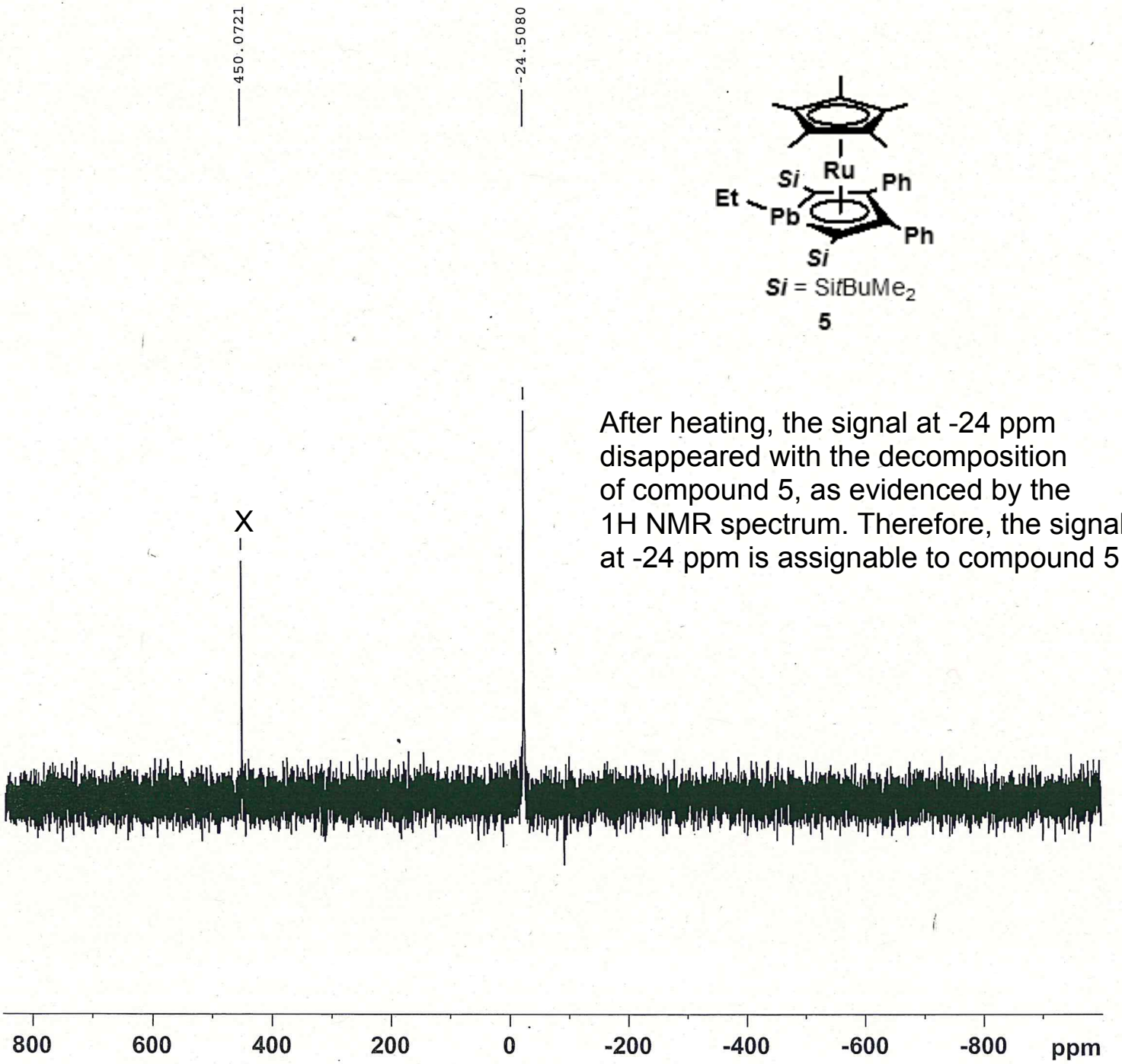
Ex 320 Et ruthenocene comp. 13C in C6D6



NAME	A13MC116MK
EXPNO	1
PROCNO	1
Date_	20140224
Time	14.49
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	C6D6
NS	1200
DS	2
SWH	40760.871 Hz
FIDRES	0.621962 Hz
AQ	0.8039582 sec
RG	203
DW	12.267 usec
DE	6.50 usec
TE	300.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.80 usec
PL1	0.00 dB
PL1W	100.47545624 W
SFO1	125.7477319 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.40 dB
PL12	19.02 dB
PL13	22.02 dB
PL2W	15.17711735 W
PL12W	0.33051354 W
PL13W	0.16564916 W
SFO2	500.0316016 MHz
SI	16384
SF	125.7326021 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

X hexane, pentane and impurities

Ex 320 Et ruthenocene comp. 207 Pb in C6D6



Si = Si*t*BuMe$_2$

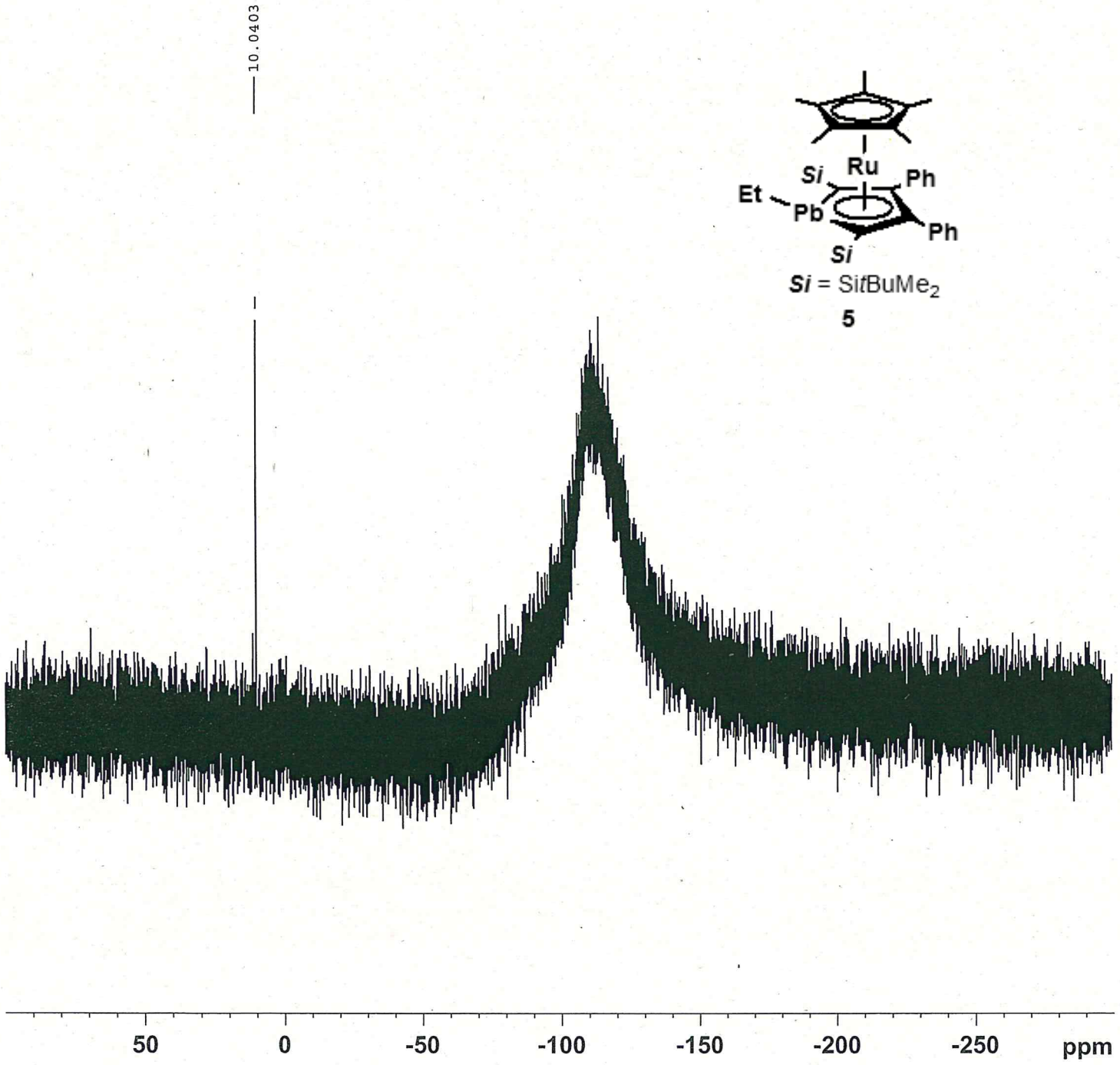
5

After heating, the signal at -24 ppm disappeared with the decomposition of compound 5, as evidenced by the 1H NMR spectrum. Therefore, the signal at -24 ppm is assignable to compound 5.

