

## Electronic Supplementary Information

### Unique properties of C,C'-linked *nido*-biscarborane tetraanion. Synthesis, structure and bonding of ruthenium monocarbollide via unprecedented cage carbon extrusion

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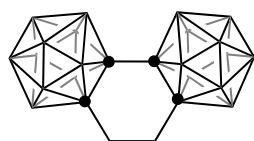
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## General Information.

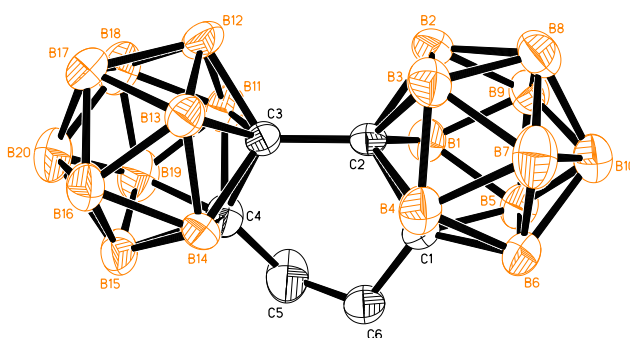
All reactions were carried out under an atmosphere of dry argon with the rigid exclusion of air and moisture in a glovebox unless otherwise specified.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a Bruker DPX 400 spectrometer at 400 MHz and 100 MHz, respectively.  $^{11}\text{B}$  NMR spectra were recorded on a Bruker DPX 300 spectrometer at 96 MHz or a Varian Inova 400 spectrometer at 128 MHz. Chemical Shifts were reported in ppm with reference 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 spectra were obtained on a Thermo Finnigan MAT 95 XL spectrometer or Waters Micromass GCT Premier. All organic solvents were freshly distilled from Na-K alloy or  $\text{CaH}_2$  immediately prior to use. 1,1'-biscarborane was prepared according to literature method.<sup>1</sup> All other chemicals were purchased from either Aldrich or Acros Chemical Co. and used as received unless otherwise specified. Elemental analyses were performed by either the Shanghai Institute of Organic Chemistry, CAS, China or MEDAC Ltd., Middlesex, U.K. X-ray photoelectron spectroscopy (XPS) analysis was measured on a VG ESCALAB 220i-XL surface analysis system (X-Ray gun of monochromatic Al-K $\alpha$  with  $h\nu = 1486.6$  eV).

**Synthesis of  $\mu$ -2,2'-( $\text{CH}_2$ )<sub>2</sub>-1,1'-(*o*- $\text{C}_2\text{B}_{10}\text{H}_{10}$ )<sub>2</sub> (2).** To a toluene/ $\text{Et}_2\text{O}$  solution (2:1, V/V, 20 mL) of 1,1'-biscarborane (**1**; 572.8 mg, 2.0 mmol) was slowly added  $n\text{BuLi}$  (2.50 mL, 1.6 M in *n*-hexane, 4.0 mmol) at 0 °C. The mixture was allowed to warm to room temperature and stirred for 30 min. The solution was then cooled to 0 °C, and 1,2-dibromoethane (0.17 mL, 2.0 mmol) was slowly added with stirring. The resulting reaction mixture was heated to reflux and stirred for overnight before quenched with water. After removal of the precipitate by filtration, the organic layer was separated, and the aqueous layer was extracted with  $\text{Et}_2\text{O}$  (20 mL x 3). The combined organic portions were dried over anhydrous  $\text{Na}_2\text{SO}_4$ . After removal of the solvent, the residue was

subjected to flash column chromatography on silica gel (230–400 mesh) using *n*-hexane as eluent to give **2** as colorless crystals (541.2 mg, 87%).

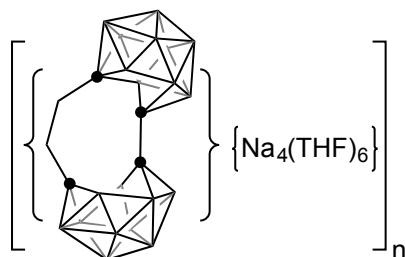


**2**: Colorless crystals. Yield: 87%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  2.67 (s, 4H) ( $\text{CH}_2$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  71.8 (cage C), 69.4 (cage C), 29.9.  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -1.8 (3B), -3.6 (2B), -9.4 (12B), -10.3 (3B). HRMS (EI): calcd for  $\text{C}_6\text{H}_{24}^{11}\text{B}_{16}^{10}\text{B}_4^+$ : 311.3804, found 311.3815. Anal. Calcd for  $\text{C}_6\text{H}_{24}\text{B}_{20}$ : C, 23.06; H, 7.74. Found: C, 22.83; H, 7.71.



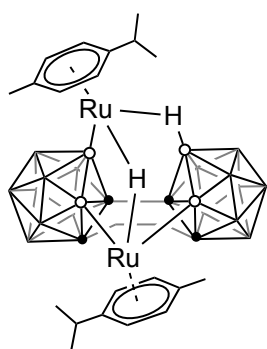
**Figure S1.** Molecular Structure of **2**.

**Synthesis of  $[(\text{CH}_2\text{C}_2\text{B}_{10}\text{H}_{10})_2\text{Na}_4(\text{THF})_6]_n$  (**3**).** To a THF (15 mL) solution of  $\mu$ -2,2'-( $\text{CH}_2$ )<sub>2</sub>-1,1'-(*o*- $\text{C}_2\text{B}_{10}\text{H}_{10}$ )<sub>2</sub> (**2**; 311 mg, 1.0 mmol) was added finely cut Na metal (115 mg, 5.0 mmol), and the mixture was stirred at room temperature for 3 days, affording a red solution. After removal of excess Na, the clear orange red solution was concentrated to about 5 mL. This solution stood at room temperature for 1 week to afford **3** as yellow crystals (713 mg, 85%).



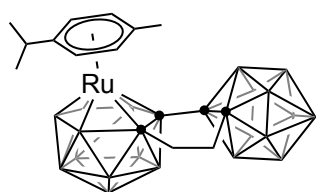
**3**: Yellow crystals. Yield: 85%.  $^1\text{H}$  NMR (400 MHz, pyridine- $d_5$ ):  $\delta$  3.65 (m, 8H) (THF), 3.62 (s, 4H) ( $\text{CH}_2$ ), 1.61 (m, 8H) (THF).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, pyridine- $d_5$ ):  $\delta$  67.8, 25.8 (THF), 43.9, 41.0 ( $\text{CH}_2$ ); the cage carbon atoms were not observed.  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz, pyridine- $d_5$ ):  $\delta$  2.5 (1B), -2.8 (1B), -8.5 (5B), -14.7 (8B), -23.5 (5B). IR (KBr,  $\text{cm}^{-1}$ ):  $\nu_{\text{BH}}$  2583 (vs), 2460 (s). Anal. Calcd for  $\text{C}_{10}\text{H}_{32}\text{B}_{20}\text{Na}_4\text{O}$  (**6** - 5 THF): C, 25.21; H, 6.77. Found: C, 25.09; H, 6.76.

**Reaction of 3 with [Ru(*p*-cymene)Cl<sub>2</sub>]<sub>2</sub>.** A THF solution (10 mL) of **3** (167.8 mg, 0.2 mmol) was added dropwise to a suspension of [Ru(*p*-cymene)Cl<sub>2</sub>]<sub>2</sub> (122.5 mg, 0.2 mmol) in THF (10 mL) at -78 °C, and the reaction mixture was stirred at this temperature for additional 1 h. Then the reaction mixture was allowed to warm to room temperature and stirred overnight to give a deep brown solution. After removal of THF under vacuo, the residue was extracted by CH<sub>2</sub>Cl<sub>2</sub> (3 x 10 mL). Removal of CH<sub>2</sub>Cl<sub>2</sub> gave a brown sticky solid. Chromatographic separation on SiO<sub>2</sub> (300–400 mesh) using *n*-hexane/CH<sub>2</sub>Cl<sub>2</sub> (50/1 to 1/2 in V/V) as eluent afforded **2** as colorless crystals (44.8 mg, 70%), **4** as black crystals (3.2 mg, 2%), **5** as yellow crystals (11.0 mg, 10%) and **6** as red orange crystals (15.7 mg, 10%).



**4:** Black crystals. Yield: 2%. <sup>1</sup>H NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ 5.45 (br, 2H), 5.40 (br, 2H), 5.19 (br, 2H), 5.06 (br, 2H) (aromatic CH), 2.96 (m, 1H), 2.56 (m, 1H) (CH), 2.33 (m, 2H) (CH<sub>2</sub>), 2.25 (s, 3H) (CH<sub>3</sub>), 2.18 (m, 2H) (CH<sub>2</sub>), 2.06 (s, 3H), 1.27 (d, *J* = 6.4 Hz, 6H), 1.23 (d, *J* = 7.2 Hz, 6H) (CH<sub>3</sub>), -16.15 (br, 1H) (RuH). <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ 89.8, 86.2, 86.1, 85.8,

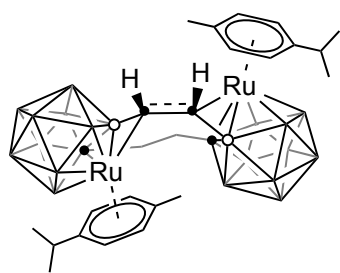
79.0 (cage C), 71.8 (cage C), 32.4, 29.8, 23.4, 23.1, 20.3, 18.7. <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ 20.7 (br, 3B), -2.7 (2B), -4.3 (4B), -9.0 (3B), -10.2 (5B), -15.6 (3B). HRMS (EI): calcd for C<sub>26</sub>H<sub>50</sub>Ru<sub>2</sub><sup>11</sup>B<sub>16</sub><sup>10</sup>B<sub>4</sub><sup>+</sup>: 783.4035, found 783.4031.



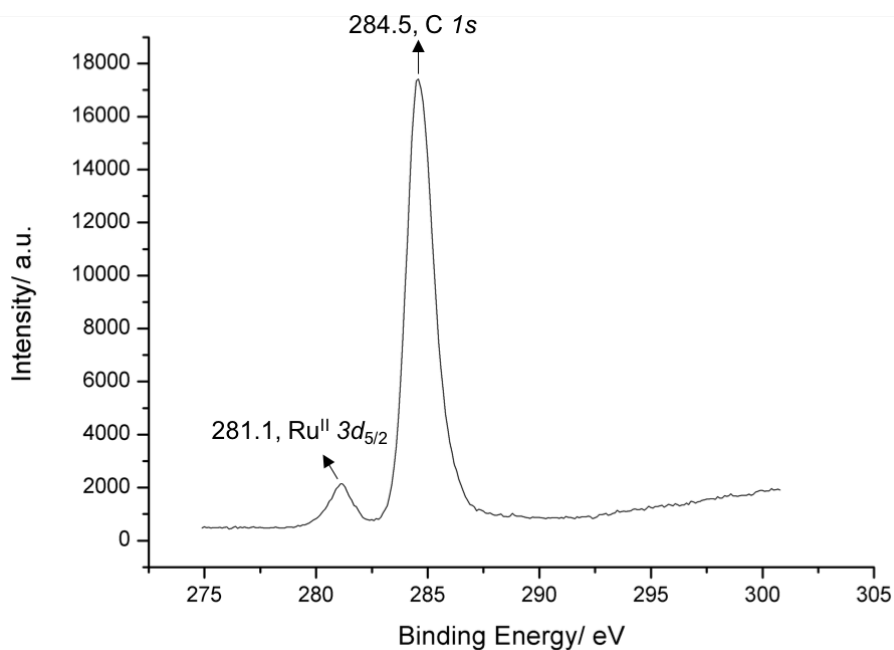
**5:** Yellow crystals. Yield: 10%. <sup>1</sup>H NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ 6.42 (d, *J* = 6.4 Hz, 1H), 6.27 (d, *J* = 6.4 Hz, 1H), 6.10 (m, 2H) (aromatic CH), 3.12 (m, 2H) (CH<sub>2</sub>), 2.95 (m, 1H) (CH), 3.10-2.91 (m, 2H) (CH<sub>2</sub>), 2.34

(s, 3H), 1.34 (d, *J* = 7.2 Hz, 3H), 1.32 (d, *J* = 6.8 Hz, 6H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ 118.2, 108.1, 104.5, 102.4, 101.2, 99.5, 80.7 (cage C), 77.3 (cage C), 39.3, 31.1, 23.7, 21.5, 17.8. <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ 9.3 (2B), 6.8 (2B), 3.8 (1B), 0.3 (1B), -1.9 (1B), -4.5 (1B), -7.0 (3B), -8.6 (1B), -9.3 (2B), -11.8 (4B), -15.8 (1B), -17.7 (1B). HRMS (EI): calcd for C<sub>16</sub>H<sub>38</sub>Ru<sup>11</sup>B<sub>16</sub><sup>10</sup>B<sub>4</sub><sup>+</sup>: 548.4000, found 548.3999. Anal. Calcd for C<sub>16</sub>H<sub>38</sub>RuB<sub>20</sub>: C, 35.08; H, 6.99.

Found: C, 34.89; H, 6.93.



**6:** Orange red crystals. Yield: 10%.  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  6.63 (br, 2H), 6.46 (br, 2H), 6.33 (br, 2H), 6.21 (m, 2H) (aromatic CH), 5.69 (br, 2H) (BCH), 2.87 (m, 2H) (CH), 2.45 (s, 6H), ( $\text{CH}_3$ ), 2.24 (d,  $J = 15.2$  Hz, 2H), 2.09 (d,  $J = 15.2$  Hz, 2H) ( $\text{CH}_2$ ), 1.46 (d,  $J = 6.8$  Hz, 6H), 1.32 (d,  $J = 7.2$  Hz, 6H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  101.5, 100.9, 84.9 (br, BC), 80.0 (cage C), 44.2, 31.7, 23.1, 21.8, 18.7.  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  12.1 (2B), 10.3 (2B), 8.2 (2B), 3.7 (3B), 2.0 (2B), -5.4 (2B), -10.3 (3B), -15.0 (2B), -17.6 (2B). HRMS (EI): calcd for  $\text{C}_{26}\text{H}_{52}\text{Ru}_2^{11}\text{B}_{16}^{10}\text{B}_4^+$ : 785.4196, found 785.4199. Anal. Calcd for  $\text{C}_{26}\text{H}_{52}\text{Ru}_2\text{B}_{20}$ : C, 39.88; H, 6.69. Found: C, 39.63; H, 6.66.



**Figure S2.** XPS spectra of **6** (C  $1s$ : 284.5 eV, Ru  $3d_{5/2}$ : 281.1 eV).

**X-ray Structure Determination.** All data were collected at 293 K on a Bruker SMART 1000 CCD diffractometer using Mo- $K_\alpha$  radiation. An empirical absorption correction was applied using the SADABS program.<sup>2</sup> 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.<sup>3</sup> All hydrogen atoms were

geometrically fixed using the riding model. Crystal data and details of data collection and refinement are given in Tables S1 and S2, respectively.

CCDC 1477943-1477947 (**2** - **6**) contain the 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](http://www.ccdc.cam.ac.uk/data_request/cif).

