Supplementary Information

Synthesis and properties of Fischer carbene complexes of N,N-dimethylaniline and anisole π-coordinated to chromium tricarbonyl

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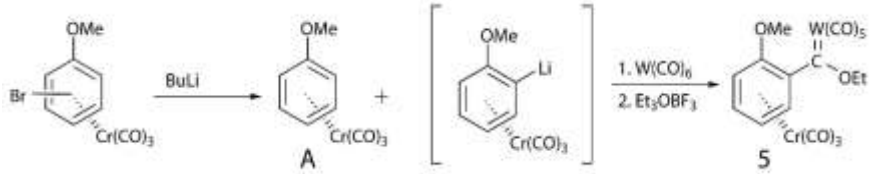
Contents

The synthesis of *o*- and *m*-bromoanisole $Cr(CO)_3$ complexes and subsequent reaction with *t*BuLi, $W(CO)_6$ and Et_3OBF_4

While only *o*-lithiation resulted from the deprotonation of $\{\eta^6$-anisole$\}Cr(CO)_3$ it was clear that this method could not be considered as a viable route to prepare *m*- and *p*-carbene isomers of anisole π-coordinated to $Cr(CO)_3$. To produce the *m*- or *p*-analogues without additional ring directing groups, it was envisaged to start with a bromo substituent on the anisole ring in either the *m*- *or p*-position. This method was used by us successfully to activate less reactive sites on thiophene when not coordinated to $Cr(CO)_3$.[1] Support of this approach came from Fischer and co-workers who showed that lithium-bromine exchange reactions could be effectively used to prepare *m*- and *p*-isomers of $M\{C(OMe)C_6H_4OMe\}(CO)_5$.[2] A challenging assignment however was to find an effective method to either (i) coordinate *m*- and *p*-bromoanisole to $Cr(CO)_3$ and thereafter introduce the carbene functionality afterwards or (ii) to prepare the *m*- or *p*-carbene complexes of anisole prior to coordination to $Cr(CO)_3$. Efforts to coordinate the *m*- or *p*-isomers of $W\{C(OEt)C_6H_4OMe\}CO)_5$ to $Cr(CO)_3$ by thermolysis or amine substitution failed and only decomposition products could be isolated.

While the synthesis of $Cr(\pi$-ArX$)(CO)_3$ for X = F and Cl is readily achieved by refluxing the halobenzene in dibutyl ether, the synthesis with X = Br and I is complicated due to instability during the thermolysis and purification procedures of the haloarene complexes. Öfele found that $Cr(\pi$-$C_6H_5X)(CO)_3$, X = Br, I) could be synthesized in low yields (28%) by amine ligand substitution from $Cr(N(picoline)_3)_3(CO)_3$ by C_6H_5X. In our case this method resulted in far smaller yields and was difficult to reproduce. Purification of the complexes required treatment with BF_3, rapid aqueous work-up and isolation by column chromatography and led to varied yields on repetition of the synthesis.[3] The procedure was modified by replacing the aqueous quenching by an extraction and filtration process through silica gel with hexane/Et_2O, affording the desired new bromoanisole complexes *m*- or *p*-$\{\eta^6$-$C_6H_4(OMe)Br\}Cr(CO)_3$ in less than 10% yields. The formation of the bromo percursors were confirmed by comparison of ^{1}H NMR spectra with literature.[4] We ascribe the low yields of the *m*- and *p*-isomers of $\{\eta^6$-$C_6H_4(OMe)Br\}Cr(CO)_3$ to the fact that much of the product was lost during the work-up and π-coordination by the Öfele method of treating the reaction mixture with BF_3-etherate and extracting with ether.[3] Hence, the lithiation was performed with *t*BuLi instead of *n*BuLi to try and improve the lithium-bromine exchange reaction.[5,6] Reaction of the lithiated anisole with $W(CO)_6$ and $[Et_3O][BF_4]$ did not give the *m*-or *p*-isomers but afforded only the *o*-isomer (**5**) in high yield. The reactions were studied by NMR spectroscopy and abandoned, as the desired *m*- or *p*-carbene isomers did not form as a result of transmetallation leading to *o*-lithiation.



Scheme S-1. *Halogen dancing* affording π-anisole $Cr(CO)_3$ and *o*-carbene product (**5**)

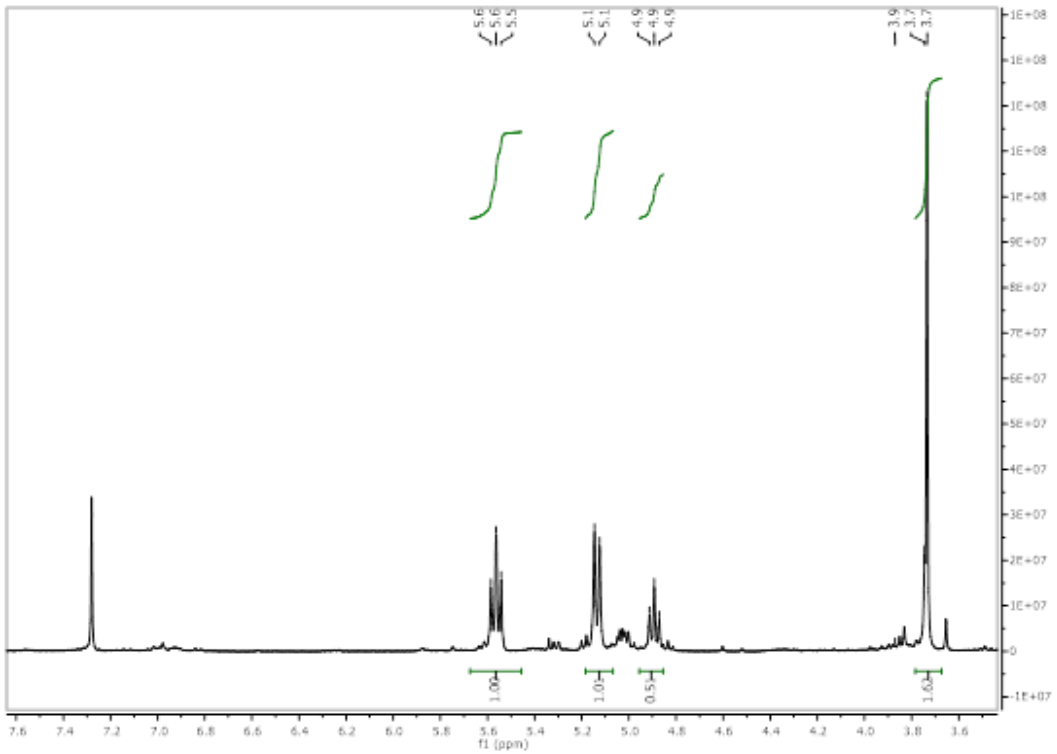


Figure S-1. ^{1}H NMR spectrum in $CDCl_3$ of π-anisole $Cr(CO)_3$ (**A**) after an early stage of litigation and reaction with $W(CO)_6$ and Et_3OBF_4

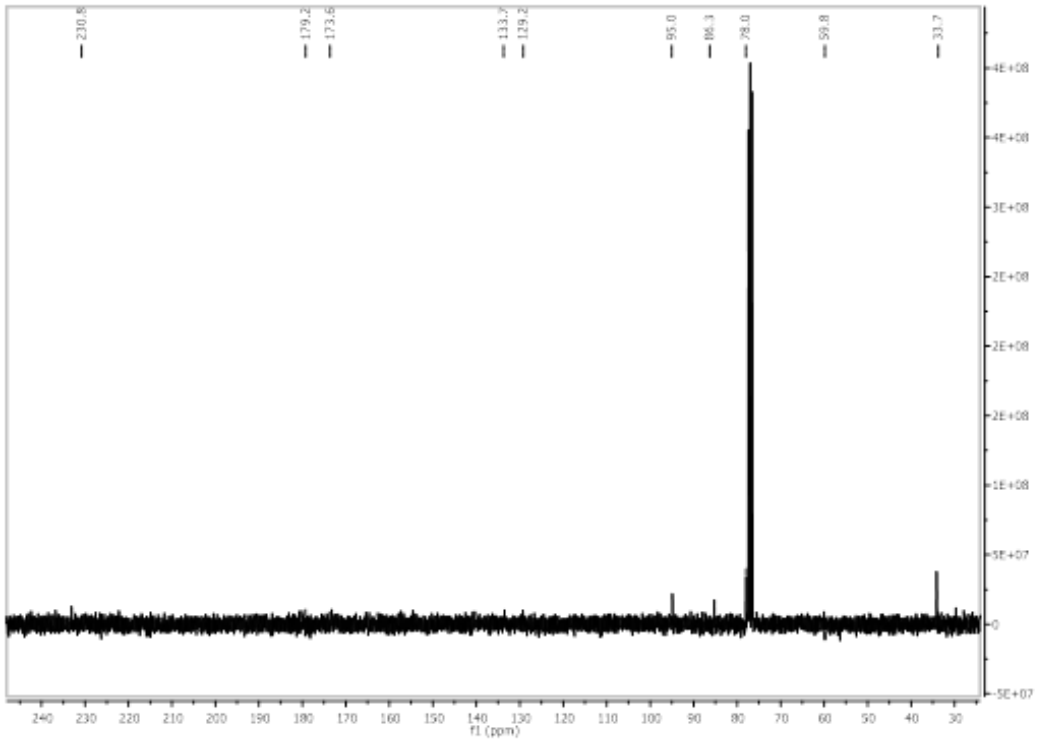


Figure S-2. ^{13}C NMR spectrum in $CDCl_3$ of π-anisole $Cr(CO)_3$ (**A**) after an early stage of litigation and reaction with $W(CO)_6$ and Et_3OBF_4.

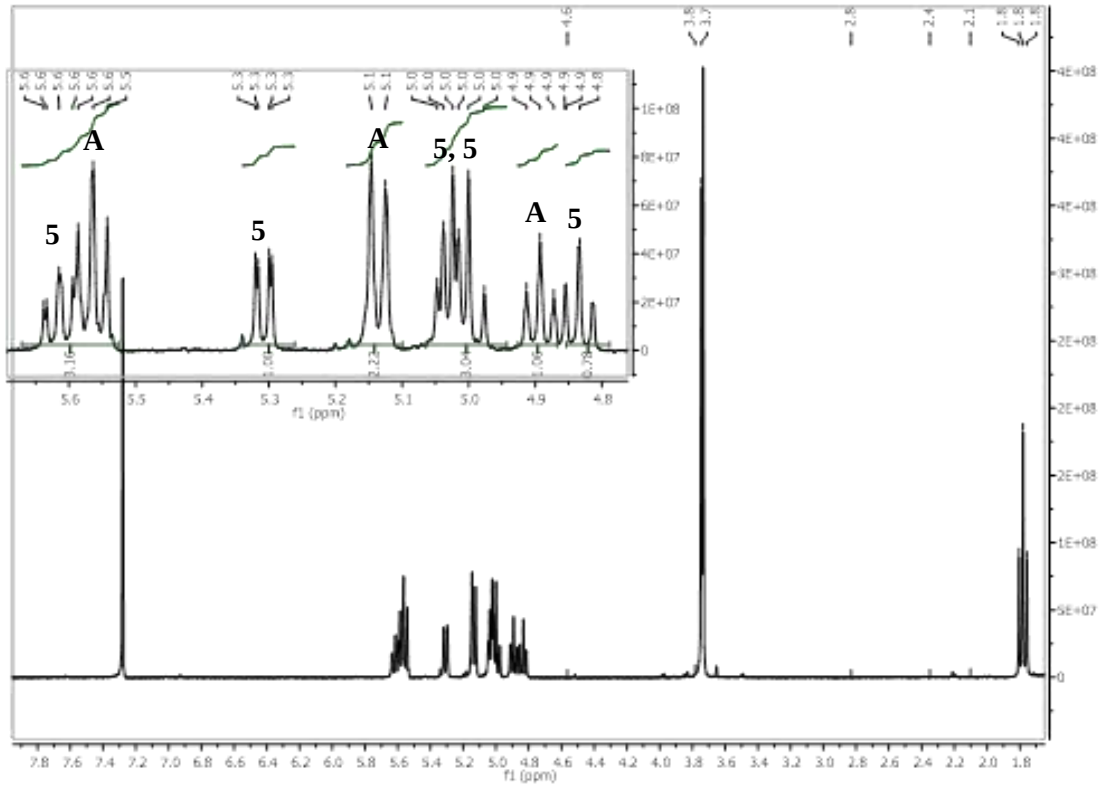


Figure S-3. ^{1}H NMR spectrum in $CDCl_3$ of the reaction mixture of **A** and **5** (1:1)

