

Electronic Supplementary Information

Metallaaromaticity Involving a d^0 Early Transition Metal Centre: Synthesis, Structure, and Aromaticity of Tantallapyridinazirine Complexes

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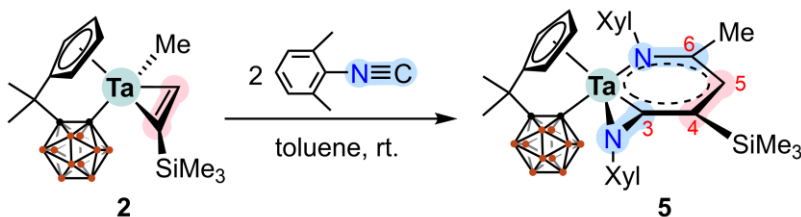
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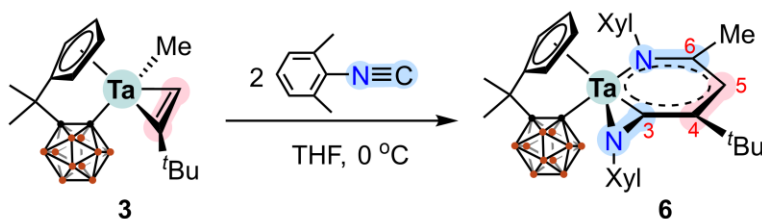
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Experimental Procedures

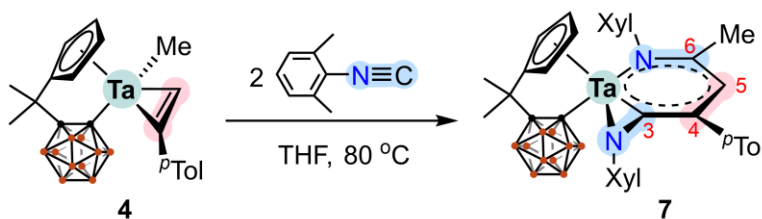
General Procedures. All reactions and manipulations were carried out under an argon atmosphere with the rigid exclusion of air and moisture using standard Schlenk techniques, or glovebox. ^1H , ^{13}C , and ^{11}B NMR spectra were recorded on a Bruker AVANCE III 400/500 NMR spectrometer at 400/500, 100/125, and 128/160 MHz, respectively. All chemical shifts were reported in δ units with references to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, and to external $\text{BF}_3\cdot\text{OEt}_2$ (0.00 ppm) for boron chemical shifts. The data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quadruplet, m = multiplet or unresolved, br = broad), coupling constant(s) in Hz, integration, and assignment. Mass spectrometry data were obtained on a Bruker Solarix 9.4T ICR Mass Spectrometer. Elemental analyses were performed by MEDAC Ltd, U.K., or the Shanghai Institute of Organic Chemistry, CAS, China. UV-visible absorption spectra were recorded on a Shimadzu UV-3600 Plus UV-Vis-NIR spectrophotometer (in the range of 300–800 nm) using 1 cm quartz cells under an argon atmosphere. All organic solvents were freshly distilled from sodium benzophenone ketyl immediately prior to use. Complexes $[\eta^5\text{-}\sigma\text{-Me}_2\text{C}(\text{C}_5\text{H}_4)(\text{C}_2\text{B}_{10}\text{H}_{10})]\text{TaMe}_3$ (**1**)¹ and $[\eta^5\text{-}\sigma\text{-Me}_2\text{C}(\text{C}_5\text{H}_4)(\text{C}_2\text{B}_{10}\text{H}_{10})]\text{TaMe}(\eta^2\text{-RC}\equiv\text{CH})$ [$\text{R} = \text{SiMe}_3$ (**2**), ^tBu (**3**), ^pTol (**4**)]² were prepared according to literature procedures. All other chemicals were purchased from either Aldrich, J&K, or Acros Chemical Co. and used as received unless otherwise specified.



Preparation of $[\eta^5\text{-}\sigma\text{-Me}_2\text{C}(\text{C}_5\text{H}_4)(\text{C}_2\text{B}_{10}\text{H}_{10})]\text{Ta}[\text{N}(\text{Xyl})\text{CC}(\text{SiMe}_3)\text{C}(\text{H})\text{C}(\text{Me})\text{N}(\text{Xyl})]$ (5). A toluene (12 mL) solution of **2** was freshly prepared from **1** (190 mg, 0.40 mmol), trimethylsilyl acetylene (40 mg, 0.40 mmol, 1.0 equiv.) and H_2 (1 atm) using the literature procedure.² To this solution, was added dropwise a toluene (2 mL) solution of xylyl isocyanide (105 mg, 0.80 mmol, 2.0 equiv.) with stirring at room temperature. The reaction mixture was stirred at room temperature for 5 days. After the reaction, the dark brown solution was filtered and concentrated to about 2 mL, to which *n*-hexane (4 mL) was slowly added. Complex **5** was obtained as dark brown crystals after this solution stood at $-30\text{ }^\circ\text{C}$ overnight (243 mg, 75%). ^1H NMR (400 MHz, C_6D_6): δ 7.12 (d, $^3J_{\text{HH}} = 7.5\text{ Hz}$, 1H, aryl CH), 7.11 (d, $^3J_{\text{HH}} = 7.5\text{ Hz}$, 1H, aryl CH), 6.95 (t, $^3J_{\text{HH}} = 7.5\text{ Hz}$, 1H, aryl CH), 6.93 (t, $^3J_{\text{HH}} = 7.5\text{ Hz}$, 1H, aryl CH), 6.83 (d, $^3J_{\text{HH}} = 7.5\text{ Hz}$, 1H, aryl CH), 6.83 (s, 1H, $\text{C}^5\text{-H}$), 6.68 (d, $^3J_{\text{HH}} = 7.5\text{ Hz}$, 1H, aryl CH), 6.11 (m, 1H, Cp-H), 5.55 (m, 1H, Cp-H), 4.59 (m, 1H, Cp-H), 4.43 (m, 1H, Cp-H), 2.77 (s, 6H, aryl CH_3), 2.19 (s, 3H, $\text{C}^6\text{-CH}_3$), 1.32 (s, 3H, bridge Me_2C), 1.29 (s, 3H, bridge Me_2C), 1.08 (s, 3H, aryl CH_3), 0.96 (s, 3H, aryl CH_3), 0.12 (s, 9H, SiMe_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ 222.4 (C^3), 156.5 (Cp C), 156.3 (aryl C), 154.0 (aryl C), 141.7 (C^6), 135.6 (aryl C), 134.1 (aryl C), 133.8 (aryl C), 130.1 (aryl C), 129.3 (aryl CH), 128.9 (aryl CH), 128.7 (aryl CH), 127.9 (C^5), 127.3 (aryl CH), 127.0 (aryl CH), 125.8 (aryl CH), 108.5 (Cp CH), 108.00 (Cp CH), 108.0 (cage C), 106.2 (Cp CH), 105.5 (Cp CH), 104.5 (cage C), 92.7 (C^4), 40.6 (bridge Me_2C), 31.9 (bridge Me_2C), 31.0 (bridge Me_2C), 26.2 ($\text{C}^6\text{-CH}_3$), 22.3 (aryl CH_3), 20.9 (aryl CH_3), 20.5 (aryl CH_3), 18.8 (aryl CH_3), 0.1 (SiMe_3). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ -2.4 (2B), -6.8 (3B), -8.8 (2B), -11.1 (3B). Anal. Calcd for $\text{C}_{34}\text{H}_{51}\text{B}_{10}\text{N}_2\text{SiTa}$ (**5**): C, 50.73; H, 6.39; N, 3.48. Found: C, 50.50; H, 6.32; N, 3.44. HRMS (APCI) calcd for $\text{C}_{34}\text{H}_{52}\text{B}_{10}\text{N}_2\text{SiTa}^+$ ($[\text{M}+\text{H}]^+$): 806.43674, Found: 806.43693. UV-Vis: $\lambda_{\text{max}} = 481\text{ nm}$.



Preparation of $[\eta^5\text{-}\sigma\text{-Me}_2\text{C}(\text{C}_5\text{H}_4)(\text{C}_2\text{B}_{10}\text{H}_{10})]\text{Ta}[\text{N}(\text{Xyl})\text{CC}(\text{tBu})\text{C}(\text{H})\text{C}(\text{Me})\text{N}(\text{Xyl})]$ (6**).** A toluene (12 mL) solution of **3** was freshly prepared from **1** (190 mg, 0.40 mmol), 3,3-dimethyl-1-butyne (66 mg, 0.80 mmol, 2.0 equiv.) and H_2 (1 atm) using the literature procedure.² After removal of toluene and excess alkyne in vacuo, THF (6 mL) was added. To this solution, was added dropwise a THF (2 mL) solution of xylyl isocyanide (105 mg, 0.80 mmol, 2.0 equiv.) with stirring at $-30\text{ }^\circ\text{C}$. The reaction mixture was stirred at $0\text{ }^\circ\text{C}$ for 7 days. After removal of THF in vacuo, and the resultant dark brown residue was recrystallized from a toluene/ether mixture to give **6** as dark brown crystals (96 mg, 30%). ^1H NMR (500 MHz, C_6D_6): δ 7.12 (d, $^3J_{\text{HH}} = 7.6\text{ Hz}$, 2H, aryl CH), 6.94 (t, $^3J_{\text{HH}} = 7.5\text{ Hz}$, 2H, aryl CH), 6.83 (s, 1H, $\text{C}^5\text{-H}$), 6.80 (d, $^3J_{\text{HH}} = 7.4\text{ Hz}$, 1H, aryl CH), 6.70 (d, $^3J_{\text{HH}} = 7.2\text{ Hz}$, 1H, aryl CH), 6.13 (m, 1H, Cp-H), 5.46 (m, 1H, Cp-H), 4.59 (m, 1H, Cp-H), 4.49 (m, 1H, Cp-H), 2.75 (s, 6H, aryl CH_3), 2.17 (s, 3H, $\text{C}^6\text{-CH}_3$), 1.31 (s, 3H, bridge Me_2C), 1.28 (s, 3H, bridge Me_2C), 1.25 (s, 9H, CMe_3), 1.03 (s, 3H, aryl CH_3), 0.98 (s, 3H, aryl CH_3). ^{13}C NMR (125 MHz, C_6D_6): δ 210.1 (C^3), 156.4 (aryl C), 155.9 (Cp C), 155.3 (aryl C), 143.7 (C^6), 135.6 (aryl C), 134.1 (aryl C), 133.8 (aryl C), 130.2 (aryl CH), 129.2 (aryl CH), 128.8 (aryl C), 128.5 (aryl CH), 127.2 (aryl CH), 126.6 (aryl CH), 125.7 (aryl CH), 123.7 (C^5), 113.2 (C^4), 108.8 (Cp CH), 107.8 (cage C), 106.9 (Cp CH), 106.7 (Cp CH), 105.1 (Cp CH), 103.6 (cage C), 40.5 (bridge Me_2C), 35.7 (CMe_3), 31.9 (bridge Me_2C), 31.7 (CMe_3), 30.9 (bridge Me_2C), 26.4 (metallacyclic CH_3), 22.4 (aryl CH_3), 20.8 (aryl CH_3), 20.4 (aryl CH_3), 19.0 (aryl CH_3). $^{11}\text{B}\{^1\text{H}\}$ (128 MHz, C_6D_6): δ -2.0 (2B), -6.3 (3B), -8.1 (2B), -10.8 (3B). Anal. Calcd for $\text{C}_{37}\text{H}_{56}\text{B}_{10}\text{N}_2\text{O}_{0.5}\text{Ta}$ (**6**·0.5ether): C, 53.81; H, 6.83; N, 3.39. Found: C, 53.95; H, 6.86; N, 3.20. HRMS (APCI) calcd for $\text{C}_{35}\text{H}_{51}\text{B}_{10}\text{N}_2\text{Ta}^-$ ($[\text{M}]^-$): 789.45303. Found: 789.45201. UV-Vis: $\lambda_{\text{max}} = 480\text{ nm}$.



Preparation of $[\eta^5\text{-}\sigma\text{-Me}_2\text{C}(\text{C}_5\text{H}_4)(\text{C}_2\text{B}_{10}\text{H}_{10})]\text{Ta}[\text{N}(\text{Xyl})\text{CC}(p\text{Tol})\text{C}(\text{H})\text{C}(\text{Me})\text{N}(\text{Xyl})]$ (7). A toluene (12 mL) solution of **4** was freshly prepared from **1** (190 mg, 0.40 mmol), *p*-tolylacetylene (47 mg, 0.40 mmol, 1.0 equiv.) and H_2 (1 atm) using the literature procedure.² After removal of the volatiles in vacuo, to the residue was added xylyl isocyanide (105 mg, 0.80 mmol, 2.0 equiv.) and THF (10 mL) at room temperature. The reaction mixture was allowed to stir at 80 °C for 12 h. After removal of THF in vacuo, the resulting dark brown residue was recrystallized from a toluene/*n*-hexane mixture at room temperature to afford **7** as dark red crystals (224 mg, 68%). ^1H NMR (500 MHz, C_6D_6): δ 7.38 (d, $^3J_{\text{HH}} = 8.1$ Hz, 2H, CH of *p*-tolyl), 7.15 (d, $^3J_{\text{HH}} = 8.6$ Hz, 1H, CH of xylyl), 7.13 (d, $^3J_{\text{HH}} = 7.0$ Hz, 1H, CH of xylyl), 7.05 (s, 1H, $\text{C}^5\text{-H}$), 6.94 (t, $^3J_{\text{HH}} = 5.6$ Hz, 1H, CH of xylyl), 6.93 (d, $^3J_{\text{HH}} = 6.7$ Hz, 2H, CH of *p*-tolyl), 6.83 (t, $^3J_{\text{HH}} = 7.6$ Hz, 1H, CH of xylyl), 6.69 (d, $^3J_{\text{HH}} = 7.3$ Hz, 1H, CH of xylyl), 6.49 (d, $^3J_{\text{HH}} = 7.4$ Hz, 1H, CH of xylyl), 6.15 (m, 1H, Cp-H), 5.51 (m, 1H, Cp-H), 4.58 (m, 1H, Cp-H), 4.42 (m, 1H, Cp-H), 2.86 (s, 3H, CH_3 of xylyl), 2.78 (s, 3H, CH_3 of xylyl), 2.17 (s, 3H, $\text{C}^6\text{-CH}_3$), 2.06 (s, 3H, CH_3 of *p*-tolyl), 1.34 (s, 3H, bridge Me_2C), 1.30 (s, 3H, bridge Me_2C), 1.02 (s, 3H, CH_3 of xylyl), 0.88 (s, 3H, CH_3 of xylyl). ^{13}C NMR (125 MHz, C_6D_6): δ 213.5 (C^3), 156.5 (Cp C), 156.2 (C of xylyl), 152.1 (C of xylyl), 145.3 (C^6), 136.4 (C of *p*-tolyl), 135.5 (C of *p*-tolyl), 134.3 (C of xylyl), 134.0 (C of xylyl), 133.9 (C of xylyl), 129.7 (CH of xylyl), 129.6 (C of xylyl), 129.3 (CH of xylyl), 129.0 (CH of *p*-tolyl), 128.5 (CH of *p*-tolyl), 128.0 (CH of xylyl), 127.3 (CH of xylyl), 126.7 (CH of xylyl), 125.9 (CH of xylyl), 122.7 (C^5), 108.8 (Cp CH), 107.9 (Cp CH), 107.8 (cage C), 106.4 (Cp CH), 105.9 (C^4), 105.6 (Cp CH), 104.7 (cage C), 40.7 (Me_2C), 31.9 (Me_2C), 31.0 (Me_2C), 26.2 (C^7), 22.4 (CH_3 of xylyl), 21.1 (CH_3 of xylyl), 20.7 (CH_3 of *p*-tolyl), 20.3 (CH_3 of xylyl), 18.8 (CH_3 of xylyl). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ -1.9 (2B), -6.2 (3B), -8.6 (2B), -10.4 (3B). Anal. Calcd for $\text{C}_{38}\text{H}_{49}\text{B}_{10}\text{N}_2\text{Ta}$ (**7**): C, 55.47; H, 6.00; N, 3.40. Found: C, 55.50; H, 5.93; N, 3.22. HRMS (APCI) calcd for $\text{C}_{38}\text{H}_{49}\text{B}_{10}\text{N}_2\text{Ta}^-$ ($[\text{M}]^-$): 823.43756. Found: 823.43523. UV-Vis: $\lambda_{\text{max}} = 491$ nm.

Crystal Data and Summary of Data Collection and Refinement

X-ray Crystallography. All single crystals were immersed in Paraton-N oil and sealed under N₂ in thin-walled glass capillaries. Data were collected at 293 K on a Bruker SMART 1000 CCD diffractometer using Mo-K α radiation. An empirical absorption correction was applied using the SADABS program.³ All structures were solved by direct methods and subsequent Fourier difference techniques and refined anisotropically for all non-hydrogen atoms by full-matrix least-squares calculations on F^2 using the SHELXTL program package.⁴ All hydrogen atoms were geometrically fixed using the riding model.

CCDC 2288668 (**5**), 2288669 (**6**) and 2288670 (**7**) contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal Data and Summary of Data Collection and Refinement for **5**, **6**, and **7·0.5** toluene.

Compound	5	6	7·0.5C₇H₈
Formula	C ₃₄ H ₅₁ B ₁₀ N ₂ SiTa	C ₃₅ H ₅₁ B ₁₀ N ₂ Ta	C _{41.5} H ₅₃ B ₁₀ N ₂ Ta
Formula weight	804.91	788.83	868.91
Crystal size, mm	0.30 x 0.20 x 0.20	0.50 x 0.40 x 0.30	0.40 x 0.30 x 0.20
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	P2 ₁ /n	P2 ₁ /c	P2 ₁ /n
<i>a</i> , Å	11.540(1)	11.579(1)	9.352(1)
<i>b</i> , Å	16.085(1)	12.987(1)	17.594(1)
<i>c</i> , Å	20.280(2)	26.895(2)	28.996(1)
β , deg	91.686(1)	97.570(2)	98.843(1)
<i>V</i> , Å ³	3762.8(3)	4008.9(5)	4714.3(4)
<i>Z</i>	4	4	4
<i>D</i> _{calcd} , Mg/m ³	1.421	1.307	1.224
Radiation (λ), Å	0.71073	0.71073	0.71073
2 θ range, deg	4.75 to 50.50	5.38 to 50.50	4.98 to 50.50
μ , mm ⁻¹	2.981	2.768	2.360
<i>F</i> (000)	1624	1592	1756
No. of obsd relfns	6809	7232	8484
No. of params refnd	433	461	523
Goodness of fit	1.030	1.046	1.194
R1	0.0289	0.0232	0.0331
wR2	0.0682	0.0542	0.0834

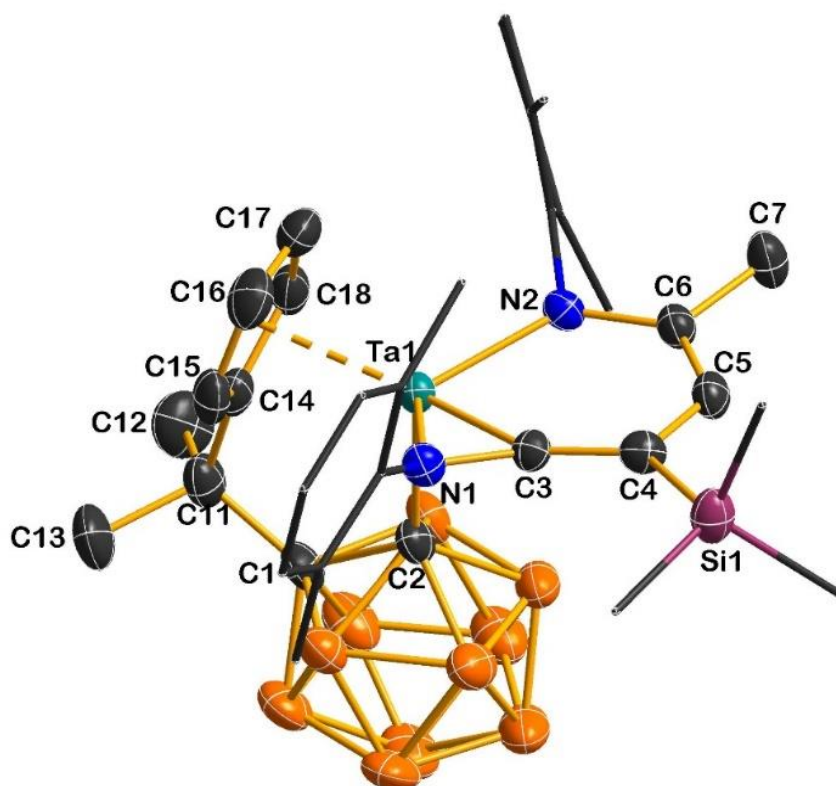


Fig. S1 Molecular structure of **5** (CCDC: 2288668). The thermal ellipsoids are set at the 50% probability level (the xyllyl and SiMe₃ groups are drawn in wireframe model and all H atoms are omitted for clarity).