BRUKER

NAME	A13MC116MH	
EXPNO	1	
PROCNO	1	
Date_	20140224	
Time	11.37	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg	
TD	65536	
SOLVENT	C6D6	
NS	1632	
DS	2	
SWH	208333.328	Hz
FIDRES	3.178914	Hz
AQ	0.1573364	sec
RG	203	
DW	2.400	usec
DE	65.00	usec
TE	300.1	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	207Pb	
P1	12.00	usec
PL1	0.00	dB
SFO1	104.5935796	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	2.40	dB
PL12	19.02	dB
PL13	22.02	dB
PL2W	15.17711735	W
PL12W	0.33051354	W
PL13W	0.16564916	W
SFO2	500.0320005	MHz
SI	65536	
SF	104.6094793	MHz
WDW	EM	
SSB	0	
LB	10.00	Hz
GB	0	
PC	1.40	

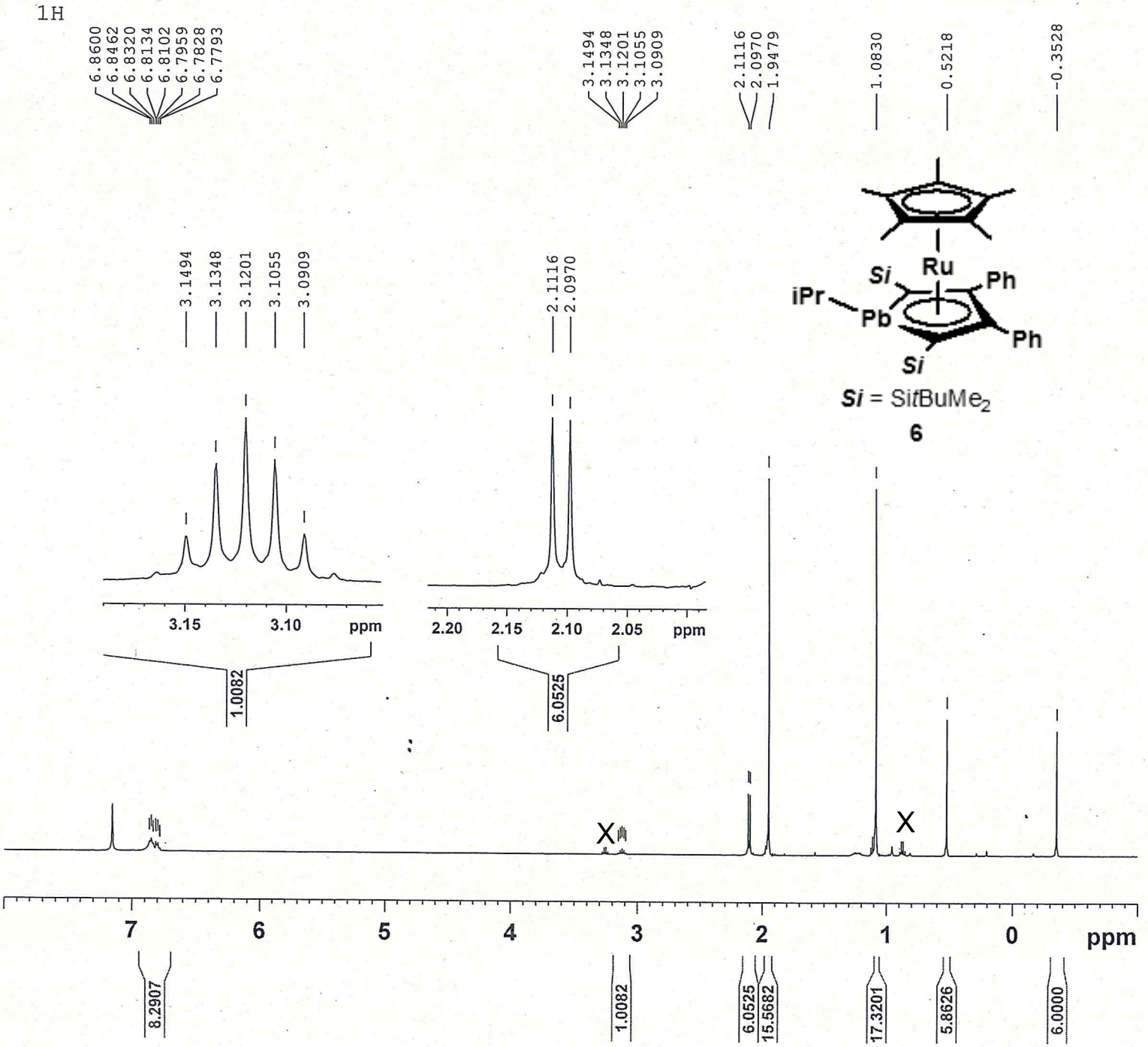
Ex 320 Et ruthenocene comp. 29Si in C6D6



NAME	A13MC116MG
EXPNO	1
PROCNO	1
Date_	20140224
Time	10.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig
TD	65536
SOLVENT	C6D6
NS	348
DS	4
SWH	39682.539 Hz
FIDRES	0.605507 Hz
AQ	0.8258036 sec
RG	203
DW	12.600 usec
DE	6.50 usec
TE	299.8 K
D1	5.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	29Si
P1	15.00 usec
PL1	3.00 dB
PL1W	37.76776123 W
SFO1	99.3319610 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.40 dB
PL12	19.02 dB
PL2W	15.17711735 W
PL12W	0.33051354 W
SFO2	500.0320001 MHz
SI	32768
SF	99.3418950 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Ex282 comp. in C6D6

