Supplementary Information

for

Microwave-assisted synthesis and characterization of $[Rh_2(OAc)_4(L)_2]$ paddlewheel complexes: a joint experimental and computational study

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Content

1D and 2D NMR spectra

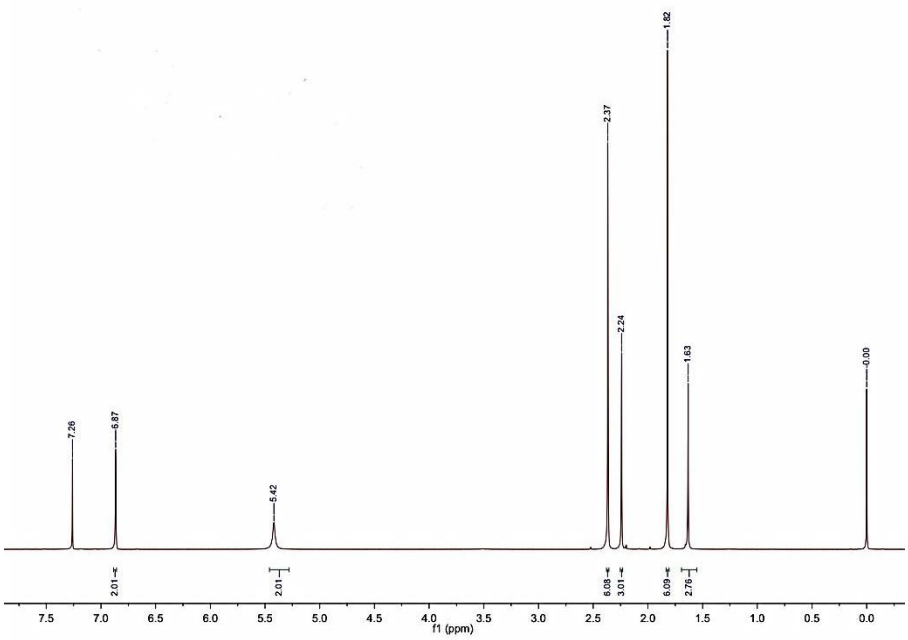

Figure S.I.8. ^{1}H NMR (in $CDCl_3$) of compound **1**.

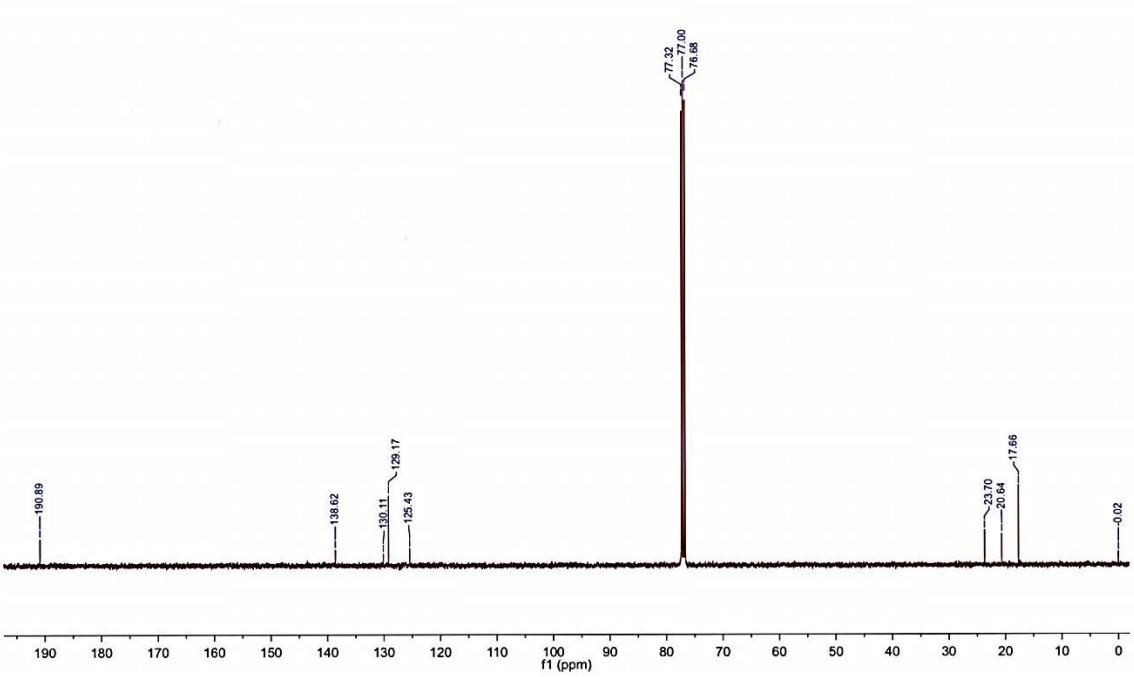

Figure S.I.9. $^{13}C\{^{1}H\}$ NMR (in $CDCl_3$) of compound **1**.

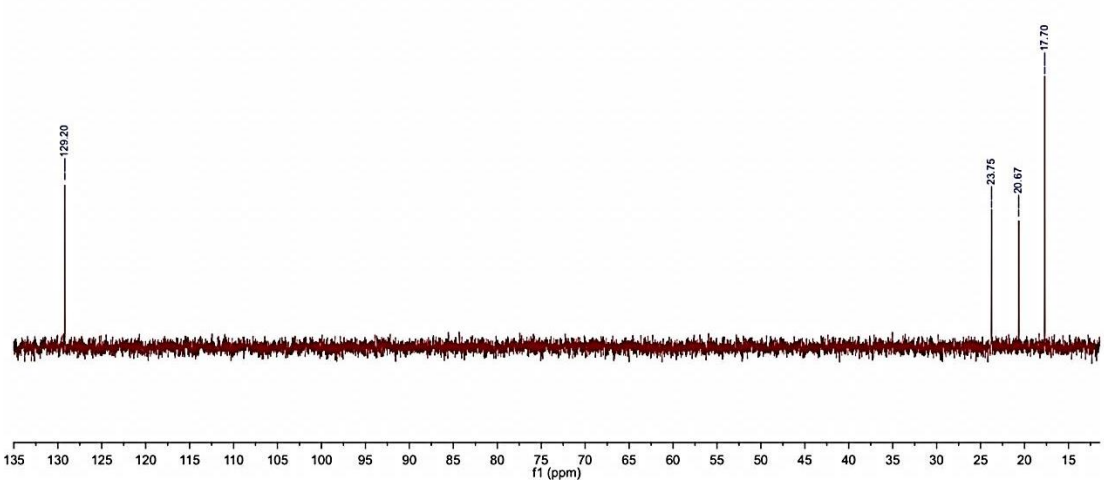

Figure S.I.10. DEPT NMR (in $CDCl_3$) of compound **1**.

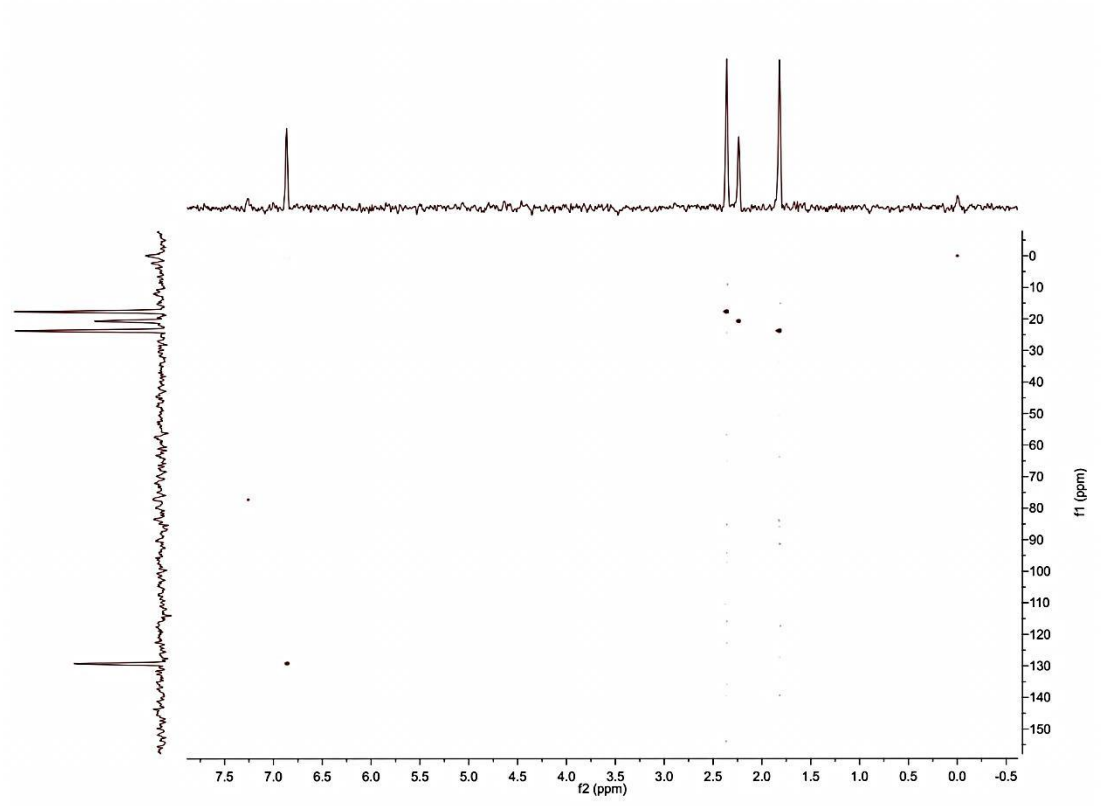

Figure S.I.14. HSQC NMR (in $CDCl_3$) of compound **1**.

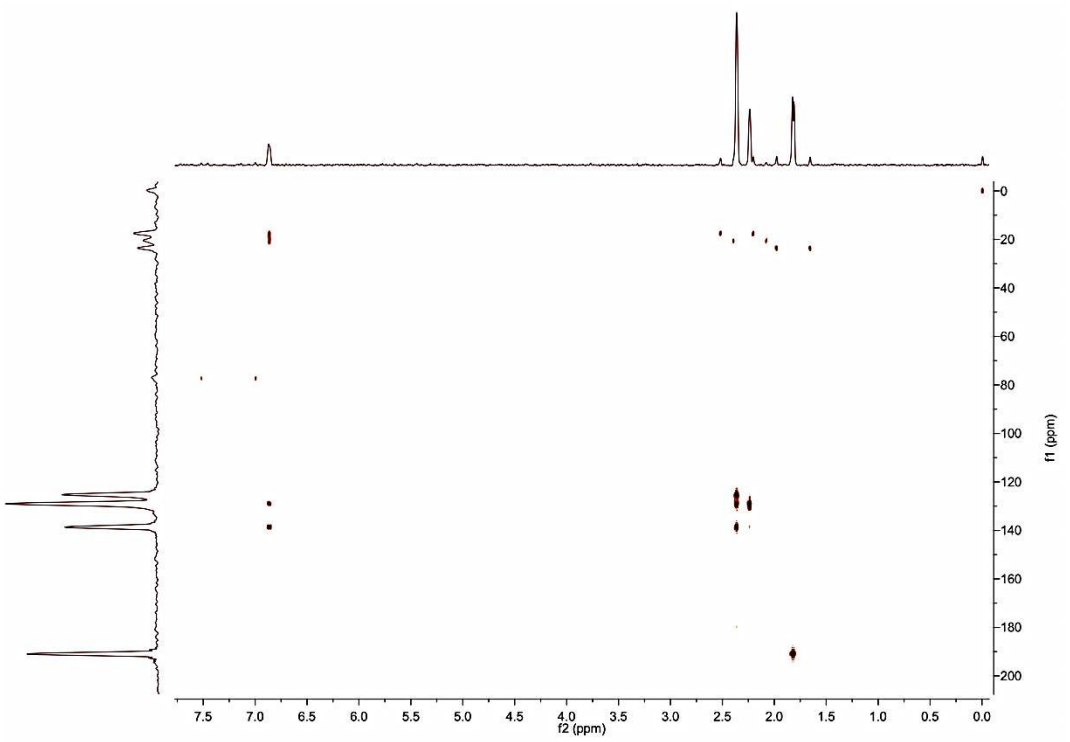

Figure S.I.15. HMBC NMR (in $CDCl_3$) of compound **1**.

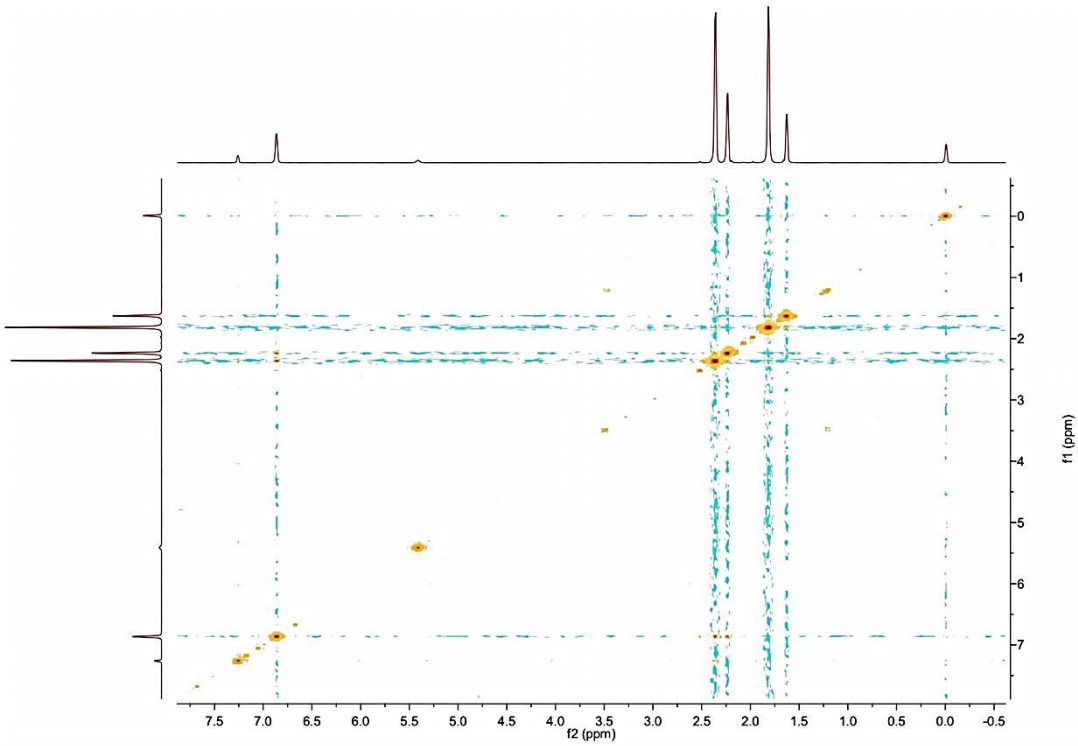

Figure S.I.16. COSY NMR (in $CDCl_3$) of compound **1**.

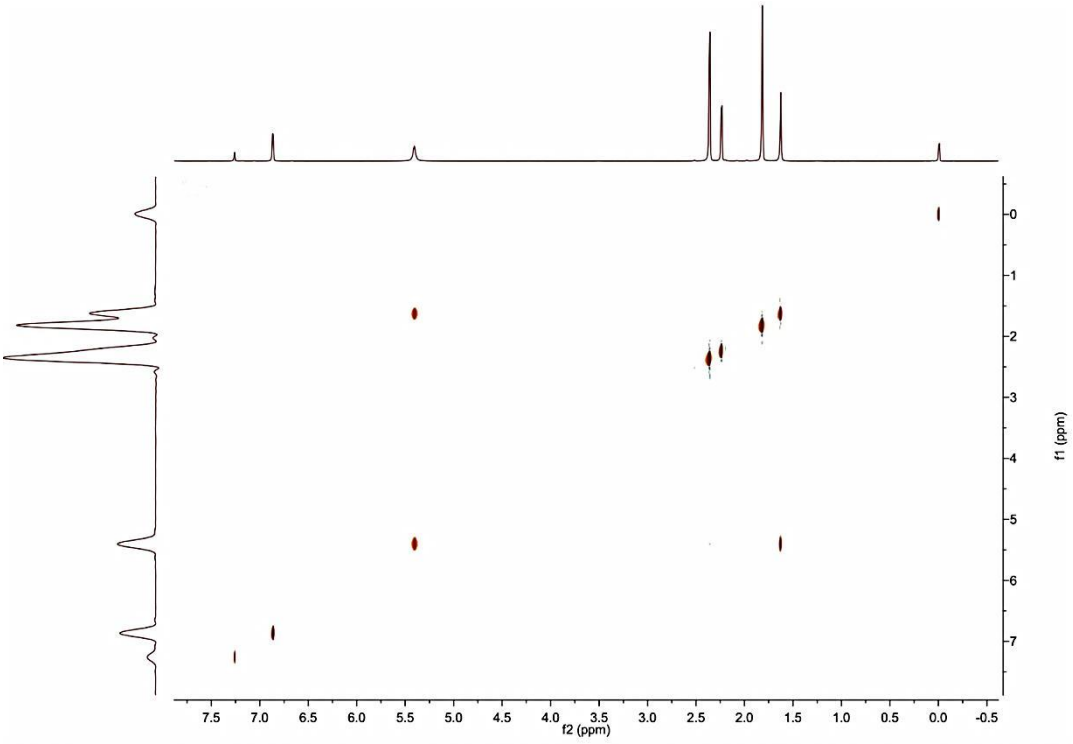

Figure S.I.17. NOESY NMR (in $CDCl_3$) of compound **1**.

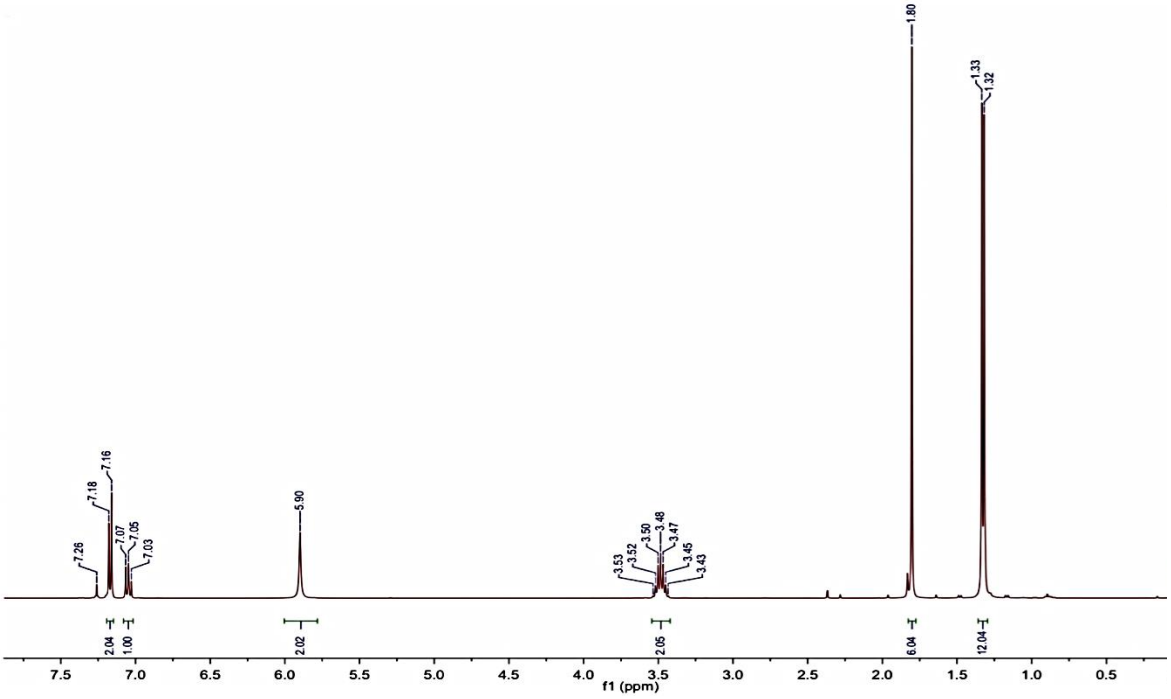

Figure S.I.1. ^{1}H NMR (in $CDCl_3$) of compound **2**.

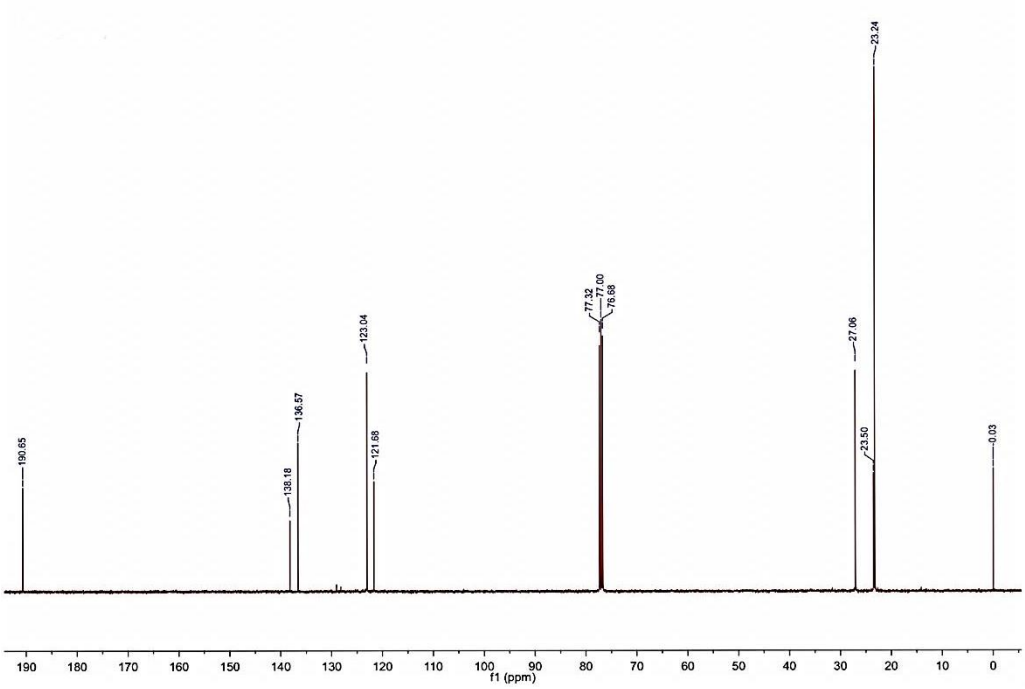

Figure S.I.2. $^{13}C\{^{1}H\}$ NMR (in $CDCl_3$) of compound **2**.

