

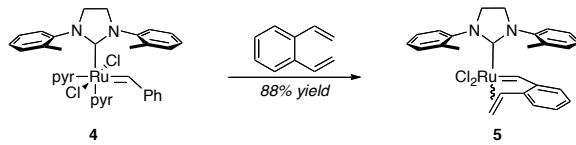
Conformations of N-Heterocyclic Carbene Ligands in Ruthenium Complexes Relevant to Olefin Metathesis

*Ian C. Stewart, Diego Benitez, Daniel J. O’Leary,¹ Ekaterina Tkatchouk, Michael W. Day, William A. Goddard, III, Robert H. Grubbs**

Supporting Information

Experimental Section: Synthesis

General. All glassware was either oven dried or flame dried, and reactions were done under an atmosphere of argon or in a nitrogen-filled glovebox unless otherwise noted. All organic solvents were dried by passage through solvent purification columns containing activated alumina. All commercial chemicals were used as obtained. Divinylbenzene was prepared according to literature procedure.² High-resolution mass spectrometry (HRMS) data were obtained on a JEOL MSRoute mass spectrometer.



Preparation of π -Complex 5. In a nitrogen-filled glovebox, a 20 mL scintillation vial was charged with **4** (0.16 g, 0.24 mmol) and benzene (4 mL). A solution of 1,2-divinylbenzene (0.034 mg, 0.26 mmol) in benzene (4 mL) was then added. The vial was capped and stored in the glovebox at r.t. for 18 h. The resulting burnt orange solution was decanted, leaving a green crystalline solid. The solid was removed from the glovebox, washed with pentane (2 x 2 mL), and dried under vacuum, yielding 0.11 g (88%). See pages S12-S29 for NMR characterization data. HR-MS (FAB+) Calculated for $C_{26}H_{26}N_2Cl_2Ru$, 538.0517; found, 538.0518.

Experimental Section: NMR Spectroscopy Experiments

NMR spectra were obtained on a Bruker Avance DPX 400 MHz NMR spectrometer equipped with a 5 mm dual $^1\text{H}/^{13}\text{C}$ Z-gradient probe. Unless otherwise specified, spectra were obtained at 23 °C. For experiments requiring low temperatures, the probe was calibrated with a sample of methanol containing a trace amount of gaseous HCl.³ 1D ^1H and ^{13}C spectra were acquired with standard pulse sequences and parameters. Details for the 2D experiments are as follows:

¹ Current address: Department of Chemistry, Bowdoin College, Brunswick, ME 04011.

² Mitchell, R. H.; Ghose, B. N.; Williams, M. E. *Can. J. Chem.* **1977**, *55*, 210.

³ Braun, S.; Kalinowski, H.-O.; Berger, S. *150 and More NMR Experiments: A Practical Course*; Wiley-VCH: Weinheim, 1998.

Gradient-enhanced 2D COSY experiment.⁴ The **cosygs** pulse program was used with the following acquisition parameters. F2 and F1 sweep widths, 7184 Hz. F2 and F1 digital resolution, 7.01 Hz/pt. 256 FIDs recorded, each consisting of 4 scans and 1024 data points (AQ = 0.071 s). A recycle delay of (D1) of 1.5 s was employed. Processing parameters: unshifted sinusoidal apodization was applied in both dimensions prior to the Fourier transformation.

2D COSYLR experiment.⁵ The **cosylr** pulse program was used with the following acquisition parameters. F2 and F1 sweep widths, 7184 Hz. F2 and F1 digital resolution, 7.01 Hz/pt. 128 FIDs recorded, each consisting of 8 scans and 1024 data points (AQ = 0.071 s). Refocusing delays of 100 ms and 200 ms were used in separate experiments. A recycle delay of (D1) of 2.0 s was employed. Zero-filling was applied once to achieve digital resolution of 3.5 Hz/pt in each dimension. Processing parameters: unshifted sinusoidal (SINE, SSB=0) apodization was applied in both dimensions prior to the Fourier transformation.

2D ROESY experiment.⁶ The **roesytp.2** pulse program was used with the following acquisition parameters. F2 and F1 sweep widths, 7184 Hz. F2 and F1 digital resolution, 3.5 Hz/pt. 256 FIDs recorded, each consisting of 16 scans and 2048 data points (AQ = 0.142 s). The 800 ms spin lock consisted of 5404 cycles of phase-shifted pairs of 74 μ s 180° pulses. A recycle delay of (D1) of 2.0 s was employed. Processing parameters: $\pi/2$ shifted sine² (QSINE, SSB=2) apodization was applied in both dimensions prior to the Fourier transformation.

Representative 2D NOESY/EXSY experiment.⁷ The **noesytp** pulse program was used with the following acquisition parameters. F2 and F1 sweep widths, 2913 Hz. F2 and F1 digital resolution, 2.8 Hz/pt. 256 FIDs recorded, each consisting of 8 scans and 1024 data points (AQ = 0.176 s). A mixing time of 800 ms was set as a simple delay. A recycle delay of (D1) of 2.0 s was employed. Processing parameters: $\pi/2$ shifted sine² (QSINE, SSB=2) apodization was applied in both dimensions prior to the Fourier transformation.

Gradient-enhanced 2D ^1H - ^{13}C HMQC experiment.⁸ The **inv4gp** pulse program was used with the following acquisition parameters. F2 sweep width, 7184 Hz, F1 sweep width, 32,895 Hz. F2 digital resolution, 7.01 Hz/pt, F1 digital resolution, 257 Hz/pt. 128 FIDs recorded, each consisting of 16 scans and 1024 data points (AQ = 0.071 s). The D2 delay was set to 3.57 ms ($1/2J = 140$ Hz). A recycle delay (D1) of 3.0 s was employed. Processing parameters: Zero-filling was applied once (SI = 2048) in F2 to achieve a digital resolution of 3.5 Hz/pt and eight times (SI = 1024) in F1 to achieve a digital resolution of 32 Hz/pt. Exponential (EM, LB = 5) apodization was applied in the F2 dimension and $\pi/3$ shifted sine² (QSINE, SSB=3) apodization was applied in the F1 dimension prior to the Fourier transformation.

2D ^1H - ^{13}C HMQC experiment without F2 decoupling.⁹ The **inv4nd** pulse program was used with the following acquisition parameters. F2 sweep width, 4789 Hz, F1 sweep width, 17605 Hz. F2 digital resolution, 4.68 Hz/pt, F1 digital resolution, 137.5 Hz/pt. 128 FIDs recorded, each consisting of 64 scans and 1024 data points (AQ = 0.107 s). The D2 delay was set to 3.57 ms ($1/2J = 140$ Hz). A recycle delay (D1) of 2.2 s was employed. Processing parameters: Zero-filling was applied eight times (SI = 1024) in F1 to achieve a digital resolution of 17.2 Hz/pt. Processing parameters: $\pi/2$ shifted sine² (QSINE, SSB=2) apodization was applied in both dimensions prior to the Fourier transformation.

⁴ Hurd, R. *J. Magn. Reson.* **1990**, *87*, 422.

⁵ Bax, A.; Freeman, R. *J. Magn. Reson.* **1981**, *44*, 542.

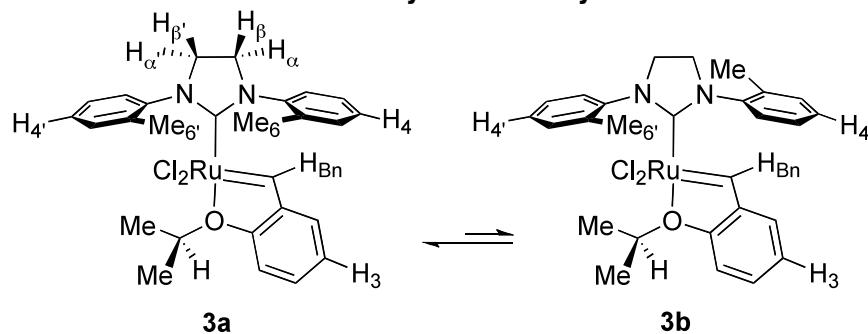
⁶ Hwang, T. -L.; Shaka, A. J. *J. Am. Chem. Soc.* **1992**, *114*, 3157.

⁷ Jeener, J.; Meier, B. H.; Bachmann, P.; Ernst, R. R. *J. Chem. Phys.* **1979**, *71*, 4546.

⁸ Hurd, R. E.; John, B. K. *J. Magn. Reson.* **1991**, *91*, 648.

⁹ Bax, A.; Griffey, R. H.; Hawkins, B. L. *J. Magn. Reson.* **1983**, *55*, 301.

NMR Analysis of Benzylidene 3



400 MHz ¹H NMR (CD₂Cl₂, 19 °C): 16.45 ppm (1H, s), 8.57 (1H, br s), 7.58-7.18 (8H, m), 6.89 (3H, app d), 4.95 (1H, sept, J = 6.1 Hz), 4.37 (2H, br s), 4.08 (2H, br s), 2.51 (6H, s), 1.47-1.22 (6H, br m).

400 MHz ¹H NMR for major isomer **3a** (CD₂Cl₂, -48 °C): 16.37 ppm (1H, s, H_{Bn}), 8.54 (1H, d, J = 7.4 Hz, H₂), 7.6-7.3 (8H, m), 7.20 (1H, t, J = 7.5 Hz), 6.9-6.8 (3H, m), 4.94 (1H, sept, J = 6.1 Hz), 4.40 (2H, m), 4.10-3.95 (2H, m), 2.51 (3H, s), 2.45 (3H, s), 1.38 (3H, d, J = 5.9 Hz), 1.23 (3H, d, J = 5.9 Hz). Minor isomer **3b**: 16.40 (1H, s).

100 MHz ¹³C NMR for major isomer **3a** (CD₂Cl₂, -48 °C):

peak #	freq. (Hz)	freq. (ppm)	intensity	intensity (absolute)
1	29752.299	295.7111	0.048685	332095.316000
2	21038.855	209.1073	0.054215	369815.912000
3	15355.857	152.6234	0.068693	468574.648000
4	14466.597	143.7849	0.083085	566745.924000
5	14256.821	141.7000	0.072214	492592.968000
6	14223.297	141.3668	0.080313	547837.092000
7	13889.728	138.0514	0.068631	468150.220000
8	13858.516	137.7412	0.084934	579357.184000
9	13270.839	131.9002	0.110824	755962.288000
10	13226.277	131.4573	0.115626	788718.888000
11	13117.935	130.3805	0.132291	902394.936000
12	13094.956	130.1521	0.109696	748267.324000
13	13021.910	129.4261	0.105835	721928.328000
14	12975.180	128.9616	0.100812	687669.788000
15	12961.729	128.8279	0.100074	682631.548000
16	12911.829	128.3320	0.113653	775261.520000
17	12863.458	127.8512	0.117171	799259.664000
18	12363.549	122.8825	0.120276	820438.720000
19	12297.960	122.2306	0.105240	717874.680000
20	11424.603	113.5503	0.109218	745004.580000
21	7562.637	75.1658	0.113104	771513.176000
22	5529.377	54.9570	0.302563	2063864.884000
23	5502.151	54.6864	0.695672	4745374.464000
24	5474.793	54.4145	0.929770	6342223.296000
25	5447.567	54.1439	0.720516	4914840.220000
26	5420.213	53.8720	0.314864	2147778.584000
27	5218.730	51.8695	0.097512	665156.928000
28	2221.267	22.0774	0.122898	838325.308000
29	2196.144	21.8277	0.127974	872945.216000
30	1962.093	19.5014	0.120911	824767.136000
31	1840.543	18.2933	0.111360	759618.572000

100 MHz ¹³C NMR for minor isomer **3b** (CD₂Cl₂, -48 °C): 297.31 ppm.

Complex 1

NOESY/EXSY 600 ms mixing time

Methyl region

-48 °C, CD₂Cl₂

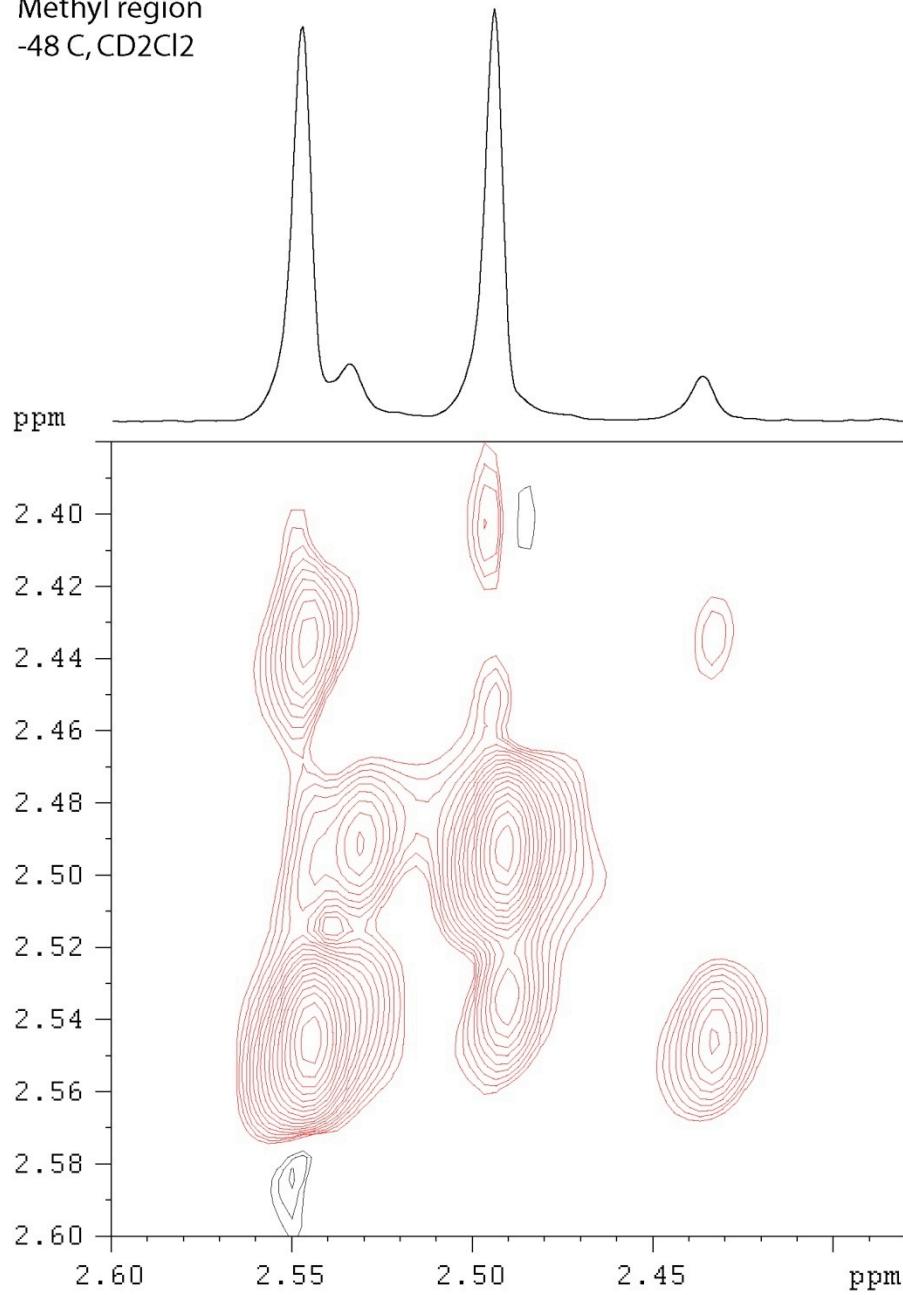


Figure S1. 400 MHz ¹H NOESY/EXSY spectrum of the methyl region for complex 3 dissolved in CD₂Cl₂ at -48 °C. Exchange between major and minor forms is evident; this data set was used to extract the magnetization exchange rate constant (k_{for}) between major and minor forms to be 3.9 s⁻¹.

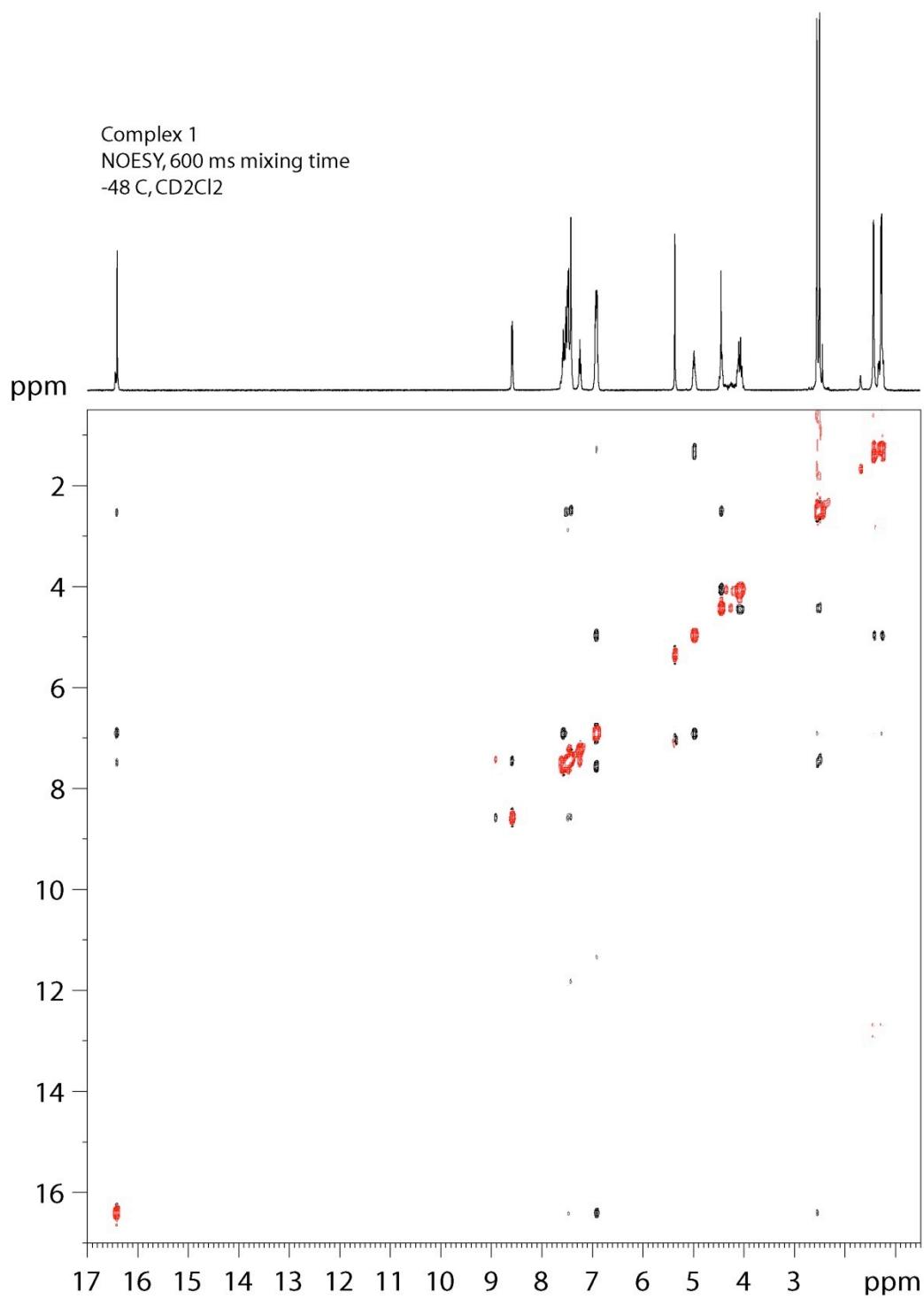


Figure S2. 400 MHz ¹H NOESY spectrum for complex **3** at -48 °C dissolved in CD₂Cl₂.

Complex 1
NOESY, 600 ms mixing time
-48 C, CD₂Cl₂

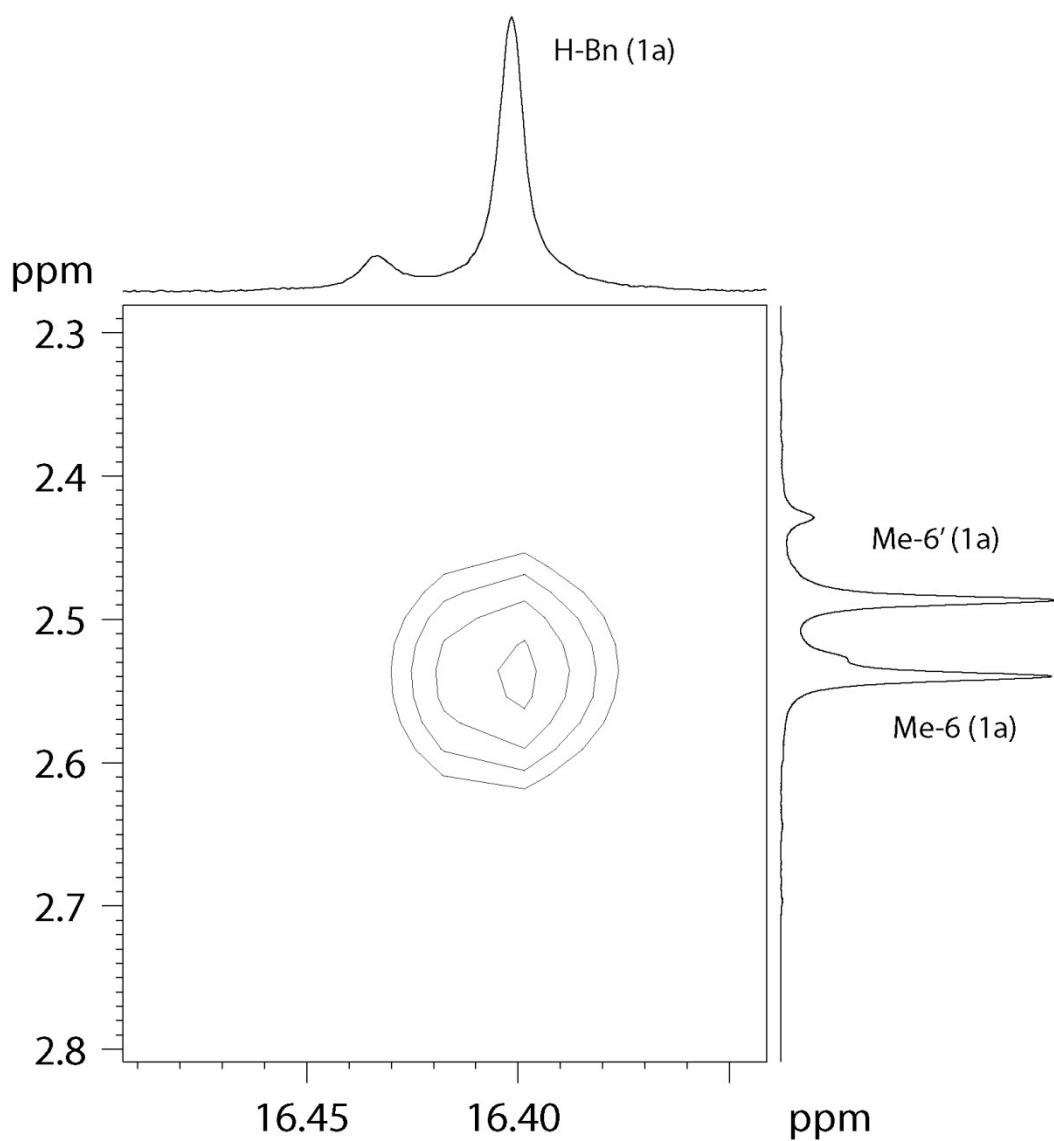


Figure S3. 400 MHz ¹H NOESY spectrum for complex **3** at -48 °C dissolved in CD₂Cl₂. Expansion plot showing NOE between H-Bn and Me-6.

Complex 1
NOESY, 600 ms mixing time
-48 °C, CD₂Cl₂

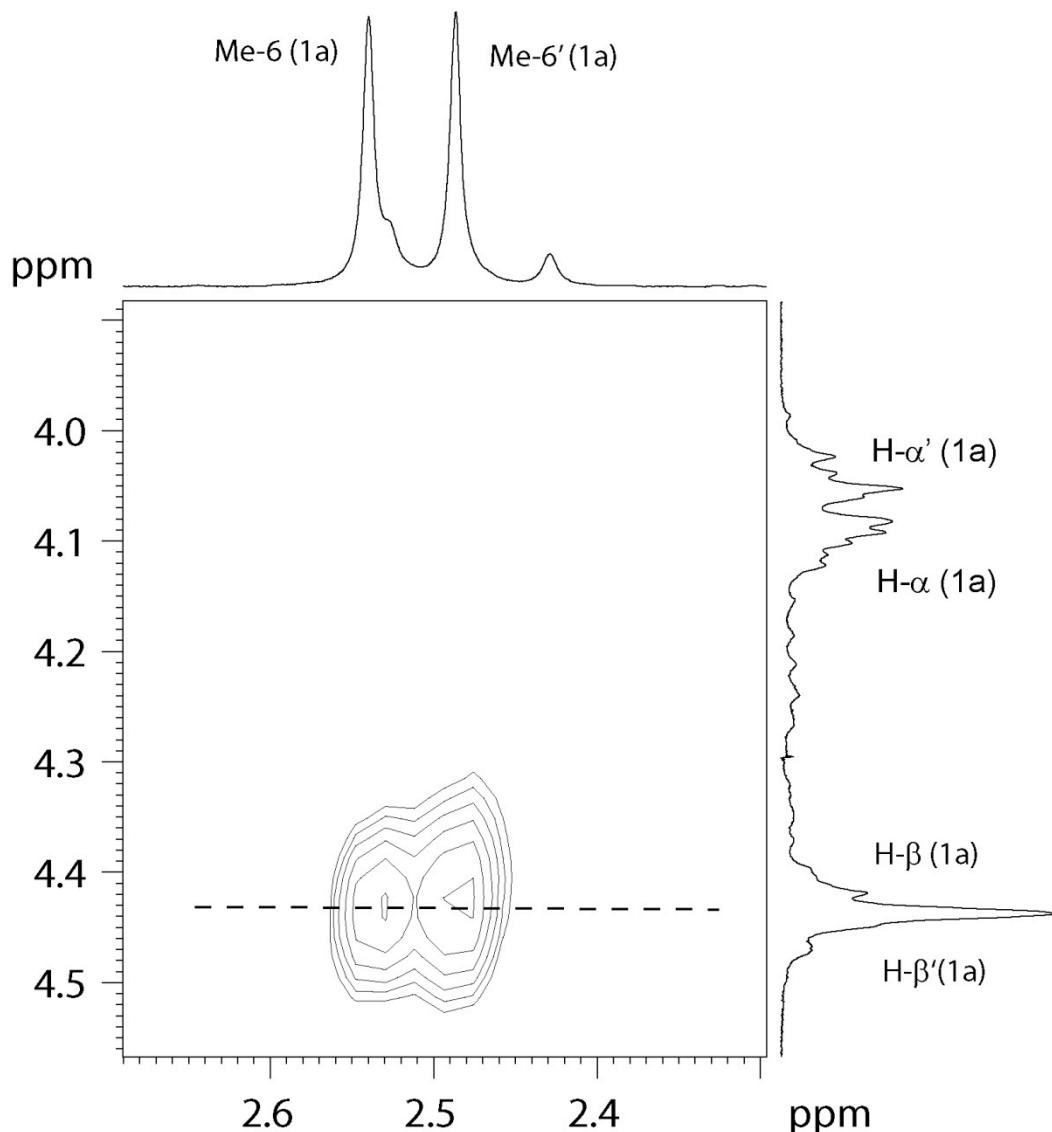


Figure S4. 400 MHz ¹H NOESY spectrum for complex 3 at -48 °C dissolved in CD₂Cl₂. Expansion plot showing NOEs between Me-6 and Me-6' and H-β and Hβ', respectively.

Complex 1
NOESY, 600 ms mixing time
-48 C, CD₂Cl₂

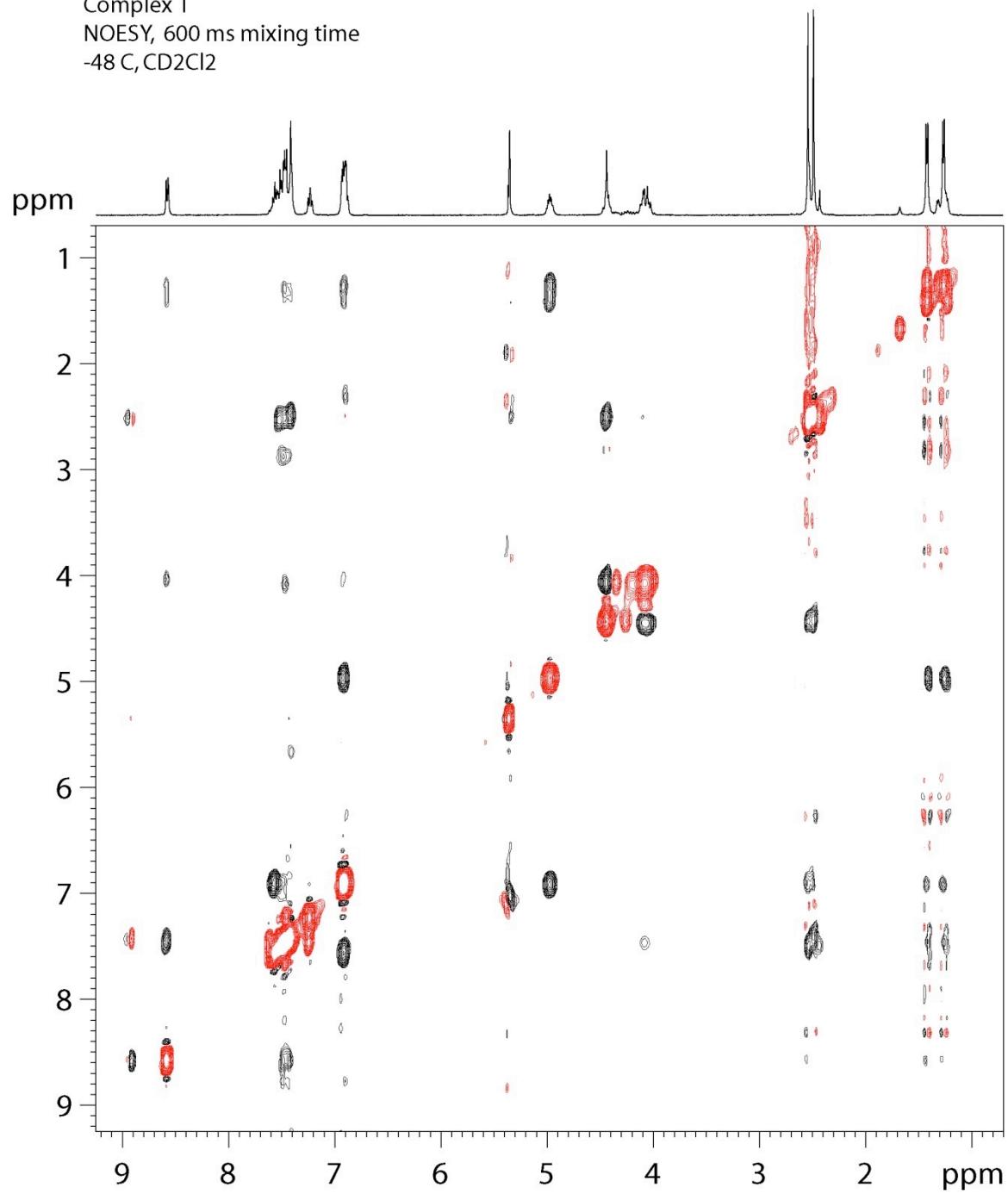


Figure S5. 400 MHz ¹H NOESY spectrum for complex 3 at -48 °C dissolved in CD₂Cl₂. Expansion plot showing region from 9-1 ppm.