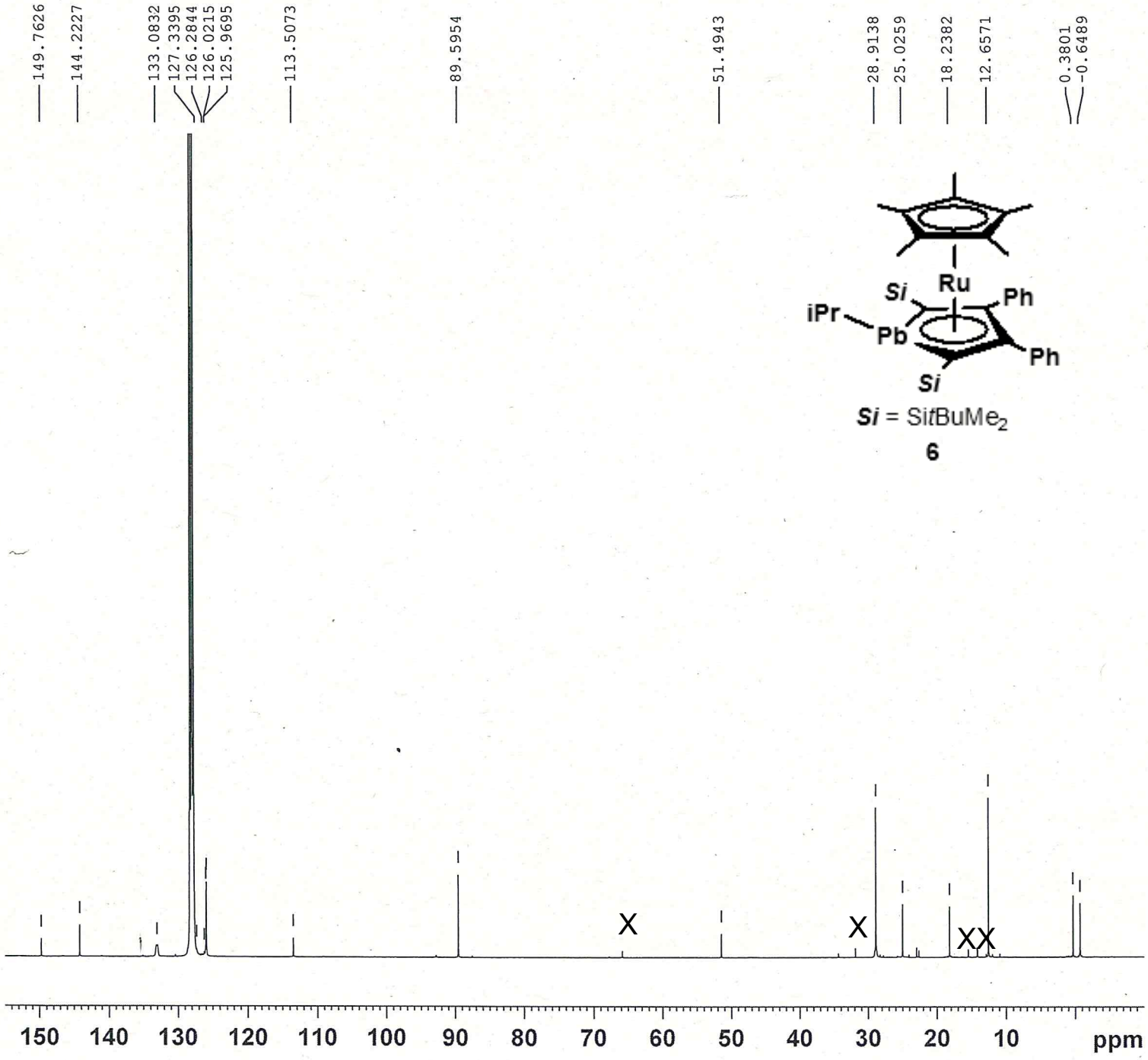
1H



NAME	A13MC116DE
EXPNO	1
PROCNO	1
Date_	20131209
Time	12.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	C6D6
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	90.5
DW	48.400 usec
DE	6.50 usec
TE	299.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 usec
PL1	2.60 dB
PL1W	15.32226563 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300023 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

X ether

Ex 285 ipro ruthenocene comp. 13C in C6D6



Si = Si*t*BuMe$_2$

6

Current Data Parameters
NAME SAITMN285-CryC
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20131211
Time	21.08
INSTRUM	spect
PROBHD	5 mm CPQNP 1H/
PULPROG	zgpg30
TD	65536
SOLVENT	C6D6
NS	14565
DS	2
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	126.99
DW	16.800 usec
DE	18.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	12.00 usec
PLW1	15.50000000 W
SFO1	100.6248425 MHz

======== CHANNEL f2 ========

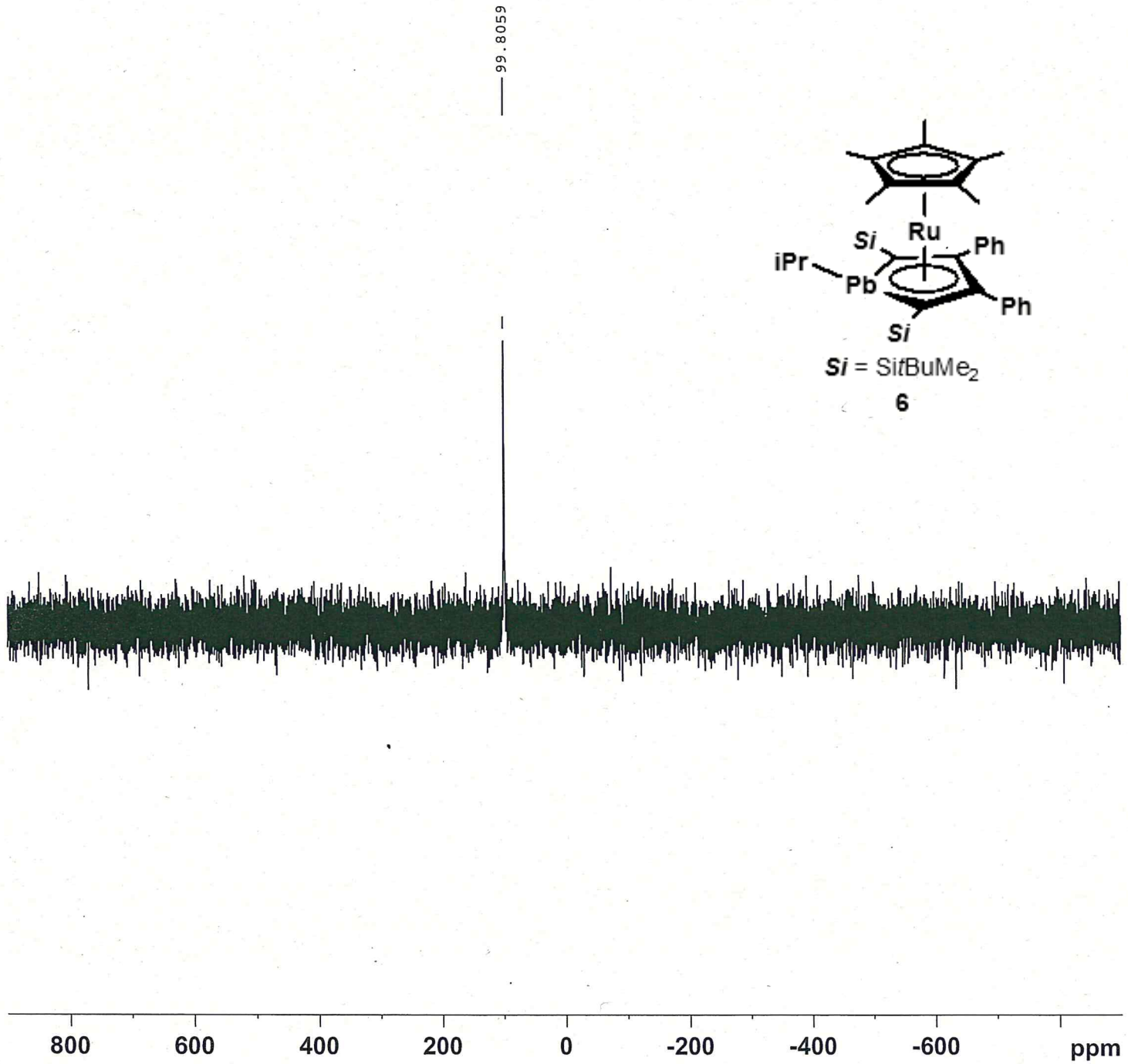
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PLW2	5.19999981 W
PLW12	0.14444000 W
PLW13	0.11700000 W
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127366 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40

X ether and impurities

Ex 285 207 Pb ipro ruthenocene comp. in C6D6



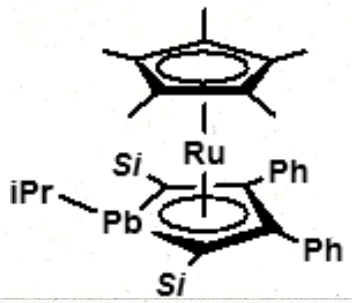
Si = Si*t*BuMe$_2$

6

NAME	A13MC116JQ	
EXPNO	1	
PROCNO	1	
Date_	20131211	
Time	14.04	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg	
TD	65536	
SOLVENT	C6D6	
NS	1020	
DS	2	
SWH	208333.328	Hz
FIDRES	3.178914	Hz
AQ	0.1573364	sec
RG	203	
DW	2.400	usec
DE	65.00	usec
TE	300.3	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	207Pb	
P1	12.00	usec
PL1	0.00	dB
SFO1	104.6092710	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	2.40	dB
PL12	19.02	dB
PL13	22.02	dB
PL2W	15.17711735	W
PL12W	0.33051354	W
PL13W	0.16564916	W
SFO2	500.0320005	MHz
SI	65536	
SF	104.6094793	MHz
WDW	EM	
SSB	0	
LB	10.00	Hz
GB	0	
PC	1.40	