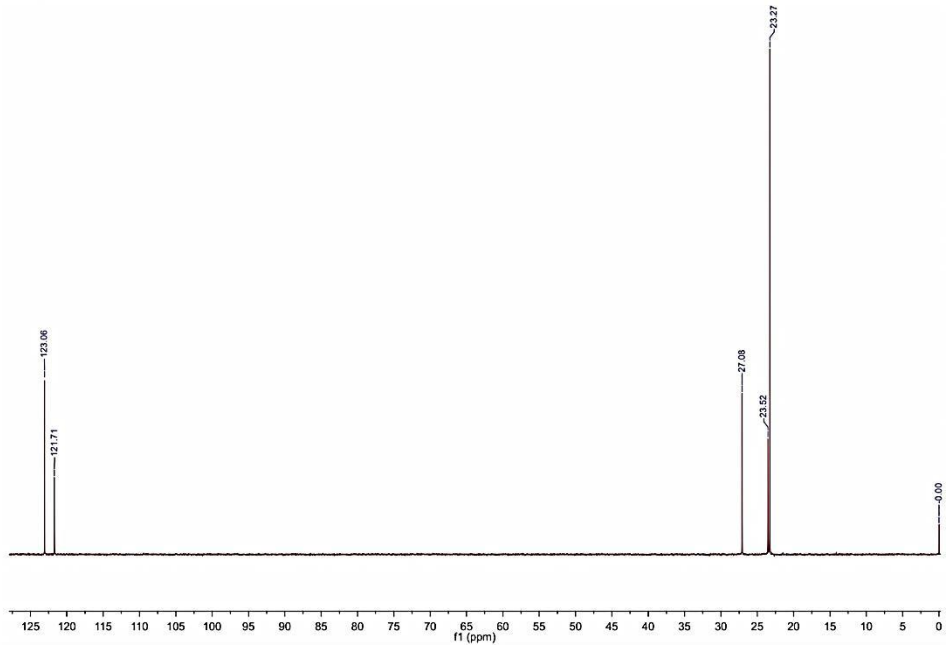

Figure S.I.3. DEPT NMR (in $CDCl_3$) of compound **2**.

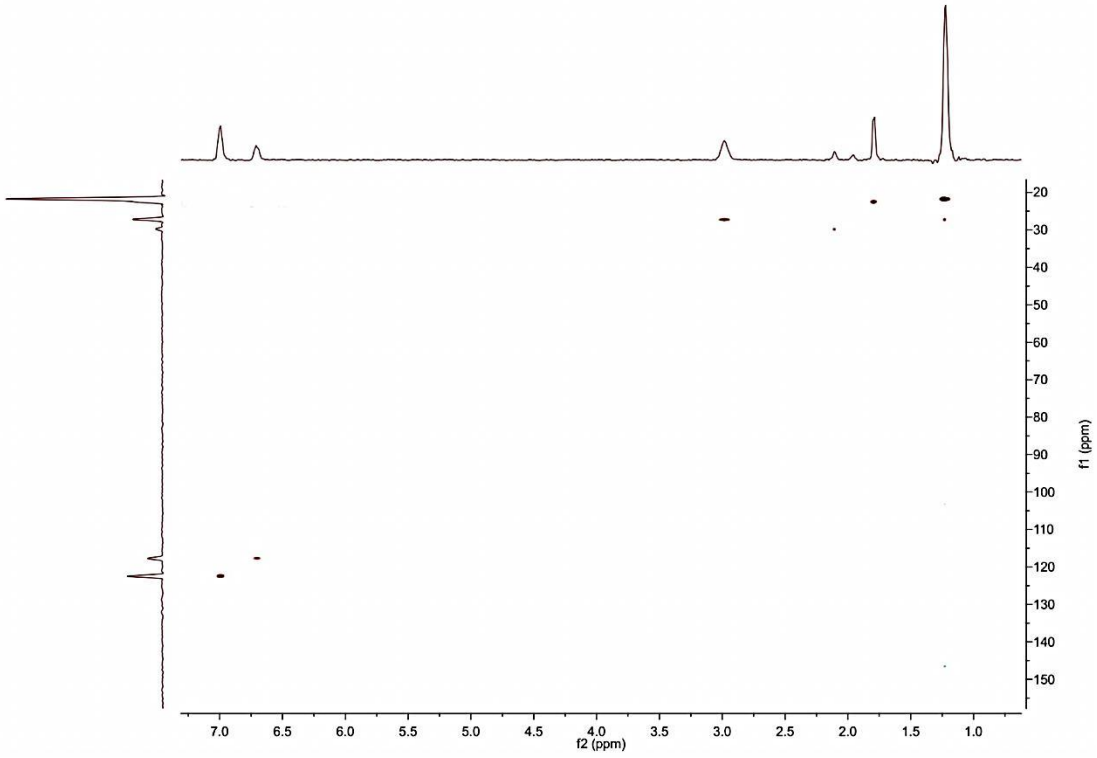

Figure S.I.4. HSQC NMR (in $CDCl_3$) of compound **2**.

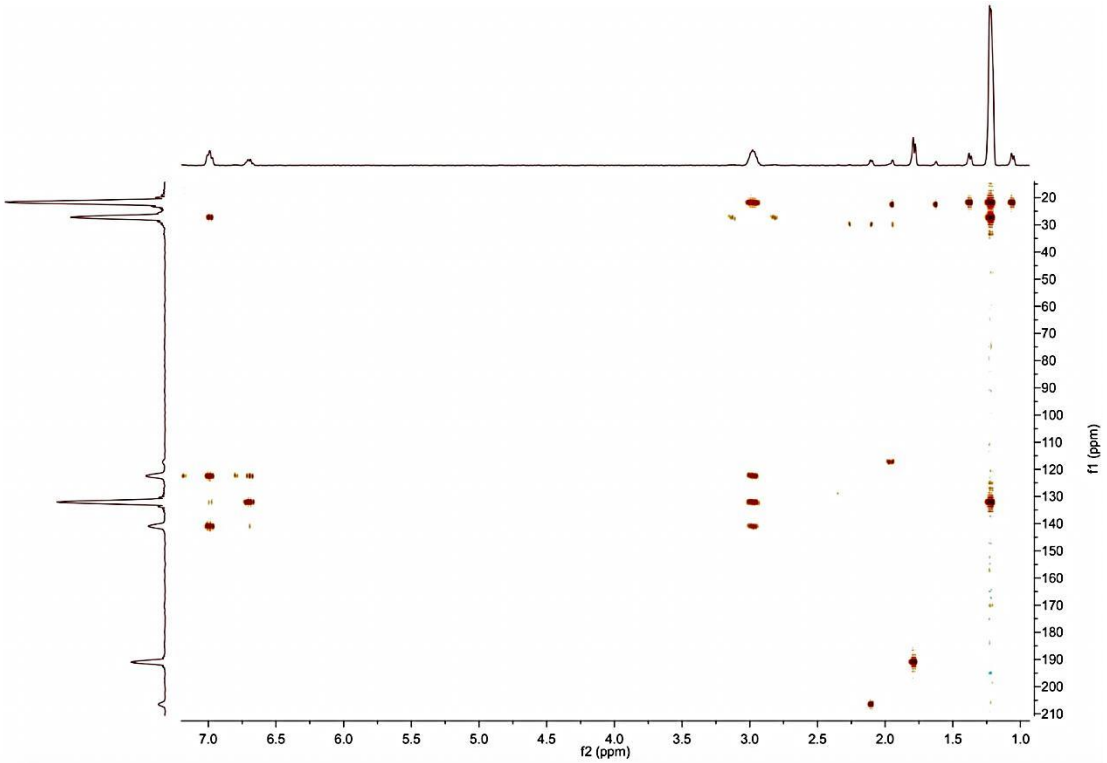

Figure S.I.5. HMBC NMR (in $CDCl_3$) of compound **2**.

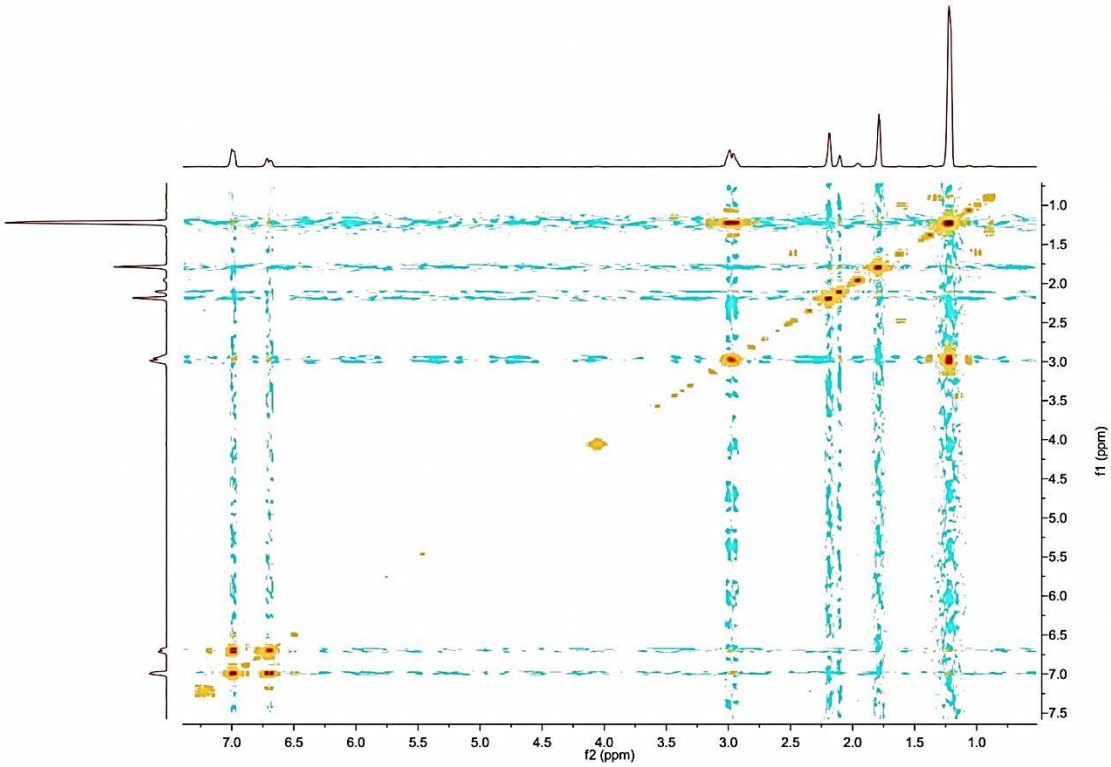

Figure S.I.6. COSY NMR (in $CDCl_3$) of compound **2**.

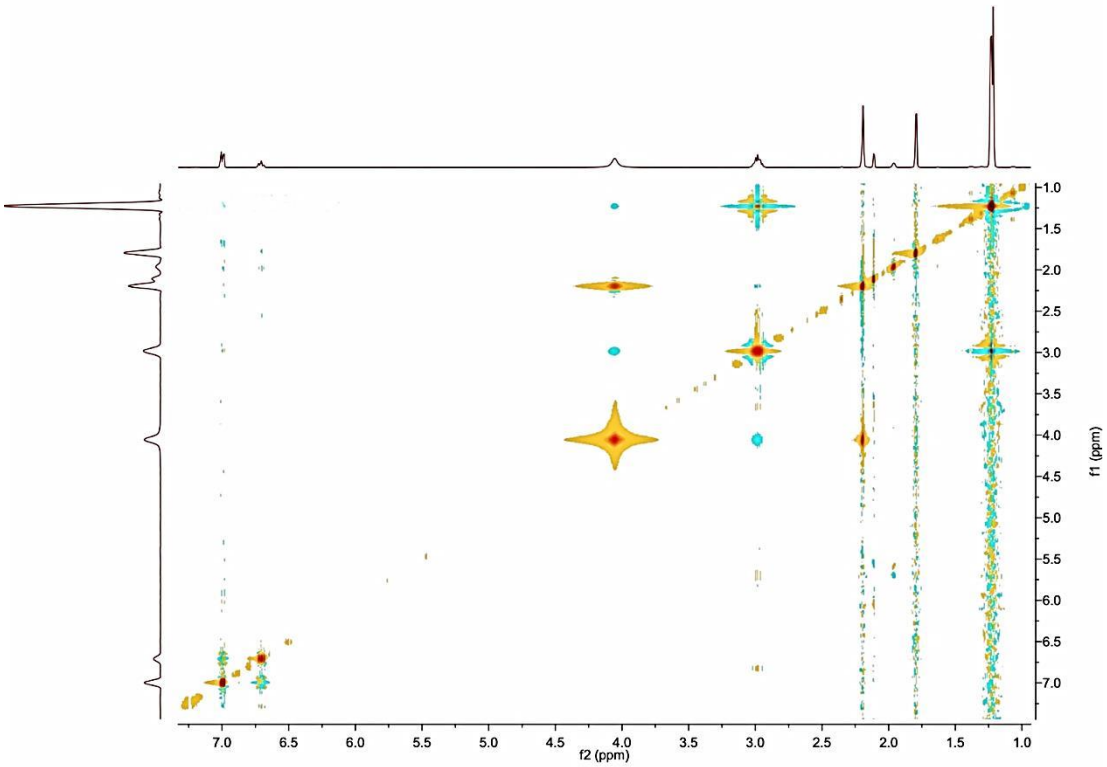

Figure S.I.7. NOESY NMR (in $CDCl_3$) of compound **2**.

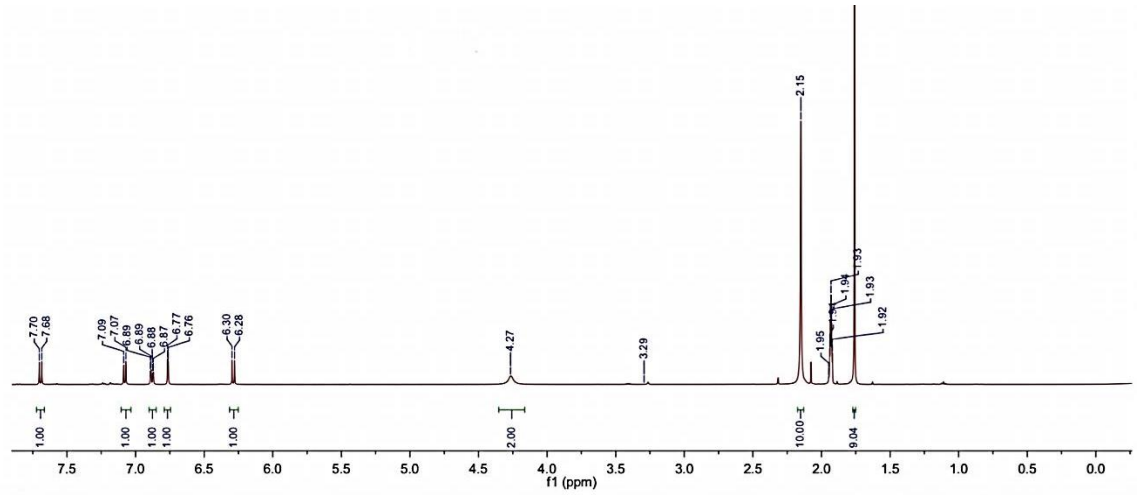

Figure S.I.18. ^{1}H NMR (in $NCCD_3$) of compound **3**.

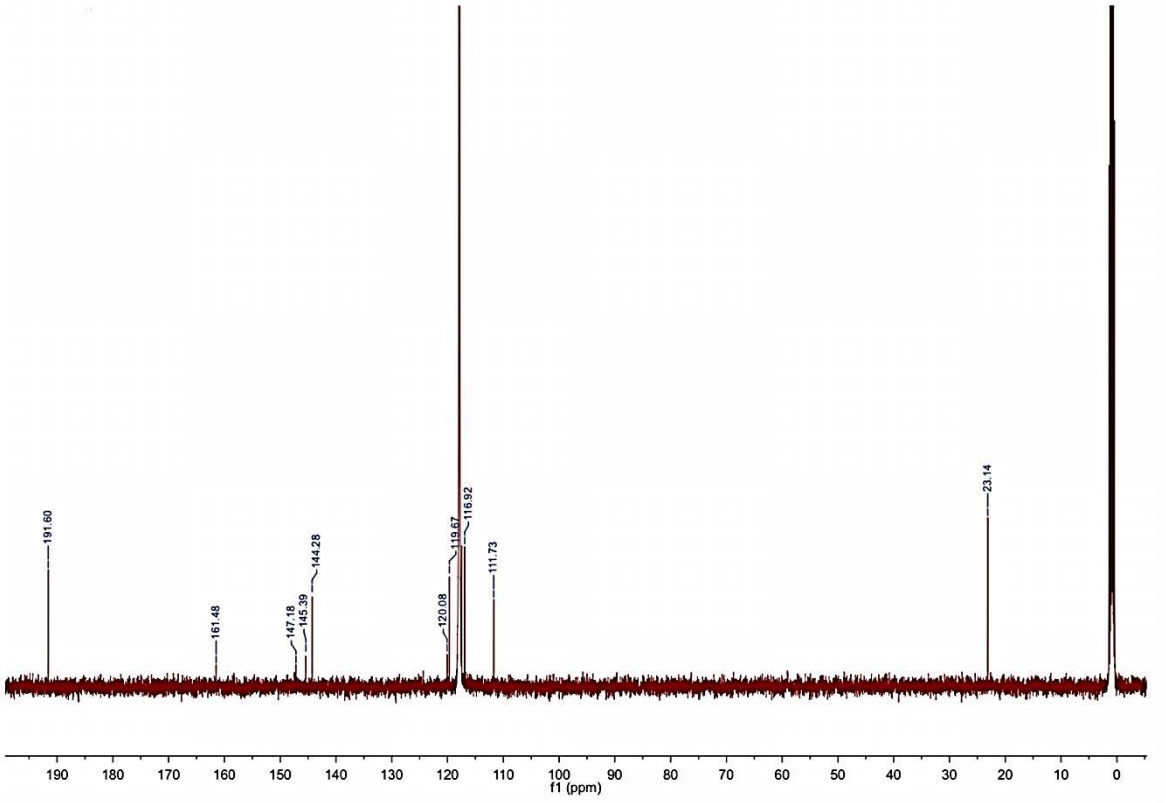

Figure S.I.19. $^{13}C\{^{1}H\}$ NMR (in $NCCD_3$) of compound **3**.

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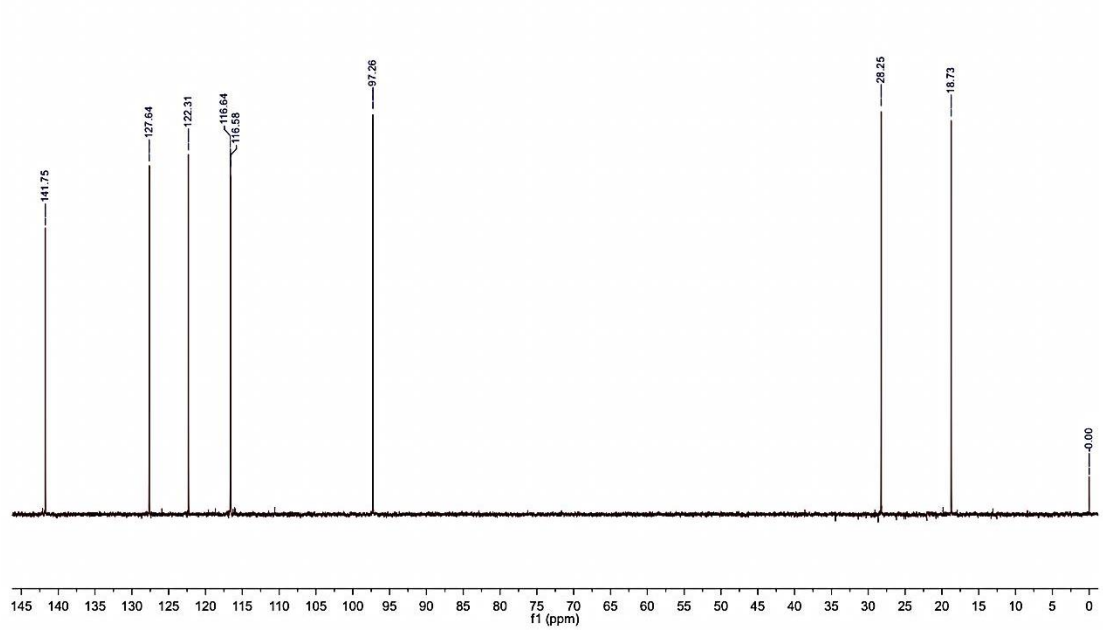


Figure S.I.20. DEPT NMR (in $NCCD_3$) of compound **3**.

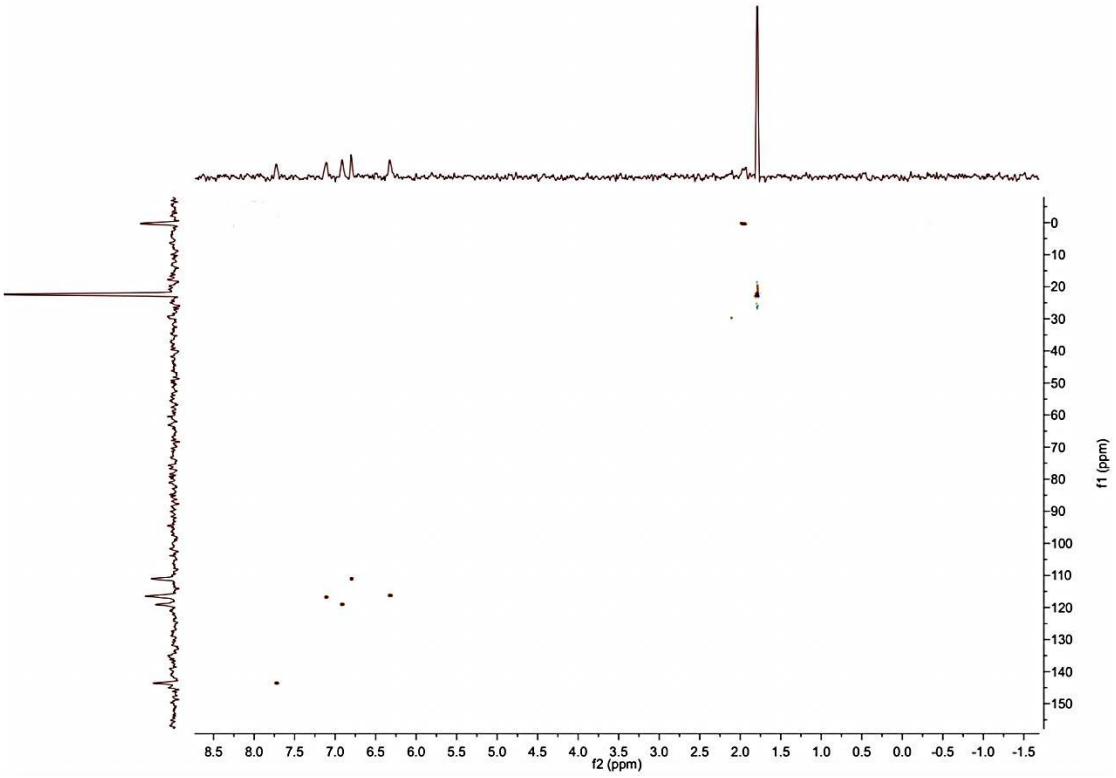


Figure S.I.21. HSQC NMR (in $NCCD_3$) of compound **3**.

