Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPORTING INFORMATION

Hetero-trimetallic Complexes Comprising Bridging Boryl and Borylene Ligands: An Experimental and Theoretical Study

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Figure S68 Optimized geometry of **5**.

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I *Supplementary Data*

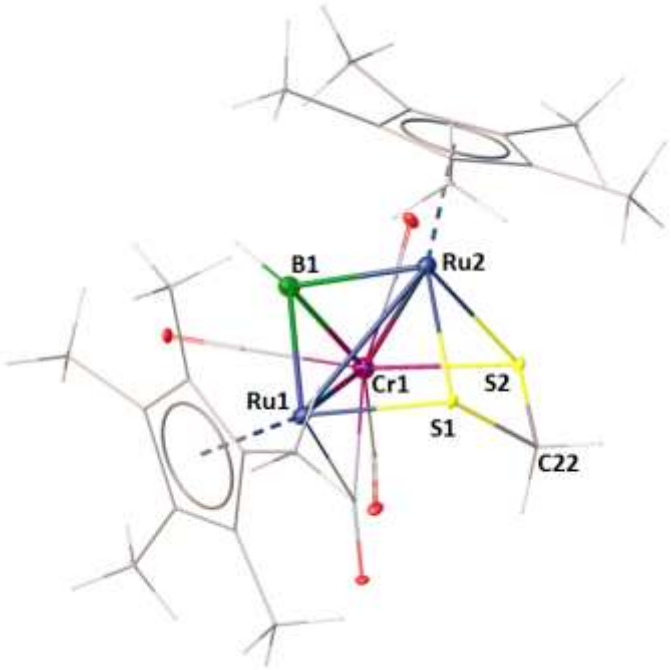

Figure S1. Molecular structure and labelling diagram for **2**. Selected bond lengths (Å) and angles (°): Ru1-B1 2.127(15), Ru2-B1 2.088(16), Cr1-B1 2.133(17), Ru1-Cr1 2.769(2), Ru2-Cr1 2.744(2), Cr1-S2 2.330(4), Ru1-S1 2.299(4), Ru2-S2 2.342(4), Ru1-Ru2 2.7802(14), C22-S1 1.803(16), C22-S2 1.846(16), S1-C22-S2 101.0(7), S1-Ru2-S2 74.51(13), Ru2-Cr1-Ru1 60.57(5), Ru2-B1-Ru1 82.5(6), C22-S1-Ru2 92.5(5), C22-S1-Ru1 109.6(6).

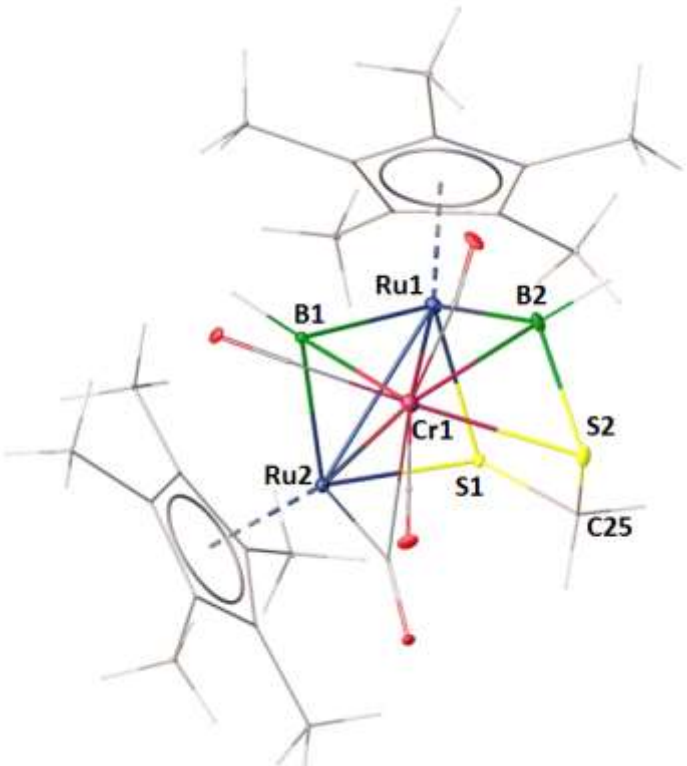

Figure S2. Molecular structure and labelling diagram for **3**. Selected bond lengths (Å) and angles (°): Ru1-B1 2.086(7), Ru2-B1 2.156(7), Cr1-B1 2.168(7), Cr1-B2 2.213(8), Ru1-Cr1 2.8000(11), Ru2-Cr1 2.7759(11), Cr1-S2 2.454(2), Ru1-S1 2.2783(17), Ru1-Ru2 2.7893(7), C25- S1 1.841(7), C25-S2 1.802(8), S1-C25-S2 113.7(4), S1-Ru1-Ru2 53.00(4), Ru2-Cr1-Ru1 60.03(2), Ru1-B2-Cr1 81.9(3), C25-S2-Cr1 106.6(2), C25 S1 Ru1 108.8(3), C25-S1-Ru2 108.8(3).

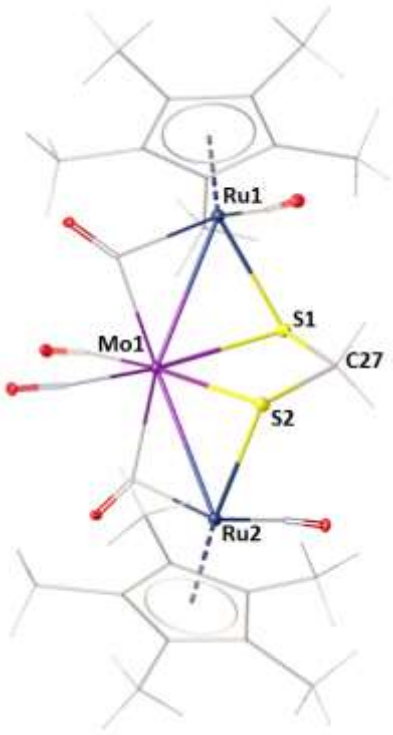

Figure S3. Molecular structures and labelling diagrams of **5**. Selected bond lengths (Å) and bond angles (°); Ru1-Mo1 2.8689(12), Ru2-Mo1 2.8703(11), Mo1-S1 2.5067(12), Ru1-S1 2.3671(11), C27-S1 1.826(4), Ru1-Mo1-Ru2 137.38(3), S1-Mo1-S2 71.43(4), S1-C27-S2 106.32(18), S1-Ru1-Mo1 56.23(3), Ru1-S1-Mo1 72.06(4).