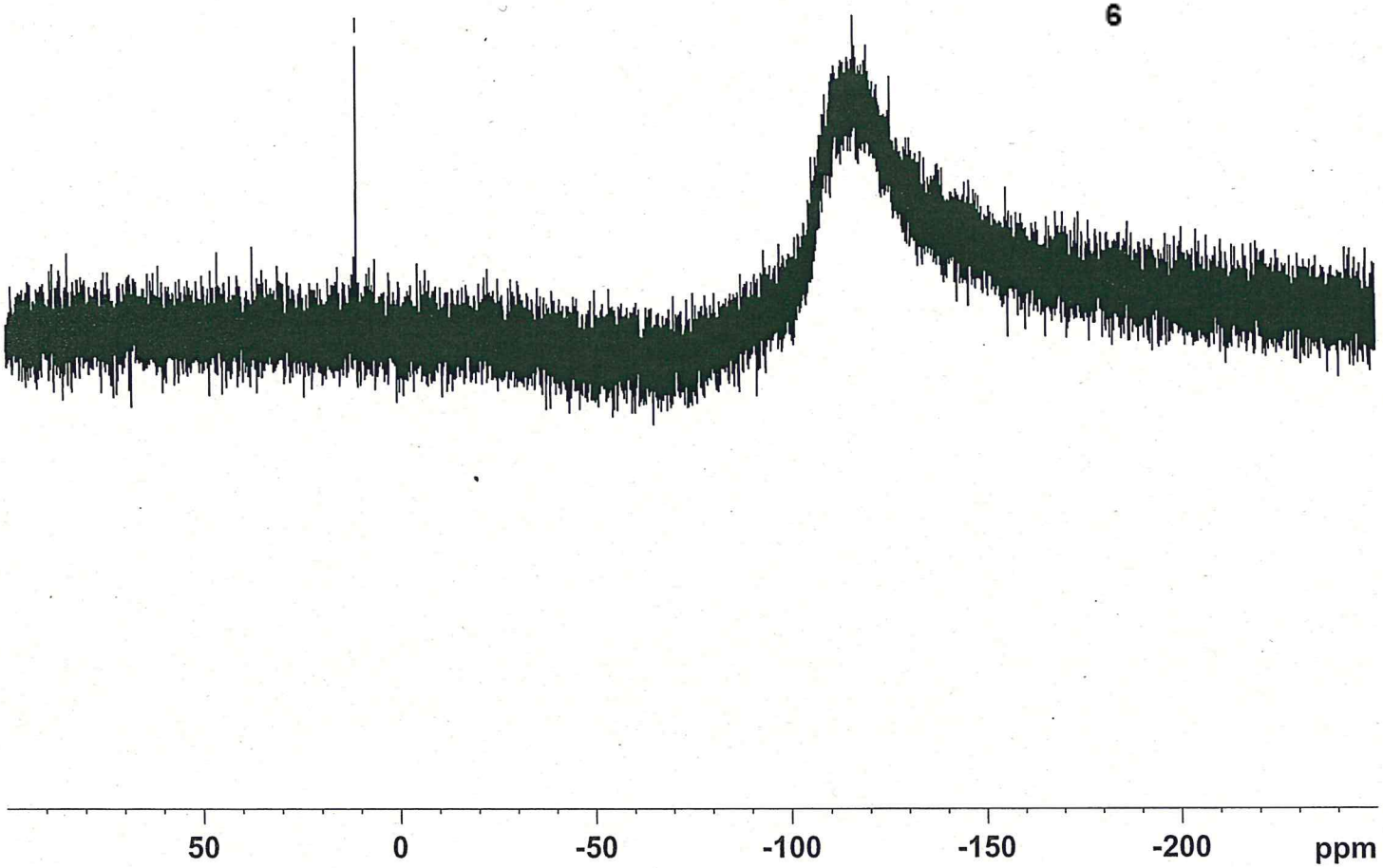
Ex 282 comp. 29Si in C6D6

10.6494



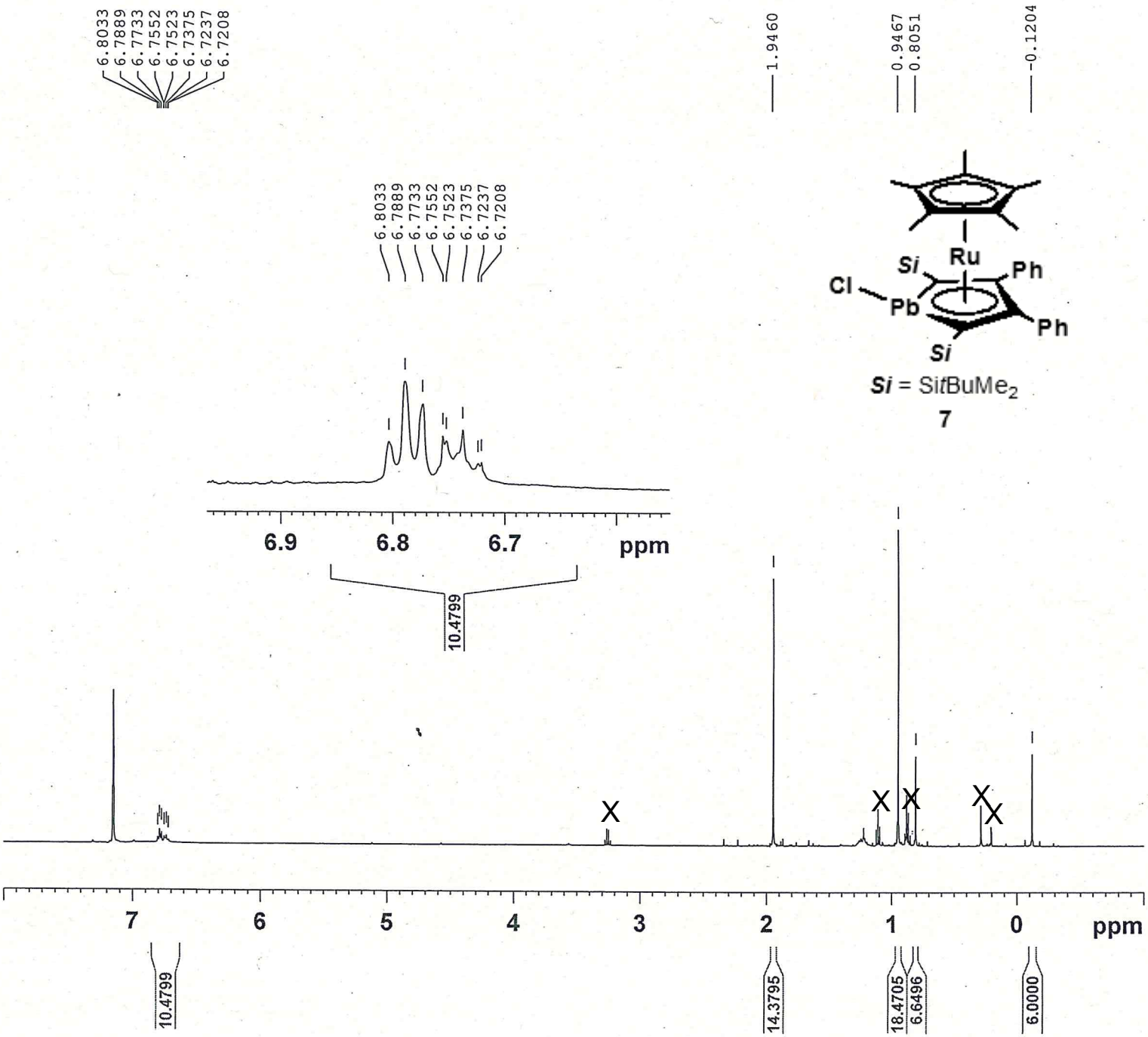
Si = Si*t*BuMe$_2$

6



NAME	A13MC116JK	
EXPNO	1	
PROCNO	1	
Date_	20131209	
Time	12.05	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgig	
TD	65536	
SOLVENT	C6D6	
NS	420	
DS	4	
SWH	39682.539	Hz
FIDRES	0.605507	Hz
AQ	0.8258036	sec
RG	203	
DW	12.600	usec
DE	6.50	usec
TE	300.0	K
D1	5.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	29Si	
P1	15.00	usec
PL1	3.00	dB
PL1W	37.76776123	W
SFO1	99.3319610	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	2.40	dB
PL12	19.02	dB
PL2W	15.17711735	W
PL12W	0.33051354	W
SFO2	500.0320001	MHz
SI	32768	
SF	99.3418950	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