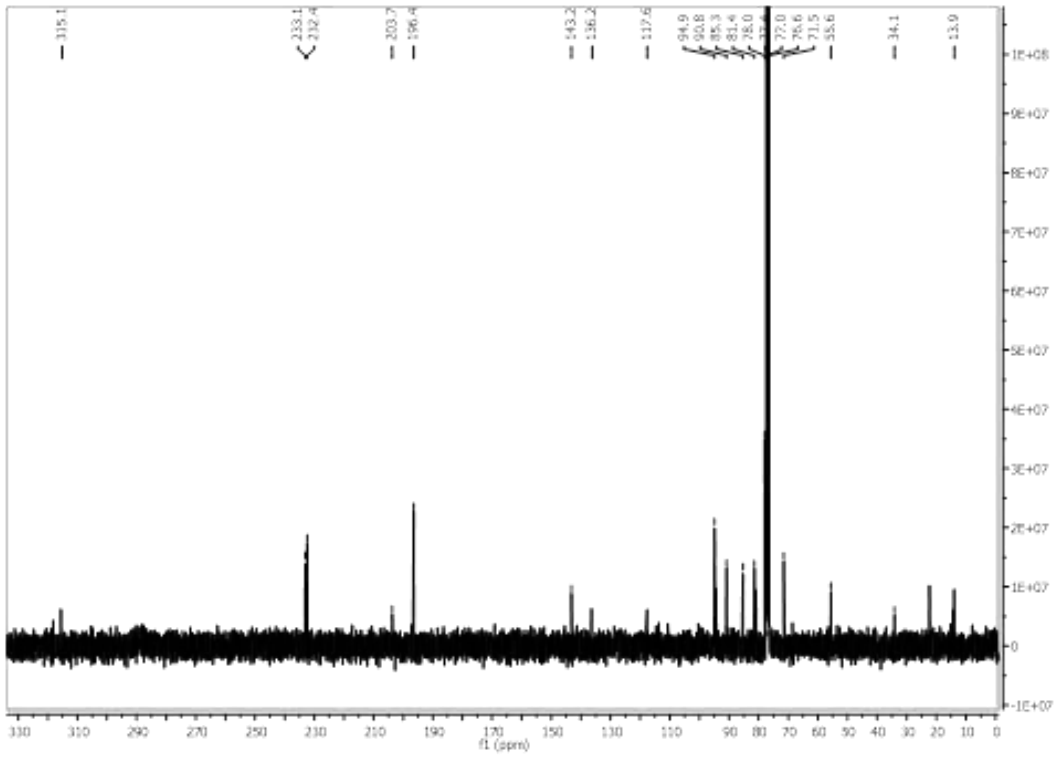


Figure S-4. ^{13}C NMR spectrum in $CDCl_3$ of the mixture of **A** and **5**

^{1}H and ^{13}C NMR spectra

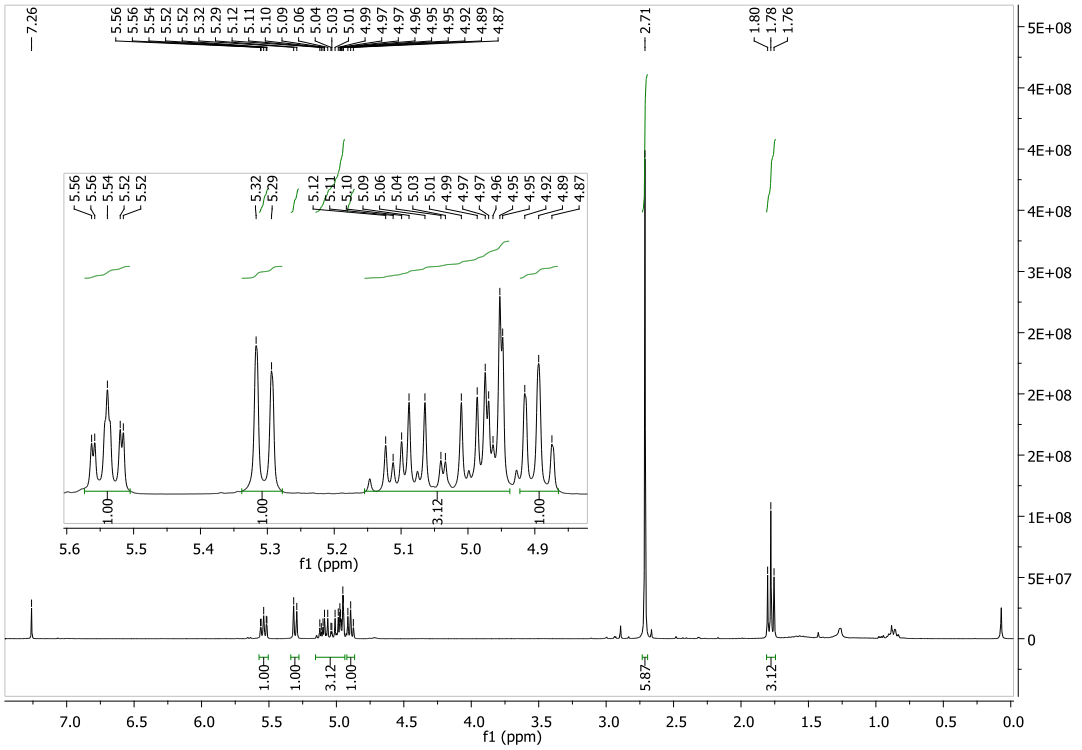


Figure S-5. ^{1}H NMR spectrum of **1** in $CDCl_3$

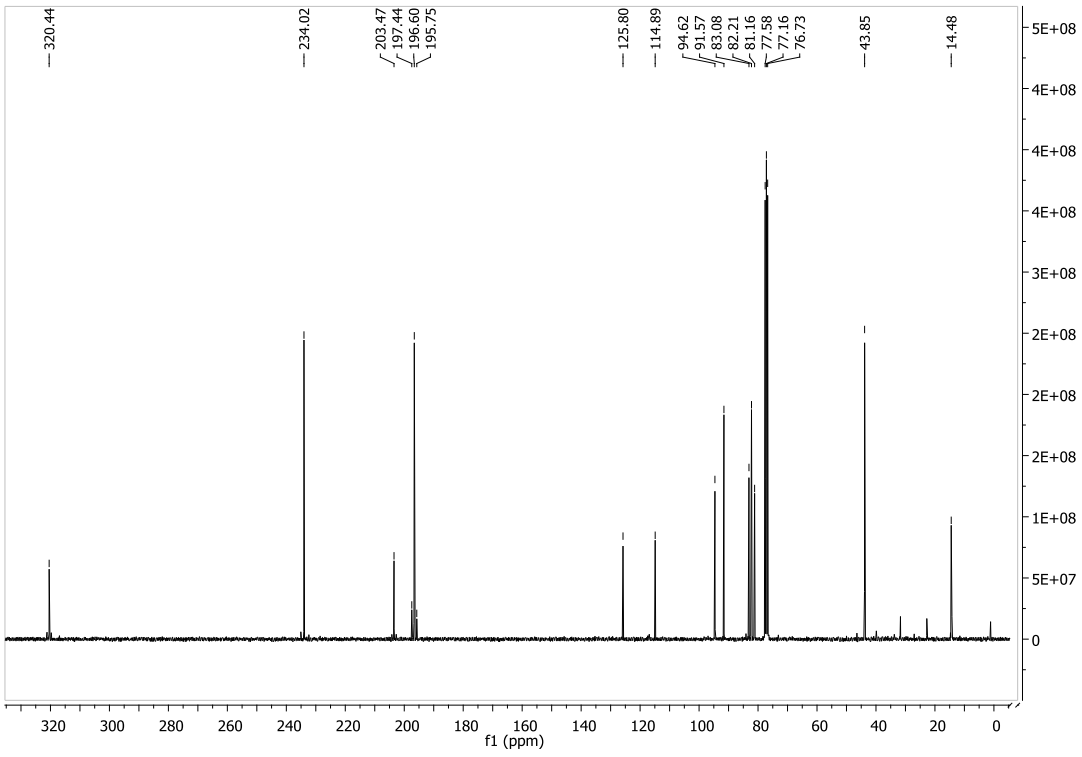


Figure S-6. ^{13}C NMR spectrum of **1** in $CDCl_3$

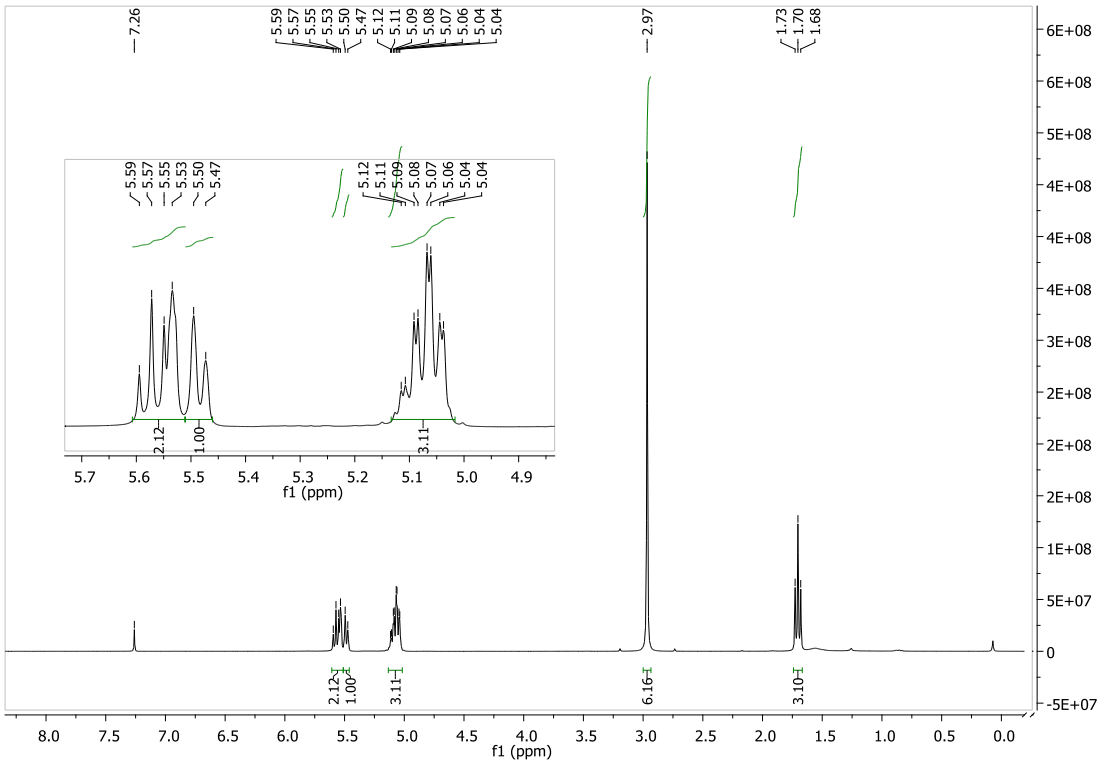


Figure S-7. ^{1}H NMR spectrum of **2** in $CDCl_3$

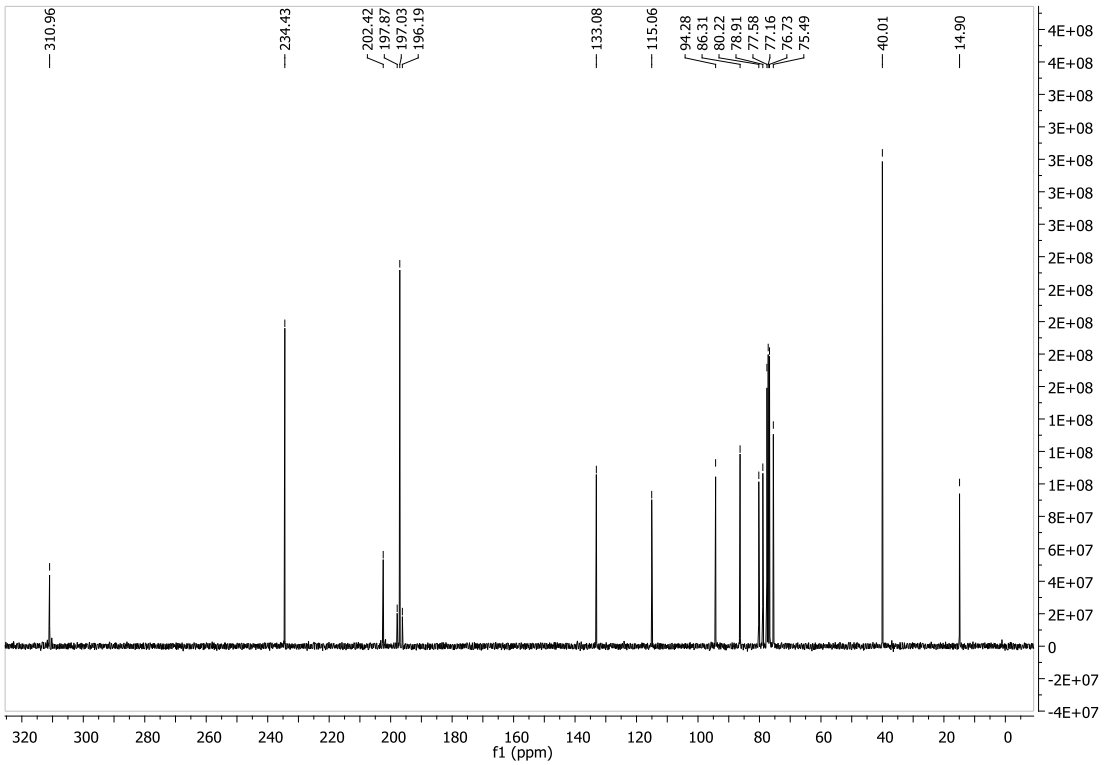


Figure S-8. ^{13}C NMR spectrum of **2** in $CDCl_3$

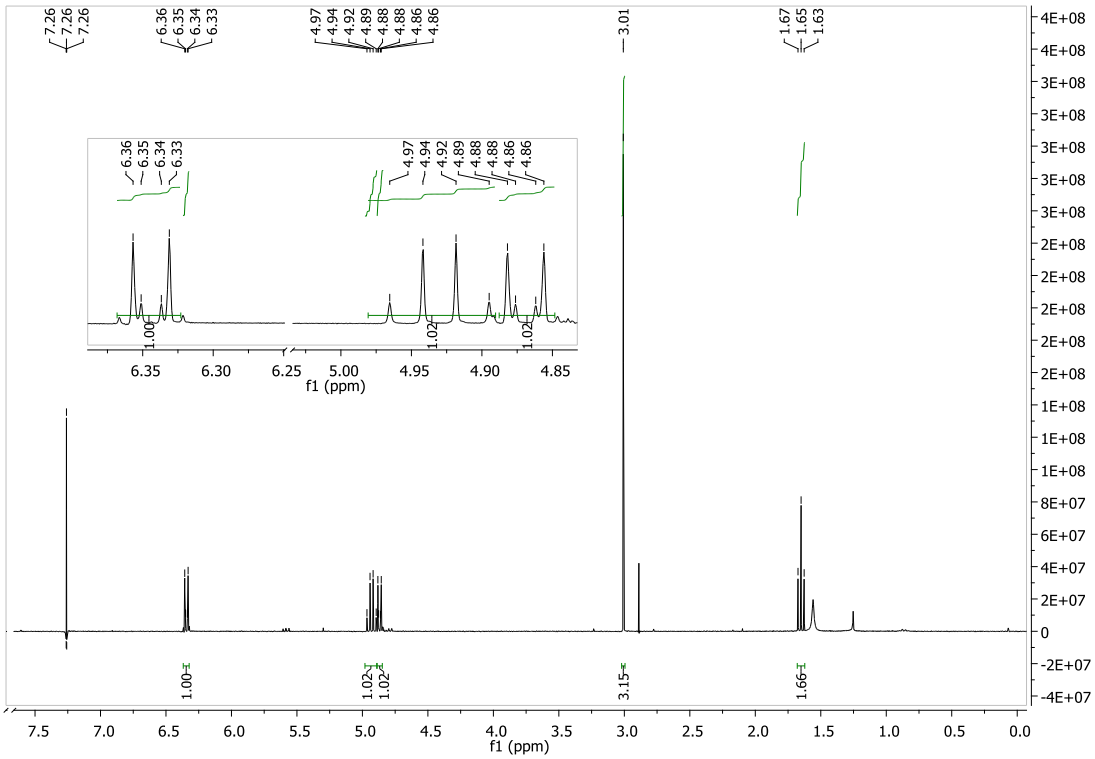


Figure S-9. ^{1}H NMR spectrum of **3** in $CDCl_3$

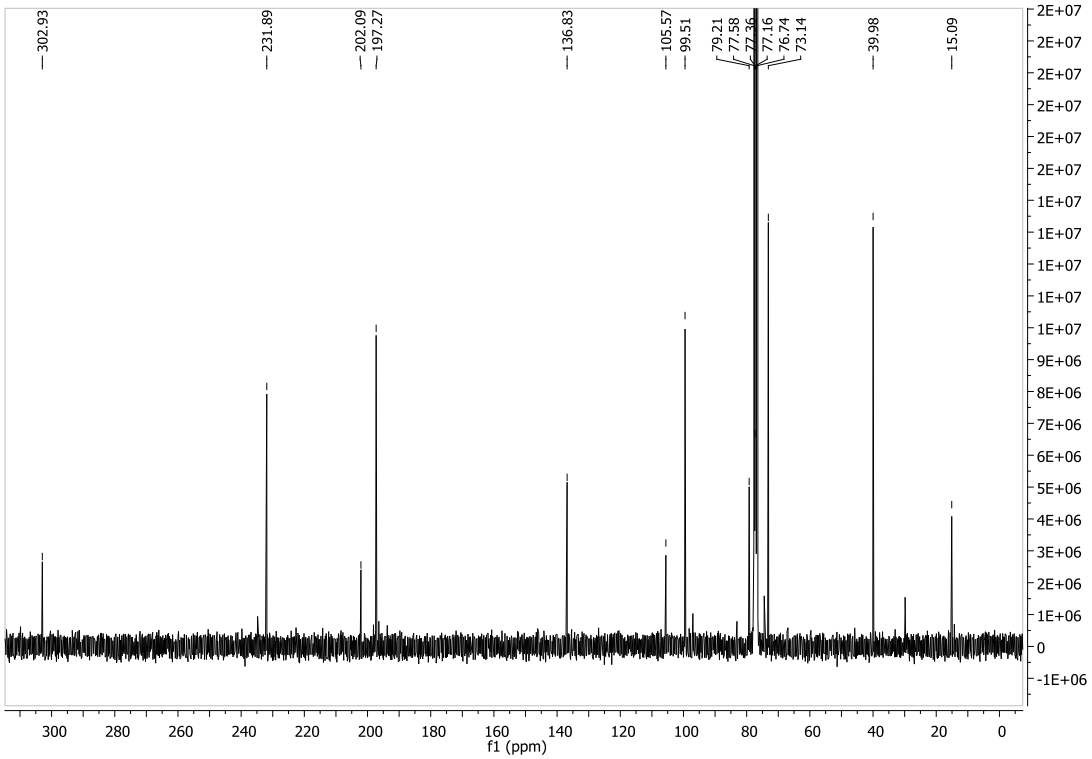


Figure S-10. ^{13}C NMR spectrum of **3** in $CDCl_3$