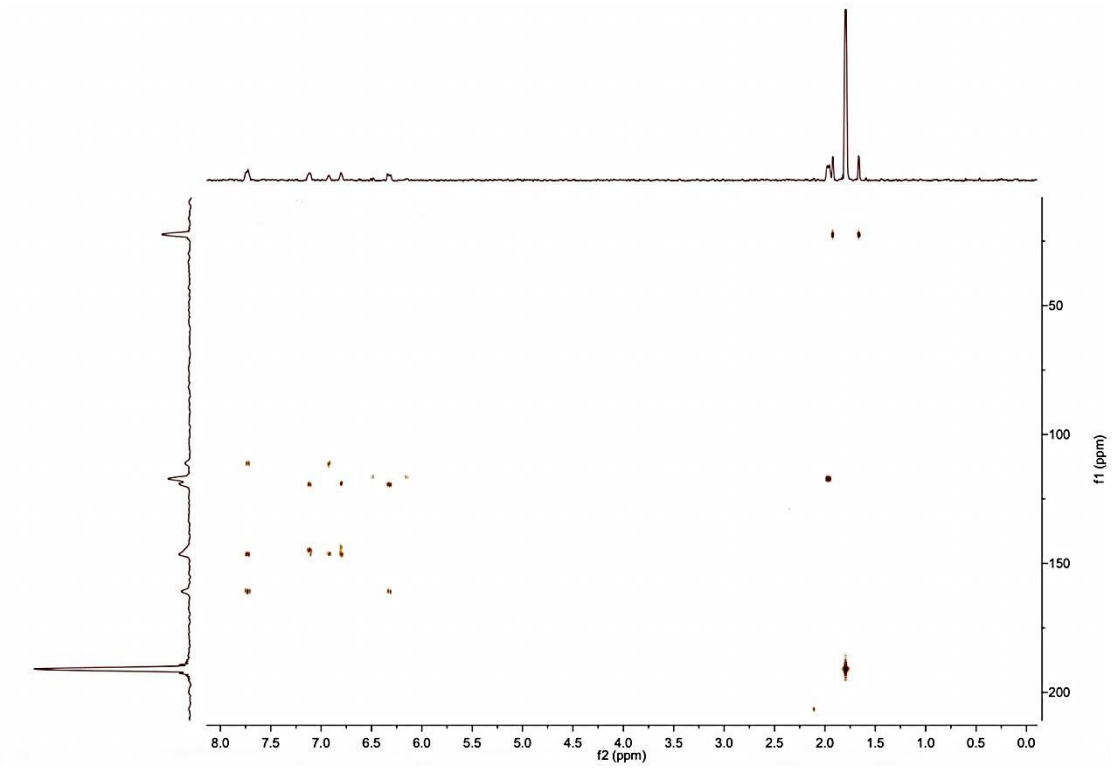


Figure S.I.22. HMBC NMR (in $NCCD_3$) of compound **3**.

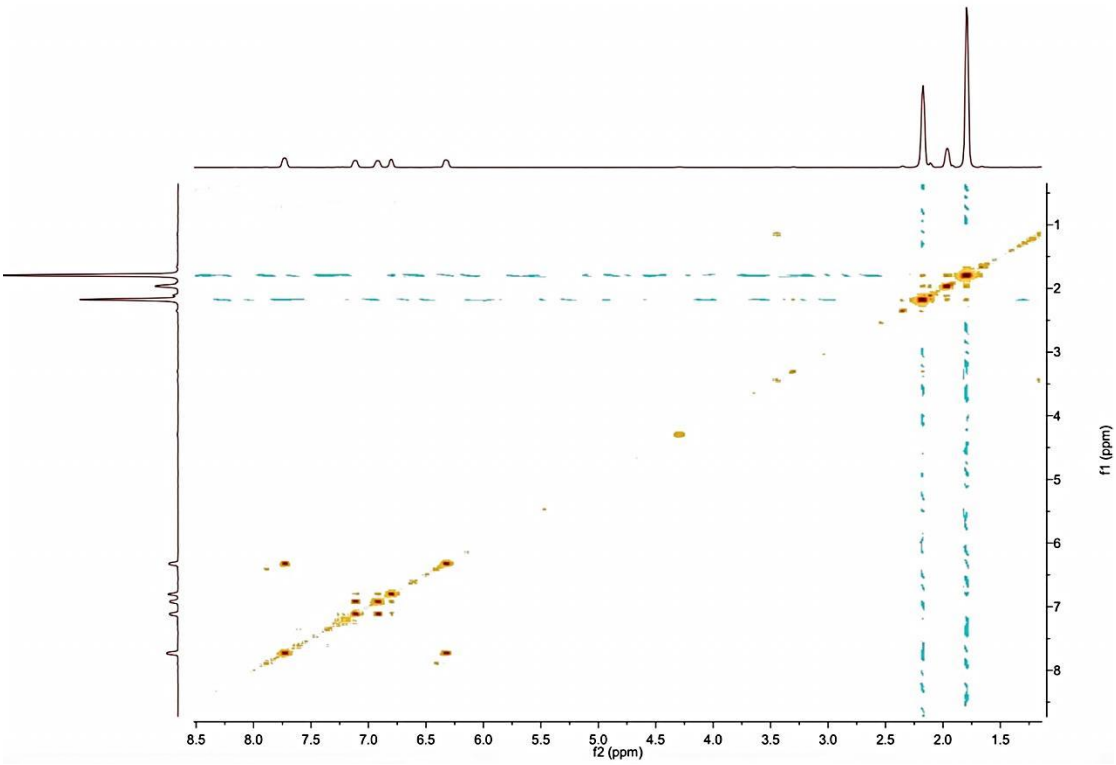


Figure S.I.23. COSY NMR (in $NCCD_3$) of compound **3**.

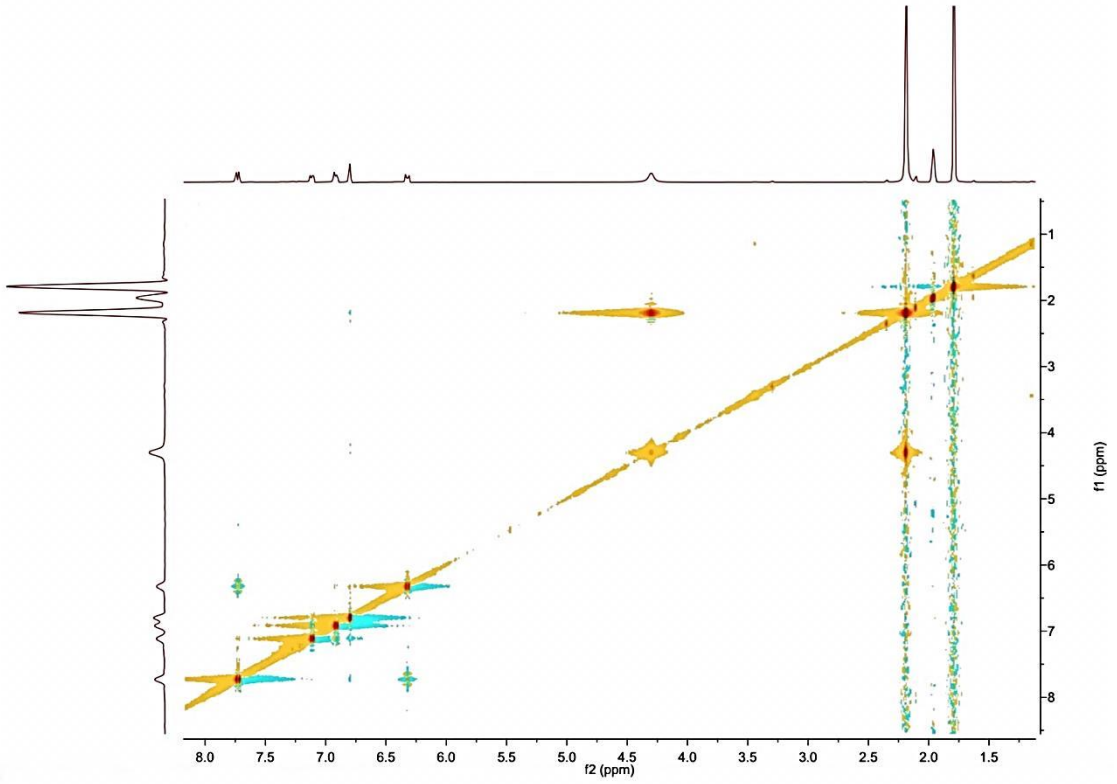


Figure S.I.24. NOESY NMR (in $NCCD_3$) of compound **3**.

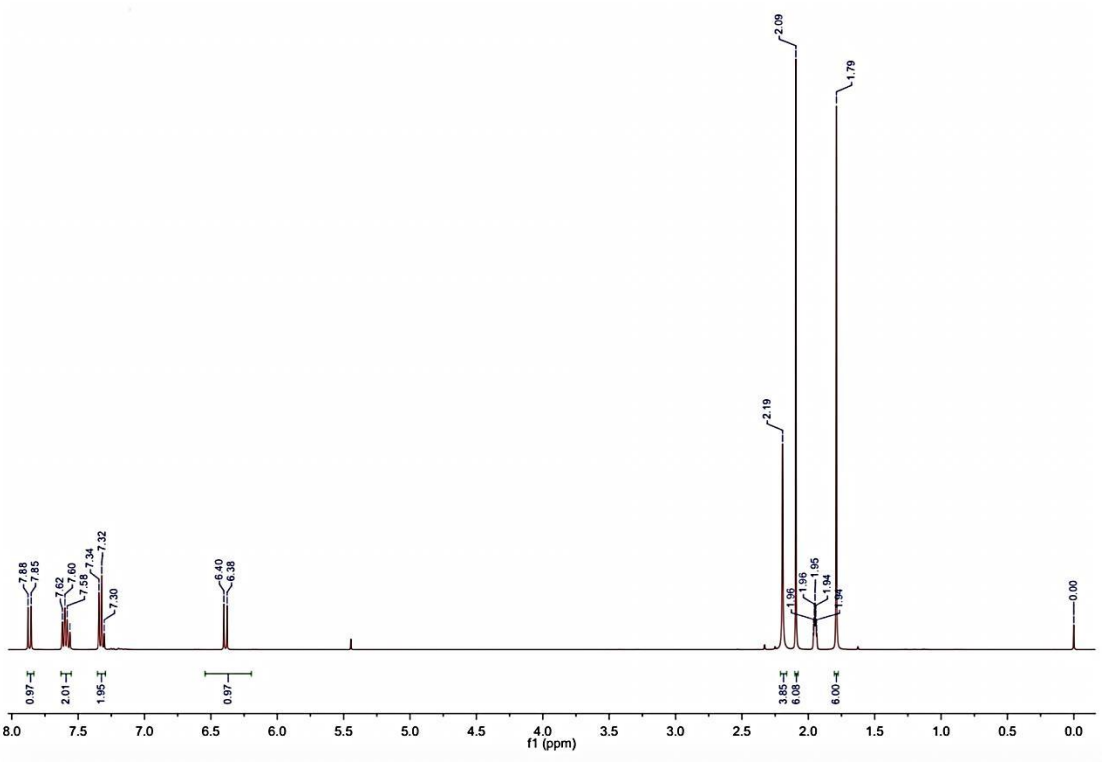


Figure S.I.25. ^{1}H NMR (in $NCCD_3$) of compound **4**.

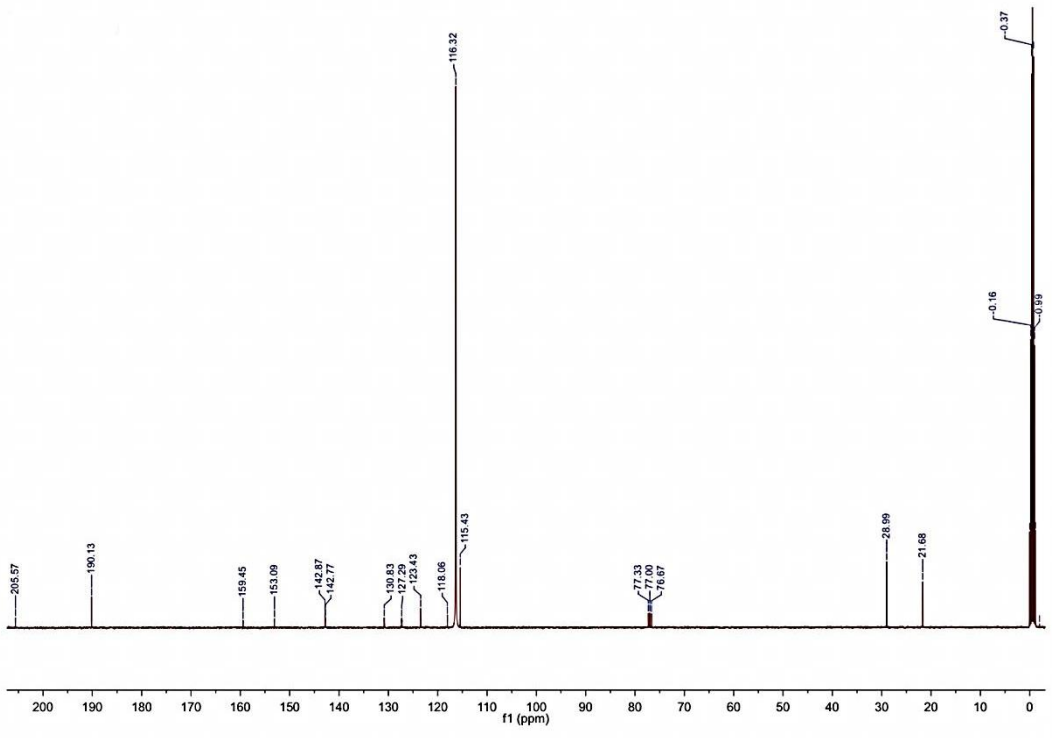


Figure S.I.26. $^{13}C\{^{1}H\}$ NMR (in $NCCD_3$) of compound **4**.

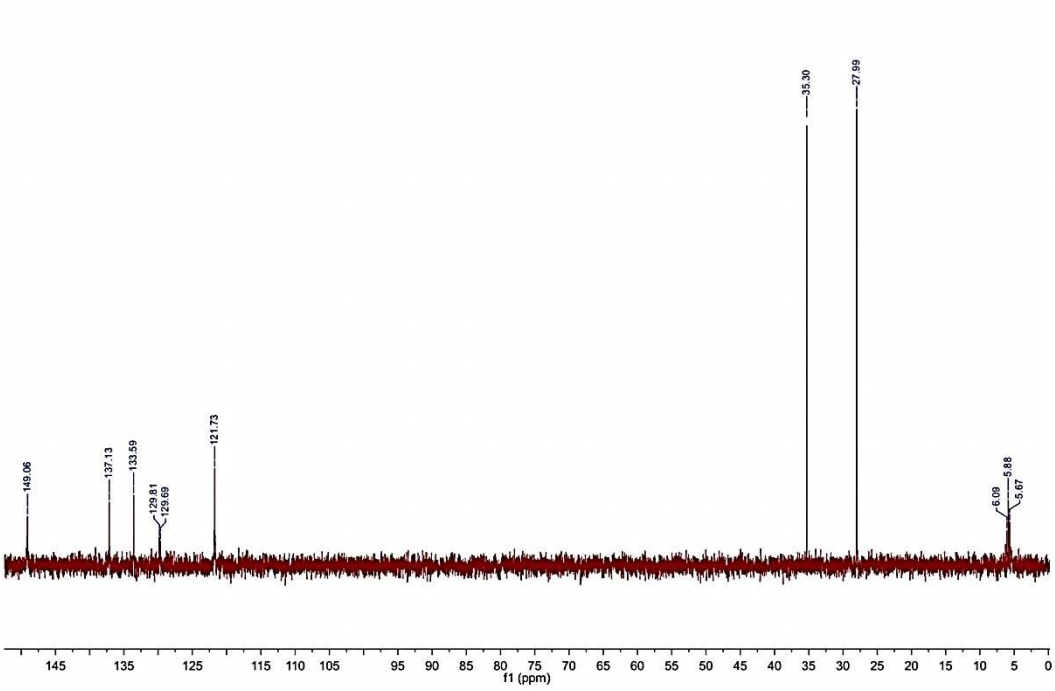


Figure S.I.27. DEPT (in $NCCD_3$) of compound **4**.

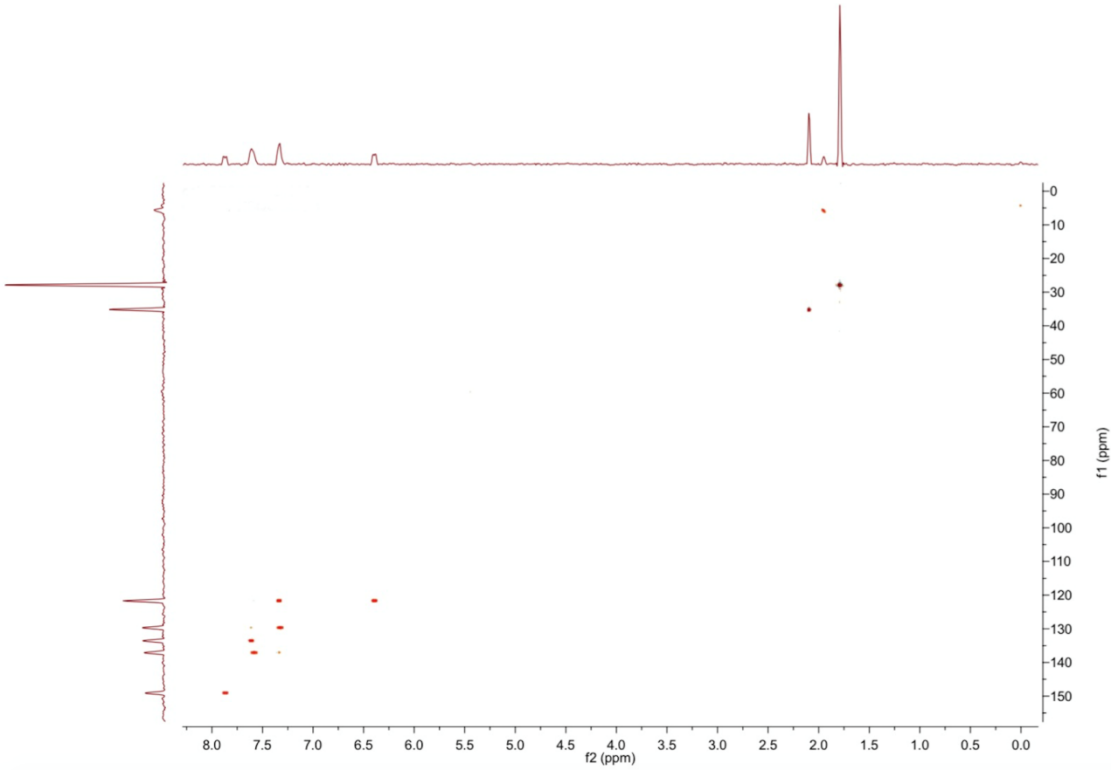


Figure S.I.28. HSQC (in $NCCD_3$) of compound **4**.

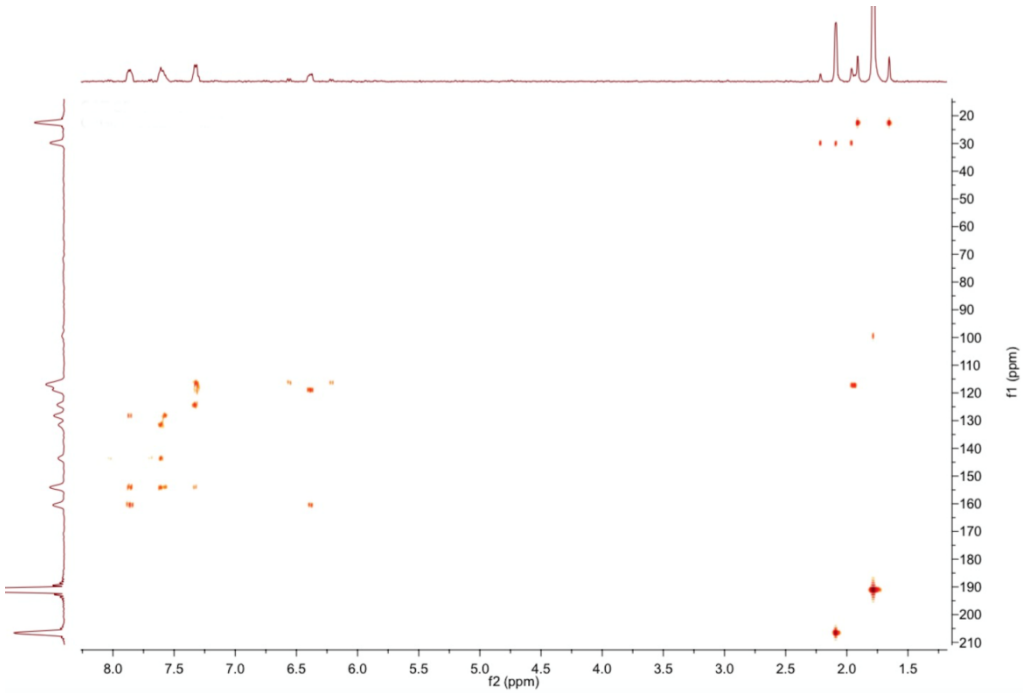


Figure S.I.29. HMBC (in $NCCD_3$) of compound **4**.

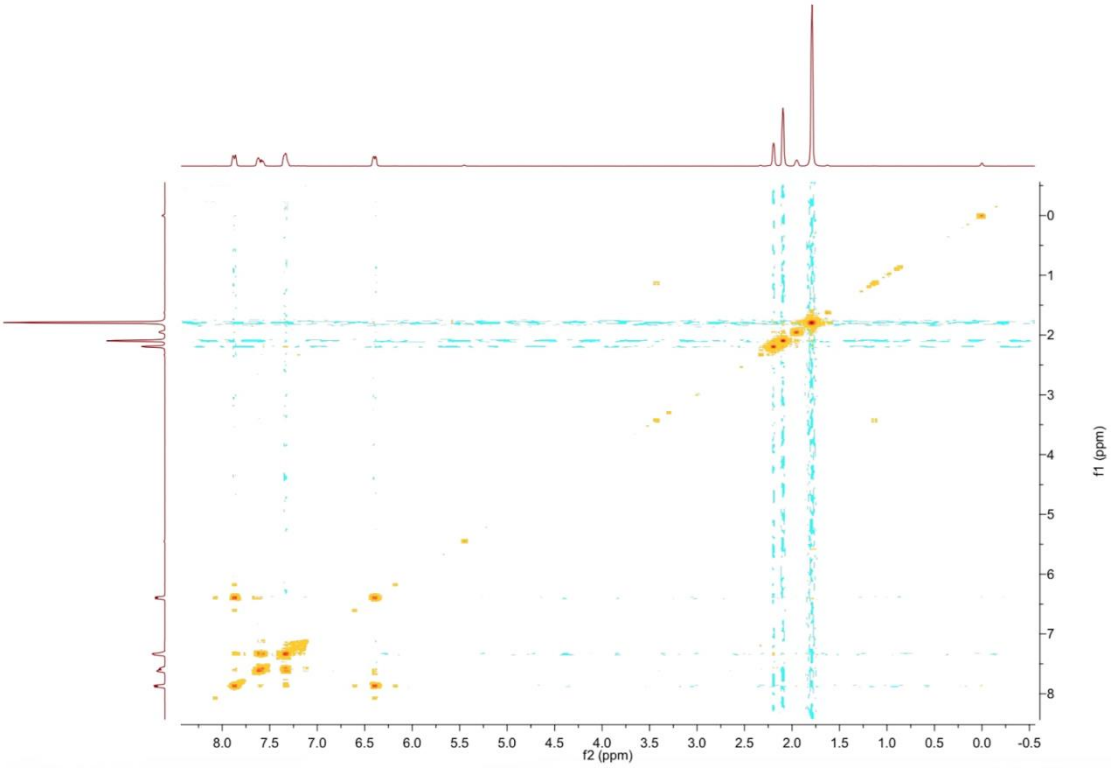


Figure S.I.30. COSY (in $NCCD_3$) of compound **4**.