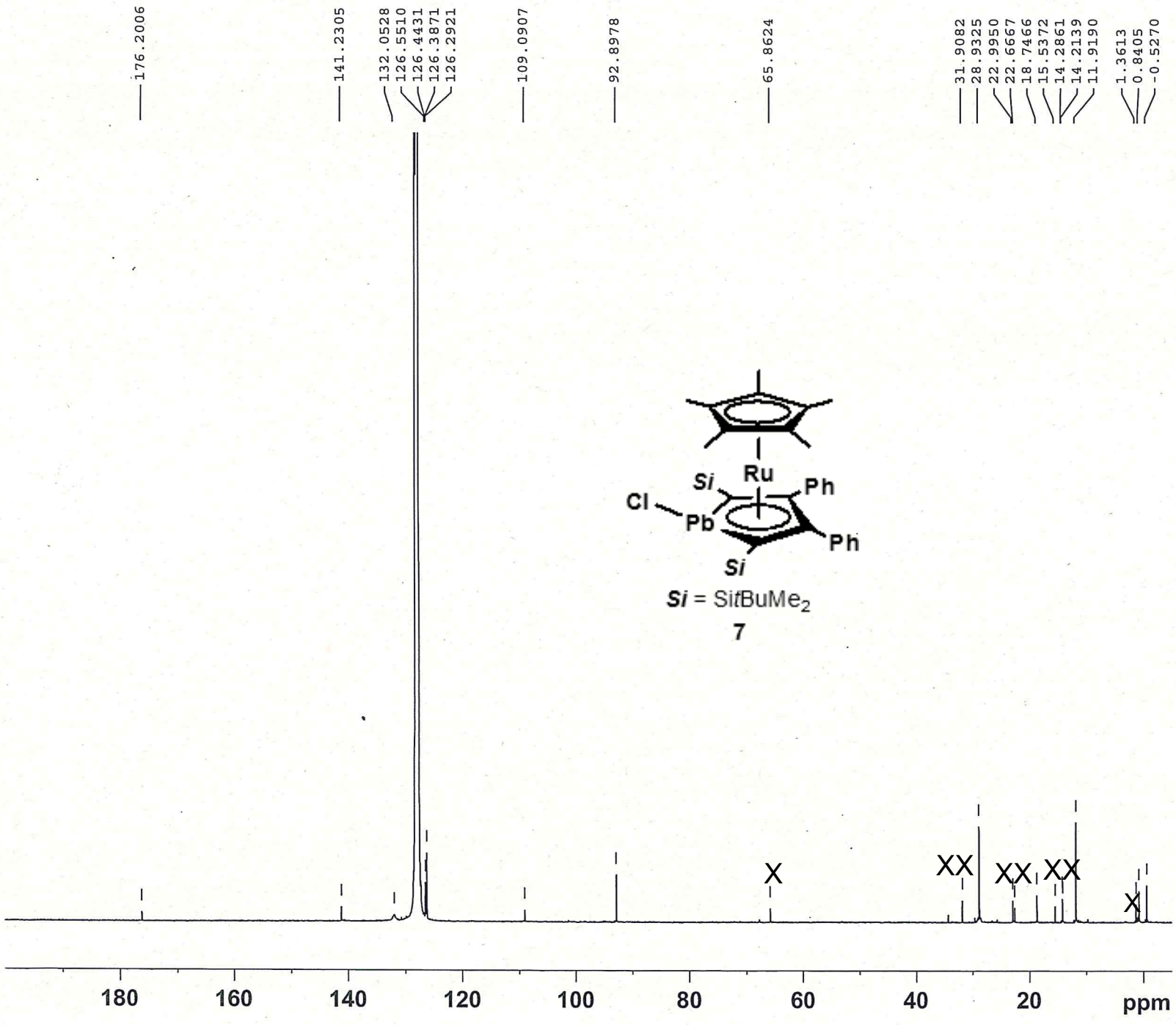
Cl ruthenocene comp. 1H in C6D6



NAME	A13MC116CT
EXPNO	1
PROCNO	1
Date_	20131029
Time	18.23
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	C6D6
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	161
DW	48.400 usec
DE	6.50 usec
TE	299.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 usec
PL1	2.60 dB
PL1W	15.32226563 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300023 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