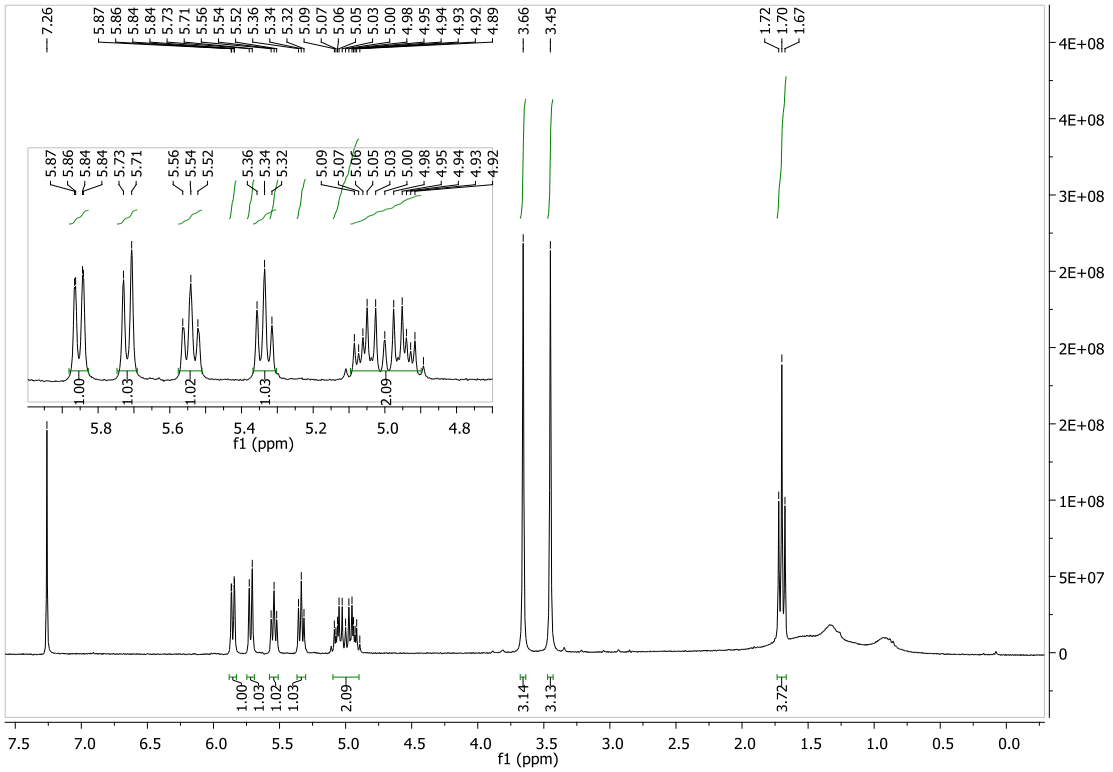


Figure S-11. ^{1}H NMR spectrum of **4** in $CDCl_3$

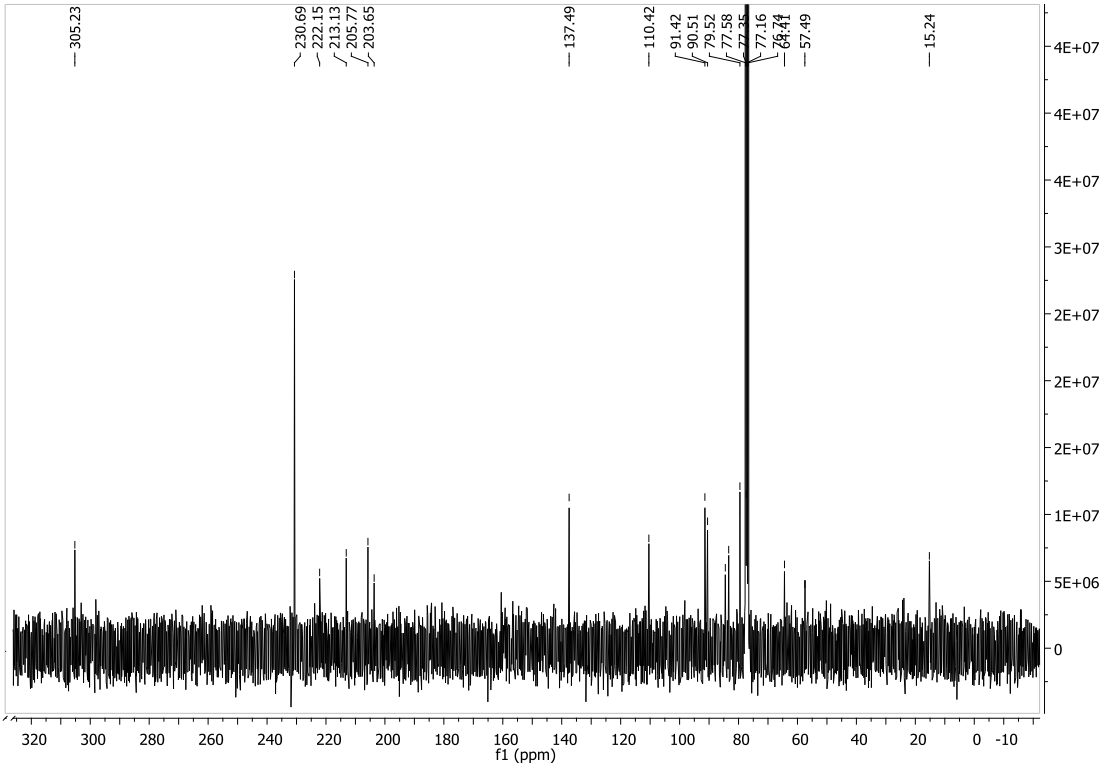


Figure S-12. ^{13}C NMR spectrum of **4** in $CDCl_3$

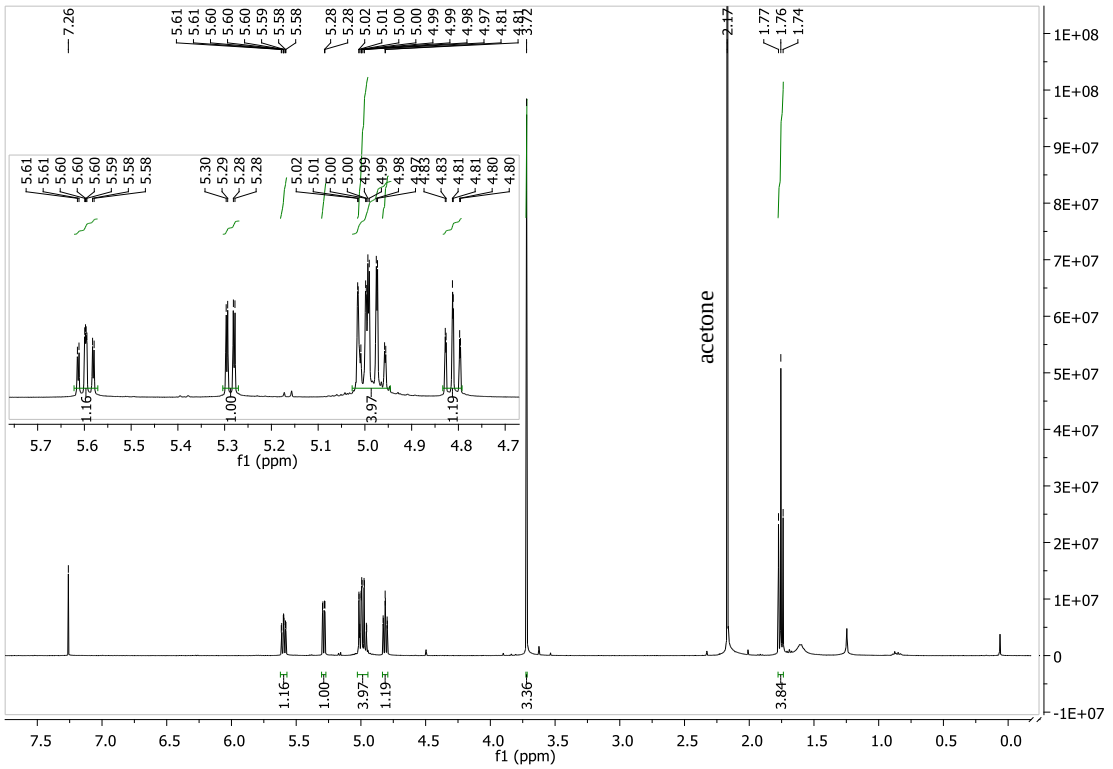


Figure S-13. ^{1}H NMR spectrum of **5** in $CDCl_3$

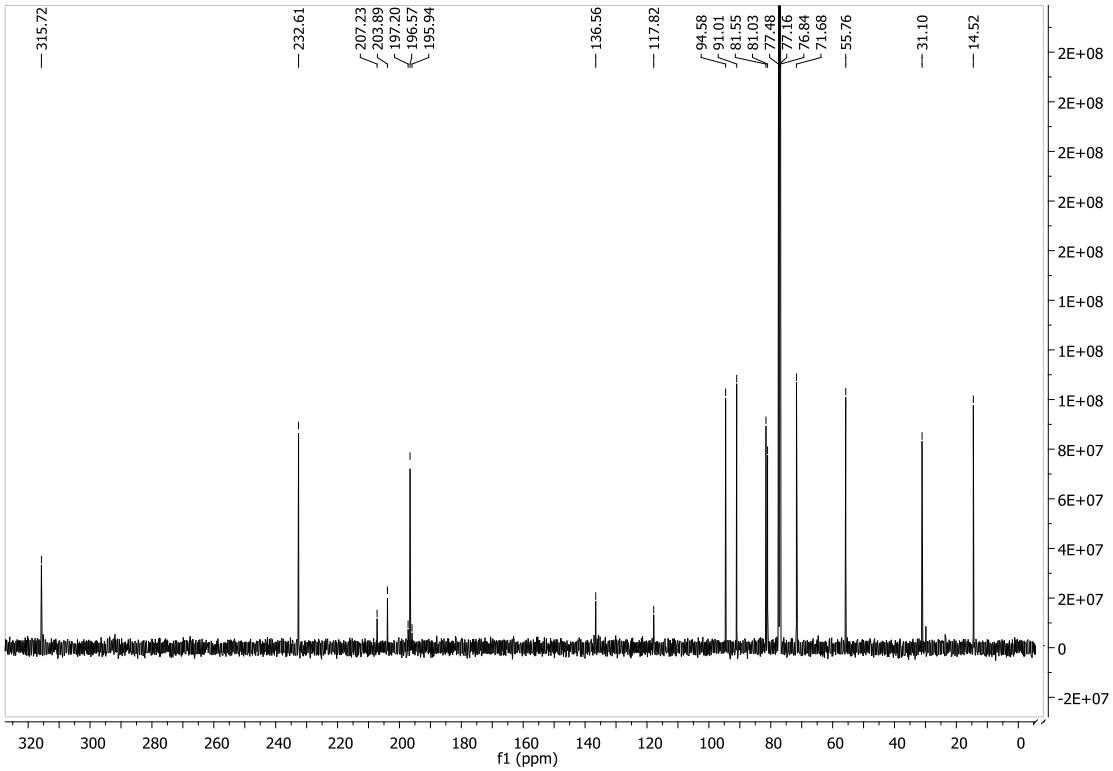


Figure S-14. ^{13}C NMR spectrum of **5** in $CDCl_3$

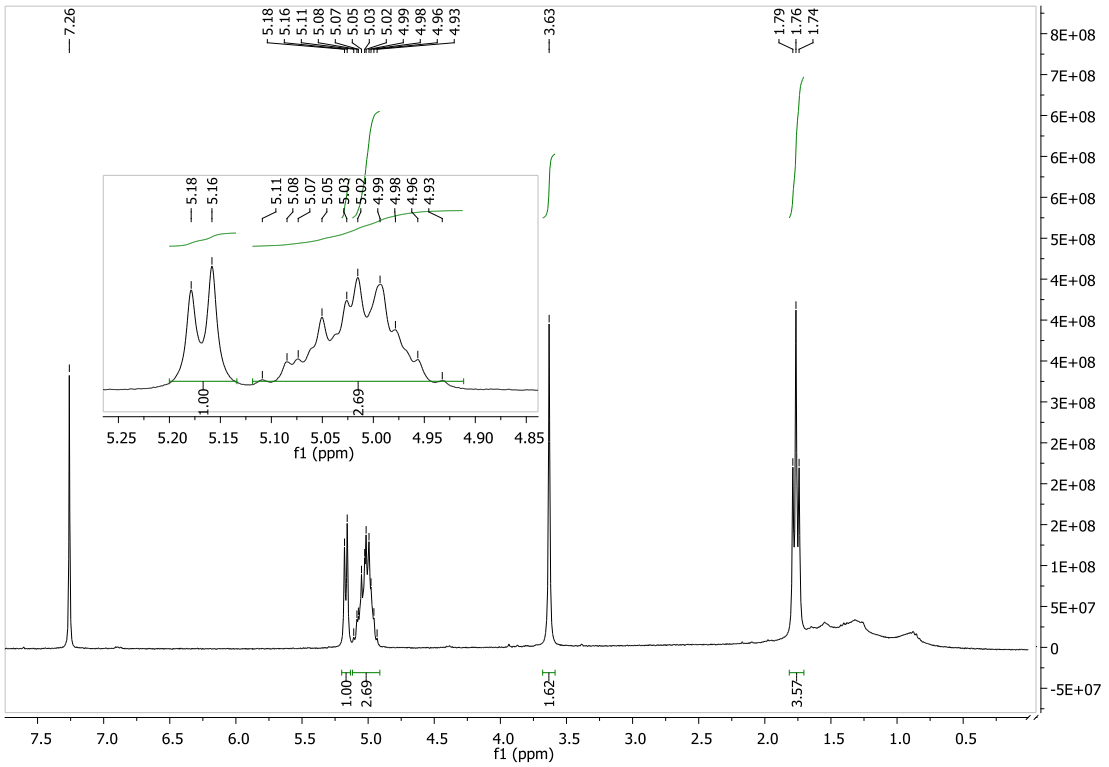


Figure S-15. ^{1}H NMR spectrum of **7** in $CDCl_3$

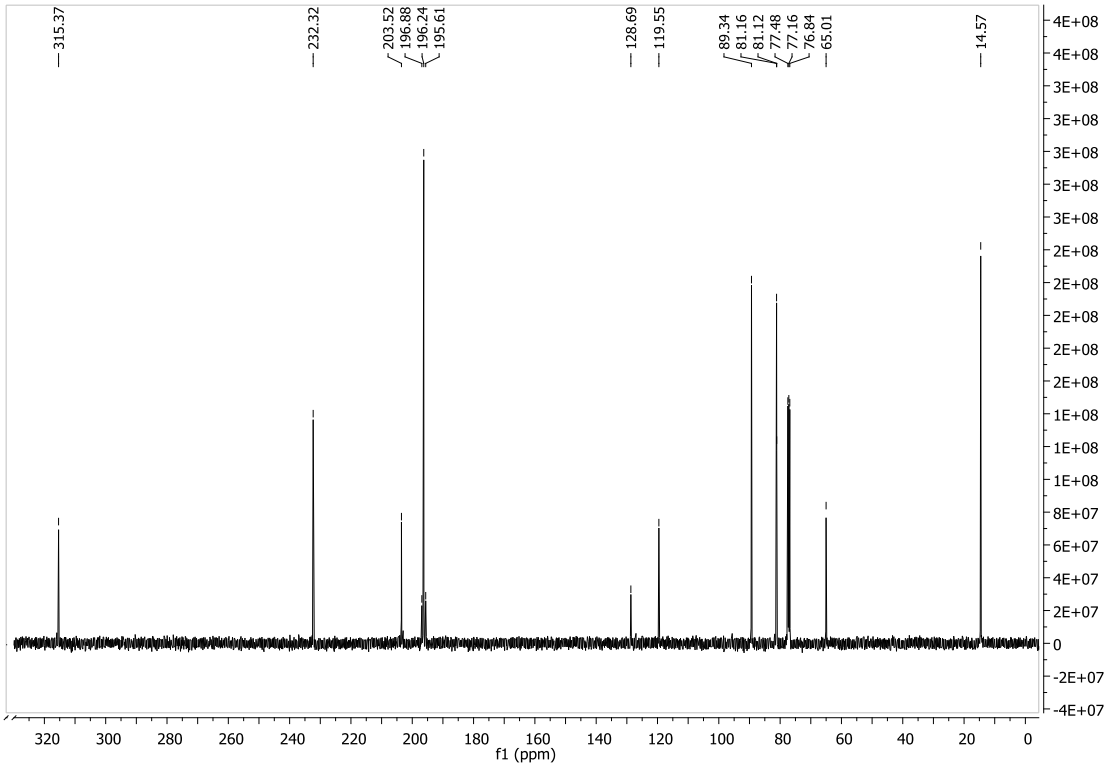


Figure S-16. ^{13}C NMR spectrum of **7** in $CDCl_3$

IR Spectroscopy

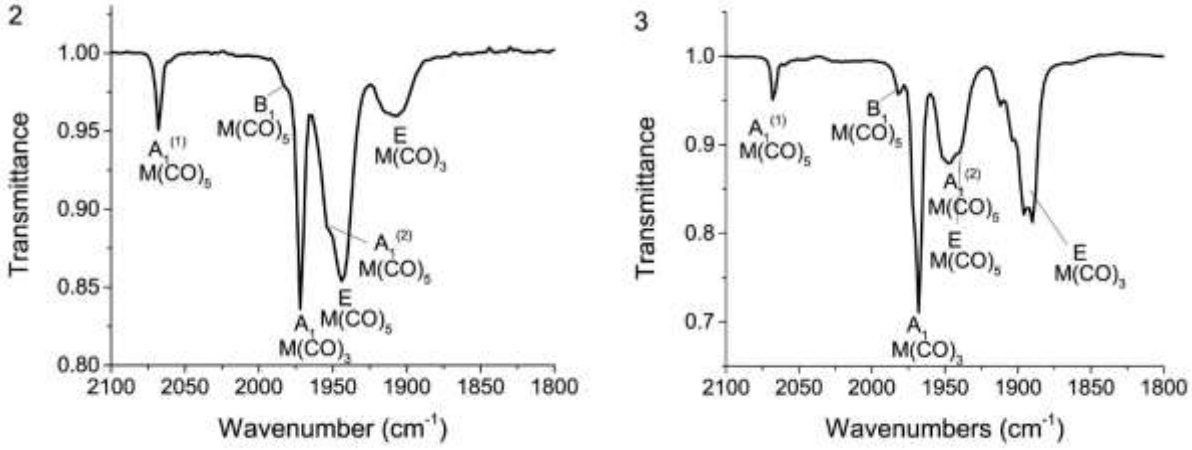


Figure S-17. FT-IR spectra of **2** (left) and **3** (right) in the carbonyl region. Recorded in hexane at 298 K