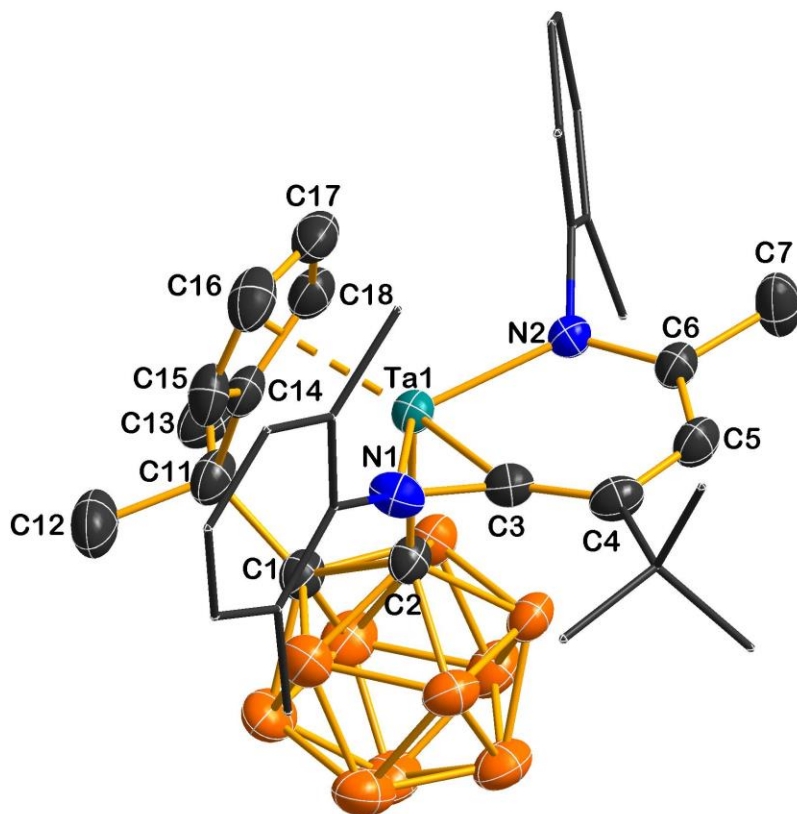


Fig. S2 Molecular structure of **6** (CCDC: 2288669). The thermal ellipsoids are set at the 50% probability level (the xylyl and *t*-butyl groups are drawn in wireframe model and all H atoms are omitted for clarity).

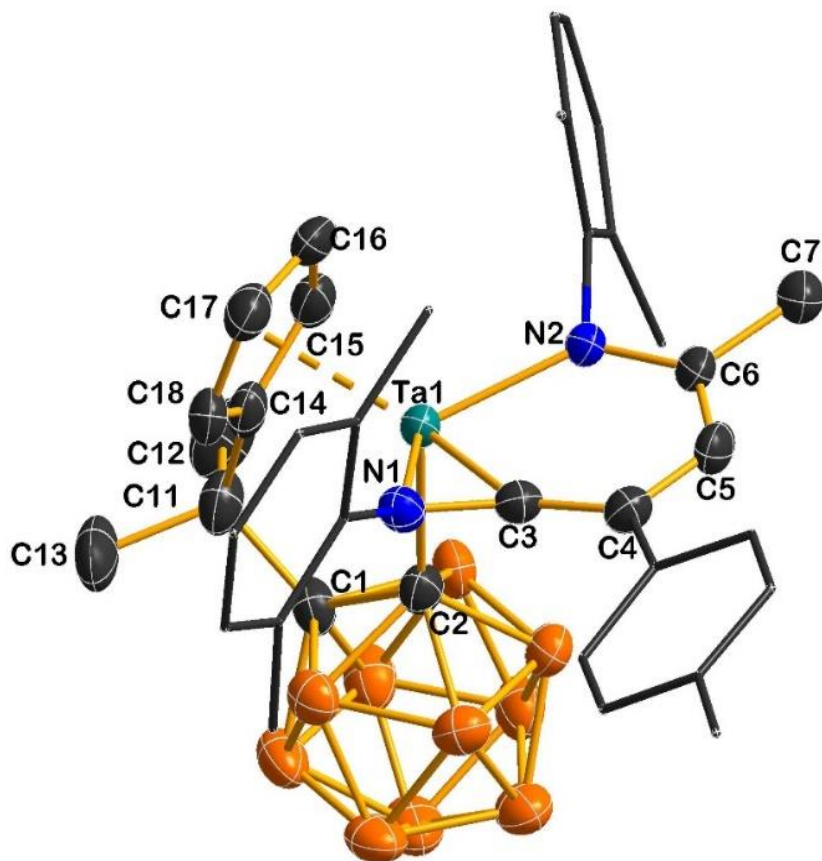


Fig. S3 Molecular structure of **7** (CCDC: 2288670). The thermal ellipsoids are set at the 50% probability level (the xylyl and *p*-tolyl groups are drawn in wireframe model and all H atoms are omitted for clarity).

Computational Details

All structures were optimized at the ω B97XD level of density functional theory (DFT).⁵ The basis set 6-31G** was applied for C, H, N, B, Si atoms while the basis set LANL2DZ was used for Ta atom.⁶⁻⁸ Frequency calculations were performed to make sure every optimized structure is a local minima, and every transition state has only one imaginary frequency. Intrinsic reaction coordinate (IRC) calculations were also carried out to ensure every transition state links two relevant intermediates.⁹ The nucleus-independent chemical shift (NICS) calculations¹⁰ were conducted using Gaussian 16¹¹ and Multiwfn¹² via the Continuous Set of Gauge Transformations (CSGT) method. ACID calculation was performed with the ACID 2.0 program.¹³

XYZ coordinates of all structures

2;

Ta	-0.59217200	-0.38004400	-0.74544700
Si	-3.76501900	0.99773900	0.76631300
C	2.48508400	-0.07898400	0.62067800
C	1.27311000	0.71844000	-0.24275900
C	2.13769800	-1.50746500	1.15350500
C	3.13726200	-2.55223800	0.62610700
H	4.12940200	-2.36955900	1.04220100
H	2.81333900	-3.54873800	0.93801600
H	3.22490800	-2.53976600	-0.46158300
C	2.19665400	-1.56834200	2.69114400
H	3.21989800	-1.41715300	3.03937700
H	1.56628400	-0.81555800	3.16614600
H	1.86358700	-2.55587800	3.02161500
C	0.73269900	-1.88000500	0.69963800
C	-0.48818300	-1.53988700	1.35563500
H	-0.58350900	-0.95020500	2.25695900
C	-1.56410800	-2.11878600	0.63736000
H	-2.60908500	-2.05969300	0.90321700
C	-1.01942000	-2.78758600	-0.48403900
H	-1.57671000	-3.31151200	-1.24794200
C	0.39063700	-2.64752700	-0.43832400
H	1.08157800	-3.03708900	-1.17216900
C	-2.23844300	0.75420100	-0.27061000
C	-1.48849000	1.41380700	-1.15577200
H	-1.54853400	2.39693800	-1.61216600
C	-4.36001200	2.77492500	0.62401000
H	-4.60643200	3.02208400	-0.41345100
H	-5.25351700	2.94776500	1.23297100
H	-3.58454700	3.47146200	0.95819200
C	-5.09188600	-0.19195000	0.15637200
H	-5.35609100	0.02240700	-0.88393100
H	-4.75554600	-1.23276600	0.20483000
H	-6.00235700	-0.10727400	0.75868400
C	-0.66981400	-0.91812200	-2.85044800
H	-1.68898100	-0.89666900	-3.25436600
H	-0.12032100	-0.10620400	-3.34944600
H	-0.20914900	-1.87018900	-3.12661200
B	1.65501300	1.24745800	1.33205400
H	0.88108700	1.04355300	2.20566300
B	3.41556300	1.03994100	1.50531800
H	3.84886700	0.70554600	2.55601600
B	4.02595300	0.33085400	0.00471500
H	4.87872600	-0.49040400	0.02176500
B	2.63620500	0.09994500	-1.07655500
H	2.48415200	-0.85414900	-1.76573300
B	1.37327700	2.40726700	0.03374000
H	0.36376000	3.02734700	0.06118500
B	2.73865400	2.63401800	1.13210100
H	2.74193200	3.50239800	1.94345300
B	4.20473700	2.06513400	0.29516200

H	5.27816000	2.53097000	0.50503900
B	3.72202000	1.47186300	-1.31688800
H	4.43278700	1.50495400	-2.26864100
B	1.97054000	1.69344500	-1.46260300
H	1.37175400	1.81434300	-2.48030400
B	2.94177700	2.91176900	-0.61476000
H	3.09096800	3.99887500	-1.07163900
C	-3.30482800	0.60602600	2.55134000
H	-3.05413900	-0.45196900	2.68054900
H	-2.43869800	1.19829600	2.86493000
H	-4.13119300	0.83517400	3.23201800

XyINC;

N	-1.81885100	-0.00220500	-0.00000900
C	-0.43061300	-0.00052400	0.00001100
C	0.24056500	-1.23168100	0.00006600
C	1.63374800	-1.20431000	0.00003500
H	2.17989600	-2.14283900	0.00004400
C	1.63079700	1.20829500	-0.00003100
H	2.17464300	2.14815800	-0.00009800
C	0.23757900	1.23229600	-0.00001400
C	-0.53158300	-2.52189000	-0.00003800
H	-1.17890300	-2.59293900	-0.87985900
H	0.14413700	-3.37954400	0.00113900
H	-1.18084400	-2.59198700	0.87840400
C	-0.53781500	2.52052700	-0.00000900
H	0.13567500	3.37992500	-0.00100500
H	-1.18712100	2.58902100	-0.87856400
H	-1.18554500	2.58989300	0.87964900
C	-2.99686600	-0.00361200	0.00002800
C	2.32426900	0.00282600	0.00001200
H	3.40953200	0.00418000	-0.00000800

TS₂;

Ta	1.03185000	-1.20925000	-0.54107200
Si	-1.46916700	-2.47421500	2.04493200
N	-2.41060700	0.86284600	-1.67275800
C	2.40685400	1.79310600	0.42312100
C	1.07290600	0.75131900	0.64540900
C	3.42372600	1.39568500	-0.69194300
C	3.51266200	2.47472100	-1.78712500
H	3.94325600	3.39223500	-1.38243300
H	4.16270800	2.11562300	-2.58952000
H	2.53989300	2.72023100	-2.21487800
C	4.84308700	1.22593600	-0.11929500
H	5.23413100	2.18733900	0.21787000
H	4.87577500	0.53700700	0.72625000
H	5.50195200	0.84458200	-0.90410900
C	2.98490300	0.08421600	-1.32625600
C	3.40381000	-1.21491200	-0.93804200
H	4.05529000	-1.45452200	-0.11048500
C	2.82157000	-2.15673800	-1.82623000

H	2.96091100	-3.22814800	-1.79132200	H	-0.45640800	4.26673400	0.94751800
C	2.05590600	-1.43762800	-2.77731300	B	-0.27061700	1.67751000	1.14013600
H	1.48701000	-1.86752800	-3.58758400	H	-1.34738200	1.32741100	0.79337900
C	2.13463200	-0.06506300	-2.45865000	B	0.15292700	2.40816700	2.70234400
H	1.61546800	0.72947700	-2.97441300	H	-0.68408400	2.61304900	3.52247300
C	0.06728400	-2.12094200	1.04800700	C	-1.02284800	-2.90432500	3.82070600
C	1.30030700	-2.60867900	0.88955600	H	-0.34362400	-3.76200100	3.85654800
H	1.90274200	-3.37192300	1.37301000	H	-0.52787000	-2.06115800	4.31241300
C	-2.64300000	-1.00807900	1.99459500	H	-1.91642100	-3.15579500	4.40189800
H	-2.73330100	-0.61081100	0.97902400				
H	-3.64376900	-1.29389200	2.33604000	2';			
H	-2.28827500	-0.19040100	2.62816500	Ta	0.63852000	-1.11253400	-0.79319200
C	-2.26378400	-3.95838600	1.19246500	Si	-1.59547300	-2.52036300	2.04700600
H	-2.45759600	-3.75265500	0.13480100	N	-2.15693700	0.77851800	-0.75919100
H	-1.60602400	-4.83185300	1.24320100	C	2.65293800	1.44850100	0.45001500
H	-3.21487100	-4.22140500	1.66762900	C	1.22690400	0.55884100	0.75179100
C	-1.29512000	0.69378500	-1.99508700	C	3.38116700	1.16009700	-0.89619200
C	-0.54864900	-2.14990200	-1.76546700	C	3.42303400	2.40666500	-1.79971100
H	-0.31095100	-3.22281100	-1.81049300	H	4.04890100	3.17964700	-1.35090100
H	-1.51382700	-2.06040000	-1.26025100	H	3.85592900	2.13386300	-2.76597600
H	-0.66481300	-1.77778300	-2.78529600	H	2.43501400	2.83542800	-1.97202700
C	-3.69293700	1.14284500	-1.21899400	C	4.84391800	0.73650700	-0.66274400
C	-4.62564600	0.09996300	-1.12580900	H	5.42378900	1.57252100	-0.26809300
C	-5.89317000	0.41784000	-0.64104700	H	4.93330100	-0.09353300	0.03986700
H	-6.63631200	-0.36919800	-0.55583700	H	5.28436100	0.43369100	-1.61659000
C	-6.21138900	1.71878100	-0.27004900	C	2.65858200	0.04093200	-1.62880100
H	-7.20342600	1.94491000	0.10743500	C	2.94721600	-1.34430400	-1.53455700
C	-5.26791800	2.73386900	-0.38641900	H	3.66679000	-1.80011100	-0.87065800
H	-5.52387300	3.74964500	-0.10164600	C	2.13452000	-2.03411300	-2.46899200
C	-3.98768000	2.46955700	-0.86647000	H	2.12231000	-3.10302100	-2.63024900
C	-4.26994600	-1.30949600	-1.51039700	C	1.35156800	-1.07542200	-3.15483400
H	-5.17114600	-1.89169100	-1.71464300	H	0.63404300	-1.28431600	-3.93355100
H	-3.62669000	-1.34104800	-2.39334900	C	1.64848300	0.20027500	-2.62319400
H	-3.73033600	-1.80711300	-0.69697300	H	1.21921300	1.13695100	-2.94858000
C	-2.95388600	3.54993800	-1.00945900	C	-0.24060100	-2.16948000	0.81876000
H	-2.58088900	3.60576100	-2.03718400	C	0.90288600	-2.71977000	0.43807200
H	-3.37003600	4.52253200	-0.74022600	H	1.49476300	-3.57667500	0.74334800
H	-2.09274000	3.35740200	-0.36431000	C	-2.50866500	-0.95311100	2.54152600
B	2.33678700	0.79029000	1.80775400	H	-2.86750200	-0.38528600	1.67828500
H	3.06507600	-0.14200700	1.88188900	H	-3.37358200	-1.19764600	3.16775400
B	2.90192900	2.47514900	1.90815500	H	-1.85322400	-0.29100900	3.11460300
H	4.05564800	2.67953900	2.07994200	C	-2.76698700	-3.73537700	1.20130000
B	1.97384100	3.41232700	0.73513700	H	-3.15629200	-3.34660000	0.25560900
H	2.48194700	4.26635500	0.09016900	H	-2.24520100	-4.67190300	0.97991400
B	0.85432900	2.29421600	-0.07390900	H	-3.62008400	-3.96824600	1.84756200
H	0.61023800	2.35893600	-1.22794300	C	-1.16135800	0.17098900	-0.70282000
B	0.65358000	0.76075900	2.31757300	C	-1.07602500	-1.98215500	-2.02619500
H	0.24175200	-0.23573400	2.80262000	H	-0.66155500	-2.92841200	-2.40054500
B	1.78691000	1.84459300	3.12395600	H	-1.94090400	-2.23396100	-1.41060900
H	2.14888500	1.63694700	4.23706200	H	-1.42287900	-1.40127000	-2.88654900
B	1.54505000	3.47376500	2.44983500	C	-3.37335500	1.44576100	-0.73329800
H	1.73434500	4.46283700	3.08235900	C	-3.37538600	2.84519200	-0.63214100
B	0.27228300	3.36345500	1.20919900	C	-4.61592400	3.47841100	-0.59192200

H	-4.64990500	4.56048100	-0.51218600	H	3.14640600	2.46189300	-3.11366600
C	-5.79696100	2.74773400	-0.65016700	C	1.18186200	1.02969300	-2.03374800
H	-6.75197500	3.26176600	-0.61390400	C	1.97015100	-0.14895200	-2.14770700
C	-5.76096700	1.36225600	-0.75931400	H	3.00896700	-0.24931800	-1.86913500
H	-6.68569500	0.79590100	-0.81004300	C	1.16355000	-1.17532300	-2.69767900
C	-4.54776300	0.67998400	-0.80780400	H	1.48223700	-2.18698700	-2.90937800
C	-2.09322500	3.62522500	-0.56913200	C	-0.12636700	-0.63627900	-2.92751600
H	-2.29078800	4.69698400	-0.63155000	H	-0.96685700	-1.16223600	-3.35855700
H	-1.55687500	3.43097700	0.36374700	C	-0.12258200	0.71909500	-2.50804600
H	-1.42110800	3.35139500	-1.38761600	H	-0.95892100	1.40078700	-2.56517700
C	-4.48857000	-0.81555300	-0.93918000	C	1.35903100	-2.09589100	0.47506100
H	-3.95685100	-1.26514600	-0.09520100	C	0.18159200	-2.01339800	1.07328300
H	-5.49308100	-1.24135000	-0.97315400	H	-0.32038300	-2.50202700	1.90168300
H	-3.95632700	-1.11228300	-1.84833200	C	2.71992400	-4.50007400	1.77134800
B	2.67074800	0.20898100	1.62059000	H	1.92159000	-5.16382600	1.42404800
H	3.24290100	-0.80143800	1.38356100	H	3.63614700	-5.09300100	1.86161600
B	3.51128100	1.75584200	1.89302400	H	2.44975400	-4.14582400	2.77133600
H	4.69457900	1.77613100	1.85335800	C	3.39219100	-3.66908300	-1.12747400
B	2.55177900	3.01712400	1.11261900	H	2.57849200	-4.26413800	-1.55570600
H	3.06944600	3.91049300	0.53110200	H	3.59656400	-2.83190400	-1.80340400
B	1.13784300	2.22393200	0.37904400	H	4.28742700	-4.29890700	-1.10261900
H	0.70146600	2.53826100	-0.67652600	C	-1.70265000	-0.22816700	0.13918100
B	1.12435600	0.28794300	2.45110500	C	-2.00598600	-1.72692300	-0.82910500
H	0.64400000	-0.72357600	2.83205000	H	-1.33674100	-2.48329700	-1.25948900
B	2.54687600	1.03798200	3.18346700	H	-2.57156600	-2.24596500	-0.05572600
H	3.06482200	0.56834100	4.14513100	H	-2.67657900	-1.37709200	-1.61434400
B	2.45823000	2.78971700	2.86467900	C	-4.06405500	0.00247100	0.44584200
H	2.92041800	3.59849900	3.60413700	C	-4.78900900	0.50382900	-0.64384100
B	0.98124300	3.09259100	1.91657800	C	-6.14451600	0.19041500	-0.72920300
H	0.36410300	4.10970200	1.96288300	H	-6.72253800	0.57013300	-1.56730700
B	0.17251500	1.53993300	1.68304800	C	-6.76047000	-0.59078300	0.24281000
H	-0.99538600	1.41986500	1.53975600	H	-7.81757700	-0.82287100	0.16391200
B	0.98214900	1.87836000	3.21603200	C	-6.02244300	-1.06248600	1.32333500
H	0.35028400	2.01719700	4.21456000	H	-6.50524700	-1.66237700	2.08988300
C	-0.86506300	-3.33073900	3.58062600	C	-4.66529100	-0.77024600	1.44885300
H	-0.32406300	-4.24540200	3.31757600	C	-4.10119300	1.35577700	-1.67817000
H	-0.16301100	-2.65659500	4.08085600	H	-4.82491900	1.80026300	-2.36513600
H	-1.64824300	-3.59596000	4.29893100	H	-3.52907800	2.15940300	-1.20286600
TS_{2-E};				H	-3.39178500	0.76905700	-2.27538900
Ta	0.19541800	-0.67568300	-0.51197200	C	-3.84653100	-1.25088000	2.61745300
Si	2.95598900	-3.04816800	0.59842500	H	-3.32508300	-0.41587800	3.09603400
N	-2.70675300	0.33626800	0.57244100	H	-4.47641900	-1.74416100	3.36114000
C	1.55613000	2.43854800	0.00595400	H	-3.07338300	-1.96253100	2.30477400
C	0.87746500	1.08363600	0.75267800	B	2.56849200	1.37077600	0.86862000
C	1.65549900	2.39219400	-1.55073000	H	3.30543600	0.67448500	0.26037500
C	0.79924600	3.49149300	-2.20457500	B	2.78110500	3.13030300	0.97716200
H	1.20065000	4.47620600	-1.96051400	H	3.71403000	3.62439600	0.43994800
H	0.82587800	3.37128600	-3.29115900	B	1.17502700	3.85988100	0.86758900
H	-0.24039100	3.46581100	-1.87574200	H	1.00252200	4.86045900	0.25609800
C	3.10300200	2.60922200	-2.03098700	B	-0.01046900	2.54455600	0.70194200
H	3.42769900	3.62748800	-1.81035900	H	-0.95345200	2.60790300	-0.00972100
H	3.80852400	1.92357100	-1.55896600	B	1.64818000	0.84510000	2.27419000
				H	1.79545900	-0.26450700	2.66130500