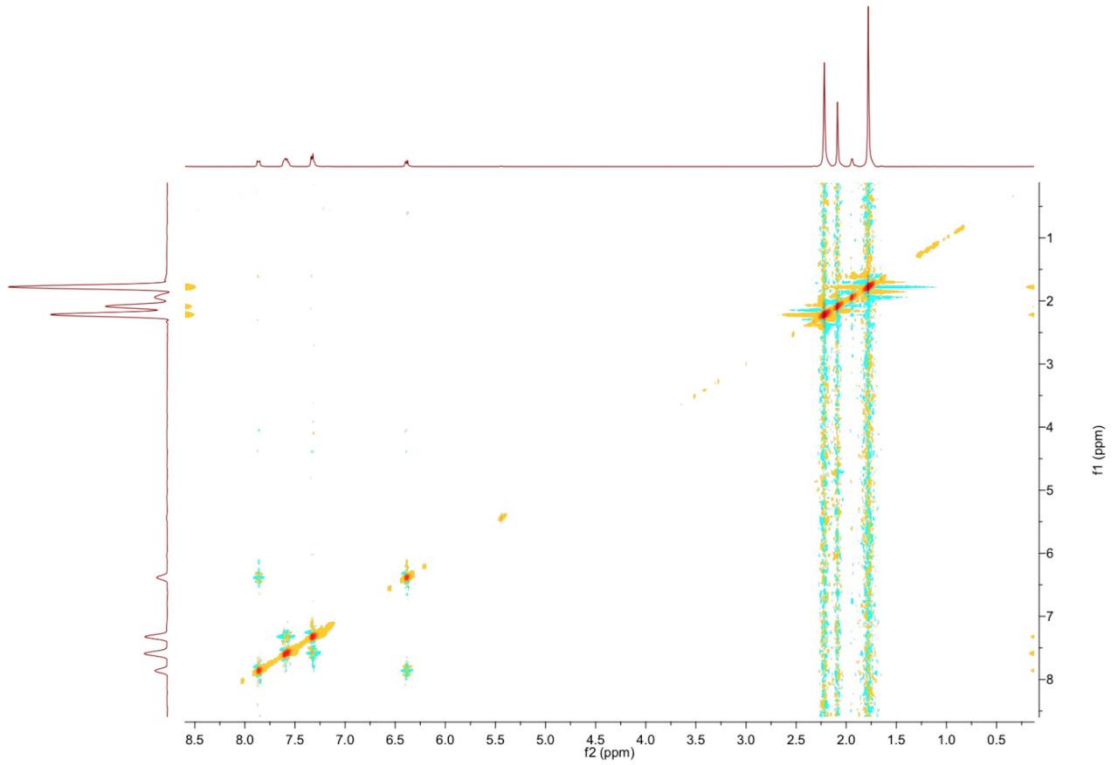


Figure S.I.31. NOESY (in $NCCD_3$) of compound **4**.

IR spectra

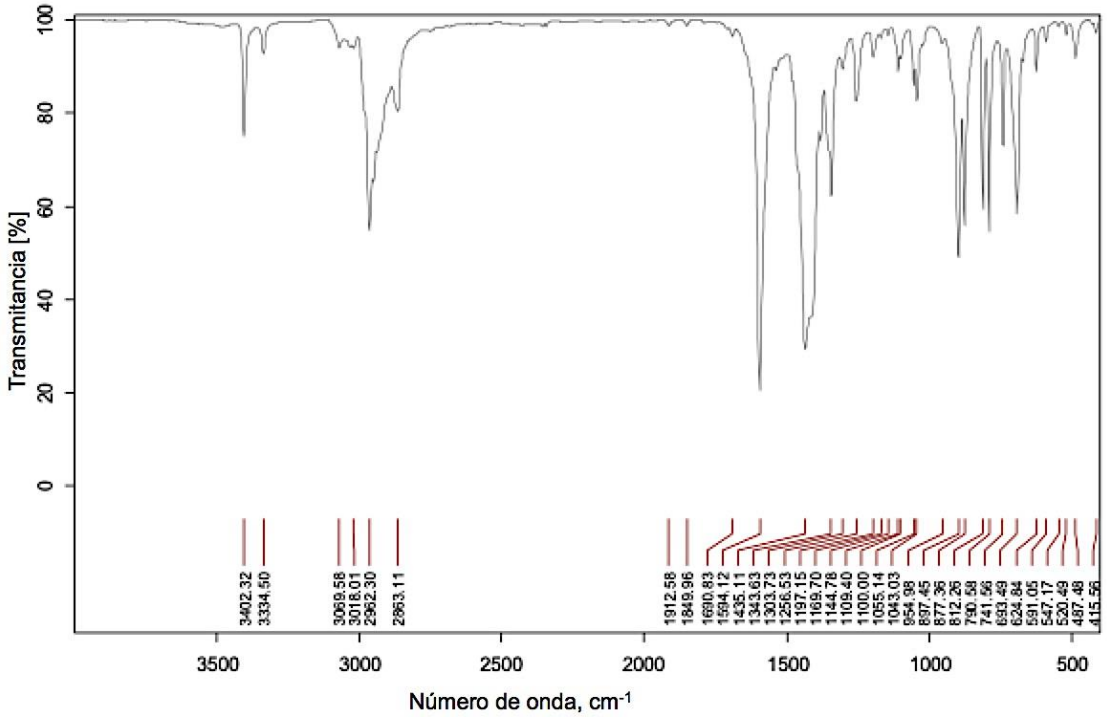


Figure S.I.32. IR spectra (in KBr) of compound **1**.

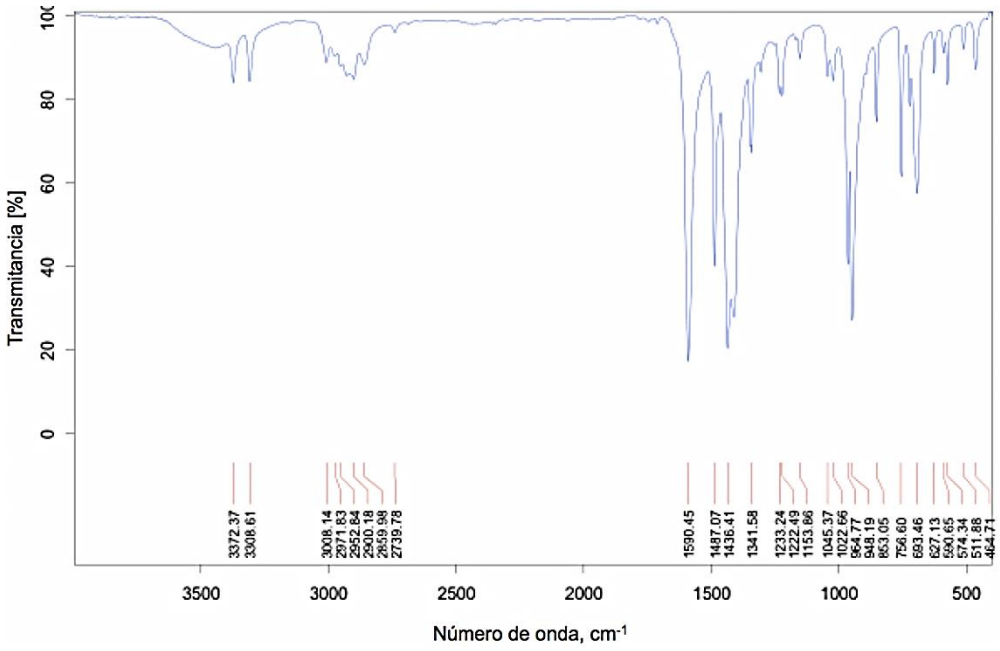


Figure S.I.33. IR spectra (in KBr) of compound **2**.

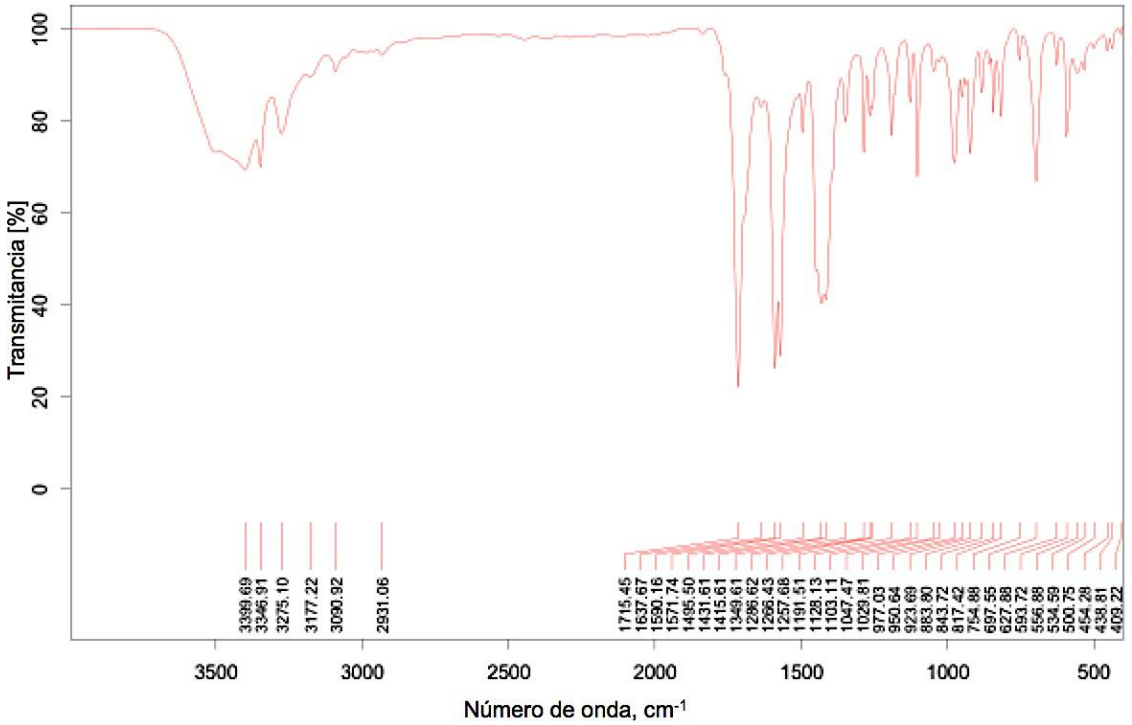


Figure S.I.34. IR spectra (in KBr) of compound **3**.

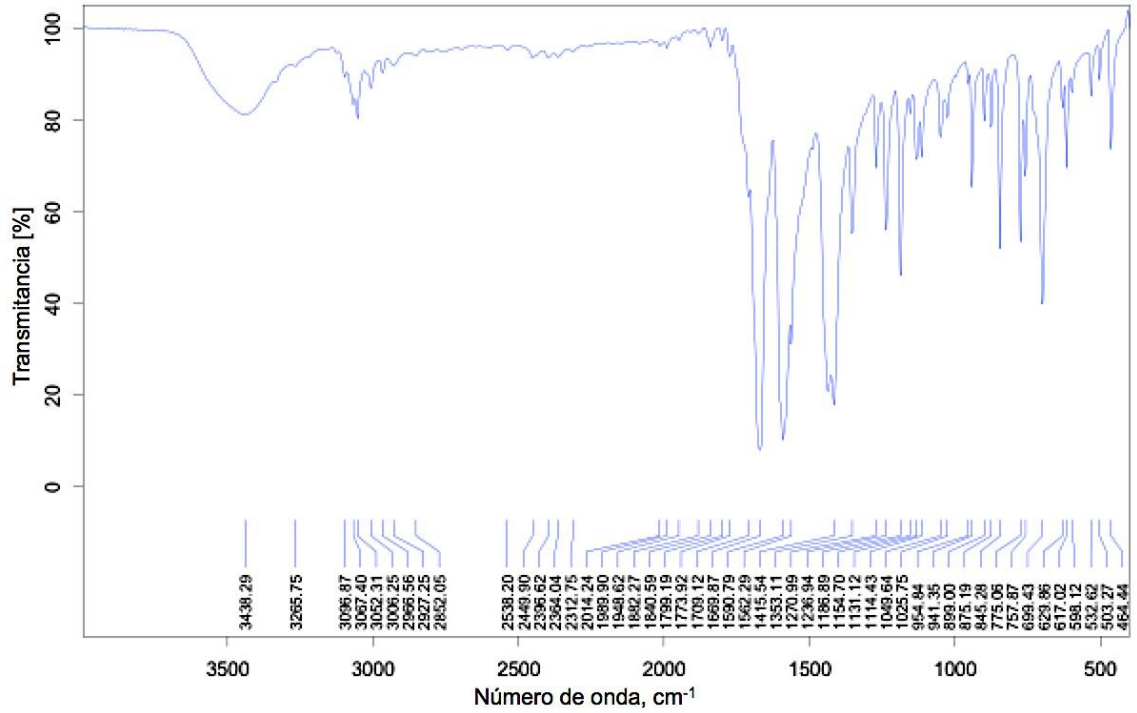


Figure S.I.35. IR spectra (in KBr) of compound **4**.

UV/Visible spectra

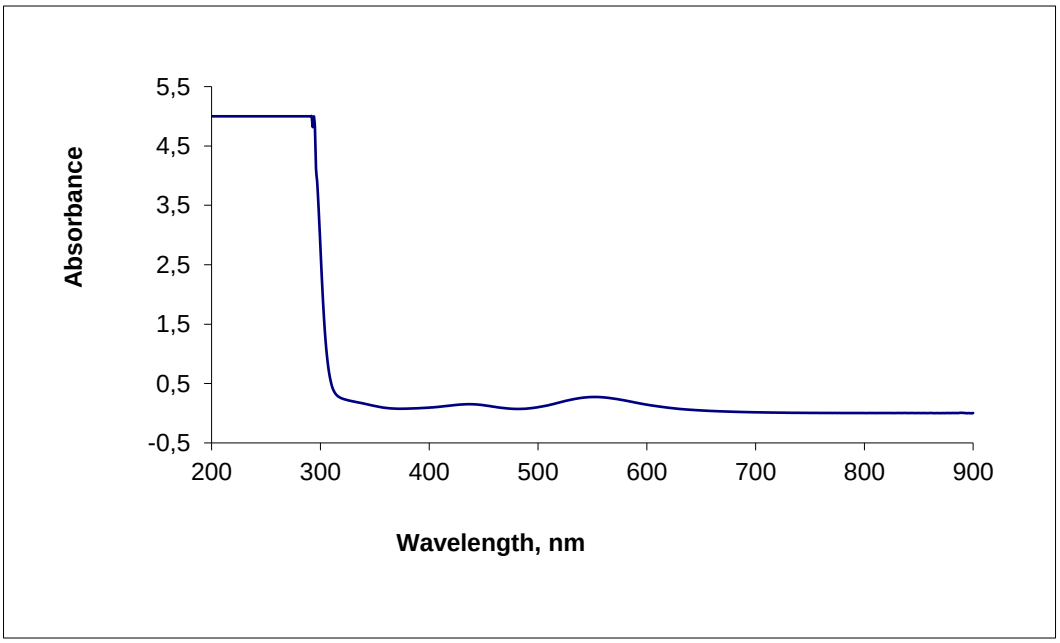


Figure S.I.36. UV-Vis spectra of a solution of compound **1** in CH_3CN (1×10^{-3} M).

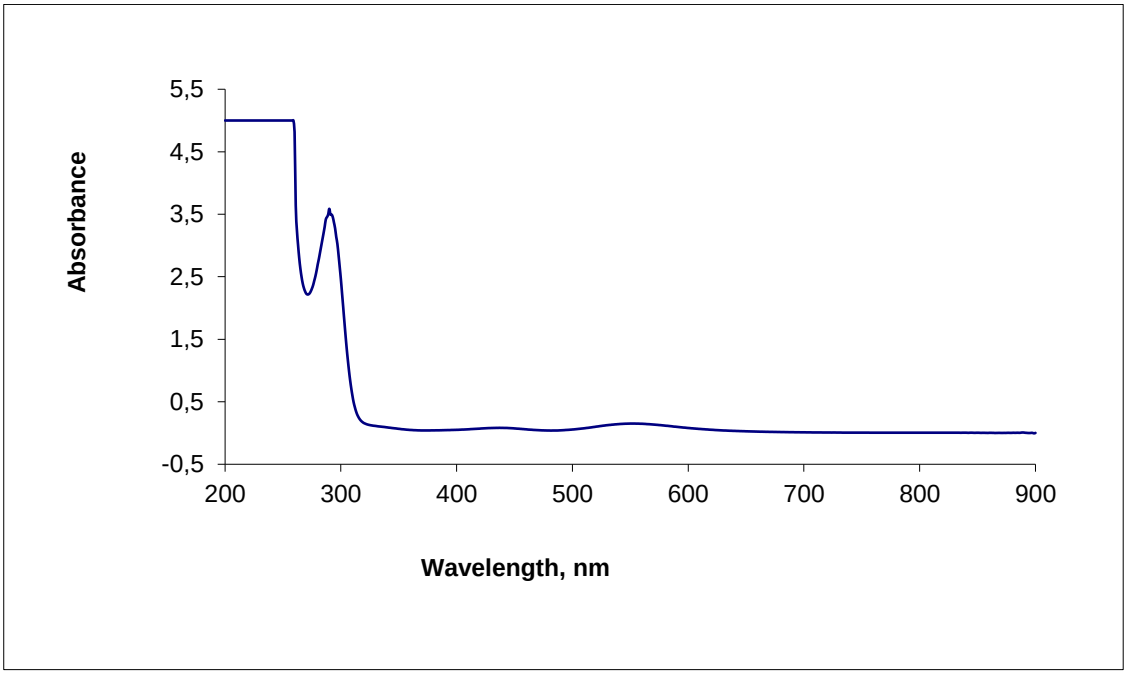


Figure S.I.37. UV-Vis spectra of a solution of compound **2** in CH_3CN (1×10^{-3} M).

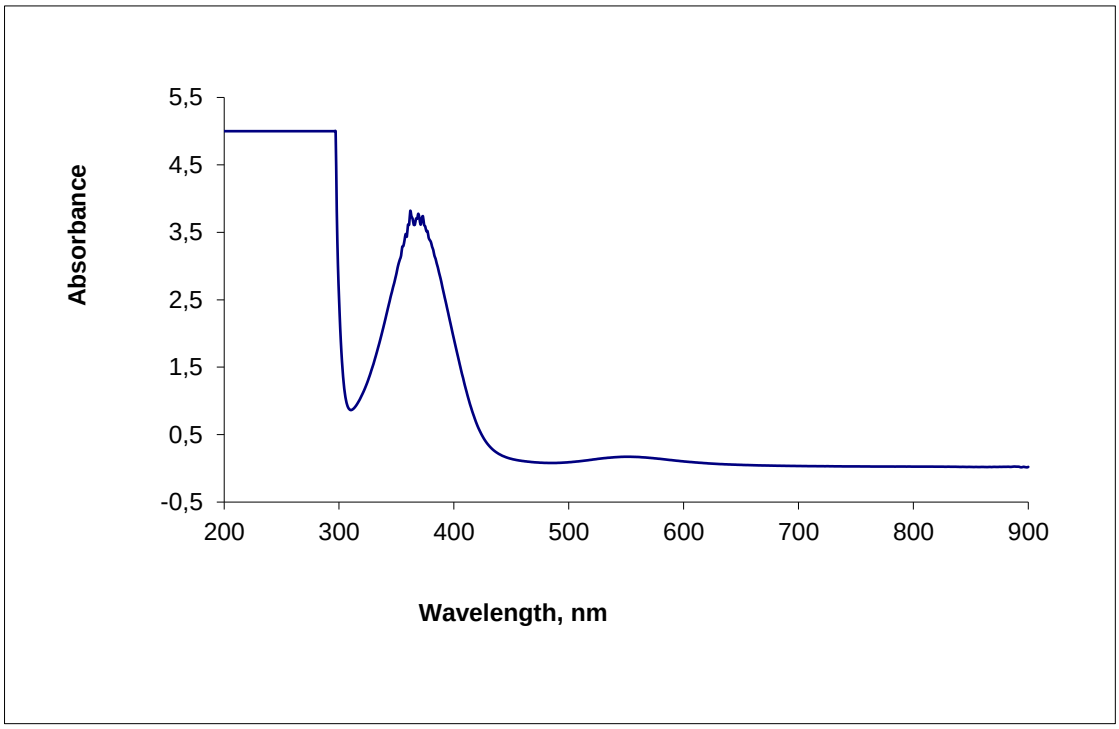


Figure S.I.38. UV-Vis spectra of a solution of compound **3** in CH_3CN (1×10^{-3} M).

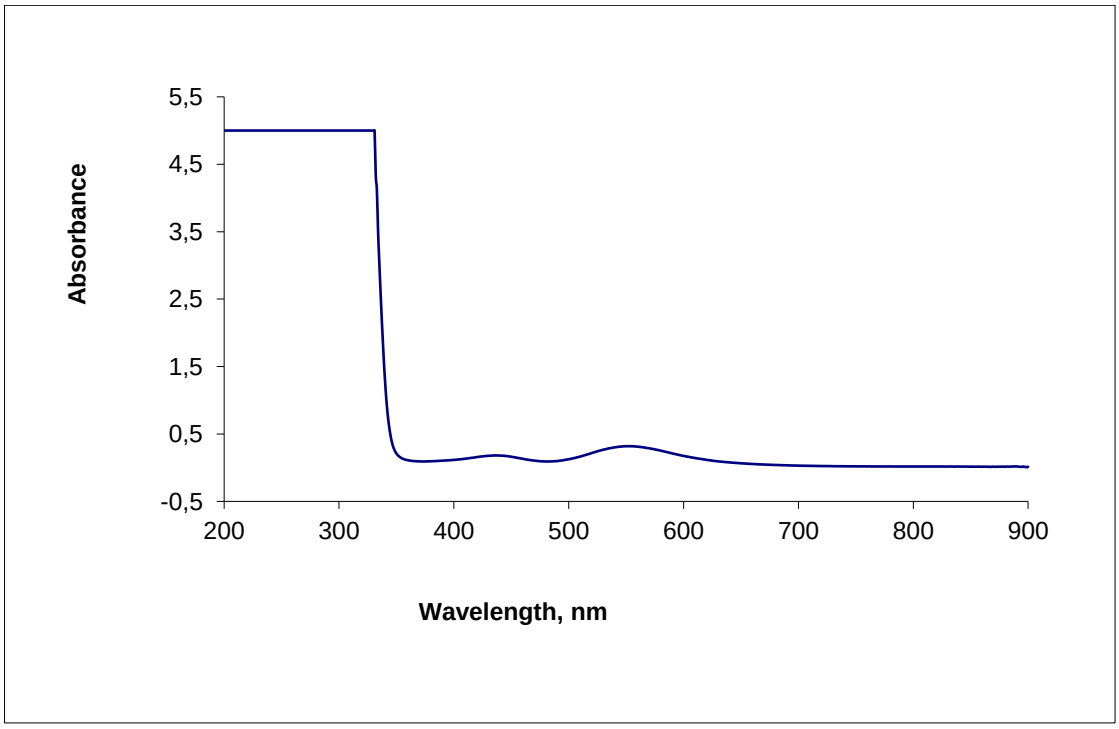
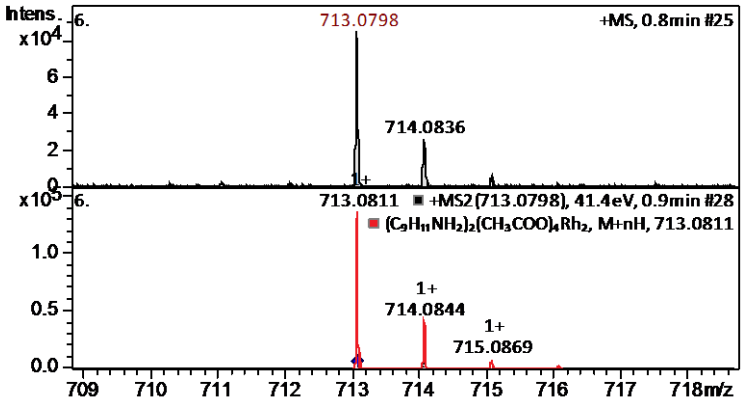
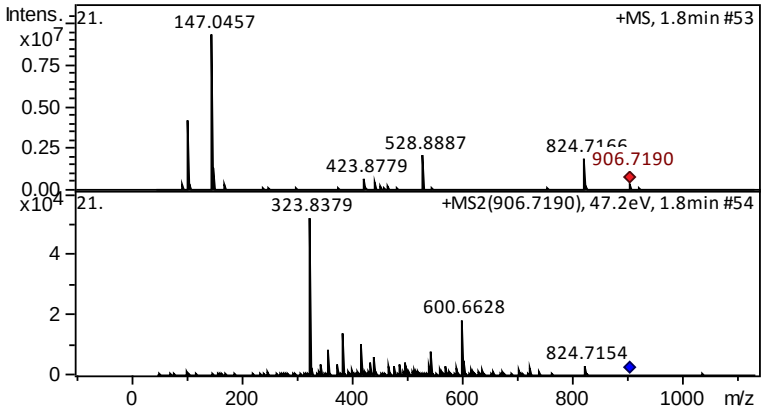


Figure S.I.39. UV-Vis spectra of a solution of compound **4** in CH_3CN (1×10^{-3} M).