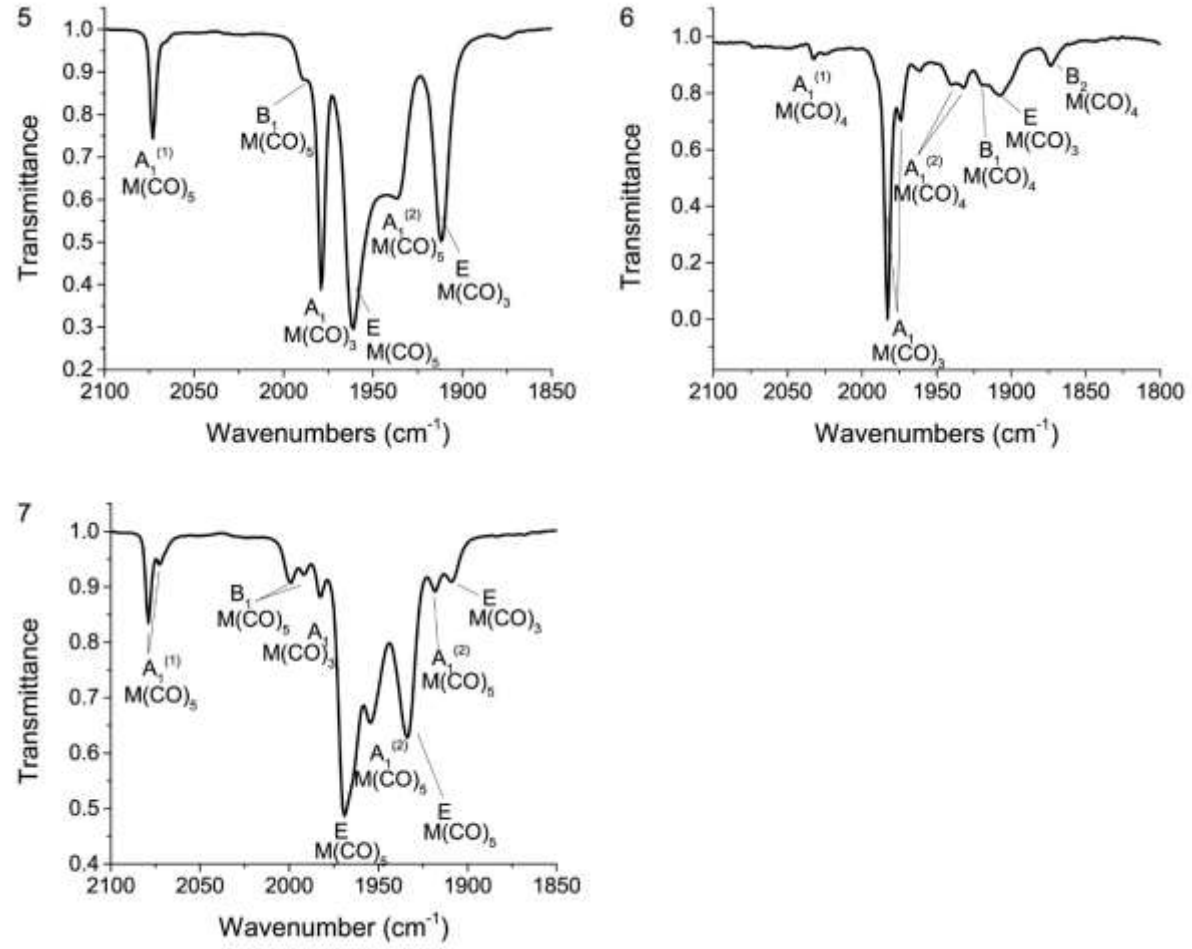
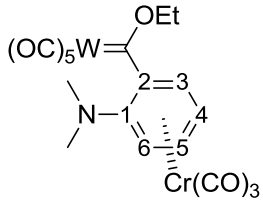


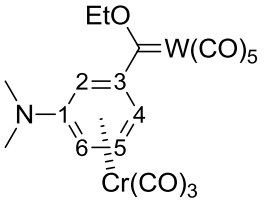
Figure S-18. FT-IR spectra of **5** (top, left), **6** (top, right) and **7** (bottom, left) in the carbonyl region. Recorded in hexane at 298 K

X-Ray Crystallography

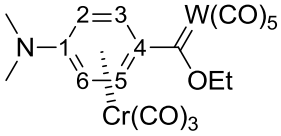
Table S-1. Selected bond lengths (Å) and bond angles (°) of the solid-state structures of **1-4**



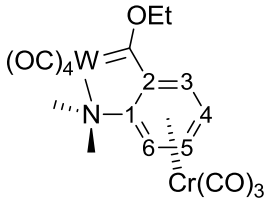
1



2



3

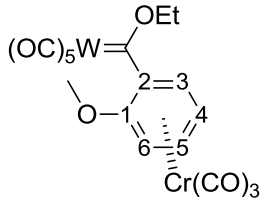
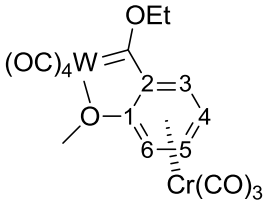
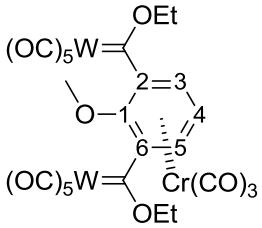


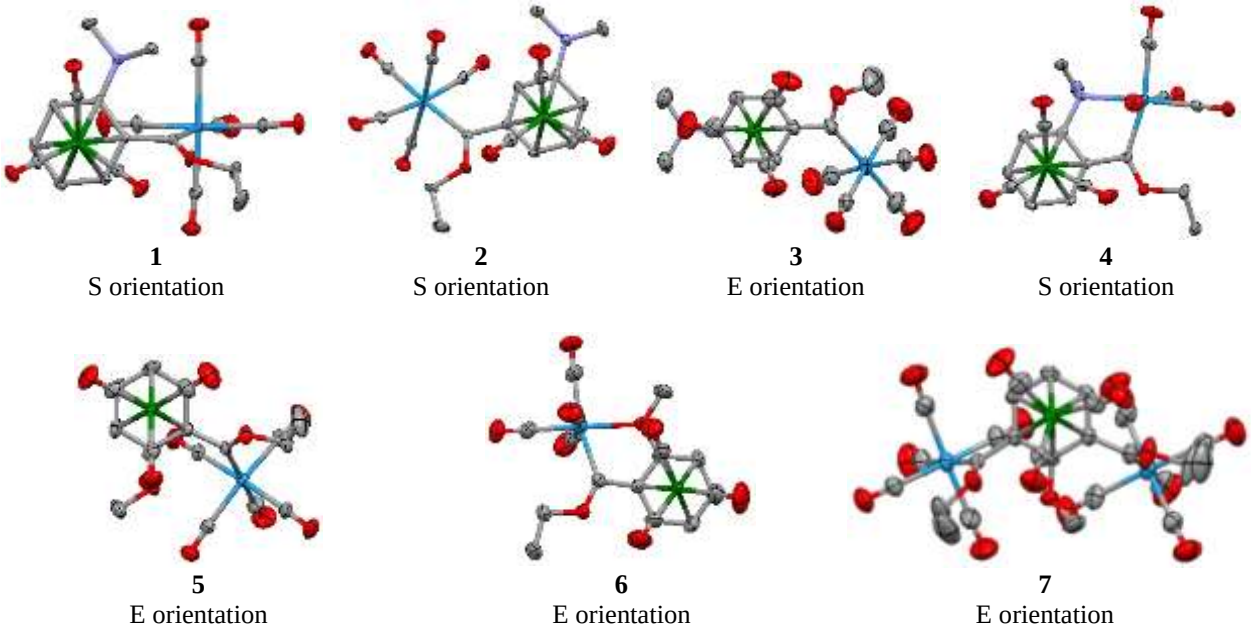
4

Bond lengths (Å)	**1**	**2***	**3**	**4**
$N–C_{Ph}$	1.387(3)	1.357(5)	1.354(3)	1.466(3)
$C_{Carb}–W$	2.165(2)	2.186(3)	2.193(3)	2.137(2)
$C_{Carb}–O$	1.318(2)	1.305(4)	1.327(4)	1.313(3)
$C_{Carb}–C_{Ph}$	1.494(3)	1.502(5)	1.485(3)	1.482(3)
C1–C2	1.420(3)	1.425(5)	1.418(3)	1.418(3)
C2–C3	1.437(3)	1.411(5)	1.399(3)	1.429(3)
C3–C4	1.399(3)	1.429(5)	1.420(3)	1.395(3)
C4–C5	1.406(4)	1.393(5)	1.415(3)	1.418(3)
C5–C6	1.403(4)	1.417(5)	1.398(3)	1.401(3)
C6–C1	1.431(3)	1.419(5)	1.422(3)	1.412(3)
$W–CO_{(ax)}$	2.039(2)	2.029(3)	2.024(4)	2.025(2)
$W–CO_{(eq)}$*	2.046	2.044	2.038	
Cr–CO*	1.844	1.840	1.841	1.857
Ph–Cr	1.710	1.722	1.715	1.698
Angles (°)				
Me1–N–Me2	111.7(2)	115.9(4)	117.8(3)	107.1(2)
Me1–N–C1	118.2(2)	119.3(3)	120.4(2)	105.3(2)
Me2–N–C1	117.3(2)	119.2(3)	120.4(2)	112.6(2)
$C_{Ph}–C_{carb}–W$	119.5(1)	123.6(2)	124.7(2)	116.8(1)
$C_{Ph}–C_{carb}–O$	106.5(2)	105.2(3)	105.4(2)	107.4(2)
$W–C_{carb}–O$	131.7(2)	130.9(3)	129.1(2)	135.7(2)
$C_{carb}–W–CO_{(ax)}$	170.51(9)	174.0(1)	174.2(1)	168.14(9)
$C_{carb}–W–CO_{(eq)}$*	91.4(9)	92.6(9)	91.7(8)	–
C6–C1–C2	117.9(2)	116.4(3)	116.4(2)	120.3(2)
C1–C2–C3	119.1(2)	122.9(3)	121.1(2)	118.9(2)
C2–C3–C4	121.9(2)	118.6(3)	122.1(2)	120.7(2)
C3–C4–C5	118.8(2)	119.3(3)	116.2(2)	119.6(2)
C4–C5–C6	120.4(2)	121.3(3)	121.9(2)	120.6(2)
C5–C6–C1	121.8(2)	120.8(3)	121.5(2)	120.0
Torsion angles (°)				
Me1–N–C1–C2	-50.1(3)	4.9(5)	6.5(4)	98.2(2)
Me2–N–C1–C6	-8.8(3)	-18.2(5)	-3.2(4)	40.9(3)
$W–C_{carb}–C_{Ph}–C\alpha1$	100.8(2)	32.0(5)	29.0(3)	4.2(3)
$O–C_{carb}–C_{Ph}–C\alpha2$	126.7(2)	26.4(4)	14.7(3)	7.7(3)

* One of the two independent molecules of the unit cell is listed.

Table S-2. Selected bond lengths (Å) and bond angles (°) of the solid-state structures of **5-7**

			
	5	**6**	**7**
Bond lengths (Å)	**5**	**6**	**7**
O–C_{Ph}	1.350(3)	1.364(4)	1.354(3)
C_{Carb1}–W1	2.168(2)	2.133(3)	2.142(2)
C_{Carb1}–OEt(1)	1.316(3)	1.318(3)	1.301(3)
C_{Carb1}–C_{Ph}	1.503(3)	1.473(4)	1.504(3)
C_{Carb2}–W2	–	–	2.144(3)
C_{Carb2}–OEt(2)	–	–	1.308(3)
C_{Carb2}–C_{Ph}	–	–	1.502(3)
W–$CO_{(ax)}$	2.034(3)	2.026(3)	2.048(3)
W–$CO_{(eq)}$*	2.046(36)	–	2.040(26)
W–$CO_{(ax)}$	–	–	2.040(4)
W–$CO_{(eq)}$*	–	–	2.045(28)
C1–C2	1.428(3)	1.414(4)	1.429(3)
C2–C3	1.422(3)	1.422(4)	1.398(3)
C3–C4	1.406(3)	1.395(5)	1.408(3)
C4–C5	1.398(4)	1.398(5)	1.390(3)
C5–C6	1.401(4)	1.406(4)	1.422(3)
C6–C1	1.409(3)	1.401(4)	1.411(3)
Cr–CO*	1.846(11)	1.385(14)	1.847(15)
Ph–Cr	1.693	1.700	
Angles (°)			
C_{Ph}–C_{carb1}–W1	122.4(1)	116.9(2)	117.9(1)
C_{Ph}–C_{carb1}–O1	105.1(2)	108.2(2)	107.0(2)
W1–C_{carb1}–O1	131.3(1)	134.7(2)	134.8(2)
C_{Ph}–C_{carb2}–W2	–	–	119.5(2)
C_{Ph}–C_{carb2}–O2	–	–	106.6(2)
W2–C_{carb2}–O2	–	–	133.5(2)
C_{carb1}–W1–$CO_{(ax)}$	173.23(9)	166.7(1)	174.5(1)
C_{carb1}–W1–$CO_{(eq)}$*	92.6(12.3)	–	90.7(13.5)
C_{carb2}–W2–$CO_{(ax)}$	–	–	175.0(1)
C_{carb2}–W2–$CO_{(eq)}$*	–	–	92.1(5.1)
C6–C1–C2	120.4(2)	121.9(3)	120.3(2)
C1–C2–C3	117.7(2)	117.8(3)	119.7(2)
C2–C3–C4	121.7(2)	120.9(3)	120.4(2)
C3–C4–C5	119.0(2)	119.5(4)	119.6(2)
C4–C5–C6	121.1(2)	121.5(3)	121.6(2)
C5–C6–C1	119.9(2)	121.9(3)	118.2(2)
Torsion angles (°)			
W1–C_{carb1}–C_{Ph}–Cα1	60.5(3)	6.1(4)	102.3(2)
O1–C_{carb1}–C_{Ph}–Cα2	54.1(2)	0.5(4)	114.0(2)
W2–C_{carb2}–C_{Ph}–Cα1	–	–	-78.2(3)
O2–C_{carb2}–C_{Ph}–Cα2	–	–	-76.9(3)



1
S orientation

2
S orientation

3
E orientation

4
S orientation

5
E orientation

6
E orientation

7
E orientation

Figure S-19. $Cr(CO)_3$ tripod conformations for **1-7**. E = eclipsed, S = staggered.