Complex 1
NOESY, 600 ms mixing time
-48 °C, CD₂Cl₂

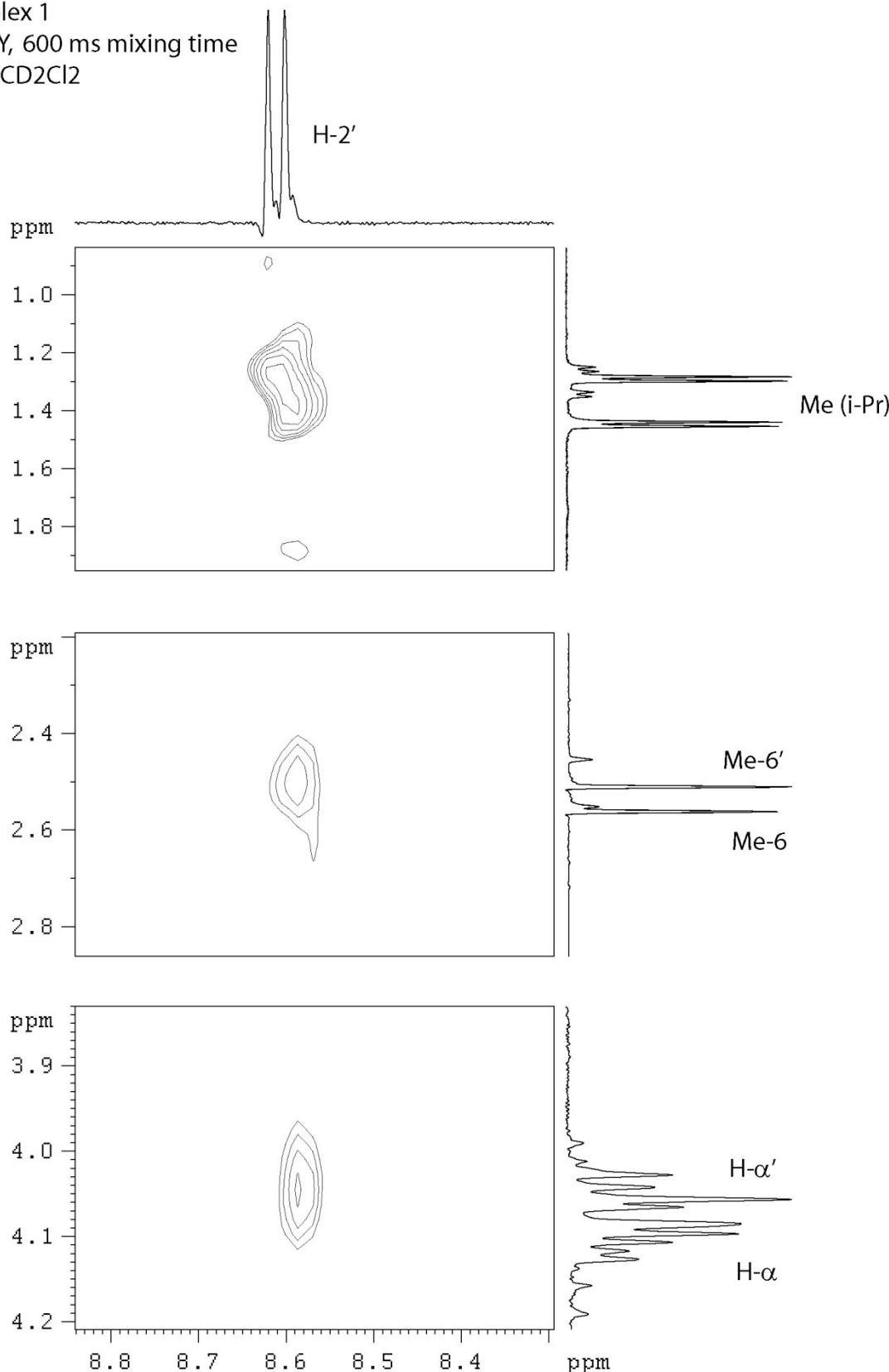


Figure S6. 400 MHz ¹H NOESY spectrum for complex 3 at -48 °C dissolved in CD₂Cl₂. Expansion plot showing H-2' NOEs.

Complex 1
cosygs
-48 °C, CD₂Cl₂

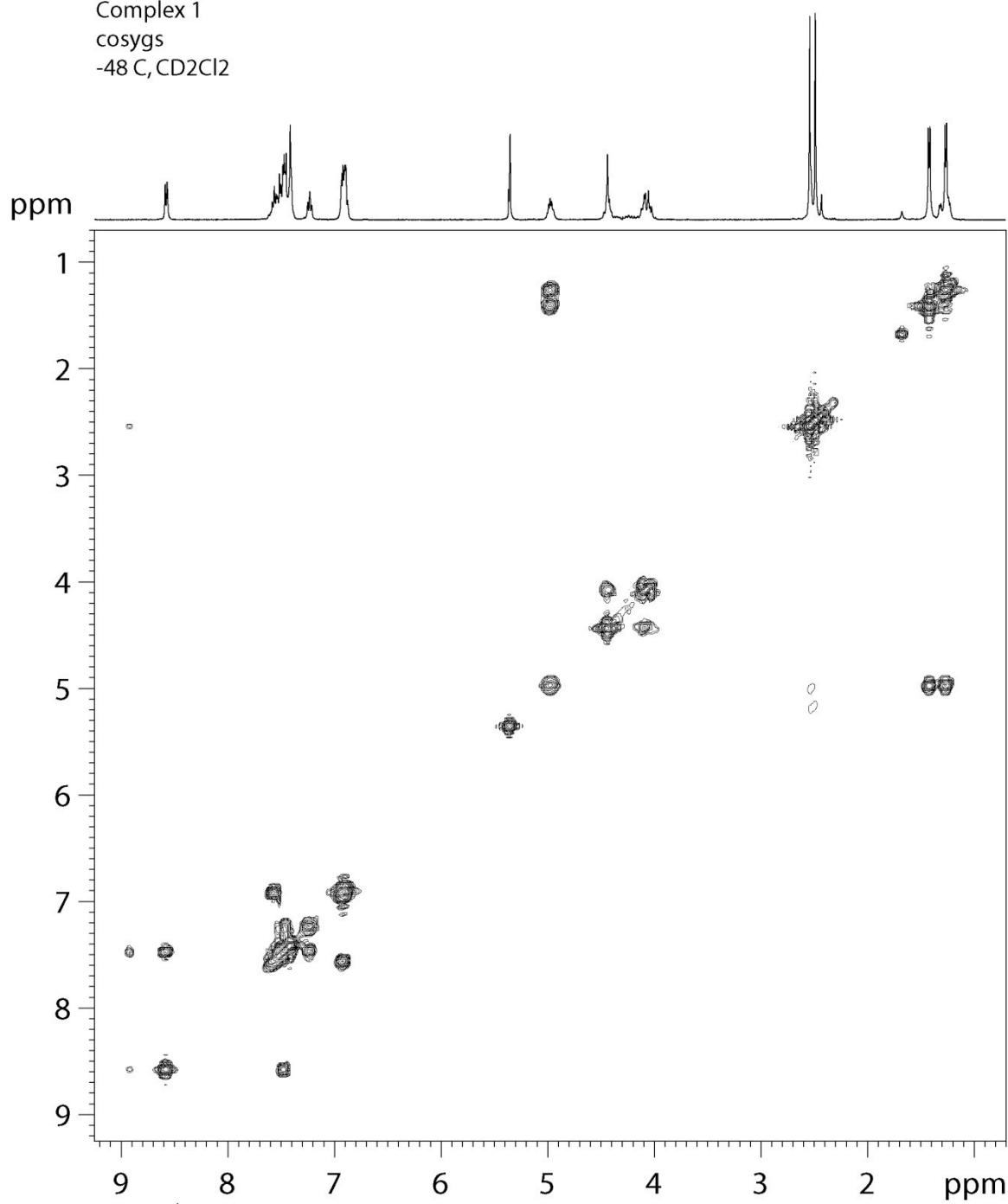


Figure S7. 400 MHz ¹H COSY spectrum for complex 3 at -48 °C dissolved in CD₂Cl₂.

Complex 1
13C spectrum
-48 °C, CD₂Cl₂

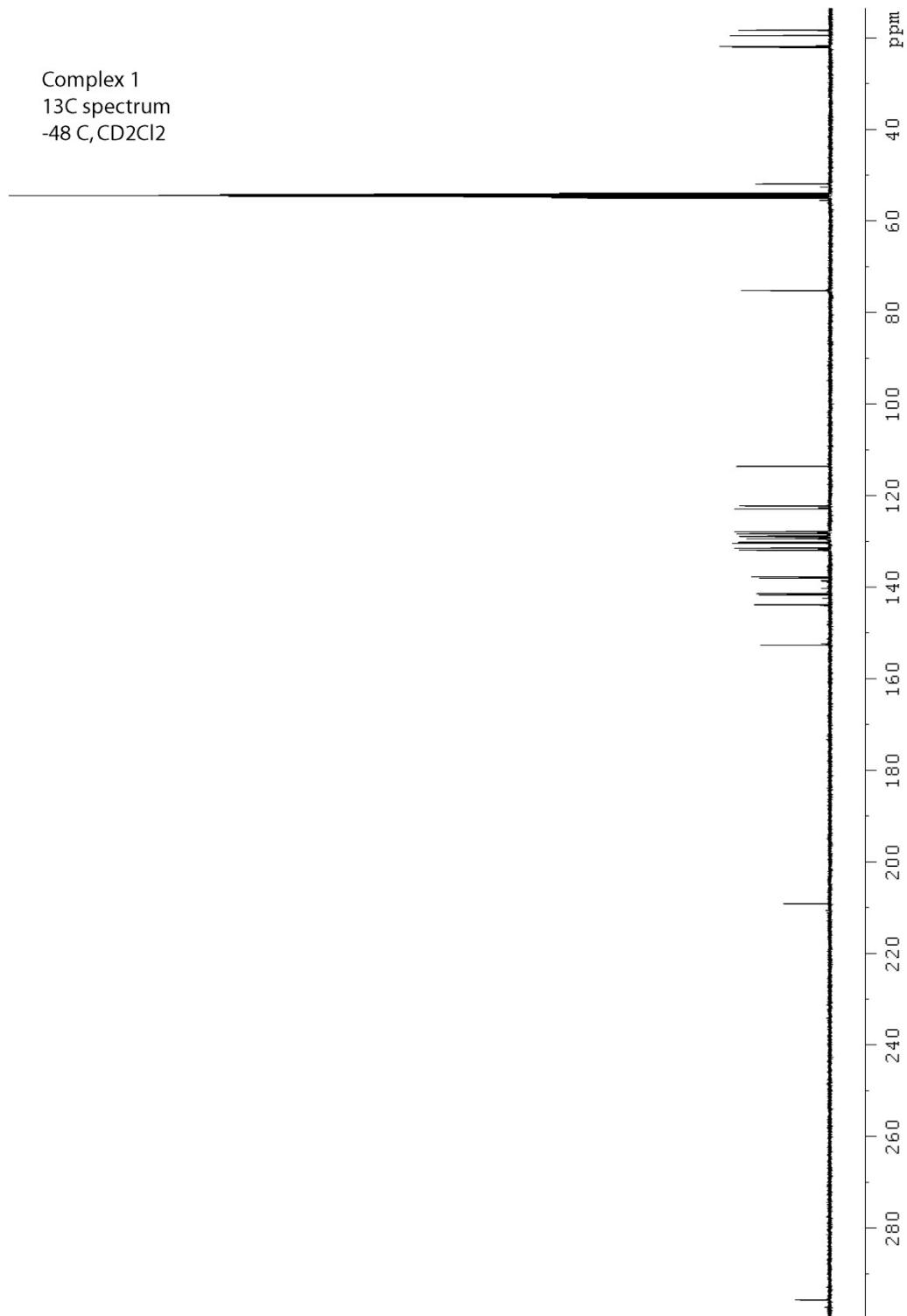


Figure S8. 100 MHz ¹³C spectrum for complex 3 at -48 °C dissolved in CD₂Cl₂.

NMR Analysis of Olefin Complex 5

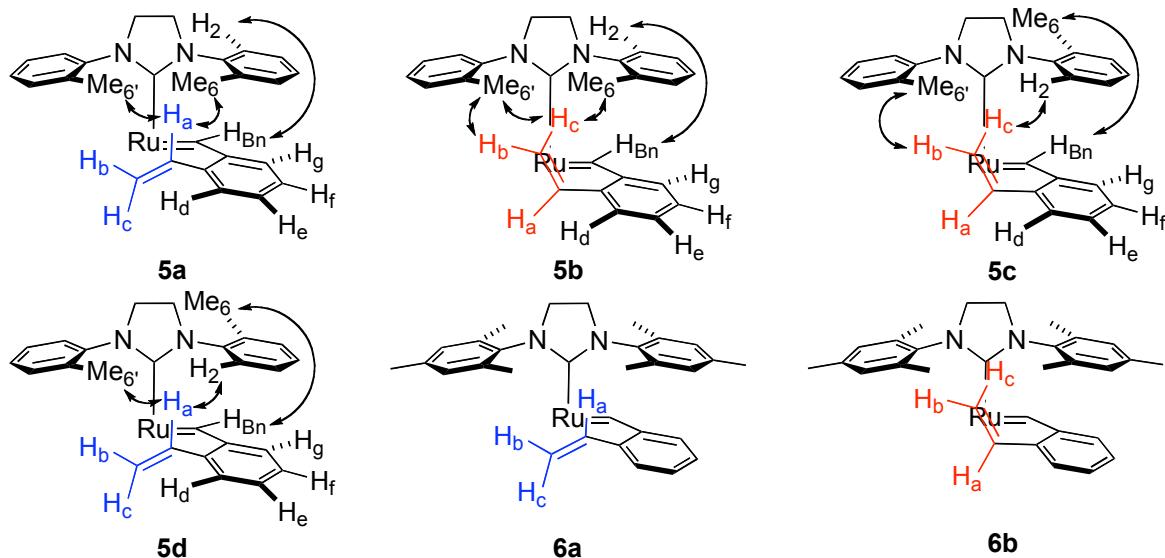


Figure S9. Naming scheme for ^1H NMR resonances in complexes **5** and **6**. Observed NOEs are indicated with double-headed arrows. Color has been used to clarify the geometry of the bound olefin (blue: side-bound, CH_2 down; red: side-bound, CH_2 up). Chloride ligands are omitted for clarity.

400 MHz ^1H selected shifts and assignments for major isomer **5a** (CD_2Cl_2 , -82°C): 15.86 ppm (1H, s, H-Bn), 8.53 (1H, d, $J = 6.8$ Hz, H-2'), 7.91 (1H, d, $J = 8.0$ Hz, H-2), 7.25 (H-3 via COSY), 7.13 (1H, t, $J = 7.4$ Hz), 7.00 (1H, t, $J = 7.4$ Hz), 6.55 (1H, d, $J = 7.9$ Hz), 6.37 (1H, d, $J = 7.9$ Hz, H-g), 4.89 (1H, dd, $J = 12.0, 9.0$ Hz, H-a), 2.55 (3H, s, Me-6'), 2.05 (1H, d, $J = 9.0$ Hz, H-b), 2.83 (1H, d, $J = 12.0$ Hz, H-c), 1.42 (3H, s, Me-6).

400 MHz ^1H selected shifts and assignments for second-most populated isomer **5b** (CD_2Cl_2 , -82°C): 15.40 ppm (1H, s, H-Bn), 8.66 (1H, d, $J = 7.8$ Hz, H-2'), 8.10 (1H, d, $J = 7.3$ Hz), 7.54 (H-3 via COSY), 7.43 (H-5' via NOESY), 7.02 (H-5 via NOESY), 6.37 (H-g via NOESY), 5.71 (dd, $J = 11.8, 10.0$ Hz, H-a), 2.98 (d, $J = 10.0$ Hz, H-b), 2.92 (d, $J = 11.8$ Hz, H-c), 2.39 (3H, s, Me-6'), 1.17 (3H, s, Me-6).

400 MHz ^1H selected shifts and assignments for third-most populated isomer **5c** (CD_2Cl_2 , -82°C): 15.32 ppm (1H, s, H-Bn), 8.75 (1H, d, $J = 7.8$ Hz, H-2'), 7.52 (H-5 via NOESY), 7.38 (H-4 via NOESY), 6.71 (H-3 via NOESY), 6.01 (1H, d, $J = 7.6$ Hz, H-2), 5.76 (dd, $J = 10, 12$ Hz, Ha), 2.905 (3H, s, Me-6), 2.83 (d, $J = 10$ Hz, Hb), 2.59 ppm (d, $J = 12$ Hz, Hc), 2.375 (3H, s, Me-6').

400 MHz ^1H selected shifts and assignments for fourth-most populated isomer **5d** (CD_2Cl_2 , -82°C): 16.01 ppm (1H, s, H-Bn), 7.235 (H-5 via NOESY), 7.08 (H-4 via NOESY), 6.22 (H-3 via NOESY), 5.61 (d, $J = 7.6$ Hz, H-2), 5.10 (dd, $J = 10, 12$ Hz, H-a), 3.03 (d, $J = 12$ Hz, H-c), 2.546 (3H, s, Me-6/6'), 2.03 (d, $J = 10$ Hz, H-b).

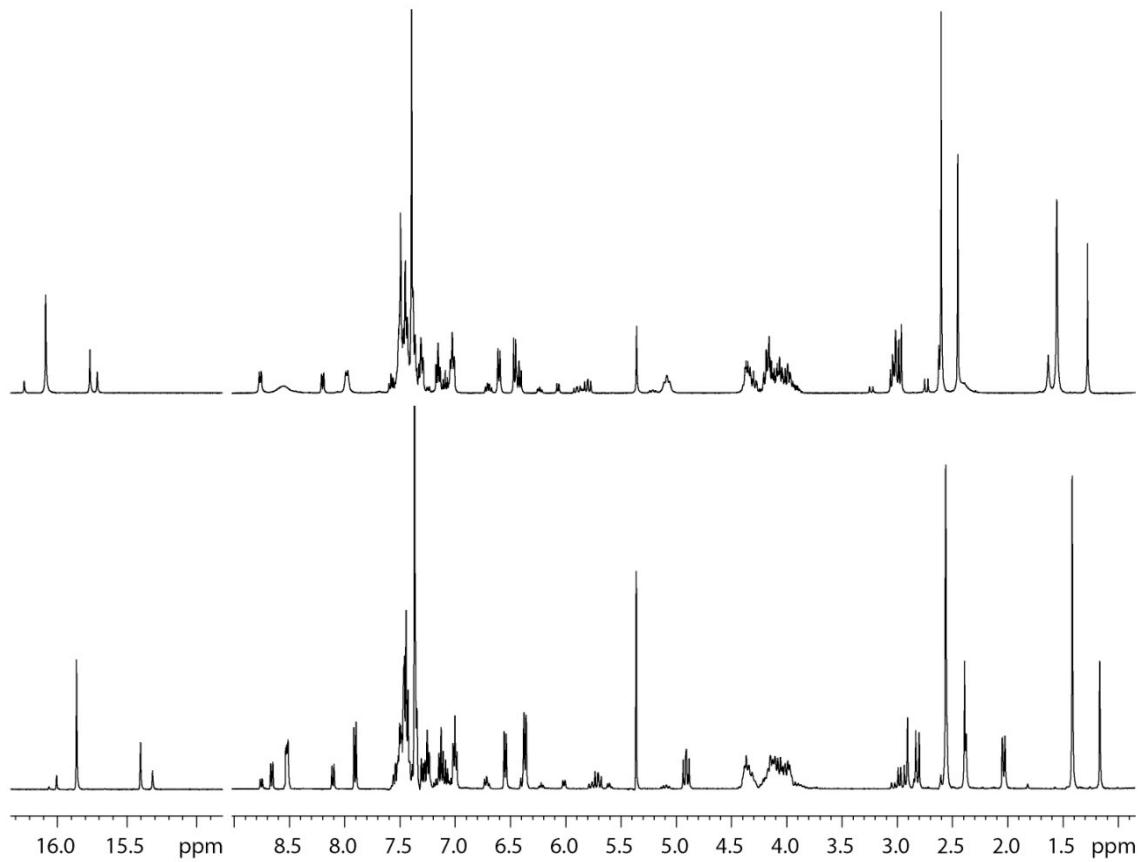


Figure S10. 400 MHz ¹H spectrum of complex 5 dissolved in CD₂Cl₂. Top: spectrum recorded at 19 °C. Bottom: spectrum recorded at -82 °C.

olefin complex
-82 deg C
COSY-gs

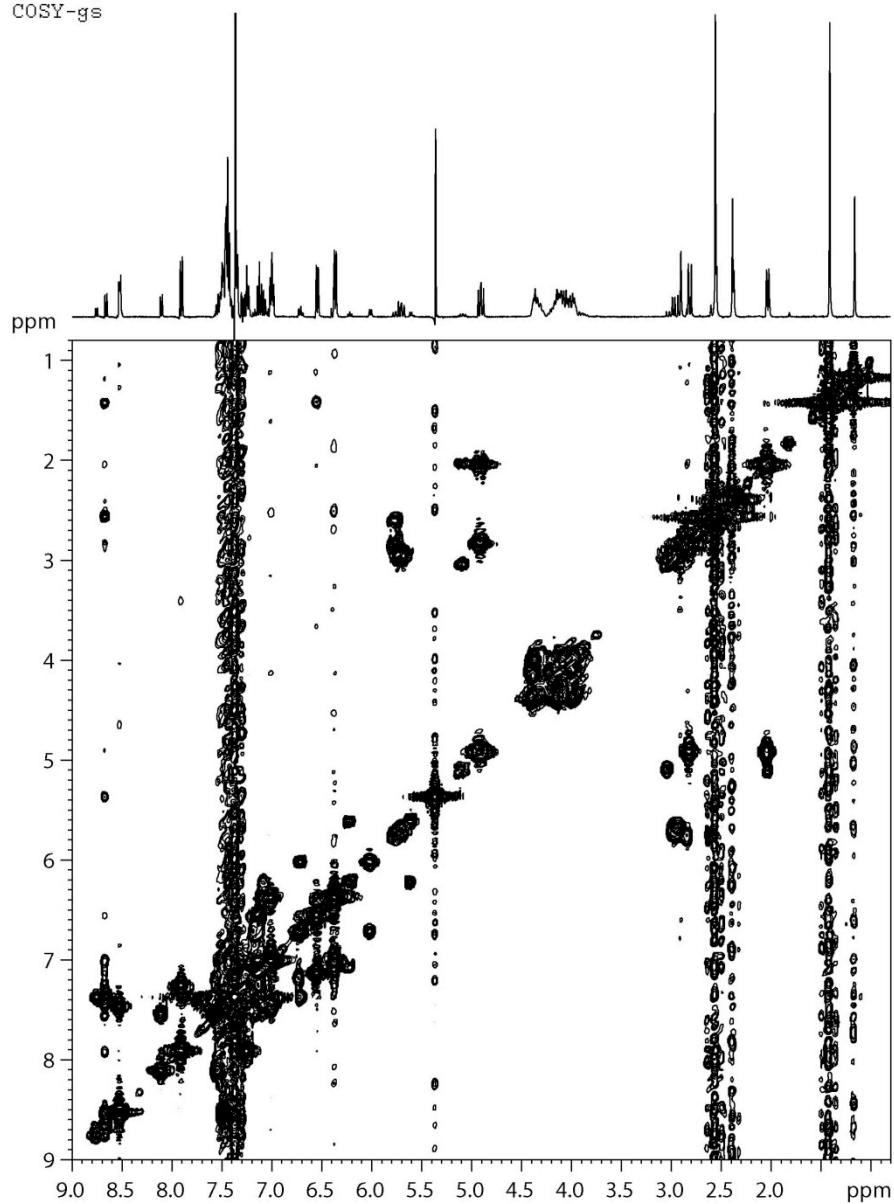


Figure S11. 400 MHz ¹H COSY spectrum for complex 5 at -82 °C dissolved in CD₂Cl₂.

olefin complex, -82 C

TOCSY-gs

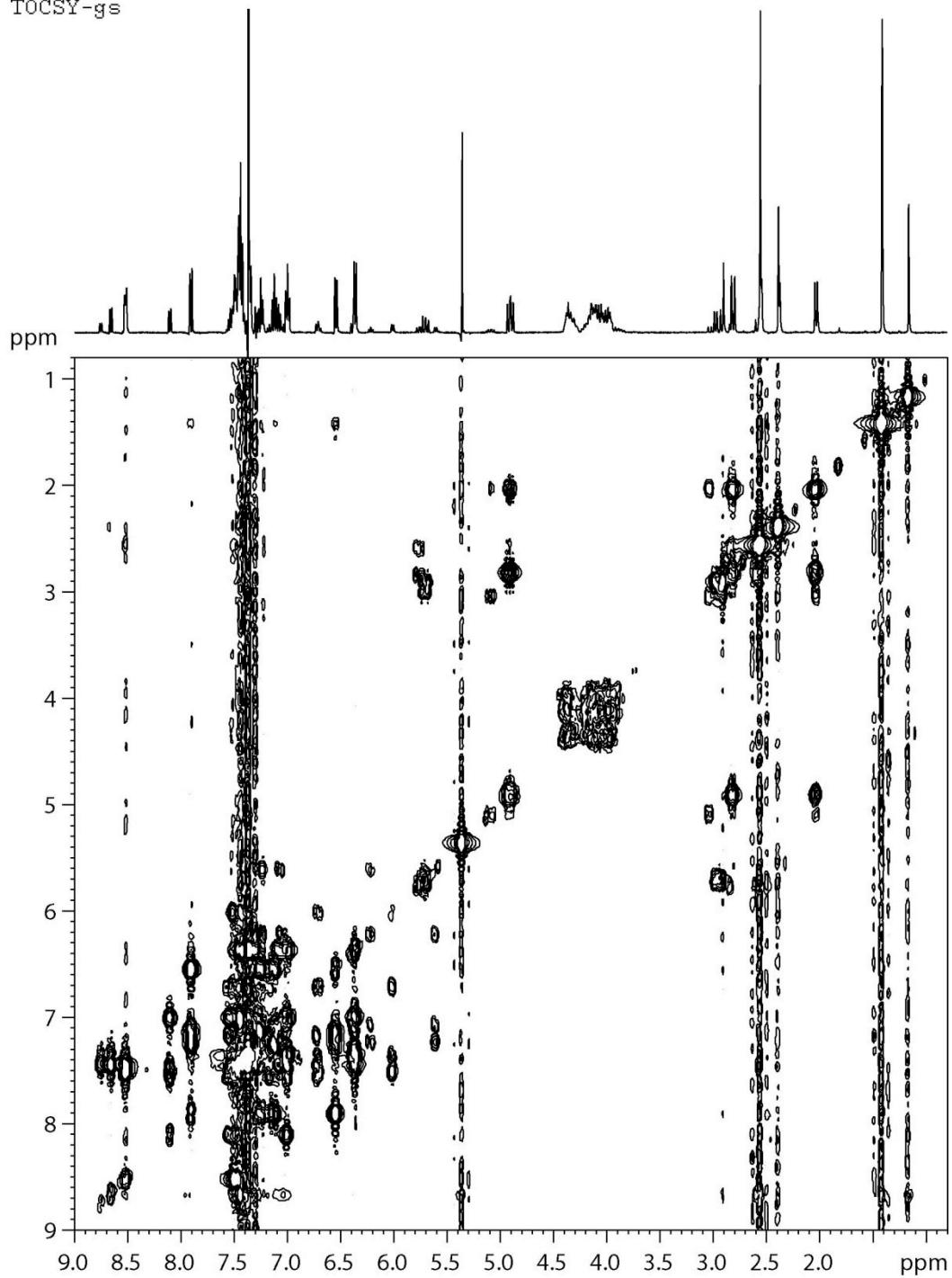


Figure S12. 400 MHz ^1H TOCSY spectrum for complex 5 at -82°C dissolved in CD_2Cl_2 .