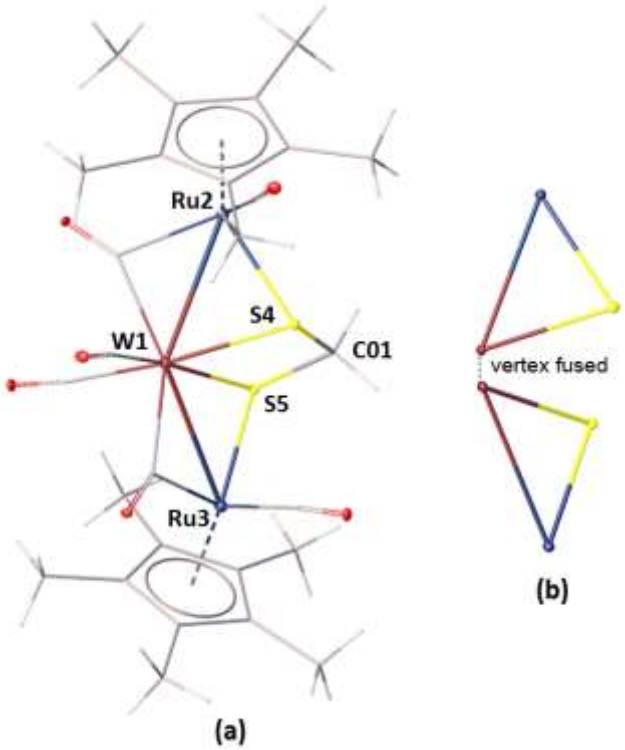

Figure S4. (a) Molecular structures and labelling diagrams of **6**. Selected bond lengths (Å) and bond angles (°); Ru2-W1 2.8706(3), Ru3-W1 2.8680(3), W1-S4 2.4994(9), W1-S5 2.5029(9), Ru2-S4 2.3735(10), Ru3-S5 2.3707(10), C01-S4 1.831(4), C01-S5 1.834(4), S4-W1-S5 71.39(3), S4-C01-S5 105.58(19), Ru2-W1-Ru3 137.379(9), S4-Ru2-W1 55.97(2), S5-Ru3-W1 56.12(2), C01-S4-Ru2 106.64(15), C01-S5-Ru3 107.64(15). (b) Fusion of two triangle {RuWS} cores of **6**.

II *Spectroscopic details*

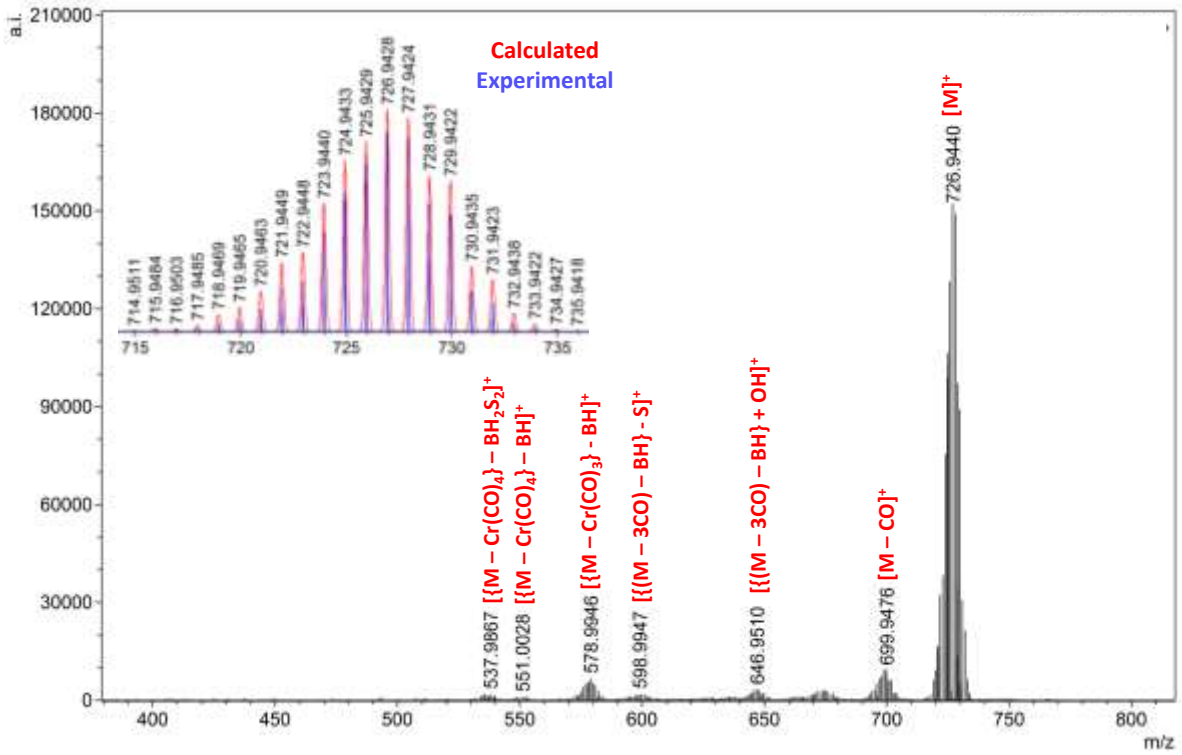

Figure S5. ESI-MS spectrum of **2** in CH_2Cl_2.