Table S-3. Crystal data and structure refinement for complexes **1-4**

	1	**2**	**3**	**4**
Empirical formula	$C_{19}H_{15}CrNO_9W$	$C_{19}H_{15}CrNO_9W$	$C_{19}H_{15}CrNO_9W$	$C_{18}H_{15}CrNO_8W$
Formula weight	637.17	637.17	637.17	609.16
Temperature	150(2) K	150(2) K	296(2) K	150(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	triclinic	monoclinic	triclinic	monoclinic
Space group	P -1	P 21/n	P -1	P 21/c
Unit cell dimensions	a = 6.8755(2) Å b = 8.5877(3) Å c = 18.8128(6) Å α = 100.8285(11)° β = 92.1596(10)° γ = 106.1381(11)°	a = 12.5295(6) Å b = 15.9703(7) Å c = 22.0120(11) Å α= 90.00° β= 103.166(2)° γ = 90.00°	a = 6.9470(2) Å b = 12.4222(3) Å c = 12.8729(3) Å α= 85.6900(9)° β= 84.1773(8)° γ = 86.7838(8)°	a = 7.8622(4) Å b = 15.4482(7) Å c = 16.4718(7) Å α= 90° β= 94.0186(17)° γ = 90°
Volume	1043.25(5) $Å^3$	4288.8(4) $Å^3$	1100.72(5) $Å^3$	1995.69(16) $Å^3$
Z	2	8	2	4
Density (calculated)	2.028 Mg/m^3	1.974 Mg/m^3	1.922 Mg/m^3	2.027 Mg/m^3
Absorption coefficient	6.081 mm^{-1}	5.917 mm^{-1}	5.763 mm^{-1}	6.349 mm^{-1}
F(000)	612	2448	612	1168
Crystal size	0.240 x 0.209 x 0.101 mm^3	0.333 x 0.095 x 0.035 mm^3	0.300 x 0.191 x 0.152 mm^3	0.191 x 0.146 x 0.099 mm^3
Theta range for data collection	2.994 to 27.097°	2.457 to 28.320°	2.210 to 27.101°	2.479 to 28.415°
Index ranges	-8<=h<=8, -10<=k<=10, -24<=l<=24	-16<=h<=16, -20<=k<=20, -28<=l<=28	-8<=h<=8, -15<=k<=15, -16<=l<=16	-10<=h<=10, -20<=k<=20, -22<=l<=22
Reflections collected	4579	9441	4848	5013
Independent reflections	4534 [R(int) = 0.0366]	8537 [R(int) = 0.0350]	4699 [R(int) = 0.0288]	4360 [R(int) = 0.0481]
Completeness to theta = 27.41°	99.8 %	99.9 %	99.9 %	99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	4579 / 0 / 283	9441 / 0 / 565	4848 / 0 / 294	5013 / 1 / 281
Goodness-of-fit on F^2	1.183	1.285	1.167	1.090
Final R indices [I>2sigma(I)]	R1 = 0.0165 wR2 = 0.0412	R1 = 0.0234 wR2 = 0.0513	R1 = 0.0193 wR2 = 0.0492	R1 = 0.0242 wR2 = 0.0335
R indices (all data)	R1 = 0.0281 wR2 = 0.0412	R1 = 0.0282 wR2 = 0.0527	R1 = 0.0201 wR2 = 0.0497	R1 = 0.0165 wR2 = 0.0319
Largest diff. peak and hole				0.403 and -0.723 $e.Å^{-3}$

Table S-4. Crystal data and structure refinement for complexes **5-7**

	5	**6**	**7**
Empirical formula	$C_{18}H_{12}O_{10}CrW$	$C_{17}H_{12}CrO_9W$	$C_{26}H_{16}CrO_{16}W_2$
Formula weight	624.13	596.12	1004.09
Temperature	296(2) K	296(2) K	296(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	triclinic	Monoclinic	monoclinic
Space group	P -1	P 21/c	P 21/n
Unit cell dimensions	a = 6.9051(2) Å b = 9.6216(2) Å c = 15.2248(4) Å α = 91.5572(8)° β = 96.2400(8)° γ = 95.4673(8)°	a = 6.9908(2) Å b = 18.3716(6) Å c = 14.9192(5) Å α = 90° β = 97.9160(10)° γ = 90°	a = 18.0230(6) Å b = 10.1401(4) Å c = 18.2221(6) Å α= 90° β = 108.2440(10)° γ = 90°
Volume	1000.22(4) $Å^3$	1897.85(10) $Å^3$	3162.78(19) $Å^3$
Z	2	4	4
Density (calculated)	2.072 Mg/m^3	2.086 Mg/m^3	2.109 Mg/m^3
Absorption coefficient	6.343 mm^{-1}	6.676 mm^{-1}	7.665 mm^{-1}
F(000)	596	1136	1888
Crystal size	0.148 x 0.137 x 0.115 mm^3	0.204 x 0.114 x 0.013 mm^3	0.218 x 0.209 x 0.119 mm^3
Theta range for data collection	2.475 to 25.242°	2.217 to 28.274°	2.328 to 30.506°
Index ranges	-9<=h<=9, -12<=k<=12, -20<=l<=20	-9<=h<=9, -24<=k<=24, -19<=l<=19	-25<=h<=25, -14<=k<=14, -26<=l<=26
Reflections collected	4968	4708	9656
Independent reflections	4919 [R(int) = 0.0271]	4203 [R(int) = 0.0446]	8378 [R(int) = 0.0478]
Completeness to theta = 27.41°	99.9 %	100 %	100 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	4968 / 0 / 273	4708 / 0 / 255	9656 / 0 / 409
Goodness-of-fit on F^2	1.260	1.127	1.065
Final R indices [I>2sigma(I)]	R1 = 0.0157 wR2 = 0.0410	R1 = 0.0239 wR2 = 0.0566	R1 = 0.0206 wR2 = 0.0449
R indices (all data)	R1 = 0.0159 wR2 = 0.0411	R1 = 0.0290 wR2 = 0.0584	R1 = 0.0279 wR2 = 0.0473
Largest diff. peak and hole	1.287 and -0.339 $e.Å^{-3}$	1.809 and -0.321 $e.Å^{-3}$	1.314 and -0.485 $e.Å^{-3}$

Cyclic voltammetry

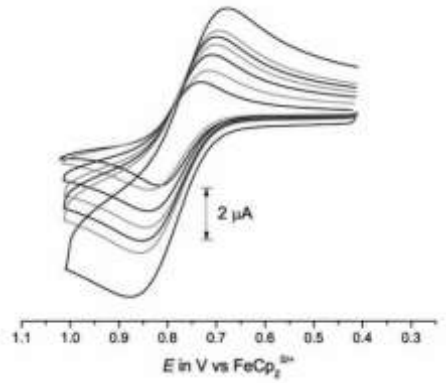


Figure S-20. Oxidation of **1** in CH_2Cl_2/0.1 M NBu_4PF_6 at scan rates of 100, 200, 400, 600, 800, 1000, 1500 and 2000 mV/s referenced against $FeCp_2^{0/+}$

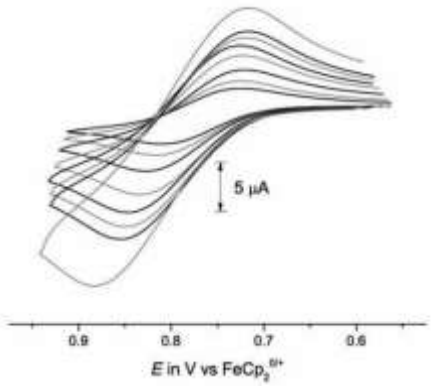


Figure S-21. Oxidation of **2** in CH_2Cl_2/0.1 M NBu_4PF_6 at scan rates of 60, 100, 200, 400, 600, 800, 1000, 1500 and 2000 mV/s referenced against $FeCp_2^{0/+}$

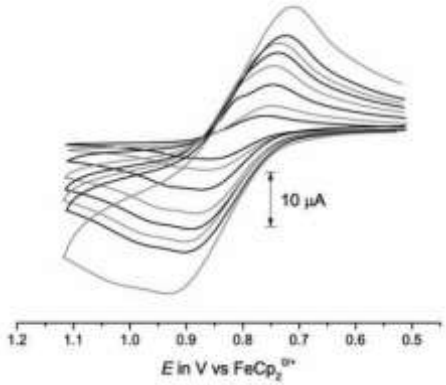


Figure S-22. Oxidation of **3** in CH_2Cl_2/0.1 M NBu_4PF_6 at scan rates of 40, 100, 200, 400, 600, 800, 1000, 1500 and 2000 mV/s referenced against $FeCp_2^{0/+}$

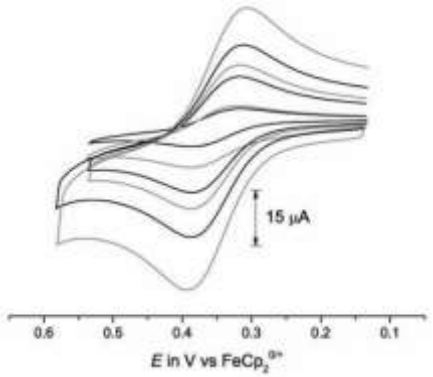


Figure S-23. Oxidation of **4** in CH_2Cl_2/0.1 M NBu_4PF_6 at scan rates of 50, 100, 200, 400, 600, 800, 1000, 1500 and 2000 mV/s referenced against $FeCp_2^{0/+}$

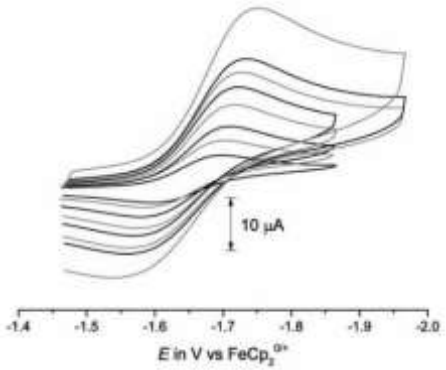


Figure S-24. Reduction of **4** in CH_2Cl_2/0.1 M NBu_4PF_6 at scan rates of 50, 100, 200, 400, 600, 800, 1000, 1500 and 2000 mV/s referenced against $FeCp_2^{0/+}$

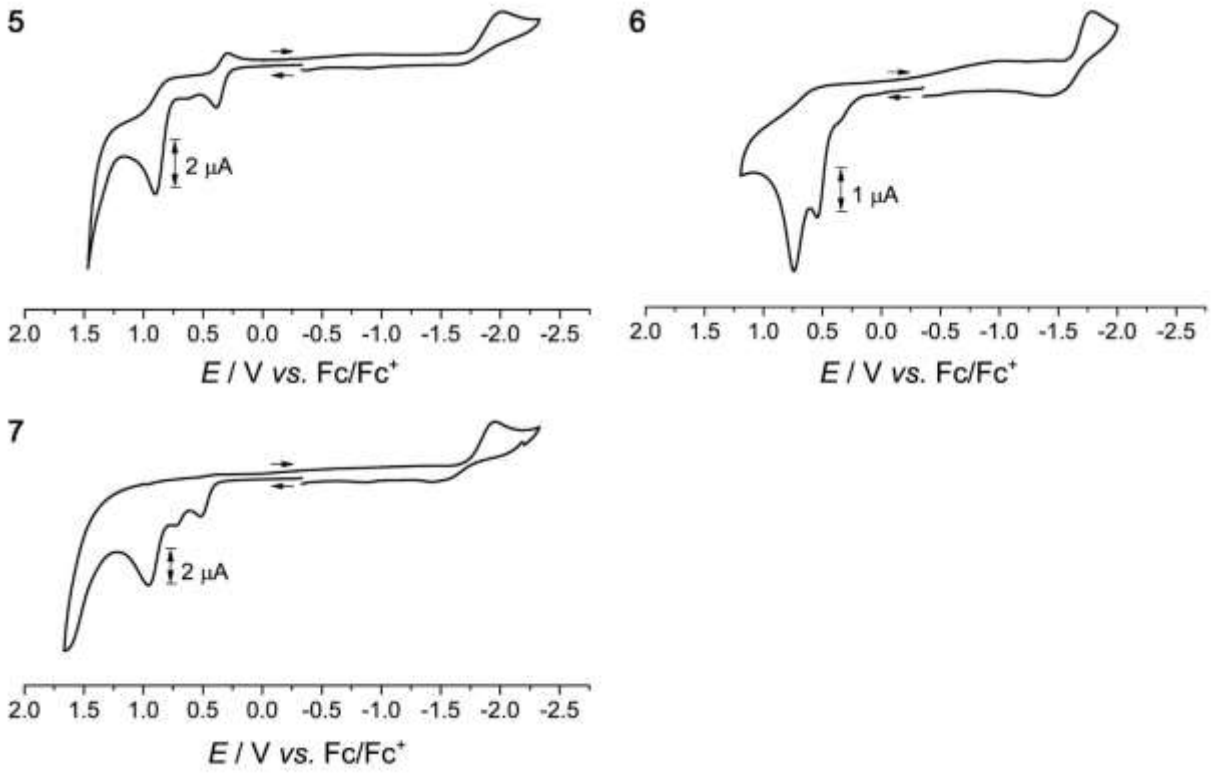


Figure S-25. Cyclovoltammograms of **5-7** in CH_2Cl_2/0.1 M NBu_4PF_6 against the ferrocene/ ferrocenium standard at 100 mV/s

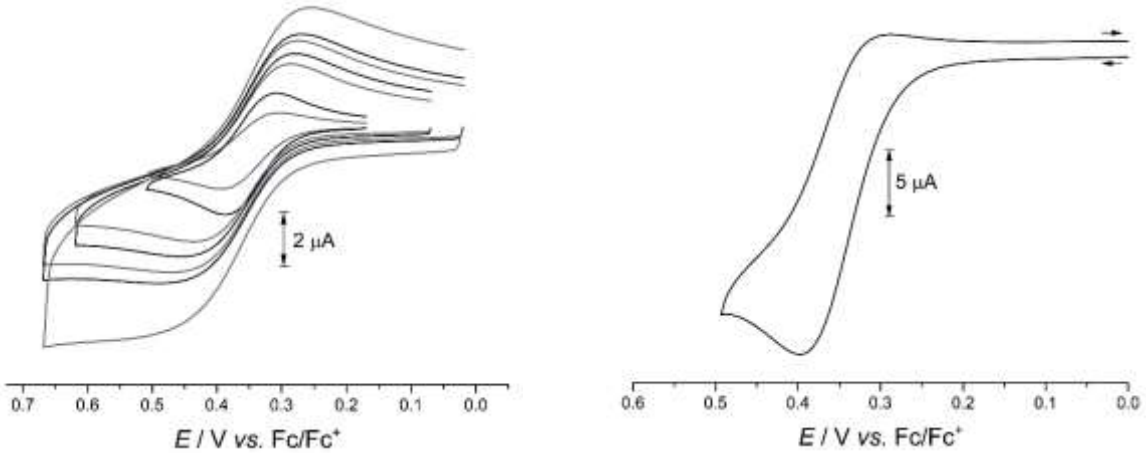


Figure S-26. Cyclovoltammograms of **5** (left) and **7** (right) in CH_2Cl_2/0.1 M NBu_4PF_6 against the ferrocene/ ferrocenium standard at multiple scan rates and 100 mV/s, respectively