B	2.84548400	2.13745800	2.43609100
H	3.87337500	1.95592200	3.00616100
B	1.96681700	3.68822900	2.44198100
H	2.36603200	4.64442600	3.02564600
B	0.23000400	3.33127000	2.26787400
H	-0.62720900	4.01906000	2.72058200
B	0.04974100	1.57105400	2.17419100
H	-0.91579700	0.96660100	2.49183200
B	1.27003800	2.27327800	3.24866300
H	1.15635400	2.18994500	4.42952800
C	4.31292200	-1.91116000	1.22697100
H	4.60151000	-1.17778800	0.46859900
H	3.99204300	-1.35731000	2.11408400
H	5.20382200	-2.49170100	1.48926500

E;

Ta	0.08929100	-0.42033300	-1.10275100
Si	1.73752000	-3.31573000	1.05169900
N	-1.96912700	-0.21036700	-0.54379800
C	1.70887300	2.12565800	0.59417400
C	0.63821800	0.80385200	0.80026000
C	2.22755300	2.39426900	-0.85200300
C	1.87233700	3.81685800	-1.32470900
H	2.42537300	4.55751100	-0.74501200
H	2.15180700	3.92593300	-2.37629500
H	0.80913200	4.04008400	-1.22238500
C	3.76015700	2.26903300	-0.93899900
H	4.23770800	3.06803900	-0.36996800
H	4.12570800	1.31790900	-0.54988200
H	4.06916700	2.36048500	-1.98398300
C	1.59844700	1.39272500	-1.80722900
C	2.15405000	0.14664200	-2.20702300
H	3.07330600	-0.28425200	-1.83876400
C	1.29405200	-0.43902800	-3.17751200
H	1.45771600	-1.37665200	-3.68681300
C	0.20318700	0.44404800	-3.37593000
H	-0.61709600	0.29456400	-4.06290700
C	0.38668000	1.56523100	-2.52681400
H	-0.28786100	2.40501100	-2.43675700
C	0.88587600	-2.14288700	-0.13728100
C	0.31182300	-2.46018000	-1.28876100
H	0.17019700	-3.36764600	-1.86972600
C	2.26575900	-4.81379200	0.02758600
H	2.97135100	-4.52629900	-0.75919200
H	2.75450300	-5.56632700	0.65564100
H	1.40435400	-5.28908800	-0.45345800
C	3.27253700	-2.63003900	1.89213100
H	3.98935000	-2.24295400	1.16115600
H	3.04368200	-1.82735400	2.59627800
H	3.76682500	-3.43707300	2.44491000
C	-1.89202400	-0.75676800	-1.70044300
C	-2.99825300	-1.25877500	-2.54896300
H	-2.97784200	-0.74724600	-3.51630200

H	-2.82565400	-2.31980800	-2.75261600
H	-3.97978800	-1.12443100	-2.08342400
C	-3.13663900	0.03198100	0.23466400
C	-3.92187900	1.15202800	-0.04929900
C	-5.04978800	1.36889800	0.74242200
H	-5.67273500	2.23722100	0.54854400
C	-5.37499000	0.49523500	1.77305000
H	-6.25292500	0.68131900	2.38306000
C	-4.57210300	-0.61087600	2.03166400
H	-4.82153700	-1.28571900	2.84514200
C	-3.43395800	-0.86198900	1.26874400
C	-3.54247700	2.09487000	-1.16067100
H	-4.19135400	2.97306000	-1.16401200
H	-2.50845200	2.43453300	-1.04443600
H	-3.62333200	1.61617400	-2.14357300
C	-2.51698700	-2.01920700	1.55363400
H	-1.50964300	-1.66022100	1.79138800
H	-2.87842400	-2.60836200	2.39898000
H	-2.41760000	-2.68429100	0.68913000
B	2.24896000	0.70810100	1.37012100
H	3.00496200	-0.00267000	0.80161500
B	2.70909900	2.32282200	1.96064800
H	3.82274200	2.69383100	1.79824400
B	1.33767600	3.39888800	1.66898000
H	1.50148200	4.51401600	1.30361400
B	0.06245300	2.42092200	0.90317600
H	-0.62078500	2.83756100	0.02680800
B	0.90380000	0.14445000	2.35195000
H	0.73996700	-1.01753800	2.49516500
B	2.20350700	1.07676000	3.10466400
H	2.98721400	0.56681200	3.84099900
B	1.62258800	2.75150500	3.28918800
H	1.99279400	3.46437100	4.16669500
B	-0.03006600	2.82915300	2.62548400
H	-0.86199100	3.58473500	3.01456000
B	-0.45269400	1.20802000	2.06123700
H	-1.56028300	0.80443000	2.00809900
B	0.50898500	1.39904700	3.53503300
H	0.05699900	1.11304300	4.59768600
C	0.48320300	-3.89975900	2.33261400
H	0.17907800	-3.09588500	3.00810200
H	-0.41533300	-4.29186100	1.84470000
H	0.91415000	-4.70439000	2.93839700

TS_E;

Ta	-0.43513200	-0.17565300	-1.12477000
Si	1.31985500	-2.81872900	1.27011100
N	-2.43701100	-0.96659700	-0.58694300
C	-0.88930400	2.74754500	0.70224400
C	-0.45678500	1.09246100	0.80678200
C	-1.15340300	3.31488900	-0.73359400
C	-2.59412000	3.83576900	-0.86780600
H	-2.74351400	4.70401000	-0.22399200

H	-2.77547200	4.14052900	-1.90213500	H	-2.65898600	4.02976900	1.93241400
H	-3.33714900	3.08834700	-0.58924500	B	-2.00058700	1.62512900	1.33675900
C	-0.22609100	4.50639800	-1.04525800	H	-2.95439200	1.34323400	0.70400700
H	-0.46508300	5.35593800	-0.40292300	B	0.62867400	0.90968000	2.10603000
H	0.82804600	4.26413100	-0.90337500	H	1.48596600	0.09870000	1.99220600
H	-0.37391500	4.80887500	-2.08569900	B	0.86298400	2.50416200	2.83301700
C	-0.90068000	2.22959200	-1.77461900	H	1.90913400	2.81788800	3.30793800
C	0.36096500	1.84435200	-2.28716500	B	-0.71021700	3.05039800	3.45851000
H	1.30508900	2.26852100	-1.99120700	H	-0.80746100	3.77314100	4.39871200
C	0.18175200	0.82214700	-3.25725800	B	-1.90720800	1.78437400	3.09519100
H	0.95853100	0.35301400	-3.84316500	H	-2.86962500	1.57754000	3.76232900
C	-1.21502900	0.61257400	-3.38247200	B	-1.06267100	0.46489600	2.26909200
H	-1.69264000	-0.08103600	-4.05941900	H	-1.41547900	-0.66553800	2.27868000
C	-1.87143700	1.47093500	-2.47279200	B	-0.25354600	1.34121600	3.58105900
H	-2.93535800	1.51413500	-2.31231800	H	-0.01510100	0.80691300	4.61788800
C	0.54601200	-1.76824600	-0.07362000	C	0.69257800	-2.61591200	3.03435800
C	0.68239500	-1.91325000	-1.38405000	H	0.85480300	-1.60493600	3.41414500
H	1.16003300	-2.64072200	-2.03657300	H	-0.36776900	-2.84738400	3.15298200
C	1.08972300	-4.62422900	0.75932100	H	1.25580600	-3.30775800	3.67225400
H	1.48277300	-4.79627400	-0.24826000	N	3.43004100	0.28312700	-0.57426300
H	1.61598400	-5.29596900	1.44607800	C	4.77464600	0.12128100	-0.27719600
H	0.03271600	-4.90869900	0.75848400	C	5.29515100	0.78757200	0.84009400
C	3.16983900	-2.44964900	1.30712300	C	6.64584400	0.59053600	1.12152200
H	3.62927500	-2.55860200	0.31996900	H	7.08216200	1.08955800	1.98128000
H	3.36592400	-1.43348900	1.66147600	C	6.87946300	-0.88352300	-0.77743400
H	3.67476800	-3.14166800	1.98988400	H	7.49695700	-1.52987300	-1.39366000
C	-2.03093600	-1.47148900	-1.67943700	C	5.53497600	-0.71954700	-1.10074100
C	-2.65652900	-2.53807000	-2.49545000	C	4.41456300	1.65636500	1.69356900
H	-2.73428500	-2.22232200	-3.53960800	H	3.60016600	1.07845300	2.14165000
H	-1.98842800	-3.40581000	-2.47771800	H	4.98625700	2.12077400	2.49899300
H	-3.64336600	-2.82810300	-2.11982500	H	3.94217000	2.44917500	1.10533900
C	-3.60588800	-1.30861600	0.16860100	C	4.90126800	-1.41119700	-2.27630400
C	-4.80691700	-0.61188700	-0.02281000	H	5.61652900	-2.07058000	-2.77177100
C	-5.90102900	-0.95047100	0.77413300	H	4.03805000	-2.00845400	-1.96389500
H	-6.83268400	-0.40815600	0.64120100	H	4.53740000	-0.68530300	-3.01133600
C	-5.81816100	-1.96376500	1.71925100	C	2.28536100	0.38011400	-0.79833300
H	-6.67618000	-2.20338700	2.33871100	C	7.43051000	-0.23425600	0.32274500
C	-4.63923300	-2.68521300	1.84692100	H	8.47977800	-0.37523500	0.56132300
H	-4.57406100	-3.50430100	2.55714900				
C	-3.52580200	-2.38254900	1.06541300	E';			
C	-4.95672000	0.44599900	-1.08043900	Ta	-0.27379700	-0.12634400	-1.06084200
H	-6.00426700	0.73414100	-1.19046100	Si	1.26836500	-2.80977900	1.52000000
H	-4.38961300	1.34394800	-0.82357700	N	-2.30890200	-0.98353200	-0.68975100
H	-4.60243700	0.09130800	-2.05376600	C	-0.86772800	2.78493200	0.73200600
C	-2.28398900	-3.21975000	1.13284500	C	-0.45526700	1.12786600	0.86295400
H	-1.39748700	-2.58775800	1.16116500	C	-1.02643000	3.35838200	-0.71510100
H	-2.28878100	-3.86846200	2.01151100	C	-2.45074100	3.89304400	-0.94521400
H	-2.19245600	-3.85637400	0.24448200	H	-2.63385300	4.76395900	-0.31380500
B	0.71042600	2.32996200	1.08050700	H	-2.56044200	4.19692200	-1.98979500
H	1.55826100	2.53455100	0.28288800	H	-3.21740700	3.15242600	-0.71523100
B	-0.10194300	3.66543500	1.91640400	C	-0.06786300	4.53944300	-0.96244900
H	0.22689600	4.77534400	1.66244000	H	-0.33911800	5.39057500	-0.33545700
B	-1.79991200	3.22514300	2.07394100	H	0.97201000	4.28568000	-0.75115100

H	-0.14331400	4.84522500	-2.00965600	B	0.73786600	2.52773200	2.97326700
C	-0.72158100	2.26991500	-1.73692000	H	1.75343000	2.83175300	3.51594500
C	0.55260000	1.89773400	-2.22086100	B	-0.87040500	3.08460200	3.49218100
H	1.48923900	2.33937300	-1.91704600	H	-1.02672000	3.80734900	4.42428700
C	0.40142400	0.85987200	-3.18732000	B	-2.05011100	1.82676200	3.04769100
H	1.19345500	0.39953400	-3.75980700	H	-3.05563000	1.62767600	3.65030600
C	-0.98879500	0.63421000	-3.33584300	B	-1.16192200	0.50099400	2.27873600
H	-1.44603300	-0.06409600	-4.02174500	H	-1.52182200	-0.62718200	2.26276300
C	-1.67051900	1.48838600	-2.44044000	B	-0.43587000	1.37231100	3.64357000
H	-2.73635900	1.53178300	-2.30622000	H	-0.27176100	0.83587800	4.69353800
C	0.56885800	-1.81886300	0.10001800	C	0.51056500	-2.57859800	3.22849400
C	0.72858600	-2.02240000	-1.18744200	H	0.61311400	-1.55328000	3.59000600
H	1.12301800	-2.80965400	-1.82517000	H	-0.54802700	-2.84301800	3.27566400
C	1.13114600	-4.63591900	1.05149500	H	1.04627600	-3.23433200	3.92541700
H	1.58632700	-4.82285700	0.07306900	N	3.08964700	0.22167200	-0.52131000
H	1.63932000	-5.26983900	1.78619000	C	4.45366300	0.06516400	-0.32946000
H	0.08540700	-4.95562700	1.00020600	C	5.08466500	0.79241200	0.68767100
C	3.10070600	-2.37637400	1.66422400	C	6.45366500	0.59004600	0.85531400
H	3.63399200	-2.54435600	0.72315800	H	6.97254000	1.13455500	1.63813200
H	3.24351800	-1.32985800	1.95021700	C	6.49349500	-1.00570900	-0.95517100
H	3.57435300	-2.99730300	2.43253400	H	7.04270100	-1.70218000	-1.58135000
C	-1.79322300	-1.49616100	-1.72884800	C	5.12643000	-0.84258500	-1.16070000
C	-2.30920700	-2.59847600	-2.57457700	C	4.30562800	1.73444900	1.56146100
H	-2.31315600	-2.30305600	-3.62777700	H	3.46208900	1.23009100	2.04227600
H	-1.61503000	-3.44094500	-2.48514100	H	4.94171900	2.15647500	2.34159100
H	-3.31235600	-2.92028800	-2.27563300	H	3.88548800	2.56069100	0.97982100
C	-3.53177900	-1.34206800	-0.03280600	C	4.37632900	-1.61346300	-2.21181400
C	-4.72157700	-0.65595700	-0.31589200	H	5.04717000	-2.27803300	-2.75956500
C	-5.87613000	-1.01297100	0.38233700	H	3.58189100	-2.21639400	-1.76019800
H	-6.79841200	-0.47810600	0.17436400	H	3.89556200	-0.94123900	-2.93075400
C	-5.86506200	-2.03354700	1.32219300	C	1.93829600	0.18929100	-0.72308300
H	-6.77052100	-2.28827200	1.86312400	C	7.15268200	-0.29567000	0.04330700
C	-4.69193300	-2.74044600	1.54607200	H	8.21798500	-0.43839400	0.19276100
H	-4.67652500	-3.56266800	2.25553400				
C	-3.51901100	-2.41841800	0.86617600	TS_{E-F};			
C	-4.80207100	0.41740000	-1.36555500	Ta	-0.26761000	-0.10036400	-0.96835100
H	-5.84387000	0.65349400	-1.59285900	Si	1.34282200	-2.74943900	1.66977000
H	-4.32098300	1.33850000	-1.02496500	N	-2.19462500	-1.08835700	-0.60391100
H	-4.31879100	0.10489600	-2.29624500	C	-0.90048000	2.88368500	0.63847400
C	-2.27389300	-3.22977000	1.05796900	C	-0.53811000	1.24096300	0.86236100
H	-1.41812600	-2.57559500	1.21491500	C	-0.98872000	3.38121600	-0.84181600
H	-2.36873600	-3.90685300	1.90985300	C	-2.39866300	3.90319200	-1.16916200
H	-2.05046600	-3.83170400	0.16920200	H	-2.61099000	4.80226100	-0.58837900
B	0.69888100	2.35310600	1.21366100	H	-2.45443900	4.15914800	-2.23085200
H	1.59382400	2.53695000	0.46237200	H	-3.17754000	3.17320700	-0.94490100
B	-0.15511800	3.69581600	1.99535900	C	-0.01124500	4.54124100	-1.10963900
H	0.19633100	4.80393500	1.76552800	H	-0.30545300	5.42733900	-0.54441000
B	-1.86414700	3.26708600	2.03816400	H	1.01561100	4.29417300	-0.83560400
H	-2.70495700	4.07909100	1.84087800	H	-0.03512500	4.78852600	-2.17470500
B	-2.02870800	1.66778800	1.28620400	C	-0.64227100	2.23232600	-1.78011600
H	-2.93791400	1.38950700	0.58718300	C	0.65238700	1.80024900	-2.15480200
B	0.53968800	0.93587200	2.23270200	H	1.57914500	2.25474000	-1.83953900
H	1.39807600	0.12062800	2.17676000	C	0.53394000	0.69213800	-3.05713500