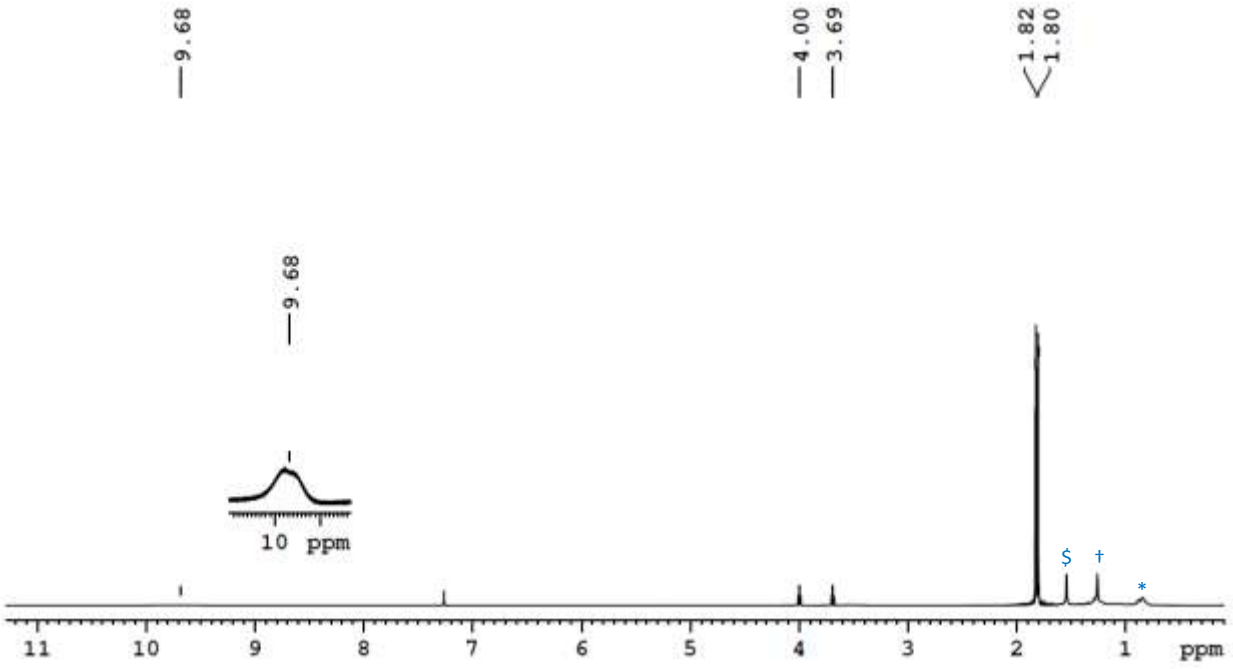

Figure S6. ^{1}H NMR spectrum of **2** in $CDCl_3$. ($$H_2O$, †Hexane, *H-Grease)

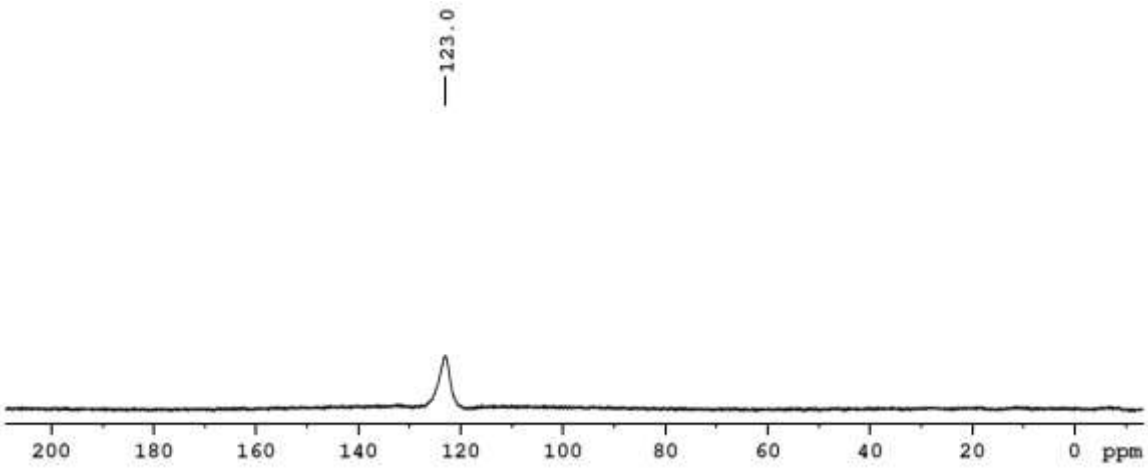

Figure S7. $^{11}B\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$.

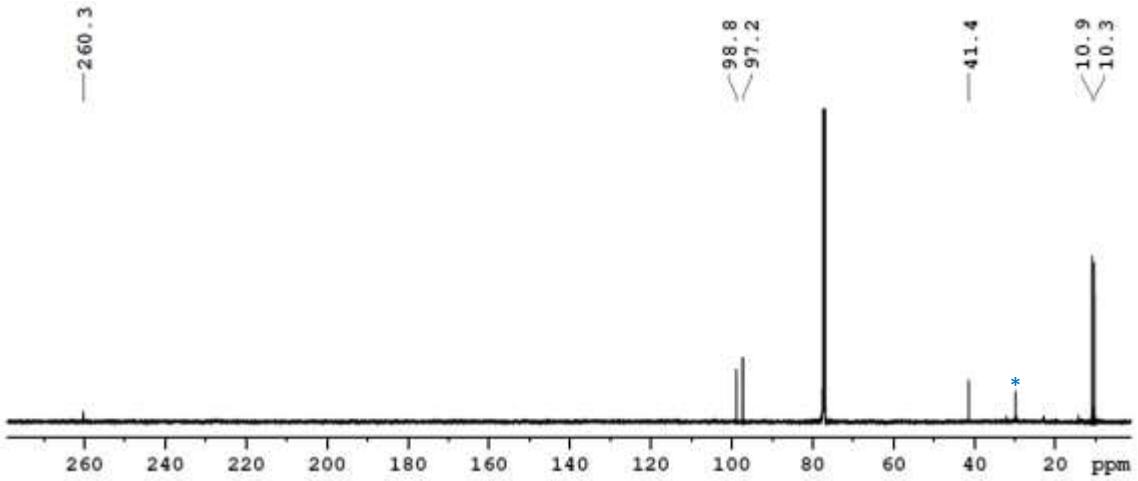

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$. (*H-Grease)

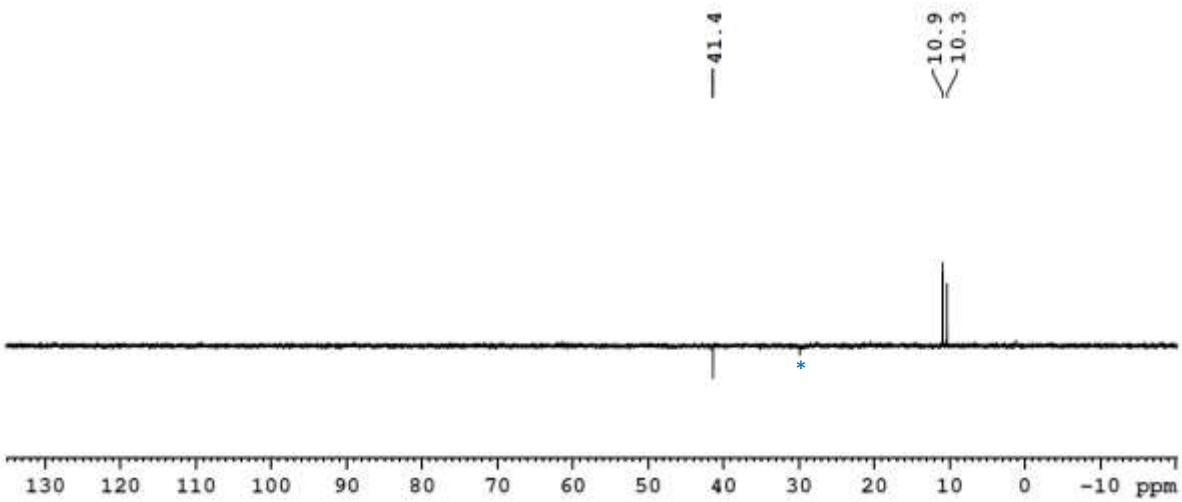

Figure S9. ^{13}C DEPT-135 NMR spectrum of compound **2** in $CDCl_3$. (*H-Grease)