IR-Spectroelectrochemistry

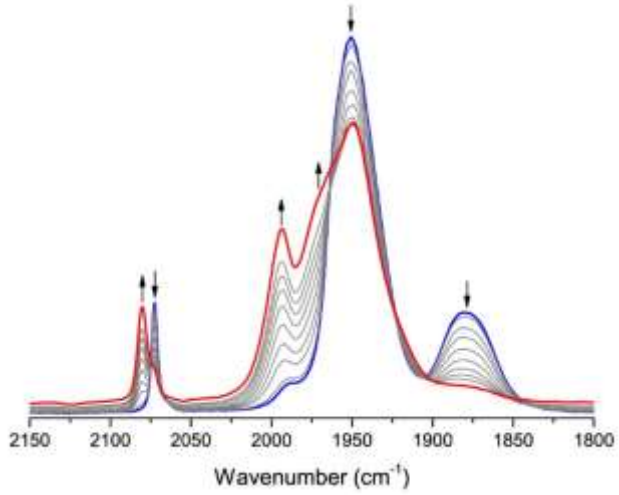


Figure S-27. IR spectroscopic changes upon the oxidation of complex **1** inside an OTTLE cell (1,2-$C_2H_4Cl_2$/NBu_4PF_6, 298 K)

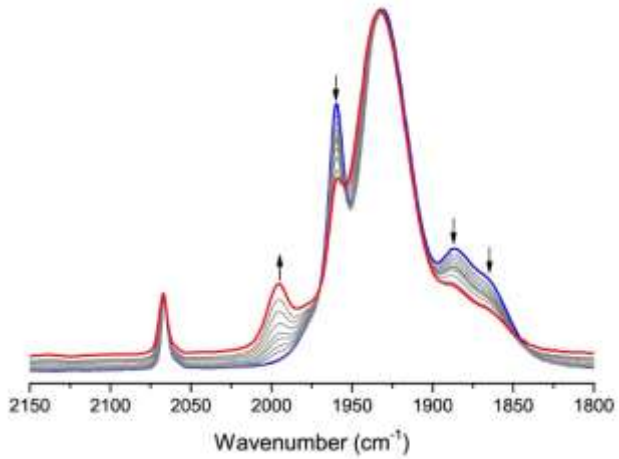


Figure S-28. IR spectroscopic changes upon the oxidation of complex **3** inside an OTTLE cell (1,2-$C_2H_4Cl_2$/NBu_4PF_6, 298 K)

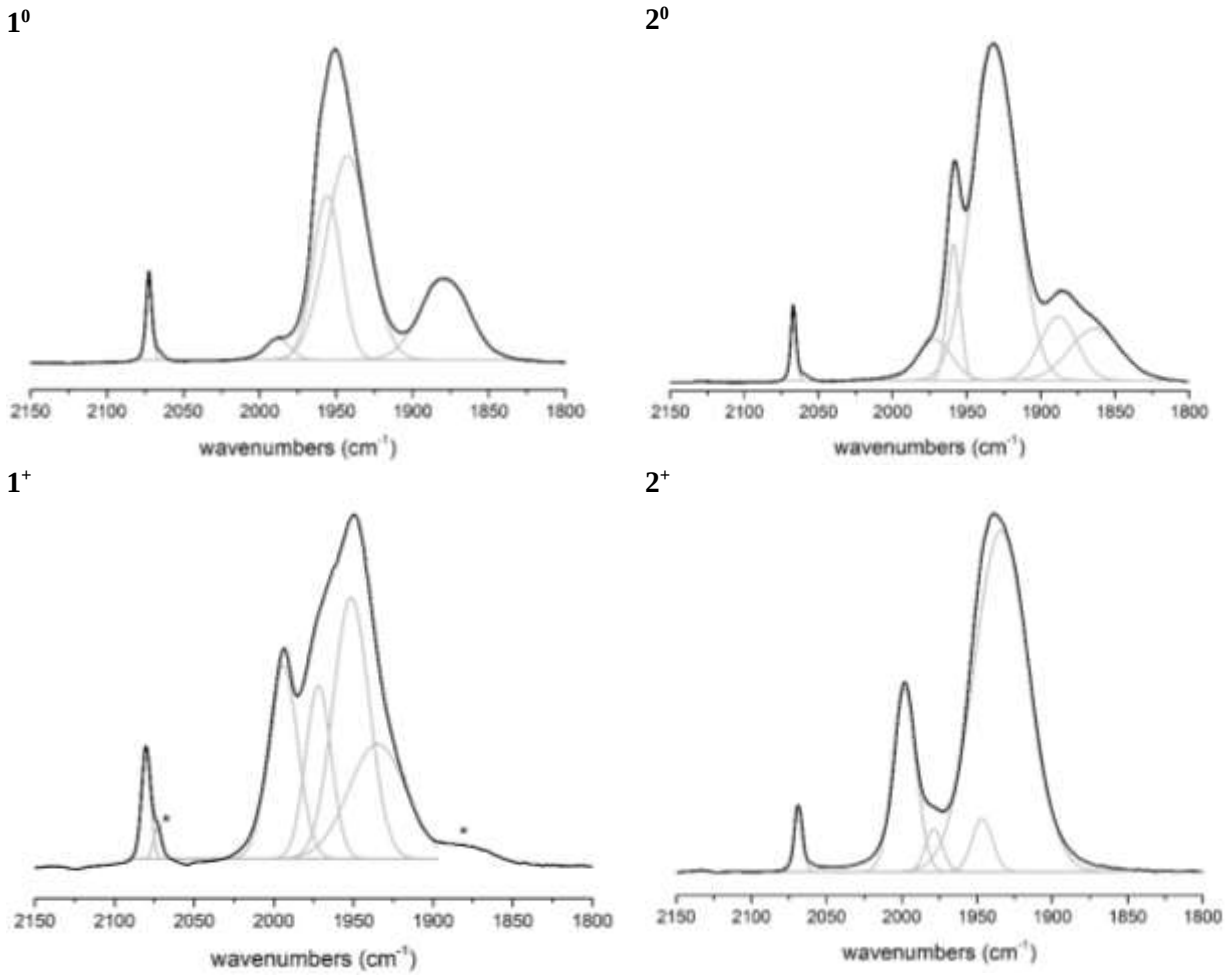
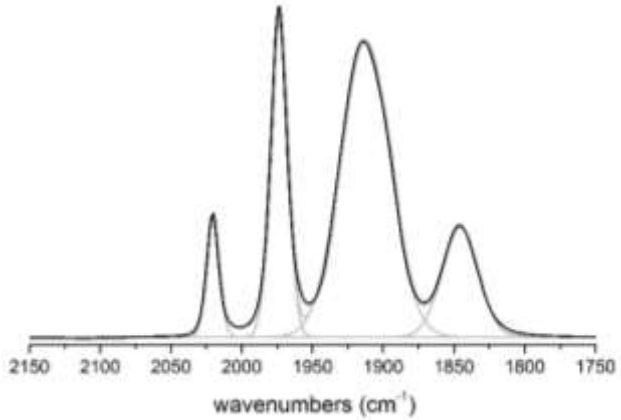


Figure S-29. Deconvoluted IR spectra of the carbonyl region of the neutral (top) and oxidised (bottom) state of **1** and **2** inside an OTTLE cell (1,2-$C_2H_4Cl_2$ / $NBuPF_6$, r.t.). * Residual peaks

4⁰



4⁺

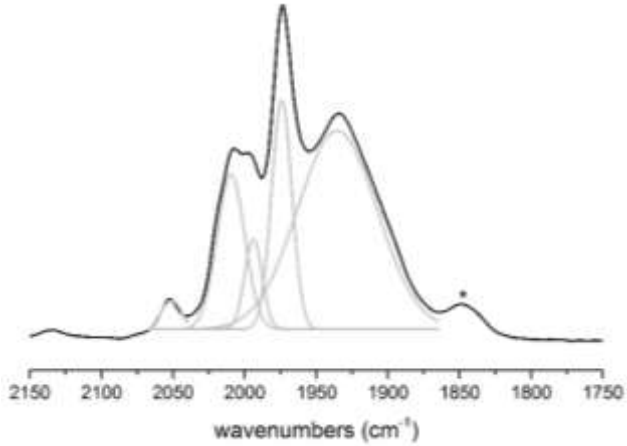


Figure S-30. Deconvoluted IR spectra of the carbonyl region of the neutral (top) and oxidised (bottom) state of **4** inside an OTTLE cell (1,2-$C_2H_4Cl_2$ / $NBuPF_6$, r.t.). * Residual peaks5

Table S-5. Deconvoluted IR spectra of the carbonyl region of the neutral and oxidised states of **1**, **2** and **4** (1,2-$C_2H_4Cl_2$ / $NBuPF_6$, r.t.)

Complex	**Bands (cm^{-1})**
1	2072, 1988, 1955, 1942, 1879
1^+	2080, 2072 (residual from neutral form), 1994, 1971, 1951, 1934
2	2067, 1972, 1959, 1931, 1888, 1863
2^+	2069, 1998, 1979, 1946, 1934
4	2020, 1973, 1912, 1846
4^+	1935, 1974, 1993, 2009, 2051

DFT calculations

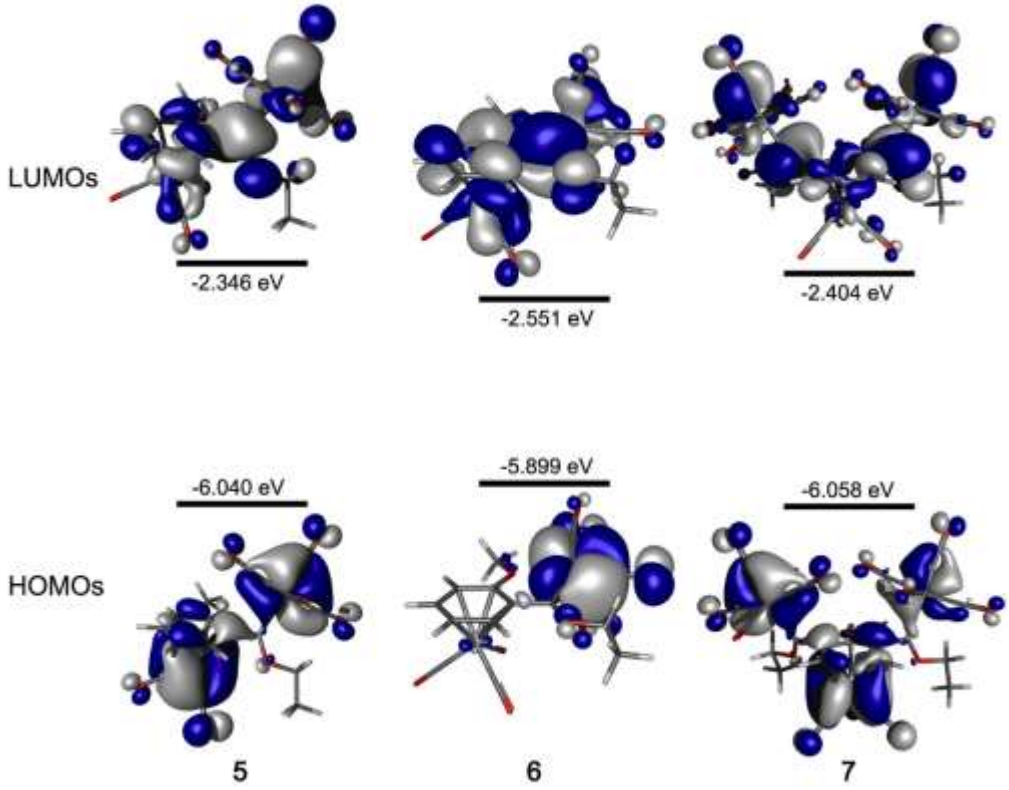


Figure S-31. Contour plots of the calculated HOMO and LUMO orbitals of the neutral complexes for **5-7**

Table S-6. Computed IR frequencies (cm^{-1}) and intensity [counts] of the carbonyl region as determined from DFT calculations of the neutral and oxidised species of **1-7**

Complex	**Bands (cm^{-1} [intensity])**
1	2129 [560] (br), 2041 [1784], 2010 [2050], 1976 [729] (br)
1^+	2152 [198] (br), 2138 [1650], 2037 [1705], 2033 [1390] (br)
2	2128 [499] (br), 2038 [1737], 2010 [2201], 1979 [511] (br)
2^+	2150 [383] (br), 2133 [1637], 2075 [776], 2024 [1518] (br)
3	2128 [565] (br), 2050 [639] (br), 2040 [1354], 2009 [1810], 1990 [625], 1978 [964] (br)
3^+	2152 [369] (br), 2134 [1863], 2070 [786], 2029 [1627] (br)
4	2091 [608] (br), 2050 [1994], 2000 [1493], 1953 [1114] (br)
4^+	2153 [510] (br), 2095 [878], 2088 [1923], 2056 [1235], 2030 [420] (br)
5	2170 [415] (br), 2066 [1570], 2042 [2502], 2031 [557] (br)
5^+	2192 [164] (br), 2174 [1867], 2121 [876], 2097 [1496], 2056 [1713] (br)
6	2134 [560] (br), 2089 [2127], 2041 [1149], 1992 [1155] (br)
6^+	2199 [404] (br), 2131 [795], 2128 [2079], 2090 [580], 2065 [414] (br)
7	2178 [580] (br), 2102 [403], 2078 [2472], 2069 [2034], 2043 [3962], 2021 [414] (br)
7^+	2194 [420] (br), 2163 [1982], 2113 [1235], 2108 [1312], 2093 [1115], 2054 [2810] (br)

Table S-7. Energy (eV) of the calculated HOMO and LUMOs of the oxidized species of **1-7**

	α-HOMO	β-HOMO	α-LUMO	β-LUMO
1^{+}	-8.825	-8.816	-5.483	-7.180
2^{+}	-8.771	-8.765	-5.953	-7.159
3^{+}	-8.638	-8.623	-5.656	-7.169
4^{+}	-9.116	-9.086	-6.184	-7.700
5^{+}	-9.133	-9.115	-5.37	-7.314
6^{+}	-9.573	-9.550	-6.137	-7.736
7^{+}	-8.980	-8.954	-5.390	-7.172

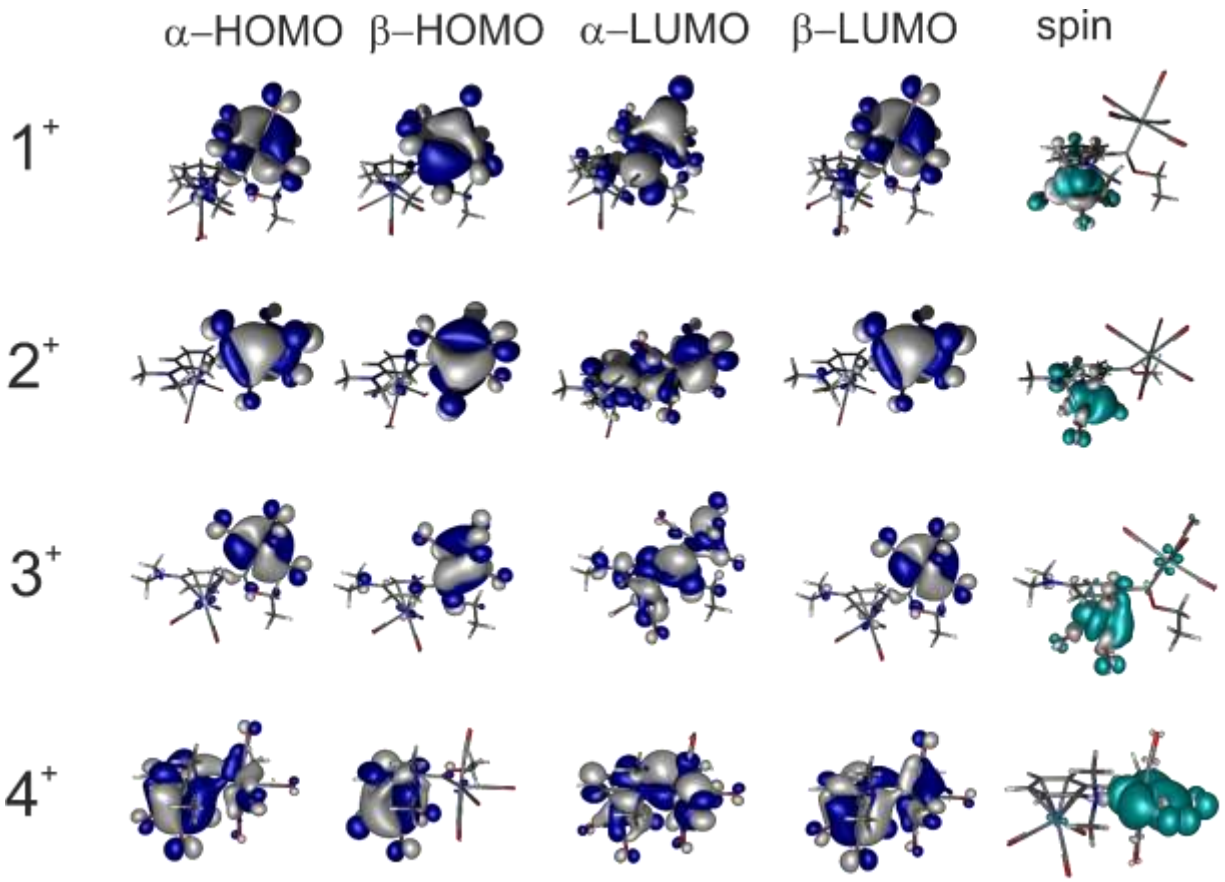


Figure S-32. Contour plots and spin densities of the calculated HOMO and LUMO orbitals of the oxidised complexes **1**$^{+}$**-4**$^{+}$