X ether, hexane, pentane and impurities

Ex 247 Cl ruthenocene comp. 13C in C6D



Si = Si*t*BuMe$_2$

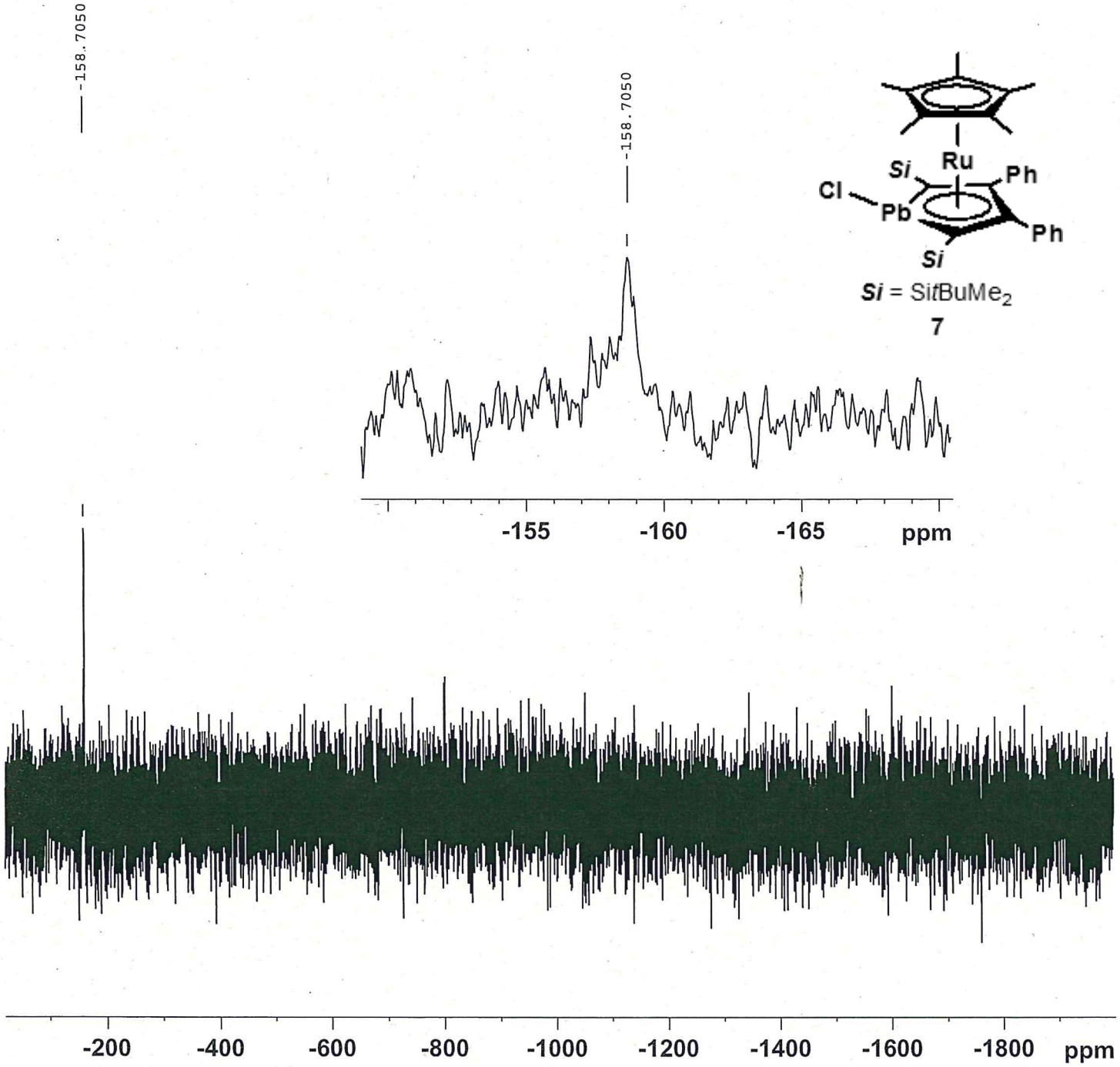
7

NAME	A11ds003MNCC	
EXPNO	2479	
PROCNO	1	
Date_	20131030	
Time	9.02	
INSTRUM	spect	
PROBHD	5 mm CPQNP 1H/	
PULPROG	zgpg30	
TD	65536	
SOLVENT	C6D6	
NS	13584	
DS	2	
SWH	29761.904	Hz
FIDRES	0.454131	Hz
AQ	1.1010548	sec
RG	126.99	
DW	16.800	usec
DE	18.00	usec
TE	300.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	12.00	usec
SI	32768	
SF	100.6127364	MHz
WDW	EM	
SSB	0	
LB	2.00	Hz
GB	0	
PC	1.40	

X ether, hexane, pentane and impurities

256

Cl ruthenocene comp. 207 Pb in C6D6

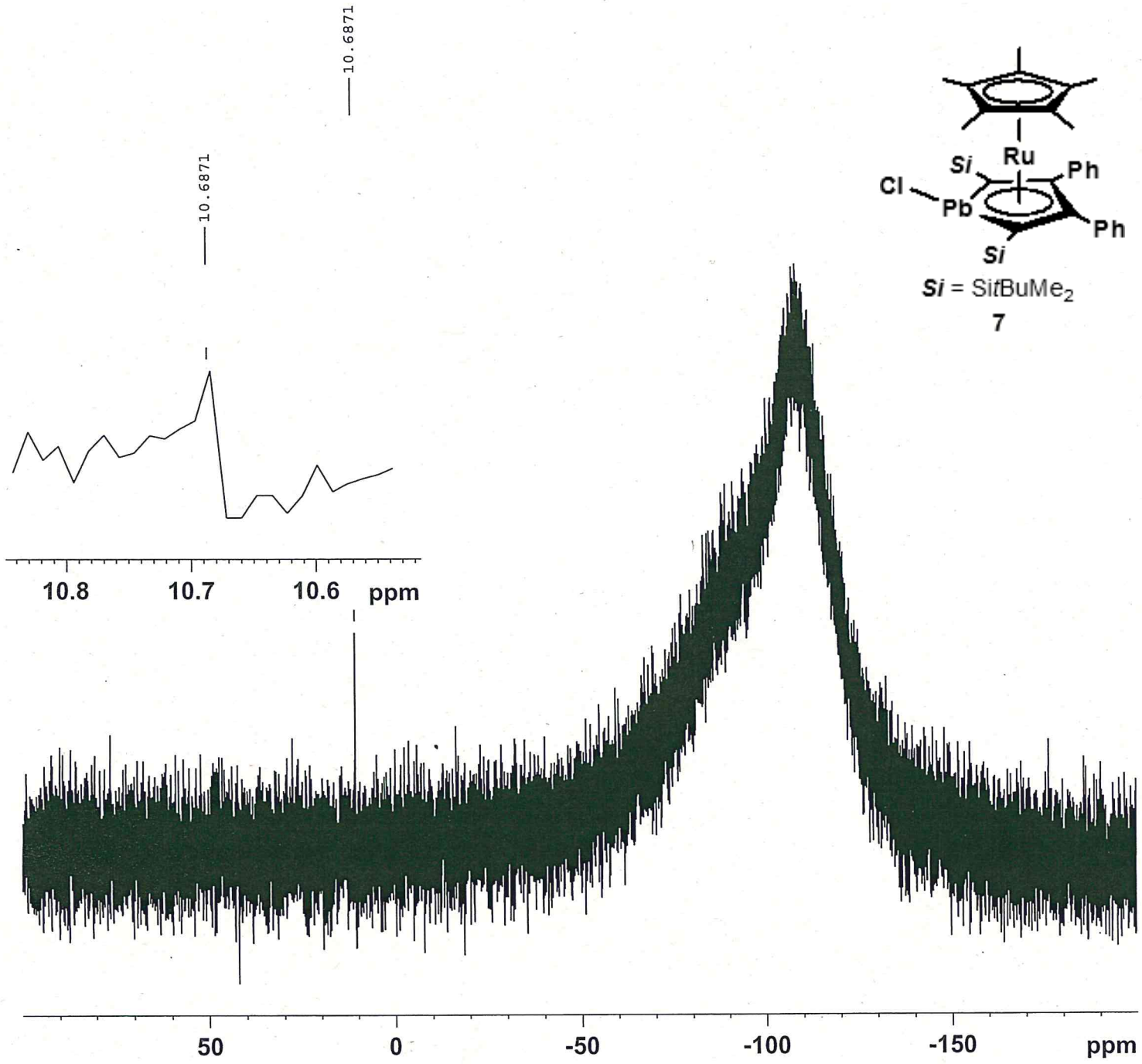


BRUKER

NAME	A13MC116HK	
EXPNO	1	
PROCNO	1	
Date_	20131106	
Time	20.09	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg	
TD	65536	
SOLVENT	C6D6	
NS	1420	
DS	2	
SWH	208333.328	Hz
FIDRES	3.178914	Hz
AQ	0.1573364	sec
RG	203	
DW	2.400	usec
DE	65.00	usec
TE	300.6	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	207Pb	
P1	12.00	usec
PL1	0.00	dB
SFO1	104.5046617	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	2.40	dB
PL12	19.02	dB
PL13	22.02	dB
PL2W	15.17711735	W
PL12W	0.33051354	W
PL13W	0.16564916	W
SFO2	500.0320005	MHz
SI	65536	
SF	104.6094793	MHz
WDW	EM	
SSB	0	
LB	10.00	Hz
GB	0	
PC	1.40	