H	1.34391600	0.20552800	-3.58023000	H	-3.21587300	1.92971600	3.53283100
C	-0.85601800	0.45400600	-3.23274100	B	-1.30459500	0.69314500	2.28243500
H	-1.29628600	-0.27527400	-3.89697500	H	-1.69009400	-0.42548400	2.31118400
C	-1.56774100	1.40079600	-2.44707700	B	-0.60492300	1.61342200	3.62824400
H	-2.63632700	1.47632000	-2.37040200	H	-0.49156400	1.12569100	4.70812900
C	0.46964100	-1.88171000	0.25542800	C	0.51778400	-2.51514300	3.34619700
C	0.17358600	-2.33747300	-0.93821400	H	0.22076100	-1.47970100	3.52562300
H	0.40474000	-3.22588400	-1.52018500	H	-0.36712900	-3.14607400	3.46085000
C	1.35712900	-4.59127700	1.25403600	H	1.23043900	-2.80027300	4.12848900
H	1.87825300	-4.78089900	0.30937900	N	3.03462500	0.04753400	-0.47489900
H	1.86213900	-5.16672600	2.03717800	C	4.41174200	-0.03176400	-0.37006100
H	0.33764400	-4.97931200	1.15852400	C	5.07164900	0.79647300	0.54702300
C	3.12867300	-2.17356600	1.83344400	C	6.45682200	0.66715400	0.63316000
H	3.71494200	-2.35315900	0.92794400	H	7.00027100	1.29117000	1.33590500
H	3.19415500	-1.11074900	2.08186000	C	6.45418900	-1.06299700	-1.05215300
H	3.60190100	-2.73306300	2.64795400	H	6.99439100	-1.78268400	-1.65961200
C	-1.52498500	-1.66472700	-1.55792200	C	5.07071600	-0.97236600	-1.17618200
C	-2.04712100	-2.59477800	-2.60176500	C	4.30596500	1.77286700	1.39526400
H	-1.28023000	-2.84153600	-3.33937200	H	3.45188300	1.29866100	1.88851400
H	-2.40931000	-3.52036200	-2.14126400	H	4.94858300	2.20804000	2.16274200
H	-2.89869400	-2.12953200	-3.10803200	H	3.90165400	2.58959900	0.78877500
C	-3.46986800	-1.43528400	-0.07788500	C	4.28658200	-1.84816700	-2.11429900
C	-4.64778100	-0.82757900	-0.54305900	H	4.94154800	-2.55626200	-2.62539700
C	-5.86771500	-1.19291800	0.02949000	H	3.51685800	-2.41244300	-1.57623200
H	-6.77575800	-0.71401100	-0.32654000	H	3.76896400	-1.25073600	-2.87273300
C	-5.93969100	-2.15159900	1.02906800	C	1.87722500	-0.01394700	-0.64073500
H	-6.89692200	-2.41816100	1.46531300	C	7.14197700	-0.24894300	-0.15734400
C	-4.77428900	-2.77275400	1.45623200	H	8.22030000	-0.33460900	-0.07085700
H	-4.81390900	-3.53514700	2.22925000				
C	-3.53833000	-2.43117600	0.91200400	F;			
C	-4.64504800	0.19676600	-1.64293500	Ta	-0.25824700	-0.48433700	-0.70791600
H	-5.65321900	0.33788600	-2.03960100	Si	1.86277000	-3.30079400	0.71593700
H	-4.29742900	1.16623500	-1.27200900	N	-2.09604800	-1.30881400	-0.13472900
H	-3.99594300	-0.10230600	-2.47034600	C	-0.98650100	2.91868000	-0.25627600
C	-2.28907200	-3.12315300	1.36606500	C	-0.70178500	1.44064000	0.54231800
H	-1.52663200	-2.38448500	1.61639700	C	-0.89974700	2.89992300	-1.81961100
H	-2.48016700	-3.74917500	2.24114600	C	-2.24813400	3.27767500	-2.45835800
H	-1.86621800	-3.75449700	0.57652500	H	-2.49769400	4.31518200	-2.23139100
B	0.64133600	2.44550600	1.20044600	H	-2.17445000	3.17256000	-3.54429800
H	1.56764700	2.56268300	0.47382800	H	-3.06855200	2.65259300	-2.10341300
B	-0.20979100	3.84359500	1.87869300	C	0.13750500	3.91470000	-2.33730400
H	0.17288100	4.93147700	1.60574700	H	-0.19213900	4.93513700	-2.13436100
B	-1.93181400	3.45576500	1.87962500	H	1.11844000	3.78309200	-1.87767100
H	-2.74102800	4.27924700	1.60991100	H	0.24261200	3.79668000	-3.41945900
B	-2.11488500	1.82245200	1.20579600	C	-0.49647800	1.51033000	-2.28658600
H	-3.00055900	1.51446700	0.48602900	C	0.83048200	0.99899700	-2.37101600
B	0.40940200	1.08514100	2.27690000	H	1.72541000	1.55174900	-2.12634700
H	1.24812400	0.24600200	2.29117500	C	0.78858500	-0.33009400	-2.86367100
B	0.61944300	2.70783300	2.94739700	H	1.63387100	-0.96834900	-3.07361400
H	1.62198000	3.01692500	3.51085600	C	-0.58335200	-0.65095800	-3.06687900
B	-0.99298000	3.32622900	3.37670700	H	-0.96046000	-1.58035800	-3.46883200
H	-1.16405300	4.09841200	4.26553300	C	-1.36230500	0.49143900	-2.73202000
B	-2.18698700	2.07472800	2.95493200	H	-2.43648900	0.55870100	-2.78302500

C	0.55663400	-2.19664300	-0.01659900	C	0.96447900	-4.52430500	1.83587900
C	-0.44192700	-2.85327700	-0.81025400	H	0.48906100	-4.00375600	2.67334000
H	-0.18141400	-3.65852900	-1.50343100	H	0.17987200	-5.05550700	1.28725400
C	2.73600900	-4.28121700	-0.64709400	H	1.65592800	-5.26762600	2.24755700
H	3.27762300	-3.62795800	-1.33910800	N	2.84475600	0.28905800	0.25006400
H	3.45887600	-4.98368900	-0.21829700	C	4.20300100	0.52438300	0.38201200
H	2.01902500	-4.86457100	-1.23464400	C	4.67434900	1.19216400	1.51979300
C	3.15858600	-2.42439500	1.76771700	C	6.04967100	1.40043500	1.60615400
H	3.95911000	-1.97086800	1.17726900	H	6.44873000	1.91363600	2.47546500
H	2.70553500	-1.64578600	2.38996500	C	6.40605100	0.29986400	-0.51307800
H	3.62374800	-3.15525800	2.43799400	H	7.08035300	-0.04333900	-1.29162100
C	-1.78507300	-2.43743000	-0.83388000	C	5.04017500	0.06683300	-0.64735900
C	-2.80583100	-3.16621900	-1.66507500	C	3.72851700	1.64935400	2.59243800
H	-2.47380300	-4.18483500	-1.87833900	H	3.17158500	0.80542300	3.01078500
H	-3.76003200	-3.20718400	-1.13286700	H	4.26996900	2.13887000	3.40394500
H	-2.98593800	-2.65837000	-2.61968100	H	2.98857700	2.35271100	2.19988700
C	-3.32614900	-1.22219700	0.57796500	C	4.46285200	-0.63815600	-1.84339100
C	-4.50283200	-0.69371200	0.02942200	H	5.25379600	-1.05590900	-2.46898500
C	-5.64231400	-0.61767500	0.83678900	H	3.79516300	-1.45070700	-1.53920000
H	-6.55269500	-0.19676600	0.41808000	H	3.87331100	0.05135400	-2.45840300
C	-5.63124400	-1.07800900	2.14347400	C	1.73431400	0.03146400	-0.00210400
H	-6.52403400	-1.00345700	2.75617300	C	6.90701300	0.96131400	0.60343500
C	-4.47617700	-1.65914300	2.65610200	H	7.97458600	1.13364600	0.69352600
H	-4.46678900	-2.04741100	3.67062100				
C	-3.32175700	-1.74961800	1.88553600	TS_{F-G};			
C	-4.60878500	-0.23754600	-1.40246400	Ta	-0.43102100	-0.63718700	-0.81829700
H	-5.58281600	-0.51250800	-1.81684900	Si	2.43807900	-3.16520500	-0.51433900
H	-4.51399100	0.85037000	-1.48791100	N	-1.82837900	-1.41184000	0.44646000
H	-3.83831000	-0.69199000	-2.02316900	C	-0.94688400	2.82570500	-0.87441000
C	-2.07981400	-2.40082400	2.43034400	C	-0.71734300	1.48894000	0.16138600
H	-1.21770100	-1.73051200	2.36106300	C	-0.98896400	2.53092600	-2.40377100
H	-2.21902200	-2.69434500	3.47366300	C	-2.33601200	2.94471700	-3.02597500
H	-1.81709300	-3.29341800	1.85270700	H	-2.44816700	4.02958600	-2.99817700
B	0.46291500	2.71399900	0.60549300	H	-2.36271400	2.62366500	-4.07099500
H	1.47578400	2.61755000	0.00163400	H	-3.18971700	2.50824000	-2.50553800
B	-0.42007400	4.24470100	0.67178000	C	0.10559300	3.30570000	-3.16200600
H	0.02950100	5.18126800	0.10199100	H	-0.10046100	4.37672000	-3.13491100
B	-2.13939000	3.86011500	0.59044300	H	1.09973400	3.14677600	-2.74081700
H	-2.88722000	4.53483400	-0.03430400	H	0.11428300	2.98425100	-4.20725700
B	-2.28419200	2.09431300	0.48005800	C	-0.78107300	1.04446200	-2.62641600
H	-3.07943500	1.57011400	-0.20980600	C	0.46494500	0.40089300	-2.86341500
B	0.05881400	1.77925800	2.03843000	H	1.43131700	0.88252300	-2.85916100
H	0.83608600	0.97949400	2.44559300	C	0.22423600	-0.96848600	-3.12417700
B	0.24040300	3.53867000	2.15006300	H	0.96911100	-1.71880800	-3.34255400
H	1.17608600	4.03264000	2.69697600	C	-1.17559400	-1.18258500	-3.02447500
B	-1.39231500	4.24854300	2.14821800	H	-1.68254400	-2.12789700	-3.16365600
H	-1.64374000	5.27150900	2.70097200	C	-1.79904700	0.06121400	-2.72567200
B	-2.56501300	2.91528500	2.02200700	H	-2.86004300	0.23516600	-2.63023500
H	-3.66068300	2.95750100	2.48098000	C	0.80961700	-2.25487300	-0.33260400
B	-1.64901000	1.40234200	1.96643400	C	-0.38712600	-3.00363700	-0.55394800
H	-2.05681100	0.36267600	2.34078000	H	-0.35302500	-3.87869900	-1.20553400
B	-1.08941400	2.72523900	3.00006600	C	2.08146500	-4.83277600	-1.33001400
H	-1.12075200	2.62678000	4.18508800	H	1.63214900	-4.71738700	-2.32294000

H	3.01756300	-5.38689600	-1.45686300	C	3.51210100	0.54726600	1.03695600
H	1.41156100	-5.45162100	-0.72463700	C	3.78865300	0.53399700	2.41679800
C	3.68171700	-2.25693000	-1.60856100	C	4.83959900	1.31999100	2.87931300
H	3.20020100	-1.75094200	-2.45195800	H	5.05957100	1.32987500	3.94281700
H	4.24625600	-1.50950500	-1.04518300	C	5.31916900	2.07001100	0.64545500
H	4.40076200	-2.97342200	-2.01991200	H	5.91623500	2.66483100	-0.04029000
C	-1.67964100	-2.63778600	-0.14447800	C	4.26676400	1.31161700	0.13198800
C	-2.87063800	-3.49399900	-0.47378900	C	2.93994800	-0.26413500	3.37010900
H	-2.55699000	-4.50030700	-0.75949800	H	2.57418900	-1.18670500	2.91261200
H	-3.52978100	-3.56326200	0.39615500	H	3.50409600	-0.51788200	4.27083700
H	-3.45756900	-3.06362900	-1.29269200	H	2.06016700	0.31258700	3.67539700
C	-2.80041100	-1.23499100	1.47166700	C	3.98218200	1.34144900	-1.34694300
C	-4.11596400	-0.84728700	1.20627700	H	4.89201800	1.14063900	-1.92041500
C	-4.98130400	-0.66844300	2.29010100	H	3.23534400	0.60039100	-1.63129500
H	-6.00297500	-0.35138800	2.09892100	H	3.61179600	2.32827700	-1.64420600
C	-4.55640800	-0.88893200	3.59073400	C	1.43190800	-0.41384300	0.02402300
H	-5.24198900	-0.74112900	4.41902700	C	5.60475000	2.08234500	2.00343800
C	-3.24655900	-1.29477900	3.83338400	H	6.42423600	2.68522000	2.38077100
H	-2.90823100	-1.45894300	4.85245100				
C	-2.35134000	-1.46807800	2.78415400	G;			
C	-4.62848900	-0.63471200	-0.19315200	Ta	-0.35687000	-0.23874400	-0.91284900
H	-5.29527400	-1.45176100	-0.49186100	Si	3.43565600	-1.03555600	-1.60657900
H	-5.19481800	0.29817400	-0.26196800	N	-1.16029700	-1.80992700	-0.00141800
H	-3.80728600	-0.58999200	-0.90759200	C	-2.05252900	2.62934800	0.06931000
C	-0.90609200	-1.80782100	3.03253000	C	-1.43877200	1.13429900	0.60998600
H	-0.26959800	-0.95861100	2.75703400	C	-1.86992300	2.94293100	-1.44185800
H	-0.73495400	-2.03745200	4.08696100	C	-3.21958600	3.13972800	-2.15799300
H	-0.57131000	-2.65618800	2.42772900	H	-3.70596800	4.04897900	-1.80186500
B	0.54887200	2.63141500	-0.08060600	H	-3.04501000	3.24333800	-3.23271600
H	1.49028600	2.29767500	-0.71366600	H	-3.90772600	2.30911100	-1.99498900
B	-0.19942800	4.23187700	-0.25556900	C	-1.05928700	4.23384600	-1.66312400
H	0.27528800	5.00114600	-1.02146200	H	-1.63331500	5.09927800	-1.32888500
B	-1.94925500	4.00504400	-0.15833700	H	-0.11312200	4.23218100	-1.12028900
H	-2.68322200	4.62110000	-0.85549000	H	-0.85249400	4.35196800	-2.73059500
B	-2.24708000	2.26383600	0.07608400	C	-1.13569900	1.78328900	-2.08935300
H	-3.13967500	1.69388300	-0.45230300	C	0.26659200	1.69812400	-2.29588000
B	0.17477800	2.03456800	1.52644500	H	1.00156000	2.40653200	-1.94327700
H	0.91251200	1.27327300	2.04883900	C	0.53275000	0.52699000	-3.04573400
B	0.51277500	3.75432000	1.28627700	H	1.50360500	0.20538700	-3.38566400
H	1.52371900	4.24660800	1.67328400	C	-0.69846800	-0.13792100	-3.28060100
B	-1.05405900	4.60371300	1.24503100	H	-0.82836300	-1.06460500	-3.82391800
H	-1.18062100	5.73035400	1.60547800	C	-1.73238100	0.64312500	-2.69341200
B	-2.33958000	3.38581100	1.44574200	H	-2.79047300	0.42784700	-2.72442000
H	-3.38981700	3.61570600	1.95378900	C	1.75903600	-1.10731200	-0.69281500
B	-1.55576600	1.81268500	1.62691500	C	0.95235700	-2.22522800	-1.11369600
H	-2.02259900	0.92023400	2.23240300	H	1.35701300	-2.76396400	-1.96528700
B	-0.81464300	3.24516600	2.35096700	C	3.98741300	0.73860800	-1.87849900
H	-0.76488300	3.36590500	3.53341100	H	4.47599400	1.12160000	-0.97916100
C	3.22277700	-3.48753600	1.16630600	H	4.71197300	0.78089800	-2.69844000
H	3.67233100	-2.57642200	1.57008200	H	3.16136100	1.41104600	-2.12523000
H	2.48286300	-3.85203400	1.88580400	C	4.76101200	-1.99766800	-0.68788300
H	4.01311100	-4.24137000	1.08210600	H	5.10109500	-1.47730400	0.20964600
N	2.46934000	-0.25542600	0.59696400	H	4.39876500	-2.98837500	-0.39380600

H	5.62311300	-2.14300100	-1.34865000
C	-0.38254000	-2.57789600	-0.87128300
C	-0.99984400	-3.74498100	-1.59728700
H	-0.27165300	-4.22642400	-2.25242400
H	-1.35521700	-4.48286300	-0.87201100
H	-1.86197100	-3.43586700	-2.19469900
C	-2.19419500	-2.46335900	0.73505800
C	-3.49990900	-2.56351400	0.24367800
C	-4.44825300	-3.22149200	1.03286000
H	-5.46876200	-3.29765900	0.66740100
C	-4.11120200	-3.76727600	2.26095800
H	-4.86520300	-4.26855400	2.85915900
C	-2.80451200	-3.66212500	2.72837100
H	-2.53671600	-4.07382200	3.69698500
C	-1.83347500	-3.01164000	1.97650100
C	-3.93723300	-1.99702000	-1.08143400
H	-4.30461900	-2.79154400	-1.74019100
H	-4.75117700	-1.27998100	-0.94065500
H	-3.12609100	-1.47989500	-1.59220600
C	-0.44265600	-2.80038900	2.49771000
H	-0.26655400	-1.72736000	2.63014400
H	-0.29771200	-3.29745100	3.45927300
H	0.31721400	-3.16618300	1.79985100
B	-0.64011800	2.59775000	1.03323200
H	0.39902100	2.83691200	0.52483300
B	-1.89918300	3.83481100	1.26217900
H	-1.67067100	4.94460000	0.91502000
B	-3.46041300	3.08040800	0.91812600
H	-4.30600100	3.66852900	0.33130900
B	-3.13881100	1.38371600	0.48196200
H	-3.72563000	0.82175500	-0.38117300
B	-0.90512600	1.33338400	2.23451900
H	0.00989300	0.68798200	2.61110300
B	-1.18441900	3.03018200	2.66124700
H	-0.45305200	3.61502300	3.39425900
B	-2.94314100	3.32224200	2.59163200
H	-3.48563500	4.12620000	3.28061700
B	-3.72793500	1.80042200	2.09862500
H	-4.82722300	1.48595200	2.42629700
B	-2.45432700	0.59366200	1.89124200
H	-2.63377300	-0.55761800	2.04638600
B	-2.32614600	1.77821600	3.19319400
H	-2.41702100	1.43839400	4.32958600
C	3.26314400	-1.91229100	-3.28043200
H	3.25524100	-3.00078000	-3.15730700
H	2.38066100	-1.63977100	-3.86690700
H	4.14492400	-1.67202300	-3.88473700
N	1.99392500	0.73296700	1.04124000
C	3.28584900	0.59095200	1.56012700
C	3.74582300	-0.56513100	2.21760500
C	5.03973200	-0.56081300	2.74422000
H	5.39884900	-1.45041200	3.25506400
C	5.38148400	1.70341200	2.01776400

H	6.00743900	2.58962900	1.95815300
C	4.08598700	1.75333800	1.51281400
C	2.86166900	-1.76724800	2.40126500
H	2.71770800	-2.32167200	1.46833600
H	3.28804000	-2.45162400	3.13879300
H	1.87229500	-1.46137900	2.74827600
C	3.51694200	3.02442600	0.94082900
H	4.23687200	3.84342400	1.01598900
H	3.23611700	2.90964300	-0.11112400
H	2.60400700	3.30096700	1.47711500
C	1.37813100	-0.04479500	0.25270400
C	5.86605800	0.54869900	2.62566600
H	6.87232600	0.52570200	3.03168800

TS_G;

Ta	-0.51812000	-0.05354100	-0.84675100
Si	4.01231000	-1.09197000	-1.20625600
N	-0.87294700	-1.83567500	-0.18831300
C	-2.65382700	2.33791700	0.22252900
C	-2.06964000	0.77964400	0.52888900
C	-2.29500300	2.95225600	-1.16802100
C	-3.54521300	3.17175600	-2.03914500
H	-4.19770000	3.91937300	-1.58495700
H	-3.23610000	3.53705900	-3.02230900
H	-4.12752200	2.26030300	-2.17763400
C	-1.61550800	4.32398100	-1.00547600
H	-2.32288400	5.04975300	-0.60101000
H	-0.75423500	4.28836700	-0.33579100
H	-1.28287800	4.67936600	-1.98457200
C	-1.34600300	2.00945300	-1.89265000
C	0.07015200	2.11243000	-1.92615800
H	0.66719700	2.83347900	-1.38878400
C	0.57664500	1.06775700	-2.72921900
H	1.62070900	0.86489600	-2.92081200
C	-0.52300600	0.30727000	-3.21479500
H	-0.46938700	-0.54400700	-3.87784100
C	-1.70967000	0.89747700	-2.70635500
H	-2.71687600	0.54821600	-2.88986000
C	2.16639300	-1.05492800	-0.72123100
C	1.37221500	-1.98851400	-1.35132400
H	1.85749900	-2.64368800	-2.07264900
C	4.18090100	-2.19452500	-2.73525200
H	3.54396800	-1.86429800	-3.56294100
H	5.21913700	-2.14484900	-3.08145000
H	3.96105800	-3.24763300	-2.53223200
C	4.62993100	0.61241600	-1.71207600
H	3.92078500	1.13470200	-2.36334100
H	4.83233900	1.24628300	-0.84639400
H	5.56433300	0.50061000	-2.27286600
C	-0.09509500	-2.09828900	-1.37641800
C	-0.68609000	-3.03155100	-2.40899100
H	-0.03746100	-3.10122500	-3.28678000
H	-0.81798900	-4.04106900	-2.00116600