**Table S1.** Crystal Data and Summary of Data Collection and Refinement for **2**, **3** and **4**.

compound	<b>2</b>	<b>3</b>	<b>4</b>
formula	C <sub>6</sub> H <sub>24</sub> B <sub>20</sub>	C <sub>30</sub> H <sub>72</sub> B <sub>20</sub> Na <sub>4</sub> O <sub>6</sub>	C <sub>26</sub> H <sub>50</sub> B <sub>20</sub> Ru <sub>2</sub>
crystal size (mm)	0.32x0.30x0.28	0.40x0.30x0.20	0.40x0.30x0.20
fw	312.45	837.04	781.03
crystal system	orthorhombic	triclinic	monoclinic
space group	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	<i>P</i> -1	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>a</i> , Å	6.982(2)	12.367(2)	10.502(1)
<i>b</i> , Å	13.129(3)	14.518(3)	34.370(3)
<i>c</i> , Å	20.440(5)	15.257(2)	10.704(2)
$\alpha$ , deg	90	66.37(1)	90
$\beta$ , deg	90	69.65(1)	113.29(1)
$\gamma$ , deg	90	81.26(1)	90
<i>V</i> , Å <sup>3</sup>	1873.1(8)	2351.7(5)	3548.3(5)
<i>Z</i>	4	2	4
<i>D</i> <sub>calcd</sub> , Mg/m <sup>3</sup>	1.108	1.182	1.458
radiation ( $\lambda$ ) Å	0.71073	0.71073	0.71073
2 $\theta$ range, deg	3.68 to 50.04	3.06 to 50.80	2.36 to 50.50
$\mu$ , mm <sup>-1</sup>	0.046	0.100	0.873
<i>F</i> (000)	640	888	1568
no. of obsd reflns	3320	8565	6415
no. of params refnd	354	557	441
goodness of fit	1.051	0.860	1.158
R1	0.0656	0.0628	0.0324
wR2	0.2022	0.1748	0.0839

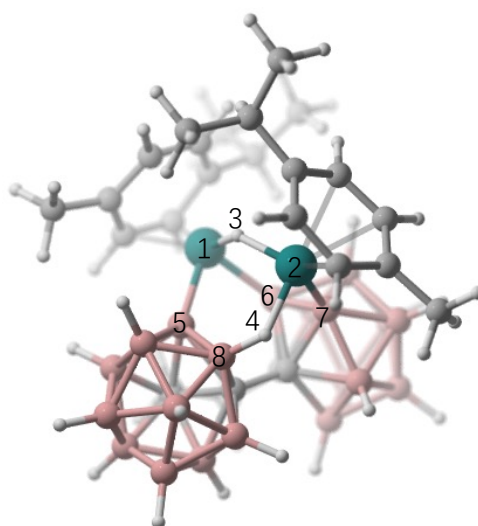
**Table S2.** Crystal Data and Summary of Data Collection and Refinement for **5** and **6**.

compound	<b>5</b>	<b>6</b>
formula	C <sub>16</sub> H <sub>38</sub> B <sub>20</sub> Ru	C <sub>26</sub> H <sub>52</sub> B <sub>20</sub> Ru <sub>2</sub>
crystal size (mm)	0.50x0.40x0.30	0.40x0.30x0.20
fw	547.73	783.02
crystal system	monoclinic	monoclinic
space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>a</i> , Å	9.193(1)	16.435(3)
<i>b</i> , Å	12.486(1)	10.493(3)
<i>c</i> , Å	28.360(2)	21.915(3)
$\beta$ , deg	95.59(1)	104.05(1)
<i>V</i> , Å <sup>3</sup>	3239.4(3)	3177.1(5)
<i>Z</i>	4	4
<i>D</i> <sub>calcd</sub> , Mg/m <sup>3</sup>	1.123	1.419
radiation ( $\lambda$ ) Å	0.71073	0.71073
2 $\theta$ range, deg	2.88 to 50.50	2.80 to 50.20
$\mu$ , mm <sup>-1</sup>	0.491	0.845
<i>F</i> (000)	1112	1584
no. of obsd reflns	5846	6518
no. of params refnd	334	487
goodness of fit	1.055	0.957
R1	0.0362	0.0765
wR2	0.0963	0.2362

## Computational Details.

All calculations were carried out with the Gaussian 09 program.<sup>4</sup> Geometry optimizations were performed at the Becke3LYP (B3LYP)<sup>5</sup> level of the density functional theory. The effective core potentials (ECPs) of Hay and Wadt with double valence basis sets (LanL2DZ)<sup>6</sup> were used to describe Ru. Polarization functions were also added for Ru ( $\zeta_f = 1.235$ ).<sup>7</sup> The 6-31g(d,p) basis set was used for all other atoms. Frequency calculations were made to determine the characteristics of all stationary points as energy minima and obtain thermal corrections. NBO analysis was also carried out using the NBO program implemented in the Gaussian 09 package.<sup>8</sup> It is noted that the optimized structures used for **4** and **6** agree well with the crystal structures (Tables S3 and S4).

**Table S3.** Comparison of the experimental and computational structures of **4**.<sup>a</sup>



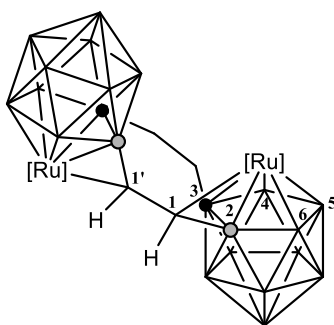
	Ru1-Ru2	Ru1-H3	Ru2-H3	Ru2-H4	Ru1-H3-Ru2
Exp.	3.125(1)	1.687(4)	1.741(5)	1.714(3)	131(2)
Calc.	3.18	1.72	1.70	1.76	136

	Ru1-B5	Ru1-B6	Ru2-B7	Ru2-B8
Exp.	2.036(3)	2.072(4)	2.218(4)	2.492(3)
Calc.	2.04	2.07	2.13	2.61

<sup>a</sup> Distances are in Å and angles are in deg.



**Table S4.** Comparison of the experimental and computational structures of **6**.<sup>a</sup>

	Ru-C1	Ru-B2	Ru-C3	Ru-B4
Exp.	2.319(6)	2.150(8)	2.307(8)	2.249(10)
Calc.	2.36	2.17	2.31	2.27
	Ru-B5	Ru-B6	C1-C1'	C1-B2
Exp.	2.249(9)	2.240(9)	1.484(1)	1.524(1)
Calc.	2.29	2.24	1.47	1.51

<sup>a</sup> Distances are in Å.

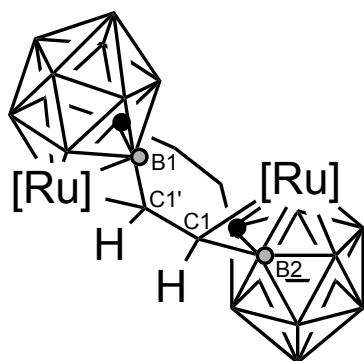
#### Energies for Possible Isomers of Complex **4**.

The calculated results show that the proposed structure of **4** bearing a bridging H atom is more energetically favored compared with the other two isomers (Table S5).

**Table S5.** Energies of all three possible isomers.

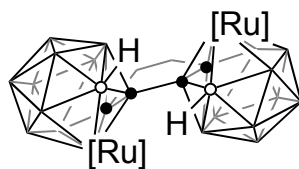
<b>4</b>	<b>4-iso1</b>	<b>4-iso2</b>
$\Delta G = 0.0$ kcal/mol	$\Delta G = 15.4$ kcal/mol	$\Delta G = 16.9$ kcal/mol

## NBO Analysis of Complex 6.



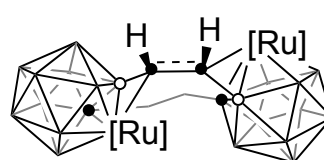
		C1-C1'		C1-B2	
Bond order		1.1458		1.0369	
	Occupancy	Coefficients		Hybrids	
Ru-C1	1.57337	Ru	C1	Ru	C1
		0.7957	0.6057	<i>d</i> 96.23%	<i>p</i> 95.10%

## Energy Comparison for 13-Vertex Bisruthenacarborane Intermediate IM-1 and 6.



**IM-1**

$\text{RuC}_2\text{B}_{10}\text{-RuC}_2\text{B}_{10}$   
 $\Delta G = 31.0 \text{ kcal/mol}$



**6**

$\text{RuCB}_{10}\text{-RuCB}_{10}$   
 $\Delta G = 0.0 \text{ kcal/mol}$

The calculated results show that **6** is thermodynamically more stable than **IM-1** by 31.0 kcal/mol.

## The Cartesian coordinates for the optimized structures

4

0 1

Ru	0.15217200	1.32899400	-0.49650500
Ru	-1.33449900	-1.38553500	0.21866900
C	2.07064100	-1.43922800	-0.54657900
C	2.95169000	-0.42331000	-1.46313400
C	3.72824400	0.71464500	-0.80956500

H	4.66806400	0.84098000	-1.35393800
H	3.13843500	1.62089900	-0.94112700
C	4.04046100	0.52669100	0.67827200
H	4.88428700	-0.15718100	0.79718900
H	4.35571600	1.48748500	1.09373400
C	-0.24277200	2.69295000	-3.82741200
H	-0.11708400	3.65821100	-4.33402200
H	-1.18734900	2.25882200	-4.16508400
H	0.56987800	2.04008800	-4.15362200
C	-0.23492500	2.88417300	-2.33433600
C	0.98734800	3.09120800	-1.61405400
H	1.92689600	3.08349600	-2.15644200
C	0.97448500	3.41439700	-0.23036000
H	1.91077500	3.63369900	0.27224000
C	-0.25888700	3.57599900	0.49030500
C	-1.42663300	3.21943900	-0.18818600
H	-2.37930700	3.23566700	0.32767800
C	-1.41176500	2.86669600	-1.57819700
H	-2.35104300	2.62519900	-2.06532900
C	-0.23776600	4.12357700	1.90930100
H	0.54483200	3.57871000	2.45096800
C	-1.55203300	3.93598200	2.67722900
H	-1.85171100	2.88487400	2.71088400
H	-2.36676400	4.51995300	2.23279200
H	-1.43077700	4.28006900	3.70872600
C	0.16209400	5.61542900	1.88545800

H	0.24886200	6.00227900	2.90608200
H	-0.59189500	6.21247400	1.35993800
H	1.12231200	5.77226300	1.38449500
C	1.91918000	-1.13651000	0.92826300
C	2.87875500	0.01502000	1.52852400
C	-1.94725300	-4.11458600	2.32915000
H	-2.78978600	-4.61723500	2.82097000
H	-1.27789900	-3.74233100	3.10670000
H	-1.41021400	-4.86333200	1.74074900
C	-2.45139000	-2.99871400	1.45493100
C	-2.69095600	-1.68241000	1.95769300
H	-2.42972900	-1.44168500	2.98161500
C	-3.24239400	-0.67738300	1.12312300
H	-3.38527900	0.31928300	1.52560600
C	-3.67921100	-0.96054000	-0.22336400
C	-3.40062500	-2.23023200	-0.73472200
H	-3.63339200	-2.47855100	-1.76291700
C	-2.70897900	-3.19238400	0.07428000
H	-2.44046700	-4.14484900	-0.37362500
C	-4.40369600	0.12018600	-1.00743200
H	-3.97632700	1.07628800	-0.67892300
C	-5.90011000	0.12194100	-0.62702600
H	-6.04258600	0.23175400	0.45261200
H	-6.37982300	-0.81299600	-0.93661800
H	-6.41934900	0.94847900	-1.12313500
C	-4.21889400	0.02273200	-2.52762700

H	-3.15970200	-0.00728800	-2.79880400
H	-4.67776300	0.88855800	-3.01606300
H	-4.70421900	-0.86893000	-2.93959100
B	3.53044400	-2.04525700	-1.25058900
H	4.46767200	-2.21791400	-0.55795200
B	2.05473300	-3.01685000	-1.21046600
H	1.98336800	-3.93489500	-0.47107100
B	0.67717000	-1.88302700	-1.37093000
B	1.12943100	-0.14689200	-1.51306900
B	3.60362400	-1.24322800	-2.81823000
H	4.66454000	-0.88606400	-3.20600900
B	3.01066900	-2.90887400	-2.69612400
H	3.64317600	-3.83179700	-3.08887600
B	1.22645300	-2.83304500	-2.77081000
H	0.57113400	-3.72241700	-3.20605600
B	0.73325400	-1.12493900	-2.96197300
H	-0.24693400	-0.82117100	-3.55839900
B	2.20861400	-0.14974300	-2.95795200
H	2.40314000	0.89390600	-3.48626500
B	2.19929100	-1.73404000	-3.77573800
H	2.26741400	-1.81766700	-4.95750200
B	1.11401600	0.46142900	1.12207400
B	0.29312900	-1.04826700	1.55357200
B	1.46172600	-2.29840800	2.11118500
H	1.33640900	-3.43111900	1.79408600
B	3.10013900	-1.63300000	2.07914500

H	4.05217800	-2.20725900	1.68853600
B	2.02241600	0.98410000	2.60981300
H	2.35124500	2.12052200	2.71414100
B	0.40194500	0.29427000	2.73480000
H	-0.55104700	0.96160400	2.97525400
B	0.54256000	-1.37714800	3.30408200
H	-0.30480300	-1.88793700	3.96441700
B	2.26042000	-1.72645300	3.60251600
H	2.64808100	-2.48056400	4.43277700
B	3.17497000	-0.25771800	3.18202900
H	4.23532900	0.06842200	3.59974800
B	1.60330200	-0.10289000	3.97111300
H	1.51557200	0.29684600	5.08593000
H	-0.25692200	-2.38758600	-0.74514900
H	-1.09396100	0.14306000	-0.49599600

**4-iso1**

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Ru	0.24758300	0.79302300	-0.92665900
Ru	-1.38882700	-0.49820600	1.41948800
C	1.22114000	-2.25249900	-0.02039400
C	1.84778500	-2.20133300	-1.52890900
C	3.09644200	-1.37423100	-1.81960300
H	3.70279500	-1.92185700	-2.54627000
H	2.76721300	-0.45018500	-2.29230200

C	3.96739200	-1.03386200	-0.60681600
H	4.58852800	-1.89264400	-0.34163300
H	4.65042800	-0.22600800	-0.88194400
C	-1.23789700	0.76758900	-4.32293600
H	-0.91955700	1.14003400	-5.30458000
H	-2.32284700	0.88648400	-4.25607100
H	-1.00633900	-0.29993000	-4.28736400
C	-0.53687600	1.52114100	-3.22446000
C	0.86102800	1.32182200	-2.96623500
H	1.41623400	0.63870100	-3.59959800
C	1.55964400	2.15204900	-2.03421900
H	2.64041900	2.08346100	-1.96568700
C	0.88350600	3.21602500	-1.33888000
C	-0.50217400	3.25259400	-1.46028900
H	-1.07710600	3.97326000	-0.88874400
C	-1.20195300	2.41798600	-2.39688500
H	-2.27480100	2.54739600	-2.51119300
C	1.69236000	4.22055800	-0.53365100
H	2.43673500	3.65025900	0.03449200
C	0.86968800	5.03930100	0.46873400
H	0.32758800	4.39468700	1.16691300
H	0.14839800	5.69314800	-0.03529800
H	1.53266600	5.68020000	1.05749000
C	2.45825300	5.15778400	-1.49396400
H	3.10333200	5.83810100	-0.92830600
H	1.76199000	5.76335100	-2.08508900

H	3.09020800	4.59817900	-2.19048000
C	1.82654200	-1.35383900	1.03465200
C	3.20374500	-0.58918800	0.63915300
C	-1.69275100	1.51639900	4.16971200
H	-2.38972700	2.22071900	4.64122300
H	-0.75258200	2.03853800	3.98437000
H	-1.49447200	0.70942300	4.87860000
C	-2.28429500	0.98849800	2.89001100
C	-2.11250900	1.67199100	1.65527200
H	-1.46728700	2.54203300	1.62081900
C	-2.80781600	1.26739400	0.48685700
H	-2.70442700	1.84288900	-0.42064800
C	-3.61278300	0.10249300	0.48464400
C	-3.77474700	-0.60075200	1.70983100
H	-4.37780800	-1.49947500	1.74591400
C	-3.12498000	-0.16636100	2.88187200
H	-3.25791500	-0.72626800	3.80201300
C	-4.33083400	-0.30273100	-0.79705500
H	-3.60852800	-0.15451200	-1.61010100
C	-5.53059700	0.63596900	-1.04962400
H	-5.22630800	1.68701300	-1.07989800
H	-6.28286500	0.52899000	-0.25995700
H	-6.00946800	0.39459500	-2.00431200
C	-4.77757500	-1.77049800	-0.83566200
H	-3.94792600	-2.45467500	-0.63983800
H	-5.17803700	-2.00815900	-1.82571300



H	-5.57414100	-1.97152300	-0.11011200
B	2.00102100	-3.66853300	-0.61470400
H	3.06105900	-3.95243100	-0.18604200
B	0.48418700	-3.75971500	0.29857200
H	0.50110300	-4.16765500	1.40636100
B	-0.47392000	-2.29378700	-0.11499400
B	0.33625200	-1.19958800	-1.25082900
B	1.59900100	-3.69180100	-2.33280900
H	2.43973300	-4.04237000	-3.09004600
B	0.69484300	-4.70109400	-1.18931900
H	0.82016900	-5.87970900	-1.15894000
B	-0.85191000	-3.86829800	-0.86838300
H	-1.84186800	-4.45890600	-0.58332600
B	-0.89517900	-2.36675200	-1.82829200
H	-1.90986700	-1.91326900	-2.24587600
B	0.63160600	-2.24575700	-2.69951300
H	0.84281400	-1.70309500	-3.73244400
B	-0.15393100	-3.83553000	-2.50442000
H	-0.62873700	-4.40687500	-3.42989500
B	1.62343400	0.35094800	0.51770900
B	0.70721100	-0.31376400	1.88696500
B	1.68902200	-1.59668700	2.72888100
H	1.17095000	-2.58146500	3.12811600
B	3.24176800	-1.78063600	1.91980100
H	3.75982000	-2.81185300	1.67937800
B	3.16972800	1.00434000	1.19331300