Mass spectrum for complex **1**.





X-Ray Diffraction Tables

Table S.I.1. Crystal data and structure refinement for compound **1**.

Identification code	shelx	
Empirical formula	C32 H50 N2 O8 Rh2	
Formula weight	796.56	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.2014(5) Å	α= 75.975(5)°.
	b = 9.2294(6) Å	β= 75.919(5)°.
	c = 11.9557(7) Å	γ= 82.881(5)°.
Volume	849.58(9) $Å^3$	
Z	1	
Density (calculated)	1.557 Mg/m^3	
Absorption coefficient	1.021 mm^{-1}	
F(000)	410	
Theta range for data collection	3.447 to 29.348°.	
Index ranges	-10<=h<=11, -12<=k<=11, -12<=l<=15	
Reflections collected	6458	
Independent reflections	3940 [R(int) = 0.0311]	
Completeness to theta = 25.242°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3940 / 2 / 211	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.0541	
R indices (all data)	R1 = 0.0553, wR2 = 0.0647	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.563 and -0.740 $e.Å^{-3}$	

Table S.I.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1764(3)	7282(4)	8133(3)	11(1)
C(2)	2974(4)	7929(4)	8460(3)	12(1)
C(3)	4389(4)	7018(4)	8721(3)	17(1)
C(4)	4606(4)	5540(4)	8631(3)	17(1)
C(5)	3417(4)	4951(4)	8269(3)	15(1)
C(6)	1974(4)	5802(4)	7997(3)	12(1)
C(7)	2819(4)	9555(4)	8556(3)	17(1)
C(8)	4408(4)	10354(4)	7887(3)	23(1)
C(9)	2390(5)	9678(5)	9854(3)	34(1)
C(10)	685(4)	5092(4)	7615(3)	15(1)
C(11)	-504(4)	4229(5)	8702(3)	26(1)
C(12)	1507(4)	4062(4)	6770(3)	24(1)
C(13)	-2695(4)	8558(4)	5332(3)	11(1)
C(14)	-4270(3)	7780(4)	5521(3)	16(1)
C(15)	-1846(3)	12130(4)	5910(3)	13(1)
C(16)	-2882(4)	13379(4)	6414(3)	17(1)
O(1)	-1922(2)	8269(3)	6173(2)	13(1)
O(2)	-2265(2)	9487(3)	4345(2)	12(1)
O(3)	-1271(2)	11049(3)	6626(2)	12(1)
O(4)	1615(2)	7742(3)	5196(2)	14(1)
Rh(1)	177(1)	9361(1)	5963(1)	10(1)
N(1)	273(3)	8156(3)	7882(2)	8(1)

Table S.I.3. Bond lengths [Å] and angles [°] for compound **1**.

C(1)-C(2)	1.394(4)
C(1)-C(6)	1.399(5)
C(1)-N(1)	1.433(4)
C(2)-C(3)	1.399(4)
C(2)-C(7)	1.520(5)
C(3)-C(4)	1.381(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.373(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.398(4)
C(5)-H(5)	0.9500
C(6)-C(10)	1.518(5)
C(7)-C(8)	1.526(5)
C(7)-C(9)	1.535(5)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.532(5)
C(10)-C(12)	1.534(4)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-O(1)	1.274(4)
C(13)-O(2)	1.279(4)
C(13)-C(14)	1.498(4)
C(14)-H(14A)	0.9800

C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-O(4)#1	1.268(4)
C(15)-O(3)	1.271(4)
C(15)-C(16)	1.503(4)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
O(1)-Rh(1)	2.034(2)
O(2)-Rh(1)#1	2.038(2)
O(3)-Rh(1)	2.037(2)
O(4)-C(15)#1	1.268(4)
O(4)-Rh(1)	2.041(2)
Rh(1)-O(2)#1	2.038(2)
Rh(1)-N(1)	2.309(3)
Rh(1)-Rh(1)#1	2.3886(5)
N(1)-H(1D)	0.911(17)
N(1)-H(1E)	0.903(17)

C(2)-C(1)-C(6)	122.2(3)
C(2)-C(1)-N(1)	119.9(3)
C(6)-C(1)-N(1)	117.9(3)
C(1)-C(2)-C(3)	117.6(3)
C(1)-C(2)-C(7)	123.4(3)
C(3)-C(2)-C(7)	119.0(3)
C(4)-C(3)-C(2)	121.4(3)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(5)-C(4)-C(3)	119.4(3)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	121.9(3)
C(4)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0
C(5)-C(6)-C(1)	117.3(3)
C(5)-C(6)-C(10)	119.8(3)

C(1)-C(6)-C(10)	122.8(3)
C(2)-C(7)-C(8)	112.0(3)
C(2)-C(7)-C(9)	111.0(3)
C(8)-C(7)-C(9)	110.4(3)
C(2)-C(7)-H(7)	107.8
C(8)-C(7)-H(7)	107.8
C(9)-C(7)-H(7)	107.8
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(11)	110.1(3)
C(6)-C(10)-C(12)	112.5(2)
C(11)-C(10)-C(12)	110.3(3)
C(6)-C(10)-H(10)	107.9
C(11)-C(10)-H(10)	107.9
C(12)-C(10)-H(10)	107.9
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5

H(12B)-C(12)-H(12C)	109.5
O(1)-C(13)-O(2)	125.5(3)
O(1)-C(13)-C(14)	117.6(3)
O(2)-C(13)-C(14)	116.8(3)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(4)#1-C(15)-O(3)	125.9(3)
O(4)#1-C(15)-C(16)	116.7(3)
O(3)-C(15)-C(16)	117.3(3)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(13)-O(1)-Rh(1)	118.5(2)
C(13)-O(2)-Rh(1)#1	119.30(19)
C(15)-O(3)-Rh(1)	118.2(2)
C(15)#1-O(4)-Rh(1)	119.4(2)
O(1)-Rh(1)-O(3)	90.19(8)
O(1)-Rh(1)-O(2)#1	176.65(9)
O(3)-Rh(1)-O(2)#1	89.88(8)
O(1)-Rh(1)-O(4)	89.94(9)
O(3)-Rh(1)-O(4)	176.42(9)
O(2)#1-Rh(1)-O(4)	89.79(8)
O(1)-Rh(1)-N(1)	87.52(9)
O(3)-Rh(1)-N(1)	87.88(9)
O(2)#1-Rh(1)-N(1)	95.83(9)
O(4)-Rh(1)-N(1)	95.71(9)
O(1)-Rh(1)-Rh(1)#1	88.83(6)
O(3)-Rh(1)-Rh(1)#1	88.86(6)
O(2)#1-Rh(1)-Rh(1)#1	87.82(6)

O(4)-Rh(1)-Rh(1)#1	87.57(6)
N(1)-Rh(1)-Rh(1)#1	175.09(6)
C(1)-N(1)-Rh(1)	120.20(18)
C(1)-N(1)-H(1D)	113.6(18)
Rh(1)-N(1)-H(1D)	101(2)
C(1)-N(1)-H(1E)	113(2)
Rh(1)-N(1)-H(1E)	100(2)
H(1D)-N(1)-H(1E)	107(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1

Table S.I.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	8(2)	15(2)	7(2)	0(1)	-2(1)	2(1)
C(2)	13(2)	13(2)	8(2)	0(2)	-2(1)	0(1)
C(3)	14(2)	23(2)	14(2)	-3(2)	-7(1)	-1(2)
C(4)	14(2)	16(2)	18(2)	0(2)	-5(1)	4(2)
C(5)	14(2)	12(2)	19(2)	-6(2)	-2(1)	2(1)
C(6)	12(2)	13(2)	9(2)	-1(2)	0(1)	-1(1)
C(7)	18(2)	16(2)	19(2)	-7(2)	-7(1)	1(2)
C(8)	26(2)	14(2)	29(2)	-6(2)	-6(2)	-6(2)
C(9)	45(2)	24(3)	31(2)	-16(2)	6(2)	-8(2)
C(10)	17(2)	11(2)	16(2)	-1(2)	-6(1)	0(1)
C(11)	22(2)	35(3)	21(2)	-1(2)	-6(2)	-12(2)
C(12)	22(2)	30(3)	25(2)	-14(2)	-9(2)	-1(2)
C(13)	9(2)	10(2)	15(2)	-8(2)	1(1)	2(1)
C(14)	13(2)	17(2)	18(2)	-6(2)	-3(1)	-3(1)
C(15)	4(2)	14(2)	21(2)	-5(2)	-1(1)	-1(1)
C(16)	16(2)	17(2)	19(2)	-9(2)	-4(1)	1(2)
O(1)	11(1)	15(1)	12(1)	-1(1)	-3(1)	-2(1)
O(2)	10(1)	14(1)	15(1)	-4(1)	-4(1)	-3(1)
O(3)	12(1)	13(1)	13(1)	-3(1)	-3(1)	2(1)
O(4)	15(1)	16(2)	10(1)	-2(1)	-3(1)	1(1)
Rh(1)	9(1)	11(1)	10(1)	-2(1)	-3(1)	0(1)
N(1)	11(1)	6(2)	7(1)	-2(1)	-2(1)	-1(1)

Table S.I.5. Hydrogen bonds for compound **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(14)-H(14A)...O(2)#2	0.98	2.58	3.558(4)	172.4
C(14)-H(14A)...O(2)#2	0.98	2.58	3.558(4)	172.4

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1 #2 -x-1,-y+2,-z+1

Table S.I.6. Crystal data and structure refinement for compound **2**.

Identification code	shelx	
Empirical formula	C26 H38 N2 O8 Rh2	
Formula weight	712.40	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.0671(11) Å	α= 69.118(9)°.
	b = 8.3981(6) Å	β= 70.302(11)°.
	c = 11.6427(14) Å	γ= 89.701(8)°.
Volume	687.89(15) $Å^3$	
Z	1	
Density (calculated)	1.720 Mg/m^3	
Absorption coefficient	1.250 mm^{-1}	
F(000)	362	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	3.493 to 29.429°.	
Index ranges	-10<=h<=11, -11<=k<=10, -16<=l<=11	
Reflections collected	5600	
Independent reflections	3196 [R(int) = 0.0287]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3196 / 2 / 183	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0300, wR2 = 0.0586	
R indices (all data)	R1 = 0.0378, wR2 = 0.0655	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.788 and -0.783 $e.Å^{-3}$	

Table S.I.7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	388(4)	-845(3)	3798(3)	15(1)
C(2)	448(4)	-2390(4)	4778(3)	17(1)
C(3)	-1145(4)	-3406(4)	5661(3)	18(1)
C(4)	-2779(4)	-2921(4)	5613(3)	18(1)
C(5)	-2774(4)	-1408(4)	4597(3)	19(1)
C(6)	-1219(4)	-352(4)	3680(3)	17(1)
C(7)	2197(4)	-2929(4)	4859(3)	21(1)
C(8)	-4486(4)	-4011(4)	6620(3)	27(1)
C(9)	-1273(4)	1251(4)	2567(3)	24(1)
C(10)	2933(4)	1693(3)	-1198(3)	15(1)
C(11)	1757(4)	2707(4)	-1867(3)	22(1)
C(12)	6622(4)	2893(3)	-315(3)	17(1)
C(13)	7574(4)	4547(4)	-479(3)	25(1)
O(1)	2419(3)	1271(2)	44(2)	18(1)
O(2)	5277(3)	2211(2)	724(2)	18(1)
O(3)	4351(3)	1335(2)	-1896(2)	17(1)
O(4)	7240(3)	2324(2)	-1226(2)	17(1)
Rh(1)	3959(1)	-46(1)	1029(1)	14(1)
N(1)	2033(3)	219(3)	2923(2)	14(1)

Table S.I.8. Bond lengths [Å] and angles [°] for compound **2**.

C(1)-C(6)	1.395(4)
C(1)-C(2)	1.403(4)
C(1)-N(1)	1.431(4)
C(2)-C(3)	1.390(4)
C(2)-C(7)	1.502(4)
C(3)-C(4)	1.391(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.393(4)
C(4)-C(8)	1.506(4)
C(5)-C(6)	1.390(4)
C(5)-H(5)	0.9500
C(6)-C(9)	1.513(4)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-O(3)	1.266(3)
C(10)-O(1)	1.272(3)
C(10)-C(11)	1.500(4)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-O(2)	1.263(3)
C(12)-O(4)	1.267(3)
C(12)-C(13)	1.509(4)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
O(1)-Rh(1)	2.031(2)

O(2)-Rh(1)	2.0333(18)
O(3)-Rh(1)#1	2.0450(19)
O(4)-Rh(1)#1	2.0506(18)
Rh(1)-O(3)#1	2.0450(19)
Rh(1)-O(4)#1	2.0506(18)
Rh(1)-N(1)	2.316(2)
Rh(1)-Rh(1)#1	2.3925(6)
N(1)-H(1E)	0.902(17)
N(1)-H(1D)	0.908(17)

C(6)-C(1)-C(2)	121.3(3)
C(6)-C(1)-N(1)	120.9(3)
C(2)-C(1)-N(1)	117.8(3)
C(3)-C(2)-C(1)	118.4(3)
C(3)-C(2)-C(7)	121.1(3)
C(1)-C(2)-C(7)	120.5(3)
C(2)-C(3)-C(4)	122.0(3)
C(2)-C(3)-H(3)	119.0
C(4)-C(3)-H(3)	119.0
C(3)-C(4)-C(5)	117.6(3)
C(3)-C(4)-C(8)	120.8(3)
C(5)-C(4)-C(8)	121.5(3)
C(6)-C(5)-C(4)	122.6(3)
C(6)-C(5)-H(5)	118.7
C(4)-C(5)-H(5)	118.7
C(5)-C(6)-C(1)	118.0(3)
C(5)-C(6)-C(9)	120.8(3)
C(1)-C(6)-C(9)	121.2(3)
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(4)-C(8)-H(8A)	109.5
C(4)-C(8)-H(8B)	109.5

H(8A)-C(8)-H(8B)	109.5
C(4)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(6)-C(9)-H(9A)	109.5
C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
O(3)-C(10)-O(1)	125.1(3)
O(3)-C(10)-C(11)	118.4(3)
O(1)-C(10)-C(11)	116.5(3)
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(2)-C(12)-O(4)	126.2(3)
O(2)-C(12)-C(13)	116.5(3)
O(4)-C(12)-C(13)	117.3(3)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(10)-O(1)-Rh(1)	119.29(18)
C(12)-O(2)-Rh(1)	118.62(17)
C(10)-O(3)-Rh(1)#1	119.51(19)
C(12)-O(4)-Rh(1)#1	118.91(18)
O(1)-Rh(1)-O(2)	90.01(8)
O(1)-Rh(1)-O(3)#1	176.00(7)
O(2)-Rh(1)-O(3)#1	89.13(8)
O(1)-Rh(1)-O(4)#1	90.25(8)

O(2)-Rh(1)-O(4)#1	176.19(7)
O(3)#1-Rh(1)-O(4)#1	90.34(8)
O(1)-Rh(1)-N(1)	88.87(8)
O(2)-Rh(1)-N(1)	85.02(8)
O(3)#1-Rh(1)-N(1)	94.94(8)
O(4)#1-Rh(1)-N(1)	98.79(8)
O(1)-Rh(1)-Rh(1)#1	88.41(6)
O(2)-Rh(1)-Rh(1)#1	88.70(6)
O(3)#1-Rh(1)-Rh(1)#1	87.66(6)
O(4)#1-Rh(1)-Rh(1)#1	87.51(6)
N(1)-Rh(1)-Rh(1)#1	173.16(6)
C(1)-N(1)-Rh(1)	126.56(17)
C(1)-N(1)-H(1E)	109.9(19)
Rh(1)-N(1)-H(1E)	103.2(18)
C(1)-N(1)-H(1D)	110.8(18)
Rh(1)-N(1)-H(1D)	98.3(18)
H(1E)-N(1)-H(1D)	106(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z

Table S.I.9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(2)	15(1)	12(1)	-7(1)	0(1)	-1(1)
C(2)	18(2)	17(2)	18(2)	-10(1)	-4(1)	3(1)
C(3)	24(2)	12(1)	18(2)	-5(1)	-6(1)	2(1)
C(4)	19(2)	16(2)	19(2)	-9(1)	-4(1)	0(1)
C(5)	18(2)	18(2)	24(2)	-11(1)	-10(1)	6(1)
C(6)	19(2)	17(2)	16(2)	-10(1)	-4(1)	2(1)
C(7)	18(2)	21(2)	22(2)	-7(1)	-7(1)	4(1)
C(8)	17(2)	22(2)	30(2)	-2(2)	-1(2)	-3(1)
C(9)	21(2)	23(2)	22(2)	-6(1)	-4(2)	6(1)
C(10)	15(2)	14(1)	18(2)	-6(1)	-7(1)	2(1)
C(11)	17(2)	27(2)	23(2)	-11(1)	-7(1)	8(1)
C(12)	14(2)	12(1)	25(2)	-6(1)	-8(1)	4(1)
C(13)	20(2)	20(2)	28(2)	-8(2)	-3(2)	-2(1)
O(1)	15(1)	21(1)	18(1)	-7(1)	-5(1)	7(1)
O(2)	18(1)	14(1)	19(1)	-7(1)	-3(1)	-1(1)
O(3)	13(1)	18(1)	17(1)	-5(1)	-5(1)	4(1)
O(4)	16(1)	13(1)	20(1)	-6(1)	-4(1)	0(1)
Rh(1)	12(1)	12(1)	14(1)	-4(1)	-3(1)	1(1)
N(1)	14(1)	15(1)	15(1)	-8(1)	-6(1)	3(1)

Table S.I.10. Hydrogen bonds for compound **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(11)-H(11C)...O(4)#2	0.98	2.62	3.457(4)	143.6
C(13)-H(13B)...O(2)#3	0.98	2.58	3.550(4)	171.1
C(11)-H(11C)...O(4)#2	0.98	2.62	3.457(4)	143.6
C(13)-H(13B)...O(2)#3	0.98	2.58	3.550(4)	171.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z #2 x-1,y,z #3 -x+1,-y+1,-z

Table S.I.11. Crystal data and structure refinement for compound **4**.

Identification code	shelx	
Empirical formula	C26 H24 O12 Rh2	
Formula weight	734.27	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 11.616(2) Å	α= 90°.
	b = 13.6577(17) Å	β= 106.927(18)°.
	c = 8.5475(15) Å	γ= 90°.
Volume	1297.3(4) $Å^3$	
Z	2	
Density (calculated)	1.880 Mg/m^3	
Absorption coefficient	1.339 mm^{-1}	
F(000)	732	
Theta range for data collection	3.502 to 29.515°.	
Index ranges	-15<=h<=14, -17<=k<=10, -8<=l<=10	
Reflections collected	6445	
Independent reflections	3033 [R(int) = 0.0262]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3033 / 0 / 183	
Goodness-of-fit on F^2	1.082	
Final R indices [I>2sigma(I)]	R1 = 0.0315, wR2 = 0.0609	
R indices (all data)	R1 = 0.0435, wR2 = 0.0674	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.620 and -1.292 $e.Å^{-3}$	

Table S.I.12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	110(3)	6559(2)	2268(4)	14(1)
C(2)	-972(3)	6279(3)	2518(4)	20(1)
C(3)	-1640(3)	6990(3)	3018(4)	22(1)
C(4)	-1257(3)	7955(3)	3250(4)	21(1)
C(5)	-184(3)	8221(3)	2971(4)	18(1)
C(6)	525(3)	7516(2)	2494(4)	15(1)
C(7)	1667(3)	7723(3)	2224(4)	19(1)
C(8)	2281(3)	7014(3)	1718(4)	18(1)
C(9)	1821(2)	6032(2)	1441(4)	14(1)
C(10)	6184(3)	4834(2)	3089(4)	14(1)
C(11)	6883(3)	4700(3)	4860(4)	19(1)
C(12)	4542(3)	3123(2)	-77(4)	12(1)
C(13)	4297(3)	2045(2)	-132(4)	21(1)
O(1)	755(2)	5835(2)	1762(3)	15(1)
O(2)	2288(2)	5334(2)	960(3)	17(1)
O(3)	5072(2)	5025(2)	2752(2)	14(1)
O(4)	3806(2)	3686(2)	310(3)	14(1)
O(5)	3219(2)	5252(2)	-2062(2)	14(1)
O(6)	4507(2)	6602(2)	411(3)	15(1)
Rh(1)	4099(1)	5150(1)	364(1)	10(1)

Table S.I.13. Bond lengths [Å] and angles [°] for compound **4**.