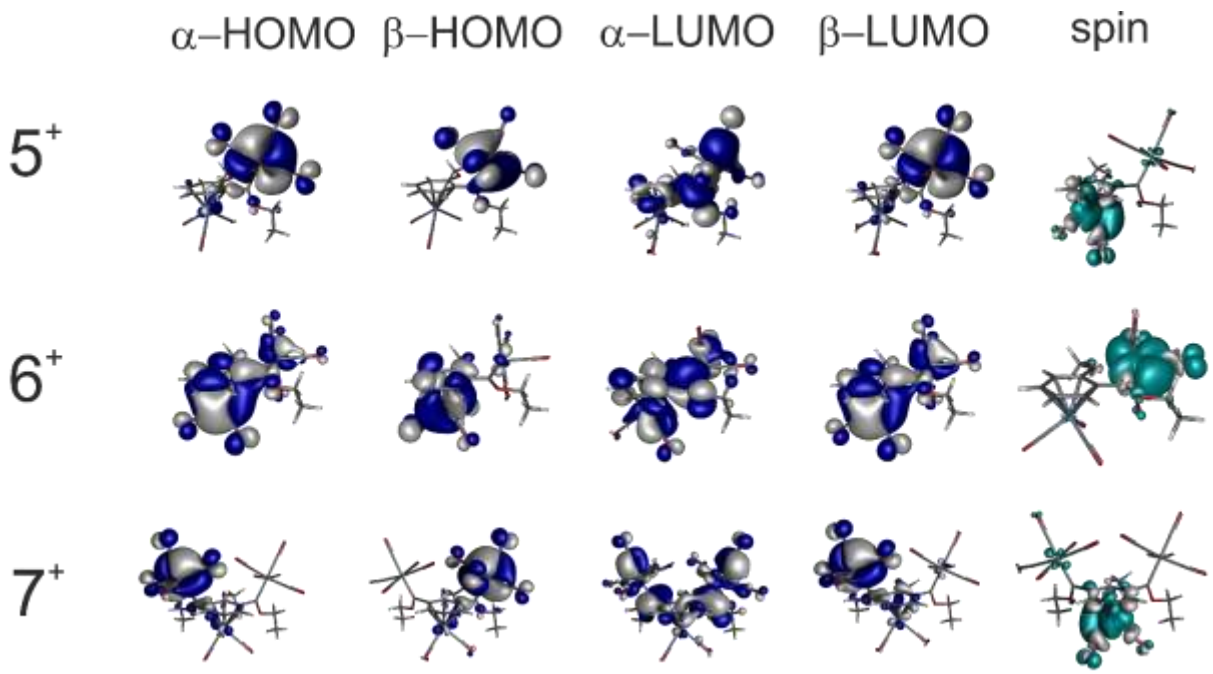


Figure S-33. Contour plots and spin densities of the calculated HOMO and LUMO orbitals of the oxidised complexes $\mathbf{5}^{+}$-$\mathbf{7}^{+}$

DFT calculated Structural Coordinates

Complex 1:

W	0.8595	2.14264	16.19429
C	1.4671	3.28851	17.77774
O	1.80495	3.9192	18.67765
C	-1.05852	2.25632	16.96979
O	-2.08763	2.39083	17.45535
C	0.51745	3.91686	15.17075
O	0.36246	4.94435	14.69212
C	2.81648	2.19239	15.51955
O	3.91098	2.27154	15.19223
C	1.30374	0.49347	17.36801
O	1.58597	-0.37871	18.0543
C	0.31824	0.78271	14.50217
O	-0.49129	-0.23409	14.4465
C	-1.39195	-0.60845	15.53755
H	-2.11279	0.199	15.64894
H	-0.80282	-0.70104	16.44664
C	-2.05531	-1.90903	15.15735
H	-2.63388	-1.80232	14.23921
H	-2.73394	-2.20168	15.96041
H	-1.318	-2.70124	15.02342
C	1.14532	0.78764	13.2475
C	1.1298	1.80915	12.24935
C	2.14795	1.75026	11.24727
H	2.13504	2.46004	10.43642
C	3.17956	0.8046	11.28904
H	3.94373	0.82543	10.52495
C	3.20514	-0.18442	12.28725
H	3.9856	-0.92986	12.31896
C	2.15502	-0.21151	13.21219
H	2.14345	-0.97732	13.97582
Cr	1.24332	-0.36258	11.17237
C	-0.30934	0.04719	10.27929
O	-1.28225	0.29282	9.69861
C	1.86667	-1.14332	9.64122
O	2.26433	-1.64973	8.67591
C	0.51573	-1.98297	11.6413
O	0.06406	-3.01184	11.9228
N	0.19096	2.80678	12.21869

C	-1.21497	2.56961	12.54229
H	-1.81868	2.66825	11.63527
H	-1.57686	3.29524	13.27195
H	-1.36953	1.56932	12.9299
C	0.38749	3.95967	11.34737
H	1.4165	4.31061	11.39535
H	-0.25944	4.76232	11.69887
H	0.12767	3.74566	10.30355

Complex 1^{+}

W	0.93683	2.12125	16.2514
C	1.52105	3.29283	17.88573
O	1.83782	3.92316	18.77813
C	-1.03877	2.41044	16.85393
O	-2.09923	2.6153	17.22112
C	0.89545	3.872	15.14387
O	0.90645	4.86412	14.57596
C	2.94071	1.96926	15.75761
O	4.05181	1.91402	15.49468
C	1.10545	0.48365	17.53531
O	1.23588	-0.38068	18.26715
C	0.3965	0.84261	14.57716
O	-0.45905	-0.14891	14.42978
C	-1.39934	-0.54171	15.4789
H	-2.07397	0.29754	15.64312
H	-0.83237	-0.72574	16.38876
C	-2.13327	-1.77421	15.00892
H	-2.69057	-1.5812	14.09166
H	-2.84488	-2.07678	15.77872
H	-1.44727	-2.60421	14.83874
C	1.22919	0.894	13.31002
C	1.11729	1.87491	12.26175
C	2.09477	1.78461	11.21243
H	1.99194	2.42189	10.34905
C	3.23087	0.96527	11.29916
H	3.97297	1.00376	10.51344
C	3.37342	0.0754	12.36725
H	4.2257	-0.58505	12.44012
C	2.34377	0.01987	13.31578
H	2.42247	-0.68309	14.13435
Cr	1.40958	-0.41356	11.29856
C	-0.34646	-0.20759	10.59689

O	-1.39749	-0.08201	10.17694
C	1.87461	-0.99386	9.52708
O	2.15659	-1.32106	8.47789
C	0.78348	-2.1145	11.9533
O	0.41238	-3.10816	12.35597
N	0.13384	2.7951	12.16675
C	-1.20877	2.63683	12.72616
H	-1.93527	2.82347	11.93238
H	-1.39084	3.34707	13.53303
H	-1.36721	1.62834	13.08787
C	0.25701	3.93044	11.25098
H	1.28016	4.29866	11.22436
H	-0.37365	4.73408	11.62626
H	-0.07195	3.67984	10.23707

Complex 2

W	0.07417	13.87056	7.77252
C	-0.47188	15.57956	8.77602
O	-0.76705	16.53667	9.33329
C	1.68388	13.7272	9.07186
O	2.56284	13.68696	9.80421
C	1.2057	15.08292	6.53794
O	1.8108	15.80169	5.88261
C	-1.59281	14.11636	6.56062
O	-2.524	14.29292	5.9196
C	-1.12687	12.82846	9.10428
O	-1.81574	12.34049	9.87805
C	0.82034	12.0758	6.64653
O	1.14464	10.89659	7.13125
C	0.86131	10.46099	8.48194
H	-0.22043	10.44501	8.60345
H	1.28906	11.1787	9.17988
C	1.45811	9.08287	8.65271
H	1.03086	8.38223	7.93517
H	1.23969	8.72168	9.65933
H	2.54156	9.10349	8.52621
C	1.24819	12.07491	5.21554
C	0.66132	12.94614	4.26982
H	-0.13818	13.58223	4.60146
C	1.11079	13.04613	2.91608
C	2.03567	12.06532	2.48662
H	2.3368	12.00652	1.45383

C	2.62397	11.17398	3.41503
H	3.35446	10.46012	3.06041
C	2.25569	11.16882	4.75659
H	2.70762	10.47336	5.44437
N	0.61562	13.99884	2.0689
C	-0.47451	14.86705	2.49657
H	-1.41842	14.32695	2.6306
H	-0.62324	15.63342	1.73979
H	-0.22184	15.37393	3.42773
C	0.84272	13.86655	0.63758
H	1.90998	13.83603	0.41201
H	0.42569	14.73507	0.1343
H	0.37115	12.96691	0.22377
Cr	0.40113	10.84059	3.54195
C	-0.27795	9.56203	4.70003
O	-0.69286	8.76491	5.42004
C	-1.33079	11.20143	2.99439
O	-2.40426	11.44433	2.65258
C	0.52416	9.54622	2.20674
O	0.62518	8.75611	1.37754

Complex 2^{+}

W	0.16068	13.8909	7.79597
C	-0.27203	15.66872	8.81042
O	-0.50255	16.63948	9.35787
C	1.83171	13.69614	9.04091
O	2.73512	13.61614	9.72948
C	1.24921	15.02285	6.45798
O	1.81904	15.68231	5.71523
C	-1.54281	14.21081	6.6606
O	-2.47839	14.41088	6.03379
C	-1.01161	12.91643	9.22251
O	-1.67459	12.4617	10.0311
C	0.69732	12.07791	6.70459
O	0.8956	10.84095	7.11658
C	0.71899	10.4081	8.49666
H	-0.35283	10.36933	8.68804
H	1.17337	11.1503	9.14938
C	1.36667	9.052	8.64759
H	0.9142	8.31736	7.98141
H	1.22968	8.70759	9.67384
H	2.43833	9.10045	8.45005

C	1.1124	12.08566	5.24672
C	0.4691	12.89152	4.28615
H	-0.38921	13.46159	4.59409
C	0.9939	13.08434	2.9618
C	1.97624	12.13614	2.54718
H	2.31818	12.1123	1.52518
C	2.61539	11.31194	3.49571
H	3.41738	10.66421	3.16784
C	2.21029	11.28497	4.82855
H	2.70835	10.64349	5.53836
N	0.50539	14.02101	2.13565
C	-0.56529	14.92233	2.5689
H	-1.51618	14.39612	2.68812
H	-0.69558	15.69454	1.81742
H	-0.30331	15.40944	3.50792
C	0.96726	14.10058	0.74846
H	2.05439	14.17847	0.70482
H	0.54847	14.99067	0.29016
H	0.64648	13.23175	0.16688
Cr	0.40414	10.7445	3.51914
C	-0.1426	9.28042	4.64923
O	-0.46181	8.40813	5.2998
C	-1.2654	10.97063	2.61072
O	-2.24915	11.12824	2.06363
C	0.7399	9.40217	2.20639
O	0.93978	8.60992	1.41571

Complex 3

W	2.27187	-0.42716	0.13177
C	3.92248	-1.51666	0.61236
O	4.85625	-2.13785	0.87718
C	3.13477	-0.07941	-1.71896
O	3.64661	0.06958	-2.73326
C	1.47852	-2.17825	-0.62928
O	1.1077	-3.1827	-1.03874
C	1.5196	-0.83452	2.01898
O	1.15828	-1.08013	3.07796
C	3.25326	1.20138	0.95018
O	3.8771	2.03221	1.43623
C	0.40784	0.70882	-0.51526
C	-0.94477	0.12045	-0.61744
C	-1.94723	0.69104	-1.45713

H	-1.72357	1.58815	-2.01245
C	-3.21014	0.11784	-1.60814
H	-3.91281	0.60319	-2.2659
C	-3.55617	-1.10753	-0.95728
C	-2.61895	-1.58458	0.00923
H	-2.85904	-2.42833	0.63502
C	-1.35235	-1.00858	0.13764
H	-0.67937	-1.44065	0.85959
N	-4.72098	-1.73746	-1.19416
C	-5.7228	-1.14401	-2.07756
H	-6.16565	-0.24339	-1.64195
H	-6.51163	-1.87136	-2.24378
H	-5.28707	-0.88997	-3.04382
C	-5.10222	-2.90986	-0.40964
H	-4.31219	-3.66081	-0.42626
H	-5.99354	-3.34676	-0.84921
H	-5.3192	-2.64912	0.63076
Cr	-2.77746	0.65985	0.61696
C	-2.7315	2.49555	0.65854
O	-2.69232	3.65202	0.69997
C	-4.51687	0.69766	1.21032
O	-5.61294	0.7212	1.58326
C	-2.21259	0.66103	2.36625
O	-1.8696	0.6812	3.47191
O	0.34675	1.92077	-1.00979
C	1.4667	2.84076	-1.09143
H	1.73527	3.11909	-0.07366
H	2.30502	2.33242	-1.5614
C	1.01712	4.03786	-1.89497
H	1.83913	4.75364	-1.95132
H	0.74311	3.74901	-2.91064
H	0.16543	4.5293	-1.42316

Complex 3^{+}

W	2.29386	-0.48531	0.04289
C	3.95094	-1.74685	0.24341
O	4.84949	-2.43734	0.34957
C	3.01494	0.01893	-1.85203
O	3.42595	0.27466	-2.88357
C	1.2775	-2.10507	-0.74172
O	0.73846	-3.02539	-1.15619
C	1.71674	-1.05795	1.95277

O	1.40813	-1.3875	3.00237
C	3.46722	1.02253	0.87731
O	4.16846	1.79035	1.34627
C	0.52725	0.75838	-0.25483
C	-0.85167	0.16802	-0.36033
C	-1.75657	0.61734	-1.35205
H	-1.47019	1.44255	-1.98769
C	-3.01144	0.01844	-1.55202
H	-3.63873	0.40045	-2.34171
C	-3.39857	-1.15099	-0.82332
C	-2.60123	-1.42392	0.3342
H	-2.91268	-2.17195	1.04566
C	-1.34011	-0.83001	0.50724
H	-0.74367	-1.14335	1.34999
N	-4.49114	-1.86224	-1.12977
C	-5.36061	-1.45652	-2.2365
H	-5.89124	-0.52695	-2.01235
H	-6.09645	-2.23601	-2.40693
H	-4.78616	-1.32925	-3.15448
C	-4.91259	-2.98712	-0.29142
H	-4.07782	-3.6622	-0.10379
H	-5.68184	-3.54499	-0.81631
H	-5.32405	-2.64824	0.66358
Cr	-2.85555	0.85644	0.59722
C	-3.05411	2.74046	0.24746
O	-3.16991	3.84688	0.0248
C	-4.70906	0.88182	1.03129
O	-5.81834	0.89189	1.28598
C	-2.55943	1.00584	2.4964
O	-2.38641	1.07571	3.61513
O	0.38483	2.04244	-0.53423
C	1.50396	2.96937	-0.62711
H	1.89027	3.11471	0.38105
H	2.27608	2.51404	-1.2443
C	0.99197	4.25911	-1.22348
H	1.81434	4.97368	-1.28324
H	0.607	4.10444	-2.23228
H	0.20678	4.69879	-0.60765