H	3.76812000	1.81887600	0.56955600
B	1.65047500	1.20010300	2.07446900
H	1.10189300	2.25340700	2.13788400
B	1.61684800	0.02843000	3.40721000
H	1.04040500	0.24065300	4.42358500
B	3.16221700	-0.86273400	3.40043700
H	3.68155500	-1.29015200	4.37779900
B	4.11954300	-0.25081000	2.03319800
H	5.29888100	-0.27269100	1.91702900
B	3.13400500	0.87217100	2.98051000
H	3.64279000	1.69174300	3.67316500
H	-1.24423300	-2.10990200	0.86247000
H	-0.77379500	-1.36082400	2.56410300

#### 4-iso2

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Ru	-0.24404900	1.30137300	-0.48983800
Ru	-0.59237000	-1.52892400	0.25382800
C	2.55387400	-0.59250400	-0.55805800
C	2.98102300	0.61487000	-1.53366600
C	3.34775400	1.97011000	-0.93210500
H	4.16331600	2.39097600	-1.52656400
H	2.48732400	2.63130700	-1.05528000
C	3.79637300	1.95337900	0.54466300
H	4.83158000	1.61065700	0.60886800
H	3.78084000	2.97889500	0.92350700

C	-1.30135900	1.71231900	-3.86344100
H	-1.95106000	2.36657100	-4.45824600
H	-1.60923000	0.68007400	-4.04231400
H	-0.27958400	1.83108400	-4.22860000
C	-1.41716300	2.07625700	-2.40780900
C	-0.64512800	3.12911000	-1.84368800
H	0.09996200	3.63685900	-2.44639800
C	-0.87857500	3.53651200	-0.50661400
H	-0.27202400	4.33606100	-0.09093000
C	-1.93031000	2.98968900	0.29272200
C	-2.62322900	1.89674700	-0.24242600
H	-3.39807700	1.41131100	0.33506900
C	-2.33869600	1.42188700	-1.55991700
H	-2.90039100	0.58749900	-1.95695600
C	-2.24178100	3.61739100	1.64495800
H	-1.27975700	3.78140700	2.14888400
C	-3.10279500	2.74109000	2.56322500
H	-2.64971300	1.75875600	2.72082600
H	-4.11223800	2.60315600	2.15810100
H	-3.21011600	3.22016900	3.54101600
C	-2.90236200	4.99861900	1.44360500
H	-3.06416300	5.48926400	2.40900800
H	-3.87500700	4.89487700	0.94943000
H	-2.28361300	5.65979600	0.82912900
C	2.37293000	-0.31275600	0.91803500
C	2.95351000	1.09589500	1.49207800

C	-0.36854400	-4.25054700	2.35991200
H	-1.00285000	-5.01504000	2.82688100
H	0.12682400	-3.69334100	3.15624800
H	0.39653400	-4.76711300	1.77374900
C	-1.20235300	-3.35237700	1.48649100
C	-1.83375600	-2.16999700	1.97270200
H	-1.64664800	-1.83687400	2.98735700
C	-2.70395200	-1.42242600	1.13504800
H	-3.17229300	-0.53436600	1.54296700
C	-3.15758600	-1.93905200	-0.13546800
C	-2.46063700	-3.02434500	-0.65176500
H	-2.68692800	-3.41678800	-1.63639500
C	-1.41692200	-3.64349400	0.11362000
H	-0.86800100	-4.46778300	-0.33265800
C	-4.40987200	-1.37217700	-0.78377300
H	-4.39120400	-0.28314900	-0.65487500
C	-5.65466800	-1.88473500	-0.02311000
H	-5.60538000	-1.63874000	1.04181500
H	-5.74102700	-2.97293800	-0.11288300
H	-6.56571900	-1.43635400	-0.43373200
C	-4.54271500	-1.67311500	-2.28356000
H	-3.65123100	-1.37600900	-2.84492200
H	-5.40196300	-1.13830300	-2.69983300
H	-4.70894100	-2.74062800	-2.46340700
B	4.11019700	-0.67276000	-1.31489800
H	5.07285700	-0.46882900	-0.66644200

B	3.08656900	-2.10796700	-1.15936500
H	3.39402200	-2.95013600	-0.39119400
B	1.38122200	-1.56532400	-1.27669500
B	1.07757400	0.15535900	-1.51688900
B	3.82143000	0.02661900	-2.90198500
H	4.66010900	0.72673300	-3.36105400
B	3.87832600	-1.73586600	-2.69921800
H	4.78869400	-2.38423500	-3.09557600
B	2.19339500	-2.31782200	-2.67873700
H	1.89633200	-3.40345700	-3.05664200
B	1.10945000	-0.92861800	-2.91006700
H	0.06901800	-1.04547700	-3.46938300
B	2.11117200	0.53642000	-2.98012200
H	1.88844100	1.55184200	-3.55202500
B	2.65939100	-0.97727700	-3.76732700
H	2.70876900	-1.08570200	-4.94811500
B	1.16073300	0.92062000	1.20907800
B	0.79584700	-0.74524000	1.60166700
B	2.34743700	-1.53893800	2.11228700
H	2.57934800	-2.65461000	1.80133600
B	3.69609000	-0.39062200	2.01560500
H	4.76100300	-0.64165200	1.57966600
B	1.88222700	1.75007200	2.64012000
H	1.81327600	2.93344700	2.70206200
B	0.55582200	0.59215000	2.81385600
H	-0.53961200	0.95231800	3.09209000

B	1.23304900	-0.95153400	3.34694200
H	0.62149600	-1.69610100	4.04247300
B	2.99023500	-0.74038100	3.57158300
H	3.62695600	-1.33707900	4.37505600
B	3.39026700	0.94044500	3.13181000
H	4.31258800	1.58236400	3.50729800
B	1.87823600	0.59159600	3.99030200
H	1.72016600	0.94441400	5.11249900
H	0.75062400	-2.33293400	-0.53328700
H	1.08742700	1.86730900	0.28712900

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Ru	-2.65842500	-0.09584900	-0.00533700
Ru	2.65841800	-0.09585500	0.00534300
B	-2.22950700	-1.74806900	-3.71254700
H	-2.05656500	-2.21724000	-4.79072100
B	-0.89265700	-1.69305500	-2.55405900
H	0.19992600	-2.09615500	-2.76972700
B	-1.54250500	-0.17245900	-3.24203200
H	-0.87550900	0.47820900	-3.98621700
B	-3.31827800	-0.38772700	-3.43171100
H	-3.91977300	0.11248900	-4.32746400
B	-3.72404100	-1.99013300	-2.75616800
H	-4.65023000	-2.62858300	-3.14088100
B	-2.23397100	-2.79094400	-2.27880800

H	-2.05560200	-3.96348000	-2.24236500
B	-3.26004100	-2.02786900	-1.04239200
H	-3.79957600	-2.73799700	-0.25289100
B	-4.00444800	-0.51834200	-1.80465600
H	-5.12889500	-0.20044600	-1.57526800
B	-2.68229700	0.62022000	-2.13267500
H	-2.74075500	1.81231500	-2.15005900
B	-1.13143100	-0.27413100	-1.53557600
B	2.22950700	-1.74766100	3.71273800
H	2.05657000	-2.21671100	4.79096500
B	0.89264900	-1.69277600	2.55425200
H	-0.19993600	-2.09585300	2.76996100
B	1.54250700	-0.17210200	3.24204700
H	0.87551800	0.47865400	3.98616100
B	3.31828000	-0.38735200	3.43174500
H	3.91977600	0.11296600	4.32744000
B	3.72403700	-1.98983500	2.75638200
H	4.65022500	-2.62824600	3.14116500
B	2.23396300	-2.79069500	2.27911700
H	2.05559400	-3.96323400	2.24280400
B	2.68230000	0.62044700	2.13259400
H	2.74076400	1.81254400	2.14986000
B	4.00444800	-0.51815400	1.80470200
H	5.12889500	-0.20029000	1.57527300
B	3.26003300	-2.02776100	1.04261100
H	3.79955500	-2.73799400	0.25319300

B	1.13142500	-0.27397000	1.53560600
C	-1.56449100	-1.87840500	-0.99740700
C	-0.49194500	0.67417300	-0.54327600
H	-0.68601800	1.69959100	-0.85981200
C	0.49193000	0.67423000	0.54321100
H	0.68599300	1.69968300	0.85964300
C	1.56448000	-1.87829600	0.99761800
C	0.77427500	-2.71458900	-0.03163900
H	1.09951700	-3.74731800	0.12123800
H	1.10004700	-2.45279800	-1.03575800
C	-0.77428700	-2.71458400	0.03194200
H	-1.09953200	-3.74732800	-0.12082000
H	-1.10005800	-2.45267700	1.03603000
C	-3.37146600	-2.10591100	2.95882200
H	-4.05599100	-2.09530600	3.81536800
H	-2.37650800	-2.36282100	3.32646200
H	-3.70971700	-2.88933400	2.27464100
C	-3.38130400	-0.76269000	2.28293200
C	-4.46819400	-0.37939300	1.45293400
H	-5.26078800	-1.09033900	1.24771700
C	-4.52952500	0.90448600	0.86251600
H	-5.37213800	1.15183100	0.22849800
C	-3.50301400	1.86695700	1.06232500
C	-2.38966600	1.44460000	1.82654600
H	-1.54910700	2.11265700	1.96663800
C	-2.32690600	0.16139500	2.43006000



H	-1.44799700	-0.10422400	3.00438300
C	-2.38089200	4.08735200	0.42858900
H	-1.61831800	3.57502200	-0.16372400
H	-1.96838100	4.29824100	1.42190200
H	-2.58095100	5.05064200	-0.04918700
C	3.37136100	-2.10626100	-2.95861700
H	4.05603700	-2.09583400	-3.81504500
H	2.37643700	-2.36310200	-3.32639300
H	3.70940900	-2.88964300	-2.27428700
C	3.38123700	-0.76296700	-2.28287200
C	2.32686600	0.16113400	-2.43007000
H	1.44794200	-0.10451300	-3.00435700
C	2.38967100	1.44439600	-1.82667700
H	1.54912700	2.11246200	-1.96681700
C	3.50305000	1.86680100	-1.06252900
C	4.52953900	0.90432000	-0.86264800
H	5.37217400	1.15170300	-0.22867300
C	4.46815300	-0.37961700	-1.45293000
H	5.26072900	-1.09056900	-1.24765700
C	2.38099600	4.08728100	-0.42898000
H	1.61842100	3.57502600	0.16339800
H	1.96847300	4.29808600	-1.42230500
H	2.58108800	5.05061200	0.04870100
C	-3.67831600	3.27416500	0.51024200
H	-4.06883400	3.16165500	-0.50857600
C	-4.73614600	4.02648200	1.34737500

H	-5.69014200	3.49120700	1.37557200
H	-4.92036600	5.01696300	0.91979700
H	-4.39444500	4.16245100	2.37959700
C	3.67840000	3.27405600	-0.51058000
H	4.06893100	3.16163000	0.50824100
C	4.73623400	4.02627100	-1.34780000
H	4.92048500	5.01678700	-0.92031700
H	5.69021700	3.49097100	-1.37596300
H	4.39451900	4.16215100	-2.38002900

### IM-1

0 1

Ru	-2.49786500	-0.36714500	0.35447100
C	-1.17174400	0.99363900	1.62887000
C	-0.96807700	1.26239700	0.20962100
C	0.07804600	0.58180600	2.38270100
H	0.37713900	-0.42004800	2.05738600
H	-0.12586100	0.54312200	3.45435900
C	1.20951100	1.57480000	2.08990900
H	0.90880600	2.57420400	2.42447600
H	2.10397700	1.31665800	2.66045800
C	-2.35109400	-2.58717600	1.19365700
C	-1.35450200	-2.40728100	0.20394700
H	-0.32631800	-2.56884900	0.48307100
C	-1.66761700	-2.01949500	-1.12713600
H	-0.86348300	-1.88590400	-1.84058000

C	-3.00286100	-1.75924700	-1.51639300
C	-3.98808700	-1.82778500	-0.48640900
H	-5.00794000	-1.53742100	-0.71106000
C	-3.67917700	-2.26616600	0.82714700
H	-4.46604700	-2.29531900	1.57139300
C	-2.02194100	-3.06512300	2.58164900
H	-2.25890200	-4.13088600	2.68148700
H	-2.59917600	-2.51714500	3.33058700
H	-0.96085500	-2.93473800	2.80863300
C	-3.44659900	-1.44153800	-2.93547200
H	-4.15869300	-0.61088700	-2.85304800
C	-2.32093700	-1.00747900	-3.87945600
H	-1.78535500	-0.13498800	-3.50038800
H	-2.74349100	-0.74464300	-4.85348400
H	-1.59831000	-1.81465800	-4.05006400
C	-4.20349500	-2.65995300	-3.51125400
H	-5.04720500	-2.95687700	-2.88060300
H	-3.53628400	-3.52367700	-3.61231100
H	-4.59516700	-2.42027000	-4.50439300
B	-2.20396600	1.69612000	-0.70133900
H	-1.95446300	1.74167600	-1.85776900
B	-3.94193800	1.31014700	-0.23977800
H	-4.64325200	0.98283500	-1.14890300
B	-4.18908600	0.71252800	1.42490300
H	-5.08227000	-0.02799700	1.70412500
B	-2.64732300	0.64694800	2.39569300

H	-2.47257600	-0.06646300	3.33687300
B	-1.72653100	2.97135700	0.64913600
H	-0.83420100	3.72784800	0.52205600
B	-3.32057100	2.96954400	-0.15031700
H	-3.59448700	3.77430200	-0.98109700
B	-4.52599100	2.40051000	1.01219700
H	-5.63740700	2.82123500	0.98651800
B	-3.73666800	1.99571800	2.56479700
H	-4.30503000	2.13806000	3.59918700
B	-2.01148400	2.33120000	2.41793000
H	-1.35015400	2.72227800	3.32561300
B	-3.14826800	3.35658600	1.57351900
H	-3.19134300	4.48325900	1.95131100
Ru	2.41465900	-0.07247400	-0.46639900
C	0.48624400	1.36546400	-0.34665200
C	1.54962600	1.64634700	0.60881700
C	2.93140900	-2.23326700	-1.42613200
C	2.02532400	-2.52925500	-0.38961200
H	1.13988300	-3.10244900	-0.63576900
C	2.27097700	-2.15711500	0.95437900
H	1.55587000	-2.44021900	1.71738900
C	3.45566500	-1.47946700	1.32613900
C	4.32532100	-1.09738400	0.27428500
H	5.20940200	-0.50975600	0.49141200
C	4.07239700	-1.46274500	-1.07275000
H	4.77041200	-1.15501700	-1.84134300

C	2.72865800	-2.74358000	-2.82597800
H	3.36694800	-3.61820300	-2.99909300
H	2.99060100	-1.98127200	-3.56277900
H	1.69131900	-3.04399500	-2.99420400
C	3.85894600	-1.18589800	2.76748100
H	4.04166000	-0.10450400	2.82790200
C	2.80256500	-1.55795100	3.81584600
H	1.85027600	-1.04842200	3.65429400
H	3.15925200	-1.27666000	4.81054300
H	2.61873500	-2.63865800	3.83182200
C	5.19033900	-1.90055900	3.09330900
H	5.99422000	-1.61070700	2.41167000
H	5.07309900	-2.98844300	3.03638300
H	5.50915800	-1.64851600	4.10908000
B	3.09216500	2.01130100	0.26894500
H	3.75376000	2.03522700	1.26137700
B	3.83791000	1.49346800	-1.32411600
H	4.96740500	1.11117000	-1.30093800
B	2.61973900	0.89090400	-2.49175700
H	2.89829900	0.08194200	-3.32306900
B	0.85756500	0.98407200	-1.91917200
H	0.01443200	0.31624500	-2.42133900
B	1.90100600	3.32929400	-0.20271800
H	1.54744900	4.13310600	0.59204200
B	3.50012900	3.18786800	-0.96803100
H	4.38514100	3.93875700	-0.71082700

B	3.27634500	2.53601000	-2.61012100
H	4.00486600	2.85086900	-3.49502600
B	1.55390900	2.24163100	-2.92555100
H	1.12917600	2.34839700	-4.03114700
B	0.62506000	2.74818800	-1.53180500
H	-0.41276000	3.28699800	-1.63791100
B	2.07232200	3.62791500	-1.91413900
H	1.87582000	4.75013200	-2.25391000