H	-1.66560200	-2.68259100	-2.74492600	H	2.94644600	2.88336800	-0.89275400
C	-1.51230800	-2.89347900	0.51100700	C	3.00518700	-0.94062600	2.80009100
C	-2.81375100	-3.29291800	0.16398400	H	3.55558400	-1.42437200	3.61059000
C	-3.38020700	-4.36870700	0.85153700	H	1.99123500	-0.72622100	3.15263900
H	-4.39041200	-4.67731700	0.59630500	H	2.91872700	-1.65601000	1.97716100
C	-2.68815000	-5.02917000	1.85546400	C	1.45015800	0.00999000	0.03992900
H	-3.15062500	-5.85787600	2.38207900	C	5.53216300	1.89350800	2.56991900
C	-1.40584600	-4.61326900	2.19442600	H	6.47943700	2.17207300	3.01997400
H	-0.86231200	-5.11487200	2.99004900				
C	-0.80248000	-3.54983100	1.52911400	G';			
C	-3.64532500	-2.59315700	-0.88091500	Ta	0.28347100	0.19640000	-0.92150000
H	-3.77923700	-3.22485900	-1.76591700	Si	-4.60694400	-0.33246200	-0.67359200
H	-4.63746500	-2.36599100	-0.48075900	N	-0.21162700	1.94501800	-0.16425100
H	-3.19824900	-1.65019500	-1.19658000	C	3.29988200	-1.20950400	-0.01395300
C	0.57840500	-3.09039800	1.88962200	C	1.96976400	-0.30195200	0.58725300
H	0.60352800	-2.00225600	1.96652400	C	3.27804500	-1.57990900	-1.53158900
H	0.90607100	-3.51917900	2.83959600	C	4.50606500	-1.01964000	-2.27434900
H	1.30606800	-3.36725700	1.11886100	H	5.41727200	-1.51026100	-1.92847200
B	-1.36037900	2.13725400	1.32056100	H	4.39542800	-1.21564300	-3.34461000
H	-0.27464700	2.46865900	0.98474800	H	4.62883400	0.05468800	-2.13004500
B	-2.68072100	3.26995400	1.65670300	C	3.29694200	-3.10652200	-1.73175900
H	-2.46729000	4.43193000	1.58162700	H	4.24913900	-3.51835800	-1.39445600
B	-4.15827500	2.57191400	0.98219600	H	2.50311100	-3.61163200	-1.17883100
H	-4.96145000	3.25492200	0.44014100	H	3.18290500	-3.33373200	-2.79528100
B	-3.73485700	1.00423600	0.24826900	C	2.02389800	-1.00949700	-2.17611700
H	-4.19974900	0.61303200	-0.76909500	C	0.82763500	-1.71425600	-2.42710600
B	-1.68683200	0.63202800	2.19088100	H	0.62293500	-2.72730200	-2.12102200
H	-0.76251400	-0.05643900	2.47824900	C	-0.09319200	-0.84982000	-3.06910000
B	-2.07925400	2.19586000	2.92983400	H	-1.09525300	-1.10183500	-3.38526200
H	-1.45303800	2.62604800	3.84327300	C	0.55924200	0.39779800	-3.27899400
B	-3.83230700	2.46191800	2.72241100	H	0.14925400	1.25074900	-3.79668400
H	-4.47561200	3.09193000	3.49893100	C	1.85575500	0.30936200	-2.71169900
B	-4.49971600	1.06473900	1.84490100	H	2.60130400	1.09238200	-2.71142000
H	-5.61475400	0.67519400	1.97967800	C	-2.85699300	0.30356900	-0.91289300
B	-3.16972100	-0.05350800	1.53763000	C	-2.45937300	1.54058500	-1.35717500
H	-3.29552400	-1.21651400	1.40771000	H	-3.20106400	2.24681500	-1.74273700
B	-3.21957300	0.83540500	3.06315400	C	-5.75276500	0.72002600	-1.73272800
H	-3.41835400	0.26956400	4.08929400	H	-5.45100400	0.70462000	-2.78485200
C	5.12949200	-1.82835800	0.11454000	H	-6.78152000	0.35031100	-1.67330200
H	5.27510200	-1.14886200	0.95659200	H	-5.75837200	1.76275100	-1.39819400
H	4.72724800	-2.77264100	0.49536100	C	-4.62528700	-2.13363400	-1.21776600
H	6.11096200	-2.03791200	-0.32524100	H	-4.27784000	-2.24730100	-2.24991700
N	1.83348400	0.91173300	0.85768600	H	-3.97358500	-2.72951900	-0.56870600
C	3.10507700	1.15764800	1.39727700	H	-5.63226800	-2.55837900	-1.15287900
C	3.69764100	2.39485300	1.07195600	C	-1.03994700	1.96245700	-1.36762900
C	4.91890600	2.73454700	1.64689800	C	-0.76502800	3.14725600	-2.27953200
H	5.38462200	3.67889900	1.37798800	H	-1.26709600	3.03625800	-3.24683600
C	4.90543900	0.70868700	2.93347400	H	-1.11758300	4.08380100	-1.82662000
H	5.36116400	0.06182800	3.67857100	H	0.30574900	3.26780800	-2.46755600
C	3.69049100	0.32285300	2.36395700	C	-0.06774000	3.11218000	0.63773000
C	3.00282300	3.32016300	0.11108500	C	1.11763800	3.87082300	0.58457400
H	1.97547000	3.50565900	0.44519500	C	1.24890600	4.98670200	1.41408600
H	3.52660600	4.27598300	0.03357800	H	2.17618200	5.55247700	1.37947000

C	0.22986200	5.37948900	2.26547700
H	0.35408100	6.24224200	2.91203800
C	-0.96123300	4.66671900	2.26426700
H	-1.78225600	4.98143600	2.90288600
C	-1.13673600	3.55052400	1.44881500
C	2.26265300	3.56744200	-0.34305800
H	2.47230400	4.43626800	-0.97605400
H	3.16983600	3.33965700	0.22278700
H	2.05536600	2.71619600	-0.98833800
C	-2.49058000	2.89650900	1.42012700
H	-3.02286100	3.06762100	2.35997300
H	-3.10326600	3.31937900	0.61361300
H	-2.43260100	1.82688100	1.24218700
B	2.15704700	-1.96107200	1.00399600
H	1.40242200	-2.75002500	0.54498900
B	3.89879000	-2.27647000	1.17713800
H	4.32408200	-3.32749500	0.83252900
B	4.74403400	-0.77689300	0.78769700
H	5.75472100	-0.78246600	0.16922100
B	3.50729900	0.42972900	0.37998900
H	3.66992600	1.19626200	-0.50457700
B	1.70702500	-0.76316100	2.20758000
H	0.60143800	-0.77520600	2.61355200
B	2.90660300	-1.99674200	2.60917600
H	2.65247300	-2.88137200	3.36195800
B	4.51409400	-1.24301700	2.47646000
H	5.44058800	-1.59068800	3.13670900
B	4.28101400	0.45078600	1.97160700
H	5.02727400	1.33137800	2.25939400
B	2.53796800	0.73259300	1.82092900
H	2.00610900	1.78222700	1.94955700
B	3.15425200	-0.30881300	3.11797600
H	3.08000300	0.02752400	4.25644100
C	-5.12249300	-0.23420000	1.13273100
H	-4.53935200	-0.93472600	1.73922400
H	-4.98071500	0.77365700	1.53635700
H	-6.17992800	-0.49685200	1.24498000
N	-1.03544600	-1.22853700	0.13913400
C	-1.52687600	-2.12105400	1.13857700
C	-1.62319000	-3.48254400	0.80920900
C	-2.12243700	-4.36381500	1.76495700
H	-2.20924500	-5.41762000	1.51651500
C	-2.38467800	-2.56507700	3.33284700
H	-2.67008700	-2.20711600	4.31809900
C	-1.90163900	-1.64248100	2.40098700
C	-1.19888800	-3.98949800	-0.54271800
H	-0.10580900	-4.01322700	-0.61294300
H	-1.56539500	-5.00509400	-0.70789900
H	-1.57435000	-3.35532800	-1.35133300
C	-1.82248200	-0.18956400	2.78536200
H	-1.42889200	-0.08678500	3.79992400
H	-1.17392300	0.38479400	2.12386400
H	-2.81761500	0.26541900	2.76873600

C	-1.64515400	-0.39306100	-0.61191900
C	-2.50087400	-3.91176700	3.02380400
H	-2.88036600	-4.61031000	3.76234400

TS_{G-5};

Ta	0.26721100	0.22180300	-0.88198300
Si	-4.53366900	-0.55034500	-0.70036400
N	-0.35094500	1.95506300	-0.21039100
C	3.35815400	-1.06020000	-0.07623300
C	1.97246000	-0.28454500	0.56486700
C	3.33470800	-1.40005600	-1.60047000
C	4.52215400	-0.75859300	-2.34304400
H	5.46183700	-1.21062000	-2.02142800
H	4.40733400	-0.93229100	-3.41665700
H	4.59183200	0.31668300	-2.17122000
C	3.42857100	-2.91840900	-1.83737000
H	4.40406400	-3.28957500	-1.51993000
H	2.66724500	-3.47639800	-1.29015500
H	3.31431500	-3.12543300	-2.90492400
C	2.04314000	-0.87894400	-2.21061000
C	0.87329700	-1.63189000	-2.44358900
H	0.71986100	-2.65771800	-2.15078500
C	-0.10358300	-0.79529600	-3.03823800
H	-1.10391000	-1.08306900	-3.32734000
C	0.49075200	0.48309200	-3.24329500
H	0.02784200	1.32841100	-3.72879500
C	1.80372300	0.44154500	-2.71252400
H	2.51294000	1.25733300	-2.71587700
C	-2.82031800	0.15106600	-0.95173700
C	-2.47767300	1.39647500	-1.52510600
H	-3.20140200	1.89966500	-2.17229400
C	-5.72057600	0.39227300	-1.82058600
H	-5.41584000	0.32833200	-2.87041600
H	-6.73354200	-0.01548800	-1.74194500
H	-5.76988100	1.45169200	-1.54727300
C	-4.48657000	-2.37925700	-1.14633000
H	-4.14092100	-2.53435800	-2.17368600
H	-3.80566800	-2.91227900	-0.47285800
H	-5.47492700	-2.84037500	-1.04854800
C	-1.23430100	2.05740000	-1.37645400
C	-0.97304200	3.28525600	-2.22498400
H	-1.58397900	3.28615200	-3.13194600
H	-1.19281400	4.20195800	-1.66448700
H	0.07784000	3.34639600	-2.52638100
C	-0.27988900	3.08828300	0.65500300
C	0.86733200	3.90210300	0.67078500
C	0.92568200	4.96947400	1.56978000
H	1.82272300	5.58246200	1.59127900
C	-0.13050000	5.25680500	2.41851600
H	-0.06337400	6.08363900	3.11828800
C	-1.28517100	4.48887300	2.34766800
H	-2.13285400	4.72387600	2.98546400
C	-1.38864900	3.41700900	1.46325800

C	2.03952200	3.70942200	-0.25286800	5;			
H	2.24321200	4.63763700	-0.79660900	Ta	0.26061900	0.15094400	-0.51203600
H	2.93930200	3.44885400	0.31063400	Si	-3.82163400	0.72687300	2.14340100
H	1.86493000	2.91949200	-0.98173000	N	-1.63187000	-0.45880600	-0.52718900
C	-2.70019800	2.68861600	1.36399900	N	0.73051500	1.84495200	0.64140200
H	-3.27055400	2.79527800	2.29081300	C	2.33780200	-2.52442700	0.11879600
H	-3.30802400	3.10093500	0.54876600	C	1.16421100	-1.47036500	0.74532000
H	-2.57323400	1.63019900	1.15093400	C	2.75611100	-2.27258500	-1.36515100
B	2.29770800	-1.92370100	0.95081900	C	4.25934600	-1.96361700	-1.48642000
H	1.59966200	-2.76153000	0.49157000	H	4.84946600	-2.83843000	-1.20805200
B	4.06492000	-2.09175700	1.08318500	H	4.48921000	-1.71097500	-2.52504300
H	4.57028000	-3.09674000	0.71032300	H	4.57118900	-1.13308700	-0.85202200
B	4.77693900	-0.52026800	0.70796000	C	2.48444500	-3.51080800	-2.23942000
H	5.77199400	-0.43178500	0.07116400	H	3.13608800	-4.33377400	-1.94036400
B	3.43854300	0.58357900	0.34360500	H	1.45342800	-3.85955800	-2.16738000
H	3.51245900	1.37353000	-0.53226200	H	2.69635800	-3.26716600	-3.28399200
B	1.77577000	-0.78635300	2.18410900	C	1.95728500	-1.09429600	-1.90210600
H	0.68424200	-0.89510100	2.61019800	C	0.68186200	-1.17242400	-2.52691300
B	3.08271800	-1.91943200	2.54024300	H	0.09428600	-2.06855000	-2.66876900
H	2.92037300	-2.83365600	3.28240400	C	0.28760400	0.13065800	-2.91088500
B	4.61780100	-1.03091300	2.39092800	H	-0.62735600	0.37820400	-3.43196900
H	5.58241300	-1.30941000	3.02858100	C	1.31589100	1.02961500	-2.51662400
B	4.23389700	0.64603500	1.92030200	H	1.35158100	2.09182200	-2.70252600
H	4.90795900	1.58258000	2.20923800	C	2.34141000	0.27194500	-1.89415200
B	2.46991600	0.78056800	1.80475100	H	3.25124100	0.68337600	-1.48101900
H	1.84962700	1.77857400	1.95532100	C	-2.81260700	-0.75175200	-1.26894700
B	3.19704400	-0.22433800	3.07329500	C	-3.31828200	-2.05831800	-1.30088100
H	3.11630600	0.08728700	4.21804800	C	-4.48113700	-2.30253900	-2.03550000
C	-5.08448200	-0.39465800	1.09403600	H	-4.88474600	-3.31101600	-2.05259500
H	-4.46846800	-1.03264700	1.73664200	C	-4.61593700	0.00571400	-2.67399800
H	-5.00246900	0.63619500	1.45357100	H	-5.12339100	0.81018300	-3.19876000
H	-6.12610200	-0.71285400	1.21145100	C	-3.46157700	0.29739900	-1.94878200
N	-0.92770300	-1.25993700	0.15566100	C	-2.66245000	-3.18481700	-0.55143900
C	-1.35077800	-2.18259700	1.15494100	H	-2.13883300	-2.82960800	0.33609600
C	-1.38645500	-3.54725400	0.82568300	H	-3.40774300	-3.92099700	-0.24009400
C	-1.82963300	-4.45498400	1.78484000	H	-1.93244400	-3.70301000	-1.18117200
H	-1.86664500	-5.51145400	1.53480600	C	-2.94362300	1.71070900	-1.90412300
C	-2.17523200	-2.67321700	3.35548300	H	-3.63539100	2.39007500	-2.40669000
H	-2.47417300	-2.33128800	4.34255400	H	-2.80218700	2.06058300	-0.87808100
C	-1.74655000	-1.72717200	2.42111400	H	-1.97534600	1.79608100	-2.40846300
C	-0.96879900	-4.02895900	-0.53746800	C	-1.44517600	0.34125900	0.54910300
H	0.12232700	-4.00748000	-0.63433100	C	-2.05683200	1.00805500	1.56131700
H	-1.29683800	-5.05789100	-0.70196500	C	-1.18901200	1.96332500	2.18459200
H	-1.39011000	-3.40447100	-1.33086800	H	-1.56443200	2.48056400	3.06279200
C	-1.73870100	-0.27215500	2.80859800	C	-3.97259300	1.39474000	3.89979800
H	-1.34348300	-0.15169200	3.82075600	H	-3.85112300	2.48251500	3.93395500
H	-1.12648300	0.33623600	2.14253700	H	-4.96011100	1.16113600	4.31148800
H	-2.75514100	0.13324500	2.79901100	H	-3.22025900	0.95028700	4.55919300
C	-1.62014300	-0.45301400	-0.57988600	C	-5.07426800	1.61335000	1.04517100
C	-2.22072200	-4.02456500	3.04713900	H	-4.83154400	2.67578000	0.93838600
H	-2.55806500	-4.74234200	3.78780200	H	-5.10836700	1.16797800	0.04598200
				H	-6.07887200	1.54043200	1.47622100
				C	0.04122800	2.38647100	1.73894000

C	0.66055400	3.56428600	2.46489100
H	1.65307100	3.33862300	2.86237300
H	0.76414500	4.44216700	1.81874900
H	0.02683600	3.84582600	3.30703700
C	1.76190200	2.73809100	0.14302900
C	1.37246900	3.71913600	-0.79316500
C	2.34544500	4.52112200	-1.38418100
H	2.04483800	5.26496800	-2.11711200
C	3.68638200	4.38666900	-1.03857000
H	4.43996100	5.00540000	-1.51511800
C	4.04134000	3.49420100	-0.03996300
H	5.07484900	3.43445500	0.29155100
C	3.08924600	2.68602100	0.59258500
C	-0.07894700	3.91655900	-1.14961300
H	-0.22582200	4.88300800	-1.63755300
H	-0.43947300	3.14352200	-1.83598800
H	-0.72127800	3.86922000	-0.26587700
C	3.51769300	1.90518000	1.80760900
H	2.72832000	1.25817400	2.18463000
H	4.40372100	1.29685000	1.61040300
H	3.78666000	2.60882600	2.60371200
B	0.76118800	-3.10145800	0.40077200
H	0.08204600	-3.32815500	-0.53605400
B	2.18342900	-4.08113400	0.80400000
H	2.43395300	-5.02061700	0.12680200
B	3.45159400	-2.97346400	1.33333600
H	4.58249900	-3.14181200	1.02323400
B	2.78843100	-1.33319200	1.24381600
H	3.42041600	-0.43203700	0.82872400
B	0.19802000	-2.31279600	1.87802700
H	-0.94311900	-2.01022800	1.97062200
B	0.83263600	-3.96329200	1.94101400
H	0.11446700	-4.89049500	2.13607900
B	2.51237700	-3.87193900	2.53149800
H	3.01530600	-4.74768100	3.15915000
B	2.90347700	-2.15332800	2.80438700
H	3.68378000	-1.77791000	3.61915400
B	1.46091000	-1.20441700	2.40447700
H	1.17517000	-0.14224300	2.84789100
B	1.28407100	-2.78112600	3.19544400
H	0.88583800	-2.86008300	4.31270400
C	-4.19301100	-1.11818300	2.12997300
H	-4.27084000	-1.49274100	1.10494500
H	-3.40682200	-1.68345200	2.64058900
H	-5.14354600	-1.32717700	2.63241100
C	-5.12654000	-1.28579600	-2.72305700
H	-6.03060700	-1.49415900	-3.28591600

NMR Spectra of New Compounds

YJT-5-183-solid-H-C6D6.1.fid

YJT-5-183-solid-H-C6D6

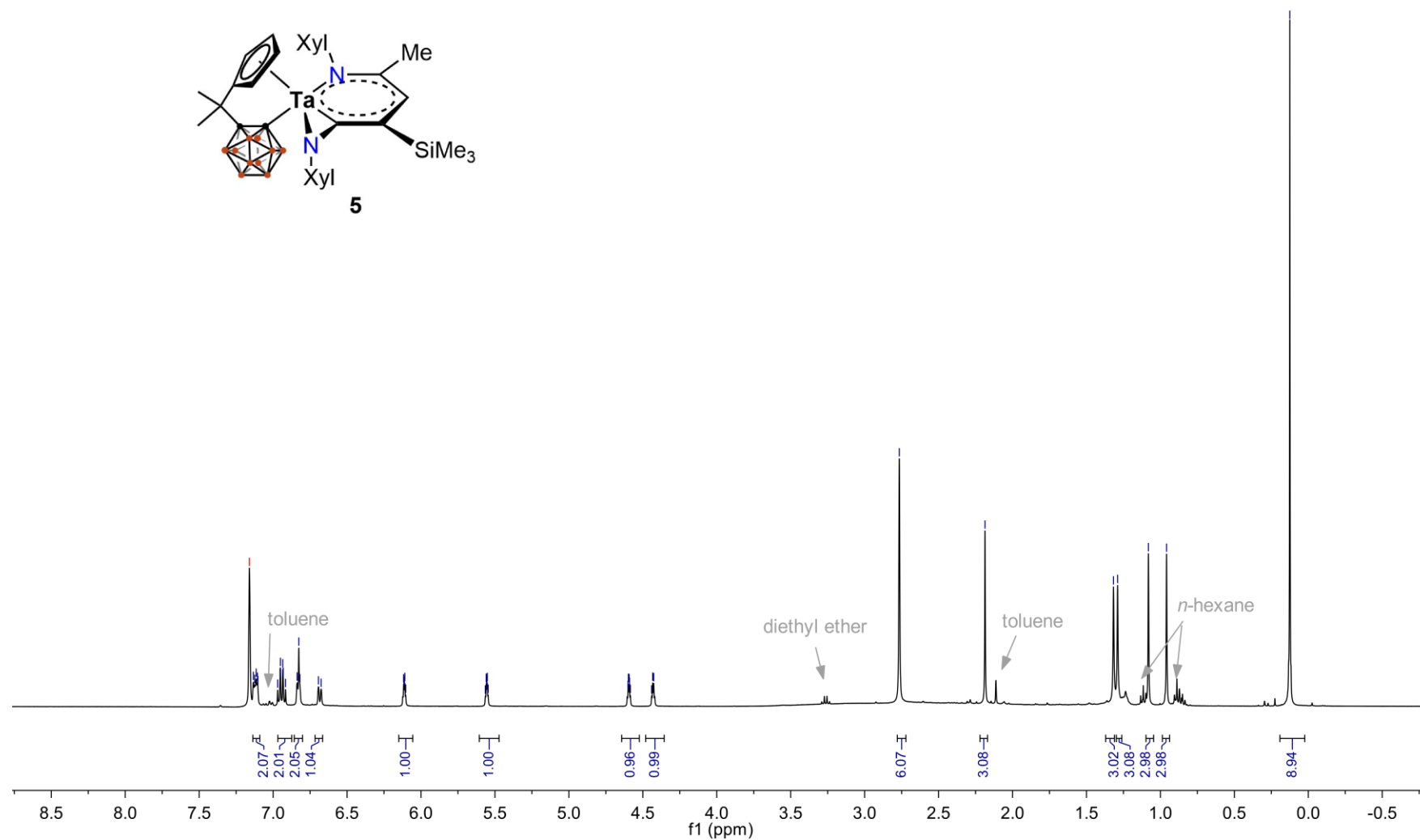
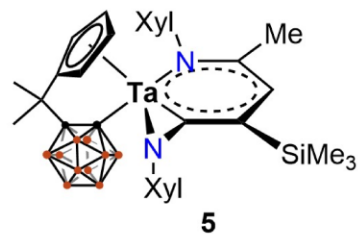


Fig. S4 ^1H NMR spectrum of compound 5 in C_6D_6 .