C(1)-O(1)	1.384(4)
C(1)-C(6)	1.387(4)
C(1)-C(2)	1.389(4)
C(2)-C(3)	1.386(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.388(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.384(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.403(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.439(4)
C(7)-C(8)	1.347(5)
C(7)-H(7)	0.9500
C(8)-C(9)	1.439(5)
C(8)-H(8)	0.9500
C(9)-O(2)	1.225(4)
C(9)-O(1)	1.371(3)
C(10)-O(3)	1.266(4)
C(10)-O(5)#1	1.272(4)
C(10)-C(11)	1.506(4)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-O(4)	1.264(4)
C(12)-O(6)#1	1.275(4)
C(12)-C(13)	1.499(4)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
O(2)-Rh(1)	2.318(2)
O(3)-Rh(1)	2.032(2)
O(4)-Rh(1)	2.027(2)
O(5)-C(10)#1	1.272(4)

O(5)-Rh(1)	2.032(2)
O(6)-C(12)#1	1.275(4)
O(6)-Rh(1)	2.037(2)
Rh(1)-Rh(1)#1	2.3863(6)

O(1)-C(1)-C(6)	121.2(3)
O(1)-C(1)-C(2)	116.6(3)
C(6)-C(1)-C(2)	122.2(3)
C(3)-C(2)-C(1)	117.9(3)
C(3)-C(2)-H(2)	121.1
C(1)-C(2)-H(2)	121.1
C(2)-C(3)-C(4)	121.7(3)
C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2
C(5)-C(4)-C(3)	119.4(3)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	120.3(3)
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.8
C(1)-C(6)-C(5)	118.5(3)
C(1)-C(6)-C(7)	117.5(3)
C(5)-C(6)-C(7)	124.0(3)
C(8)-C(7)-C(6)	120.7(3)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	121.1(3)
C(7)-C(8)-H(8)	119.4
C(9)-C(8)-H(8)	119.4
O(2)-C(9)-O(1)	115.4(3)
O(2)-C(9)-C(8)	127.0(3)
O(1)-C(9)-C(8)	117.6(3)
O(3)-C(10)-O(5)#1	126.0(3)
O(3)-C(10)-C(11)	118.0(3)
O(5)#1-C(10)-C(11)	116.1(3)
C(10)-C(11)-H(11A)	109.5

C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(4)-C(12)-O(6)#1	125.2(3)
O(4)-C(12)-C(13)	118.0(3)
O(6)#1-C(12)-C(13)	116.8(3)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(9)-O(1)-C(1)	121.7(3)
C(9)-O(2)-Rh(1)	132.6(2)
C(10)-O(3)-Rh(1)	118.56(19)
C(12)-O(4)-Rh(1)	118.92(19)
C(10)#1-O(5)-Rh(1)	118.95(19)
C(12)#1-O(6)-Rh(1)	119.59(19)
O(4)-Rh(1)-O(3)	88.87(9)
O(4)-Rh(1)-O(5)	90.74(9)
O(3)-Rh(1)-O(5)	176.45(8)
O(4)-Rh(1)-O(6)	176.17(8)
O(3)-Rh(1)-O(6)	90.22(9)
O(5)-Rh(1)-O(6)	89.94(9)
O(4)-Rh(1)-O(2)	87.39(8)
O(3)-Rh(1)-O(2)	93.65(8)
O(5)-Rh(1)-O(2)	89.86(8)
O(6)-Rh(1)-O(2)	96.37(8)
O(4)-Rh(1)-Rh(1)#1	88.79(6)
O(3)-Rh(1)-Rh(1)#1	88.50(6)
O(5)-Rh(1)-Rh(1)#1	87.97(6)
O(6)-Rh(1)-Rh(1)#1	87.47(6)
O(2)-Rh(1)-Rh(1)#1	175.58(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

Table S.I.14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	13(2)	14(2)	14(2)	-2(1)	5(1)	1(1)
C(2)	18(2)	19(2)	25(2)	-2(2)	10(1)	-2(1)
C(3)	14(2)	30(2)	24(2)	-3(2)	9(1)	-1(1)
C(4)	20(2)	22(2)	23(2)	-8(2)	9(1)	5(1)
C(5)	20(2)	14(2)	19(2)	-5(1)	4(1)	2(1)
C(6)	15(2)	13(2)	16(2)	-3(1)	4(1)	-1(1)
C(7)	21(2)	13(2)	24(2)	-1(1)	8(1)	-3(1)
C(8)	14(2)	18(2)	23(2)	2(2)	7(1)	-5(1)
C(9)	11(1)	19(2)	12(2)	4(1)	3(1)	1(1)
C(10)	20(2)	9(2)	16(2)	0(1)	6(1)	1(1)
C(11)	23(2)	17(2)	16(2)	2(1)	4(1)	4(1)
C(12)	16(2)	11(2)	11(2)	2(1)	4(1)	0(1)
C(13)	22(2)	11(2)	32(2)	0(2)	15(1)	0(1)
O(1)	15(1)	13(1)	20(1)	-2(1)	10(1)	1(1)
O(2)	13(1)	17(1)	22(1)	-2(1)	9(1)	1(1)
O(3)	13(1)	16(1)	14(1)	1(1)	6(1)	2(1)
O(4)	17(1)	8(1)	20(1)	0(1)	10(1)	1(1)
O(5)	12(1)	16(1)	12(1)	1(1)	3(1)	2(1)
O(6)	14(1)	8(1)	26(1)	1(1)	10(1)	-1(1)
Rh(1)	10(1)	8(1)	13(1)	1(1)	6(1)	1(1)

Table S.I.15. Hydrogen bonds for compound **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...O(5)#2	0.95	2.53	3.277(4)	135.5
C(8)-H(8)...O(6)	0.95	2.33	3.151(4)	144.5
C(11)-H(11A)...O(3)#3	0.98	2.52	3.489(4)	168.6
C(13)-H(13A)...O(3)#4	0.98	2.61	3.379(4)	135.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x,-y+1,-z #3 -x+1,-y+1,-z+1

#4 -x+1,y-1/2,-z+1/2

Computational Methodology

Our theoretical calculations were done using Gaussian09 series of programs.[1] We have optimized the geometries at gas-phase with no constraints nor model systems but the real ligands for each complex at the DFT level of theory with the Berny algorithm. We have chosen the pure local functional of Truhlar and Zhao M06-L [2] in conjunction with a mix of triple-ζ quality basis sets: the LANL08 relativistic pseudopotential [3] for Rh atoms and 6-311G for all of the rest of atoms. We also calculated the harmonic frequencies after each geometry optimization in order to check all of them were positive (ensuring us that we found local minima on the potential energy surface) and for obtaining thermal and entropic corrections to the electronic energy at 298K.

For the report of bond energies, we also have calculated the Basis Set Superposition Error (BSSE) by using the counterpoise correction (CP) proposed, first by Boys and Bernardi,[4] already implemented in Gaussian. In this regard, considering a supermolecule AB, made up of two interacting systems A and B, we can write the dissociation energy as

$$E_{dis}(AB) = E_{AB}^{AB}(AB) - E_{A}^{A}(A) - E_{B}^{B}(B) \quad (1)$$

where $E_{Y}^{Z}(X)$ represents the energy of the system X at the geometry Y with the basis set Z. When a complete basis set is used, Ec. (1) is exact itself. However, for the basis sets we have chosen, our bonding energies contain a BSSE that is defined as

$$\delta_{AB}^{BSSE} = E_{AB}^{A}(A) - E_{AB}^{AB}(A) + E_{AB}^{B}(B) - E_{AB}^{AB}(B) \quad (2)$$

which depends on the basis set and the geometry of AB. So, we have reported BSSE-corrected bonding energies with the CP procedure by using the following equation:

$$E_{dis}^{CP}(AB) = E_{dis}(AB) + \delta_{AB}^{BSSE} \quad (3)$$

On the other hand, the dissociation energy can be decomposed into two terms: the bonding energy, E_{bond}, and deformation energy, E_{def}. The second one can be understood as the energy necessary to deform A and B from their geometries when isolated to the geometry they adopt within the supermolecule AB. Thus, we can write:

$$E_{dis}(AB) = E_{bond} + E_{def} \quad [\text{or } E_{dis}^{CP}(AB) = E_{bond}^{CP} + E_{def}] \quad (4)$$

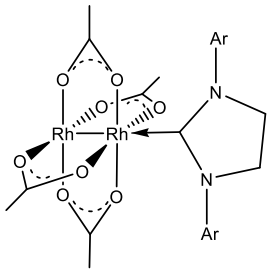
where

$$E_{bond} = E_{AB}^{AB}(AB) - E_{AB}^{A}(A) - E_{AB}^{A}(B)$$

and

$$E_{def} = E_{AB}^{A}(A) - E_{A}^{A}(A) - E_{AB}^{B}(B) - E_{B}^{B}(B)$$

Therefore, our reported dissociation and bonding energies are BSSE-corrected by using Eqs. (3) and (4).



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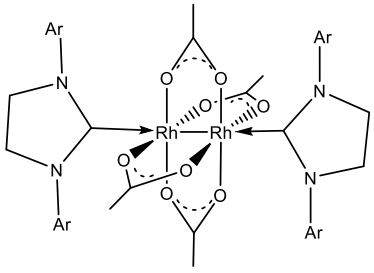

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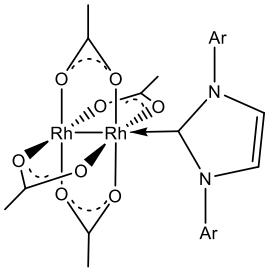

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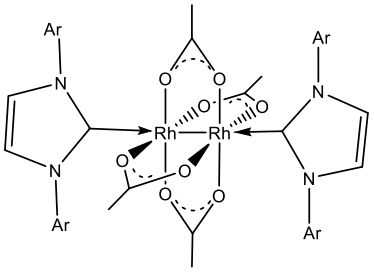

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Table S.I.16. Interaction energies (in kcal·mol^{-1}) for the complexes [$Rh_2(OAc)_4(L)$], L = IDip, **5'**; L = SIDip, **6'**, and [$Rh_2(OAc)_4(L)_2$], L = IDip, **5**; L = SIDip, **6**, calculated at the M06-L/(6-311G,LANL08) level.[a] (IDip = 1,3-bis[diisopropylphenyl]imidazol-2-ylidene and SIDip = 1,3-bis[diisopropylphenyl]-4,5-dihydroimidazol-2-ylidene)

Complex	ΔH^0_R	ΔG^0_R	E_{Dissoc}	E_{Bond}	E_{Def}
5'	-51.35	-30.86	-45.53	-55.73	10.20
5	-35.92	-18.82	-23.36	-30.13	6.77
6'	-53.64	-31.54	-48.00	-56.22	8.22
6	-36.24	-19.81	-22.22	-30.58	8.36

[a] These energies are BSSE corrected by means of the counterpoise method.

Tabla S.I.17. Cartesian coordinates (x y z) of all of the studied compounds calculated at the M06-L/(6-311G,LANL208) level.

Binuclear Rhodium Acetate Complex
E (scf) = -1133.07366441 a.u.
All of the frequencies are positive

Rh	0.000000	0.000000	1.205690
Rh	0.000000	0.000000	-1.205690
O	-2.081981	-0.004191	1.146415
O	-2.081286	-0.003800	-1.149584
C	-2.683210	0.000000	-0.002152
C	-4.173256	0.030446	0.002479
H	-4.520378	1.022791	0.296121
H	-4.562176	-0.198417	-0.985635
H	-4.562078	-0.676725	0.733181
O	-0.003800	2.081286	1.149584
O	-0.004191	2.081981	-1.146415
O	2.081981	0.004191	1.146415
O	2.081286	0.003800	-1.149584
O	0.004191	-2.081981	-1.146415
O	0.003800	-2.081286	1.149584
C	0.000000	-2.683210	0.002152
C	2.683210	0.000000	-0.002152
C	0.000000	2.683210	0.002152
C	0.030446	4.173256	-0.002479
H	-0.198417	4.562176	0.985635
H	1.022791	4.520378	-0.296121
H	-0.676725	4.562078	-0.733181
C	4.173256	-0.030446	0.002479
H	4.520378	-1.022791	0.296121
H	4.562176	0.198417	-0.985635
H	4.562078	0.676725	0.733181
C	-0.030446	-4.173256	-0.002479
H	-1.022791	-4.520378	-0.296121
H	0.676725	-4.562078	-0.733181
H	0.198417	-4.562176	0.985635

Coumarin
E (scf) = -496.938125287 a.u.
All of the frequencies are positive

C	-1.983472	1.978854	0.000000
C	-0.596235	1.893259	0.000000
C	0.000000	0.634555	0.000000
C	-0.768058	-0.546354	0.000000
C	-2.170610	-0.429539	0.000000
C	-2.774101	0.818999	0.000000
H	-2.456564	2.952898	0.000000
H	0.034130	2.771247	0.000000
C	-0.068226	-1.799159	0.000000
H	-2.770436	-1.332569	0.000000
H	-3.853021	0.900492	0.000000
C	1.286735	-1.848081	0.000000
C	2.102358	-0.657395	0.000000
H	-0.649068	-2.715385	0.000000
H	1.829672	-2.781870	0.000000
O	1.384237	0.584570	0.000000
O	3.327631	-0.592777	0.000000

Dip-aniline
E (scf) = -523.399856281 a.u.
All of the frequencies are positive

C	1.197093	1.628589	0.106695
C	-0.000083	2.332710	-0.000020
C	-1.197191	1.628604	-0.106737

NH_2-coumarin
E (scf) = -552.285319187 a. u.
All of the frequencies are positive

C	2.103676	-1.266245	-0.000051
C	0.767724	-1.635473	-0.000062
C	-0.215674	-0.650373	-0.000019

C	-1.226398	0.232569	-0.107901	C	0.128725	0.713422	0.000030
C	-0.000030	-0.470998	0.000053	C	1.486687	1.072160	0.000026
C	1.226396	0.232606	0.107893	C	2.488750	0.096027	-0.000006
H	2.128342	2.175190	0.194666	H	2.870943	-2.032254	-0.000065
H	-0.000025	3.415628	-0.000037	H	0.471304	-2.675185	-0.000096
H	-2.128506	2.175083	-0.194778	C	-0.945210	1.667151	0.000068
N	0.000086	-1.859650	0.000257	H	1.752575	2.123996	0.000057
H	-0.851826	-2.380217	-0.061384	C	-2.240774	1.265960	0.000061
H	0.852223	-2.379973	0.060793	C	-2.621385	-0.126484	0.000019
C	-2.532399	-0.539883	-0.184419	H	-0.699399	2.723903	0.000096
H	-2.373966	-1.403144	-0.848943	H	-3.060037	1.970118	0.000085
C	-3.688887	0.258945	-0.786848	O	-1.544976	-1.060012	-0.000026
H	-3.421008	0.687537	-1.754465	O	-3.764551	-0.581587	-0.000034
H	-4.560182	-0.384142	-0.928793	N	3.824571	0.438690	0.000041
H	-3.994828	1.076497	-0.129194	H	4.114658	1.397048	-0.000005
C	-2.931407	-1.073748	1.204169	H	4.539052	-0.262524	-0.000263
H	-3.818380	-1.709918	1.143906				
H	-2.127953	-1.647795	1.670257				
H	-3.161146	-0.237613	1.869488				
C	2.532431	-0.539823	0.184493				
H	2.374127	-1.402892	0.849269				
C	3.688920	0.259226	0.786559				
H	3.421293	0.687668	1.754310				
H	4.560486	-0.383582	0.928117				
H	3.994318	1.076927	0.128833				
C	2.931391	-1.074023	-1.204040				
H	3.818385	-1.710156	-1.143676				
H	2.127955	-1.648185	-1.670022				
H	3.161077	-0.238018	-1.869526				

Mes-NH_2

E (scf) = -405.488723497 a.u.

All of the frequencies are positive

C	-0.377878	1.223225	-0.000134
C	1.016118	1.193330	-0.001552
C	1.740065	-0.005075	-0.001791
C	1.011403	-1.197599	-0.001716
C	-0.384859	-1.222224	-0.000159
C	-1.087076	0.001102	0.000878
H	1.552321	2.138921	-0.002738
H	1.544631	-2.144606	-0.003037
N	-2.473962	0.005389	0.001878
H	-2.990000	0.862735	0.002142
H	-2.994550	-0.849261	0.002247
C	-1.132184	2.520107	-0.000605

Rh_coumarin (1)

E (scf) = -1630.04264650 a.u.

All of the frequencies are positive

Rh	2.780874	0.462439	0.377248
Rh	0.554656	-0.316110	-0.226956
O	1.981236	1.049462	2.216327
O	-0.122482	0.320811	1.648788
C	0.732594	0.844870	2.474417
C	0.236462	1.210486	3.833726
H	0.340324	0.352933	4.502090
H	-0.817041	1.478264	3.798281
H	0.824084	2.027593	4.244965
O	3.171384	-1.421368	1.160118
O	1.074999	-2.165940	0.577549
O	3.451708	-0.172191	-1.488276

H	-1.778579	2.619325	-0.880987	O	1.346008	-0.891168	-2.070255
H	-1.777157	2.620775	0.880649	O	0.162721	1.604117	-0.985899
H	-0.452138	3.371850	-0.001827	O	2.282719	2.309876	-0.452727
C	-1.142975	-2.516773	-0.000533	C	1.104794	2.498760	-0.945078
H	-1.788090	-2.616000	0.880858	C	2.603321	-0.696409	-2.315164
H	-1.789789	-2.614557	-0.880841	C	2.256334	-2.335037	1.082628
H	-0.465275	-3.370435	-0.001843	C	2.591994	-3.697931	1.587933
C	3.243054	-0.003936	0.002341	H	3.438157	-3.653496	2.268257
H	3.648893	0.455524	0.908972	H	2.857101	-4.343374	0.748061
H	3.640022	-1.019101	-0.052749	H	1.729707	-4.142434	2.080837
H	3.653429	0.554161	-0.844363	C	3.103243	-1.082859	-3.667041
				H	2.967840	-0.249662	-4.360083
				H	2.539341	-1.929568	-4.051161
				H	4.163980	-1.317848	-3.626929
				C	0.793206	3.854693	-1.487067
				H	0.627978	4.552974	-0.664073
				H	-0.099151	3.824647	-2.106143
				H	1.636786	4.230631	-2.063346
				C	-7.350147	-1.115965	-0.266709
				C	-6.070883	-1.616160	-0.483002
				C	-4.986421	-0.759404	-0.329658
				C	-5.144744	0.590427	0.037135
				C	-6.452189	1.068298	0.248520
				C	-7.542921	0.225827	0.098309
				H	-8.204344	-1.770880	-0.381893
				H	-5.893601	-2.644407	-0.765333
				C	-3.962171	1.391149	0.169092
				H	-6.589463	2.106023	0.530695
				H	-8.544421	0.600925	0.263021
				C	-2.728887	0.867690	-0.052103
				C	-2.562444	-0.506112	-0.430656
				H	-4.070408	2.433369	0.448793
				H	-1.820386	1.444886	0.025525
				O	-3.720350	-1.289570	-0.555381
				O	-1.491965	-1.098942	-0.673542

Rh_coumarin (2)
E (scf) = -2127.00113733 a.u.
All of the frequencies are positive

Rh	-1.130028	0.408940	-0.224528
Rh	1.131642	-0.410260	0.226441
O	-0.338292	1.372456	-1.906558
O	1.789708	0.603961	-1.478966
C	0.919579	1.259944	-2.184413
C	1.405838	1.925246	-3.424743

Rh_dip_aniline (1)
E (scf) = -1656.52003078 a.u.
All of the frequencies are positive

Rh	2.521376	-0.082501	0.770873
Rh	0.379999	0.064656	-0.403466
O	2.533307	-2.123409	0.288112
O	0.577708	-1.954107	-0.909651
C	1.592989	-2.619367	-0.444028
C	1.689288	-4.063614	-0.812089

H	1.109383	1.298768	-4.318062	H	2.493878	-4.190010	-1.596853
H	2.517946	2.020558	-3.402488	H	0.711638	-4.420039	-1.219271
H	0.918038	2.922466	-3.538110	H	1.995329	-4.661806	0.087771
O	-1.470528	-1.322796	-1.344883	O	3.426455	0.350878	-1.063150
O	0.658850	-2.086297	-0.939709	O	1.410880	0.570139	-2.151406
O	-1.788147	-0.618397	1.467873	O	2.356118	1.948991	1.181369
O	0.339959	-1.347790	1.921478	O	0.308331	2.087619	0.146887
O	1.472223	1.334466	1.333697	O	-0.547981	-0.448151	1.390083
O	-0.670189	2.071989	0.954709	O	1.453619	-0.505504	2.520895
C	0.511720	2.193867	1.466932	C	0.167670	-0.620828	2.459129
C	-0.917964	-1.261268	2.186327	C	1.303627	2.594012	0.810713
C	-0.510116	-2.195189	-1.465012	C	2.710368	0.603239	-2.108159
C	-0.802885	-3.434707	-2.245869	C	3.425427	0.989058	-3.361092
H	-1.573993	-3.244630	-2.988612	H	4.411453	0.531540	-3.388978
H	-1.162456	-4.216990	-1.573487	H	3.559267	2.072674	-3.388179
H	0.102257	-3.801926	-2.723847	H	2.848544	0.700812	-4.236578
C	-1.417082	-1.913671	3.439528	C	1.196697	4.033537	1.198239
H	-1.635024	-1.113662	4.204109	H	0.589383	4.130413	2.100923
H	-0.646359	-2.608463	3.835614	H	0.706452	4.607662	0.410860
H	-2.374864	-2.446365	3.224693	H	2.181476	4.444040	1.405414
C	0.804502	3.433449	2.247681	C	-0.563478	-1.005871	3.702537
H	1.163612	4.215833	1.575169	H	-0.327806	-2.043815	3.964988
H	1.575938	3.243547	2.990127	H	-1.636371	-0.913106	3.552192
H	-0.100544	3.800446	2.726011	H	-0.245730	-0.387380	4.537431
C	9.106120	-0.946547	-0.069261	C	-4.287333	-1.191004	0.633742
C	7.852182	-1.522165	0.104148	C	-4.841753	-0.003079	1.084579
C	6.735580	-0.693099	0.142690	C	-4.319345	1.213746	0.645327
C	6.838919	0.704907	0.007482	C	-3.240177	1.257897	-0.240583
C	8.121193	1.259038	-0.167087	C	-2.702770	0.034210	-0.691836
C	9.242801	0.443971	-0.202610	C	-3.208408	-1.203864	-0.255435
H	9.983184	-1.580129	-0.101793	H	-4.695872	-2.135826	0.970076
H	7.717583	-2.589651	0.208491	H	-5.678560	-0.015450	1.772588
C	5.628883	1.474420	0.067849	H	-4.750523	2.142921	1.002786
H	8.215855	2.334344	-0.267330	N	-1.551684	0.065906	-1.552927
H	10.224265	0.878971	-0.344300	H	-1.497306	0.885326	-2.147694
C	4.421489	0.876948	0.236223	H	-1.436390	-0.772032	-2.114927
C	4.305244	-0.549388	0.366914	C	-2.703548	2.593397	-0.725728
H	5.696845	2.553076	-0.021631	H	-1.665659	2.467473	-1.041735
H	3.492926	1.425219	0.294013	C	-2.654407	3.649779	0.380948
O	5.498432	-1.301152	0.314586	H	-2.107274	3.272498	1.246198
O	3.263952	-1.209760	0.522344	H	-2.145270	4.547153	0.021471
C	-9.104572	0.944917	0.069693	H	-3.653324	3.949747	0.707900
C	-7.850627	1.520569	-0.103547	C	-3.526874	3.097580	-1.924625
C	-6.733985	0.691545	-0.141791	H	-3.127442	4.038891	-2.310171