## Reference

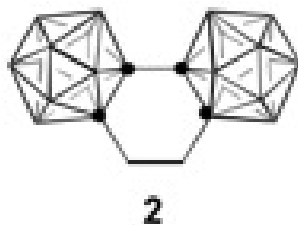
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7.260

2.668

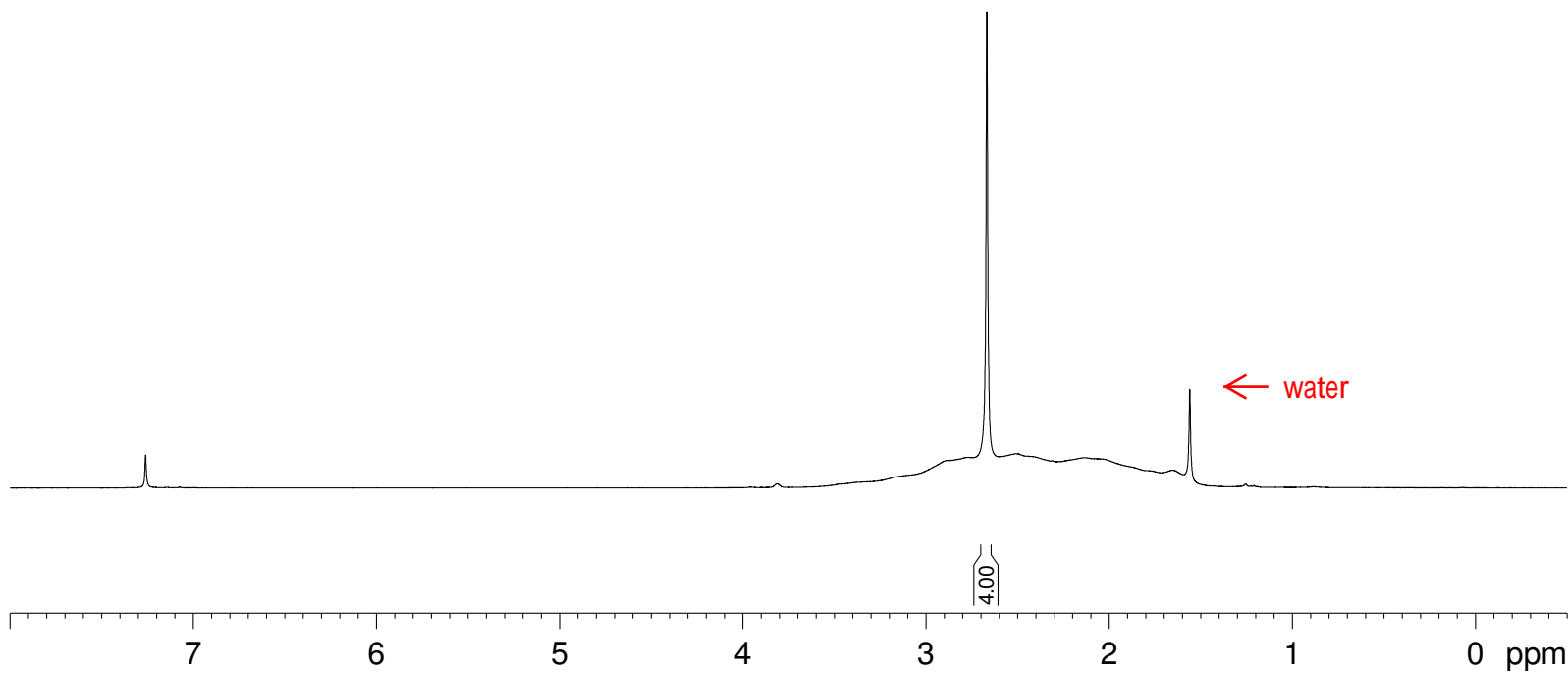
1.560

ZD-biscarborane-(CH<sub>2</sub>)<sub>2</sub>-311-CDCl<sub>3</sub>-



```
NAME ZD-biscarborane-(CH2)2-311-CDCl3-H
EXPNO 1
PROCNO 1
Date_ 20130218
Time 19.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 50.8
DW 60.800 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1
```

```
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -1.00 dB
PL1W 13.56617069 W
SFO1 400.1924713 MHz
SI 32768
SF 400.1900150 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```

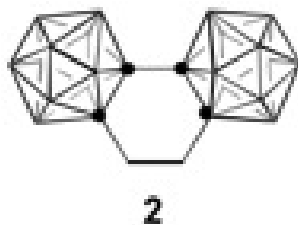




77.48  
77.16  
76.84  
71.78  
69.39

29.89

ZD-biscarborane-(CH<sub>2</sub>)<sub>2</sub>-311-CDCl<sub>3</sub>-C



```

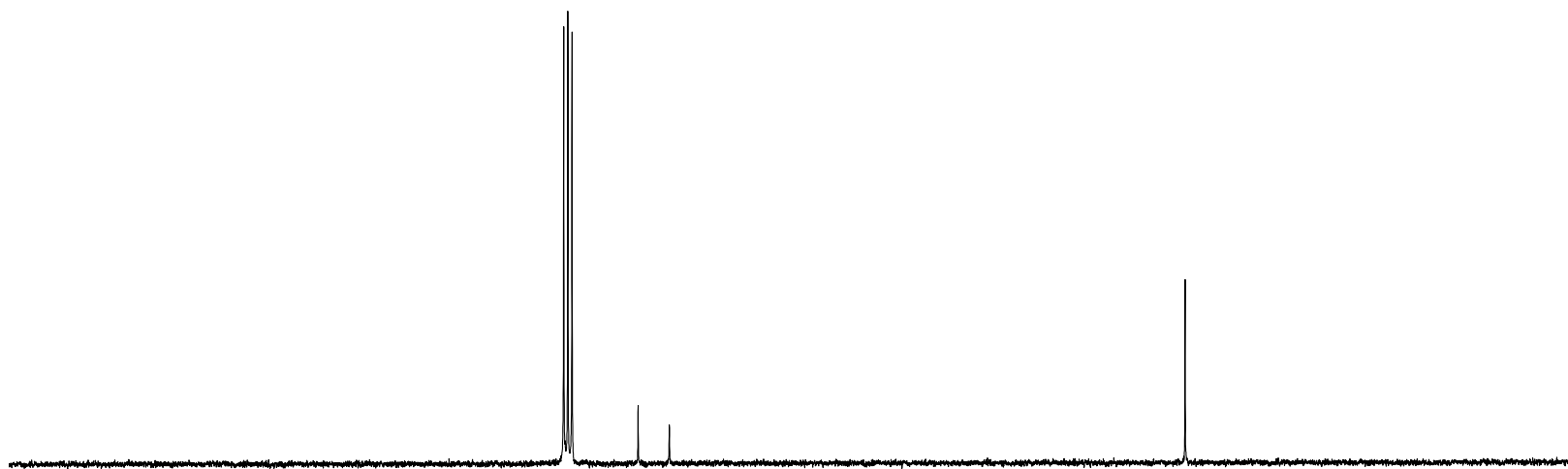
NAME      ZD-biscarborane-(CH2)2-311-CDCl3-C
EXPNO     1
PROCNO    1
Date_     20130218
Time      19.25
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         450
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         181
DW         20.800 usec
DE         6.50 usec
TE         296.2 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1       13C
P1         9.90 usec
PL1        -2.00 dB
PL1W       55.33689499 W
SFO1       100.6379183 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -1.00 dB
PL12       15.16 dB
PL13       18.62 dB
PL2W       13.56617069 W
PL12W      0.32844096 W
PL13W      0.14806664 W
SFO2       400.1916008 MHz
SI         32768
SF         100.6278441 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



110 100 90 80 70 60 50 40 30 20 10 ppm

ZD-biscarborane-(CH<sub>2</sub>)<sub>2</sub>-311-CDCl<sub>3</sub>-B (de

```

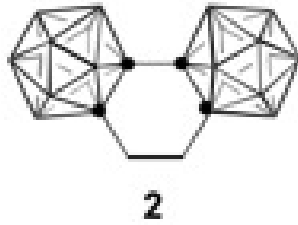
NAME      ZD-biscarborane-(CH2)2-311-CDCl3-B (de
EXPNO     1
PROCNO    1
Date_     20130218
Time      19.15
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgdc
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        25510.203 Hz
FIDRES     0.389255 Hz
AQ         1.2845556 sec
RG         203
DW         19.600 usec
DE         6.50 usec
TE         296.2 K
D1         5.0000000 sec
D11        0.0300000 sec
TD0        1
    
```

```

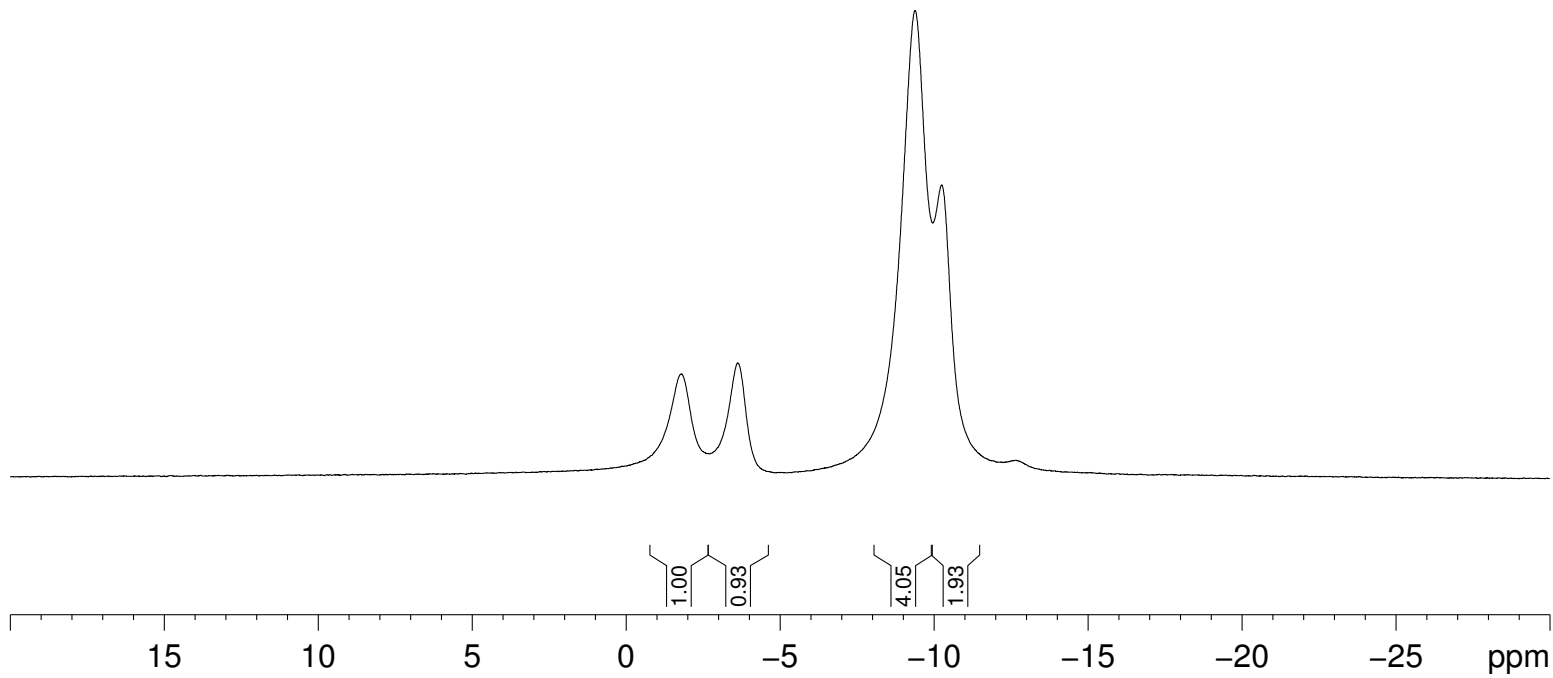
===== CHANNEL f1 =====
NUC1      11B
P1         7.60 usec
PL1        -3.00 dB
PL1W       55.13059616 W
SFO1      128.3968556 MHz
    
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2        -1.00 dB
PL12       15.16 dB
PL2W       13.56617069 W
PL12W      0.32844096 W
SFO2      400.1916008 MHz
SI         32768
SF         128.3968847 MHz
WDW        EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40
    
```

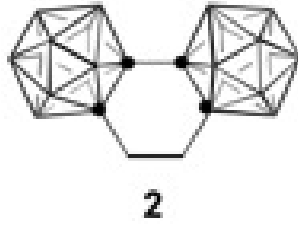


— -1.79  
— -3.62  
  
— -9.38  
— -10.25



ZD-biscarborane-(CH<sub>2</sub>)<sub>2</sub>-311-CDCl<sub>3</sub>-B(c)

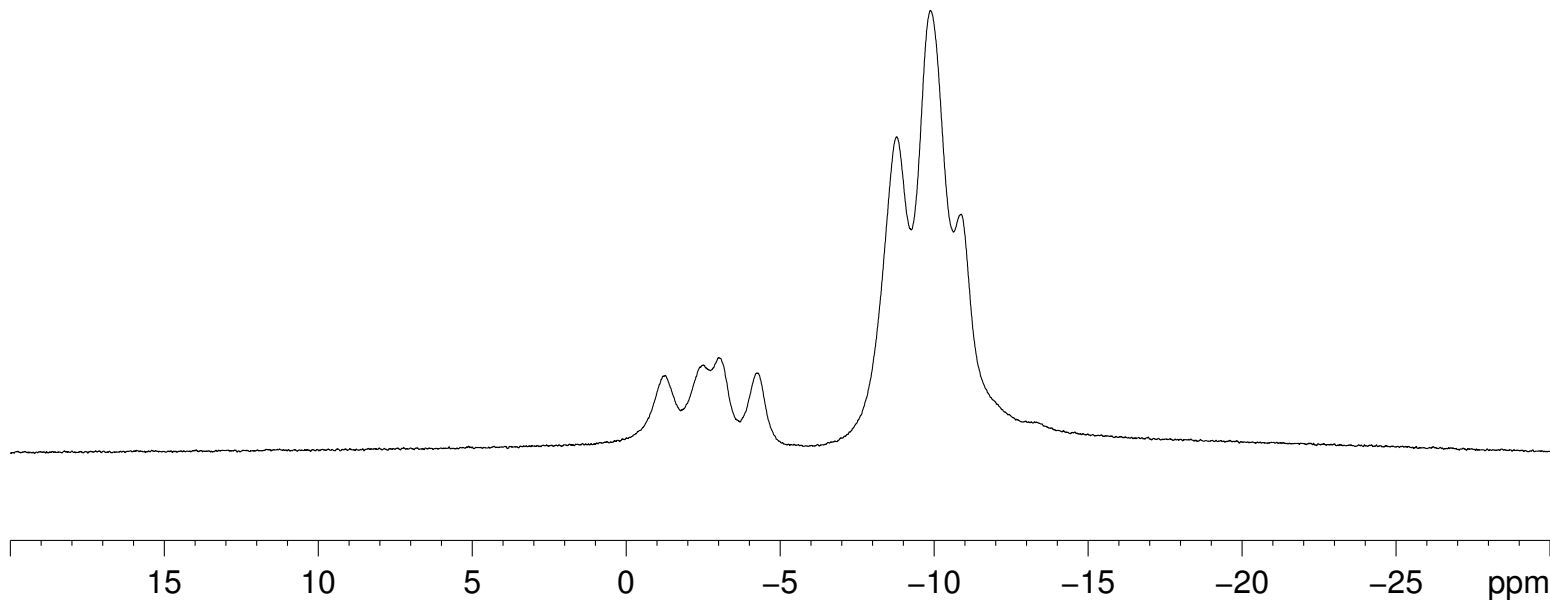
— -1.27      — -8.78  
 — -2.50      — -9.88  
 — -3.01      — -10.87  
 — -4.27



```

NAME      ZD-biscarborane-(CH2)2-311-CDCl3-B(c)
EXPNO     1
PROCNO    1
Date_     20130218
Time      19.16
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH       25510.203 Hz
FIDRES    0.389255 Hz
AQ         1.2845556 sec
RG         161
DW         19.600 usec
DE         6.50 usec
TE         295.9 K
D1         5.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      11B
P1         7.60 usec
PL1        -3.00 dB
PL1W       55.13059616 W
SF01      128.3968556 MHz
SI         32768
SF         128.3968865 MHz
WDW        EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40
  