olefin complex, -82 C

COSYLR

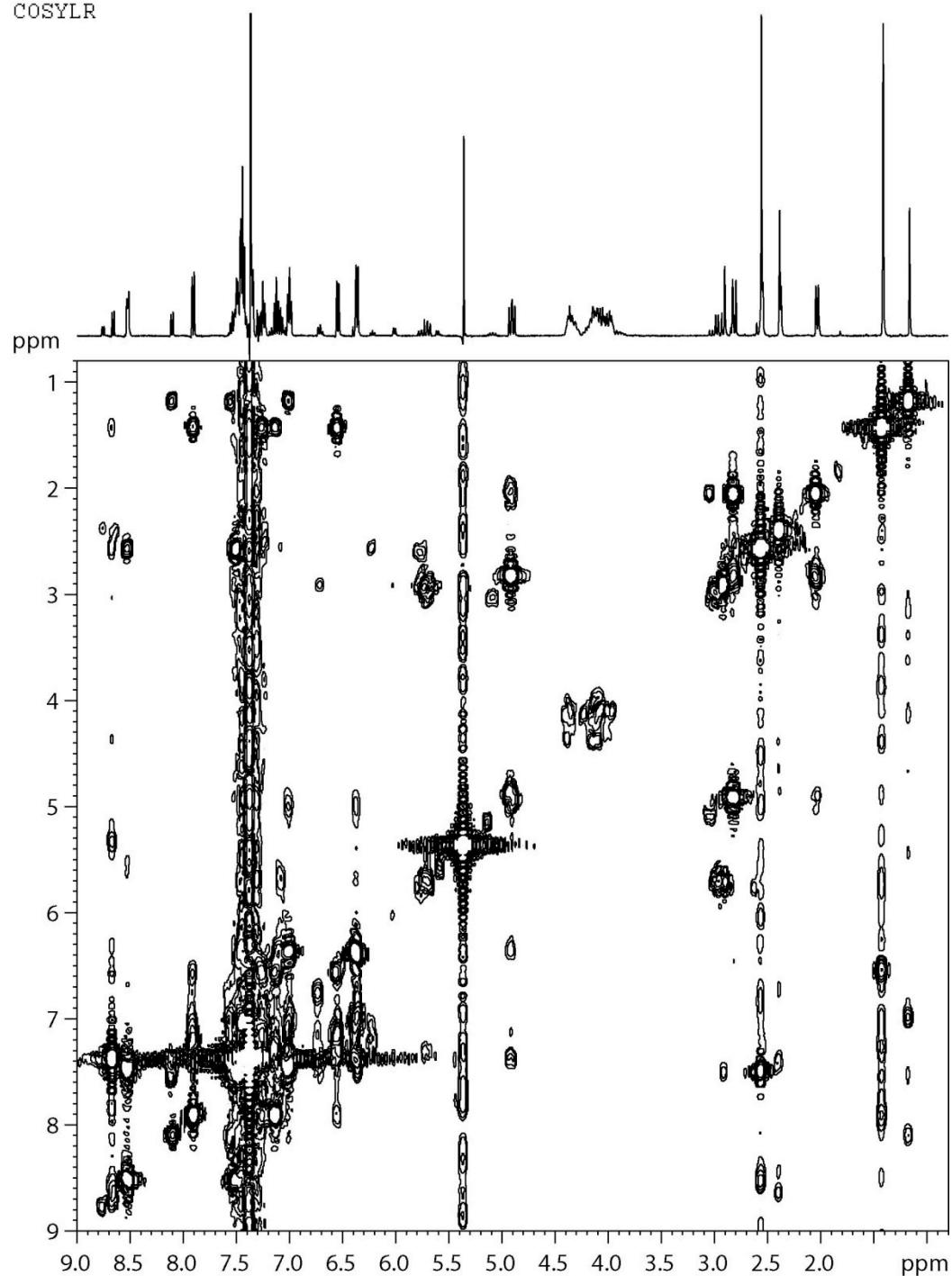


Figure S13. 400 MHz ¹H COSY-LR spectrum for complex 5 at -82 °C dissolved in CD₂Cl₂.

olefin complex
-82 deg C
COSYLR

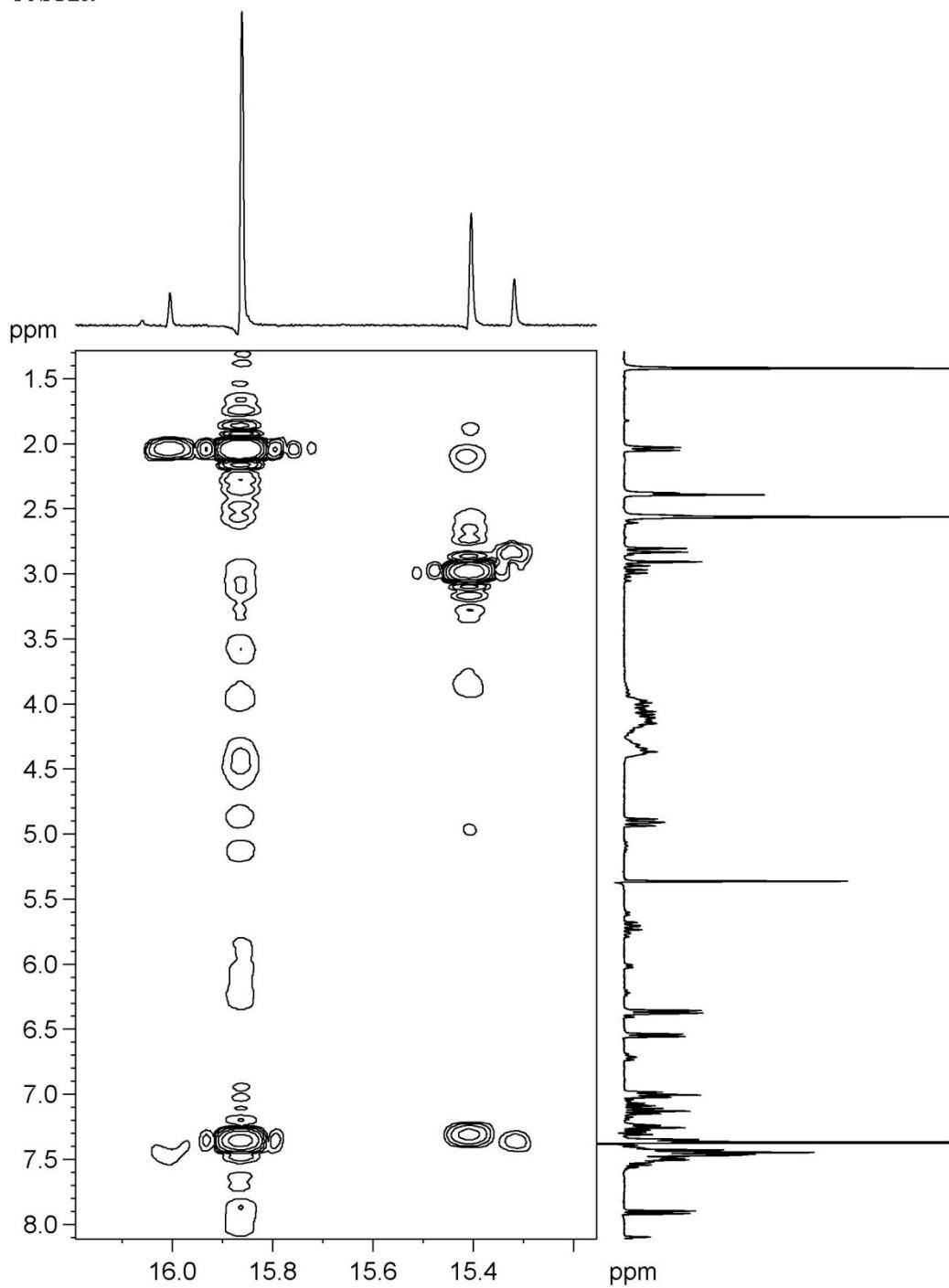


Figure S14. 400 MHz ¹H COSY-LR spectrum (expansion plot) for complex 5 at -82 °C dissolved in CD₂Cl₂.

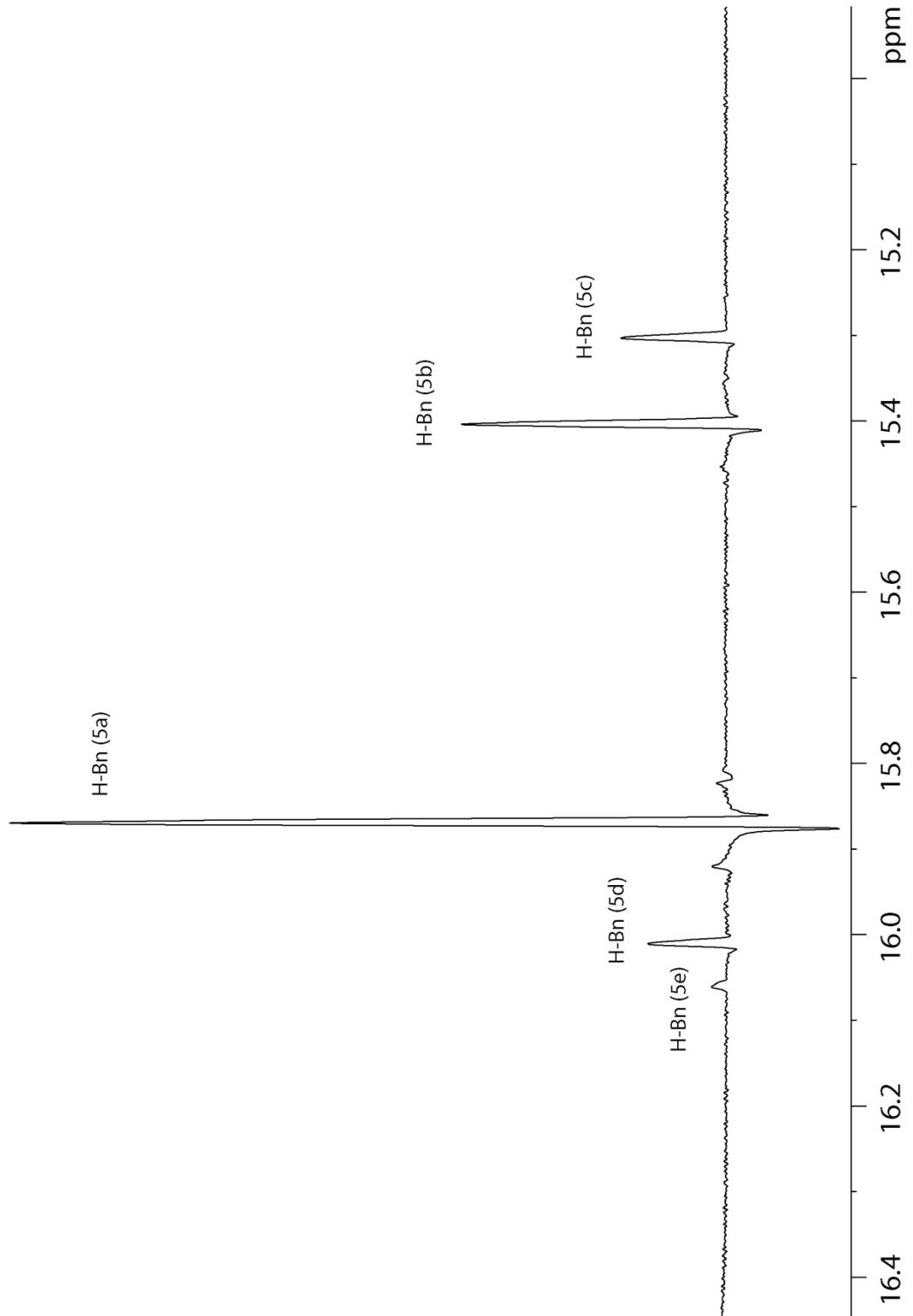


Figure S15. 400 MHz ¹H spectrum (expansion plot) for complex 5 at -82 °C dissolved in CD₂Cl₂.

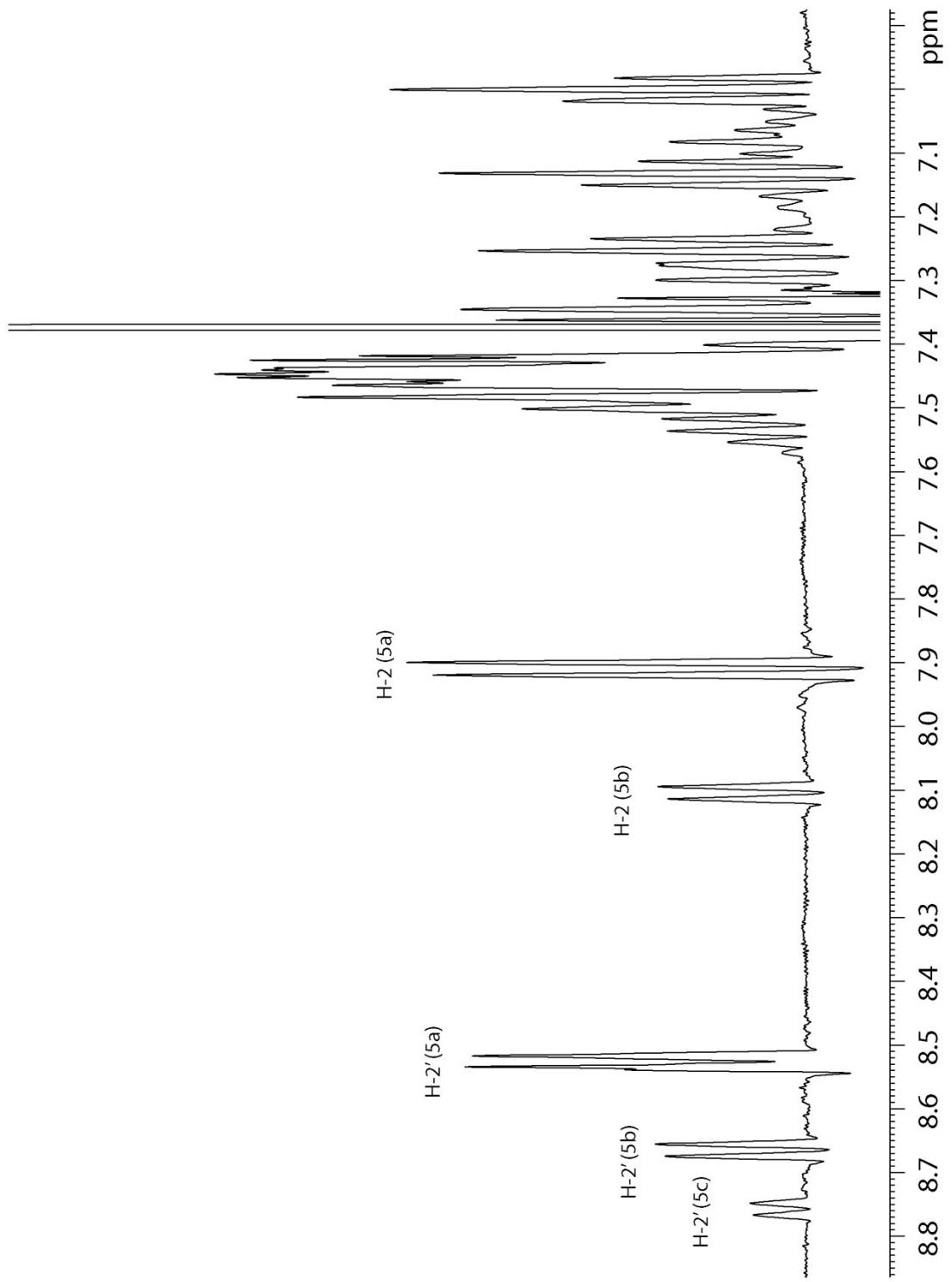


Figure S16. 400 MHz ¹H spectrum (expansion plot) for complex **5** at -82 °C dissolved in CD₂Cl₂.

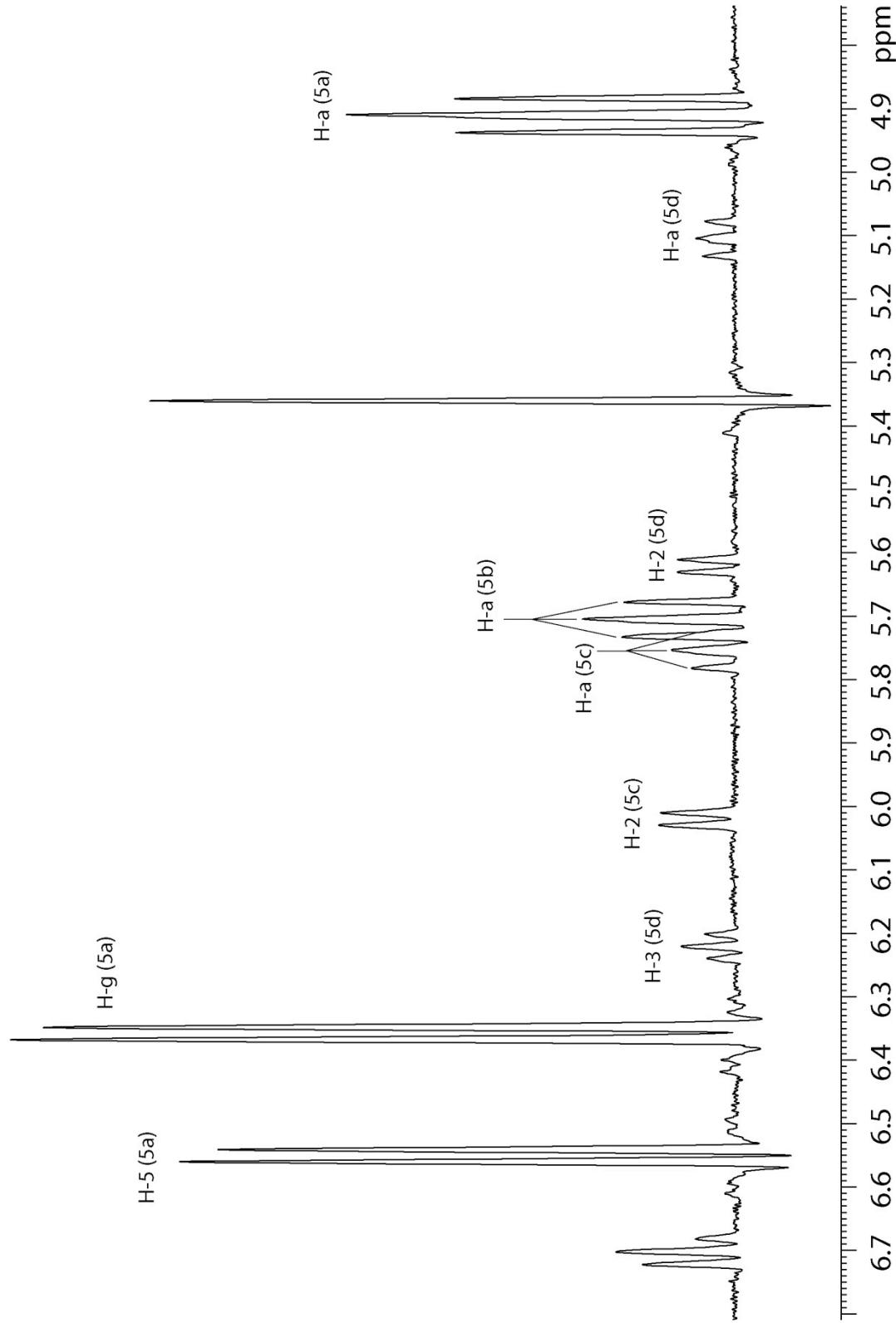


Figure S17. 400 MHz ^1H spectrum (expansion plot) for complex 5 at -82 °C dissolved in CD_2Cl_2 .

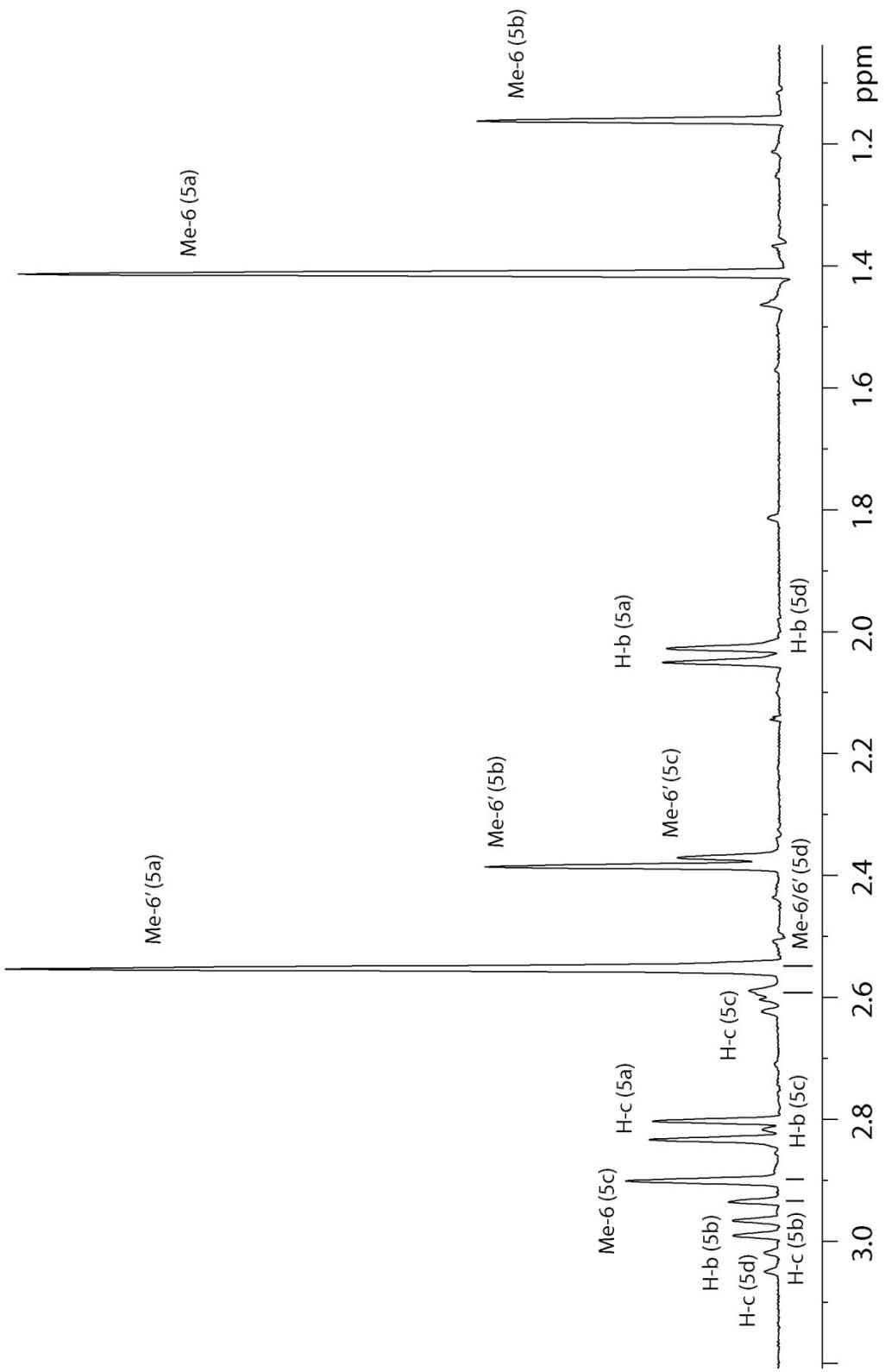


Figure S18. 400 MHz ^1H spectrum (expansion plot) for complex 5 at -82°C dissolved in CD_2Cl_2 .

Complex 5
ROESY, 300 ms mixing time
-82 °C, CD₂Cl₂

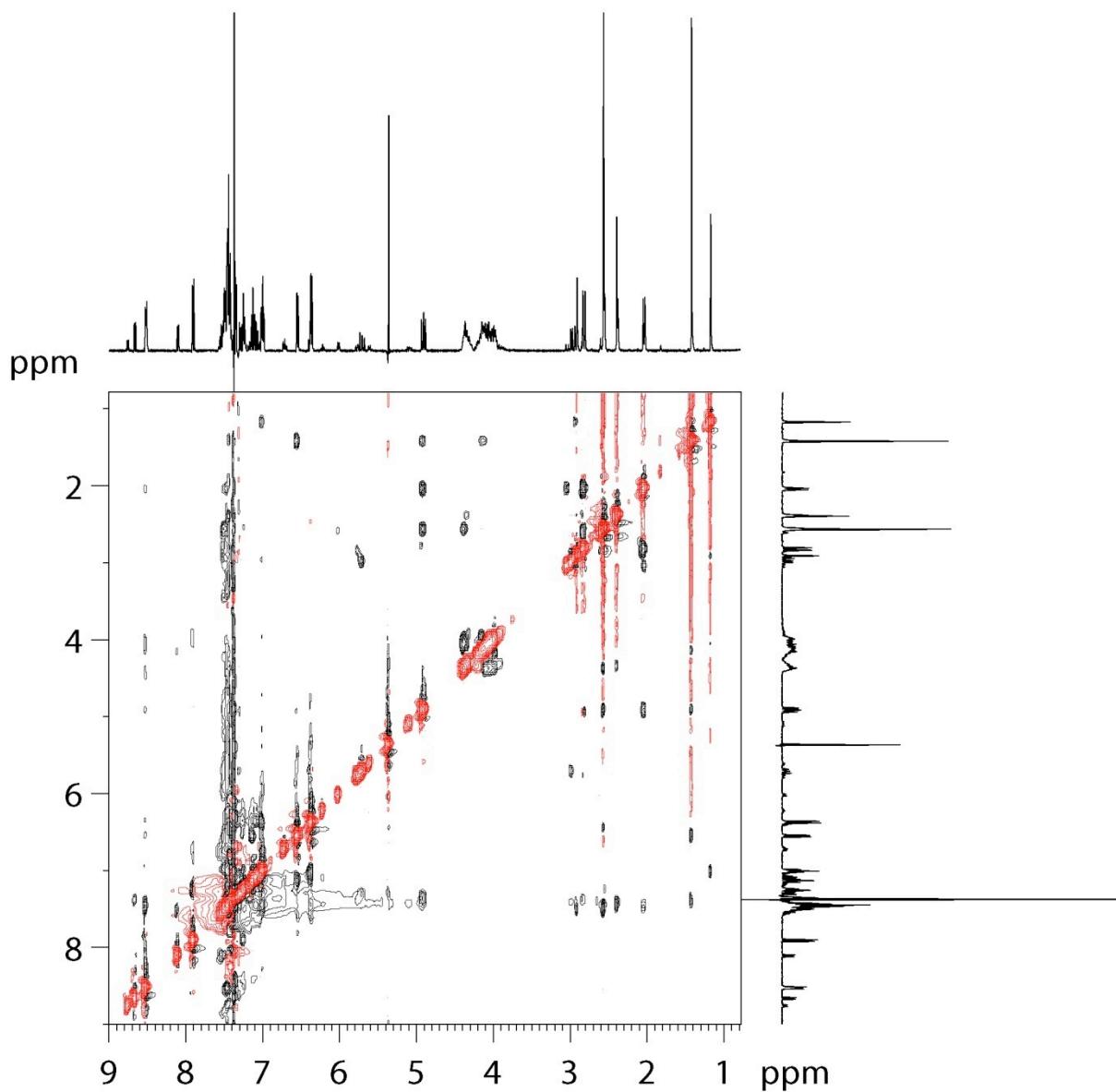


Figure S19. 400 MHz ¹H ROESY experiment for complex **5** at -82 °C dissolved in CD₂Cl₂.

Complex 5
ROESY, 300 ms mixing time
-82 °C, CD₂Cl₂

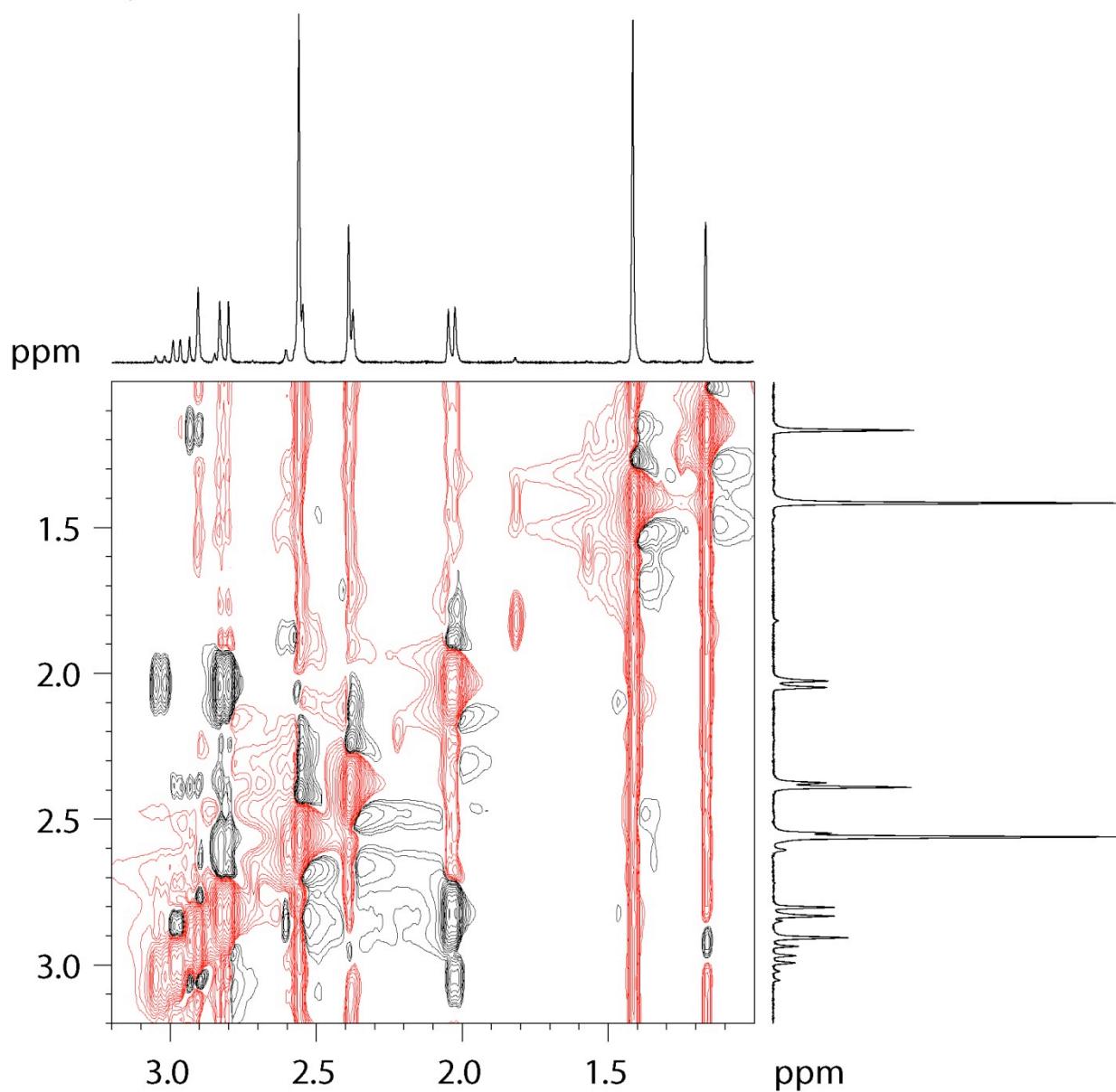


Figure S20. 400 MHz ¹H ROESY experiment for complex **5** at -82 °C dissolved in CD₂Cl₂.