Complex 4

W	-1.77827	-0.25109	0.11615
Cr	2.90111	-0.03972	0.07545
O	-3.58247	-2.78282	0.85707
O	-3.62684	0.19172	-2.46764
O	-3.8831	1.687	1.39609
O	-0.6018	-0.29244	3.10163
O	-0.1373	2.41634	-0.65822
O	2.67973	-1.95245	2.37475
O	2.57996	2.20198	2.04946
O	5.8418	-0.04944	0.65323
N	-0.07394	-1.67689	-0.88976
C	-2.9393	-1.85939	0.59408
C	-2.90773	-0.00417	-1.59106
C	-3.09622	0.97038	0.91831
C	-0.95964	-0.32046	2.00959
C	-0.23077	1.11332	-0.57569
C	2.73384	-1.22662	1.47737
C	2.69988	1.34202	1.29102
C	4.7089	-0.04765	0.43276
C	1.01852	0.51601	-1.10569
C	2.12126	1.30605	-1.55979
H	2.04506	2.38132	-1.52539
C	3.28192	0.70522	-2.03899
H	4.10887	1.3147	-2.37354
C	3.39817	-0.70381	-2.02419
H	4.31152	-1.17799	-2.35293
C	2.32831	-1.49457	-1.5902
H	2.43161	-2.5686	-1.60028
C	1.12606	-0.89046	-1.15568
C	0.1868	-2.87565	-0.04461
H	0.51994	-2.57089	0.94137
H	0.92908	-3.53697	-0.49588
H	-0.74293	-3.42892	0.05277
C	-0.567	-2.1604	-2.22416
H	-1.50914	-2.68212	-2.07542
H	0.15488	-2.84594	-2.67521
H	-0.7208	-1.31335	-2.88779
C	-1.21463	3.29022	-0.2141
H	-2.11688	3.00734	-0.75453
H	-1.3636	3.11704	0.85066
C	-0.80139	4.71267	-0.50535

H	-1.59761	5.38521	-0.18125
H	0.10978	4.97654	0.03384
H	-0.63833	4.86375	-1.57347

Complex 4^{+}

W	-1.78104	-0.23873	0.05872
Cr	2.83319	-0.01785	0.00978
O	-3.66323	-2.83337	0.66147
O	-3.2905	0.17459	-2.7441
O	-4.03829	1.6027	1.35096
O	-0.4997	-0.32048	3.00681
O	-0.13177	2.42331	-0.62602
O	2.4405	-1.76314	2.43893
O	2.68882	2.4242	1.79766
O	5.7799	-0.2924	0.63145
N	-0.09937	-1.6871	-0.88139
C	-3.00898	-1.92808	0.46348
C	-2.73045	-0.0018	-1.76725
C	-3.22389	0.95534	0.8836
C	-0.9202	-0.32951	1.94995
C	-0.2065	1.12182	-0.5912
C	2.56514	-1.10207	1.51196
C	2.75883	1.49667	1.13564
C	4.66616	-0.19009	0.40617
C	0.99609	0.5182	-1.1541
C	2.10201	1.2982	-1.63175
H	2.02478	2.3742	-1.61659
C	3.26237	0.68512	-2.09391
H	4.09484	1.28469	-2.43296
C	3.38208	-0.72378	-2.02913
H	4.30269	-1.20334	-2.32959
C	2.30284	-1.51288	-1.60324
H	2.41179	-2.58654	-1.58752
C	1.11352	-0.89905	-1.16042
C	0.1583	-2.86453	0.00376
H	0.48011	-2.53932	0.98568
H	0.91202	-3.5269	-0.4237
H	-0.76404	-3.43215	0.09926
C	-0.56593	-2.22303	-2.20905
H	-1.51874	-2.72912	-2.07258
H	0.15908	-2.93492	-2.60826
H	-0.6869	-1.40663	-2.91582

C	-1.19434	3.28182	-0.10288
H	-2.11478	3.02199	-0.62652
H	-1.29739	3.06206	0.96016
C	-0.79559	4.71611	-0.34597
H	-1.57546	5.37229	0.04364
H	0.13719	4.95688	0.16408
H	-0.68285	4.91823	-1.41141

Complex 5

W	3.48327	5.08619	11.97831
C	3.92316	7.06568	11.97351
O	4.15977	8.1882	11.9743
C	2.37347	5.36199	13.68269
O	1.76807	5.52775	14.637
C	1.87432	5.59428	10.81126
O	1.00898	5.96939	10.16514
C	4.65853	4.81604	10.30308
O	5.33355	4.69318	9.3932
C	5.16708	4.87569	13.12158
O	6.12403	4.88263	13.75007
C	2.81079	2.98452	11.96623
O	3.11727	1.98704	12.73257
Cr	0.87564	0.5741	10.41073
C	2.45724	-0.0786	9.78122
O	3.45855	-0.49513	9.38869
C	0.01746	-0.75219	9.50606
O	-0.52376	-1.59885	8.93916
C	1.02769	-0.57222	11.81703
O	1.12256	-1.30868	12.69959
C	1.63947	2.56113	11.14387
C	1.59337	2.63052	9.72189
C	0.41164	2.28331	9.04428
H	0.3815	2.27749	7.9651
C	-0.74152	1.92191	9.76931
H	-1.63868	1.65256	9.2278
C	-0.73339	1.90254	11.16778
H	-1.61511	1.61749	11.7241
C	0.4709	2.17108	11.83853
H	0.5081	2.10677	12.91816
O	2.71966	2.98249	9.10357
C	2.75507	2.95671	7.68116
H	3.76305	3.25717	7.40689

H	2.03484	3.66025	7.25824
H	2.55821	1.9492	7.30691
C	4.12671	2.07704	13.76289
H	3.87138	2.91478	14.41263
H	5.08005	2.27178	13.27092
C	4.13636	0.77199	14.50713
H	3.17116	0.58192	14.97954
H	4.89814	0.8188	15.28792
H	4.37603	-0.05847	13.84114

Complex 5^+

W	3.3283	5.18771	12.10223
C	3.65885	7.23856	12.15434
O	3.83376	8.35943	12.17631
C	2.08496	5.36622	13.74649
O	1.39713	5.44636	14.64813
C	1.76984	5.5997	10.8445
O	0.91726	5.87811	10.13601
C	4.60016	5.03629	10.47616
O	5.2894	4.9372	9.57806
C	4.95394	5.03301	13.36082
O	5.86289	5.04527	14.04642
C	2.89997	3.10182	11.97805
O	3.40047	1.99671	12.46367
Cr	0.76522	0.65228	10.75523
C	2.40099	-0.2546	10.43646
O	3.37914	-0.78365	10.22205
C	0.01733	-0.73999	9.72562
O	-0.42456	-1.58437	9.11133
C	0.17976	-0.39308	12.2319
O	-0.18749	-1.008	13.108
C	1.68235	2.71211	11.18982
C	1.72917	2.55575	9.777
C	0.56335	2.15573	9.09348
H	0.59695	1.96256	8.03069
C	-0.6745	2.08872	9.77171
H	-1.56752	1.82849	9.21737
C	-0.74018	2.30347	11.14224
H	-1.68194	2.21999	11.66873
C	0.45116	2.55289	11.85187
H	0.42094	2.66884	12.92857
O	2.90352	2.736	9.20377

C	3.03323	2.59669	7.78892
H	4.06601	2.85141	7.56816
H	2.36576	3.28814	7.27084
H	2.83572	1.56712	7.48147
C	4.56792	2.01288	13.32019
H	4.33111	2.62896	14.18886
H	5.38144	2.47809	12.76167
C	4.88211	0.5945	13.70359
H	4.05401	0.1377	14.24833
H	5.75695	0.58891	14.35601
H	5.11158	-0.01374	12.82737

Complex 6

W	1.80093	-0.29483	0.02483
C	2.99616	-1.87994	0.39257
O	3.67174	-2.79044	0.5983
C	3.26849	0.8993	0.45066
O	4.15045	1.61334	0.70663
C	2.55655	-0.24089	-1.87458
O	3.08202	-0.15075	-2.88902
C	1.41175	-0.2014	2.03147
O	1.31857	-0.08706	3.1679
C	0.19347	1.05135	-0.52619
O	0.07196	2.34659	-0.55377
Cr	-2.90684	-0.07822	0.0316
C	-2.32246	-0.87142	1.57731
O	-1.96403	-1.36744	2.55115
C	-4.60091	-0.5751	0.49174
O	-5.67144	-0.87882	0.78682
C	-3.18121	1.4677	0.97441
O	-3.35927	2.43476	1.57041
C	-1.02781	0.4345	-1.05492
O	-0.04747	-1.62286	-0.5323
C	-1.12932	-0.9784	-1.02332
C	-2.28956	-1.63815	-1.45139
H	-2.38787	-2.71044	-1.37752
C	-3.35444	-0.87552	-1.96438
H	-4.25565	-1.38424	-2.27942
C	-3.25691	0.52126	-2.08284
H	-4.08409	1.09497	-2.47732
C	-2.12348	1.16892	-1.5864
H	-2.06155	2.24773	-1.60781

C	-0.11462	-3.05517	-0.39766
H	-0.93451	-3.32433	0.2684
H	0.83097	-3.35895	0.03702
H	-0.24092	-3.51062	-1.37922
C	1.14476	3.18838	-0.08317
H	2.00314	3.02902	-0.73757
H	1.40305	2.86822	0.92729
C	0.66438	4.61171	-0.12072
H	0.40344	4.91277	-1.13693
H	1.46295	5.26493	0.23639
H	-0.20519	4.74978	0.52452

Complex 6^+

W	1.80888	-0.23785	0.02916
C	3.07412	-1.87384	0.4007
O	3.7515	-2.75632	0.60887
C	3.39816	0.94006	0.37982
O	4.30598	1.60102	0.56841
C	2.33935	-0.15094	-1.95645
O	2.66118	-0.06204	-3.04121
C	1.32718	-0.24859	2.044
O	1.11684	-0.22062	3.15701
C	0.18327	1.09279	-0.52006
O	0.08358	2.3842	-0.54837
Cr	-2.83	-0.07772	-0.0022
C	-2.29287	-0.90076	1.57037
O	-1.95276	-1.42338	2.52822
C	-4.56724	-0.56246	0.45108
O	-5.63361	-0.85941	0.7182
C	-3.08754	1.51071	0.94564
O	-3.22298	2.48746	1.51501
C	-0.99134	0.45456	-1.07387
O	0.00611	-1.5852	-0.4552
C	-1.0884	-0.96103	-0.99791
C	-2.22044	-1.65091	-1.44472
H	-2.30536	-2.72318	-1.35296
C	-3.3002	-0.90667	-1.95908
H	-4.198	-1.43028	-2.25987
C	-3.22069	0.49124	-2.10608
H	-4.06123	1.0443	-2.50214
C	-2.10225	1.16722	-1.62029
H	-2.05681	2.24682	-1.6527

C	-0.10227	-2.98862	-0.14745
H	-0.97541	-3.16057	0.4811
H	0.79613	-3.25448	0.40045
H	-0.15804	-3.56371	-1.07159
C	1.14541	3.22111	-0.02903
H	2.00695	3.1032	-0.6901
H	1.39676	2.85658	0.9703
C	0.65269	4.63916	-0.002
H	0.39585	4.9843	-1.0044
H	1.44265	5.28433	0.38631
H	-0.21958	4.74102	0.64484

Complex 7

W	4.75199	4.43593	4.47135
C	2.87268	4.69917	5.20691
O	1.8143	4.84627	5.61827
C	4.79661	2.6307	5.4561
O	4.7587	1.64587	6.03309
C	5.40712	5.39687	6.16753
O	5.67016	5.94432	7.13365
C	4.55694	6.26438	3.55352
O	4.40034	7.28308	3.06437
C	3.85024	3.52871	2.86284
O	3.26346	3.05044	2.00771
C	6.77429	4.25243	3.64952
O	7.37219	3.30925	2.99926
W	9.0511	9.2662	7.0657
C	8.12235	10.75567	8.0933
O	7.59282	11.59209	8.67051
C	10.71835	9.7366	8.15831
O	11.58563	10.08379	8.81873
C	8.49023	7.9249	8.52657
O	8.1821	7.19618	9.34752
C	7.25779	9.01431	6.09739
O	6.22945	8.9475	5.60418
C	9.65211	10.63619	5.65476
O	9.99251	11.41143	4.88923
C	9.90213	7.61166	5.90394
O	10.9408	6.8668	6.07195
Cr	9.75416	5.93785	2.89592
C	9.76841	4.85416	1.42877
O	9.78777	4.1768	0.49714

C	10.93124	4.77301	3.66899
O	11.69832	4.03896	4.11693
C	11.20269	6.79489	2.20035
O	12.12008	7.33248	1.75465
C	7.68048	5.44964	3.6673
O	8.58934	5.2253	5.92673
C	8.47164	5.87148	4.76022
C	9.15536	7.12438	4.70068
C	9.03746	7.92257	3.55248
H	9.56942	8.86363	3.50649
C	8.26612	7.51065	2.45379
H	8.20699	8.12025	1.5634
C	7.63629	6.26432	2.50485
H	7.06341	5.9189	1.6534
C	8.57147	3.80334	5.97882
H	7.55212	3.41828	5.91679
H	8.99476	3.53606	6.94466
H	9.18079	3.38086	5.17855
C	6.73372	2.04003	2.72184
H	6.32094	1.6582	3.6552
H	5.92284	2.23174	2.01946
C	7.77099	1.12281	2.14003
H	8.18482	1.53553	1.21886
H	7.30125	0.16525	1.9078
H	8.58235	0.94447	2.84752
C	11.8363	7.03697	7.19517
H	12.34504	7.99207	7.06106
H	11.23441	7.06748	8.10404
C	12.79979	5.88463	7.19337
H	12.27668	4.93431	7.31012
H	13.48958	6.00405	8.03087
H	13.37977	5.85935	6.26971

Complex 7^{+}

W	4.75171	4.51036	4.35886
C	2.77882	4.79002	4.93625
O	1.69901	4.93734	5.25265
C	4.65581	2.68282	5.31152
O	4.54127	1.69291	5.86261
C	5.28082	5.44329	6.11644
O	5.52692	5.9616	7.09988

C	4.64709	6.36649	3.48009
O	4.55267	7.39811	3.00642
C	4.00219	3.62205	2.64812
O	3.53874	3.14981	1.72312
C	6.79399	4.26928	3.7524
O	7.49606	3.27206	3.27764
W	9.05358	9.17656	7.14434
C	8.0742	10.6037	8.29298
O	7.53423	11.37832	8.92254
C	10.74719	9.68304	8.20741
O	11.62898	10.02948	8.83901
C	8.59603	7.74397	8.57034
O	8.35569	6.94617	9.34232
C	7.25797	8.88907	6.20358
O	6.24138	8.78762	5.69358
C	9.50255	10.63273	5.75343
O	9.74633	11.42485	4.97324
C	9.96175	7.65689	5.95178
O	11.06107	6.95396	5.99931
Cr	9.82415	5.93468	2.95288
C	9.7575	4.66159	1.57097
O	9.74015	3.90008	0.72922
C	10.95274	4.66475	3.78612
O	11.61672	3.88642	4.27612
C	11.14051	6.7443	1.86085
O	11.91186	7.23982	1.19535
C	7.69433	5.48188	3.75899
O	8.59885	5.32625	6.03639
C	8.47084	5.92948	4.86362
C	9.17051	7.16923	4.77222
C	9.09715	7.9346	3.59907
H	9.65036	8.8634	3.54036
C	8.29043	7.52471	2.52242
H	8.22408	8.12243	1.62305
C	7.62341	6.30953	2.61101
H	7.02883	5.96338	1.77386
C	8.42169	3.92323	6.21943
H	7.37507	3.64025	6.10923
H	8.7477	3.72719	7.23786
H	9.04182	3.36517	5.51649
C	6.91416	1.9596	3.10449
H	6.67054	1.5749	4.09625
H	5.99077	2.07133	2.5361

C	7.91522	1.09177	2.39535
H	8.15599	1.48682	1.4077
H	7.49094	0.09448	2.26692
H	8.83725	0.99357	2.97047
C	12.02158	7.14044	7.06466
H	12.45371	8.13534	6.94709
H	11.48257	7.09508	8.0121
C	13.06046	6.06051	6.95217
H	12.61753	5.06938	7.0599
H	13.79517	6.1911	7.74853
H	13.58655	6.11099	5.99761

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