```



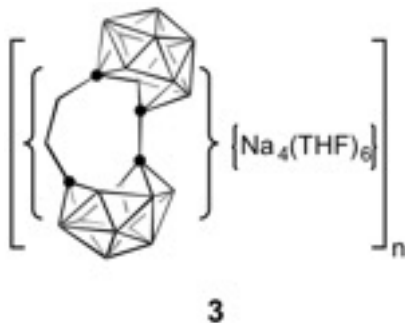
8.720  
7.591  
7.213

4.686

3.665  
3.650  
3.634  
3.622

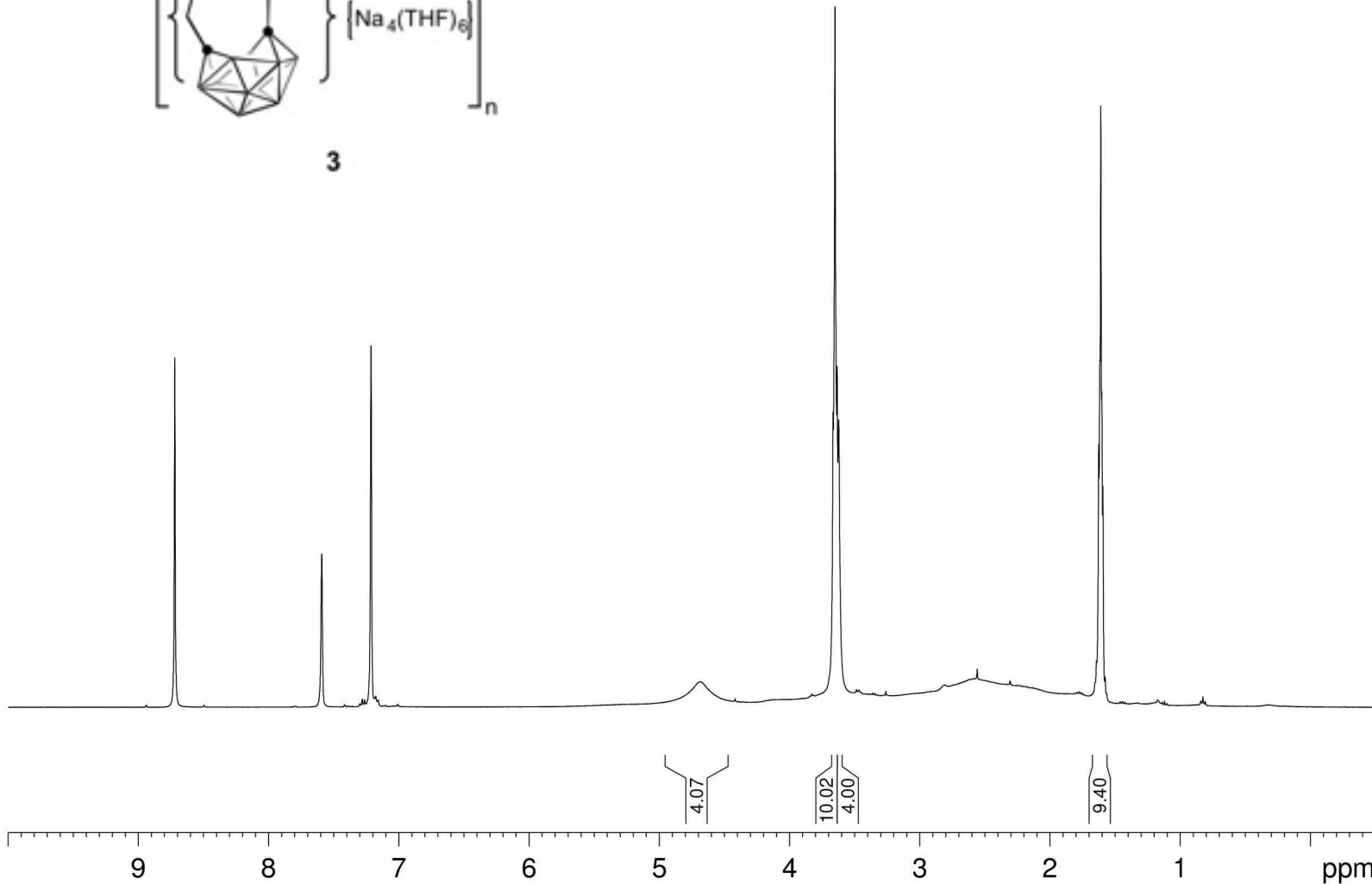
1.625  
1.617  
1.609  
1.602  
1.593

ZD-433-Pyr-H



NAME ZD-433-Pyr-H  
EXPNO 1  
PROCNO 1  
Date\_ 20130225  
Time 18.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT Pyr  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 45.2  
DW 60.800 usec  
DE 6.50 usec  
TE 294.9 K  
D1 1.00000000 sec  
TD0 1

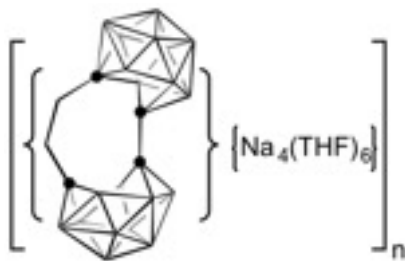
===== CHANNEL f1 =====  
NUC1 1H  
P1 14.00 usec  
PL1 -1.00 dB  
PL1W 13.56617069 W  
SFO1 400.1924713 MHz  
SI 32768  
SF 400.1899995 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



150.11  
149.84  
149.57

135.85  
135.60  
135.35

123.78  
123.53  
123.28



3

67.83

43.92  
40.98

25.77

ZD-433-Pyr-C

```

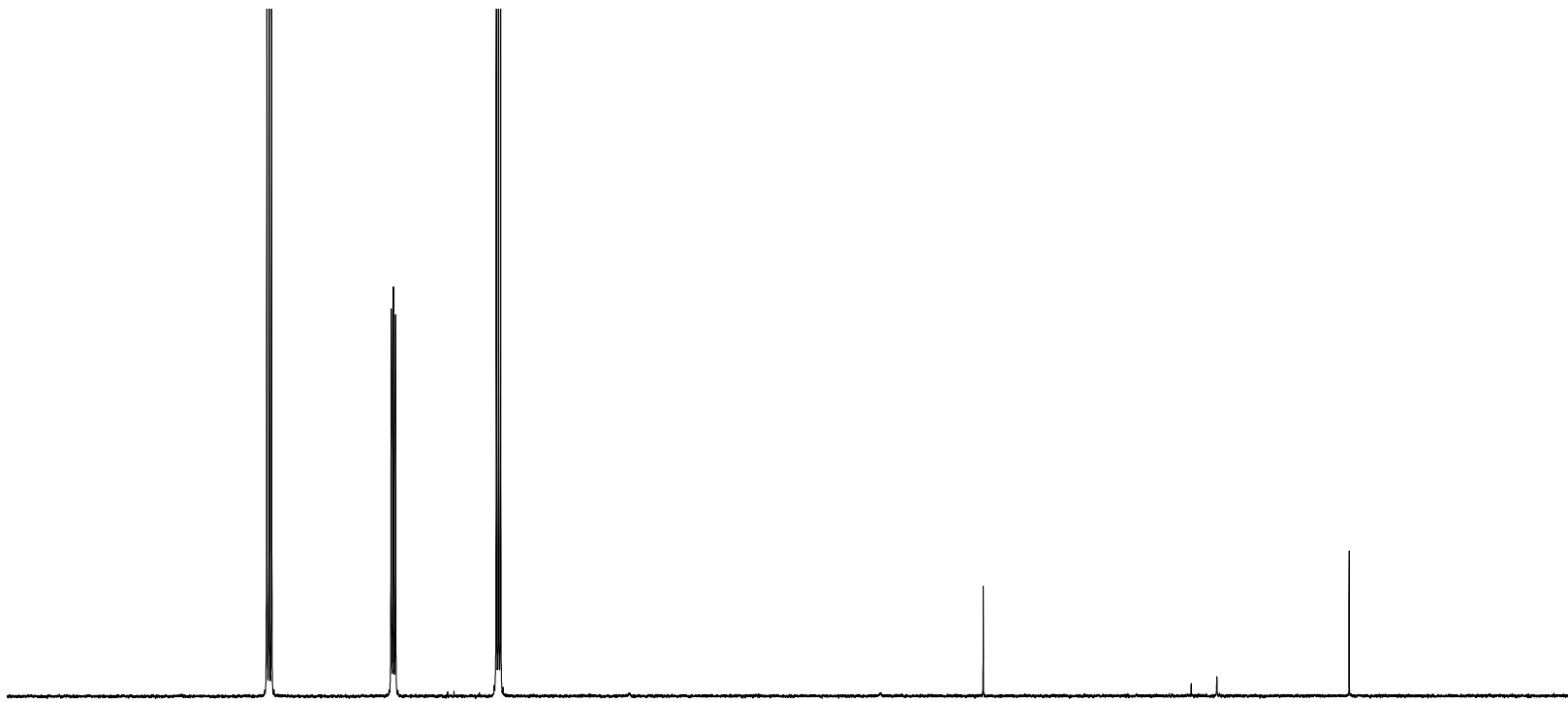
NAME      ZD-433-Pyr-C
EXPNO     1
PROCNO    1
Date_     20130225
Time      19.02
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   Pyr
NS        975
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        2050
DW        20.800 usec
DE        6.50 usec
TE        295.5 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

```

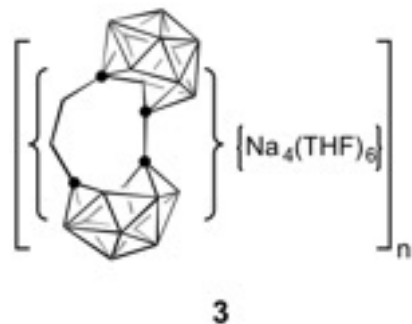
===== CHANNEL f1 =====
NUC1      13C
P1        9.90 usec
PL1       -2.00 dB
PL1W      55.33689499 W
SFO1      100.6379183 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -1.00 dB
PL12      15.16 dB
PL13      18.62 dB
PL2W      13.56617069 W
PL12W     0.32844096 W
PL13W     0.14806664 W
SFO2      400.1916008 MHz
SI        32768
SF        100.6278389 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm



— -6.96  
 — -8.19  
 — -10.28  
 — -15.21  
 — -24.43

ZD-433-Pyr-B (de)

```

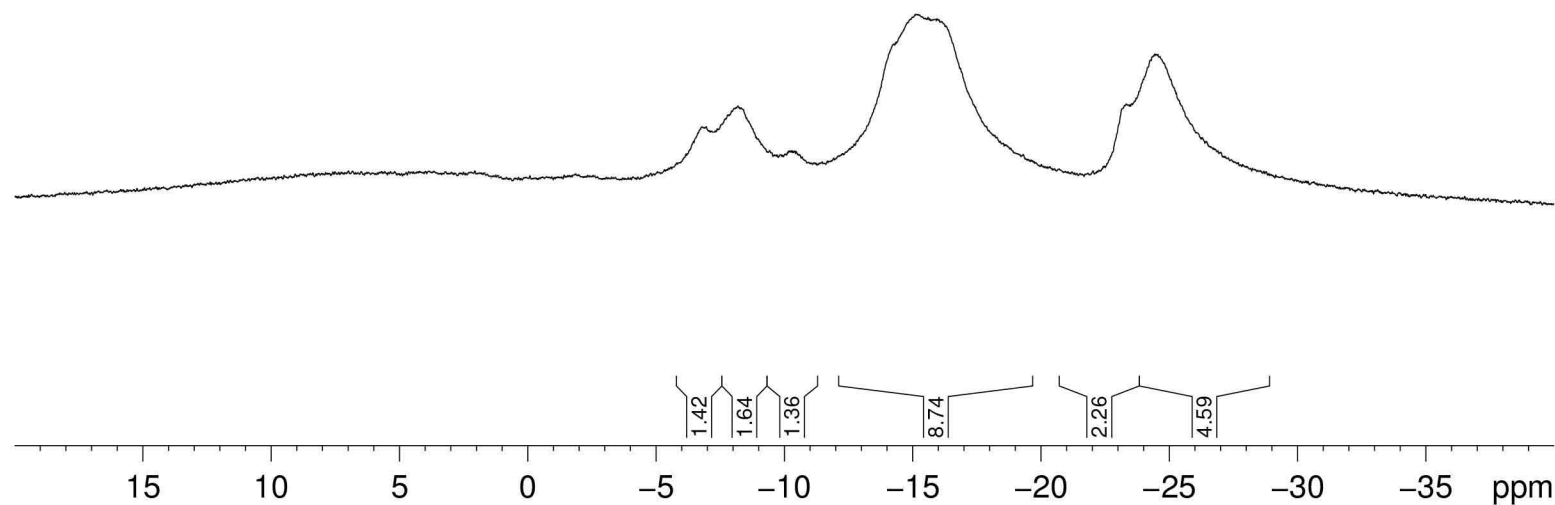
NAME      ZD-433-Pyr-B (de)
EXPNO     1
PROCNO    1
Date_     20130224
Time      18.32
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgdc
TD        65536
SOLVENT   CD2C12
NS        12
DS        0
SWH       25510.203 Hz
FIDRES    0.389255 Hz
AQ        1.2845556 sec
RG        287
DW        19.600 usec
DE        6.50 usec
TE        296.0 K
D1        5.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

```

===== CHANNEL f1 =====
NUC1      11B
P1        7.60 usec
PL1       -3.00 dB
PL1W      55.13059616 W
SFO1      128.3968556 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -1.00 dB
PL12      15.16 dB
PL2W      13.56617069 W
PL12W     0.32844096 W
SFO2      400.1916008 MHz
SI        32768
SF        128.3968847 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40
  
```



ZD-433-Pyr-B (c)

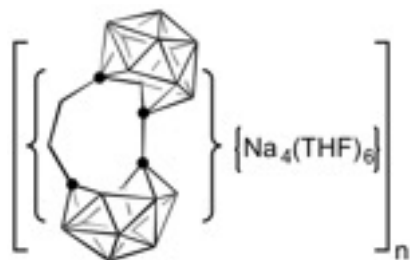
```

NAME      ZD-433-Pyr-B(c)
EXPNO     1
PROCNO    1
Date_     20130224
Time      18.33
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CD2Cl2
NS         12
DS         0
SWH        25510.203 Hz
FIDRES     0.389255 Hz
AQ         1.2845556 sec
RG         161
DW         19.600 usec
DE         6.50 usec
TE         295.9 K
D1         5.00000000 sec
TD0        1
    