Complex 5
ROESY, 300 ms mixing time
-82 °C, CD₂Cl₂

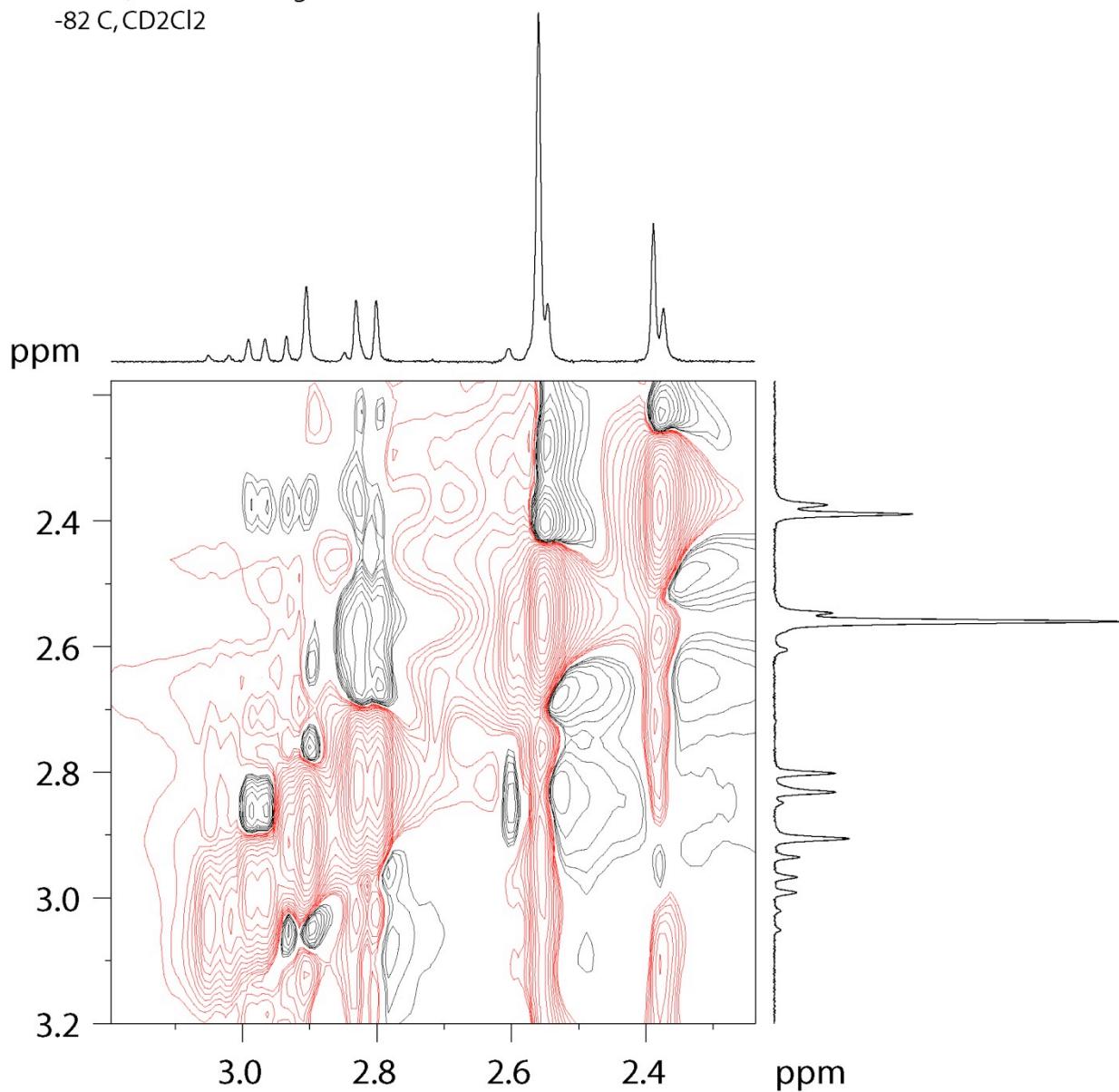


Figure S21. 400 MHz ¹H ROESY experiment for complex 5 at -82 °C dissolved in CD₂Cl₂.

Complex 5
ROESY, 300 ms mixing time
-82 °C, CD₂Cl₂

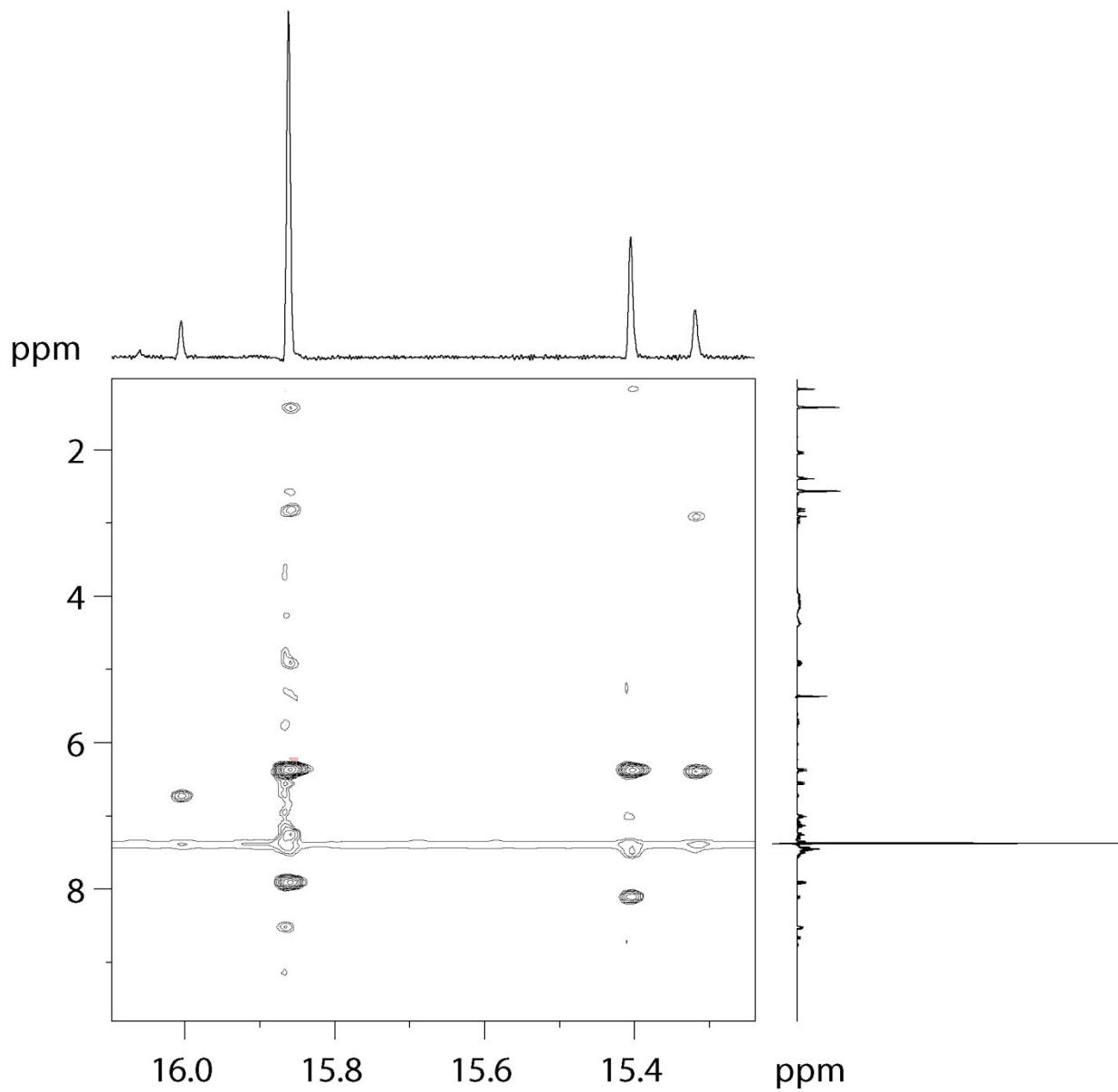


Figure S22. 400 MHz ¹H ROESY experiment for complex **5** at -82 °C dissolved in CD₂Cl₂.

Complex 5
ROESY, 300 ms mixing time
-82 °C, CD₂Cl₂

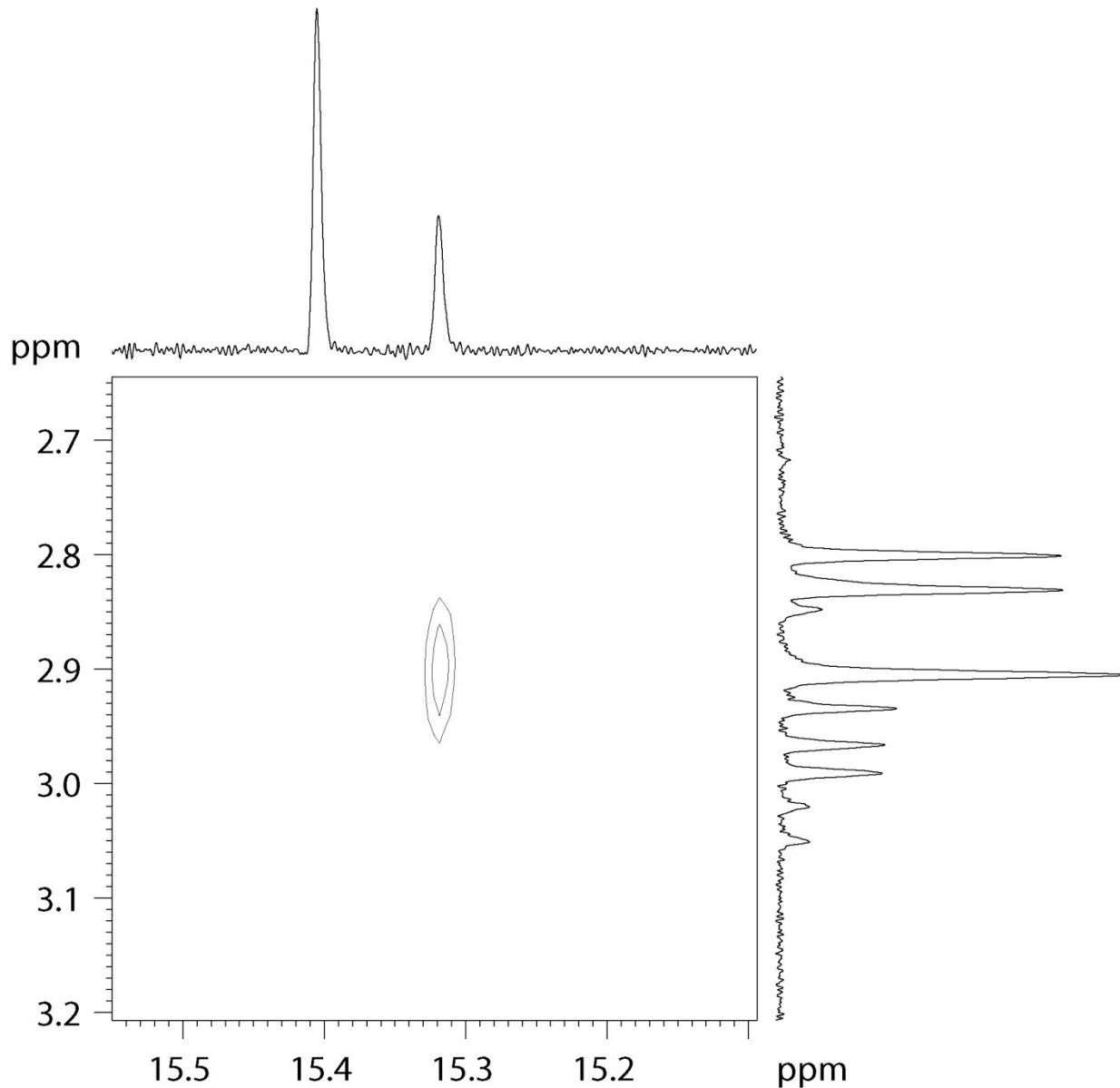


Figure S23. 400 MHz ¹H ROESY experiment for complex 5 at -82 °C dissolved in CD₂Cl₂.

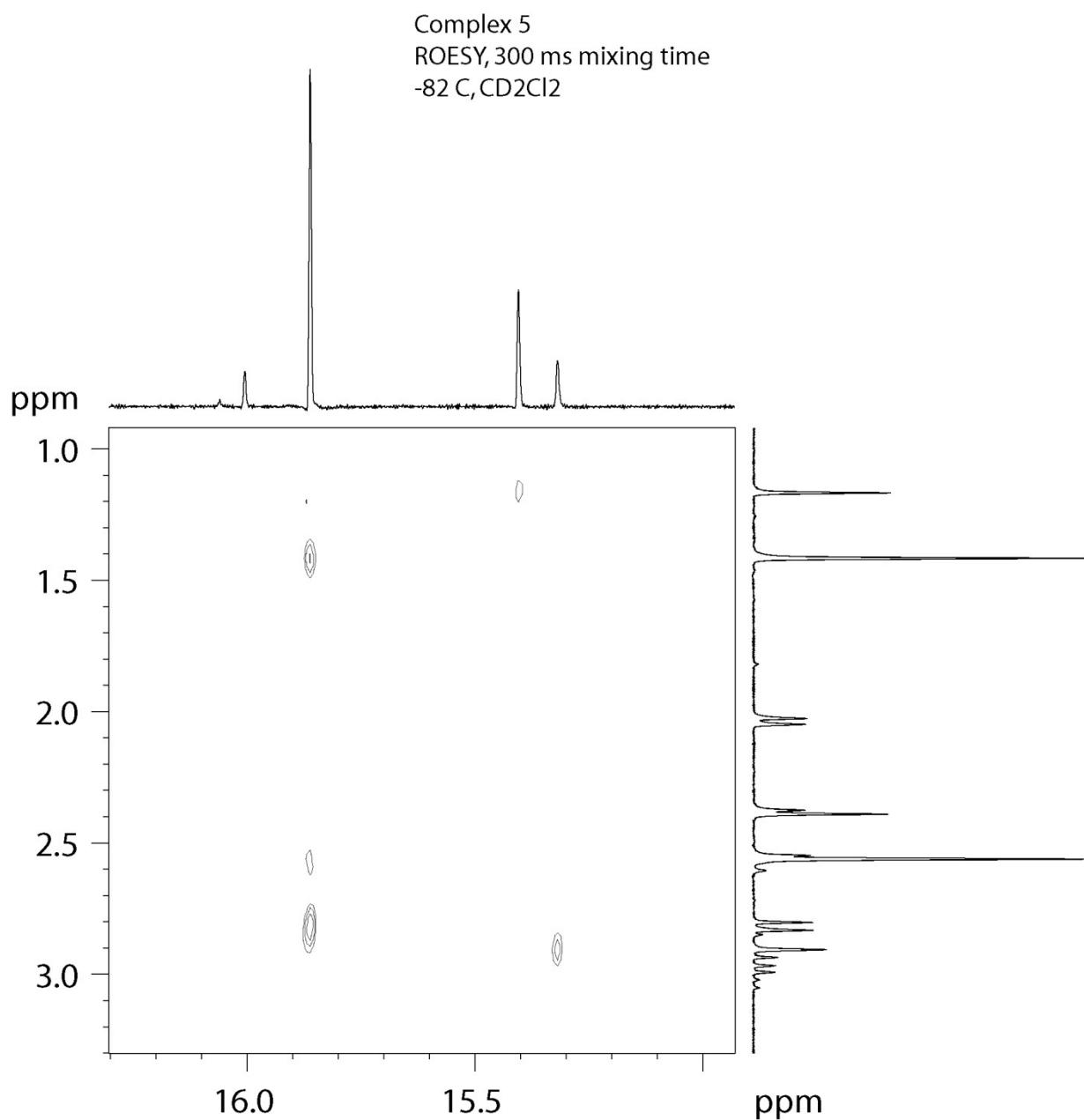


Figure S24. 400 MHz ¹H ROESY experiment for complex **5** at -82 °C dissolved in CD₂Cl₂.

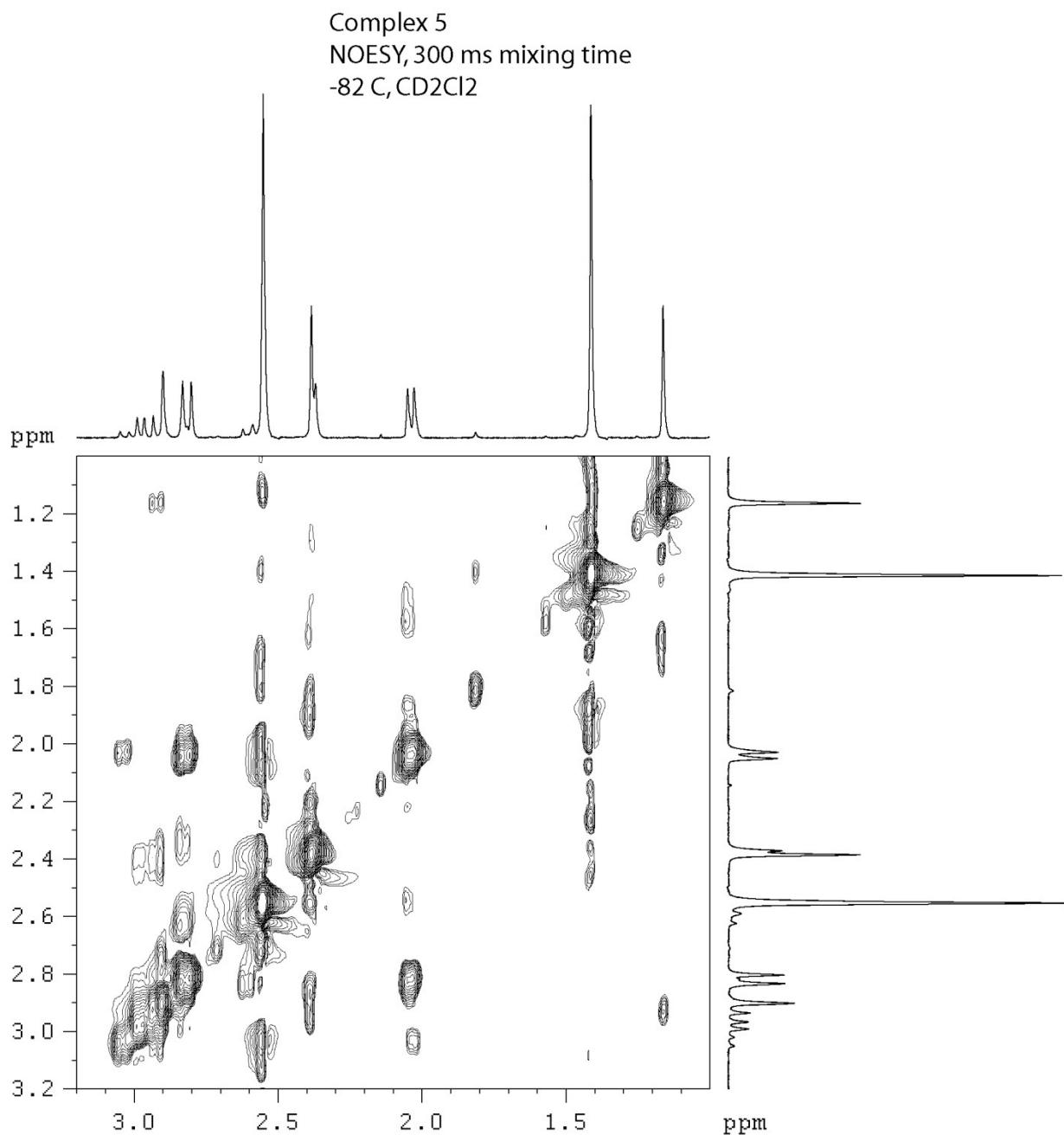


Figure S25. 400 MHz ¹H NOESY experiment for complex **5** at -82 °C dissolved in CD₂Cl₂.

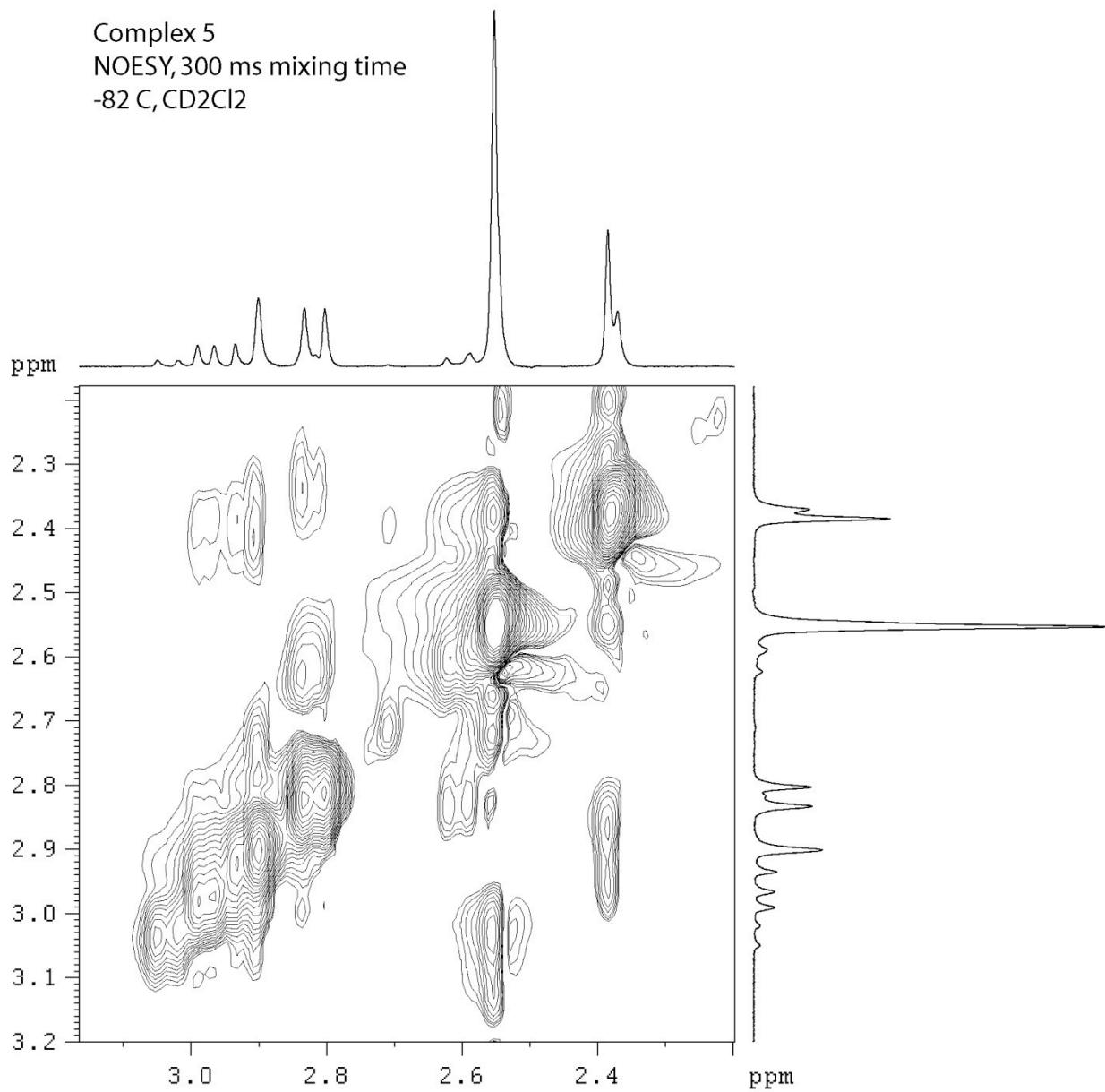


Figure S26. 400 MHz ¹H NOESY experiment for complex **5** at -82 °C dissolved in CD₂Cl₂.

Computational Section

Electronic Energies, Solvation and Thermodynamic Corrections

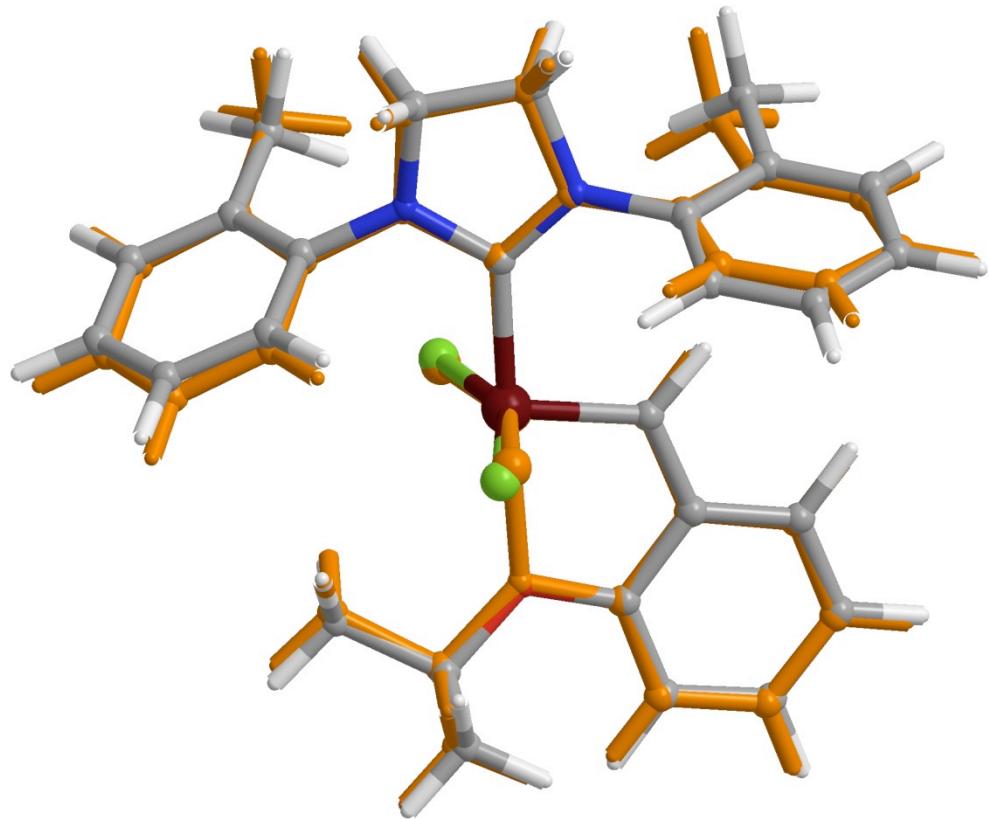
Geometry/Energy	SP Gas Phase LACV3P**+(2f)	LACVP** CH ₂ Cl ₂	B3LYP/LACVP** gas phase Optimization Analytic Hessian		
	E _{SCF}	V _{solv}	H _{vib}	ZPE	S _{vib}
B3LYP/B3LYP					
3d	-2246.426644	-14.2813	19.373	321.483	127.25056
3b	-2246.426976	-14.3458	19.393	321.469	127.60973
3c	-2246.427469	-14.6046	19.341	321.625	127.32037
3a	-2246.427469	-14.3899	19.37	321.595	127.70626
B3LYP/M06					
3d	-2245.40703	-14.6177	19.373	321.483	127.25056
3b	-2245.407782	-14.6894	19.393	321.469	127.60973
3c	-2245.407088	-14.9578	19.341	321.625	127.32037
3a	-2245.407882	-14.745	19.37	321.595	127.70626
M06-L/M06					
3d	-2245.406645	-15.3701	19.373	321.483	127.25056
3b	-2245.407311	-15.0758	19.393	321.469	127.60973
3c	-2245.407679	-15.5123	19.341	321.625	127.32037
3a	-2245.408321	-15.4764	19.37	321.595	127.70626

Complex	Geometry MO6-L/ LACVP+**	Geometry MO6-L/ LACVP+**	Geometry B3LYP/LACVP+**		
	Single Point Energy Gas Phase MO6/LACV3P++*(2f)	MO6/LACVP+** CH ₂ Cl ₂	Analytic Hessian		
	E _{SCF}	V _{solv}	H _{vib}	ZPE	S _{vib}
5a	-2129.677242	-23.2186	16.745	286.031	113.7118
5b	-2129.677569	-21.4698	17.305	286.142	113.7135
5c	-2129.675997	-21.8468	16.575	286.197	111.4614
5d	-2129.674211	-22.7799	16.648	286.02	112.1315
5e	-2129.671264	-20.8354	16.188	285.981	113.4256
5f	-2129.669191	-23.0595	16.084	285.981	112.4291
5g	-2129.668002	-21.1299	16.111	286.037	112.0403
5h	-2129.67639	-15.3855	16.384	285.842	115.4433
5i	-2129.675931	-15.5148	16.884	285.829	114.6841
5j	-2129.675945	-15.5397	16.763	286.01	113.2571
5k	-2129.663656	-22.4721	16.13	285.866	112.3851
5l	-2129.674172	-15.35	16.865	285.84	114.0773