C	-6.837285	-0.706460	-0.019310	H	-3.534683	2.373156	-2.744051
C	-8.119570	-1.260627	0.155077	H	-4.566790	3.266708	-1.631454
C	-9.241219	-0.445593	0.203164	C	-2.635088	-2.542107	-0.701579
H	-9.981670	1.578463	0.102002	H	-1.737461	-2.381833	-1.300381
H	-7.716049	2.588050	-0.207975	C	-3.651117	-3.301938	-1.567290
C	-5.627202	-1.475922	-0.079334	H	-3.953340	-2.719465	-2.440972
H	-8.214205	-2.335927	0.255423	H	-3.231675	-4.248020	-1.918245
H	-10.222689	-0.880629	0.331854	H	-4.556523	-3.529188	-1.001147
C	-4.419800	-0.878413	-0.247512	C	-2.183629	-3.391539	0.490316
C	-4.303592	0.547921	-0.365464	H	-1.736720	-4.322702	0.146250
H	-5.695131	-2.554571	0.010249	H	-1.444136	-2.852079	1.085141
H	-3.491200	-1.426649	-0.305027	H	-3.024972	-3.647696	1.142216
O	-5.496825	1.299632	-0.313516				
O	-3.262293	1.208321	-0.520769				

Rh_dip_aniline (2)
E (scf) = -2179.95985822 a.u.
All of the frequencies are positive

Rh	1.130986	0.008045	-0.448696
Rh	-1.134752	-0.080556	0.494004
O	1.375807	1.808142	0.613354
O	-0.728966	1.690567	1.529495
C	0.424554	2.260145	1.362782
C	0.679879	3.531405	2.106409
H	1.390455	3.351254	2.915520
H	-0.242858	3.919340	2.529734
H	1.127807	4.271909	1.444886
O	1.755653	-1.075594	1.236553
O	-0.370847	-1.175092	2.107596
O	0.740455	-1.778438	-1.460746
O	-1.385442	-1.867120	-0.591319
O	-1.750937	1.031985	-1.174414
O	0.364309	1.084832	-2.074240
C	-0.902544	1.362618	-2.092285
C	-0.424006	-2.332672	-1.319011
C	0.901145	-1.424555	2.142753
C	1.417730	-2.201116	3.310936
H	2.452685	-1.933654	3.513804
H	1.383385	-3.270226	3.088705
H	0.801688	-2.022831	4.189247
C	-0.681540	-3.597093	-2.073346
H	-1.309064	-3.387313	-2.942056
H	-1.221144	-4.307692	-1.449122
H	0.252040	-4.034028	-2.418182
C	-1.418329	2.151212	-3.252681

Rh_NH_2_coumarin (1)
E (scf) = -1685.40176289 a.u.
All of the frequencies are positive

Rh	-2.414046	0.250921	1.189509
Rh	-0.815286	-0.108957	-0.614317
O	-1.991156	2.290041	1.031692
O	-0.434098	1.949215	-0.626387
C	-1.098740	2.706242	0.197951
C	-0.778403	4.164544	0.196365
H	0.117550	4.343426	0.794803
H	-0.575778	4.512690	-0.814608
H	-1.596482	4.731271	0.633052
O	-0.846886	0.030787	2.549229
O	0.650384	-0.371684	0.852444
O	-2.710712	-1.820842	1.195460
O	-1.241013	-2.148717	-0.543140
O	-2.357481	0.173880	-1.995551
O	-3.874679	0.458784	-0.291988
C	-3.555578	0.402520	-1.540771
C	-2.099562	-2.569551	0.341089
C	0.334781	-0.249345	2.106085
C	1.421076	-0.480117	3.103129
H	1.248093	0.111518	3.998973
H	1.433010	-1.532340	3.395435
H	2.391336	-0.243077	2.671061
C	-2.416470	-4.028246	0.337712
H	-3.171040	-4.237352	-0.423735
H	-1.531377	-4.611699	0.093027
H	-2.815017	-4.332203	1.301881
C	-4.631631	0.647095	-2.546323

H	-1.319919	3.219612	-3.046387	H	-4.633794	1.701387	-2.831412
H	-2.471902	1.935298	-3.417646	H	-4.456442	0.060934	-3.445785
H	-0.841902	1.931715	-4.148590	H	-5.605054	0.411321	-2.123851
C	5.657986	-1.215769	1.043515	C	2.410275	-1.800882	-1.473685
C	6.199070	-0.013712	1.494505	C	3.640500	-1.930389	-0.847867
C	5.752380	1.190920	0.956393	C	4.376573	-0.785768	-0.554899
C	4.776309	1.219546	-0.044005	C	3.900275	0.497655	-0.885128
C	4.264852	-0.010338	-0.504390	C	2.655876	0.608351	-1.525846
C	4.678978	-1.240235	0.047377	C	1.918803	-0.530902	-1.818015
H	5.991816	-2.148684	1.481195	H	1.802652	-2.677132	-1.667949
H	6.956031	-0.015202	2.269930	H	4.037587	-2.896333	-0.569223
H	6.161291	2.123672	1.324920	C	4.711472	1.623982	-0.519605
N	3.221661	-0.008240	-1.479273	H	2.247419	1.589811	-1.740048
H	3.193086	0.803480	-2.082765	C	5.896650	1.458634	0.118513
H	3.140700	-0.858294	-2.024187	C	6.415916	0.156316	0.461534
C	4.283284	2.525133	-0.645939	H	4.353256	2.619278	-0.760407
H	3.211643	2.413544	-0.848908	H	6.516689	2.295505	0.404629
C	4.409439	3.714818	0.305945	O	5.594059	-0.954460	0.087657
H	3.960052	3.490220	1.274619	O	7.473439	-0.095995	1.032666
H	3.902046	4.587530	-0.112144	N	0.596713	-0.407330	-2.334416
H	5.453254	3.995412	0.471959	H	0.432268	0.422358	-2.895097
C	5.014277	2.822381	-1.967286	H	0.242358	-1.235346	-2.801541
H	4.617808	3.723504	-2.441871				
H	4.930094	2.000157	-2.683626				
H	6.080690	2.978076	-1.782679				
C	4.060517	-2.538218	-0.442126				
H	2.998374	-2.345692	-0.632731				
C	4.718070	-3.001193	-1.755037				
H	4.706840	-2.225007	-2.525701				
H	4.209568	-3.880733	-2.158383				
H	5.765258	-3.264455	-1.582098				
C	4.110565	-3.661936	0.592716				
H	3.530496	-4.520047	0.244817				
H	3.693767	-3.331050	1.544745				
H	5.131716	-4.011638	0.768844				
C	-5.573119	1.418034	-1.021507				
C	-6.156121	0.274401	-1.562783				
C	-5.773751	-0.981436	-1.098214				
C	-4.823166	-1.120394	-0.082143				
C	-4.272431	0.051367	0.473340				
C	-4.618044	1.332076	-0.005826				
H	-5.854865	2.391994	-1.403515				
H	-6.894708	0.361363	-2.350853				
H	-6.213126	-1.869337	-1.536737				

N	-3.258814	-0.062150	1.474542
H	-3.284679	-0.914191	2.019755
H	-3.164474	0.743826	2.080814
C	-4.405867	-2.486922	0.435616
H	-3.345320	-2.433444	0.706389
C	-4.510664	-3.586486	-0.621821
H	-3.987800	-3.297819	-1.535237
H	-4.063239	-4.511423	-0.250162
H	-5.549896	-3.809443	-0.878040
C	-5.222100	-2.864284	1.684190
H	-4.883478	-3.814931	2.103650
H	-5.151905	-2.105448	2.468700
H	-6.280662	-2.964379	1.428910
C	-3.952027	2.565677	0.576760
H	-2.907986	2.308284	0.784633
C	-4.625353	2.985933	1.895787
H	-4.673863	2.167640	2.620032
H	-4.087745	3.814979	2.363047
H	-5.653387	3.309678	1.710614
C	-3.910832	3.748627	-0.390108
H	-3.292511	4.549445	0.023242
H	-3.486676	3.451827	-1.350350
H	-4.905041	4.167056	-0.569819

Rh_NH_2_coumarin (2)

E (scf) = -2237.71848391 a.u.

All of the frequencies are positive

Rh	-0.858124	-0.217541	0.852838
Rh	0.858137	0.512993	-0.726887
O	-0.431961	-2.194163	0.316676
O	1.172980	-1.514397	-1.185043
C	0.474336	-2.422399	-0.582360
C	0.706573	-3.845871	-0.973154
H	-0.035607	-4.149758	-1.714607
H	1.693403	-3.965561	-1.412696
H	0.597292	-4.500667	-0.111089
O	-2.218245	-0.081354	-0.739573
O	-0.600755	0.606982	-2.220689
O	-1.183312	1.807480	1.302344
O	0.440866	2.487628	-0.178617
O	2.222465	0.366343	0.859963
O	0.602899	-0.309101	2.344962
C	1.826963	-0.014645	2.031027
C	-0.474488	2.715672	0.711501
C	-1.822935	0.300844	-1.910068

Rh_Mes_NH_2 (1)

E (scf) = -1538.60639799 a.u.

One negative frequency at -7.56 cm^{-1}

Rh	0.254809	0.045227	-0.395331
Rh	2.356870	-0.073517	0.848574
O	-0.135002	1.847545	0.601049
O	1.847941	1.732163	1.754911
C	0.731569	2.300916	1.459790
C	0.417245	3.606511	2.110074
H	-0.684705	3.669167	2.329233
H	1.017910	3.711183	3.046893
H	0.686005	4.456250	1.409795
O	-0.634067	-1.011034	1.176655
O	1.336962	-1.092131	2.359692
O	0.744883	-1.746447	-1.333989
O	2.702790	-1.886955	-0.142709
O	3.224426	0.961682	-0.755093
O	1.239075	1.105034	-1.908078
C	2.512736	1.326097	-1.768020
C	1.861857	-2.333162	-1.006194
C	0.078195	-1.338489	2.211904

C	-2.866322	0.416329	-2.972921	C	-0.628235	-2.034543	3.328162
H	-3.534128	-0.443984	-2.942421	H	-1.472515	-2.604716	2.941997
H	-3.477907	1.303045	-2.793021	H	0.058506	-2.683025	3.867055
H	-2.409826	0.501808	-3.955190	H	-1.015352	-1.300568	4.033051
C	-0.705482	4.138370	1.105433	C	2.194811	-3.602256	-1.718086
H	0.044579	4.443583	1.838291	H	2.659592	-3.373599	-2.684508
H	-0.606177	4.793722	0.242459	H	2.902326	-4.190293	-1.138481
H	-1.687754	4.255977	1.555195	H	1.292975	-4.178032	-1.916126
C	2.872546	-0.143481	3.089973	C	3.210966	2.055500	-2.865999
H	3.471775	-1.038182	2.908148	H	3.783532	2.931651	-2.436721
H	3.551647	0.707553	3.055455	H	3.966619	1.373507	-3.346929
H	2.418681	-0.222273	4.074035	H	2.476390	2.405725	-3.623913
C	-4.003680	-2.153311	0.910309	C	-3.457563	1.253036	-0.879097
C	-5.133001	-2.162366	0.106501	C	-4.700555	1.220636	-0.244827
C	-5.943133	-1.031314	0.059459	C	-5.303818	0.014167	0.146183
C	-5.639282	0.117097	0.814200	C	-4.619566	-1.178831	-0.105289
C	-4.492451	0.107009	1.624597	C	-3.375113	-1.194691	-0.739107
C	-3.679331	-1.017805	1.675204	C	-2.813269	0.030201	-1.131668
H	-3.336929	-3.007403	0.923191	H	-5.207257	2.155967	-0.042532
H	-5.395733	-3.023206	-0.492332	H	-5.061621	-2.121511	0.203112
C	-6.524769	1.240242	0.701727	N	-1.523019	0.033494	-1.749381
H	-4.217978	1.000987	2.174256	H	-1.344153	0.846183	-2.338791
C	-7.616938	1.197467	-0.102096	H	-1.306295	-0.817156	-2.255950
C	-7.952998	0.035600	-0.889372	C	-2.806984	2.548330	-1.263829
H	-6.303525	2.132736	1.277427	H	-1.834755	2.663547	-0.775191
H	-8.294134	2.033825	-0.196186	H	-2.643765	2.621744	-2.346065
O	-7.059823	-1.073736	-0.764989	H	-3.429306	3.397010	-0.980642
O	-8.911472	-0.097905	-1.647362	C	-2.639356	-2.478997	-0.986458
N	-2.453737	-0.980547	2.384973	H	-2.488469	-2.678547	-2.054539
H	-2.400474	-0.308539	3.139893	H	-1.650883	-2.458099	-0.520944
H	-2.073259	-1.879657	2.653502	H	-3.185469	-3.326613	-0.578847
C	4.276569	2.074696	-0.816377	C	-6.654142	0.010139	0.804141
C	5.443718	1.837901	-0.106567	H	-7.452553	0.214313	0.083779
C	6.055376	0.591334	-0.201580	H	-6.872394	-0.955232	1.263234
C	5.511778	-0.429952	-1.003656	H	-6.727518	0.773499	1.582161
C	4.331660	-0.170344	-1.718439				
C	3.716330	1.071948	-1.628281				
H	3.765858	3.025995	-0.720443				
H	5.886631	2.594830	0.525813				
C	6.196966	-1.690448	-1.031032				
H	3.874455	-0.961992	-2.301306				
C	7.330817	-1.890117	-0.314151				
C	7.915509	-0.860816	0.511547				
H	5.786383	-2.488480	-1.640786				

H	7.858231	-2.832860	-0.323475
O	7.219390	0.387300	0.528614
O	8.934612	-0.944818	1.193520
N	2.459038	1.287532	-2.244861
H	2.189994	2.255908	-2.367186
H	2.269668	0.736428	-3.072482

Rh_Mes_NH_2 (2)

E (scf) = -1944.13382732 a.u.

All of the frequencies are positive

Rh	-0.574171	1.085715	-0.006900
Rh	0.574171	-1.085715	-0.006900
O	0.784366	1.657010	-1.504953
O	1.868708	-0.368995	-1.486608
C	1.697341	0.841180	-1.919766
C	2.619235	1.338488	-2.985885
H	3.095327	2.264647	-2.663514
H	3.377873	0.595940	-3.216119
H	2.053251	1.568566	-3.889889
O	0.791435	1.665845	1.477758
O	1.858035	-0.369554	1.483595
O	-1.858035	0.369554	1.483595
O	-0.791435	-1.665845	1.477758
O	-0.784366	-1.657010	-1.504953
O	-1.868708	0.368995	-1.486608
C	-1.697341	-0.841180	-1.919766
C	-1.698609	-0.849101	1.900154
C	1.698609	0.849101	1.900154
C	2.652002	1.349929	2.936353
H	2.307249	2.296661	3.343427
H	2.765483	0.617165	3.734273
H	3.637238	1.498488	2.490664
C	-2.652002	-1.349929	2.936353
H	-3.637238	-1.498488	2.490664
H	-2.307249	-2.296661	3.343427
H	-2.765483	-0.617165	3.734273
C	-2.619235	-1.338488	-2.985885
H	-2.053251	-1.568566	-3.889889
H	-3.095327	-2.264647	-2.663514
H	-3.377873	-0.595940	-3.216119
C	0.696554	-4.776202	1.240015
C	-0.114959	-5.913756	1.220176
C	-0.535876	-6.505225	0.025596
C	-0.119228	-5.923546	-1.178528
C	0.690356	-4.787909	-1.210919

carbene1

E (scf) = -1161.04750425 a.u.

All of the frequencies are positive

C	0.000000	0.000000	0.264262
C	0.274672	-0.709165	-2.022793
C	-0.274672	0.709165	-2.022793
H	1.315647	-0.764515	-2.364032
H	-0.312804	-1.409538	-2.618624
H	0.312804	1.409538	-2.618624
H	-1.315647	0.764515	-2.364032
N	-0.207823	1.059864	-0.570039
N	0.207823	-1.059864	-0.570039
C	-0.585989	2.372769	-0.145650
C	-1.909536	2.617365	0.259884
C	0.386672	3.392931	-0.174717
C	-2.250652	3.924481	0.633273
C	0.000000	4.683546	0.197911
C	-1.310357	4.948444	0.593924
H	-3.262616	4.137229	0.959643
H	0.727335	5.486138	0.186813
H	-1.593818	5.954270	0.881310
C	0.585989	-2.372769	-0.145650
C	1.909536	-2.617365	0.259884
C	-0.386672	-3.392931	-0.174717
C	2.250652	-3.924481	0.633273
C	0.000000	-4.683546	0.197911
C	1.310357	-4.948444	0.593924
H	3.262616	-4.137229	0.959643
H	-0.727335	-5.486138	0.186813
H	1.593818	-5.954270	0.881310
C	1.829949	3.055904	-0.506859
H	1.825408	2.255015	-1.255477
C	-2.928273	1.497364	0.368203
H	-2.535382	0.627355	-0.168298
C	2.928273	-1.497364	0.368203
H	2.535382	-0.627355	-0.168298
C	-1.829949	-3.055904	-0.506859
H	-1.825408	-2.255015	-1.255477

C	1.098394	-4.226226	0.012307	C	2.618971	4.231334	-1.084530
H	-0.429938	-6.344395	2.166421	H	2.111703	4.679816	-1.941762
H	-0.437534	-6.361351	-2.120677	H	2.775179	5.016217	-0.340047
N	1.868708	-3.029866	0.003920	H	3.606814	3.899343	-1.411037
H	2.418794	-2.864939	0.839333	C	2.522935	2.492478	0.745304
H	2.420911	-2.877957	-0.832525	H	2.576023	3.255732	1.526821
C	1.122873	-4.134175	2.527485	H	1.972781	1.637679	1.144617
H	2.210331	-4.170840	2.668751	H	3.542861	2.171564	0.514279
H	0.822251	-3.083113	2.561419	C	-4.279031	1.862196	-0.255030
H	0.674122	-4.639030	3.383309	H	-4.771562	2.671631	0.289709
C	1.110998	-4.154425	-2.504463	H	-4.169828	2.179936	-1.294730
H	0.800735	-3.106396	-2.547165	H	-4.951878	1.001294	-0.232449
H	2.198655	-4.182992	-2.645854	C	-3.087450	1.085699	1.839649
H	0.665985	-4.670822	-3.355239	H	-2.130061	0.758530	2.249575
C	-1.414429	-7.724751	0.026560	H	-3.449046	1.926312	2.439222
H	-2.376154	-7.530904	-0.457446	H	-3.803498	0.266241	1.940531
H	-0.953092	-8.557869	-0.511277	C	-2.618971	-4.231334	-1.084530
H	-1.622364	-8.064663	1.042341	H	-2.111703	-4.679816	-1.941762
C	-0.690356	4.787909	-1.210919	H	-2.775179	-5.016217	-0.340047
C	0.119228	5.923546	-1.178528	H	-3.606814	-3.899343	-1.411037
C	0.535876	6.505225	0.025596	C	-2.522935	-2.492478	0.745304
C	0.114959	5.913756	1.220176	H	-2.576023	-3.255732	1.526821
C	-0.696554	4.776202	1.240015	H	-1.972781	-1.637679	1.144617
C	-1.098394	4.226226	0.012307	H	-3.542861	-2.171564	0.514279
H	0.437534	6.361351	-2.120677	C	4.279031	-1.862196	-0.255030
H	0.429938	6.344395	2.166421	H	4.771562	-2.671631	0.289709
N	-1.868708	3.029866	0.003920	H	4.169828	-2.179936	-1.294730
H	-2.420911	2.877957	-0.832525	H	4.951878	-1.001294	-0.232449
H	-2.418794	2.864939	0.839333	C	3.087450	-1.085699	1.839649
C	-1.110998	4.154425	-2.504463	H	2.130061	-0.758530	2.249575
H	-0.800735	3.106396	-2.547165	H	3.449046	-1.926312	2.439222
H	-2.198655	4.182992	-2.645854	H	3.803498	-0.266241	1.940531
H	-0.665985	4.670822	-3.355239				
C	-1.122873	4.134175	2.527485				
H	-2.210331	4.170840	2.668751				
H	-0.822251	3.083113	2.561419				
H	-0.674122	4.639030	3.383309				
C	1.414429	7.724751	0.026560				
H	0.953092	8.557869	-0.511277				
H	1.622364	8.064663	1.042341				
H	2.376154	7.530904	-0.457446				

Rh_carbene1 (1)

E (scf) = -2294.20602459 a.u.

All of the frequencies are positive

Rh_carbene1 (2)

E (scf) = -3455.31475607 a.u.