YJT-5-183-solid-C-C6D6.1.fid
 YJT-5-183-solid-C-C6D6

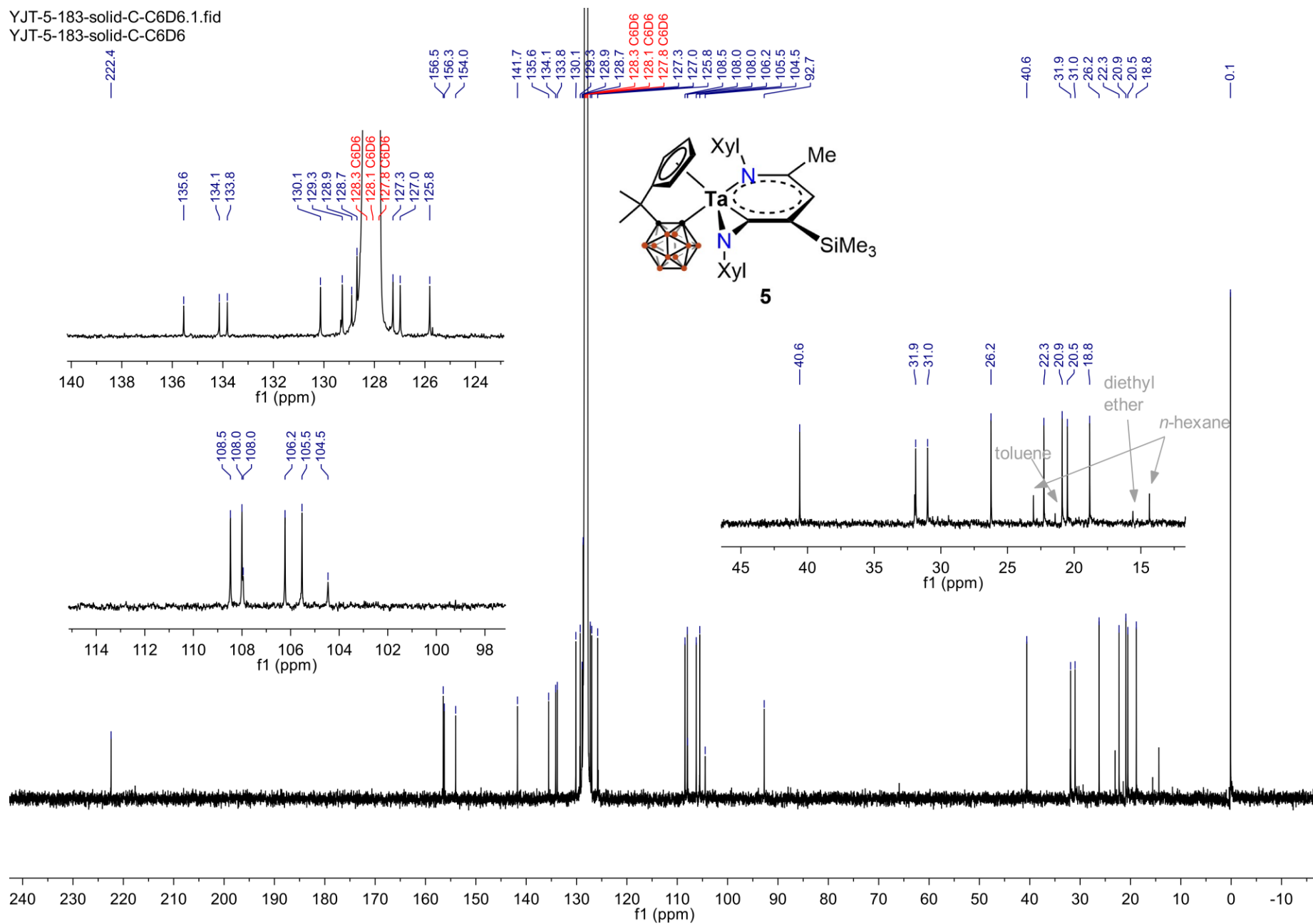


Fig. S5 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound 5 in C_6D_6 .

YJT-5-183-solid-B(de)-C6D6.1.fid
YJT-5-183-solid-B(de)-C6D6

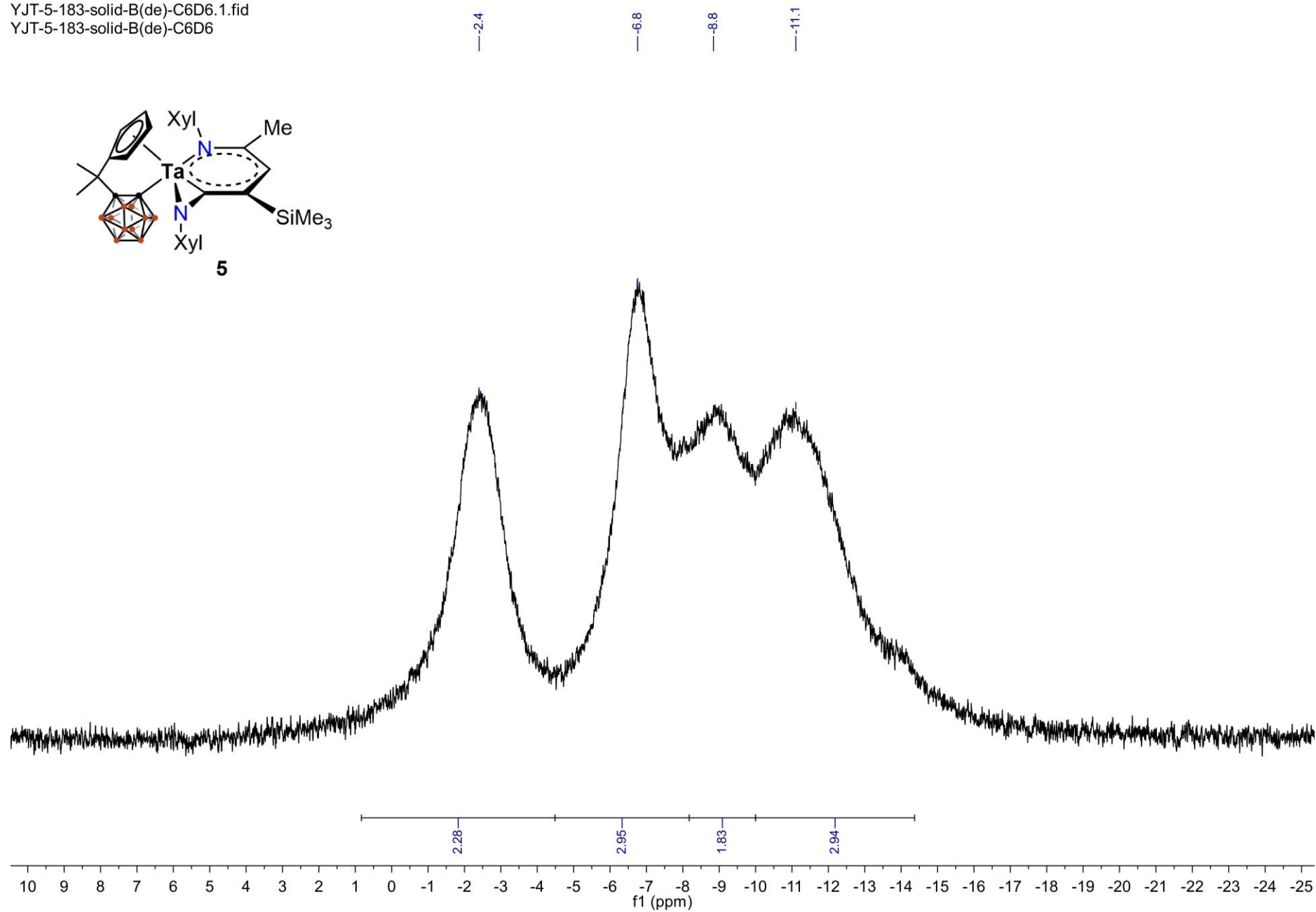


Fig. S6 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **5** in C_6D_6 .

YJT-5-183-solid-B(c)-C6D6.1.fid
YJT-5-183-solid-B(c)-C6D6

— -1.8
— -2.6
— -6.1
— -7.3
— -8.3
— -9.8
— -11.2

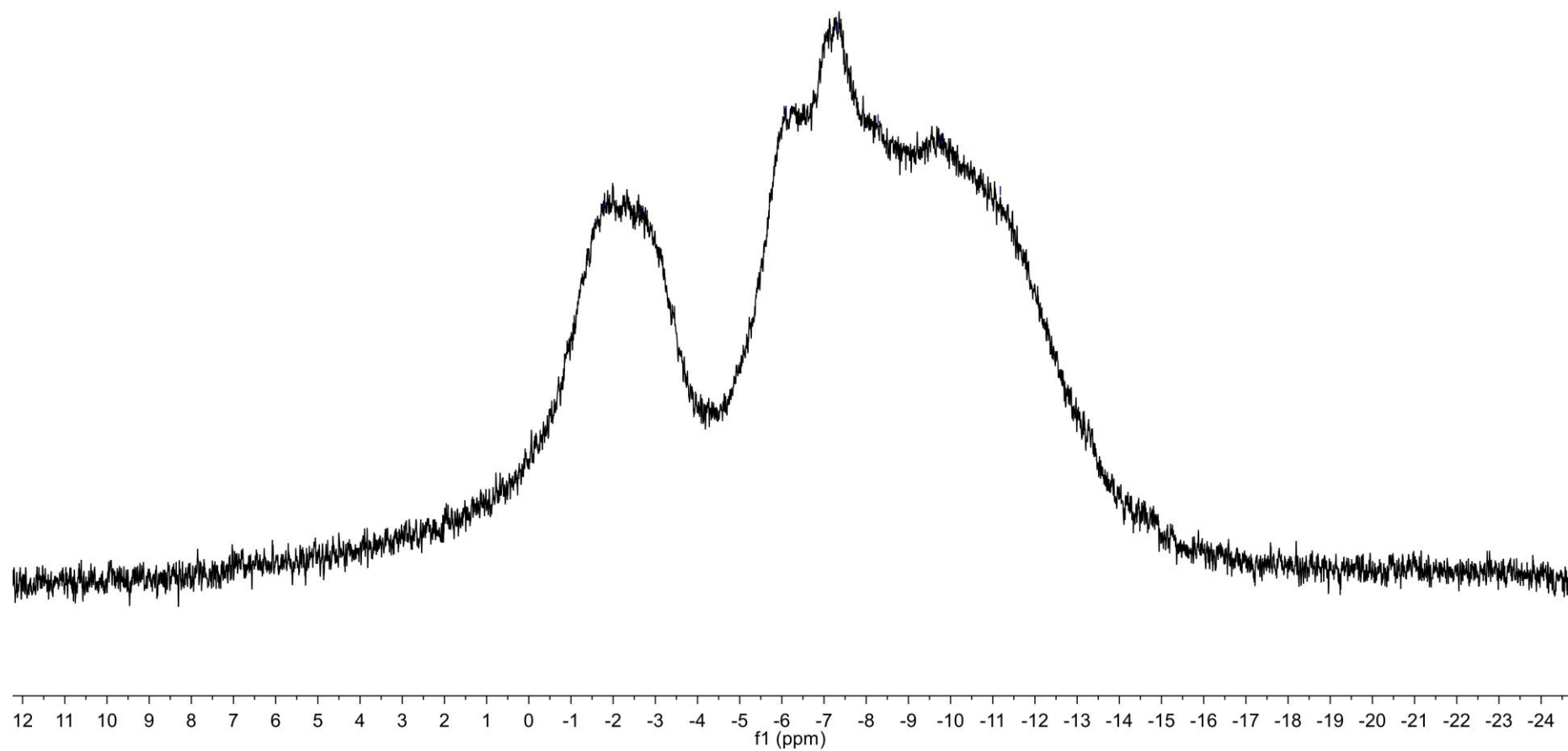
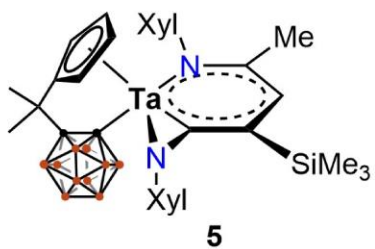


Fig. S7 ¹¹B NMR spectrum of compound 5 in C₆D₆.

YJT-7-115-solid-1-H-C6D6 6.1.fid

YJT-7-115-solid-1-H-C6D6 6

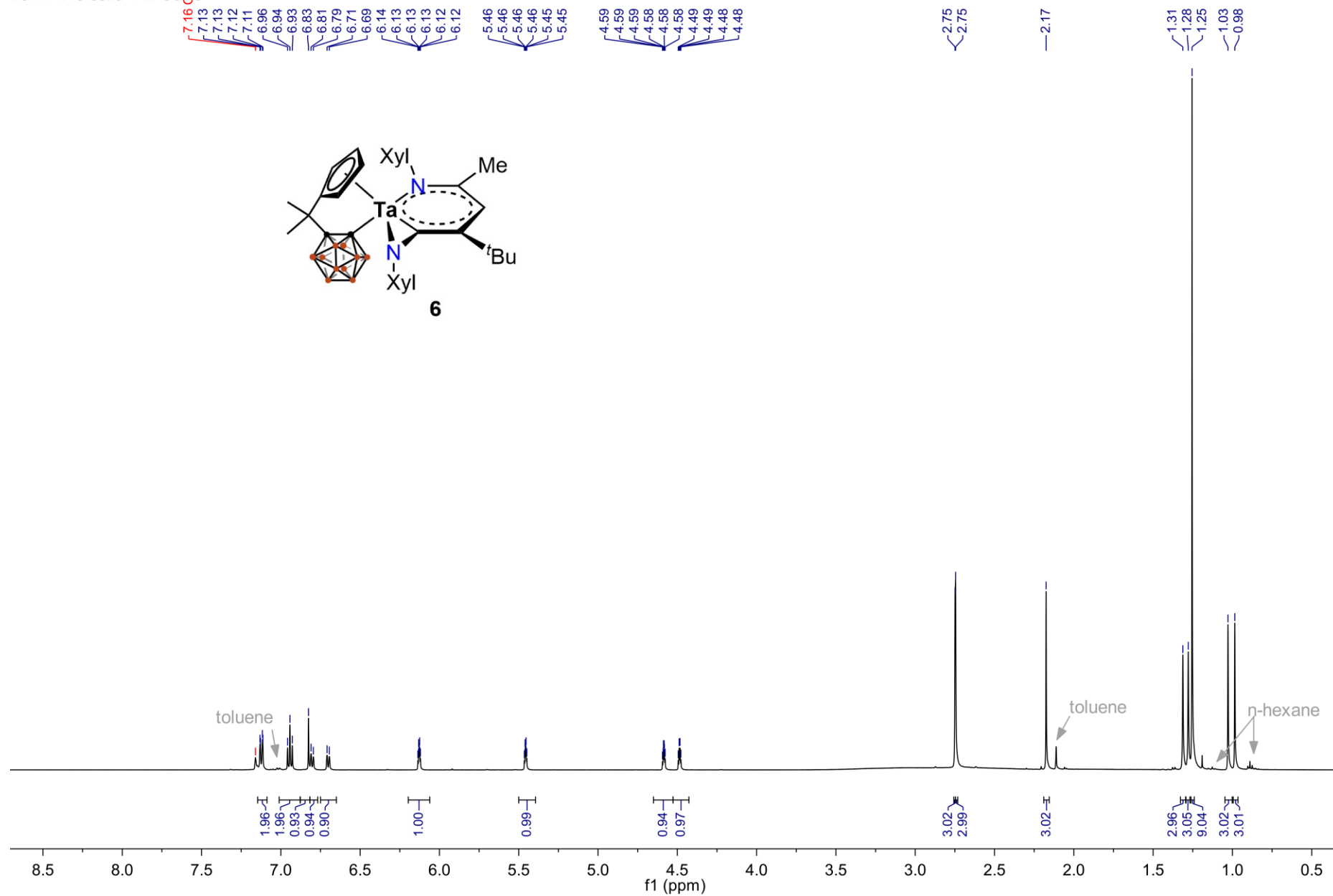


Fig. S8 ^1H NMR spectrum of compound **6** in C_6D_6 .

YJT-7-115-solid-1-C-C6D6.1.fid
YJT-7-115-solid-1-C-C6D6

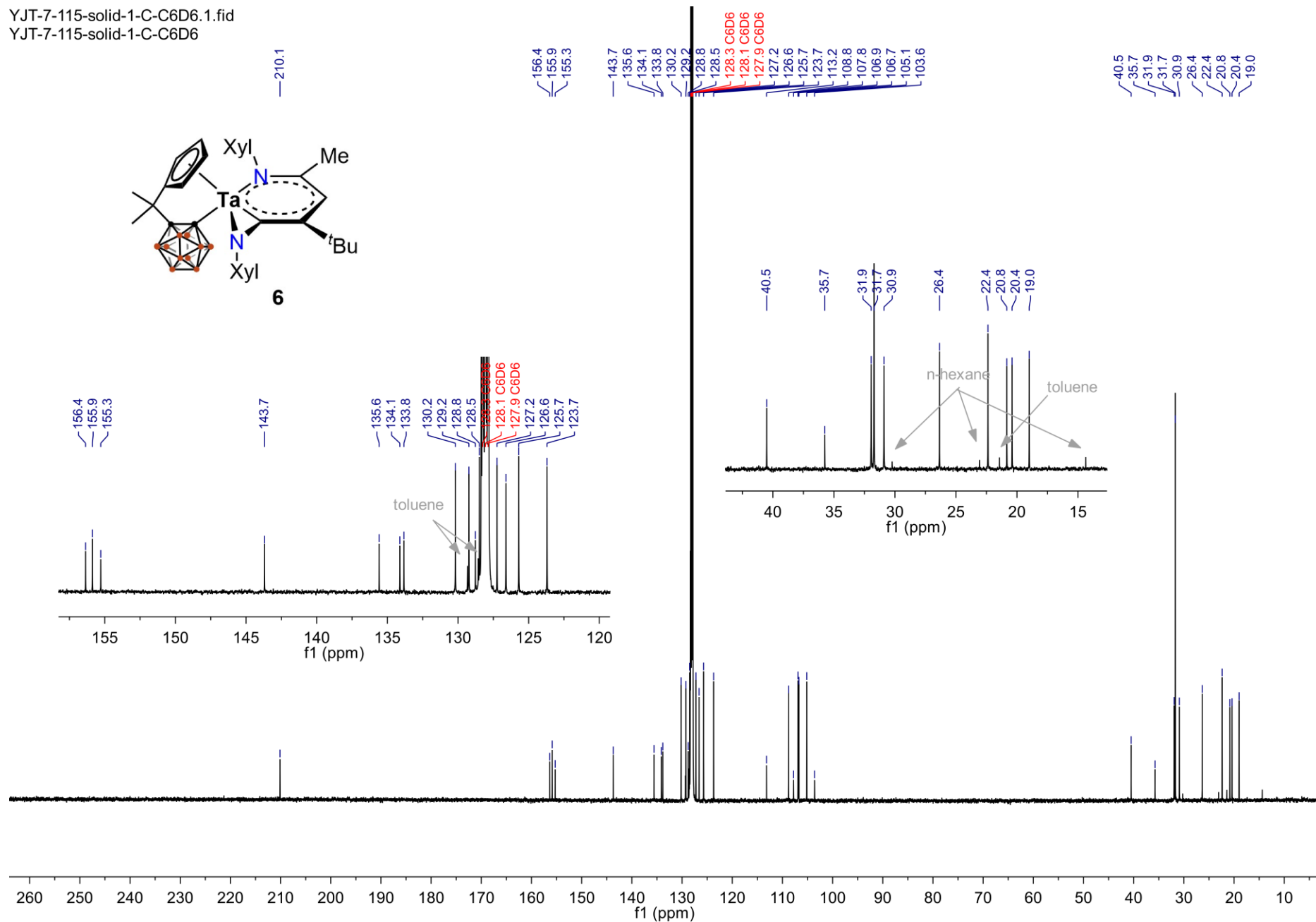


Fig. S9 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **6** in C_6D_6 .