256

Cl ruhtenocene comp. 29Si in C6D6



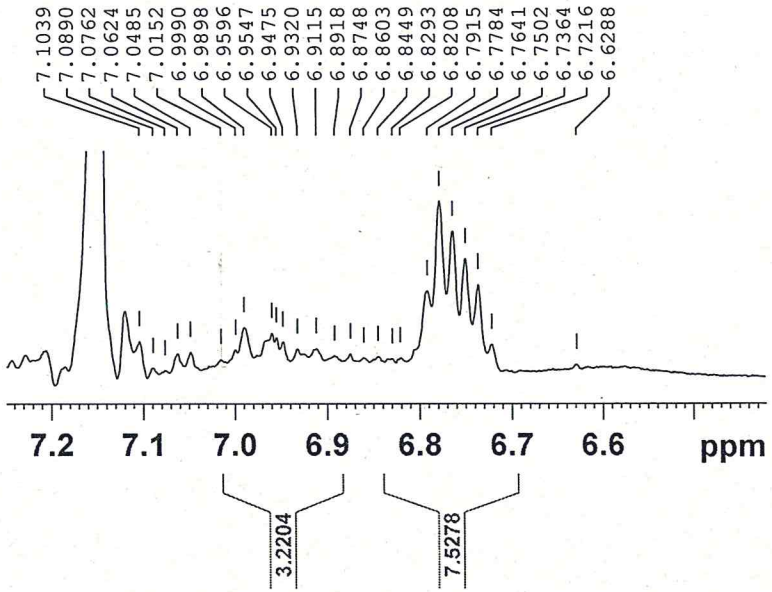
Si = Si*t*BuMe$_2$

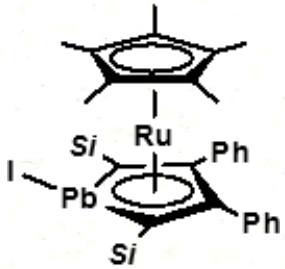
7

BRUKER

NAME	A13MC116HI	
EXPNO	1	
PROCNO	1	
Date_	20131106	
Time	12.39	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgig	
TD	65536	
SOLVENT	C6D6	
NS	868	
DS	4	
SWH	39682.539	Hz
FIDRES	0.605507	Hz
AQ	0.8258036	sec
RG	203	
DW	12.600	usec
DE	6.50	usec
TE	300.1	K
D1	5.00000000	sec
D11	0.03000000	sec
TD0	1	
========	CHANNEL f1 ========	
NUC1	29Si	
P1	15.00	usec
PL1	3.00	dB
PL1W	37.76776123	W
SFO1	99.3319610	MHz
========	CHANNEL f2 ========	
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	2.40	dB
PL12	19.02	dB
PL2W	15.17711735	W
PL12W	0.33051354	W
SFO2	500.0320001	MHz
SI	32768	
SF	99.3418950	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

Ex 198 recry form Et2O 1H in C6D6

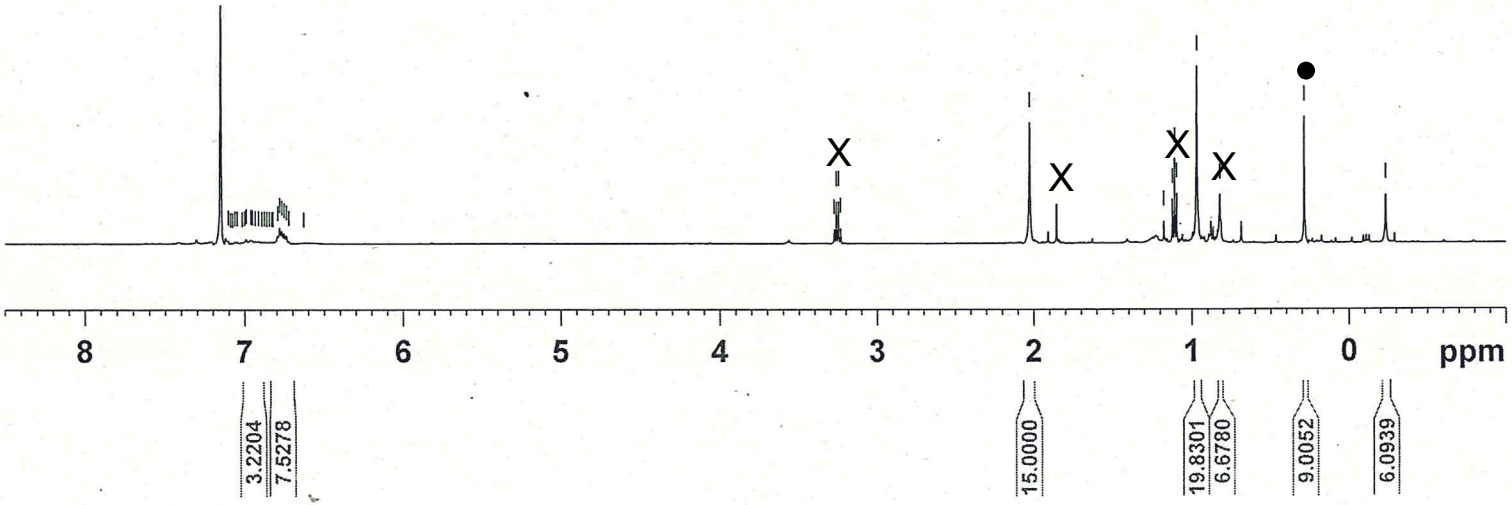




Si = Si*t*BuMe$_2$

8

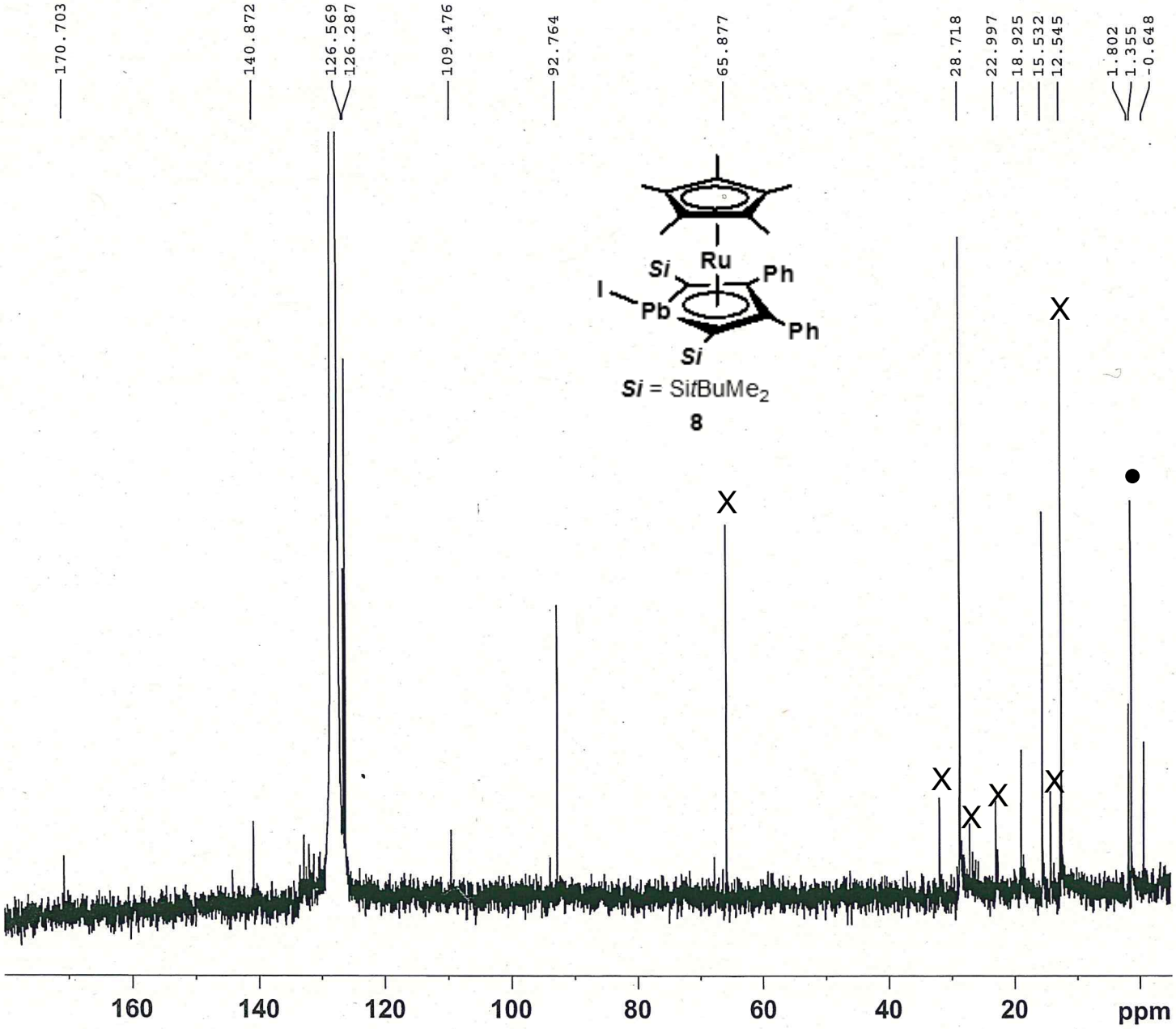
NAME	A13MC116BP
EXPNO	1
PROCNO	1
Date_	20130724
Time	14.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	C6D6
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	161
DW	48.400 usec
DE	6.50 usec
TE	300.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 usec
PL1	2.60 dB
PL1W	15.32226563 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1299784 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