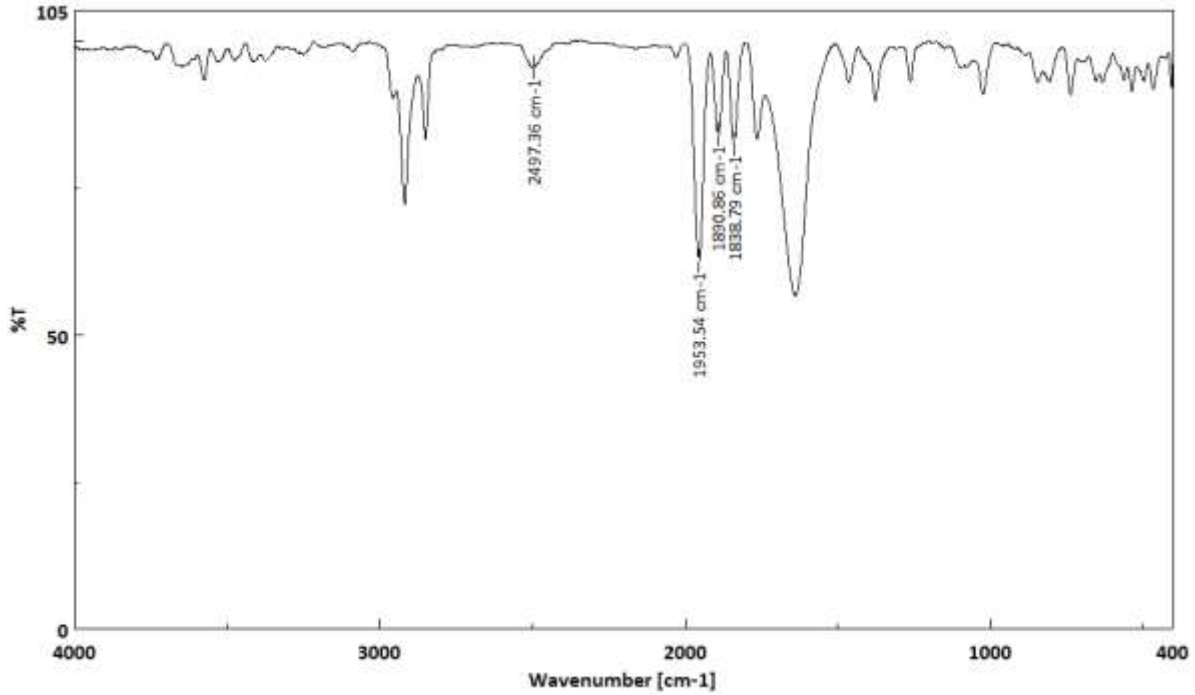

Figure S10. IR spectrum of **2** in CH_2Cl_2.

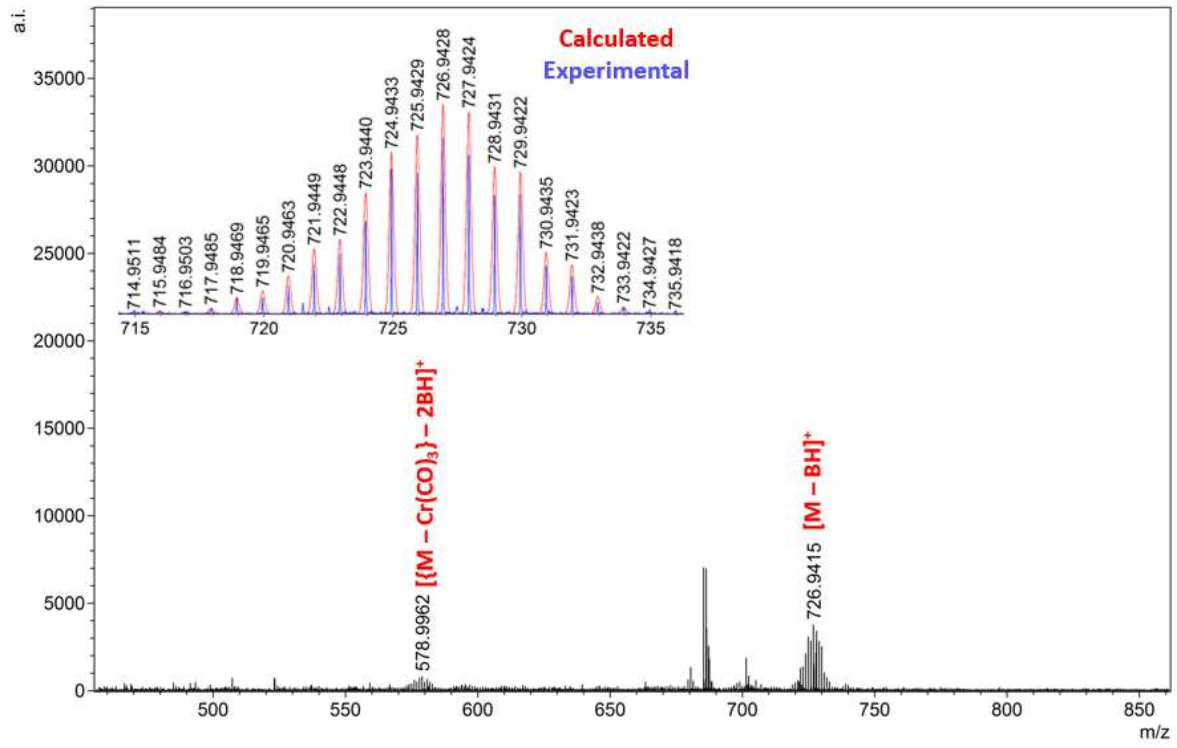

Figure S11. ESI-MS spectrum of **3** in CH_2Cl_2.