```

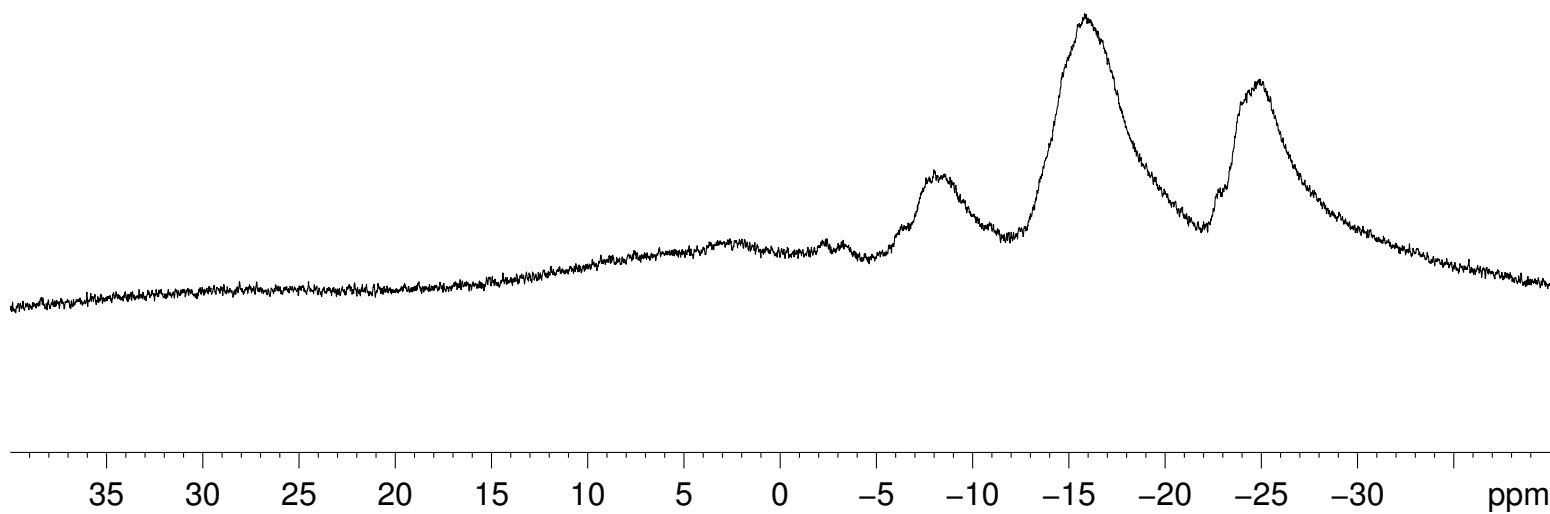
```

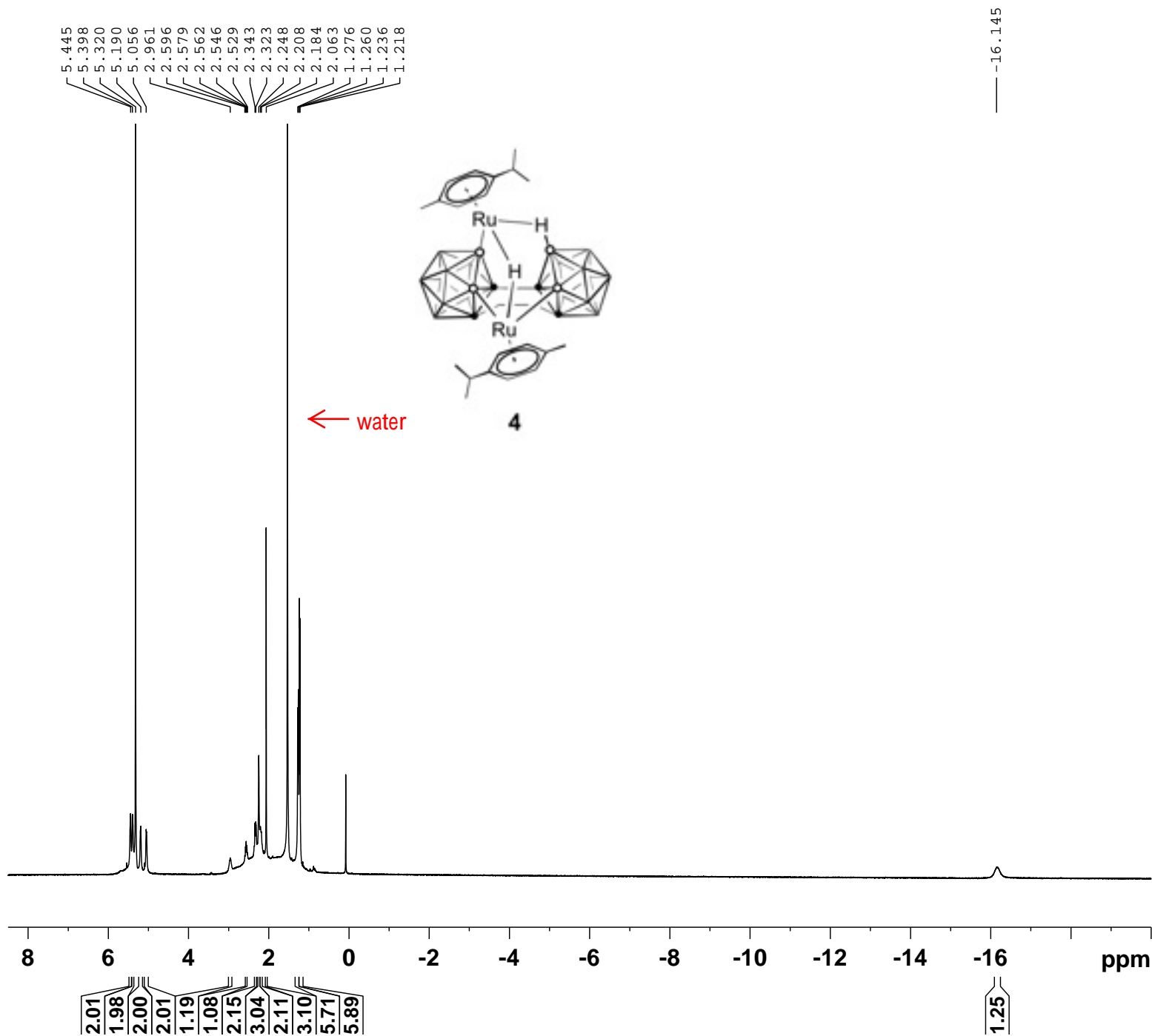
===== CHANNEL f1 =====
NUC1      11B
P1        7.60 usec
PL1       -3.00 dB
PL1W      55.13059616 W
SFO1      128.3968556 MHz
SI         32768
SF         128.3968865 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
    
```

— -7.99  
 — -15.82  
 — -24.90



3





```

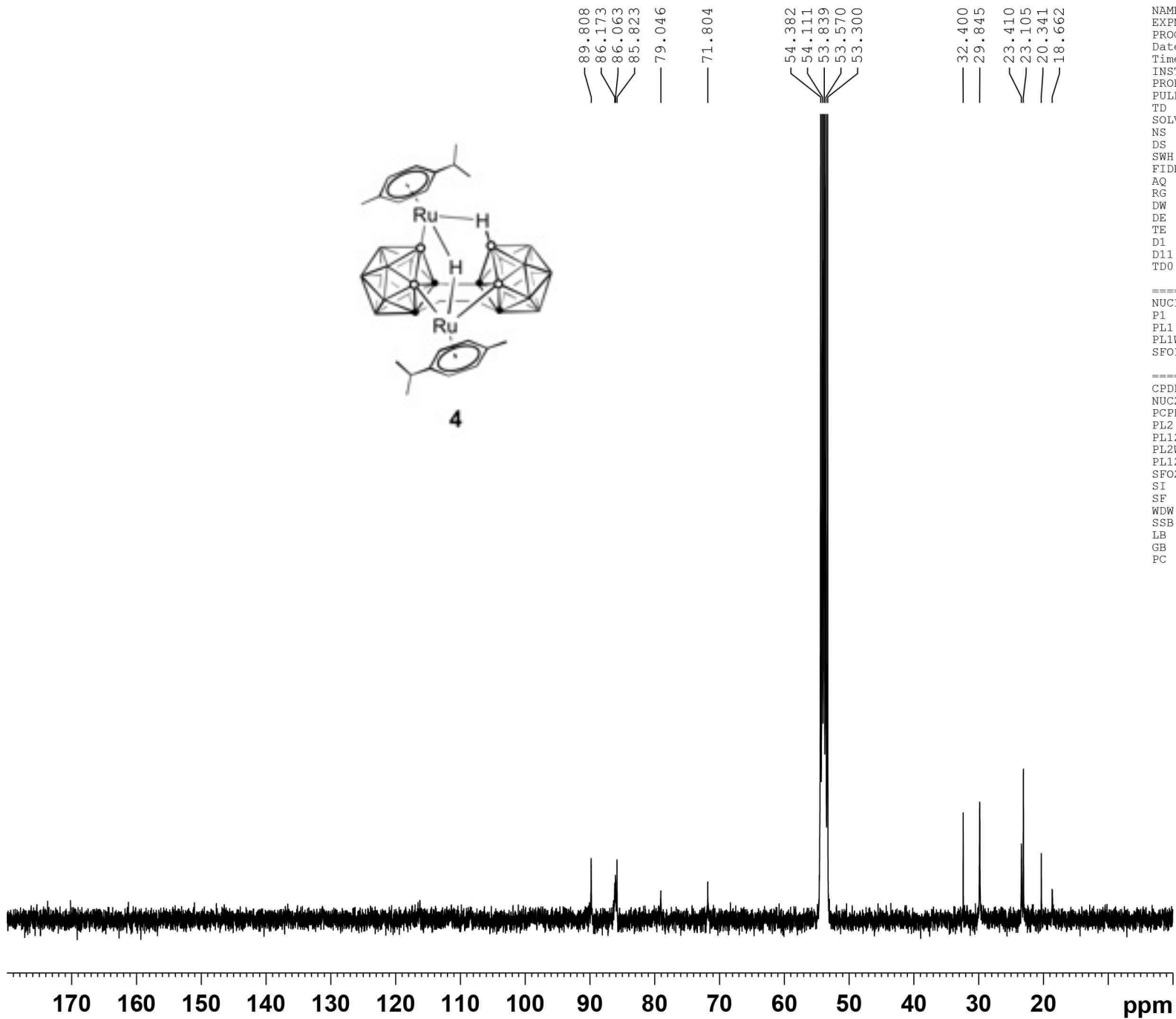
NAME      ZD-177-1-CD2Cl2-H
EXPNO     1
PROCNO    1
Date_     20110510
Time      15.41
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CD2Cl2
NS         128
DS         2
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         228
DW         20.800 usec
DE         6.50 usec
TE         297.0 K
D1         1.00000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1       1H
P1         14.00 usec
PL1        -1.00 dB
PL1W       13.56617069 W
SFO1       400.1908004 MHz
SI         32768
SF         400.1900192 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

-16.145





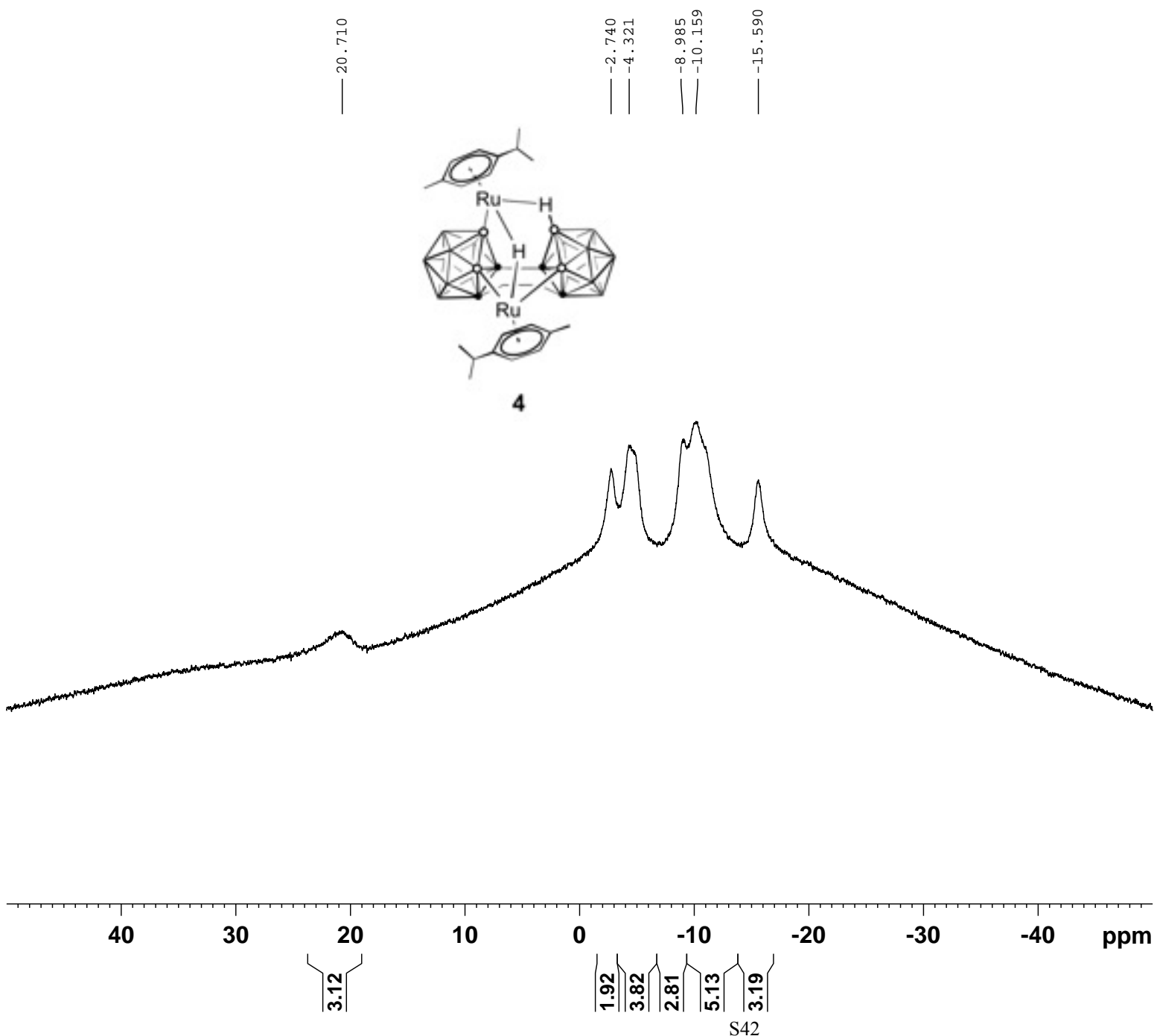
```

NAME      ZD-1-77-1-CD2C12-C
EXPNO     1
PROCNO    1
Date_     20110509
Time      22.55
INSTRUM   spect
PROBHD    5 mm PADUL 13C
PULPROG   zgdc
TD         131072
SOLVENT   CD2C12
NS         31278
DS         0
SWH       29761.904 Hz
FIDRES    0.227065 Hz
AQ         2.2020595 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE         294.7 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.68 usec
PL1        -0.60 dB
PL1W       41.24164963 W
SFO1       100.6227690 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2         0.00 dB
PL12       15.66 dB
PL2W       8.31434441 W
PL12W      0.22585411 W
SFO2       400.1320007 MHz
SI         131072
SF         100.6127271 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40

```



```

NAME      ZD-1-77-1-CD2C12-B(de)
EXPNO     1
PROCNO    1
Date_     20110510
Time      12.05
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgdc
TD         65536
SOLVENT   CDC13
NS         200
DS         0
SWH        25510.203 Hz
FIDRES     0.389255 Hz
AQ         1.2845556 sec
RG         456
DW         19.600 usec
DE         6.50 usec
TE         297.4 K
D1         5.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      11B
P1        7.60 usec
PL1       -3.00 dB
PL1W      55.13059616 W
SFO1      128.3968556 MHz
  
```

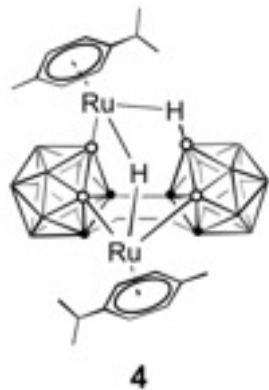
```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2        -1.00 dB
PL12      15.16 dB
PL2W      13.56617069 W
PL12W     0.32844096 W
SFO2      400.1916008 MHz
SI         32768
SF         128.3968863 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
  