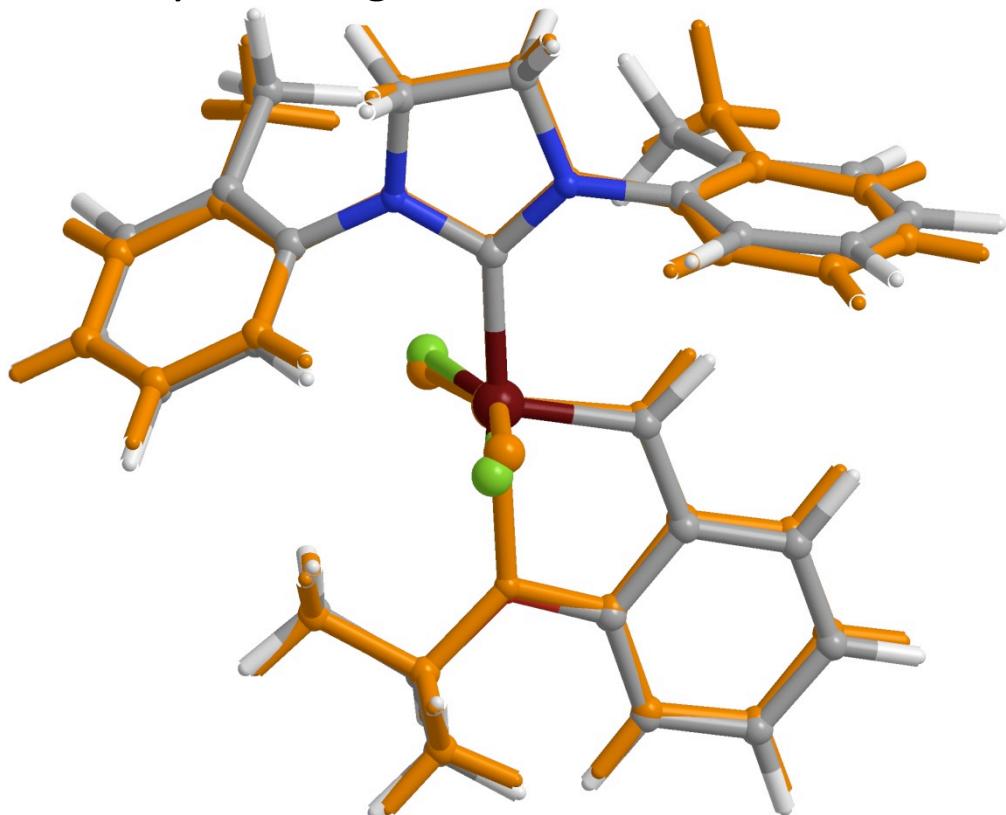
	Geometry B3LYP/ LACVP+**	Geometry B3LYP/ LACVP+**	Geometry B3LYP/ LACVP+**		
Complex	Single Point Energy Gas Phase MO6/LACV3P**++(2f)	MO6/LACVP+** CH ₂ Cl ₂	Gas Phase Optimization Analytic Hessian		
	E _{SCF}	Vsolv	Hvib	ZPE	Svib
5a	-2129.675324	-21.7887	16.745	286.031	113.7118
5b	-2129.676886	-21.0393	17.305	286.142	113.7135
5c	-2129.676278	-21.0802	16.575	286.197	111.4614
5d	-2129.674062	-21.3056	16.648	286.02	112.1315
5e	-2129.672999	-20.7455	16.188	285.981	113.4256
5f	-2129.674483	-21.9691	16.084	285.981	112.4291
5g	-2129.671134	-21.7221	16.111	286.037	112.0403
5h	-2129.675494	-15.0037	16.384	285.842	115.4433
5i	-2129.674838	-15.068	16.884	285.829	114.6841
5j	-2129.67511	-15.3562	16.763	286.01	113.2571
5k	-2129.671676	-21.7432	16.13	285.866	112.3851
5l	-2129.674077	-15.0605	16.865	285.84	114.0773

	Geometry B3LYP/ LACVP+**	Geometry B3LYP/ LACVP+**	Geometry B3LYP/ LACVP+**		
Complex	Single Point Energy Gas Phase B3LYP/LACV3P**++(2f)	B3LYP/LACVP+** CH ₂ Cl ₂	Gas Phase Optimization Analytic Hessian		
	E _{SCF}	Vsolv	Hvib	ZPE	Svib
5a	-2130.623446	-21.9926	16.745	286.031	113.7118
5b	-2130.625229	-21.1875	17.305	286.142	113.7135
5c	-2130.625273	-21.2182	16.575	286.197	111.4614
5d	-2130.622654	-21.4997	16.648	286.02	112.1315
5e	-2130.621468	-21.0416	16.188	285.981	113.4256
5f	-2130.622153	-22.2292	16.084	285.981	112.4291
5g	-2130.620668	-21.9096	16.111	286.037	112.0403
5h	-2130.628653	-14.8596	16.384	285.842	115.4433
5i	-2130.627521	-14.87	16.884	285.829	114.6841
5j	-2130.628004	-15.1605	16.763	286.01	113.2571
5k	-2130.619641	-21.9885	16.13	285.866	112.3851
5l	-2130.627643	-14.8966	16.865	285.84	114.0773

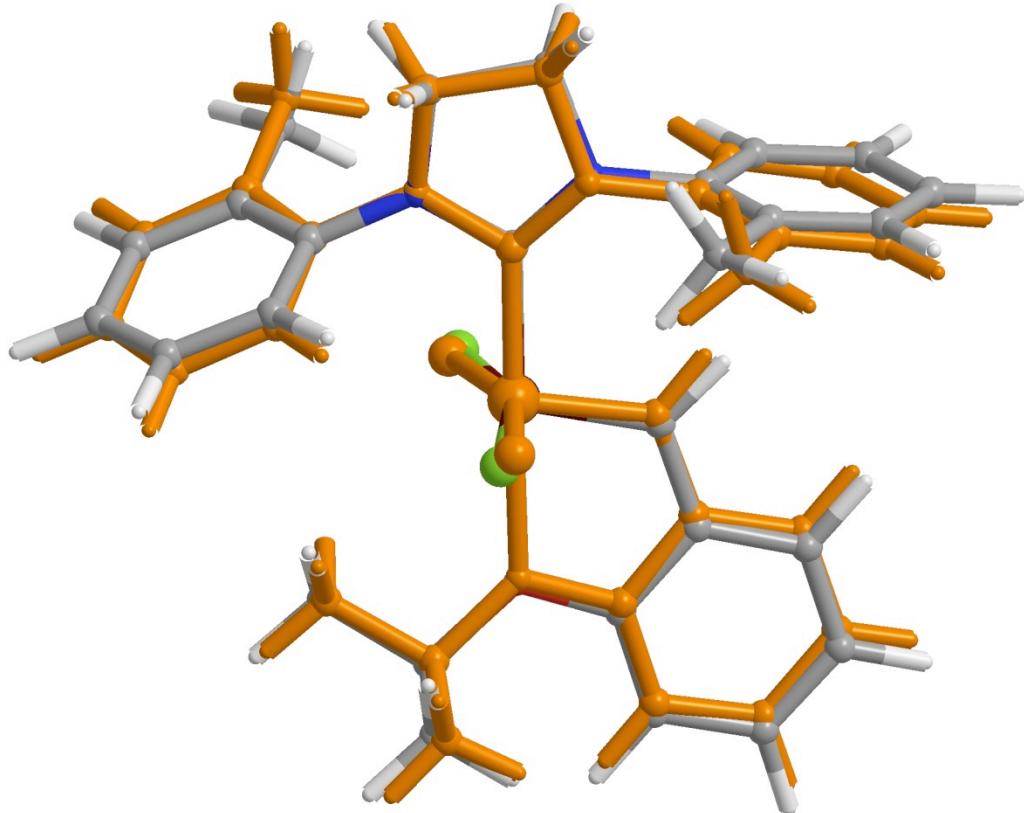
3a X-Ray in Orange, B3LYP minimized in color.



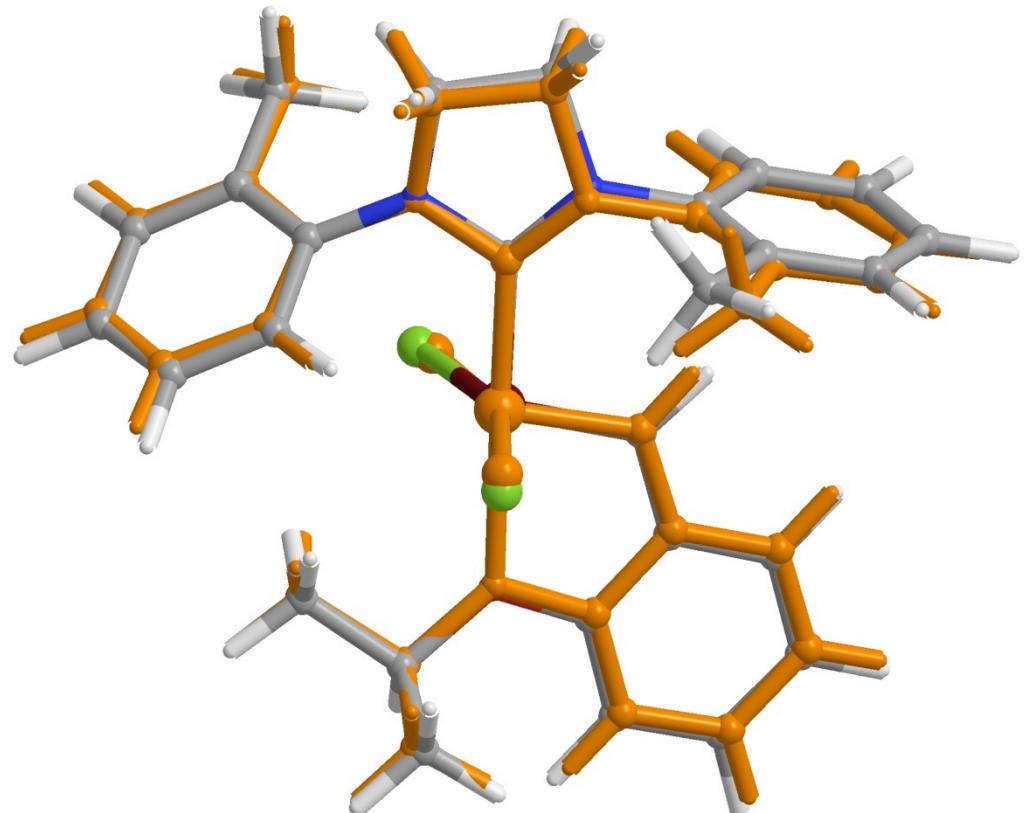
3a X-Ray in Orange, M06-L minimized in color.



3b X-Ray in Orange, B3LYP minimized in color.



3b X-Ray in Orange, M06-L minimized in color.



XYZ coordinates

a) B3LYP optimized geometries

3a				C3	2.1041763864	-0.3505597370	-1.9600898547
N1	0.3180701199	0.1904840695	-0.5470926453	N4	0.7892397781	-0.7823388313	-2.4785651558
C2	1.7922907050	0.1706389742	-0.5551975006	C5	-0.4185062405	1.0829754677	0.3355048737
C3	2.0919360378	-0.4900344041	-1.9025352467	C6	-1.6969704634	2.5935528972	2.2919465561
N4	0.7895516591	-1.0929907171	-2.2593440820	C7	-1.1871656120	2.1916716191	-0.0290029518
C5	-0.3934350378	1.0271296225	0.3746583835	C8	-0.2617893202	0.7150404201	1.6882476370
C6	-1.7163180278	2.7630905413	2.1068424411	C9	-0.9164771759	1.4924779516	2.6488462170
C7	-1.0939109238	2.1267060203	-0.1322441175	C10	-1.8362232333	2.9441986131	0.9512351012
C8	-0.3379945197	0.7772647514	1.7610123226	H11	-0.8201940952	1.2187270984	3.6964808895
C9	-1.0080469088	1.6691522726	2.6051420415	H12	-2.4392433133	3.7999550404	0.6623451942
C10	-1.7658377413	2.9903116449	0.7334941884	C13	-0.2370341988	-0.4196285307	-1.6622764021
H11	-0.9887675854	1.4856525004	3.6766132920	Ru14	-2.2075929064	-0.7173977250	-1.7278265411
H12	-2.3136153639	3.8373816403	0.3310824151	Cl15	-2.1762253203	-2.0474972082	0.2750453956
C13	-0.2359445121	-0.5760932998	-1.5267195861	Cl16	-2.5339130118	1.2458359582	-3.1078888297
Ru14	-2.2134733840	-0.7377174266	-1.6842049046	C17	-2.3611138533	-2.0238483226	-3.0182518429
Cl15	-2.4090555664	-1.7766981823	0.4764194849	C18	-1.5173258759	-2.4879438505	-3.5261146999
Cl16	-2.2958670979	1.0475266978	-3.3163383342	C19	0.7878931482	-1.7562360519	-3.5289134116
C17	-2.3379257082	-2.2396418787	-2.7428927886	C20	0.9320126643	-3.6687747350	-5.5415285992
H18	-1.4815244461	-2.8278132572	-3.0749978520	C21	0.9850989760	-3.1010019125	-3.2024538659
C19	0.7192734697	-1.7935740012	-3.5075675902	C22	0.6760770295	-1.3364962000	-4.8675126647
C20	0.7091168105	-3.0994350650	-5.9630155537	C23	0.7469295590	-2.3230629740	-5.8601306212
C21	1.1711719427	-3.1266470033	-3.5690009416	C24	1.0535549416	-4.0633256827	-4.2087349018
C22	0.2730235390	-1.1238151835	-4.6498455925	H25	0.6539675453	-2.0252062718	-6.9014632091
C23	0.2611059872	-1.7811723463	-5.8789908765	H26	1.1962585510	-5.1090796273	-3.9529935322
C24	1.1565782166	-3.7599706921	-4.8182893443	H27	2.7310031887	0.0348151803	-2.7682578250
H25	-0.0998308586	-1.2641430978	-6.7630832388	H28	1.7572641011	1.7290948539	-1.3536222576
H26	1.4930289710	-4.7915766992	-4.8880782303	H29	2.3005993704	0.6805307666	-0.0251288207
H27	2.3797338064	0.2362890882	-2.6734036833	H30	2.6209925608	-1.2014783743	-1.4966638222
H28	2.1900120169	1.1861103756	-0.4768085147	C31	-3.6668956620	-2.4920303211	-3.4248051837
H29	2.1744680762	-0.4190871469	0.2853381924	C32	-6.2214537551	-3.3425854078	-4.1905884823
H30	2.8731867020	-1.2510813931	-1.8402731889	C33	-3.8315875956	-3.4411535613	-4.4513019315
C31	-3.6314613581	-2.7212127074	-3.1715950625	H34	-4.8233467235	-1.9772860441	-2.7859074333
C32	-6.1633378124	-3.6031328896	-3.9783517474	C35	-6.0966092667	-2.4022142158	-3.1644140313
C33	-3.7688996773	-3.8330714301	-4.0239353474	C36	-5.0982580248	-3.8656641010	-4.8363667023
C34	-4.8045237790	-2.0571531212	-2.7298041037	H37	-6.9854383782	-2.0189261705	-2.6791789843
C35	-6.0662553133	-2.4974288975	-3.1295221860	H38	-7.2154316865	-3.6693024196	-4.4836171527
C36	-5.0236001263	-4.2746031249	-4.4280909786	O39	-4.5509609476	-1.0557710867	-1.8166693136
H37	-6.9677188382	-2.0006710954	-2.7933391508	C40	-5.6080989597	-0.5482977896	-0.9414544476
H38	-7.1484719659	-3.9418477667	-4.2872957039	H41	-6.4601390238	-0.3036202690	-1.5864232623
O39	-4.5616277232	-0.9862926646	-1.9208100916	H42	-2.9434109630	-3.8334171853	-4.9400509701
C40	-5.6552523147	-0.3097201532	-1.2190355015	H43	-5.2147973415	-4.5972354750	-5.6299092362
H41	-6.4497967940	-0.1493517577	-1.9572522607	C44	-5.0776284286	0.7329919787	-0.3169483150
H42	-2.8687025134	-4.3388455396	-4.3634015512	H45	-4.2352220440	0.5198288296	0.3476930294
H43	-5.1183975782	-5.1337238044	-5.0849683525	H46	-5.8724845103	1.1986623265	0.2753840814
C44	-5.1170651136	1.0410391079	-0.7731126393	H47	-4.7513197696	1.4338097506	-1.0888854111
H45	-4.3353970195	0.9164373439	-0.0177317545	C48	-5.9810821723	-1.6104569226	0.0887019252
H46	-5.9324781713	1.6225273933	-0.3297654417	H49	-5.1021236330	-1.8648970367	0.6867397550
H47	-4.7052449760	1.5933750097	-1.6209902483	H50	-6.3538789044	-2.5239916572	-0.3823165413
C48	-6.1441947730	-1.1735225813	-0.0598401153	H51	-6.7651889924	-1.2234946279	0.7483457150
H49	-5.3212384819	-1.3512614722	0.6373755242	H52	-2.1953989288	3.1733311711	3.0641488051
H50	-6.5217123557	-2.1411075257	-0.4011079841	H53	0.9846472365	-4.4082492969	-6.3359974953
H51	-6.9555451140	-0.6579506508	0.4652689057	H54	-1.2875126798	2.4425869733	-1.0794336180
H52	-2.2312522360	3.4305066129	2.7925458233	H55	0.5496635690	-0.4889384526	2.0962037060
H53	0.7059805317	-3.6178754085	-6.9180186845	H56	1.6142688627	-0.3698745721	1.8597557950
H54	-0.1009062082	-0.1094578525	-4.5529145147	H57	0.1850725254	-1.3818177389	1.5801022749
C55	1.6259067562	-3.8681290316	-2.3333308687	H58	0.4711704447	-0.6576366909	3.1735344326
H56	2.6212666888	-3.5445681046	-2.0022655183	H59	1.0587284004	-3.3843220693	-2.1563302702
H57	1.6846524713	-4.9424411771	-2.5281067625	C60	0.4675566404	0.1145358035	-5.2228469863
H58	0.9398440198	-3.706848612	-1.4961745616	H61	1.2901556395	0.7396788458	-4.8553665802
H59	-1.1175695021	2.2885271453	-1.2049747968	H62	-0.4539445452	0.5055879999	-4.7779343978
C60	0.3744077700	-0.4221080046	2.3362356576	H63	0.4111804073	0.2408013916	-6.3073060611
H61	1.4594010967	-0.2671934157	2.3966042070	3c			
H62	0.1806235951	-1.3116702598	1.7311539885	N1	0.2637518788	0.7958344589	-1.1148951479
H63	0.0207800939	-0.6239831085	3.3508107590	C2	1.7363437320	0.8287627508	-1.1874865762
3b			C3	2.0040712592	0.0100253931	-2.4511747564	
N1	0.2990338462	0.3559206087	-0.6756831056	C4	0.7339782540	-0.7299921445	-2.6178839831
C2	1.7049788465	0.7129320450	-0.9400510149	C5	-0.3869197799	1.4687955230	-0.0252237708
C7			C6	-1.5409537966	2.7488607290	2.1601976733	
C8			C7	-0.5858455986	2.8629001575	-0.0832029981	
C9			C8	-0.7446047809	0.7329350993	1.1083693760	
C9			C9	-1.3328724817	1.3724005512	2.2007184660	

C10	-1.1666839272	3.4782761445	1.0304741083	Ru17	-2.1908463099	-0.7424834115	-1.7095804205	
C11	-0.2350533454	3.6667703926	-1.3100168933	Cl18	-1.9685722822	-2.3084541732	0.1286004291	
H12	-1.6165581465	0.7941468208	3.0752648798	Cl19	-2.6833520159	1.3175681684	-2.8466944638	
H13	-1.3418428116	4.5507706990	1.0020578811	C20	-2.3944589984	-1.9169586336	-3.1150382652	
H14	-0.5658796123	4.7027373961	-1.1971123543	H21	-1.5795806273	-2.2685858425	-3.7455968745	
H15	-0.7270152617	3.2412395039	-2.1895722242	H22	0.9793111317	3.3153872773	-1.5990431136	
C16	-0.2732033354	-0.2112616094	-1.8624552776	C23	0.7927897720	-1.9214943925	-3.4430596004	
Ru17	-2.1980460573	-0.6812610975	-1.7135543608	C24	0.8785118827	-3.7063893411	-5.5722609189	
Cl18	-1.7370887847	-2.4368678090	-0.1105172551	C25	0.9627713254	-3.2913345484	-3.1682380273	
Cl19	-2.9012019771	1.4898669608	-2.4622527781	C26	0.6834994004	-1.4502406572	-4.7542268695	
C20	-2.4288443639	-1.5805857136	-3.3043903360	C27	0.7214776096	-2.3430000565	-5.8241381618	
H21	-1.6416094625	-1.7202369490	-4.0459978606	C28	0.9974413358	-4.1679656901	-4.2607760483	
H22	0.8451692689	3.6872100336	-1.5005342152	H29	0.6256404631	-1.9767111759	-6.8419397123	
C23	0.7240155992	-1.9191504699	-3.4153820668	H30	1.1189847446	-5.2320755222	-4.0745638058	
C24	0.8344054274	-4.2708266395	-4.9028072793	H31	2.3762499733	0.3351629543	-2.9615719920	
C25	0.6153907113	-3.1580934660	-2.7754050019	H32	2.1997572178	1.5386198354	-0.8796975396	
C26	0.8844436330	-1.8329120373	-4.8129326303	H33	2.0714586104	0.0398238087	0.0671329734	
C27	0.9413612881	-3.0323556939	-5.5351966297	H34	2.9015750856	-1.0171856448	-1.9350217838	
C28	0.6616928475	-4.3354693494	-3.5197537421	C35	-3.7064553734	-2.4175171762	-3.4570200905	
H29	1.0579267953	-2.9874310768	-6.6155602878	C36	-6.2713677869	-3.3475842824	-4.0831633012	
H30	0.5660857181	-5.2942274240	-3.0194709868	C37	-3.9111893912	-3.2861719828	-4.5457977107	
C31	0.9546865434	-0.5047995444	-5.5312925320	C38	-4.8279234587	-2.0250839781	-2.6829314993	
H32	1.9694867221	-0.0872524800	-5.5222696265	C39	-6.1060995045	-2.4890638923	-2.9929595921	
H33	0.2897759278	0.2333923474	-5.0727414184	C40	-5.1830339066	-3.7508481288	-4.8612957423	
H34	0.6651706704	-0.6180728077	-6.5798589025	H41	-6.9682742510	-2.1990216471	-2.4057601990	
H35	2.1904443924	0.6510534736	-3.3209400553	H42	-7.2692151409	-3.7059158472	-4.3212346454	
H36	2.1069851573	1.8540427832	-1.2571706985	O43	-4.5207857974	-1.1740690534	-1.663222015	
H37	2.1624349918	0.3666752049	-0.2867901039	C44	-5.5342635305	-0.7715998456	-0.6856348295	
H38	2.8392564493	-0.6865170161	-2.3462353648	H45	-6.4384126384	-0.5260103372	-1.2547853459	
C39	-3.7259180810	-2.1042455591	-3.6658192750	H46	-3.0495251710	-3.5860245411	-5.1366011136	
C40	-6.2670465799	-3.0775259329	-4.3227806064	H47	-5.3306209177	-4.4210655295	-5.7025653386	
C41	-3.9523787106	-2.7557221980	-4.8931018927	C48	-5.0182596544	0.4911258765	-0.0126555550	
C42	-4.8138567937	-1.9512929797	-2.7685218029	H49	-4.1248788529	0.2775838661	0.5819323331	
C43	-6.0797127129	-2.4388188209	-3.0941837433	H50	-5.7910920148	0.8800912199	0.6589856217	
C44	-5.2123235056	-3.2403506589	-5.2245658727	H51	-4.7726194890	1.2543507260	-0.7545261755	
H45	-6.9159617914	-2.3314532753	-2.4149333978	C52	-5.7912187044	-1.9134003256	0.2938013335	
H46	-7.2554073025	-3.4535165896	-4.5724976057	H53	-4.8639220636	-2.1657268723	0.8149022127	
O47	-4.4921563874	-1.2899346492	-1.6205401719	H54	-6.1563589718	-2.8117971555	-0.2111128976	
C48	-5.4612102793	-1.1532827187	-0.5318132796	H55	-6.5438762843	-1.6057798854	1.0277568758	
H49	-6.4166155141	-0.8785675349	-0.9937600248	H56	-0.7205938033	-0.2992168435	1.3445339338	
H50	-3.1169320222	-2.8718946053	-5.5786187934	H57	-2.1270746699	3.5069339264	2.7777344237	
H51	-5.3765014568	-3.7405397651	-6.1739761005	H58	0.9111365510	-4.4130742323	-6.3972014032	
C52	-4.9842192556	0.0011725070	0.3362075970	H59	0.5436767794	-0.3860497774	-4.9216460135	
H53	-4.0382518481	-0.2478026536	0.8261728424	C60	1.0805509278	-3.8017884250	-1.7533233812	
H54	-5.7311249768	0.1985122320	1.1125860548	H61	1.9458341034	-3.3655437714	-1.2398732304	
H55	-4.8437856786	0.9045110254	-0.2618519263	H62	1.2012400524	-4.8883456736	-1.7452573770	
C56	-5.5729698040	-2.4730810553	0.2258406492	H63	0.1947916256	-3.5456061124	-1.1617714477	
H57	-4.5979457791	-2.7407569016	0.6415682366	5a				
H58	-5.9064377722	-3.2883222047	-0.4220700978	Ru1	0.0342766102	-0.0055620779	0.0383319671	
H59	-6.2955170795	-2.3698864649	1.0424767552	Cl2	0.0731184928	2.4347608302	0.0605164592	
H60	-0.5768867588	-0.3390719522	1.1186947372	Cl3	-2.4205673215	0.2192085497	0.0393459201	
H61	-1.9949924301	3.2590750157	3.0054499213	N4	-0.3244873369	-0.0086016652	-2.1111598391	
H62	0.8783036536	-5.1823782701	-5.4925978157	N5	-0.8622257489	-3.0022741479	-0.2345831360	
H63	0.4584108615	-3.1809748797	-1.7020482294	C6	-0.3892937798	-1.8559012890	-0.7638967615	
3d								
N1	0.2927545260	0.5915238339	-0.9360385202	C7	-1.0240022064	-3.2257809938	-2.5745567501	
C2	1.7647105823	0.5364556847	-0.8633116581	H8	-0.4320059020	-3.7614966987	-3.3202722305	
C3	2.1021441823	-0.2906415925	-2.1016220978	H9	-1.9842445059	-2.9452770148	-3.0238144299	
N4	0.8198395478	-0.9759767707	-2.3677378863	C10	-1.1937834789	-4.0127980832	-1.2679878342	
C5	-0.4137305682	1.3761547600	0.0396527501	H11	-2.2142240818	-4.3756381664	-1.1189063568	
C6	-1.6447505560	2.9019623563	2.0147981976	H12	-0.5081100996	-4.8648407545	-1.1995299468	
C7	-0.5633578354	2.7629896483	-0.1689073898	C13	0.0493563211	-0.9752970160	-3.0366159273	
C8	-0.8519246315	0.7699652663	1.2203602487	C14	1.1616083758	-1.1736649305	-3.8844434847	
C9	-1.4781630509	1.5323185660	2.2071038353	C15	1.4803492802	-0.1492361555	-4.7855345243	
C10	-1.1879140870	3.5035593744	0.8408580918	H16	2.3372627309	-0.2766507908	-5.4426073056	
C11	-0.0995628430	3.4316116835	-1.4389856980	C17	0.7354127946	1.0321941133	-4.8441351984	
H12	-1.8246579260	1.0546548470	3.1188749253	C18	-0.3568625271	1.2109003725	-3.9962526183	
H13	-1.3232211515	4.5726650407	0.6971965012	H19	-0.9339121688	2.1295570292	-4.0200707649	
H14	-0.3146363008	4.5033399581	-1.4091375268	C20	-0.7103326298	0.2000967000	-3.0994223230	
H15	-0.6149049402	2.9973595226	-2.3013027790	C21	1.9965978372	-2.4334332648	-3.8417208234	
C16	-0.2285962825	-0.3865496782	-1.7325963852	H22	2.0923826447	-2.8218245051	-2.8232556757	
				H23	3.0014010492	-2.2428770069	-4.2294765516	