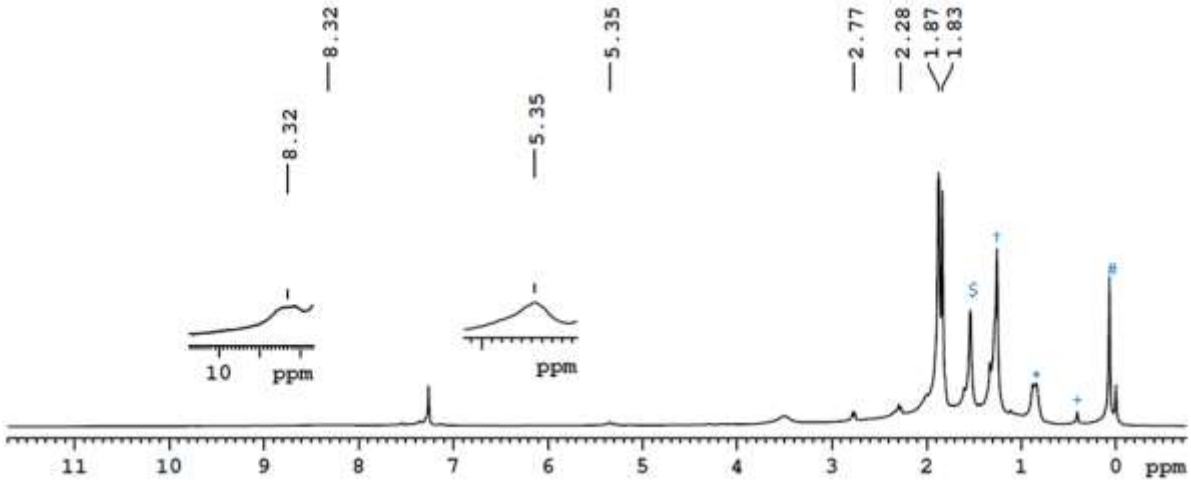

Figure S12. ^{1}H NMR spectrum of **3** in $CDCl_3$. ($H_2O, †Hexane, *H-Grease, +inseparable impurity, #Silicone grease)

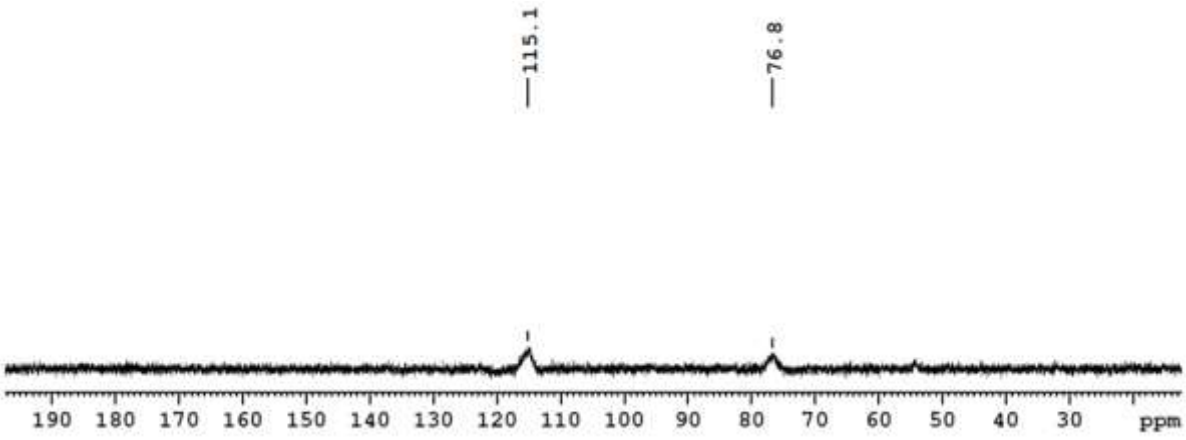

Figure S13. $^{11}B\{^{1}H\}$ NMR spectrum of **3** in $CDCl_3$.

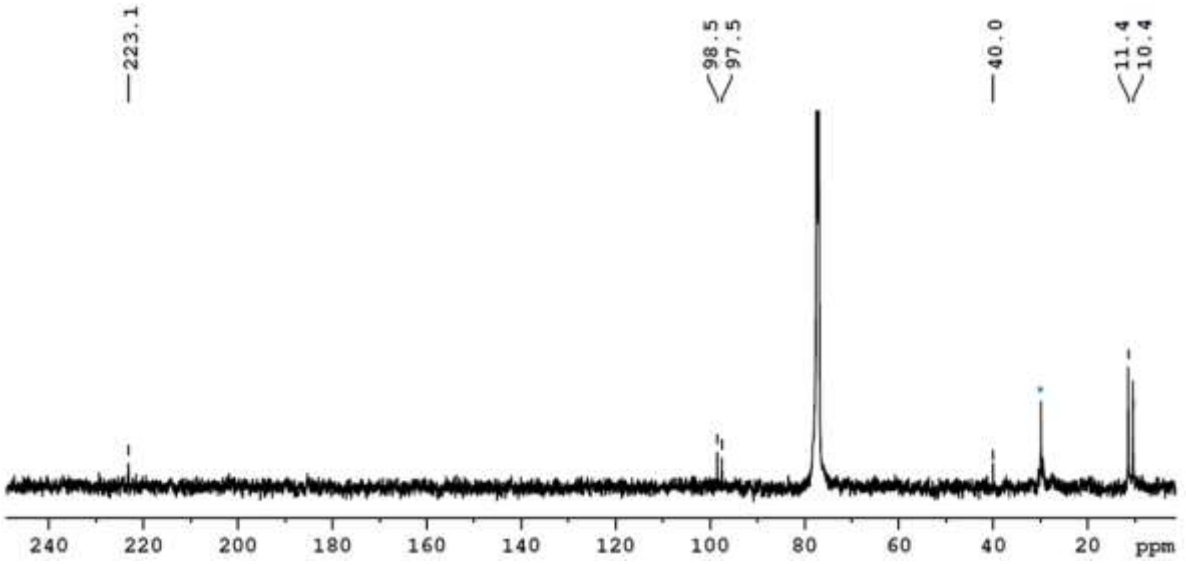

Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in $CDCl_3$. (*H-Grease)