```

— 20.43

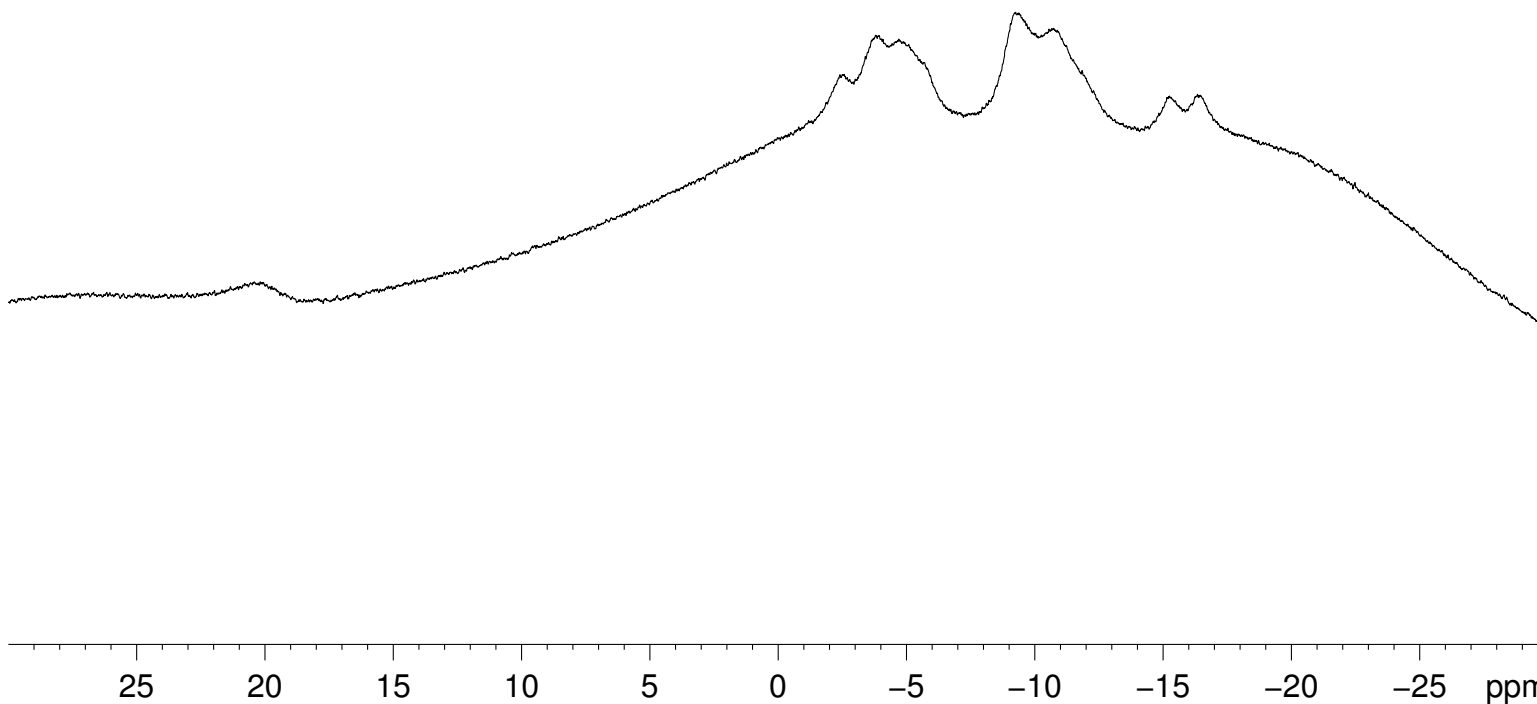
— -2.48  
— -3.80  
— -4.52  
  
— -9.26  
— -10.72  
  
— -15.13  
— -16.26

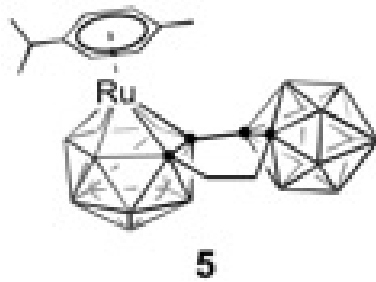
ZD-1-77-1-CD2Cl2-B (cou)



```
NAME      ZD-1-77-1-CD2Cl2-B (cou)
EXPNO     1
PROCNO    1
Date_     20110510
Time      13.56
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   THF
NS         800
DS         0
SWH        25510.203 Hz
FIDRES     0.389255 Hz
AQ         1.2845556 sec
RG         456
DW         19.600 usec
DE         6.50 usec
TE         297.0 K
D1         5.00000000 sec
TD0        1
```

```
===== CHANNEL f1 =====
NUC1      11B
P1         7.60 usec
PL1        -3.00 dB
PL1W      55.13059616 W
SFO1      128.3968556 MHz
SI         32768
SF         128.3968865 MHz
WDW        EM
SSB         0
LB         3.00 Hz
GB         0
PC         1.40
```





6.432  
6.416  
6.278  
6.262  
6.109  
6.103  
6.099  
6.088  
5.322  
5.320  
5.318

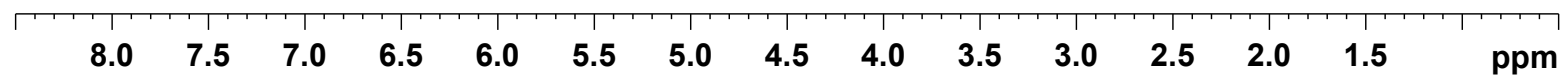
3.130  
3.122  
3.110  
3.099  
3.016  
2.999  
2.982  
2.964  
2.947  
2.930  
2.913  
2.627  
2.616  
2.605  
2.590  
2.580  
2.568  
2.536  
2.513  
2.499  
2.490  
2.478  
2.452  
2.344  
1.348  
1.330  
1.327  
1.310

← water

```

NAME          1D_1H-2
EXPNO         1
PROCNO        1
Date_         20110508
Time          15.29
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CD2Cl2
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            114
DW            60.800 usec
DE            6.50 usec
TE            296.7 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            14.00 usec
PL1           -1.00 dB
PL1W         13.56617069 W
SFO1         400.1924713 MHz
SI            32768
SF           400.1900200 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



1.00  
1.01  
2.03

S44

2.02  
1.22  
2.22  
3.13  
6.29

ZD-1-79-2-CD2C12-C

```

NAME      ZD-1-79-2-CD2C12-C
EXPNO     1
PROCNO    1
Date_     20110508
Time      22.46
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CD2C12
NS         11332
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         181
DW         20.800 usec
DE         6.50 usec
TE         297.5 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

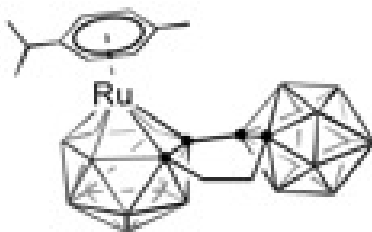
===== CHANNEL f1 =====
NUC1      13C
P1        9.90 usec
PL1       -2.00 dB
PL1W      55.33689499 W
SFO1      100.6379183 MHz
  
```

```

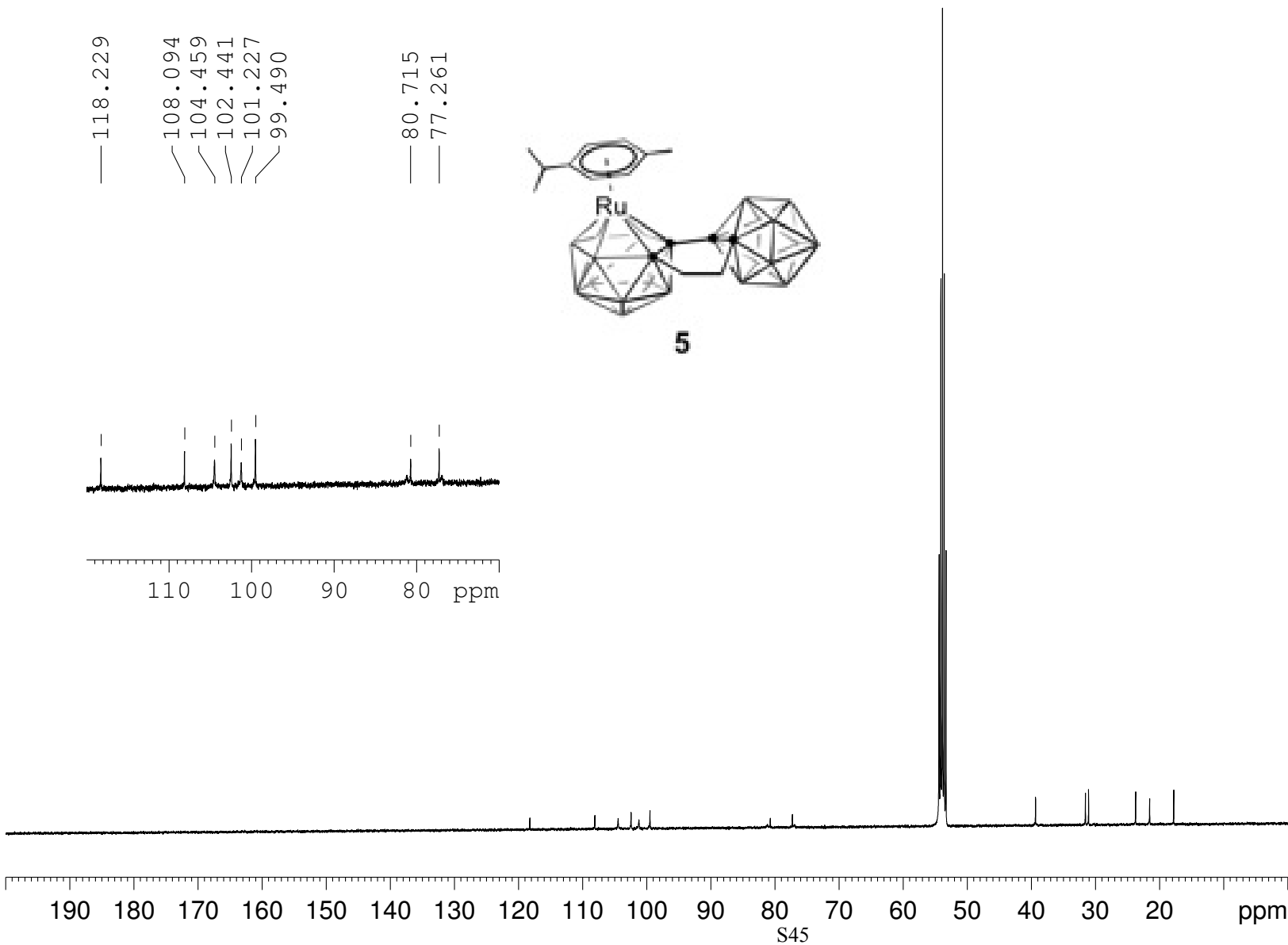
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -1.00 dB
PL12      15.16 dB
PL13      18.62 dB
PL2W      13.56617069 W
PL12W     0.32844096 W
PL13W     0.14806664 W
SFO2      400.1916008 MHz
SI        32768
SF        100.6278149 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

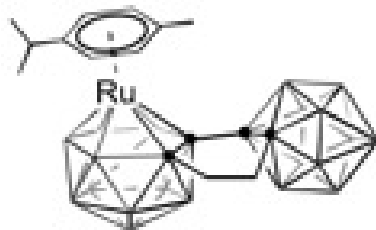
118.23  
 108.09  
 104.46  
 102.44  
 101.23  
 99.49  
 80.72  
 77.26  
 54.38  
 54.11  
 53.84  
 53.57  
 53.30  
 39.34  
 31.54  
 31.06  
 23.72  
 21.53  
 17.77

118.229  
 108.094  
 104.459  
 102.441  
 101.227  
 99.490  
 80.715  
 77.261



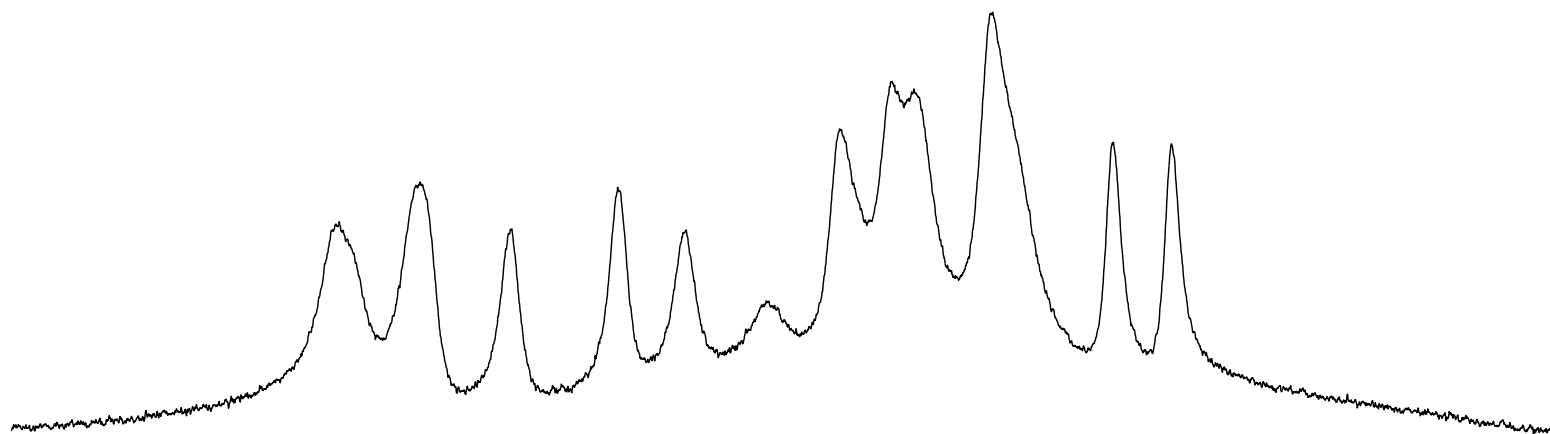
5





5

— 9.372  
 — 6.774  
 — 3.804  
 — 0.278  
 — -1.856  
 — -4.547  
 — -6.959  
 — -8.629  
 — -9.325  
 — -11.831  
 — -15.820  
 — -17.723



15 10 5 0 -5 -10 -15 -20 -25 ppm

2.00 1.85 1.26 1.08 1.04 1.12 2.12 1.32 1.94 4.16 1.09 1.02

```

NAME      ZD-1-79-2-CD2C12-B(de)
EXPNO     1
PROCNO    1
Date_     20110508
Time      15.33
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgdc
TD         65536
SOLVENT   CD2C12
NS         32
DS         0
SWH       25510.203 Hz
FIDRES    0.389255 Hz
AQ         1.2845556 sec
RG         287
DW         19.600 usec
DE         6.50 usec
TE         297.2 K
D1         5.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      11B
P1         7.60 usec
PL1        -3.00 dB
PL1W      55.13059616 W
SFO1      128.3968556 MHz
  
```

```

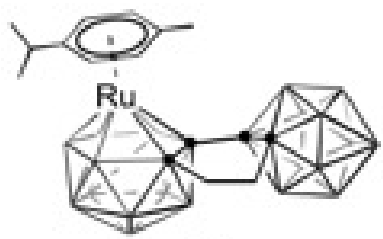
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      90.00 usec
PL2         -1.00 dB
PL12       15.16 dB
PL2W      13.56617069 W
PL12W      0.32844096 W
SFO2      400.1916008 MHz
SI         32768
SF         128.3969291 MHz
WDW        EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40
  
```

ZD-1-79-2-CD2Cl2-B (cou)

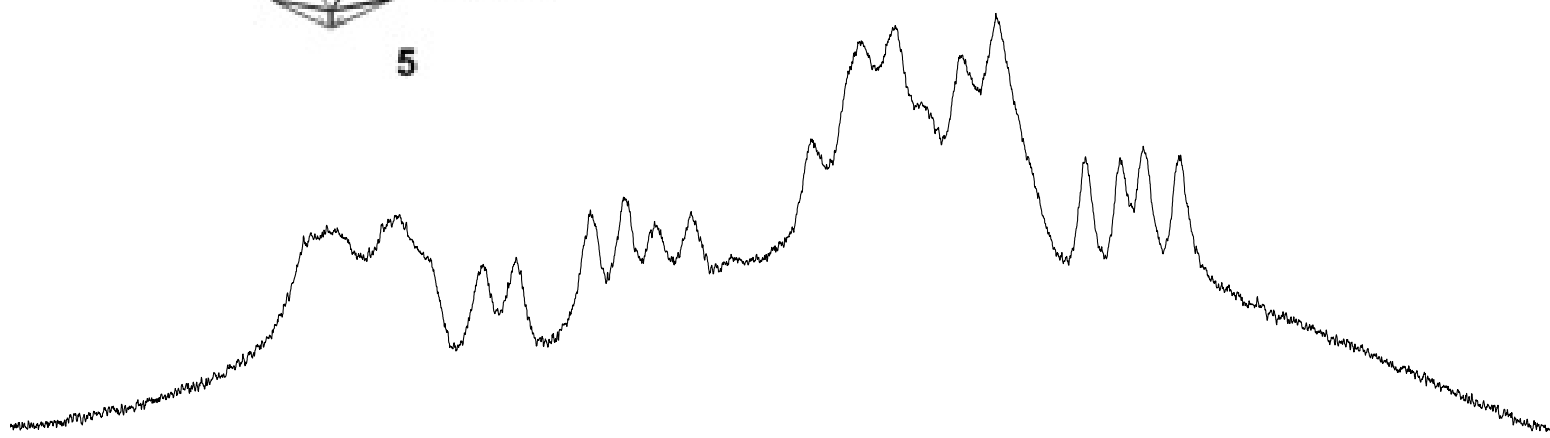
```
NAME      ZD-1-79-2-CD2Cl2-B (cou)
EXPNO     1
PROCNO    1
Date_     20110508
Time      15.43
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CD2Cl2
NS         64
DS         0
SWH        25510.203 Hz
FIDRES     0.389255 Hz
AQ         1.2845556 sec
RG         456
DW         19.600 usec
DE         6.50 usec
TE         296.6 K
D1         5.00000000 sec
TDO        1
```

```
===== CHANNEL f1 =====
NUC1      11B
P1         7.60 usec
PL1        -3.00 dB
PL1W      55.13059616 W
SFO1      128.3968556 MHz
SI         32768
SF         128.3968865 MHz
WDW        EM
SSB         0
LB         3.00 Hz
GB         0
PC         1.40
```