All of the frequencies are positive

Rh	-0.260696	3.165847	-0.096913	Rh	1.261988	-0.051030	-0.066674
Rh	-0.081266	0.680402	0.051967	Rh	-1.273244	0.022753	0.039162
O	-0.247189	3.208957	1.994650	O	1.241123	-0.078836	2.045583
O	-0.053812	0.919403	2.143020	O	-1.056125	-0.002067	2.137893
C	-0.153160	2.110154	2.659396	C	0.116087	-0.054078	2.682373
C	-0.186450	2.201995	4.151446	C	0.174906	-0.080464	4.178346
H	-1.219730	2.138877	4.500170	H	-0.206624	0.858366	4.583113
H	0.370705	1.383778	4.601815	H	-0.454364	-0.881918	4.567571
H	0.216549	3.158136	4.476842	H	1.199276	-0.221743	4.513423
O	-2.330137	2.980488	-0.068098	O	1.202830	2.053293	-0.080862
O	-2.194003	0.693350	0.120466	O	-1.089216	2.109709	0.077110
O	-0.273190	2.940101	-2.174897	O	1.042574	-0.055921	-2.164375
O	-0.155889	0.643331	-2.054580	O	-1.253625	0.064235	-2.071681
O	1.992122	0.960171	0.007744	O	-1.214594	-2.082906	0.020153
O	1.827122	3.251782	-0.101922	O	1.080753	-2.138771	-0.084609
C	2.498915	2.153073	-0.041495	C	-0.082023	-2.703034	-0.039973
C	-0.240918	1.767172	-2.705858	C	-0.128730	0.014377	-2.708317
C	-2.854779	1.806465	0.050737	C	0.072715	2.674533	0.010851
C	-4.343244	1.710499	0.148963	C	0.111926	4.168538	0.044158
H	-4.805702	2.621642	-0.294722	H	1.141167	4.516904	0.033345
H	-4.703759	0.776234	-0.354121	H	-0.428709	4.579035	-0.811121
H	-4.643204	1.647651	1.235498	H	-0.396095	4.535455	0.938004
C	-0.305711	1.681297	-4.197185	C	-0.186972	0.030489	-4.204301
H	0.483002	2.289366	-4.640879	H	0.161465	-0.924638	-4.601191
H	-0.204087	0.650434	-4.525791	H	-1.205742	0.203484	-4.541288
H	-1.258167	2.080230	-4.549618	H	0.470269	0.806206	-4.598918
C	3.989437	2.239586	-0.027355	C	-0.117966	-4.196693	-0.034199
H	4.380354	1.790119	0.887296	H	-0.050922	-4.560565	0.995254
H	4.405053	1.665240	-0.857077	H	-1.057457	-4.551637	-0.453470
H	4.314376	3.275414	-0.094483	H	0.734643	-4.595571	-0.580695
C	0.113957	-1.424929	-0.020399	C	-3.495236	0.110421	-0.052510
C	1.032756	-3.586847	-0.407408	C	-5.753416	-0.530761	-0.516802
C	-0.480203	-3.673646	-0.537609	C	-5.656081	0.986540	-0.603213
H	1.567343	-3.919636	-1.296879	H	-6.116039	-0.996027	-1.435770
H	1.425716	-4.139189	0.447774	H	-6.385325	-0.876750	0.307925
H	-0.808319	-3.885979	-1.559000	H	-5.835513	1.366960	-1.612826
H	-0.938184	-4.406611	0.123159	H	-6.333525	1.509203	0.075451
N	-0.915173	-2.301164	-0.151813	N	-4.242124	1.241055	-0.204771
N	1.262866	-2.130865	-0.203201	N	-4.343065	-0.932825	-0.262866
C	-2.317873	-2.095265	0.061849	C	-3.841346	2.599159	0.012982
C	-2.793682	-1.956685	1.379260	C	-3.608720	3.045848	1.329437
C	-3.176916	-2.104880	-1.046854	C	-3.725120	3.456286	-1.091431
C	-4.177451	-1.916615	1.571888	C	-3.358866	4.407576	1.520885
C	-4.556808	-2.075181	-0.804370	C	-3.480013	4.814701	-0.851864

C	-5.054706	-2.001081	0.490720	C	-3.321941	5.292334	0.443652
H	-4.574246	-1.810258	2.573028	H	-3.179573	4.779563	2.522610
H	-5.245809	-2.088944	-1.646361	H	-3.394624	5.495560	-1.692818
H	-6.125141	-1.986078	0.659741	H	-3.138561	6.347066	0.615888
C	2.632419	-1.718638	-0.076995	C	-4.075829	-2.330638	-0.099208
C	3.375325	-1.483422	-1.246783	C	-3.868209	-3.119620	-1.244093
C	3.214996	-1.655296	1.200141	C	-4.095690	-2.887474	1.192339
C	4.742521	-1.221416	-1.115490	C	-3.733048	-4.501753	-1.077025
C	4.585419	-1.381203	1.283097	C	-3.938293	-4.273419	1.313484
C	5.347656	-1.179358	0.137571	C	-3.775756	-5.078348	0.189992
H	5.335761	-1.038678	-2.005511	H	-3.577741	-5.128820	-1.949222
H	5.056117	-1.329217	2.258994	H	-3.948785	-4.723210	2.300869
H	6.409058	-0.975169	0.221255	H	-3.668455	-6.151455	0.301933
C	-2.659149	-2.051610	-2.471873	C	-3.758321	2.939467	-2.519199
H	-1.566164	-1.986299	-2.434571	H	-3.895144	1.854007	-2.487162
C	-1.823960	-1.796301	2.538324	C	-3.582282	2.061576	2.485561
H	-0.974876	-1.222003	2.169990	H	-3.143589	1.134429	2.108347
C	2.731031	-1.467113	-2.621063	C	-3.735118	-2.511048	-2.627426
H	1.655811	-1.629632	-2.493911	H	-3.770043	-1.421997	-2.523443
C	2.413081	-1.850621	2.473016	C	-4.265740	-2.036345	2.437025
H	1.355073	-1.927502	2.205265	H	-4.266477	-0.986756	2.132085
C	-3.061391	-3.291671	-3.276069	C	-4.903961	3.560518	-3.328207
H	-2.720011	-4.218777	-2.800643	H	-5.874721	3.381611	-2.859131
H	-4.148984	-3.359479	-3.372564	H	-4.779363	4.643577	-3.415070
H	-2.641695	-3.256748	-4.284676	H	-4.934605	3.149496	-4.340428
C	-3.146818	-0.774087	-3.164338	C	-2.406739	3.191123	-3.204361
H	-4.235431	-0.765611	-3.264169	H	-2.193874	4.261466	-3.280149
H	-2.848638	0.108450	-2.597427	H	-1.600171	2.715691	-2.644632
H	-2.720405	-0.695755	-4.165818	H	-2.408524	2.780136	-4.217293
C	-1.304128	-3.150248	3.039944	C	-4.997792	1.745038	2.990621
H	-2.120928	-3.784751	3.385574	H	-5.503267	2.649873	3.341585
H	-0.767711	-3.694689	2.251908	H	-5.613843	1.299877	2.204203
H	-0.609088	-3.010656	3.873285	H	-4.959840	1.035469	3.821943
C	-2.408296	-0.981258	3.692326	C	-2.680486	2.509995	3.635468
H	-2.813115	-0.032988	3.332670	H	-1.675445	2.745050	3.272321
H	-3.204914	-1.514535	4.224065	H	-3.072504	3.386084	4.160862
H	-1.627096	-0.758766	4.418902	H	-2.591831	1.700828	4.364641
C	2.822281	-3.141653	3.197241	C	-5.598182	-2.333956	3.139197
H	2.683306	-4.024195	2.568005	H	-6.452573	-2.165668	2.478820
H	3.876727	-3.107521	3.485920	H	-5.639693	-3.375660	3.470453
H	2.228675	-3.279615	4.107229	H	-5.721775	-1.699734	4.020552
C	2.557920	-0.642400	3.407239	C	-3.089245	-2.219665	3.404597
H	3.576796	-0.561617	3.797262	H	-3.089513	-3.219894	3.848352
H	2.307824	0.282110	2.887108	H	-2.141961	-2.059791	2.890571

H	1.878485	-0.744024	4.261826	H	-3.154696	-1.491000	4.218510
C	3.294813	-2.575805	-3.520886	C	-4.876587	-2.956697	-3.552143
H	4.363138	-2.427645	-3.702272	H	-4.854846	-4.039583	-3.706079
H	3.175396	-3.565134	-3.072630	H	-5.856692	-2.706483	-3.138603
H	2.792684	-2.580667	-4.491485	H	-4.791080	-2.481361	-4.532515
C	2.903891	-0.094427	-3.284898	C	-2.373082	-2.861738	-3.244021
H	2.477108	0.69084	-2.660541	H	-1.564080	-2.547517	-2.584027
H	3.960204	0.133048	-3.455966	H	-2.280864	-3.938410	-3.416151
H	2.399769	-0.072375	-4.254232	H	-2.247789	-2.358753	-4.206286
				C	3.488977	-0.101603	0.053553
				C	5.735534	0.557421	0.551135
				C	5.653171	-0.960384	0.623491
				H	6.089133	1.019207	1.475161
				H	6.366492	0.917527	-0.268792
				H	5.823164	-1.347779	1.632035
				H	6.344218	-1.470514	-0.050947
				N	4.247261	-1.224851	0.203836
				N	4.321897	0.948820	0.292788
				C	3.866260	-2.586159	-0.027577
				C	3.657327	-3.027560	-1.349553
				C	3.752800	-3.453534	1.069792
				C	3.436749	-4.392661	-1.553640
				C	3.537952	-4.814649	0.817763
				C	3.405854	-5.286152	-0.483171
				H	3.276949	-4.760643	-2.560043
				H	3.454653	-5.502933	1.652714
				H	3.247376	-6.343289	-0.665067
				C	4.060880	2.349620	0.138286
				C	3.834905	3.129989	1.285882
				C	4.126455	2.921652	-1.144965
				C	3.727256	4.516144	1.130924
				C	3.999296	4.311545	-1.254817
				C	3.820077	5.107041	-0.126928
				H	3.556126	5.135886	2.005193
				H	4.043746	4.771322	-2.236613
				H	3.736696	6.183197	-0.228783
				C	3.759536	-2.946807	2.501560
				H	3.880513	-1.859234	2.480134
				C	3.628575	-2.037254	-2.500438
				H	3.173742	-1.117780	-2.123066
				C	3.659559	2.509485	2.658937
				H	3.699209	1.421621	2.546030
				C	4.286731	2.079724	-2.396166
				H	4.323775	1.029168	-2.096791

C	4.903550	-3.556549	3.321515
H	5.877473	-3.362683	2.865097
H	4.792252	-4.641504	3.402039
H	4.916544	-3.149854	4.335882
C	2.403089	-3.223877	3.167366
H	2.207401	-4.298108	3.234394
H	1.596473	-2.759695	2.598378
H	2.384890	-2.818252	4.182327
C	5.044620	-1.701329	-2.990889
H	5.562931	-2.598518	-3.342852
H	5.649317	-1.254501	-2.196618
H	5.006343	-0.987486	-3.818539
C	2.742766	-2.494470	-3.659180
H	1.744364	-2.760476	-3.300162
H	3.159478	-3.353838	-4.193201
H	2.634301	-1.679317	-4.378902
C	5.585078	2.408775	-3.143908
H	6.465209	2.256299	-2.514117
H	5.594307	3.450922	-3.475694
H	5.690443	1.778608	-4.030470
C	3.066637	2.242392	-3.313644
H	3.046170	3.237066	-3.769996
H	2.145418	2.095048	-2.750092
H	3.094165	1.499749	-4.116751
C	4.771526	2.947638	3.622321
H	4.742108	4.028469	3.788828
H	5.764107	2.704834	3.235149
H	4.658257	2.460371	4.593944
C	2.279173	2.855468	3.235978
H	1.489016	2.530173	2.558823
H	2.175141	3.933079	3.395408
H	2.132092	2.360426	4.199260

carbene2

E (scf) = -1159.84513690 a.u.

All of the frequencies are positive

C	0.000000	0.000000	0.295176
N	0.000000	1.070452	-0.591336
N	0.000000	-1.070452	-0.591336
C	0.026728	2.446835	-0.178121
C	-1.166910	3.191809	-0.236369
C	1.241638	2.998866	0.259691
C	-1.113129	4.536683	0.143717
C	1.242374	4.347280	0.640605
C	0.081382	5.110090	0.576370

Rh_carbene2 (1)

E (scf) = -2293.00798194 a.u.

All of the frequencies are positive

Rh	0.005226	0.676275	0.027497
Rh	-0.002058	3.167306	-0.038240
O	0.026230	0.828350	2.129228
O	0.014085	3.130590	2.053132
C	0.022805	2.007055	2.682912
C	-0.003271	2.054494	4.177531
H	0.525428	1.203095	4.601138
H	0.434209	2.985125	4.530704
H	-1.037205	2.014155	4.527380

H	-2.012648	5.138255	0.108375	O	2.108122	0.820638	0.020265
H	2.163358	4.798674	0.990732	O	2.078086	3.120879	-0.044517
H	0.102992	6.152938	0.870056	O	-0.029895	0.718950	-2.078261
C	-0.026728	-2.446835	-0.178121	O	-0.027592	3.022087	-2.124098
C	1.166910	-3.191809	-0.236369	O	-2.083047	3.106176	-0.027257
C	-1.241638	-2.998866	0.259691	O	-2.094119	0.806572	0.047900
C	1.113129	-4.536683	0.143717	C	-2.682167	1.966563	0.011795
C	-1.242374	-4.347280	0.640605	C	-0.053654	1.866099	-2.692306
C	-0.081382	-5.110090	0.576370	C	2.686038	1.985696	-0.004105
H	2.012648	-5.138255	0.108375	C	4.180126	1.994087	0.016414
H	-2.163358	-4.798674	0.990732	H	4.545770	1.497507	0.916904
H	-0.102992	-6.152938	0.870056	H	4.572848	1.431789	-0.832406
C	2.500231	2.160214	0.385402	H	4.550233	3.014976	-0.015414
H	2.365263	1.254145	-0.214705	C	-0.130252	1.829817	-4.185266
C	-2.476870	2.520487	-0.613721	H	-1.081664	2.250047	-4.515903
H	-2.261298	1.761545	-1.374054	H	0.660792	2.442982	-4.617011
C	2.476870	-2.520487	-0.613721	H	-0.046174	0.808632	-4.546897
H	2.261298	-1.761545	-1.374054	C	-4.176369	1.960235	0.018017
C	-2.500231	-2.160214	0.385402	H	-4.546549	1.490606	0.930936
H	-2.365263	-1.254145	-0.214705	H	-4.557009	2.975423	-0.050880
C	3.750266	2.879074	-0.130810	H	-4.554560	1.364350	-0.814156
H	3.620008	3.229965	-1.156854	C	-0.001097	-1.432136	-0.044500
H	4.007875	3.742833	0.487559	N	-1.084956	-2.282108	-0.135714
H	4.607510	2.201805	-0.110564	N	1.075678	-2.281075	-0.199849
C	2.680480	1.721318	1.847198	C	-2.480066	-1.956904	0.033360
H	2.786610	2.592585	2.500541	C	-3.295480	-1.899151	-1.102772
H	1.816839	1.143126	2.180587	C	-2.967214	-1.741504	1.334391
H	3.574912	1.103507	1.959949	C	-4.668910	-1.702551	-0.906060
C	-3.512820	3.481590	-1.197788	C	-4.343651	-1.546681	1.480004
H	-3.873279	4.189573	-0.447084	C	-5.191095	-1.547165	0.372710
H	-3.109711	4.055931	-2.034914	H	-5.327077	-1.660232	-1.767202
H	-4.381234	2.925250	-1.556478	H	-4.755859	-1.382239	2.468114
C	-3.047670	1.786201	0.612313	H	-6.256915	-1.402901	0.508838
H	-2.317557	1.091322	1.032132	C	2.473750	-1.950999	-0.078116
H	-3.318601	2.503217	1.392628	C	3.025577	-1.867354	1.209838
H	-3.945565	1.222685	0.342926	C	3.228327	-1.755801	-1.241621
C	-3.750266	-2.879074	-0.130810	C	4.404213	-1.654469	1.308526
H	-3.620008	-3.229965	-1.156854	C	4.606011	-1.554219	-1.093495
H	-4.007875	-3.742833	0.487559	C	5.192015	-1.517932	0.167770
H	-4.607510	-2.201805	-0.110564	H	4.862527	-1.590673	2.288644
C	-2.680480	-1.721318	1.847198	H	5.217823	-1.410961	-1.977818
H	-2.786610	-2.592585	2.500541	H	6.260798	-1.363966	0.264325
H	-1.816839	-1.143126	2.180587	C	-2.023278	-1.692851	2.522235
H	-3.574912	-1.103507	1.959949	H	-1.077795	-1.273126	2.170078

C	3.512820	-3.481590	-1.197788	C	-2.732476	-1.958372	-2.511111
H	3.873279	-4.189573	-0.447084	H	-1.645087	-2.057889	-2.444661
H	3.109711	-4.055931	-2.034914	C	2.168187	-1.997344	2.455481
H	4.381234	-2.925250	-1.556478	H	1.132206	-1.782054	2.177097
C	3.047670	-1.786201	0.612313	C	2.593569	-1.697549	-2.618293
H	2.317557	-1.091322	1.032132	H	1.506663	-1.730113	-2.496777
H	3.318601	-2.503217	1.392628	C	-1.744850	-3.098925	3.074742
H	3.945565	-1.222685	0.342926	H	-1.306309	-3.751353	2.315653
C	0.003016	0.677667	-1.937427	H	-2.666598	-3.568212	3.431454
C	-0.003016	-0.677667	-1.937427	H	-1.046227	-3.048016	3.914149
H	0.011591	1.390215	-2.743375	C	-2.508344	-0.759599	3.631401
H	-0.011591	-1.390215	-2.743375	H	-3.397176	-1.143867	4.140190
				H	-2.739039	0.232066	3.234534
				H	-1.723598	-0.644163	4.382823
				C	-3.275487	-3.159598	-3.294587
				H	-4.362620	-3.103285	-3.398714
				H	-3.040345	-4.104284	-2.798531
				H	-2.848040	-3.190828	-4.299559
				C	-3.023541	-0.642044	-3.246972
				H	-2.652225	0.208255	-2.673153
				H	-4.097329	-0.508461	-3.408369
				H	-2.535954	-0.633393	-4.225008
				C	3.021872	-2.888749	-3.485303
				H	2.751705	-3.841558	-3.023859
				H	4.104920	-2.891977	-3.638829
				H	2.546921	-2.843835	-4.468271
				C	2.926579	-0.367134	-3.306641
				H	3.998386	-0.275359	-3.504840
				H	2.616759	0.471974	-2.682572
				H	2.406642	-0.292978	-4.264466
				C	2.234627	-3.428638	3.009827
				H	3.261665	-3.688286	3.282729
				H	1.889211	-4.159863	2.275091
				H	1.613158	-3.530384	3.902564
				C	2.548463	-0.976066	3.530785
				H	2.565175	0.034701	3.118577
				H	3.527018	-1.187988	3.970691
				H	1.812995	-1.000313	4.339383
				C	-0.685843	-3.604441	-0.361400
				C	0.666660	-3.603881	-0.400101
				H	-1.408087	-4.394300	-0.458108
				H	1.382326	-4.393560	-0.537907

Rh_carbene2 (2)

E (scf) = -3452.91283052 a.u.

One negative frequency at -23.06 cm^{-1}

Rh	-1.270615	0.011879	0.006792
Rh	1.267035	-0.036742	-0.038336
O	-1.098428	0.023193	2.107358
O	1.199573	-0.054217	2.072585
C	0.058474	-0.053127	2.680103
C	0.071786	-0.157770	4.174037
H	-0.443625	-1.067570	4.488217
H	1.093626	-0.178256	4.543928
H	-0.460745	0.685090	4.616098
O	-1.190212	-2.093781	0.048149
O	1.108059	-2.129691	-0.003581
O	-1.209734	0.036555	-2.105171
O	1.086727	-0.075248	-2.137758
O	1.190711	2.065574	-0.094396
O	-1.106312	2.103637	-0.022735
C	0.051901	2.676705	-0.076821
C	-0.068201	0.014436	-2.711954
C	-0.050051	-2.703528	0.035062
C	-0.070754	-4.198234	0.041150
H	-1.000029	-4.561786	0.474733
H	-0.007206	-4.569006	-0.986098
H	0.793706	-4.584587	0.578932
C	-0.075954	0.101646	-4.206777
H	0.513548	0.961042	-4.531741
H	0.385763	-0.788025	-4.637416
H	-1.093023	0.196707	-4.578085
C	0.071870	4.171153	-0.096382
H	-0.038853	4.552014	0.923116
H	1.016686	4.532635	-0.495568
H	-0.769643	4.551517	-0.673651
C	3.495625	-0.046529	0.082731
N	4.319280	-1.151101	0.215822
N	4.365578	0.997993	0.347931
C	3.949164	-2.528018	0.018279
C	3.829893	-3.353435	1.144202
C	3.747644	-2.997862	-1.291027
C	3.601426	-4.718779	0.929742
C	3.512984	-4.366457	-1.454929
C	3.464487	-5.224939	-0.358118
H	3.515547	-5.382490	1.783812
H	3.357660	-4.762789	-2.451028
H	3.292931	-6.284883	-0.508917
C	4.078815	2.405973	0.238268

C	4.314698	3.030891	-0.996598
C	3.624256	3.102056	1.368518
C	4.101409	4.412684	-1.074946
C	3.448225	4.484641	1.247738
C	3.687563	5.135438	0.040243
H	4.266568	4.923797	-2.016475
H	3.109186	5.055411	2.104504
H	3.541854	6.207353	-0.034166
C	3.760563	-2.047244	-2.474510
H	3.389267	-1.080965	-2.123001
C	3.857579	-2.804232	2.559567
H	3.966377	-1.716920	2.505507
C	4.717170	2.239125	-2.228410
H	5.108325	1.270726	-1.900238
C	3.344217	2.390058	2.678265
H	3.217263	1.326107	2.463132
C	5.187842	-1.846332	-3.007684
H	5.858174	-1.471860	-2.229890
H	5.601325	-2.787784	-3.382038
H	5.194467	-1.124862	-3.829705
C	2.813852	-2.486337	-3.592065
H	3.162690	-3.389273	-4.102099
H	1.811963	-2.675265	-3.197138
H	2.738270	-1.693316	-4.339932
C	5.034205	-3.365974	3.366535
H	4.965181	-4.453780	3.457141
H	5.992327	-3.134489	2.895131
H	5.045818	-2.949008	4.376530
C	2.521272	-3.089571	3.260774
H	1.691167	-2.680734	2.682962
H	2.359823	-4.164260	3.386448
H	2.505756	-2.632920	4.253736
C	4.528434	2.550803	3.643869
H	5.453996	2.166936	3.208395
H	4.689331	3.604198	3.893089
H	4.345386	2.008483	4.575104
C	2.041756	2.863754	3.330242
H	2.085211	3.916556	3.623078
H	1.197286	2.728447	2.651629
H	1.843062	2.284169	4.234647
C	5.817981	2.924704	-3.042983
H	5.468938	3.859284	-3.489611
H	6.692008	3.154169	-2.429150
H	6.140118	2.276378	-3.861629

C	3.475328	1.963136	-3.090021
H	2.714444	1.422648	-2.526434
H	3.036790	2.903352	-3.440742
H	3.737190	1.364340	-3.967997
C	5.631046	-0.799948	0.556531
C	5.660133	0.550823	0.638525
H	6.394194	-1.544603	0.693747
H	6.457494	1.238958	0.853965
C	-3.488049	0.061883	-0.096363
N	-4.307427	1.171632	-0.213142
N	-4.369890	-0.977141	-0.336263
C	-3.926607	2.547426	-0.027909
C	-3.813863	3.364891	-1.160353
C	-3.711313	3.024501	1.276348
C	-3.575561	4.730246	-0.957184
C	-3.467114	4.392995	1.428846
C	-3.423509	5.243943	0.326079
H	-3.494754	5.388177	-1.816191
H	-3.302358	4.795605	2.420916
H	-3.245000	6.303892	0.468404
C	-4.089111	-2.383088	-0.202834
C	-4.257540	-2.969465	1.060669
C	-3.701940	-3.115505	-1.334305
C	-4.066108	-4.352535	1.165186
C	-3.540829	-4.497136	-1.186086
C	-3.728306	-5.112960	0.049283
H	-4.187075	-4.832426	2.130403
H	-3.254518	-5.093588	-2.044930
H	-3.598741	-6.185287	0.144203
C	-3.726954	2.085961	2.469896
H	-3.390046	1.104437	2.125147
C	-3.862060	2.806218	-2.571489
H	-3.982777	1.720766	-2.508197
C	-4.583950	-2.147397	2.294135
H	-4.764726	-1.115213	1.981617
C	-3.459524	-2.446195	-2.673418
H	-3.385730	-1.368565	-2.503740
C	-5.149616	1.935259	3.031741
H	-5.844135	1.564145	2.273814
H	-5.530148	2.895616	3.392974
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C	-2.748033	2.512003	3.565363
H	-3.057856	3.435520	4.063408
H	-1.745457	2.658851	3.154691

H	-2.690072	1.731521	4.327794
C	-5.040848	3.375708	-3.370049
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H	-5.996432	3.157737	-2.887222
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C	-2.530328	3.069946	-3.289169
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H	-2.354284	4.141746	-3.420080
H	-2.533800	2.610587	-4.280980
C	-4.628067	-2.710314	-3.634035
H	-5.575558	-2.359797	-3.218199
H	-4.731067	-3.780551	-3.837890
H	-4.469710	-2.200875	-4.587867
C	-2.130041	-2.888061	-3.294675
H	-2.127180	-3.954092	-3.539307
H	-1.304114	-2.686673	-2.610860
H	-1.945870	-2.339310	-4.221410
C	-5.850940	-2.643956	2.999276
H	-5.727518	-3.663928	3.373847
H	-6.711335	-2.639326	2.325559
H	-6.087757	-2.006203	3.854626
C	-3.379086	-2.128355	3.244785
H	-2.493821	-1.751200	2.732147
H	-3.165564	-3.132497	3.624654
H	-3.574666	-1.477837	4.102734
C	-5.629327	0.826543	-0.519785
C	-5.668686	-0.524599	-0.595410
H	-6.391006	1.575258	-0.642333
H	-6.474798	-1.208791	-0.790168

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