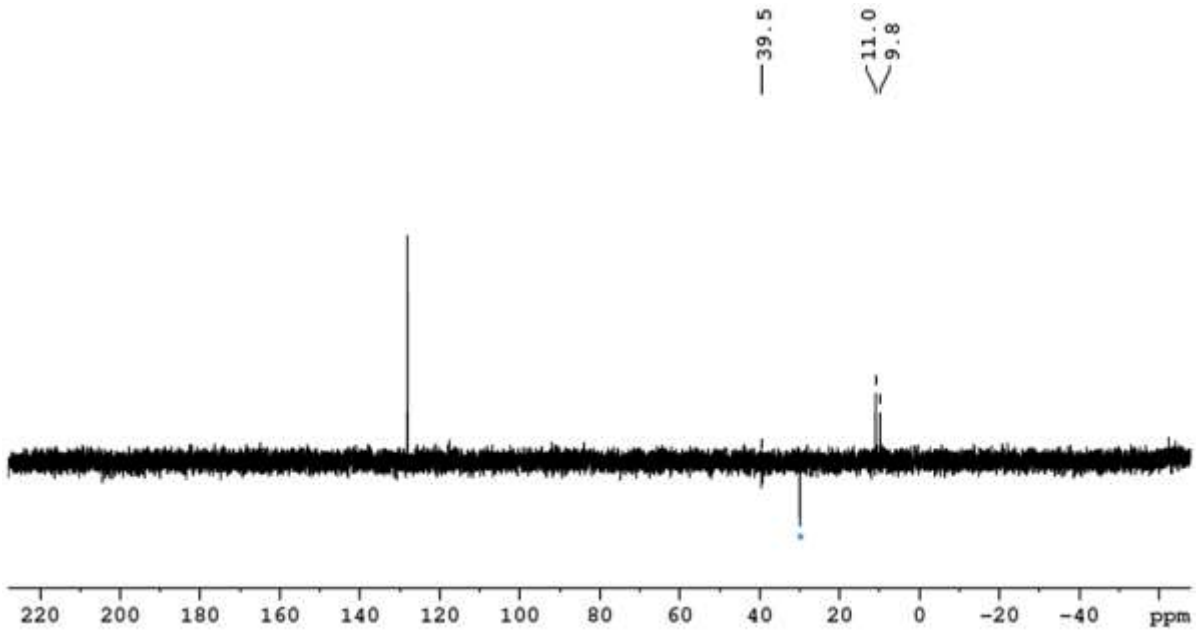

Figure S15. ^{13}C DEPT-135 NMR spectrum of compound **3** in C_6D_6. (*H-Grease)

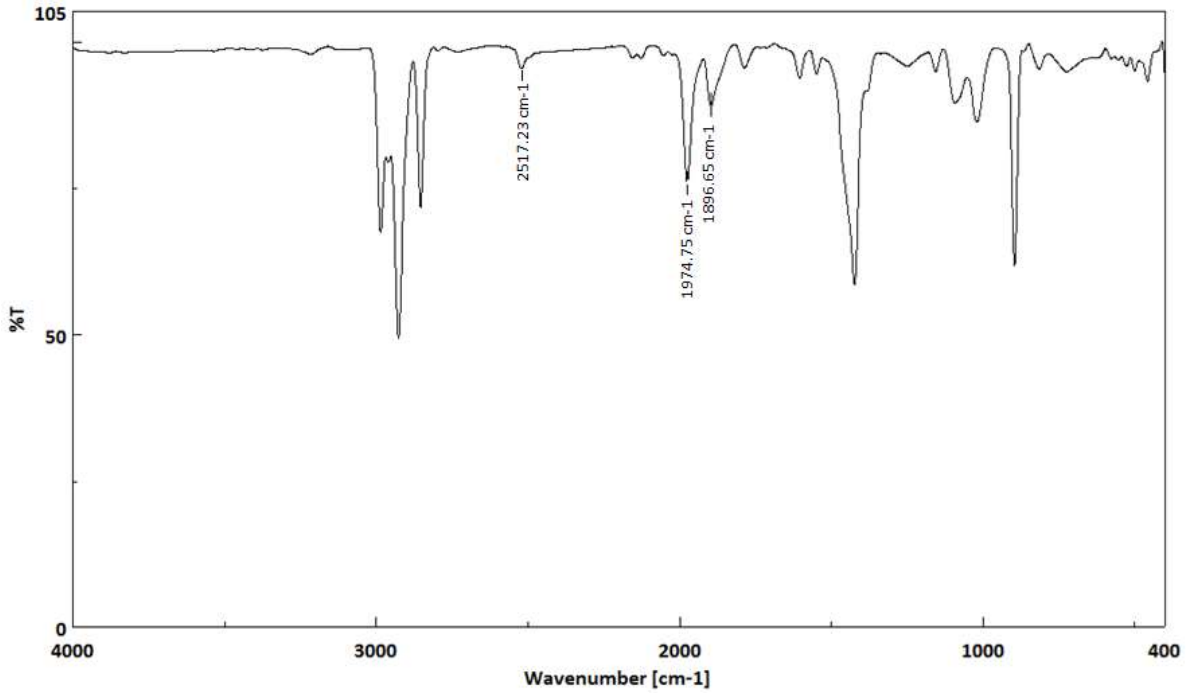

Figure S16. IR spectrum of **3** in CH_2Cl_2.

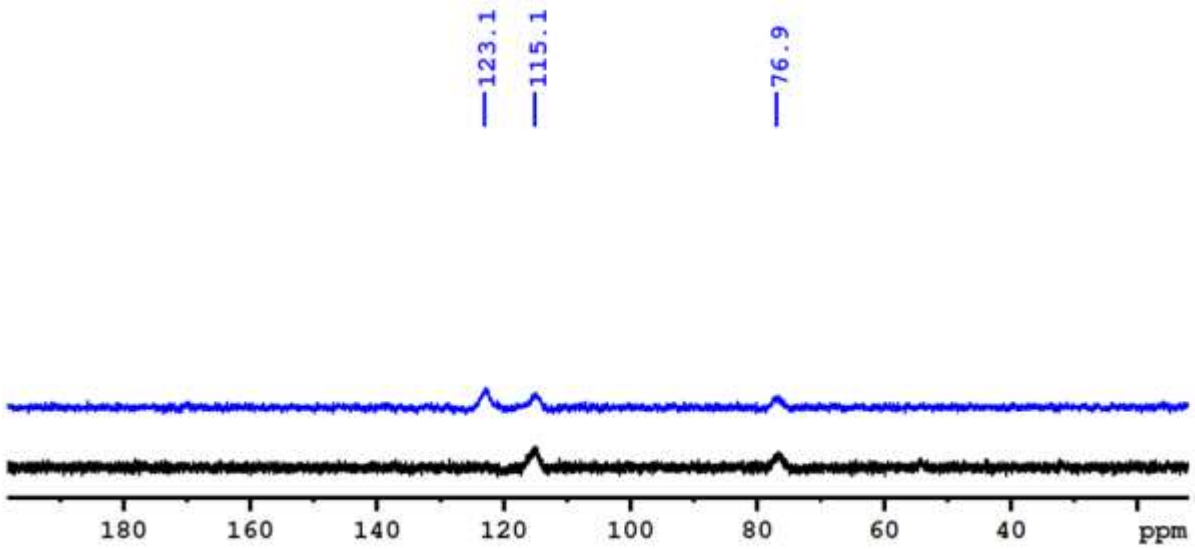

Figure S17. Stacked $^{11}B\{^1H\}$ NMR spectrum of **3** (bottom) and after 24 h (top) that contains mixture of **2** and **3** in $CDCl_3$.