H24	1.5607633871	-3.2317717993	-4.4571132518	H37	-0.0246672917	-1.0859152090	-0.2168083276
C25	-1.0904429271	-3.3265139948	1.1458847681	H38	0.0362592018	3.8982698183	-0.1317206807
C26	-0.2244626338	-4.2210341357	1.8062356192	H39	-2.1494679146	0.1926487454	-0.3349244183
C27	-0.5408998432	-4.5793708869	3.1250265360	H40	-2.1296807160	2.6748071384	-0.2883717849
H28	0.1203090216	-5.2594550591	3.6565092710	H41	8.4695629535	-0.0088172038	-0.8482710629
C29	-1.6723867774	-4.0738897069	3.7666831188	H42	6.5918919852	1.7362584169	4.4749260593
C30	-2.5154935421	-3.1841735525	3.0962546667	H43	2.6892082519	7.2741310137	1.3767026546
H31	-3.3939520554	-2.7783712206	3.5891486842	H44	5.5048248132	4.3852129719	4.0862625036
C32	-2.2270550402	-2.8144584251	1.7823326286	H45	0.7806265512	2.6536715382	4.5038661394
C33	1.0081714434	-4.7957213472	1.1471010870	H46	2.4901078777	2.1943566269	4.4689188222
H34	0.7891332287	-5.7488429407	0.6479760638	H47	1.4394863394	1.7931158281	3.1095667843
H35	1.7849877549	-4.9926540843	1.8914140064	H48	6.5873370842	-0.5903151448	4.7434982371
H36	1.4237179134	-4.1158478217	0.3991156647	H49	5.8539622634	-2.0209959002	4.0235566442
C37	0.0665390441	-0.3830920469	1.8480641191	H50	5.0177962383	-0.4607580737	3.9418930398
H38	-0.8245276316	-0.1570726817	2.4398349739	H51	7.2337742574	2.9210103750	3.3144190372
C39	1.2591538331	-0.8468729740	2.5256590310	C52	1.2063536394	0.6789893897	-0.0725388039
C40	1.3700639364	-1.0136173543	3.9196994319	H53	2.8057549874	-0.5795826559	-0.9014547265
H41	0.5260229345	-0.7697745111	4.5588394748	H54	0.4521055273	6.8384550571	2.3929325919
C42	2.5584800348	-1.4980298116	4.4626830526	H55	8.7358250057	-2.2041889722	0.3105745861
H43	2.6522092582	-1.6299779301	5.5366306392	H56	4.4609638400	5.5187156401	1.5178419180
C44	3.6339935669	-1.8190116010	3.6232810415	H57	7.0975761996	1.7764419088	0.2002690189
H45	4.5580082843	-2.1964616458	4.0525978771				
C46	3.5350024162	-1.6484343552	2.2365365099				
H47	4.3802920999	-1.8860204972	1.5957904201	C1	-0.0633323032	0.1544674600	-0.1581419339
C48	2.3536920037	-1.1504109042	1.6852898550	C2	0.0850100967	2.9579338111	-0.3199209650
C49	2.1458761137	-0.8972299126	0.2325319860	C3	-1.2202529250	0.9193567533	-0.3450015817
H50	2.2609156932	-1.7521156794	-0.4308474515	H4	4.7374228944	3.1511108612	4.7463622108
C51	2.2104197565	0.3849225015	-0.3051026838	Ru5	4.0881366159	1.6742594758	0.0504867738
H52	2.4533938208	1.2401814211	0.3141564023	C16	4.4399902152	0.6276428915	-2.1019901068
H53	2.3297604790	0.5275318420	-1.3759565967	C17	5.5224663407	3.5113115209	-0.7252205142
H54	-1.5657578253	0.3207570844	-2.4403417425	C8	3.1667313632	0.0607579157	1.3352312468
H55	-2.8512228061	-2.1073567473	1.2453580149	N9	4.4578515020	3.4030131970	2.6621319349
H56	1.0166857355	1.8123045618	-5.5456581851	N10	5.8500629614	1.7251795131	2.4586605658
H57	-1.8906613748	-4.3700714958	4.7890288197	C11	3.4026394348	5.5795133185	2.2079502839
				C12	2.0647740500	3.7056713782	3.0356639858
				C13	2.5910692732	2.7559289827	-0.0786746147
				C14	3.2870212803	4.2297673486	2.6006077718
C1	-0.0089609191	0.0000413645	-0.1820153152	C15	4.7739084289	2.3345726619	1.8965986631
C2	0.0139068537	2.8120670865	-0.1342026481	C16	0.923338860	4.5066274815	3.0676857669
C3	-1.2052635618	0.7235465301	-0.2507420851	C17	1.0148742634	5.8422917194	2.6718290702
H4	4.6252020406	3.0558761924	4.8697452420	C18	6.5742827541	0.6116842323	1.9078173751
Ru5	4.0888568598	1.6950403255	0.0393584695	C19	8.0317680256	-1.5210732108	0.8603906929
C16	4.5451371262	0.8485469814	-2.1763037617	C20	6.6726226435	-0.5810110163	2.6588564774
C17	5.4457111811	3.6669802937	-0.5178230035	C21	7.4134967384	-1.6349946825	2.1087041494
C8	3.2853933468	-0.1196870431	1.1280576312	C22	2.7430484780	0.5039705271	2.2315247578
N9	4.3102865457	3.2202572078	2.7748644133	C23	3.9428807427	-0.6833489314	1.4917615820
N10	5.7788256960	1.6207913719	2.5065594534	C24	2.7118492096	3.8292364206	-0.2463792034
C11	3.4887022841	5.3672700574	1.9753698672	C25	-0.0239827386	4.0896030077	3.3953930991
C12	1.9726610530	3.8809158787	3.1932746238	H26	7.4954792657	-2.5651667333	2.6657487582
C13	2.5361724461	2.7043869044	-0.0197449763	C27	7.200864423	0.7370353114	0.6622785199
C14	3.2295351634	4.1511744146	2.6180811517	C28	1.2554341233	2.1971735043	-0.1292770829
C15	4.6986215074	2.2273213209	1.9499252208	C29	7.9206542611	-0.3367919720	0.1334912988
C16	0.9859501914	4.8737008951	3.0931277207	C30	6.0115203672	-0.7437385107	4.0086263989
C17	1.2355328283	6.0878081918	2.4507555912	C31	6.4611749377	2.5551316435	3.5191547917
C18	6.5608725552	0.5759592898	1.9051876034	C32	2.2397790064	6.3638455028	2.2495109592
C19	8.1317264243	-1.4181259293	0.7544838064	C33	5.3087262040	3.4931143405	3.8728224410
C20	6.6897695967	-0.6611342769	2.5746774010	C34	-1.1477435325	2.3173678925	-0.4222051567
C21	7.4881720619	-1.6435278905	1.9746089642	C35	2.4624789397	0.0695066344	0.1365850844
H22	2.8818867855	0.1767431621	2.0910628724	C36	-0.1266421076	-0.9292787072	-0.1103899336
H23	4.1051404133	-0.8324159974	1.1526206535	H37	0.1560917134	4.0392539567	-0.3979847603
H24	2.6076268053	3.7864610479	-0.1494442494	H38	-2.1821666799	0.4231216750	-0.4392213648
H25	0.0072345996	4.6860275475	3.5275327975	H39	-2.0520219345	2.8985446714	-0.5779368909
H26	7.5947891613	-2.6064974757	2.4682078207	C40	4.7141932964	6.1683663134	1.7490895710
C27	7.2110256259	0.8126882540	0.6881315888	H41	8.3826764121	-0.2395934460	-0.8435628512
C28	1.2232492591	2.0924894719	-0.0587422555	H42	6.7949839079	1.9441219220	4.3597574106
C29	7.9880642748	-0.1918140474	0.1068631115	H43	2.3014982504	7.4039710291	1.9402407361
C30	1.6592956129	2.5622285824	3.8594611885	H44	5.6294547708	4.5221982719	4.0473930584
C31	5.9972608165	-0.9450618957	3.8881227162	H45	5.4157158110	6.2912975800	2.5848351251
C32	6.3304536270	2.3921037710	3.6418572402	H46	4.5563532701	7.1581036005	1.3118453866
C33	2.4894572725	6.3362310556	1.8859926349	H47	6.6361167279	-0.3420283924	4.8175173588
C34	5.1787691806	3.3486321132	3.9685962854	H48	5.8441185913	-1.8016547198	4.2303541070
C35	-1.1950314175	2.1252379798	-0.2234400899	H49	5.0474584185	-0.2284651644	4.0533451742

H50	7.3244622505	3.0916360359	3.1051068058	H4	4.8883315051	3.4900558654	4.7497022541
C51	1.1747238448	0.7886084608	-0.0364400898	Ru5	4.0574909514	1.6773396335	-0.0537227769
H52	5.1920139597	5.5275415088	1.0011748057	Cl6	4.4955597947	0.7447171080	-2.2290264509
H53	2.7251021826	-0.6521878506	-0.6313885716	Cl7	5.2741737379	3.6811388207	-0.7509670452
H54	0.1349535119	6.4792669023	2.6918003945	C8	3.3365935943	-0.1798674988	1.0450341402
H55	8.5908909003	-2.3606025147	0.4572835356	N9	4.3317885521	3.1337024472	2.7242081095
H56	2.0145835747	2.6650041695	3.3416478452	N10	5.9702443639	1.7556629622	2.2689013218
H57	7.1122056386	1.6680409028	0.1105134638	C11	3.4034896071	5.2393890211	1.9037182297
				C12	2.0420610292	3.7845223276	3.3249469827
				C13	2.4913432481	2.6715452812	-0.0175247483
				C14	3.2282853404	4.0460168523	2.6130824413
Ru1	0.0268242017	0.0026622846	-0.0026516268	C15	4.7802943492	2.2299065985	1.8205876409
Cl2	-0.0288942420	2.4426084691	-0.0153747311	C16	1.0327511841	4.7575190521	3.2857129587
Cl3	-2.4198948690	0.1334213735	-0.1655434274	C17	1.1967688264	5.9486073705	2.5753215064
N4	-0.0495782224	-2.0086750787	-2.1746282927	C18	6.7267444612	0.6432197656	1.7537320115
N5	-0.7639638354	-3.0225130766	-0.3683394180	C19	8.2218641454	-1.5574339809	0.9194975570
C6	-0.2519591474	-1.8648171714	-0.8373173001	C20	6.4057427868	-0.6440902963	2.2065353497
C7	-0.6828772485	-3.2380614980	-2.6993560898	C21	7.1443877637	-1.7493734989	1.789474751
H8	-0.0500188986	-3.7252604997	-3.4439649780	C22	3.0212860076	0.0879007105	2.0491483882
H9	-1.6442515683	-2.9826025361	-3.1629250912	C23	4.1538540435	-0.8888215501	0.9675851673
C10	-0.8525949920	-4.0614110593	-1.4222138312	C24	2.5458321820	3.7495953463	-0.1775178983
H11	-1.8103925950	-4.5837914813	-1.3716011266	C25	0.1058972264	4.5748313563	3.8232876683
H12	-0.0468510468	-4.7942437139	-1.2817689797	C26	6.8814115377	-2.7447068175	2.1333867523
C13	0.3320149083	-0.9465585186	-3.0643909107	C27	7.8451492869	0.8613985870	0.9238240838
C14	1.5048304113	-1.0844150937	-3.8391859592	C28	1.1798349163	2.0581777434	0.0452232123
C15	1.8353312515	-0.0354711931	-4.7068795594	C29	8.5644584610	-0.2704607646	0.5059323221
H16	2.7382565180	-0.1161197625	-5.3072661332	C30	1.8419510533	2.4980956270	4.0898198021
C17	1.0429502129	1.1125147173	-4.8028126227	C31	6.3368289491	2.2910972368	3.5978437127
C18	-0.1104275626	1.2301963745	-4.028856770	C32	2.3834162554	6.1908437370	1.8787509841
H19	-0.7257516878	2.1224577794	-4.0811364443	C33	5.3475150837	3.4446979914	3.7584663918
C20	-0.4762416167	0.1925248907	-3.1680937408	C34	-1.2432222258	2.0863528178	0.0848359130
C21	2.3896196287	-2.3071960083	-3.7528936184	C35	2.4904772812	-0.0138295344	-0.0396294952
H22	2.4464111861	-2.6942759398	-2.7310275545	C36	-0.0701390585	-1.1231805434	0.0146407734
H23	3.4043632803	-2.0730784442	-4.0868551399	H37	-0.0126041113	3.8616434847	0.0590805641
H24	2.0211352723	-3.1212357418	-4.3913868311	H38	-2.2000169665	0.1518314609	0.0726508537
C25	-0.9375761729	-3.4311218290	0.9975710049	H39	-2.1810987891	2.6341104825	0.0964281181
C26	0.1926559371	-3.7851727919	1.7427771224	C40	8.2863885155	2.2419778633	0.5107132161
C27	0.0586516383	-4.2713260299	3.0431897923	H41	9.4150645385	-0.1288555474	-0.1549490708
H28	0.9408257779	-4.5324892543	3.6193963665	H42	6.2056986763	1.5108002868	4.3591601249
C29	-1.2179343924	-4.4096138687	3.5916172507	H43	2.5161509828	7.1104698601	1.3169452082
C30	-2.3431574639	-4.0684167450	2.8383348428	H44	5.8008254558	4.4191217407	3.5394958214
H31	-3.3332983073	-4.1794235991	3.2727897517	H45	0.9320968200	2.5449731425	4.6942082978
C32	-2.2359806066	-3.5819775195	1.5262314627	H46	2.6819389293	2.2825423656	4.7591677649
C33	-3.4705174541	-3.2446393196	0.7270844833	H47	1.7462885098	1.6458932922	3.4074558187
H34	-3.3753978310	-2.2629324337	0.2536803835	H48	7.5111902616	2.7571898406	-0.0645214206
H35	-4.3529220417	-3.2349164608	1.3729121579	H49	9.1932662113	2.1855492578	-0.0967259194
H36	-3.6535655788	-3.9878048650	-0.0605371646	H50	8.5087072165	2.8662760158	1.3850080176
C37	-0.0848457915	-0.3208414289	1.8143362931	H51	7.3816279741	2.6124856948	3.6087633255
H38	-1.0516903451	-0.1773592352	2.3046196880	C52	1.1634514144	0.6459877295	0.0406915314
C39	1.0792088665	-0.6111568736	2.6237371694	H53	2.6999862398	-0.5716188067	-0.9484309126
C40	1.0782107140	-0.6632629214	4.0307357245	H54	0.3988396625	6.6859662564	2.5674885175
H41	0.1601601889	-0.4608245901	4.5754942147	H55	8.8021946108	-2.4079366739	0.5733785284
C42	2.2542349686	-0.9791396934	4.7083957830	H56	4.3215240101	5.3872889245	1.3432759007
H43	2.2629658986	-1.0192377109	5.7937038887	H57	5.5705792085	-0.7701130771	2.8892837754
H44	3.4272434483	-1.2485972138	3.9902968023				
H45	4.3405050040	-1.4963151423	4.5241503276				
C46	3.4378796009	-1.1932861049	2.5904395386				
H47	4.3558026792	-1.3916229568	2.0432529519	Ru1	-0.0140207355	0.0717919189	0.0221151166
C48	2.2687960194	-0.8622057577	1.9045222830	Cl2	-0.2381226728	2.4975098946	0.0396521722
C49	2.1636638672	-0.7547849952	0.4218865060	Cl3	-2.4672120180	0.0483425350	-0.0550335553
H50	2.3499203974	-1.6661046542	-0.1441127851	N4	-0.2257763148	-1.8824420483	-2.1966766101
C51	2.2158636604	0.4684286871	-0.2351367426	N5	-0.4192403347	-3.0360175836	-0.3446040017
H52	2.3736412449	1.3905512673	0.3110154022	C6	-0.2060585244	-1.7951737467	-0.8451205868
H53	2.4031538048	0.5125791986	-1.3047987580	C7	-0.3668842929	-3.2716229831	-2.6793269507
H54	1.3340253270	1.9138338077	-5.4758755367	H8	0.5998354464	-3.6323892638	-3.0557423765
H55	-1.3794670117	0.2672204139	-2.5686112090	H9	-1.0986592790	-3.3318590644	-3.4886651190
H56	-1.3398948111	-4.7842382220	4.6040856306	C10	-0.8132816865	-3.9941179446	-1.4080136193
H57	1.1763290766	-3.6688116152	1.2985022904	H11	-1.8999175643	-4.1411287367	-1.3709505587
				H12	-0.3235824054	-4.9597952386	-1.2657642280
				C13	0.1259540648	-0.8352921517	-3.1177448773
C1	-0.0541793802	-0.0369682879	0.0410201329	C14	1.4818920663	-0.5664405218	-3.3468632159
C2	-0.0325961533	2.7756999306	0.0649614581	C15	1.8641965512	0.4057634264	-4.2705284902
C3	-1.2531489926	0.6846193811	0.0706307979	H16	2.9160543598	0.6173367870	-4.4374004531

C17	0.8780535482	1.0990138525	-4.9760136692	C30	6.5551138546	2.6354046863	3.4313410908
C18	-0.4703845383	0.8081974055	-4.7644883378	C31	2.1020069430	6.1663623015	2.1266068449
H19	-1.2291833073	1.3507273230	-5.3217186116	C32	5.3570441176	3.5183638825	3.7967990769
C20	-0.8824855231	-0.1675295892	-3.8438118626	C33	-1.1561052945	2.6275075020	-0.1580312803
C21	-2.3459238845	-0.4741384207	-3.6483050010	C34	2.2767103325	0.1121398385	0.3488829168
H22	-2.5750360254	-1.5200055518	-3.8883528103	H35	-0.4005312540	-0.6592059148	0.3976163265
H23	-2.9578870626	0.1555115934	-4.2993929331	H36	0.2905608147	4.2144043770	-0.3912738938
H24	-2.6481173785	-0.3002082848	-2.6099512579	H37	-2.3501922663	0.8462444438	0.0859535950
C25	-0.6773057293	-3.4191992600	1.0156878217	H38	-2.0157336719	3.2744249353	-0.3074992219
C26	0.2125564791	-4.3046497904	1.6566788601	C39	4.5185654461	5.9594605194	1.3902346111
C27	-0.1193517783	-4.7389562477	2.9479214939	C40	8.4659527813	2.3952784962	0.6500991436
H28	0.5583194211	-5.4138991532	3.4647827777	H41	9.5653198143	0.0451609610	-0.0845198307
C29	-1.2902218704	-4.3165568961	3.5807046537	H42	6.8514471914	1.9573861925	4.2366220813
C30	2.1581216611	-3.4381205399	2.9281582886	H43	2.0970591864	7.1657233327	1.6990945924
H31	-3.0693692651	-3.1001509125	3.4129191246	H44	5.6207546862	4.5737169525	3.9051365817
C32	-1.8549343828	-2.9934841437	1.6404395995	H45	5.3286114968	6.1015199272	2.1173559881
C33	1.4816069080	-4.7894338458	0.9947714078	H46	4.3106016104	6.9336116983	0.9394353593
H34	1.2915670767	-5.6411335632	0.3277104134	H47	7.6409817572	3.0718948261	0.4181163064
H35	2.2036155971	-5.1230796989	1.7451815890	H48	9.1247235336	2.3661123500	-0.2216406988
H36	1.9500571093	-4.0029438496	0.3970035727	H49	9.0487282770	2.8100401109	1.4842014110
C37	-0.0164230461	-0.3564213386	1.8209714736	H50	7.4294430578	3.2216858066	3.1293599118
H38	-0.9441622847	-0.2188885465	2.3824696023	C51	1.0460155081	0.9300014842	0.2134587831
C39	1.1798966256	-0.7531684153	2.5344070717	H52	4.8953349267	5.2876548994	0.6109735918
C40	1.2415019246	-0.9824411016	3.9222480454	H53	2.4283849408	-0.6625258261	-0.3973672500
H41	0.3542162726	-0.8339037125	4.5313856029	H54	0.0558234524	6.2910619348	2.7869602074
C42	2.4364841734	-1.4122099409	4.4965205270	H55	8.8788813561	-2.2567513704	0.4914280327
H43	2.4915368967	-1.5955660991	5.5655732913	H56	5.5930159004	-0.6713857704	2.7666464991
C44	3.5677016802	-1.6147542188	3.6942472907	H57	2.1174409211	2.6173462568	3.6564185771
5h							
H47	4.4059920511	-1.5211044113	1.7040820988	Ru1	0.0154852729	-0.0086303080	-0.0018839757
C48	2.3294061091	-0.9343838976	1.7339896122	Cl2	0.0306103960	2.4485313773	-0.0907522306
C49	2.1701515816	-0.6047265052	0.2914464986	N3	-2.9019614493	0.6075232957	0.0067647172
H50	2.4220879092	-1.3893864318	-0.4191731118	N4	-2.3578075571	0.0189363568	2.0425830504
C51	2.1218462694	0.7171406453	-0.1417045768	C5	-1.8734506626	0.2312498340	0.7999903095
H52	2.2309100363	1.5357034960	0.5599689553	C6	-4.2129331550	0.5607028308	0.6873724529
H53	2.2865874099	0.9685769320	-1.1849688158	H7	-4.8447497763	-0.2003288111	0.2159215374
H54	1.1578216417	1.8642280693	-5.6943131212	H8	-4.7230523133	1.5249894454	0.6170173407
H55	-1.5204836155	-4.6704921380	4.5818029426	C9	-3.8259228682	0.2003599964	2.1307665121
H56	-2.5049356985	-2.2974504894	1.1181733719	H10	-4.0717173333	0.9948519197	2.8420801642
H57	2.2320701469	-1.1279696218	-2.7972493331	H11	-4.2911968481	-0.7283756940	2.4765260052
5g							
C1	-0.2473588965	0.4053299843	0.2416929970	C13	-2.5612567590	-0.2169254943	-2.2678509845
C2	0.1320509405	3.1561691210	-0.2038957842	C14	-2.5287043350	-0.0163073574	-3.6502077727
C3	-1.3441892441	1.2560825667	0.0629744933	H15	-2.3087053322	-0.8499321537	-4.3105326749
H4	4.8533586184	3.1936237408	4.7157973139	C16	-2.7910814584	1.2521696905	-4.1679679000
Ru5	4.0396238095	1.5585989868	0.0595343157	C17	-3.0731752574	2.3127351058	-3.3034575450
Cl6	4.2820606140	0.2307085102	-1.9393588365	H18	-3.2595844449	3.3024485250	-3.7128158992
Cl7	5.4828442057	3.2212455961	-0.9972746201	C19	-3.0997859597	2.1452431252	-1.9125792987
C8	3.0624323241	0.0926617497	1.4926704534	C20	-3.3764046594	3.3235113774	-1.0104630062
N9	4.4501888770	3.3254614642	2.6404267245	H21	-4.4217455835	3.3445657432	-0.6740388800
N10	6.0372821600	1.8641380697	2.2806683382	H22	-3.1901585175	4.2605843327	-1.5423280364
C11	3.2781398395	5.4051650403	2.0473855604	C24	-1.6528843331	-0.4424183015	3.2035915713
C12	2.0997114778	3.6153013988	3.2280450119	C25	-1.2774126066	-1.7887978372	3.2805399868
C13	2.6220138732	2.7439734336	-0.0946887928	C26	-0.6444773455	-2.2706017416	4.4270939625
C14	3.2484786927	4.1080121741	2.6004923972	H27	-0.3436342689	-3.3126385962	4.4785817460
C15	4.8489828152	2.3272612622	1.8197921118	C28	-0.3994215240	-1.4075175681	5.4979552759
C16	0.9435393138	4.3923099533	3.2957042758	C29	-0.7739351623	-0.0643978569	5.4113179673
C17	0.9484626746	5.6735111879	2.7409288319	H30	-0.5657594468	0.6066454125	6.2411540350
C18	6.8128543855	0.7730167167	1.7503696163	C31	-1.4034356377	0.4496622168	4.2674183763
C19	8.3021119878	-1.4140214413	0.8614602128	C32	-1.7622968948	1.9156229618	4.1844143938
C20	6.4492699309	-0.5304862875	2.1157070673	H33	-1.5735669352	2.3194053836	3.1851011637
C21	7.1824113258	-1.6279488499	1.6672730166	H34	-1.1751670548	2.4954526097	4.9021651950
H22	2.7542759941	0.6136474898	2.3938973064	H35	-2.8202380329	2.0891837116	4.4206864716
H23	3.7682036894	-0.7203087713	1.6236748315	C36	1.0158569927	-0.0048800460	1.5542668748
H24	2.8184449874	3.7782235624	-0.3868013763	H37	0.6796050302	0.5232494764	2.4493076325
H25	0.0510479916	3.9991755546	3.7726466038	C38	2.3132077890	-0.6394749313	1.6272284364
H26	6.8828174461	-2.6340925157	1.9444417755	C39	3.0223939743	-0.7903648753	2.8383449693
C27	7.9699536351	1.0088333549	0.9778567705	H40	2.6138501297	-0.3641573415	3.7506371688
C28	1.2422229934	2.3097665170	-0.0167365038	C41	4.2128275255	-1.5103458959	2.8631579358
C29	8.6870607405	-0.1136559827	0.5354884195	H42	4.7526107189	-1.6407122419	3.7965750105

C43	4.7081187068	-2.0810629883	1.6813654252	H56	-1.8780462953	1.9409388070	-1.7475742625
H44	5.6334626201	-2.6499520402	1.7043582441	H57	-1.1973029689	2.6875194637	3.1451347584
C45	4.0268090762	-1.9213151939	0.4711785994			5j	
H46	4.4252929936	-2.3576745448	-0.4406902504				
C47	2.8403981311	-1.1832155783	0.4291994605	Ru1	0.0207897153	0.0013724838	0.0032577337
C48	2.0790280993	-0.9496467033	-0.8181380593	Cl2	0.0241745083	2.4899670233	-0.0306404843
H49	1.8003466969	-1.8317878544	-1.3884187536	N3	-2.9408980731	0.3190656520	0.0120677788
C50	1.8830306106	0.2951231327	-1.3688124281	N4	-2.2813036769	0.4746687109	2.0921925566
H51	2.3326350970	1.1904311636	-0.9540932565	C5	-1.8597210889	0.2697043677	0.8241139484
H52	1.4651641852	0.3857460221	-2.3684259115	C6	-4.1541418817	0.7748177885	0.7233269237
Cl53	-0.6059469483	-2.3714820404	-0.2512981959	H7	-5.0324388770	0.2036032423	0.4161660070
H54	0.0881634527	-1.7752329133	6.3966764999	H8	-4.3271151376	1.8360178169	0.5023691597
H55	-2.7726071098	1.4212394815	-5.2410651843	C9	-3.7606137449	0.5395019450	2.1814441948
H56	-1.4563151398	-2.4314965333	2.4249120874	H10	-4.0790742352	1.3432643023	2.8487997489
H57	-2.3697455836	-1.1981074782	-1.8459735865	H11	-4.1411024128	-0.4140981186	2.5704754813
				C12	-2.9406426444	0.2130960764	-1.4230201604
		5i		C13	-3.5466722702	-0.9098812433	-2.0280443560
Ru1	0.0257366252	-0.0043931716	0.0025045404	C14	-3.5783452697	-0.9509714943	-3.4280000624
Cl2	0.0123001568	2.4773009417	-0.0126446442	H15	-4.0299707783	-1.8111327865	-3.9155946425
N3	-2.9360355508	0.2623638001	0.0123727731	C16	-3.0320211312	0.0742905481	-4.2048090069
N4	-2.2851360728	0.5541932395	2.0763671627	C17	-2.4385277557	1.1752997248	-3.5879666678
C5	-1.8562128908	0.2732052335	0.8301773982	H18	-2.0106652999	1.9782915312	-4.1808899787
C6	-4.1544860716	0.7707564598	0.6779115293	C19	-2.4010452010	1.2494614237	-2.1930064496
H7	-5.0218375931	0.1500936755	0.4429901526	C20	-4.1178315256	-2.0448852175	-1.2139047586
H8	-4.3539199086	1.7944899190	0.3370812370	H21	-5.0240831332	-1.7444669408	-0.6663717499
C9	-3.7557605189	0.7139757145	2.1563263449	H22	-3.3802406128	-2.4010592760	-0.4859206410
H10	-4.002294155	1.6250871145	2.7050739735	H23	-4.3925348197	-2.8826701033	-1.8645828513
H11	-4.1979640886	-0.1425422650	2.6802440784	C24	-1.5409051962	0.2291874868	3.2943629782
C12	-2.9184174090	0.0902843256	-1.4149679190	C25	-1.1812209625	-1.0837514590	3.6149367950
C13	-3.5372775005	-1.0451525568	-1.9819045803	C26	-0.5132417485	-1.3509734247	4.8100053984
C14	-3.5457016130	-1.1464709800	-3.3787135320	H27	-0.2257101008	-2.3686404906	5.0535531710
H15	-4.0047042236	-2.0188132542	-3.8369230315	C28	-0.2178654657	-0.3028932146	5.6829390686
C16	-2.9625144893	-0.1685781930	-4.1892782944	C29	-0.5773872117	1.0053081108	5.3526521938
C17	-2.3544062765	0.9448637230	-3.6101427029	H30	-0.3300584943	1.8168301876	6.0307518140
H18	-1.8995020145	1.7121094333	-4.2297188232	C31	-1.2422404315	1.3032565414	4.1540335658
C19	-2.3405916031	1.0795436389	-2.2189601104	C32	-1.5842395232	2.7263060148	3.7879451987
C20	-4.1384386039	-2.1355646556	-1.1295149125	H33	-1.2743578624	2.9544018976	2.7614404002
H21	-5.0622432074	-1.8108731958	-0.6337743382	H34	-1.0872579160	3.4242587342	4.4652195423
H22	-3.4290706790	-2.4516705168	-0.3592187729	H35	-2.6617666875	2.9178171010	3.8583384438
H23	-4.3878268286	-3.0060115012	-1.7424058636	C36	1.0974255066	0.0486836512	1.5083622958
C24	-1.5235511770	0.5736811766	3.2908500578	H37	0.8231465093	0.6250826767	2.3941542949
C25	-1.3280147835	-0.6164396819	4.0208494236	C38	2.3819831766	-0.6134203077	1.5334456701
C26	-0.6317964028	-0.5196133292	5.2352204165	C39	3.1443493188	-0.7597584910	2.7119958830
H27	-0.4619013772	-1.4232426554	5.8152323963	H40	2.7903200638	-0.3080886150	3.6347779061
C28	-0.1535152851	0.7048432392	5.7092078506	C41	4.3166424173	-1.5076896418	2.6920924501
C29	-0.3584133700	1.8718849897	4.9689707300	H42	4.8967978528	-1.6365382378	3.6009315331
H30	0.0191087386	2.8254444232	5.3257061749	C43	4.7430861686	-2.1083828793	1.4981505312
C31	-1.0487845828	1.8031972779	3.7573704287	H44	5.6553515458	-2.6980606281	1.4882479941
C32	-1.8190177828	-1.9507985314	3.5118742337	C45	4.0119767534	-1.9503767793	0.3184200672
H33	-1.5268547145	-2.7522249640	4.1958522001	H46	4.3589485061	-2.4077437452	-0.6040194468
H34	-1.4112258963	-2.1805475978	2.5213874675	C47	2.8425258231	-1.1840821051	0.3197592070
H35	-2.9123036329	-1.9740944289	3.4257887301	C48	2.0359420247	-0.9376914655	-0.8944597353
C36	1.1117018118	-0.0368153439	1.5022602453	H49	1.7378799134	-1.8123670059	-1.4661573539
H37	0.8354384417	0.4774411113	2.4240630777	C50	1.8203450866	0.3167696791	-1.4223044904
C38	2.4020214870	-0.6889067797	1.4891619448	H51	2.2943590887	1.2054717723	-1.0203481541
C39	3.1729107686	-0.8769719024	2.6568615910	H52	1.3685744758	0.4153461164	-2.4064694550
H40	2.8191640789	-0.4678553312	3.5995962508	C53	-0.5946871097	-2.3573757711	-0.1389057273
C41	4.3558774633	-1.6067812346	2.5993728020	H54	0.2969547890	-0.5007633153	6.6189660444
H42	4.9438652037	-1.7650677188	3.4987548447	H55	-3.0700574899	0.0081339594	-5.2886736875
C43	4.7830866150	-2.1504600603	1.3787215650	H56	-1.4037101042	-1.8782625552	2.9099430773
H44	5.7038029457	-2.7258509715	1.3384753690	H57	-1.9415185846	2.0953289269	-1.6928987551
C45	4.0412179199	-1.9532519041	0.2108790559			5k	
H46	4.3883028597	-2.3667138298	-0.7320880869				
C47	2.8619161897	-1.2034107035	0.2511200989	Ru1	0.0412755896	0.0455568759	0.0009237470
C48	2.0449646223	-0.9171317997	-0.9475476389	Cl2	0.0906746294	2.4792050768	-0.0533286713
H49	1.7397366347	-1.7711299460	-1.5461116667	Cl3	-2.3900851600	0.3016862922	-0.1040707106
C50	1.8252956009	0.3540801685	-1.4264830980	N4	-0.3604671740	-1.8834827956	-2.2180736756
H51	2.3011968659	1.2272187765	-0.9939097032	N5	-0.7984912158	-2.9736122586	-0.3720332432
H52	1.3643171871	0.4910073434	-2.4014616976	C6	-0.3583108470	-1.7957427562	-0.8651394139
Cl53	-0.5779698748	-2.3569122937	-0.2285019030	C7	-0.9430471909	-3.1474396242	-2.7157027820
H54	0.3798019678	0.7452167784	6.6550833552	H8	-0.2922317495	-3.5932789223	-3.4734019592
H55	-2.9822959099	-0.2819845125	-5.2696664709	H9	-1.9257366490	-2.9613398487	-3.1627568917