YJT-7-115-solid-1-B(de)-C6D6.1.fid
YJT-7-115-solid-1-B(de)-C6D6

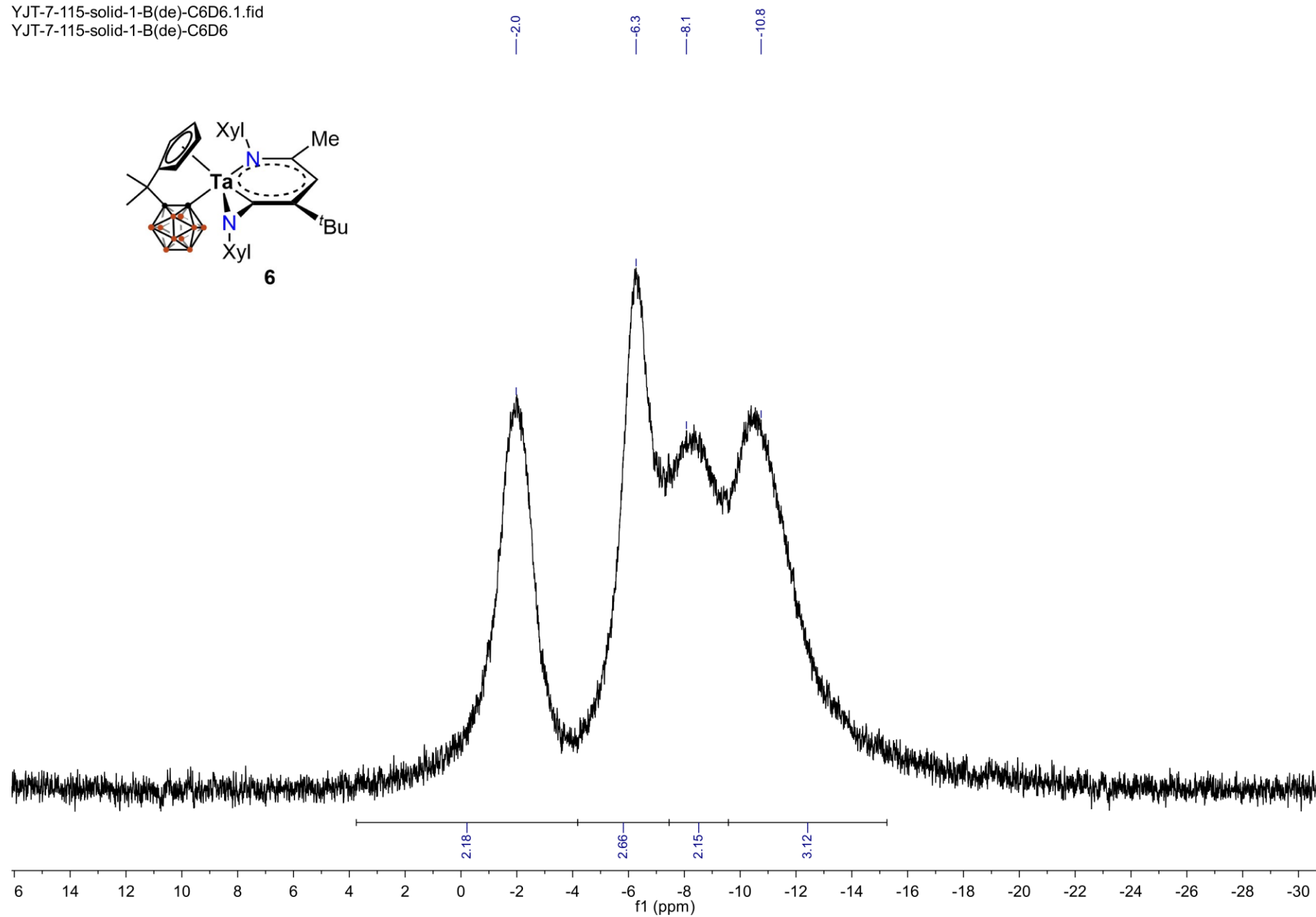


Fig. S10 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **6** in C_6D_6 .

YJT-7-115-solid-1-B(c)-C6D6.2.fid
YJT-7-115-solid-1-B(c)-C6D6

— -1.5
— -2.4

— -5.7
— -6.8
— -8.0
— -9.6
— -10.9

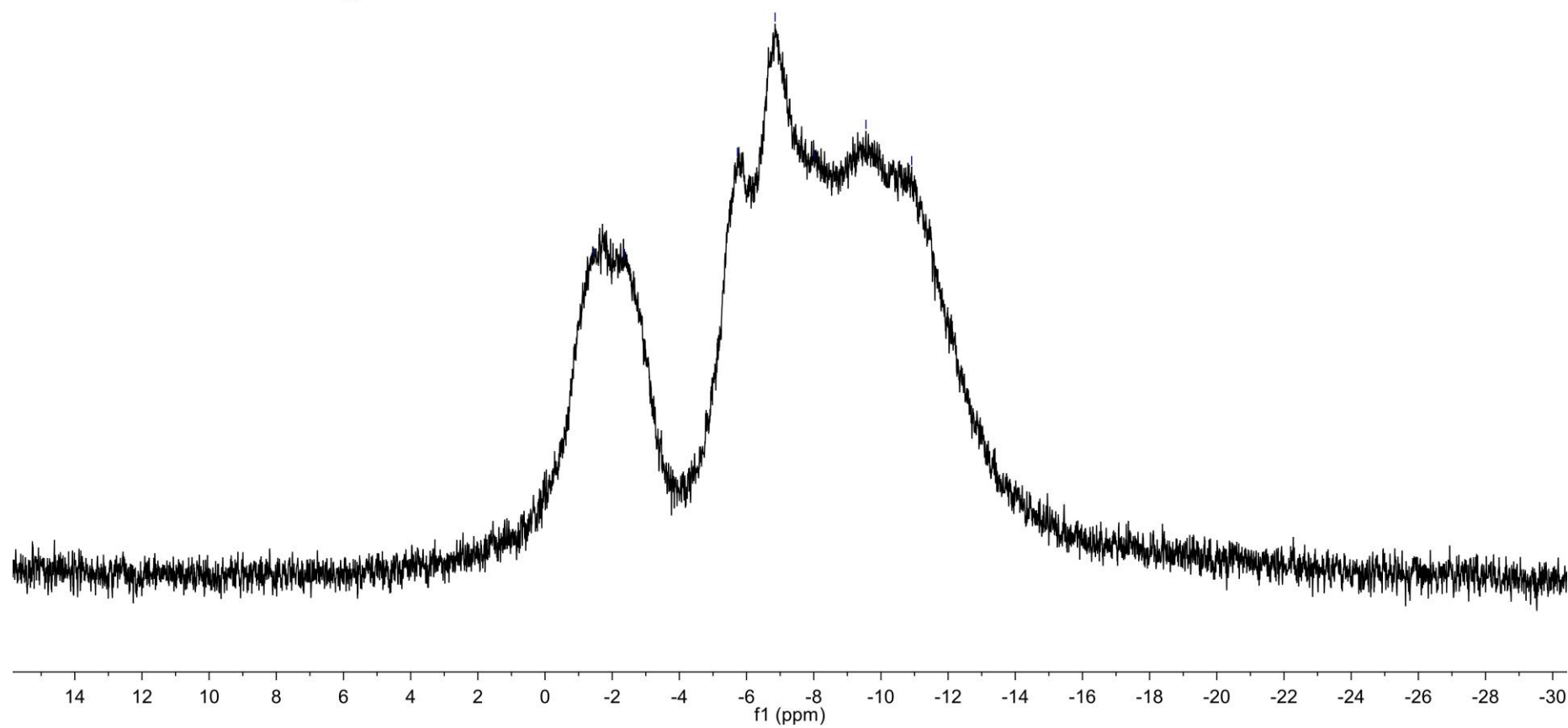
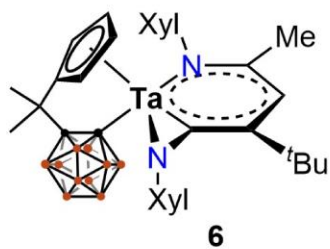


Fig. S11 ^{11}B NMR spectrum of compound **6** in C_6D_6 .

YJT-7-114-solid-H-C6D6.2.fid

YJT-7-114-solid-H-C6D6

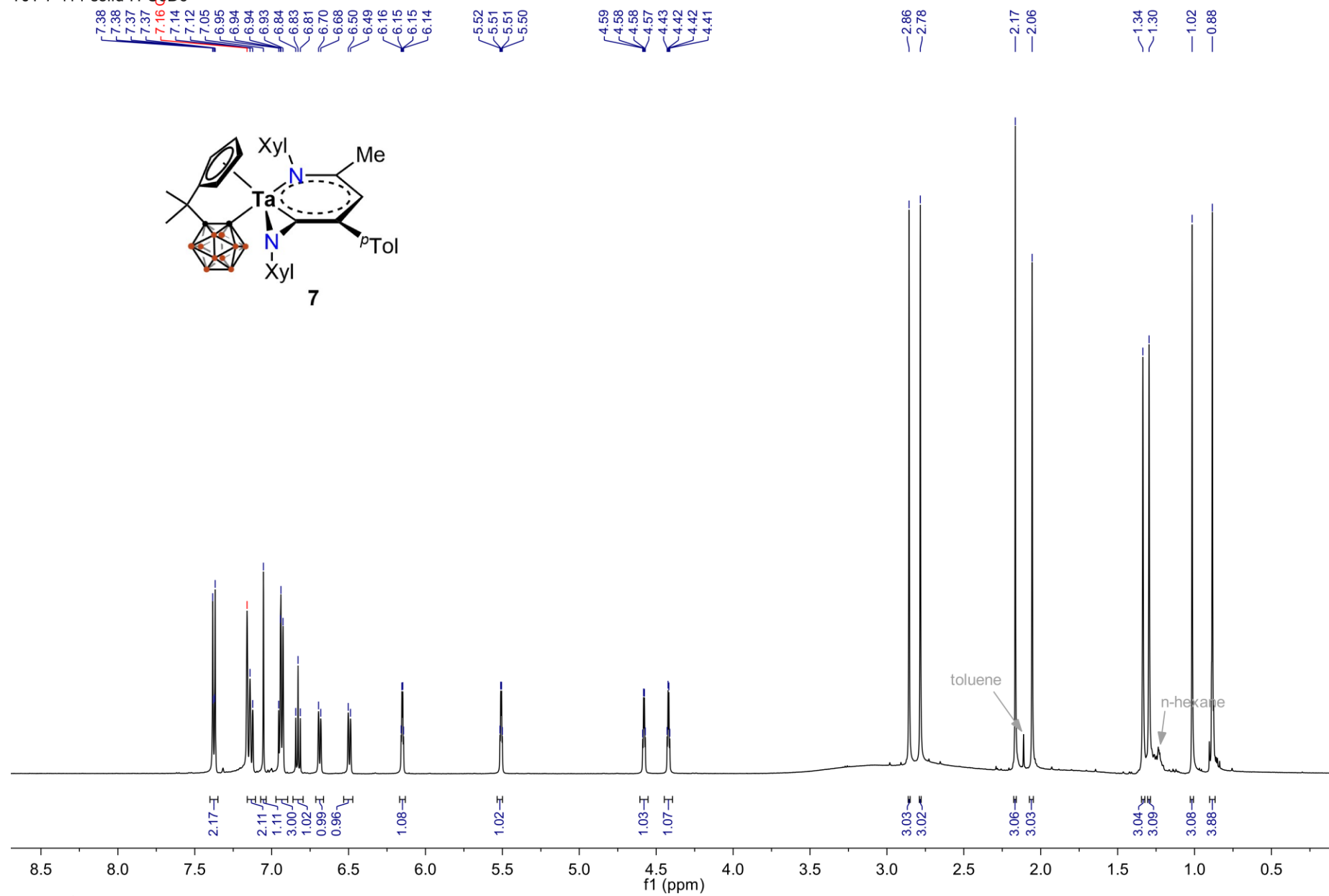


Fig. S12 ^1H NMR spectrum of compound 7 in C_6D_6 .

YJT-7-114-solid-C-C6D6.1.fid
YJT-7-114-solid-C-C6D6

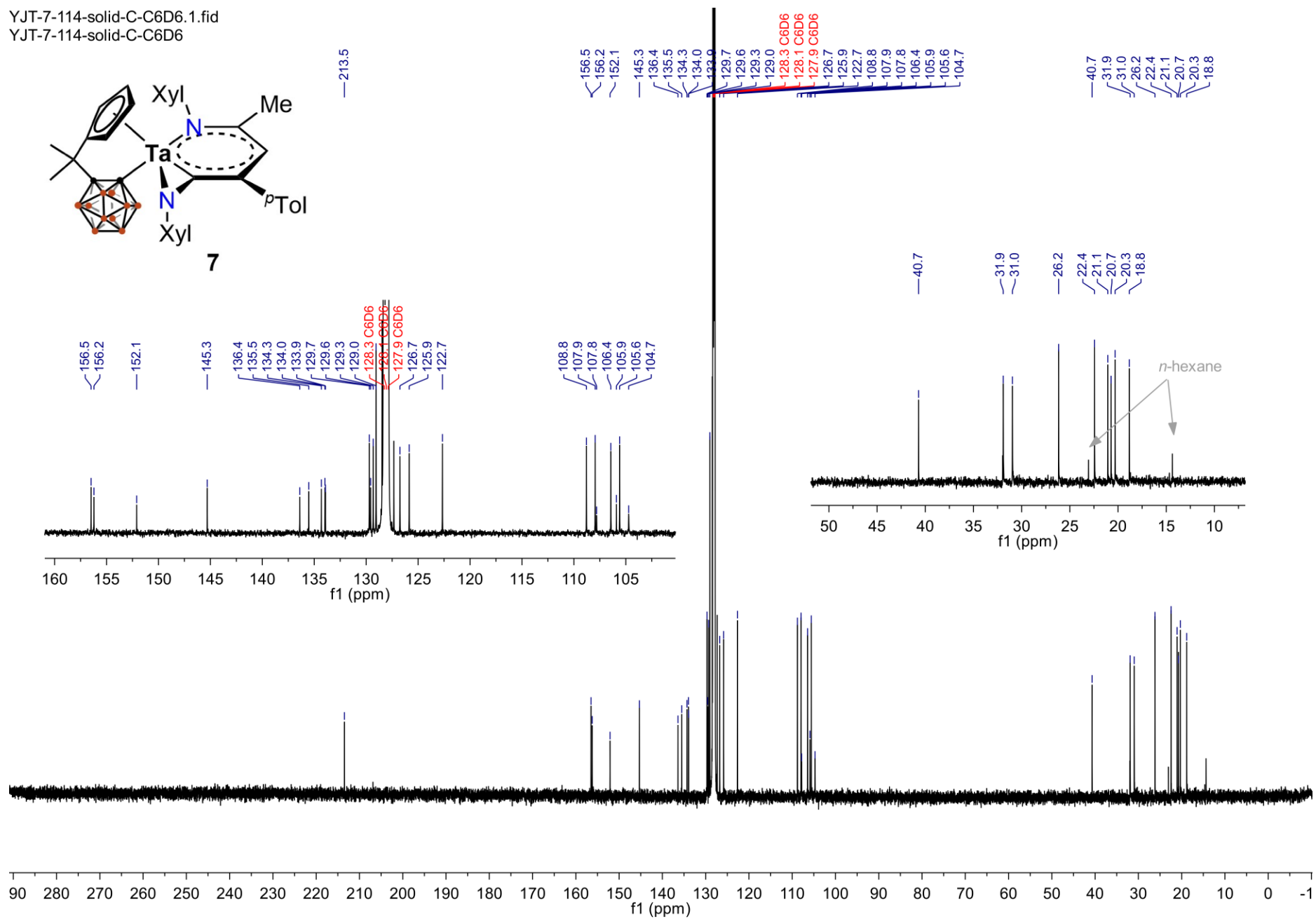


Fig. S13 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **7** in C_6D_6 .

YJT-7-126-solid-B(de)-C6D6.1.fid
YJT-7-126-solid-B(de)-C6D6

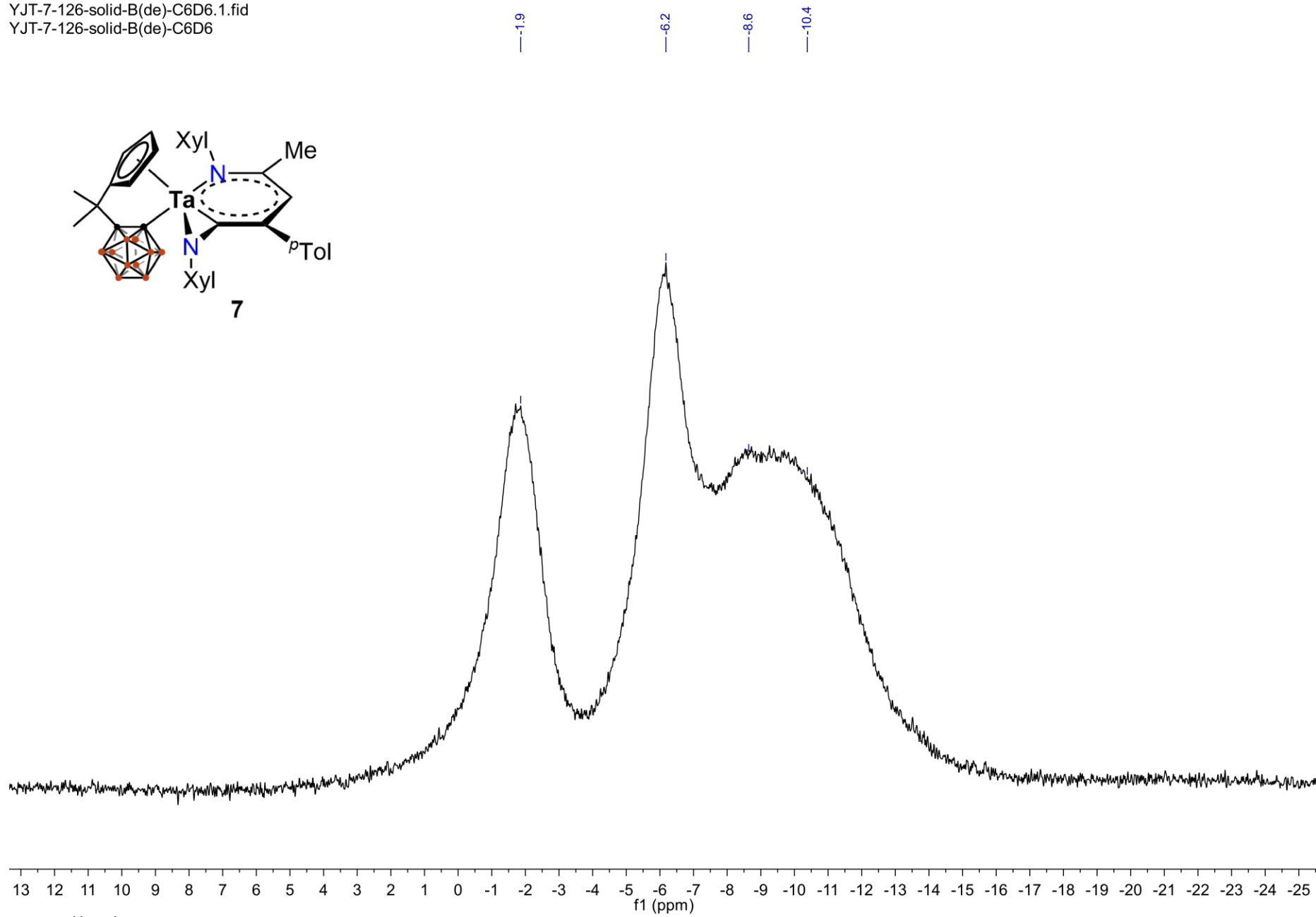


Fig. S14 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **7** in C_6D_6 .