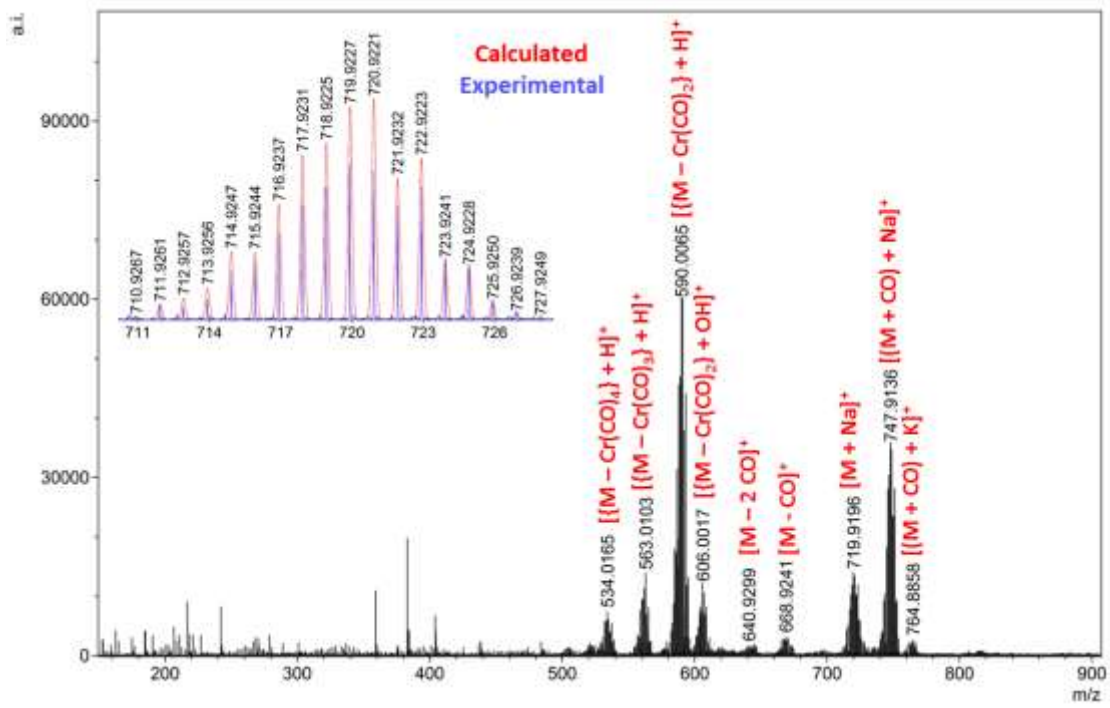

Figure S18. ESI-MS spectrum of **4** in CH_2Cl_2.

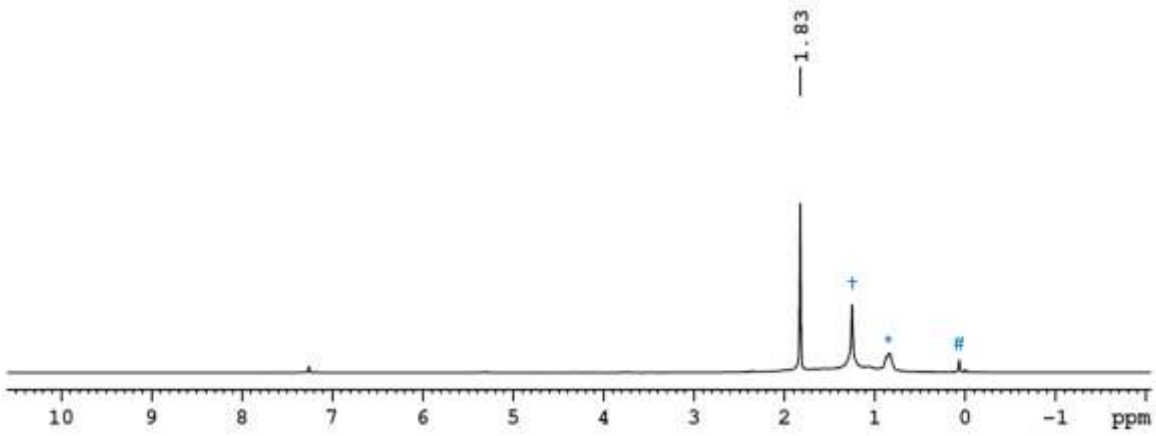

Figure S19. ^{1}H NMR spectrum of **4** in $CDCl_3$. (†Hexane, *H-Grease, #Silicone grease)

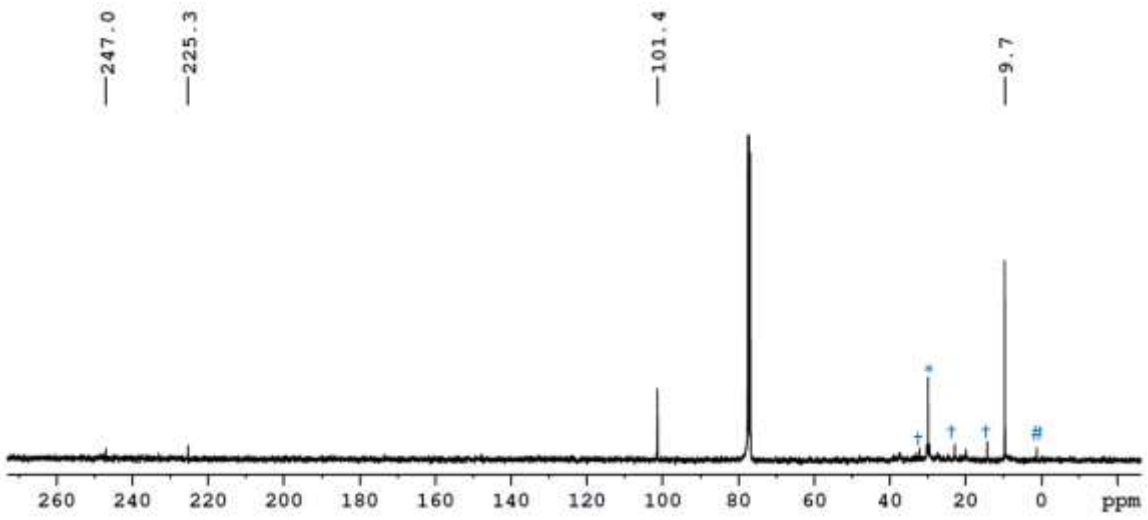

Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in $CDCl_3$. (*H-Grease, †Hexane, #Silicone grease)