C10	-1.0366179684	-3.9817271922	-1.4325398726	H23	-2.6465449019	3.2707529826	-0.3464171500
H11	-2.0139189743	-4.4527576057	-1.3006917438	C24	-1.6075907934	0.0146370708	3.2917788901
H12	-0.2667993950	-4.7617910856	-1.3752032261	C25	-1.4348167477	-1.2122577915	3.9597705042
C13	0.1090297449	-0.8801254636	-3.1340914438	C26	-0.7561107016	-1.1867318875	5.1883505604
C14	1.4905712987	-0.8004904857	-3.3608297438	H27	-0.6004999854	-2.1221538721	5.7196371869
C15	2.0107908287	0.1189927459	-4.2700332455	C28	-0.2796484979	0.0058634117	5.7377128349
H16	3.0826128804	0.1797331147	-4.4331951483	C29	-0.4710284521	1.2145599855	5.0629236651
C17	1.1354121788	0.9551130831	-4.9669927664	H30	-0.1000296462	2.1457729266	5.4805643084
C18	-0.2400188236	0.8560314036	-4.7576672438	C31	-1.1405087225	1.2154872459	3.8383494738
H19	-0.9129706406	1.5116893377	-5.3035793739	C32	-1.9457870261	-2.5069188584	3.3771021990
C20	-0.7913359759	-0.0632872629	-3.8509113097	H33	-1.6591569370	-3.3521519310	4.0087617174
C21	-2.2874160527	-0.1578625063	-3.6811736634	H34	-1.5507856659	-2.6721744706	2.3694092129
H22	-2.6905280913	-1.0379734795	-4.2001236818	H35	-3.0403360798	-2.5069521694	3.2998548845
H23	-2.7738972404	0.7221303844	-4.1104472385	C36	1.0967600944	-0.0508009426	1.5004164188
H24	-2.5684915444	-0.2155345801	-2.6257670162	H37	0.8207017264	0.4775087851	2.4141018429
C25	-0.8490497877	-3.4156099969	0.9931267398	C38	2.3776645263	-0.7213152747	1.5033623838
C26	0.3272368597	-3.8826206399	1.5896582471	C39	3.1355153323	-0.9120113578	2.6790805510
C27	0.3056424676	-4.4078184495	2.8812228621	H40	2.7813290673	-0.4884830533	3.6151715793
H28	1.2246948720	-4.7551404842	3.3428713116	C41	4.3045392354	-1.6652547068	2.6387600579
C29	-0.9069063703	-4.4721885111	3.5706668707	H42	4.8816314268	-1.8261952298	3.5446776110
C30	-2.0809899308	-4.0203029822	2.9648081277	C43	4.7306795734	-2.2301000341	1.4273916265
H31	-3.0211174177	-4.0778433958	3.5073559693	H44	5.6398507397	-2.8243651434	1.4005477173
C32	-2.0866123897	-3.4930300762	1.6638765587	C45	4.0019832662	-2.0306523401	0.2516078844
C33	-3.3749179892	-3.0421736699	1.0207142455	H46	4.3476544274	-2.4616083104	-0.6840567577
H34	-3.2770401884	-2.0388589677	0.5947313092	C47	2.8373013735	-1.2576976038	0.2745730017
H35	-4.1858854523	-3.0316542536	1.7544254029	C48	2.0339835455	-0.9717290457	-0.9330891257
H36	-3.6769809327	-3.7215394030	0.2123079181	H49	1.7220252761	-1.8282358323	-1.5246194541
C37	-0.0576087174	-0.3178692334	1.8107235142	C50	1.8373433222	0.2965341271	-1.4286644201
H38	-1.0046215036	-0.1256241704	2.3225686043	H51	2.3211327305	1.1675899339	-1.0009040157
C39	1.0952251163	-0.7101340037	2.5940349524	H52	1.3842307488	0.4322402028	-2.4072190171
C40	1.1042996425	-0.8195555140	3.9974371881	CI53	-0.5887473707	-2.3953125029	-0.1869687069
H41	0.2074129724	-0.5785829153	4.5615272105	H54	0.2388327419	-0.0095641147	6.6924975344
C42	2.2619850651	-1.2447377844	4.6471457902	H55	-2.8865468529	1.1000623918	-5.2759663391
H43	2.2776968242	-1.3318953160	5.7296396619	H56	-2.3813398790	-1.3693341750	-1.7834175991
C44	3.4064413608	-1.5647594523	3.9043588623	H57	-1.2822447487	2.1384093008	3.2828427874

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Ru1	0.0218736106	-0.0194932372	-0.0063911491
Cl2	0.0284945605	2.4403123367	-0.0947058042
N3	-2.9080613935	0.5228943516	0.0034566699
N4	-2.3524429919	0.0613457704	2.0664607223
C5	-1.8655230540	0.2323719503	0.8170617226
C6	-4.2128922244	0.3636085456	0.6801478386
H7	-4.6667377876	-0.5873156979	0.3726794405
H8	-4.8951478234	1.1767262148	0.4233074347
C9	-3.8007539638	0.3642706105	2.1526462791
H10	-3.9428347667	1.3428230690	2.6294108093
H11	-4.3192161066	-0.3920296797	2.7475992166
C12	-2.8603982745	0.6943398792	-1.4239067135
C13	-2.5953483599	-0.4097730695	-2.2420020274
C14	-2.5948858844	-0.2659806722	-3.6321694491
H15	-2.3808919895	-1.1245446874	-4.2618470563
C16	-2.8798063796	0.9770672804	-4.1964755065
C17	-3.1555422819	2.0715063068	-3.3721285863
H18	-3.3651326230	3.0399237556	-3.8190378657
C19	-3.1518318736	1.9611162182	-1.9757998358
C20	-3.4232621387	3.1665643556	-1.1095818707
H21	-4.3958606434	3.1005860284	-0.6048235088
H22	-3.4334500150	4.0772230544	-1.7146936274

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				N4	0.8341035595	-0.8249879186	-2.4415666569
				C5	-0.4257223933	1.0528269764	0.3076150274
				C6	-1.9718714518	2.2907166261	2.2621712755
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N1	0.3100655054	0.3316094838	-0.6512650524	C7	-1.4293368136	1.9501615764	-0.0614204099
C2	1.7189778867	0.6555700416	-0.8789302962	C8	-0.1736220373	0.7559605460	1.6618550097
C3	2.1114542908	-0.3796519786	-1.9185563837	C9	-0.9613805682	1.3977055534	2.6205993052
N4	0.8089418905	-0.7782961383	-2.4650989774	C10	-2.2098738749	2.5647768742	0.9184403776
C5	-0.4469350761	1.0140657846	0.3409739891	H11	-0.7978736755	1.1600914934	3.6704598687
C6	-1.9801170281	2.3079009426	2.2673537574	H12	-2.9979716826	3.2534481703	0.6233782990
C7	-1.4249786270	1.9305144032	-0.0482895312	C13	-0.213632051	-0.3866654987	-1.6912590360
C8	-0.2156049154	0.7239335169	1.6998779057	Ru14	-2.1571568276	-0.6498992270	-1.7634101035
C9	-0.9970551709	1.3921796937	2.6452073791	Cl15	-2.0773484969	-1.8197667662	0.3544614603
C10	-2.1978006820	2.5753333824	0.9188844165	Cl16	-2.6250319897	1.2264550412	-3.2604244287
H11	-0.8511275453	1.1595991596	3.6987752464	C17	-2.3297665965	-2.0130586153	-3.0060430814
H12	-2.9665166641	3.2799216616	0.6106647070	H18	-1.4907780207	-2.5289878664	-3.4827166642
C13	-0.2246131571	-0.4167956968	-1.6613940899	C19	0.8000825136	-1.8198270692	-3.4572078461
Ru14	-2.1651503602	-0.6839056349	-1.7445410579	C20	0.7742809451	-3.7799728937	-5.4192253515
Cl15	-2.1638346528	-1.8050724001	0.4109094704	C21	0.9909484750	-3.1570028721	-3.1041789024
Cl16	-2.4565109380	1.1418108123	-3.3263952054	C22	0.6075930861	-1.4290838040	-4.7932739238
C17	-2.3514108423	-2.0809950049	-2.9464499858	C23	0.5945978713	-2.4399978503	-5.7624935209
H18	-1.5207975368	-2.6066125906	-3.4274294016	C24	0.9756468079	-4.1449252802	-4.0870689121
C19	0.7716277063	-1.7586469050	-3.4955968241	H25	0.4387956164	-2.1631624725	-6.8038425195
C20	0.7593991493	-3.6369862589	-5.5354639420	H26	1.1115811445	-5.1880695097	-3.8153890913
C21	0.8384918535	-3.1222567484	-3.1543977450	H27	2.8450011647	-0.1863697494	-2.6147303657
C22	0.6921687525	-1.3381885015	-4.8216823411	H28	1.8907763692	1.6345508092	-1.3547558841
C23	0.6798992074	-2.2803938490	-5.8496814720	H29	2.2966770285	0.6194960952	0.0479557074
C24	0.8353200221	-4.0488000552	-4.2034598288	H30	2.5405039752	-1.3557104176	-1.3102345546
H25	0.6054969070	-1.9565738233	-6.8841050406	C31	-3.6367716770	-2.4361818072	-3.4343251195
H26	0.8766768305	-5.1105121294	-3.9659295068	C32	-6.2061604234	-3.1862470480	-4.2573201351
H27	2.7540737987	0.0173454220	-2.7102842592	C33	-3.8150057544	-3.3521165399	-4.4879148950
H28	1.8073642823	1.6844866948	-1.2570776587	C34	-4.7897165671	-1.9069186113	-2.8009072578
H29	2.2986149952	0.5809168835	0.0464000962	C35	-6.0689524623	-2.2834403970	-3.2010057488
H30	2.6194794822	-1.2492044764	-1.4729481628	C36	-5.0884049809	-3.7220639991	-4.9032491385
C31	-3.6627150696	-2.5121963177	-3.3538486340	H37	-6.9484869538	-1.8820848640	-2.7083007823
C32	-6.2388695884	-3.2778366499	-4.1421574169	H38	-7.2049301658	-3.4742749546	-4.5764098652
C33	-3.8489732573	-3.4729670073	-4.3653396929	O39	-4.5041815479	-1.0253509796	-1.8167993582
C34	-4.8116075674	-1.9448844557	-2.7462192139	C40	-5.5434231028	-0.5425013860	-0.9175816119
C35	-6.0940582341	-2.3267380054	-3.1300165770	H41	-6.3854741311	-0.2219215894	-1.5489337160
C36	-5.1256136700	-3.8526129064	-4.7618146968	H42	-2.9280865517	-3.7558006754	-4.9743565622
H37	-6.9699995525	-1.8927632281	-2.6592125379	H43	-5.216248036	-4.4233215293	-5.7229032926
H38	-7.2400401560	-3.5716922604	-4.4481006127	C44	-4.9381709936	0.6503924649	-0.2179216455
O39	-4.5180537861	-1.0188799735	-1.8063045585	H45	-4.0927336618	0.3319677198	0.4042783381
C40	-5.5556240571	-0.4673017892	-0.9454679119	H46	-5.6827068771	1.1253093370	0.4285127426
H41	-6.3825398418	-0.1601414563	-1.6031933651	H47	-4.5785787982	1.3835346902	-0.9477448547
H42	-2.9655359146	-3.9032073348	-4.8353527748	C48	-5.9440105348	-1.6554794707	0.0277464779
H43	-5.2595745175	-4.5901659281	-5.5479297162	H49	-5.0676637594	-1.9730493912	0.6024178043
C44	-4.9271392695	0.7442461496	-0.3001471060	H50	-6.3401361079	-2.5257429743	-0.5041036966
H45	-4.0994511292	0.4344110718	0.3498016811	H51	-6.7134235128	-1.3017385175	0.7209822098
H46	-5.6662374517	1.2723930881	0.3102864216	H52	-2.5762041777	2.7608533698	3.0341236879
H47	-4.5367524194	1.4290809712	-1.0607418559	H53	0.7596660617	-4.5409277557	-6.1960076749
C48	-5.9954868809	-1.5168631177	0.0538248310	H54	-1.5920187630	2.1595108177	-1.1168921350
H49	-5.1350195784	-1.8233756833	0.6575579513	C55	0.8348582808	-0.2743457005	2.0657422208
H50	-6.4074523588	-2.4057957887	-0.4328167554	H56	1.8565963908	0.1260024276	2.1041592627
H51	-6.7641825232	-1.1054657477	0.7153684145	H57	0.8278456122	-1.1169366720	1.3653089935
H52	-2.5803803810	2.8005461427	3.0284268647	H58	0.6096452708	-0.6660074681	3.0611015991
H53	0.7548045445	-4.3803360933	-6.3291669885	H59	1.1132888336	-3.4113213033	-2.0530584279
H54	0.6114231543	-0.2735537973	-5.0263884501	C60	0.3840961312	0.0069103743	-5.1487637510
C55	0.8080749798	-3.5519751589	-1.7189867145	H61	1.1532096771	0.6556119206	-4.7132515995
H56	1.6351278321	-3.1287587807	-1.1354871849	H62	-0.5769436118	0.3694427300	-4.7568297572
H57	0.8618578510	-4.640048275	-1.6305268792	H63	0.3881883228	0.1512770836	-6.2323279088
H58	-0.1166179090	-3.2144205013	-1.22070067754	3c			
H59	-1.5736286357	2.1297384562	-1.1085877087	N1	0.3187390951	0.6381886341	-0.9697285031
C60	0.7604956851	-0.3318265918	2.1143633723	C2	1.7778464608	0.5748015765	-0.8797677616
H61	1.8017552688	0.0146733236	2.0810153953	C3	2.1233494136	-0.3089672192	-2.0640493960
H62	0.6747221342	-1.2046276205	1.4565691476	N4	0.8526132750	-0.9990690272	-2.3117161958
H63	0.5648302561	-0.6629679013	3.1375324566	C5	-0.4290450933	1.4707650892	-0.0952290215
3b							
N1	0.3232486292	0.3868422357	-0.6997224975	C6	-1.9601617612	3.0849720130	1.5728620532
C2	1.7498556056	0.6429285718	-0.8991719278	C7	-0.3839385255	2.8665798772	-0.2744877101
C3	2.1291626861	-0.4831007332	-1.8415190687	C8	-1.2208457974	0.8917409699	0.8975743265
				C9	-1.9931532295	1.7024468681	1.7307304702
				C10	-1.1601973320	3.6526145072	0.5804976329

C11	0.3935652434	3.4872646948	-1.3936809302	C18	-1.9754504493	-2.5203691940	0.0884177830
H12	-2.6169865165	1.2489056739	2.4973221204	C19	-2.6219571229	1.4048852008	-2.5045555779
H13	-1.1610135727	4.7319734703	0.4373918244	C20	-2.3875674450	-1.8298062275	-3.1586604908
H14	0.0141802426	4.4866165210	-1.6226735686	H21	-1.5929970842	-2.1142236972	-3.8555163509
H15	0.3121234593	2.8812378521	-2.3032994698	H22	1.3244031469	3.6484580357	-1.2264037537
C16	-0.2008989885	-0.3806204967	-1.7177385983	C23	0.7811358210	-1.9281025232	-3.4496612174
Ru17	-2.1215408334	-0.7647128944	-1.6685312858	C24	0.7080054257	-3.8141981922	-5.4838912550
C18	-1.8156030437	-2.5357724398	-0.0176059234	C25	0.8799087554	-3.2880317531	-3.1092231256
C19	-2.6728856111	1.4482610991	-2.4794388608	C26	0.6776101729	-1.5124088218	-4.7785001063
C20	-2.3908546050	-1.7784921666	-3.1953134675	C27	0.6376802723	-2.4571085286	-5.8015876245
H21	-1.6066856951	-2.0451423271	-3.9100319057	C28	0.8306959972	-4.2182761948	-4.1553019624
H22	1.4612637851	3.5957481742	-1.1600086069	H29	0.5450916369	-2.1371844902	-6.8359968207
C23	0.7826186149	-1.9342564323	-3.3806500609	H30	0.8951835631	-5.2779476748	-3.9144814015
C24	0.7237946939	-3.7787689577	-5.4478139596	H31	2.2210526220	0.4766556052	-3.1531865206
C25	0.9245841875	-3.2905443253	-3.0983893908	H32	2.1593961833	1.6626334068	-1.0576387104
C26	0.5946858728	-1.4659062485	-4.6942500881	H33	2.1729869497	0.1578036329	-0.1102953331
C27	0.5750080423	-2.4173624336	-5.7202933524	H34	2.9378968979	-0.8241094624	-2.1749369261
C28	0.8896140171	-4.2202897868	-4.1365587349	C35	-3.7057862451	-2.2868748325	-3.5102875148
H29	0.4224523986	-2.0823268214	-6.7448707677	C36	-6.2963008619	-3.1180465924	-4.1743605634
H30	0.9866848304	-5.2806404110	-3.9196204401	C37	-3.9425567014	-3.0433987214	-4.6736437916
C31	0.3205186403	-0.0152025933	-4.9534835063	C38	-4.8103130510	-1.9658831926	-2.6799299941
H32	1.1423180081	0.6336846556	-4.6257947368	C39	-6.1001877283	-2.3748576222	-3.0084884345
H33	-0.5736202023	0.3199013102	-4.4058348494	C40	-5.2260154139	-3.4591534116	-5.0059167565
H34	0.1562810515	0.1715777424	-6.0177575894	H41	-6.9442501063	-2.1203834118	-2.3763077539
H35	2.4203751079	0.2744059331	-2.9496508502	H42	-7.3039482334	-3.4352118983	-4.4320248064
H36	2.2251477897	1.5718730919	-0.9374112367	O43	-4.4724199203	-1.2310130350	-1.5970525918
H37	2.0698029005	0.1221791015	0.0791995744	C44	-5.4572009595	-0.9118730555	-0.5711669569
H38	2.9173236619	-1.0317864086	-1.8531469666	H45	-6.3397234092	-0.5142411493	-1.0950177049
C39	-3.7026054627	-2.2700395249	-3.5249858694	H46	-3.0919705645	-3.2924913107	-5.3067923313
C40	-6.2769816595	-3.1912527718	-4.1317999050	H47	-5.3983073979	-4.0430232943	-5.9055236672
C41	-3.9398258117	-3.0290929206	-4.6864717287	C48	-4.8134591613	0.1641317499	0.2690087919
C42	-4.7977052811	-1.9936972495	-2.6675585313	H49	-3.9096837948	-0.2392344053	0.7428783492
C43	-6.0796948831	-2.4468770186	-2.9668164820	H50	-5.5007330564	0.4892439782	1.0560893594
C44	-5.2151290398	-3.4894677851	-4.9901837619	H51	-4.5266814291	1.0277982967	-0.3385883597
H45	-6.9162788395	-2.2274464772	-2.3118980915	C52	-5.7931758784	-2.1548759176	0.2271128337
H46	-7.2780022256	-3.5448949921	-4.3666771653	H53	-4.8859246746	-2.5313827552	0.7103382572
O47	-4.4577442421	-1.2553886379	-1.5872414617	H54	-6.2044833346	-2.9549562559	-0.3942879338
C48	-5.4178724758	-1.0043989733	-0.5208778520	H55	-6.5308681849	-1.9110302722	0.9980795821
H49	-6.3362342340	-0.6363418790	-1.0031507300	H56	-1.1178557641	-0.2634097131	1.0487445817
H50	-3.0956773295	-3.2485128560	-5.3389291576	H57	-2.5450888138	3.6029103954	2.3126783275
H51	-5.3872562609	-4.0771368557	-5.8873963372	H58	0.6750267269	-4.5610968375	-6.2735484216
C52	-4.7920627874	0.0813454177	0.3201525572	H59	0.5929297095	-0.4488156609	-4.9926302018
H53	-3.8639325706	-0.2976237195	0.7663175927	C60	1.0145438209	-3.7191896797	-1.6834840905
H54	-5.4710159511	0.3710708143	1.1280513606	H61	1.8006966614	-3.1575606464	-1.1652841037
H55	-4.5492280370	0.9628796443	-0.2811235111	H62	1.2523928266	-4.7839399427	-1.6149570502
C56	-5.6662312726	-2.2784627879	0.2602621567	H63	0.0887466529	-3.5375140111	-1.1212105738
H57	-4.7225427944	-2.6270990107	0.6924726008				5a
H58	-6.0722456598	-3.0806123611	-0.3619914557	Ru1	-0.2615848491	0.0731731266	0.0305075382
H59	-6.3771240759	-2.0839002767	1.0694806989	C12	-0.4964788982	2.5304121477	-0.0429251563
H60	-1.2212319625	-0.1929827008	1.0098467370	C13	-2.7585997777	0.0320175260	-0.0577294986
H61	-2.5640891408	3.7249218587	2.2114607915	N4	-0.3759828265	-2.0120583583	-2.0577359866
H62	0.6999640354	-4.4970948588	-6.2647587937	N5	-0.8492408972	-3.0063759216	-0.1765362494
H63	1.0301698219	-3.5986616174	-2.0610105233	C6	-0.4839474305	-1.8301507905	-0.7173314143
				C7	-0.9973826468	-3.2669614240	-2.4909191739
				H8	-0.4184636410	-3.7526026519	-3.2806125767
				H9	-2.0031940550	-3.0541936897	-2.8767195881
				C10	-1.0305750007	-4.0586845307	-1.1922592034
				H11	-1.9807140866	-4.5740504062	-1.0274751254
				H12	-0.2201790717	-4.7979140983	-1.1286562814
				C13	0.2132443835	-1.0571831341	-2.9266393772
				C14	1.3475849674	-1.4163741228	-3.6861123034
				C15	1.9505554004	-0.4137698975	-4.4551282173
				H16	2.8337865447	-0.6670204917	-5.0395429720
				C17	1.4730941189	0.8983483374	-4.4526335514
				C18	0.3639642841	1.2364414906	-3.677924473
				H19	-0.0013103496	2.2583828867	-3.6407294872
				C20	-0.2791961962	0.2516256683	-2.9269170291
				C21	1.9369126055	-2.7961198377	-3.6545777064
				H22	1.8435596529	-3.2619633973	-2.6660964627
				H23	2.9996179932	-2.7677749990	-3.9113789468
				H24	1.4571006480	-3.4706776924	-4.3756195358

C25	-0.8713069354	-3.3180496804	1.2132726157	H38	0.2156150540	3.9896940563	0.1292644348
C26	0.1451102959	-4.1274360456	1.7585826190	H39	-1.8308405160	0.2301699876	0.6292457150
C27	0.0823636730	-4.4027576260	3.1302486439	H40	-1.8802194137	2.7082900521	0.5619808787
H28	0.8693954801	-5.0086236698	3.5766325992	H41	7.8667959926	-0.6404550946	-0.8724674868
C29	-0.9357941130	-3.8855211242	3.9308062353	H42	6.4450576562	1.7449388956	4.4468537454
C30	-1.9190255637	-3.0685791115	3.3709563306	H43	2.1024282419	7.1281464960	1.5050196460
H31	-2.7044851804	-2.6453674069	3.9915534753	H44	5.2578997218	4.3257050548	4.1345477901
C32	-1.8920885480	-2.7891753288	2.0052985342	H45	0.7496289092	1.8853407683	3.8440244969
C33	1.2849784108	-4.6541615810	0.9377342696	H46	2.4476380871	1.9027326144	4.3441616676
H34	1.0467259713	-5.6172913771	0.4676866514	H47	2.0203425562	1.4229519360	2.7020540803
H35	2.1670789153	-4.8138751906	1.5647982363	H48	6.3938402840	-0.4071324828	4.8955503415
H36	1.5687266878	-3.9586049649	0.1391138332	H49	5.4209571694	-1.7621386291	4.3399102384
C37	-0.1391828292	-0.2992812796	1.8447584889	H50	4.8271660325	-0.1046605355	4.1397657446
H38	-0.9882935530	-0.0394919112	2.4920522398	H51	7.0734688601	2.9822390743	3.3335299702
C39	1.0559834645	-0.8573282067	2.4265493607	C52	1.4542561797	0.7979944442	-0.0257749480
C40	1.2303290561	-1.1559179985	3.7909871969	H53	2.9225528346	-0.1493624813	-1.3496866449
H41	0.4435066805	-0.9054767612	4.4996497116	H54	-0.0274371242	6.3286992037	2.5206370621
C42	2.3891272319	-1.8067280476	4.2090492879	H55	7.8869431912	-2.7441437062	0.4769403376
H43	2.5254474055	-2.0568978881	5.2580557363	H56	4.1109462862	5.6157317586	1.5069910124
C44	3.3711100340	-2.1617485251	3.2757196076	H57	6.9591252998	1.4499179557	0.1224041337
H45	4.2666490363	-2.6821431765	3.6080014364				
C46	3.2193589753	-1.8453029338	1.9207338634				
H47	3.9966179037	-2.1096332554	1.2053873530	C1	0.1312320297	0.5865551634	0.2545400316
C48	2.0746145439	-1.1726477229	1.4949639628	C2	0.3848308283	3.3553702599	-0.1842522376
C49	1.8206942704	-0.7297412044	0.1083374999	C3	-0.994448124	1.4198409691	0.2758052602
H50	2.0518179739	-1.4404731860	-0.6898364556	H4	4.4990024374	2.8939594391	4.6572191384
C51	1.8022028689	0.6448034899	-0.2182378286	Ru5	4.3481412197	1.8297524392	-0.1319321774
H52	2.0270523803	1.3971519613	0.5339868586	C16	4.8962211682	0.7126440332	-2.2318199005
H53	1.9630188222	0.9557089097	-1.2494824760	C17	5.9144636608	3.6683115632	-0.7327485540
H54	-1.1735687748	0.4912243490	-2.3457450437	C8	3.5223171088	0.0554767961	0.9240519619
H55	-2.6229081676	-2.1304973992	1.5357747684	N9	4.3831823029	3.3630866861	2.5981751112
H56	1.9803449377	1.6565672208	-5.0434119812	N10	5.8856721472	1.7924805978	2.4036173852
H57	-0.9485544448	-4.1054663940	4.9955707416	C11	2.8723546492	5.2243219737	2.0922799272
				C12	2.0261252088	3.1758718908	3.1301787373
				C13	2.8898612974	2.9847692641	-0.2794275788
				C14	3.0711326814	3.9211495128	2.5758790740
C1	0.2784983892	0.0864036142	0.2074184995	C15	4.8285700935	2.3779948533	1.7868776779
C2	0.2231477138	2.9019718490	0.1454836979	C16	0.7469450751	3.7195309092	3.2089973532
C3	-0.9150374090	0.7826739129	0.4323525388	C17	0.5257384591	5.0135166278	2.7327297917
H4	4.3486092428	2.9117003836	4.7118301004	C18	6.4633528839	0.5637448192	1.9891754840
Ru5	4.3153812735	1.8197092147	-0.1577524115	C19	7.3162618769	-1.9135109645	1.0532398926
C16	5.0715842650	0.9361729967	-2.2981102237	C20	6.4348024164	-0.5401528121	2.8695770125
C17	5.6917835689	3.8526267500	-0.51080401091	C21	6.8872726480	-1.7684272348	2.3747540321
C8	3.7152813694	-0.1751207950	0.6281242412	H22	3.2580104446	0.2742893897	1.9583165354
N9	4.2547026183	3.2440700788	2.6211723417	H23	4.2571832221	-0.7358290346	0.7793567551
N10	5.7186937271	1.6436089561	2.4524361605	H24	3.0906613554	4.0359790433	-0.5294474388
C11	3.1644204786	5.3075975232	1.9474851896	H25	-0.0703492705	3.1355972685	3.6240669434
C12	1.8688513693	3.5353502245	3.0339390665	H26	6.8588091464	-2.6359729363	3.0322587871
C13	2.7351658694	2.8152848495	-0.1981768246	C27	6.9104366018	0.4330312932	0.6722186745
C14	3.0735029296	4.0283086333	2.4977260418	C28	1.5269445600	2.5328671554	-0.1610146866
C15	4.6965012838	2.2647224508	1.8103192597	C29	7.3162510708	-0.8144016097	0.1966374082
C16	0.7632430636	4.3939737902	3.0365669566	C30	5.8782393840	-0.4515466034	4.2598494532
C17	0.8471003656	5.6827692518	2.5065605337	C31	6.3583631454	2.5935443391	3.5369593994
C18	6.3893129946	0.4918497391	1.9675457245	C32	1.5738707325	5.7480337716	2.1778926182
C19	7.4801425473	-1.8268262604	0.8945009147	C33	5.1104403789	3.3810200177	3.8805406813
C20	6.3727652477	-0.6850933549	2.7447232734	C34	-0.8698776827	2.7941572903	0.0417992779
C21	6.9401704458	-1.8338855581	2.1831395739	C35	2.6503359176	0.3777321772	-0.1179736729
H22	3.4782299386	-0.1388915973	1.6913945668	H36	0.0229436082	-0.4852960146	0.4057742729
H23	4.5201321244	-0.8516520132	0.3425256972	H37	0.4950905957	4.4251264197	-0.3482944441
H24	2.8172755676	3.8939062566	-0.3839670096	H38	-1.9763897907	0.9915309093	0.4635904845
H25	-0.1807297125	4.0329297479	3.4415824780	H39	-1.7550601242	3.4257051625	0.0461327818
H26	6.9217013474	-2.7592292712	2.7566701326	H40	4.0069235155	6.0030689064	1.5061662866
C27	6.9503117634	0.5163234264	0.6884464590	H41	7.6123095342	-0.9156414095	-0.8431685806
C28	1.4353669558	2.2112298510	-0.0418628486	H42	6.7250677569	1.9653634039	4.3514007175
C29	7.4785823806	-0.6537054774	0.1415774104	H43	1.3911242772	6.7530771371	1.8018465382
C30	1.7648235209	2.1197998936	3.5127771341	H44	5.3117903267	4.4087363130	4.1948766205
C31	5.7208945352	-0.7396155182	4.0944285492	H45	4.7306350663	6.2953034171	2.2773301778
C32	6.1826127293	2.4046695266	3.6157784435	H46	3.6508256914	6.9176703017	1.0254344269
C33	2.0416236431	6.1353297606	1.9418889462	H47	6.6191614693	-0.0977008576	4.9884894803
C34	4.9851447784	3.2931309661	3.8984410330	H48	5.5449551315	-1.4343060535	4.6047084051
C35	-0.9430786854	2.1826911391	0.3953618763	H49	5.0203725732	0.2301091692	4.3128831299
C36	2.7759913366	0.2100323790	-0.3291701011	H50	7.1767028113	3.2426477342	3.1960720731