YJT-7-126-solid-B(c)-C6D6.1.fid
YJT-7-126-solid-B(c)-C6D6

— -1.3
— -2.1

— -5.5
— -6.7

— -8.5
— -9.3
— -10.2

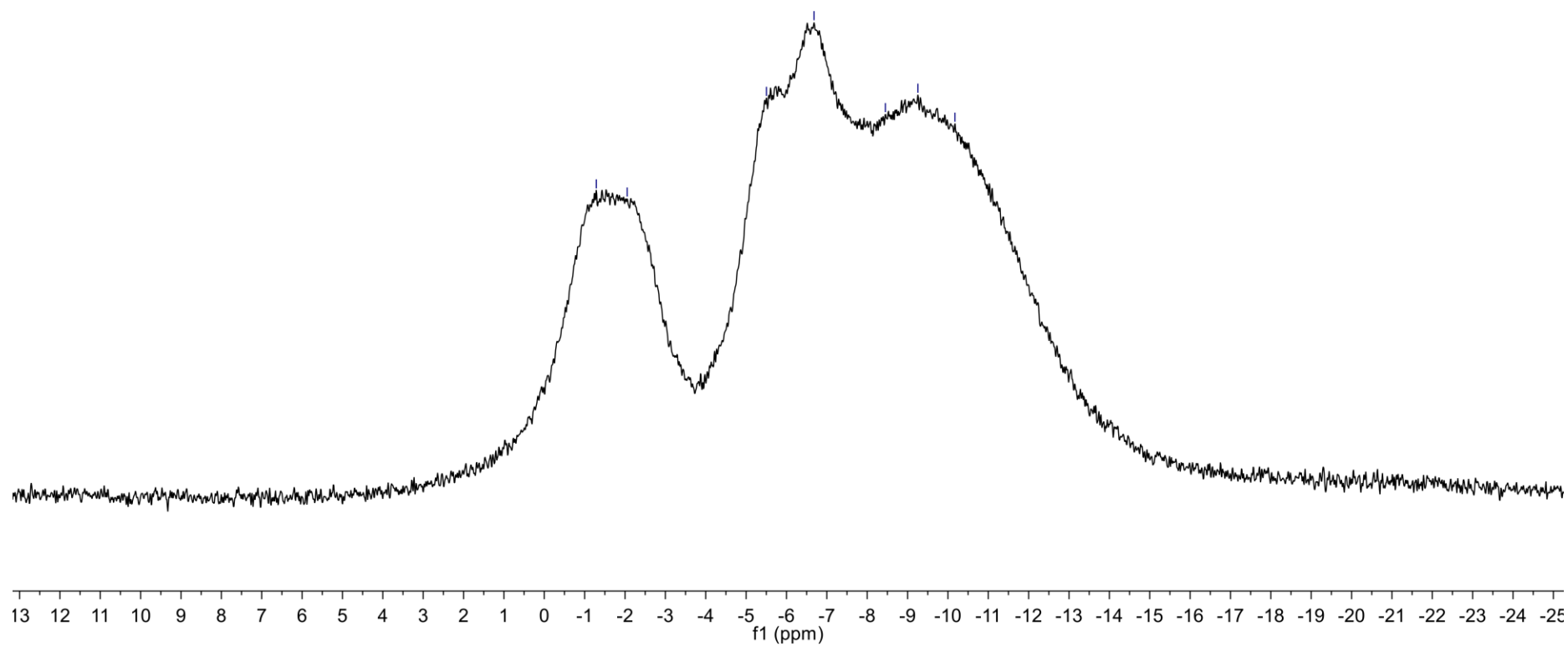
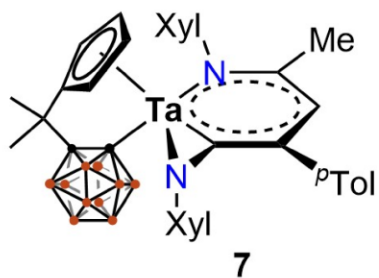


Fig. S15 ^{11}B NMR spectrum of compound 7 in C_6D_6 .

Mass Spectra of New Compounds

Bruker 9.4T FTICR MS Analysis Report

Analysis Info

Sample Name:	YJT5183	Reference No.:	szwx344
Applicant Name:	Yang Jinting	Analysis Created:	20201008
Analysis Path	0003.D	Instrument:	solarix XR
Parameters:	4.5kV, APCI II with DIP		
Method:	Broad_60-1000_XR_9_4T_newshimming_20170915		

Acquisition Parameter

Polarity	Positive	Pulse Program	Basic	No. of Laser Shots	20
Broadband Low Mass	57.7 m/z	Source Accumulation	0.000 sec	Calibration Date	Thu Jan 16 2020
Broadband High Mass	2000.0 m/z	Ion Accumulation Time	0.020 sec	Date Acquisition Size	1048576
Acquisition Mode	Serial MS	Time of flight to Detector	0.001 sec	Size Apodization	Sine-Squared

Accurate Mass Measurement

Molecular formula :	C ₃₄ H ₅₁ B ₁₀ N ₂ SiTa
Abundant Isotopic (theoretical) [M+H] ⁺ :	806.43674
Monoisotopic (theoretical) [M+H] ⁺ :	--
(experimental) [M+H] ⁺ :	806.43693
Error (ppm) :	0.2

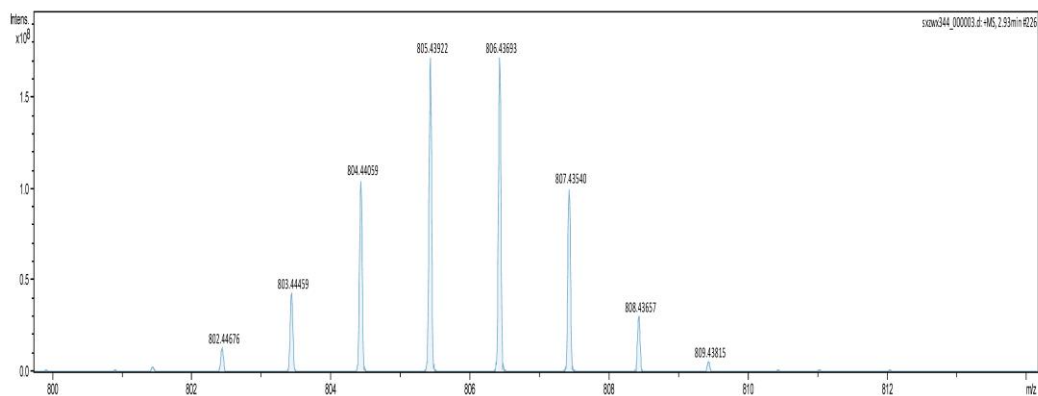


Fig. S16 High resolution mass spectrum showing [M+H]⁺ mass peak of compound 5.

Bruker 9.4T FTICR MS Analysis Report

Analysis Info

Sample Name:	YJT7115	Reference No.:	axzwx513
Applicant Name:	Yang Jingting	Analysis Created:	20220629
Analysis Path	0001.D	Instrument:	solarix XR
Parameters:	4.5kV, APCI II with DIP		
Method:	Broad_60-1000_XR_9_4T_newshimming_20170915		

Acquisition Parameter

Polarity	Positive	Pulse Program	Basic	No. of Laser Shots	20
Broadband Low Mass	57.7 m/z	Source Accumulation	0.000 sec	Calibration Date	Thu Jan 16 2020
Broadband High Mass	2000.0 m/z	Ion Accumulation Time	0.020 sec	Date Acquisition Size	1048576
Acquisition Mode	Serial MS	Time of flight to Detector	0.001 sec	Size Apodization	Sine-Squared

Accurate Mass Measurement

Molecular formula :	C ₃₅ H ₅₁ B ₁₀ N ₂ Ta
Abundant Isotopic (theoretical) [M]:	789.45303
Monoisotopic (theoretical) [M]:	--
(experimental) [M]:	789.45201
Error (ppm) :	-1.3

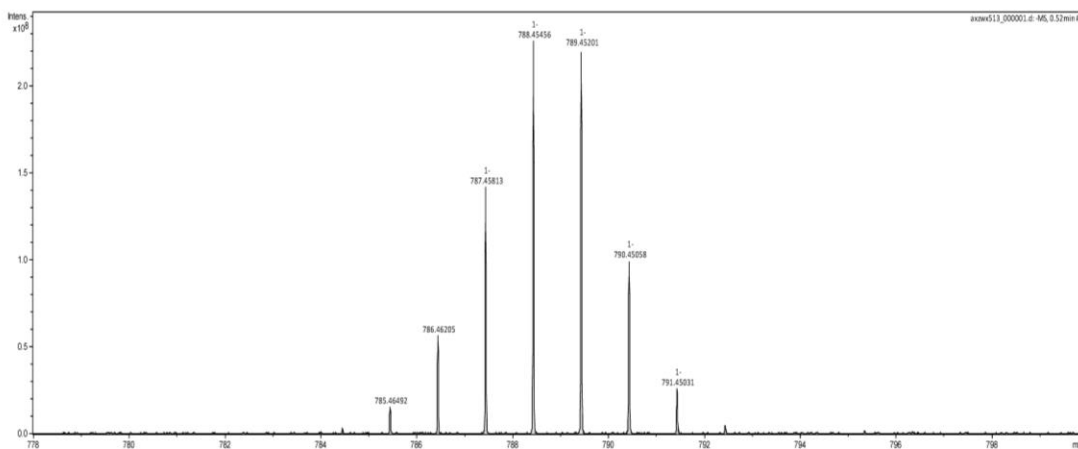


Fig. S17 High resolution mass spectrum showing $[M]^+$ mass peak of compound **6**.

Bruker 9.4T FTICR MS Analysis Report

Analysis Info

Sample Name:	YJT7114	Reference No.:	axzwx512
Applicant Name:	Yang Jingting	Analysis Created:	20220629
Analysis Path	0001.D	Instrument:	solarix XR
Parameters:	4.5kV, APCI II with DIP		
Method:	Broad_60-1000_XR_9_4T_newshimming_20170915		

Acquisition Parameter

Polarity	Positive	Pulse Program	Basic	No. of Laser Shots	20
Broadband Low Mass	57.7 m/z	Source Accumulation	0.000 sec	Calibration Date	Thu Jan 16 2020
Broadband High Mass	2000.0 m/z	Ion Accumulation Time	0.020 sec	Date Acquisition Size	1048576
Acquisition Mode	Serial MS	Time of flight to Detector	0.001 sec	Size Apodization	Sine-Squared

Curate Mass Measurement

Molecular formula :	C ₃₈ H ₄₉ B ₁₀ N ₂ Ta
Abundant Isotopic (theoretical) [M]:	823.43756
Monoisotopic (theoretical) [M]:	--
(experimental) [M]:	823.43523
Error (ppm) :	-2.8

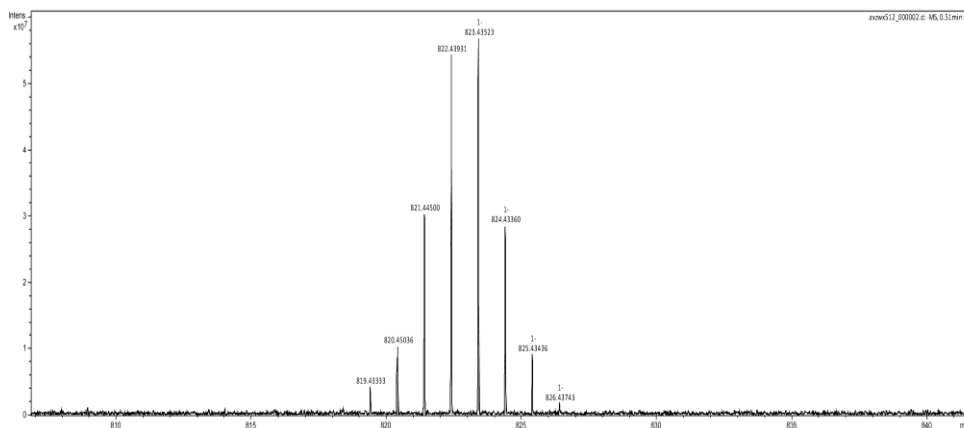


Fig. S18 High resolution mass spectrum showing (M⁺) mass peak of compound 7.

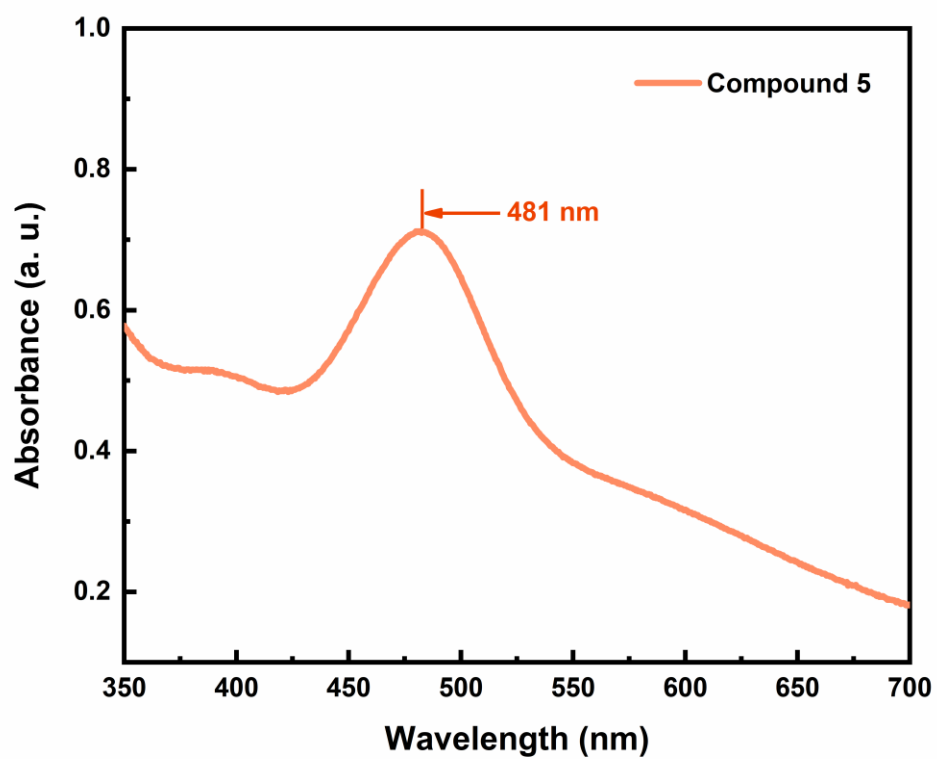


Fig. S19 UV-visible spectrum of compounds **5** in THF.

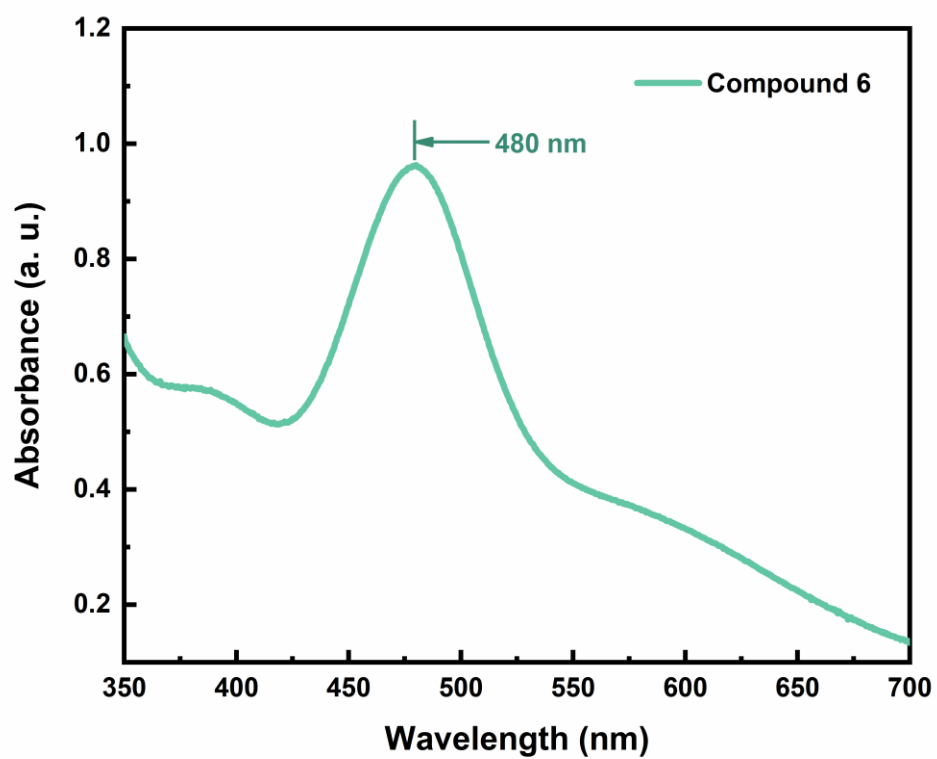


Fig. S20 UV-visible spectrum of compounds **6** in THF.

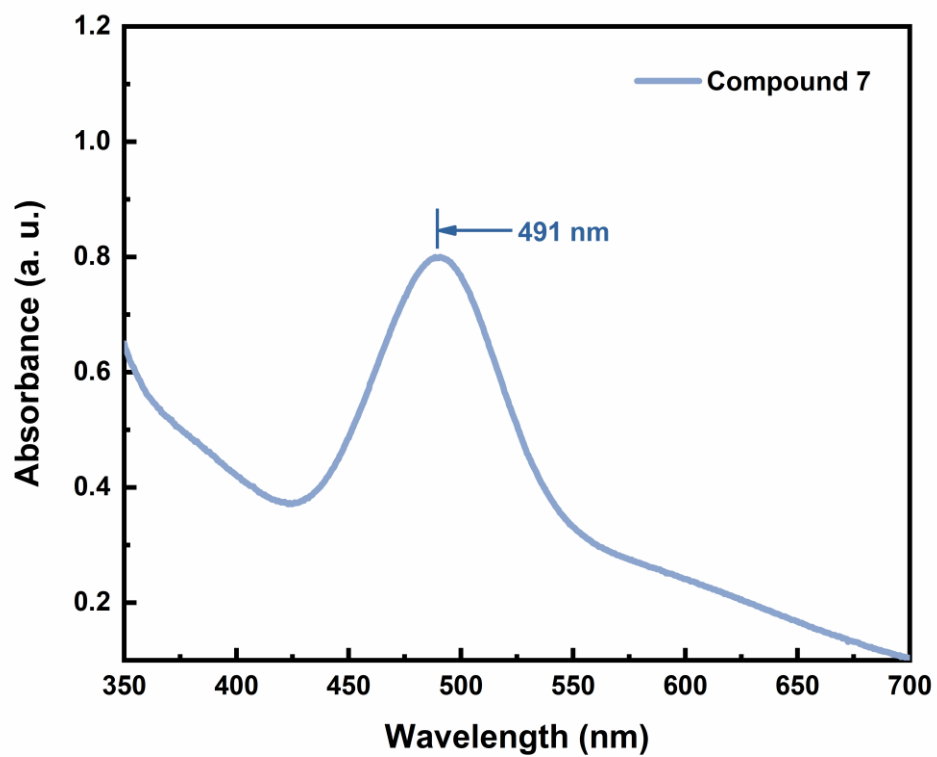


Fig. S21 UV-visible spectrum of compounds 7 in THF.

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