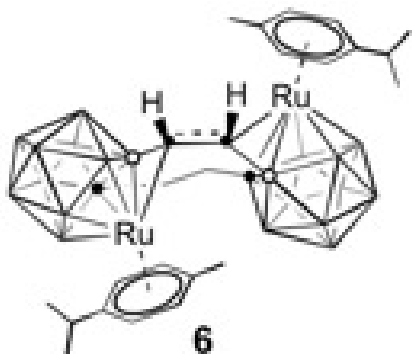
9.72  
7.36  
4.64  
3.56  
1.16  
0.09  
-0.92  
-2.11  
-6.00  
-7.64  
-8.74  
-10.92  
-12.00  
-14.92  
-16.04  
-16.79  
-18.01



5



15 10 5 0 -5 -10 -15 -20 -25 ppm



6.625  
6.464  
6.326  
6.207  
5.686  
5.320

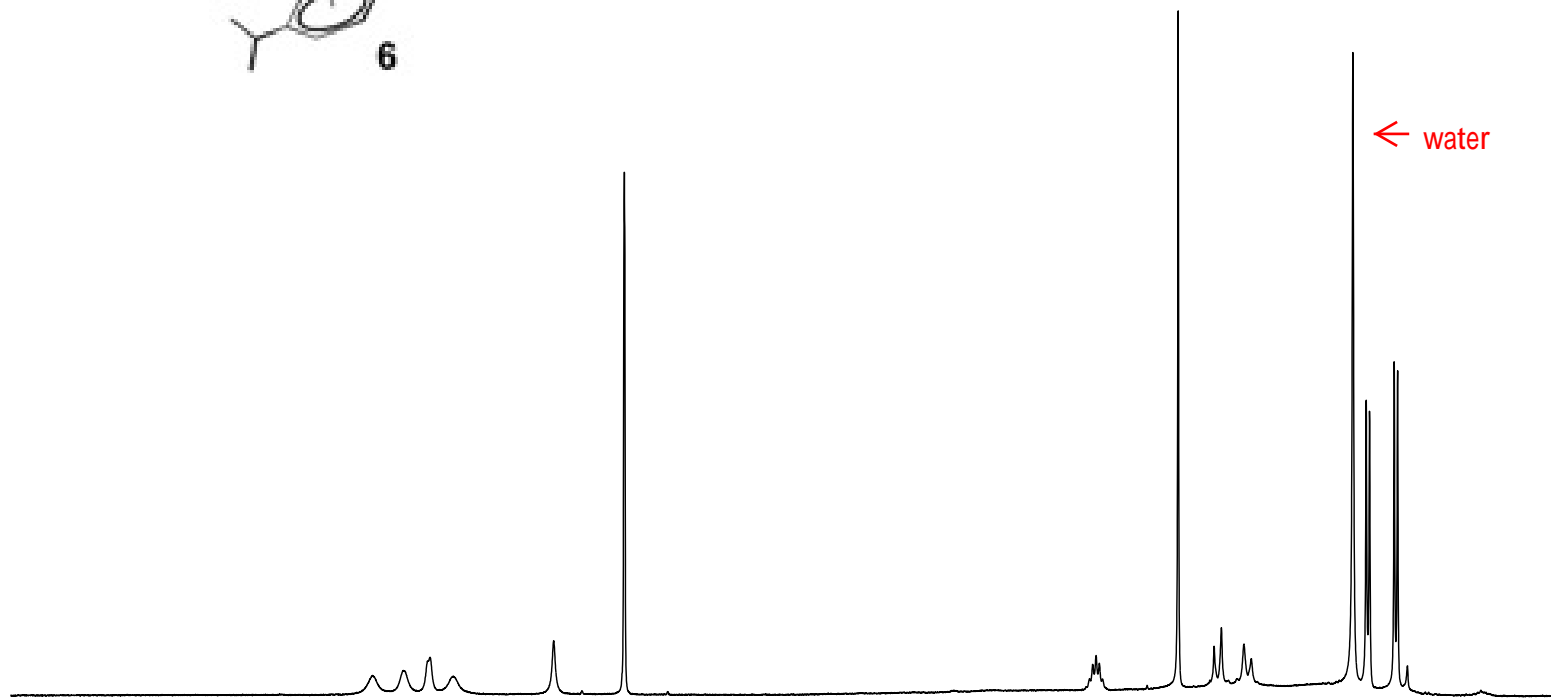
2.908  
2.891  
2.874  
2.857  
2.841  
2.448  
2.262  
2.224  
2.107  
2.069  
1.542  
1.473  
1.456  
1.328  
1.310

```

NAME      ZD-1-67-3-CD2C12-H
EXPNO     1
PROCNO    1
Date_     20110326
Time      21.14
INSTRUM   spect
PROBHD    5 mm PADUL 13C
PULPROG   zg30
TD         65536
SOLVENT   CD2C12
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         203
DW         60.800 usec
DE         6.50 usec
TE         295.0 K
D1         1.00000000 sec
TD0        1
  
```

```

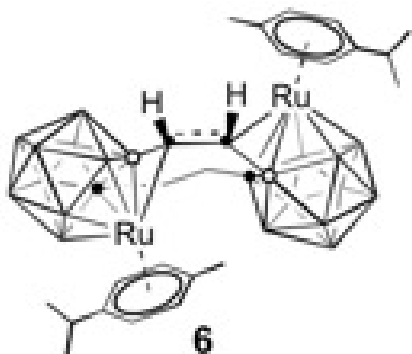
===== CHANNEL f1 =====
NUC1      1H
P1        14.83 usec
PL1       0.00 dB
PL1W      8.31434441 W
SFO1      400.1324710 MHz
SI        32768
SF        400.1300156 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```



8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm

2.00 2.04 2.09 2.06 2.06 2.07 6.57 2.17 2.08 6.49 6.58





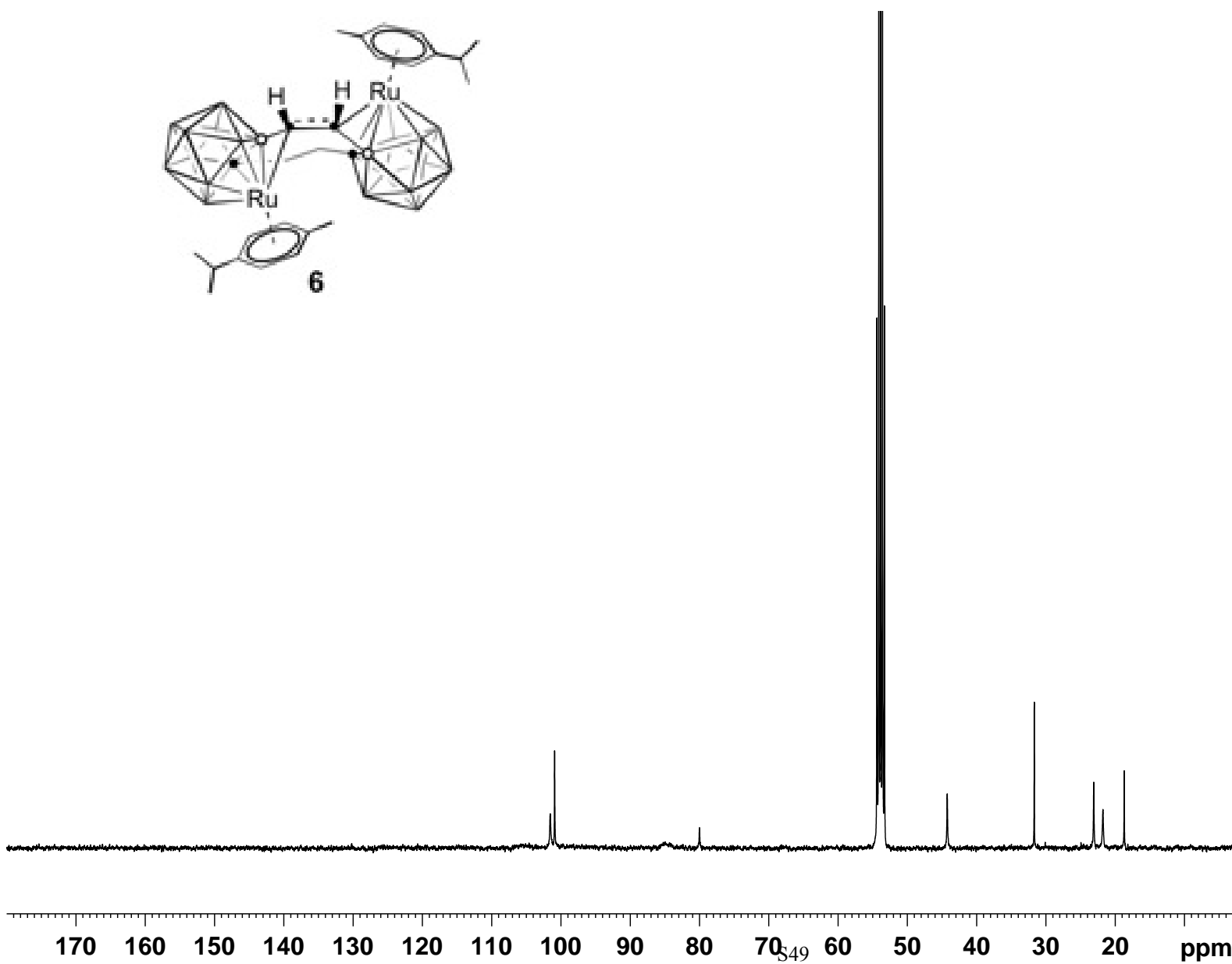
101.536  
100.899

84.895  
80.000

54.380  
54.111  
53.841  
53.570  
53.299  
44.235

31.671

23.096  
21.771  
18.694



```

NAME      ZD-1-67-3-CD2C12-C
EXPNO     1
PROCNO    1
Date_     20110326
Time      21.20
INSTRUM   spect
PROBHD    5 mm PADUL 13C
PULPROG   zgdc
TD         131072
SOLVENT   CD2C12
NS         17799
DS         0
SWH        29761.904 Hz
FIDRES     0.227065 Hz
AQ         2.2020595 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE         295.0 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

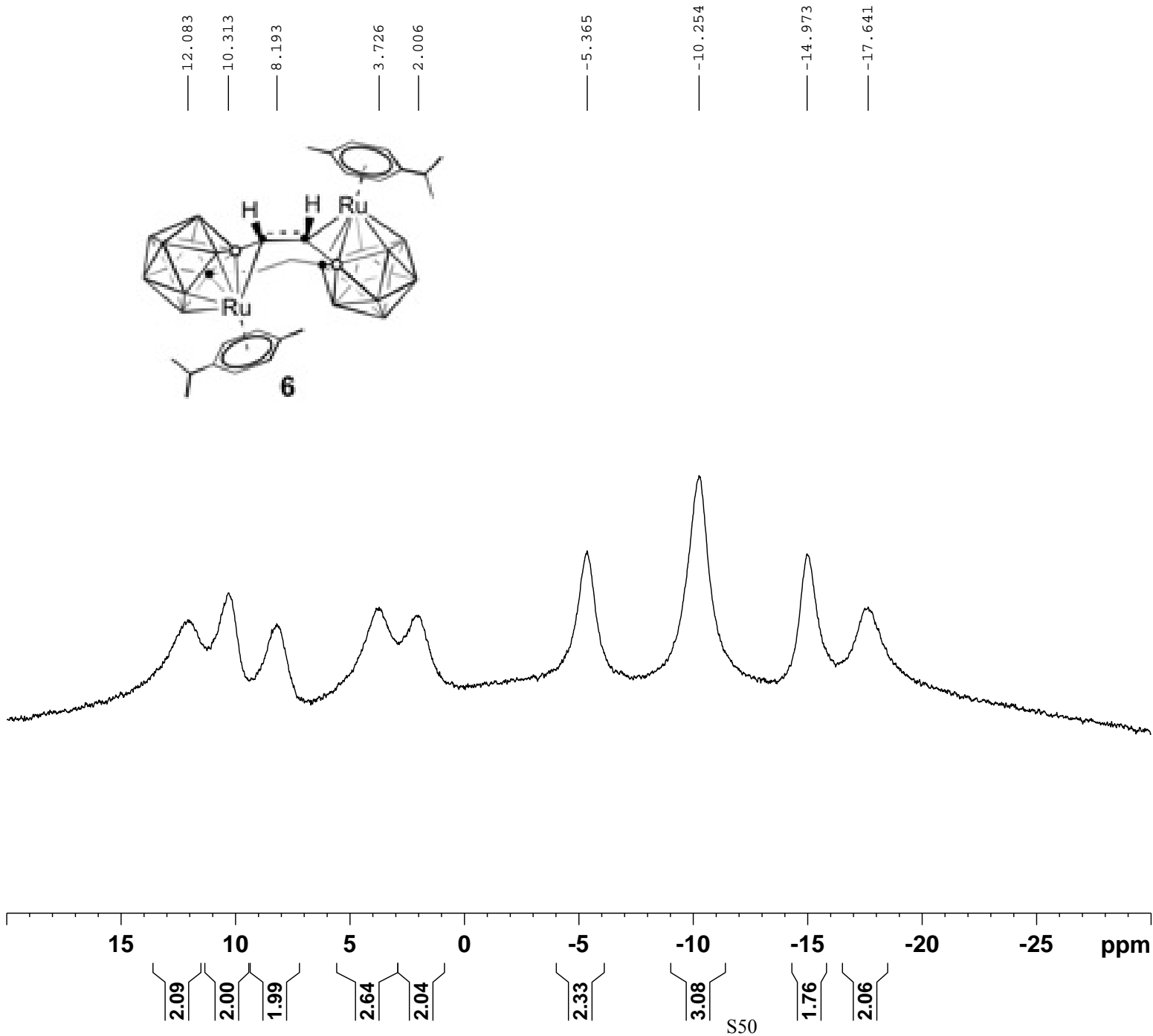
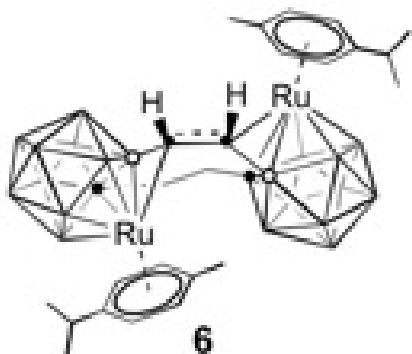
===== CHANNEL f1 =====
NUC1       13C
P1         9.68 usec
PL1        -0.60 dB
PL1W       41.24164963 W
SFO1       100.6227690 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2         0.00 dB
PL12       15.66 dB
PL2W       8.31434441 W
PL12W      0.22585411 W
SFO2       400.1320007 MHz
SI         131072
SF         100.6127279 MHz
WDW        EM
SSB         0
LB         3.00 Hz
GB         0
PC         1.40

```



```

NAME      ZD-1-67-3-CD2C12-B(de)
EXPNO     1
PROCNO    1
Date_     20110327
Time      13.59
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgdc
TD         65536
SOLVENT   CDCl3
NS         64
DS         0
SWH       25510.203 Hz
FIDRES    0.389255 Hz
AQ         1.2845556 sec
RG         362
DW         19.600 usec
DE         6.50 usec
TE         297.5 K
D1         5.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

===== CHANNEL f1 =====
NUC1      11B
P1         7.60 usec
PL1        -3.00 dB
PL1W      55.13059616 W
SFO1      128.3968556 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2        -1.00 dB
PL12       15.16 dB
PL2W      13.56617069 W
PL12W     0.32844096 W
SFO2      400.1916008 MHz
SI         32768
SF         128.3968863 MHz
WDW        EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40

```

ZD-1-67-3-CD2Cl2-B (cou)

```
NAME      ZD-1-67-3-CD2Cl2-B (cou)
EXPNO     1
PROCNO    1
Date_     20110327
Time      14.10
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         400
DS         0
SWH        25510.203 Hz
FIDRES     0.389255 Hz
AQ         1.2845556 sec
RG         456
DW         19.600 usec
DE         6.50 usec
TE         297.2 K
D1         5.00000000 sec
TDO        1
```

```
===== CHANNEL f1 =====
NUC1      11B
P1         7.60 usec
PL1        -3.00 dB
PL1W      55.13059616 W
SF01      128.3968556 MHz
SI         32768
SF         128.3968865 MHz
WDW        EM
SSB         0
LB         3.00 Hz
GB         0
PC         1.40
```

12.03  
10.74  
9.61

2.79

-4.88  
-5.92

-9.81  
-10.85

-14.53  
-15.61

-18.18