C51	1.3907315292	1.1385933364	0.0300082764	Ru5	4.2699955473	2.0688009532	-0.2122598827
H52	4.5678125599	5.4095552101	0.7701489591	Cl6	4.8621512539	1.5720943186	-2.5252638267
H53	2.7761429964	-0.1548936324	-1.0623983243	Cl7	5.3774317330	4.2754349168	-0.3981035342
H54	-0.4701074638	5.4475514641	2.7843021306	C8	3.9287561963	-0.0438732640	0.3862772783
H55	7.6296047578	-2.8898605305	0.6930092858	N9	4.3442091338	3.2795259464	2.6365602292
H56	2.2263458791	2.1658343972	3.4871481669	N10	5.8914793130	1.7707562245	2.3360002777
H57	6.9327646173	1.3105685867	0.0234928004	C11	3.1393442962	5.3465938285	2.1566875630
				C12	1.9718798133	3.4171873936	3.1138797390
		5d		C13	2.5916420564	2.8683370097	-0.0492319169
Ru1	-0.2877519252	0.0986446830	-0.0662279191	C14	3.1324721080	4.0214694685	2.5942379177
Cl2	-0.6132707451	2.5410283578	-0.1997530790	C15	4.7907446198	2.3451770937	1.7781908251
Cl3	-2.7463092142	-0.0185268174	-0.4698545906	C16	0.8132181089	4.1987629722	3.1891072785
N4	-0.1057791654	-1.9585859836	-2.1725120684	C17	0.8075093897	5.5252237012	2.7542422269
N5	-0.7685527916	-2.9887624284	-0.3614146728	C18	6.4357107060	0.4889383092	2.0084746471
C6	-0.3504141605	-1.8001519317	-0.8505723394	C19	7.4200309161	-2.0653925460	1.4974862079
C7	-0.6438438888	-3.2268122900	-2.6738698432	C20	6.1150275913	-0.5770912532	2.8614698952
H8	0.0023020654	-3.6669954194	-3.4371297720	C21	6.6019589608	-1.8549598156	2.6115050551
H9	-1.6346157967	-3.0454024465	-3.1119102969	H22	3.7349539719	-0.1377329827	1.4535663669
C10	-0.7216441004	-4.0397477836	-1.3947793705	H23	4.7871572427	-0.6034511404	0.0142861726
H11	-1.6096556344	-4.6752512774	-1.3350949447	H24	2.5455958822	3.9621774774	-0.1209635337
H12	0.1681100790	-4.6697780631	-1.2382339647	H25	-0.0985810298	3.7500858839	3.5797454141
C13	0.5538261452	-0.9858768019	-2.9686788561	H26	6.3377854592	-2.6781941553	3.2698604214
C14	1.7811673578	-1.3196406356	-3.5815924661	C27	7.2713263040	0.3036137024	0.8966097474
C15	2.4493478577	-0.3048098575	-4.2765153929	C28	1.3766799210	2.1052557580	0.0801448602
H16	3.4038449080	-0.5369339690	-4.7462879310	C29	7.7429096854	-1.0001091899	0.6611791027
C17	1.9423567326	0.9949499459	-4.3402877073	C30	1.9807110151	1.9755335101	3.5203918925
C18	0.7383921450	1.3071958876	-3.7099725063	C31	6.1854231655	2.3156860886	3.6722258578
H19	0.3467693243	2.3199500573	-3.7246648828	C32	1.96666259987	6.0978567473	2.2262011906
C20	0.0320999613	0.3091812211	-3.0364503680	C33	5.2830339707	3.5330517152	3.7360571514
C21	2.3948726130	-2.6841023321	-3.4645546072	C34	-0.9613869966	1.7605913160	0.5910985299
H22	2.2108159892	-3.1341768585	-2.4810914769	C35	2.9080238495	0.3131437764	-0.4941475873
H23	3.4772229984	-2.6345117815	-3.6121019110	H36	0.5997010188	-1.2233540921	-0.0011340018
H24	2.0068705818	-3.3845208287	-4.2156092185	H37	-0.0203085827	3.7052882519	0.4902743358
C25	-0.6075106221	-3.3932477188	1.0020934759	H38	-1.6178722795	-0.2940697486	0.6308491591
C26	0.6687053545	-3.7972731851	1.4059742728	H39	-1.9420769462	2.1542302674	0.8463924888
C27	0.8873057187	-4.2408630152	2.7072809010	C40	7.6238582369	1.4173023025	-0.0357805671
H28	1.8848630629	-4.5326283912	3.0253704111	H41	8.3812463020	-1.1682260547	-0.2038844931
C29	-0.1843416032	-4.2725346807	3.6019117154	H42	5.9428630529	1.5714486088	4.4436113120
C30	-1.4562885497	-3.8795088931	3.1871043967	H43	1.9598094918	7.1235316027	1.8682023805
H31	-2.2879321120	-3.9109883494	3.8885634137	H44	5.8225391025	4.4696897416	3.5389391215
C32	-1.7049542583	-3.4450026340	1.8755567549	H45	1.0067633950	1.6631893282	3.9063418309
C33	-3.0763339869	-3.0573943594	1.4267043250	H46	2.7377320674	1.7668276167	4.2875546084
H34	-3.0888330892	-2.0524894392	0.9857918871	H47	2.2213711912	1.3346223542	2.6604207332
H35	-3.7855565927	-3.0887655270	2.2575092330	H48	6.9421115016	1.4542848686	-0.8991856024
H36	-3.4447988138	-3.7339587961	0.6459003023	H49	8.6269131062	1.2743456747	-0.4482740961
C37	-0.3902053062	-0.2838015305	1.7481035701	H50	7.5699498340	2.3998950520	0.4406793816
H38	-1.3562802035	-0.1460823050	2.2546946236	H51	7.2498998784	2.5544378159	3.7533073887
C39	0.7671117400	-0.6736242805	2.5143801735	C52	1.5491051343	0.7114813371	-0.0734860962
C40	0.7808734678	-0.9076801682	3.9025191354	H53	3.0350847089	0.0656426929	-1.5494387094
H41	-0.1259091278	-0.7510480265	4.4833253892	H54	-0.1068416571	6.1098780917	2.8194841475
C42	1.9483172750	-1.3635026664	4.5107407990	H55	7.8064845797	-3.0587665975	1.2841221706
H43	1.9645057074	-1.5576413755	5.5802689879	H56	4.0536294548	5.7516442549	1.7291486481
C44	3.0982624380	-1.5929019635	3.7452791191	H57	5.4515303647	-0.4003389232	3.7067029461
H45	4.0016096550	-1.9602339311	4.2272159471				
C46	3.0983639439	-1.3535176113	2.3668280113				
H47	3.9985047066	-1.5266584401	1.7796101005	Ru1	-0.6645672743	0.0071515223	-0.0065608625
C48	1.9416214326	-0.8768311591	1.7519244606	Cl2	-1.4692244153	2.3278621606	0.4109936289
C49	1.8241066385	-0.5561373925	0.3139663945	Cl3	-3.0688374429	-0.6239077283	-0.0817035393
H50	2.1769229481	-1.3125986463	-0.3926709490	N4	-0.1966483616	-2.0321118493	-2.2200958234
C51	1.7656958377	0.7828644000	-0.1185210840	N5	-0.6686897316	-3.0556445747	-0.3426237198
H52	1.8533801795	1.5976478060	0.5957803967	C6	-0.4293439726	-1.8496046785	-0.8873952795
H53	2.0219418742	1.0356553801	-1.1464866106	C7	-0.2247097298	-3.4613541156	-2.5829424318
H54	2.4997173231	1.7642218528	-4.8683620650	H8	0.7930085385	-3.8398019483	-2.7462406157
H55	-0.9299651398	0.5285960709	-2.5670776735	H9	-0.7963152321	-3.6053625817	-3.5035292256
H56	-0.0269799338	-4.5996664887	4.6270071255	C10	-0.8676075644	-4.0913612135	-1.3627772638
H57	1.4917966818	-3.7382372433	0.6935405756	H11	-1.9460694785	-4.2546694755	-1.4919427326
				H12	-0.4080519587	-5.0371369571	-1.0613521440
				C13	0.5391977956	-1.1229868275	-3.0429691337
C1	0.4700842074	-0.1500872280	0.1174360805	C14	1.8027565007	-1.5326366899	-3.4977119873
C2	0.1064367001	2.6301440293	0.3865303564	C15	2.5748001477	-0.7021860257	-4.3027910058
C3	-0.7783850507	0.3772503207	0.4660256109	H16	3.5526630192	-1.0340826401	-4.6414712138
H4	4.7461467216	3.6346397535	4.6848742544	C17	2.0827483717	0.5544743076	-4.6614772943

C18	0.8293800762	0.9569694201	-4.2087549410	C31	1.4400358919	5.5794288272	2.4701374609
H19	0.4420948959	1.9338096533	-4.4916134627	C32	5.3231291132	3.5755536951	3.7270325935
C20	0.0265531380	0.1364122661	-3.3981221464	C33	-0.8419968581	2.4989451639	0.2708087982
C21	-1.3064617615	0.6223967691	-2.9277008334	C34	2.8662696629	0.4595923509	-0.3125925536
H22	-1.9893890369	-0.1899271860	-2.6648230612	H35	0.3632086635	-0.6992190181	0.2590221157
H23	-1.7868198695	1.2422747959	-3.6906083693	H36	0.3386667729	4.2818199814	-0.0465449058
H24	-1.2282184925	1.2828730666	-2.0456534289	H37	-1.7493630113	0.5677770437	0.5857865434
C25	-0.5668658157	-3.3928646604	1.0376043180	H38	-1.7772404726	3.0396630010	0.3948279193
C26	0.6521378532	-3.9450955500	1.4816074142	C39	3.7744600984	6.1371758495	1.6481241443
C27	0.7589271449	-4.2673829195	2.8388896756	C40	7.9852385350	1.2931857734	-0.0510257637
H28	1.6985507525	-4.6727484760	3.2104993456	H41	8.2360875599	-1.4108520515	-0.0456031597
C29	-0.3009590409	-0.4044433286	3.7200068659	H42	6.9984727971	2.1941834458	4.0741574466
C30	-1.4945262464	-3.4898207461	3.2569431987	H43	1.1294888961	6.5846712236	2.1911942104
H31	-2.3162024346	-3.3001023162	3.9425797064	H44	5.4848490673	4.6251173191	3.9892312908
C32	-1.6330492587	-3.1660880855	1.9062831358	H45	4.5083559921	6.4711279680	2.3922820155
C33	1.8037461368	-4.1485719085	0.5421181159	H46	3.2887971864	7.0290666148	1.2444163274
H34	1.6518119034	-5.0125249070	-0.1184767529	H47	7.2479743517	1.9531223489	-0.5216082701
H35	2.7323135935	-4.3206385391	1.0926905414	H48	8.5185111058	0.7764338649	-0.8518589270
H36	1.9563080355	-3.2751454429	-0.1056066564	H49	8.6917624695	1.9522114579	0.4678429749
C37	-0.4069540128	-0.3970303057	1.7879926996	H50	7.3807963679	3.5597466773	2.9974917103
H38	-1.2813275565	-0.3454232296	2.4507739050	C51	1.5512238683	1.0766154759	-0.0383273619
C39	0.8954130479	-0.6521192750	2.3387047672	H52	4.3481552557	5.6505279380	0.8470626975
C40	1.1672571059	-0.9314229662	3.6922292472	H53	3.0012457703	0.0283586184	-1.3061093119
H41	0.3571715592	-0.9075160053	4.4180958491	H54	-0.5100832630	5.0224093226	3.1932452806
C42	2.4616515900	-1.2734300874	4.0731006468	H55	7.3625678496	-3.0413846264	1.5961165754
H43	2.6811106779	-1.5057387046	5.1119235034	H56	5.4637905518	0.1750947391	3.7341262501
C44	3.4820283660	-1.3419807068	3.1142479450	H57	2.5472272145	2.0004521360	3.4334528402
H45	4.4872325328	-1.6245130882	3.4187215809				
C46	3.2286128782	-1.0367884577	1.7729862132				
H47	4.0325572245	-1.0709145544	1.0396207288	Ru1	-0.0831921701	-0.0406581110	0.0560452989
C48	1.9418678826	-0.6615150283	1.3857503150	Cl2	-0.2973168130	2.4626015226	0.0999237851
C49	1.5582948633	-0.2539513845	0.0220034873	N3	-2.9802351716	0.4771129559	0.0035074673
H50	1.9583587941	-0.8558180107	-0.7971358983	N4	-2.5084877227	-0.1460488319	2.0419936079
C51	1.1803553384	1.0779240070	-0.2680116444	C5	-1.9863118465	0.1067058832	0.8349591540
H52	1.2283854297	1.8508842883	0.4953090480	C6	-4.3030862613	0.3411269517	0.6233774690
H53	1.2543643118	1.4324831660	-1.2965551331	H7	-4.8138692305	-0.5361165854	0.2043531727
H54	2.6712384428	1.2135628487	-5.2941845942	H8	-4.9245071620	1.2221897834	0.4380157687
H55	-0.1862051681	-4.2906110633	4.7729385896	C9	-3.9468705849	0.1614590114	2.0983709518
H56	-2.5319923053	-2.6940000297	1.5114315755	H10	-4.1126310724	1.0774689795	2.6823100197
H57	2.1943695608	-2.5034729332	-3.2048734838	H11	-4.4937766921	-0.6564944941	2.5764703602
				C12	-2.7350174390	0.8082505236	-1.3592177185
				C13	-2.0415407283	-0.1080723798	-2.1586374432
				C14	-1.6535133973	0.2449573666	-3.4535706188
C1	0.3650035891	0.3873583496	0.2054660499	C15	-1.1016293956	-0.4669280552	-4.0627192384
C2	0.3373258296	3.1959810041	0.0192648078	C16	-1.9854985880	1.5027884465	-3.9521896819
C3	-0.8260373732	1.1035570451	0.3776993813	C17	-2.6940190636	2.4020655714	-3.1522498633
H4	4.8035983595	3.0879634465	4.5666368384	H18	-2.9187687667	3.3971917108	-3.5317178550
Ru5	4.4220519881	2.0681071634	-0.2652069348	C19	-3.0713008255	2.0880239825	-1.8422457576
Cl6	5.1049251393	1.0856672980	-2.3765718916	C20	-3.7047192909	3.1174513503	-0.9596019558
Cl7	5.7248804158	4.1047926246	-0.8214687774	H21	-4.7867910366	2.9711098635	-0.8468531268
C8	3.8085909883	0.1400131551	0.6644062111	H22	-3.5550559910	4.1198323241	-1.3689020190
N9	4.4956040465	3.4723598060	2.5126569010	H23	-3.2484474701	3.0945505688	0.0377920244
N10	6.1556102408	2.0857811651	2.1336349841	C24	-1.720622301	-0.4182140685	3.1995183648
C11	2.7734749502	5.2030220194	2.2496392535	C25	-1.2479737614	-1.7167884455	3.3943792655
C12	2.2177245268	3.0061303986	3.1732666869	C26	-0.4148190698	-1.9945867963	4.4774867730
C13	2.8536330607	3.0823607911	-0.2459515019	H27	-0.0259887249	-2.9998541841	4.6154720702
C14	3.1377117525	3.8958432133	2.6093566793	C28	-0.0713064777	-0.9718902055	5.3628456574
C15	4.9734395719	2.5553990214	1.6463923571	C29	-0.5426714770	0.3254060109	5.1528555943
C16	0.9011005581	3.4040690867	3.3856827797	H30	-0.2426612533	1.1263876732	5.8260680819
C17	0.5163724072	4.6999807257	3.0351421753	C31	-1.3666772489	0.6360835684	4.0624651156
C18	6.5656567509	0.7216927581	1.9700536958	C32	-1.7748467166	2.0484485491	3.7740991070
C19	7.1443047405	-1.9834627073	1.7177609023	C33	-1.6117032194	2.2996899641	2.7167739764
C20	6.0913647458	-0.1916660902	2.9210032451	H34	-1.1935039871	2.7514591889	4.3758195729
C21	6.3823064524	-1.5469856773	2.8049601718	H35	-2.8332206463	2.2313166513	3.9976380292
H22	3.5700429189	0.2497384110	1.7210221552	C36	1.0079148804	-0.0591973994	1.5622943673
H23	4.6103451685	-0.5601232493	0.4304403894	H37	0.7432194589	0.4721490176	2.4871718947
H24	2.9366162930	4.1633122253	-0.4239278253	C38	2.2673049208	-0.7514780009	1.5228745299
H25	0.1815585646	2.7080814395	3.8087571949	C39	3.0563265946	-1.0119994456	2.6629224857
H26	6.0031625763	-2.2542006581	3.5378665660	H40	2.7417592585	-0.6186246249	3.6277612672
C27	7.3816696024	0.3137213197	0.9044261362	C41	4.1960345118	-1.7997433644	2.5490430075
C28	1.5481768861	2.4885196489	-0.1042940159	H42	4.7985469367	-2.0196736224	3.4263279919
C29	7.6341654083	-1.0640477554	0.7915658874	C43	4.5625040059	-2.3280505166	1.3024933593

H44	5.4511660373	-2.9496030138	1.2216170858	H57	-1.3719063369	2.7222716359	3.1918194368
C45	3.8052893292	-2.0579545801	0.1614275596			5j	
H46	4.1058776624	-2.4582366479	-0.8043825821	Ru1	-0.0577712458	0.1322736286	0.0614279124
C47	2.6708318286	-1.2488626850	0.2556534576	Cl2	-0.0528336843	2.6519502037	0.2880677263
C48	1.8431859770	-0.8627341189	-0.8946959666	N3	-3.0099174691	0.3524242884	0.0360164913
H49	1.5739855199	-1.6511879326	-1.5970472416	N4	-2.3958529237	0.4365804785	2.1276738351
C50	1.6422304176	0.4681099190	-1.2562095857	C5	-1.9509793399	0.3292821209	0.8679408292
H51	2.1566477352	1.2841208025	-0.7540575258	C6	-4.2599358168	0.6501532326	0.7470008047
H52	1.2210471027	0.7074108755	-2.2307756855	H7	-5.0814676981	0.0209789737	0.3944589792
C153	-0.6006398220	-2.4931077870	-0.0169370524	H8	-4.5306771268	1.7019234856	0.5811109490
H54	0.5817373251	-1.1785460831	6.2075248286	C9	-3.8658113876	0.3729193635	2.1932959032
H55	-1.6848969395	1.7935155924	-4.9555972714	H10	-4.2603685165	1.1104325962	2.8988806899
H56	-1.4972027776	-2.4795225272	2.6606021266	H11	-4.1691381454	-0.6294163632	2.5308725446
H57	-1.8223647532	-1.0997246841	-1.7636135245	C12	-2.8761704891	0.1793659430	-1.3714931238
		5i		C13	-3.4895716287	-0.9230221693	-1.9995061412
Ru1	-0.0513429430	0.0984082132	0.0556835699	C14	-3.2359343574	-1.1107522630	-3.3623993351
Cl2	-0.0638173927	2.6082969031	0.3077041836	H15	-3.6819795860	-1.9703528613	-3.8592248778
N3	-3.0051345152	0.2636614783	0.0305393767	C16	-2.3861612940	-0.2640784539	-4.0771020634
N4	-2.3896666867	0.5724083265	2.0979329213	C17	-1.7756679376	0.8100279653	-3.4331666560
C5	-1.9445168545	0.3208044242	0.8615583284	H18	-1.1115089814	1.4780929131	-3.9759337671
C6	-4.2538578114	0.6560578060	0.6963664668	C19	-2.0302233567	1.0401827586	-2.0790853104
H7	-5.0703198843	-0.0274920895	0.4463913655	C20	-4.2987053152	-1.9185621137	-1.2281273965
H8	-4.5371979367	1.6663894307	0.3723036323	H21	-5.3253332703	-1.5771967160	-1.0416326663
C9	-3.8583203569	0.6044090695	2.1700006803	H22	-3.8254543844	-2.1293873132	-0.2615920143
H10	-4.1952257267	1.4762802930	2.7389344562	H23	-4.3687026328	-2.8624052605	-1.7748423935
H11	-4.2255650847	-0.3003735049	2.6764875021	C24	-1.5735198786	0.2081154684	3.2680470855
C12	-2.8663472745	0.0354939244	-1.3674168046	C25	-1.0836564582	-1.0798722076	3.4981527956
C13	-3.4984469492	-1.0758722395	-1.9586958129	C26	-0.2122692960	-1.3058383500	4.5629988523
C14	-3.2414419883	-1.3190918730	-3.3117916827	H27	0.1935339842	-2.3001397564	4.7304709855
H15	-3.6977672684	-2.1902079213	-3.7783282085	C28	0.1526954874	-0.2413213982	5.3900102987
C16	-2.3689755505	-0.5175119796	-4.0508543657	C29	-0.3454399707	1.0408263738	5.1495214468
C17	-1.7399378106	0.5671121391	-3.4434998026	H30	-0.0384073690	1.8696333631	5.7846644205
H18	-1.0576690071	1.1986324151	-4.0071696642	C31	-1.2143482678	1.2972153246	4.0798244834
C19	-1.9997182711	0.8540537660	-2.1007719098	C32	-1.6766998209	2.6825070684	3.7520235346
C20	-4.3135500797	-2.0347710791	-1.1482442498	H33	-1.3465047854	2.9640869884	2.7425433956
H21	-5.3285949179	-1.6685585256	-0.9474865347	H34	-1.2762592537	3.4104812335	4.4619662104
H22	-3.8228737819	-2.2291187137	-0.1862553511	H35	-2.7699471912	2.7675541399	3.7675470692
H23	-4.4126651423	-2.9908454600	-1.6687808288	C36	1.0600002970	0.0753795544	1.5465139991
C24	-1.5591376639	0.5893094280	3.2553848560	H37	0.8427283600	0.6524892230	2.4554646365
C25	-1.1698039545	-0.6289426260	3.8423089488	C38	2.2992578048	-0.6500079790	1.4992640499
C26	-0.2935090088	-0.5642766811	4.9339463088	C39	3.1056200420	-0.8986564395	2.6297207845
H27	0.0347690342	-1.4931158923	5.3973504566	H40	2.8169312362	-0.4777007666	3.5915172010
C28	0.1827297784	0.6582284527	5.4118576341	C41	4.2314871948	-1.7044504266	2.5084207225
C29	-0.2126269466	1.8530586067	4.8069575727	H42	4.8494252503	-1.9148761753	3.3774405511
H30	0.1736874236	2.8047343396	5.1607975995	C43	4.5653743763	-2.2597872948	1.2642835258
C31	-1.0903771179	1.8168130794	3.7234200868	H44	5.4440176267	-2.8946462705	1.1781409249
C32	-1.6029365119	-1.9381876059	3.2617479586	C45	3.7915009811	-1.9977487505	0.1319845156
H33	-1.2986746426	-2.7727561644	3.8984890805	H46	4.0708952928	-2.4169871265	-0.8319803388
H34	-1.1641896817	-2.0918581612	2.2645486539	C47	2.6700181614	-1.1707780341	0.2333628875
H35	-2.6899751038	-1.9941724819	3.1279657477	C48	1.8252500564	-0.7814250229	-0.9045339614
C36	1.0611008013	-0.0028497264	1.5438738681	H49	1.5071262413	-1.5748598199	-1.5795868980
H37	0.8382522718	0.5443167748	2.4686731871	C50	1.6568844252	0.5457015666	-1.2967847589
C38	2.3085335834	-0.7144889980	1.4818291018	H51	2.2104551953	1.3596188227	-0.8340656269
C39	3.1079522973	-0.9842634280	2.6124897186	H52	1.2218091714	0.7599665245	-2.2716876984
H40	2.8035223861	-0.5965813282	3.5833182995	C53	-0.7854112039	-2.2250465259	-0.2005655852
C41	4.2512163522	-1.7632467818	2.4780387631	H54	0.8375767809	-0.4059475635	6.2188180651
H42	4.8657711050	-1.9870235676	3.3460315980	H55	-2.1942026126	-0.4543266937	-5.1299968559
C43	4.6084972210	-2.2726409597	1.2211334033	H56	-1.3442470885	-1.8747168778	2.7999573609
H44	5.5014993606	-2.8854647003	1.1238926992	H57	-1.5874351865	1.8911781783	-1.5637512424
C45	3.8392850971	-1.9924594526	0.0898661441			5k	
H46	4.1368431096	-2.3760767574	-0.8835012985	Ru1	-0.6071963558	0.1115658653	-0.0201559137
C47	2.7004170353	-1.1915772450	0.2050016059	Cl2	-1.2122131423	2.5008982639	0.2853916959
C48	1.8611915598	-0.7852494290	-0.9311167071	Cl3	-3.0520643742	-0.2662568128	-0.2081209891
H49	1.5460035998	-1.5675700615	-1.6203956576	N4	-0.4652816408	-1.8666231048	-2.2634701719
C50	1.6794392901	0.5458332174	-1.2921383660	N5	-0.8304995570	-2.9658496688	-0.3934065186
H51	2.2184604147	1.3559571116	-0.8063159178	C6	-0.5491326834	-1.7493448770	-0.9072980545
H52	1.2411135612	0.7788535742	-2.2613315657	C7	-0.9384623383	-3.1903266024	-2.7011063763
C153	-0.7474664485	-2.2545269988	-0.3494564616	H8	-0.3300514156	-3.5734295084	-3.5238021184
H54	0.8731868553	0.6767637134	6.2518749090	H9	-1.9749908366	-3.0933587710	-3.0477382304
H55	-2.1719004750	-0.7529174402	-5.0936039027	C10	-0.8443577976	-4.0128129434	-1.4295842300

H11	-1.6970031773	-4.6821683699	-1.2841830773	C24	-1.6667870326	0.1087332888	3.2515749109
H12	0.0790798356	-4.6091938485	-1.3608232833	C25	-1.2587176665	-1.0716060582	3.8955192625
C13	0.4866168204	-1.1379427684	-3.0462333589	C26	-0.3621936457	-0.9401590217	4.9662532834
C14	1.6733008879	-1.8091704762	-3.3828233215	H27	-0.0146675185	-1.8419533748	5.4674996441
C15	2.6573746818	-1.1746600942	-4.1321986283	C28	0.0960444276	0.3090034577	5.3853534410
H16	3.5748388003	-1.6994793301	-4.3849773737	C29	-0.3400333796	1.4696717373	4.7418244154
C17	2.4547431611	0.1471263732	-4.5412745253	H30	0.0257312757	2.4440969998	5.0533060801
C18	1.2771608572	0.8073247356	-4.2015882473	C31	-1.2247174006	1.3665481704	3.6691666335
H19	1.1237462223	1.8354763367	-4.5240945412	C32	-1.7185462435	-2.4152049419	3.4281682430
C20	0.2615826536	0.1850498282	-3.4530688597	H33	-1.4465882847	-3.1944700531	4.1449080883
C21	-0.9831222180	0.9302849050	-3.0903163923	H34	-1.2709741740	-2.6684149783	2.4575321777
H22	-1.7894079544	0.2667905514	-2.7625479241	H35	-2.8038113651	-2.4440527632	3.2816142983
H23	-1.3480346871	1.5212111968	-3.9361670288	C36	1.0349812872	-0.1003721318	1.5196034141
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H28	2.2782757180	-4.2899531757	2.6727010069	C41	4.2553953414	-1.8321368844	2.4102810967
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C32	-1.5038293945	-3.5783343393	1.9061757421	C45	3.8035020067	-2.0789208101	0.0318533031
C33	-2.9469195669	-3.3399413642	1.6034328390	H46	4.0814112719	-2.4727857249	-0.9433260106
H34	-3.1282955595	-2.3014052711	1.2988504053	C47	2.6682319193	-1.2751338258	0.1598873939
H35	-3.5723792722	-3.5729340996	2.4684142477	C48	1.8084650439	-0.8853290108	-0.9647809691
H36	-3.2863420883	-3.9575488149	0.7634416379	H49	1.5296164852	-1.6684204985	-1.6693851159
C37	-0.4463813590	-0.3316414314	1.7751460988	C50	1.5772641983	0.4465968672	-1.3042526974
H38	-1.3576581823	-0.2968154490	2.3891573049	H51	2.0976722477	1.2646875910	-0.8116081370
C39	0.8226948534	-0.6067061104	2.3947206072	H52	1.1230076258	0.6876239855	-2.2637007965
C40	1.0184936955	-0.8799429552	3.7624129350	C153	-0.5557518049	-2.5552078437	-0.0255432602
H41	0.1717648071	-0.8440548286	4.4447352282	H54	0.7986886546	0.3758661314	6.2128305664
C42	2.2889948840	-1.2231123983	4.2178149332	H55	-1.7306993930	1.3914666746	-5.0411379491
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C44	3.3620493680	-1.2998042636	3.3199925744	H57	-1.5254482371	2.2471076525	3.1045075937
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H50	1.9647086683	-0.9734422690	-0.6734739412				
C51	1.3305462467	1.0400757937	-0.2625112013				
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H57	0.5476431504	-4.6239187905	4.4400247680				

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H10	-3.9566950466	1.5020969676	2.5107216131
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C13	-2.1193183458	-0.3539873345	-2.1473599762
C14	-1.7347189220	-0.0800446006	-3.4625136785
H15	-1.2141743730	-0.8412674772	-4.0386789851
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C19	-3.0733278416	1.8880478556	-1.9328731370
C20	-3.6799246738	2.9814485782	-1.1100837996
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H22	-3.4742115301	3.9565746896	-1.5585563746
H23	-3.2512714978	2.9868610859	-0.1009980182