● silicone grease

X ether and impurities

Ex 198 Iplumbole Ru 13C



Si = Si*t*BuMe$_2$

8

Current Data Parameters

NAME	A11ds003MNCC
EXPNO	1989
PROCNO	1

F2 - Acquisition Parameters

Date_	20130724
Time	16.18
INSTRUM	spect
PROBHD	5 mm CPQNP 1H/
PULPROG	zgpg30
TD	65536
SOLVENT	C6D6
NS	896
DS	2
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	126.99
DW	16.800 usec
DE	18.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	12.00 usec
PLW1	15.50000000 W
SFO1	100.6248425 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PLW2	5.19999981 W
PLW12	0.14444000 W
PLW13	0.11700000 W
SFO2	400.1316005 MHz

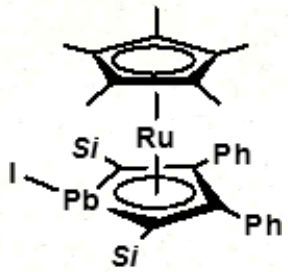
F2 - Processing parameters

SI	32768
SF	100.6127376 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40

● silicone grease

X ether and impurities

Ex 326 iodoruthenocene comp. 207Pb in C6D6

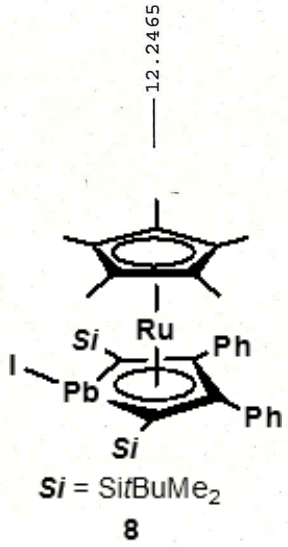


Si = Si*t*BuMe$_2$

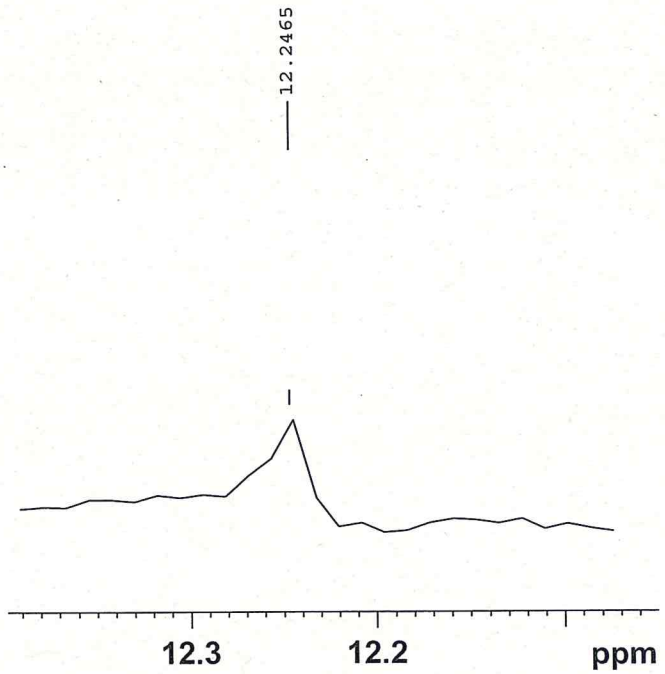
8

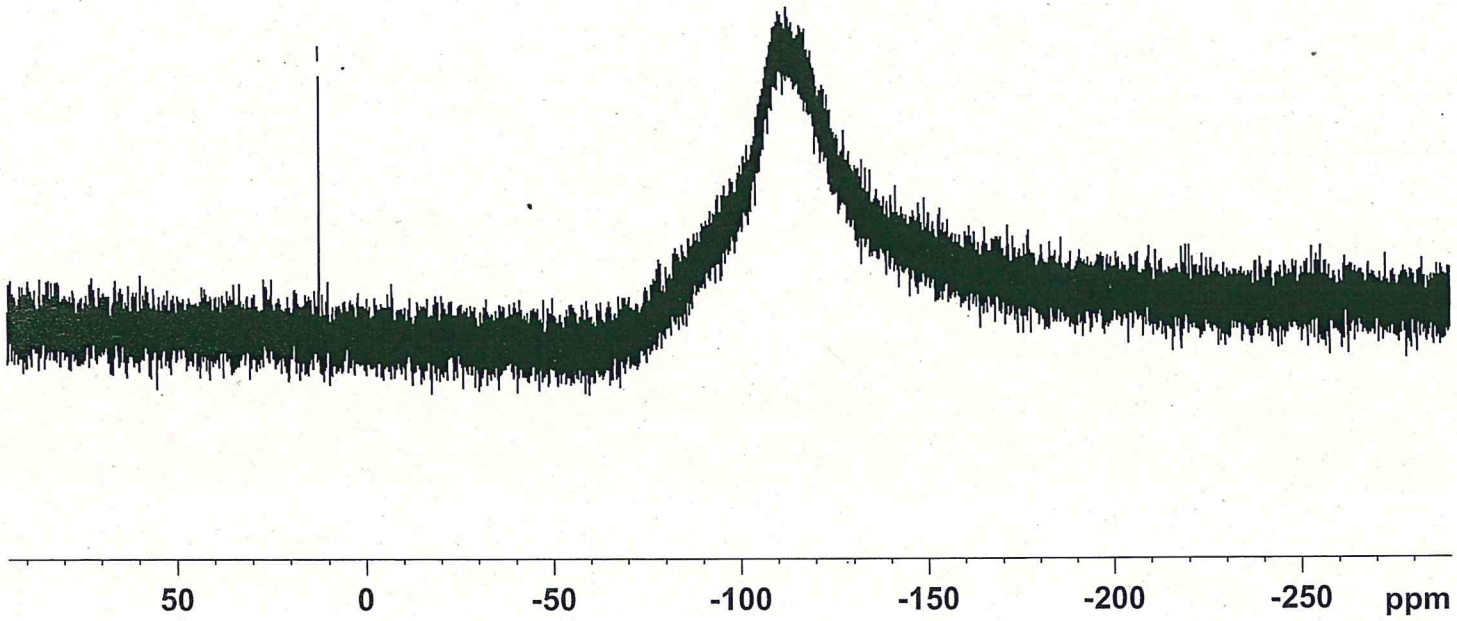
NAME	A13MC116NE	
EXPNO	1	
PROCNO	1	
Date_	20140306	
Time	17.35	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg	
TD	65536	
SOLVENT	C6D6	
NS	2000	
DS	2	
SWH	208333.328	Hz
FIDRES	3.178914	Hz
AQ	0.1573364	sec
RG	203	
DW	2.400	usec
DE	65.00	usec
TE	302.1	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	207Pb	
P1	12.00	usec
PL1	0.00	dB
SFO1	104.5935796	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	2.40	dB
PL12	19.02	dB
PL13	22.02	dB
PL2W	15.17711735	W
PL12W	0.33051354	W
PL13W	0.16564916	W
SFO2	500.0320005	MHz
SI	65536	
SF	104.6094793	MHz
WDW	EM	
SSB	0	
LB	10.00	Hz
GB	0	
PC	1.40	

Ex 326 iodoruthenocene comp. 29Si in C6D6



8





NAME	A13MC116ND
EXPNO	1
PROCNO	1
Date_	20140306
Time	12.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig
TD	65536
SOLVENT	C6D6
NS	1068
DS	4
SWH	39682.539 Hz
FIDRES	0.605507 Hz
AQ	0.8258036 sec
RG	203
DW	12.600 usec
DE	6.50 usec
TE	299.8 K
D1	5.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	29Si
P1	15.00 usec
PL1	3.00 dB
PL1W	37.76776123 W
SFO1	99.3319610 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.40 dB
PL12	19.02 dB
PL2W	15.17711735 W
PL12W	0.33051354 W
SFO2	500.0320001 MHz
SI	32768
SF	99.3418950 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40