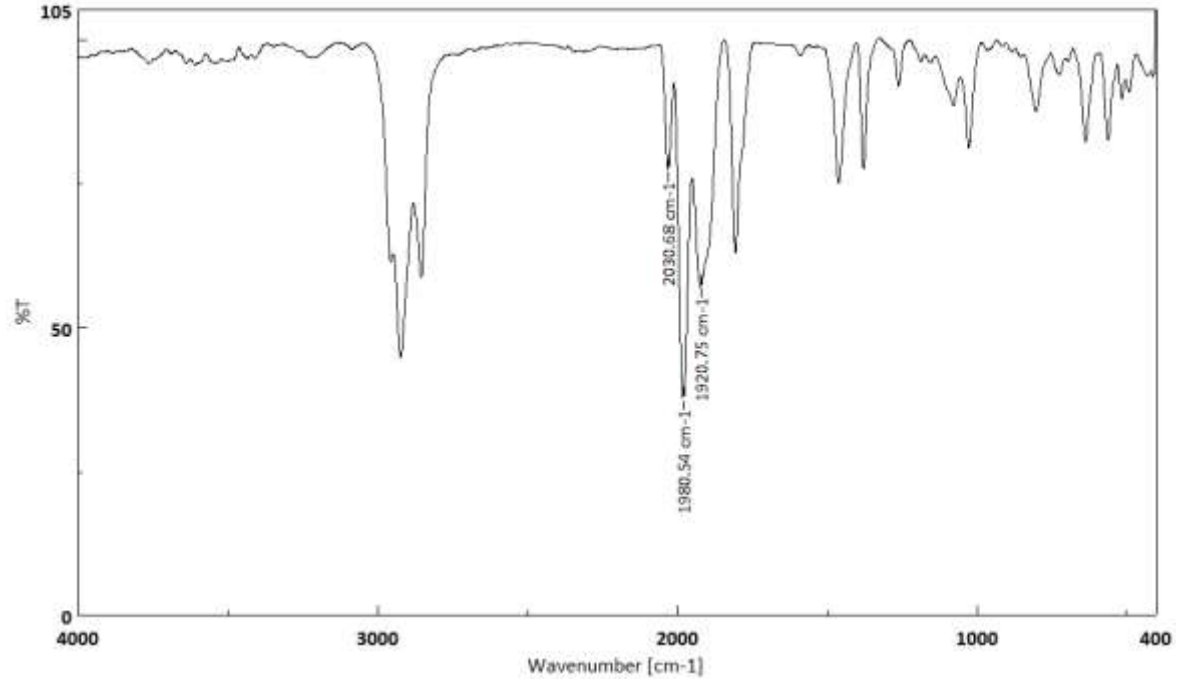

Figure S21. IR spectrum of **4** in CH_2Cl_2.

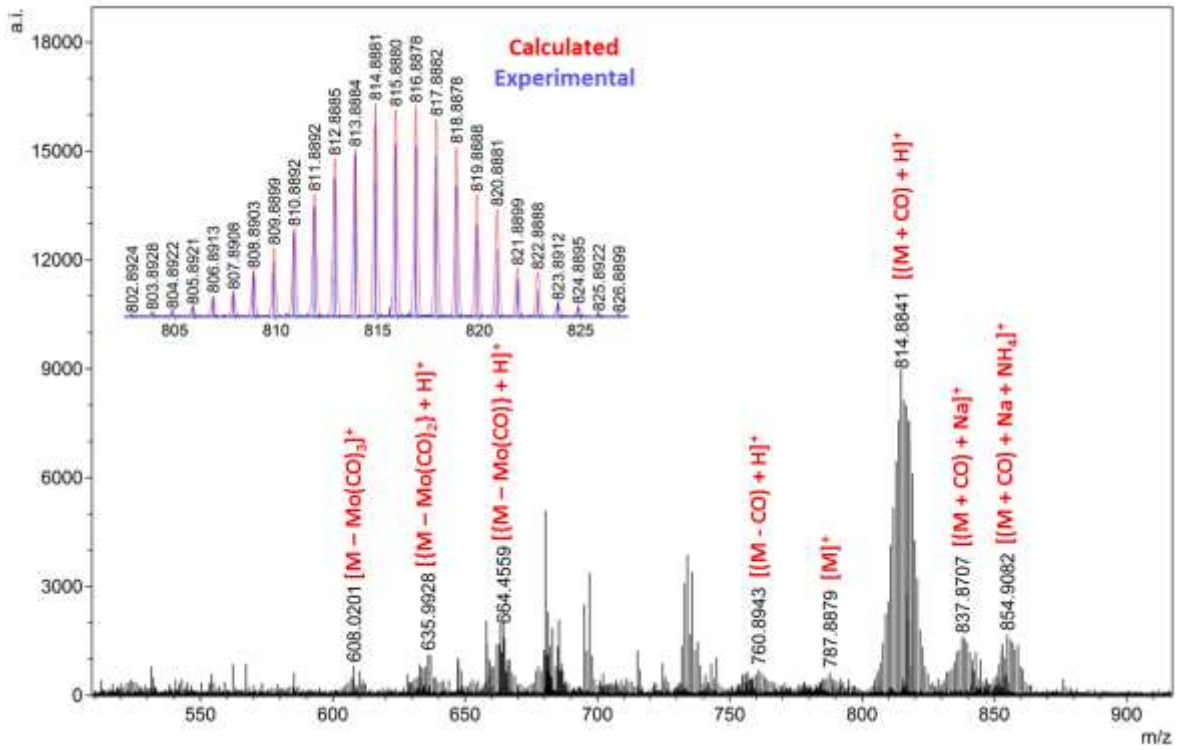

Figure S22. ESI-MS spectrum of **5** in CH_2Cl_2.

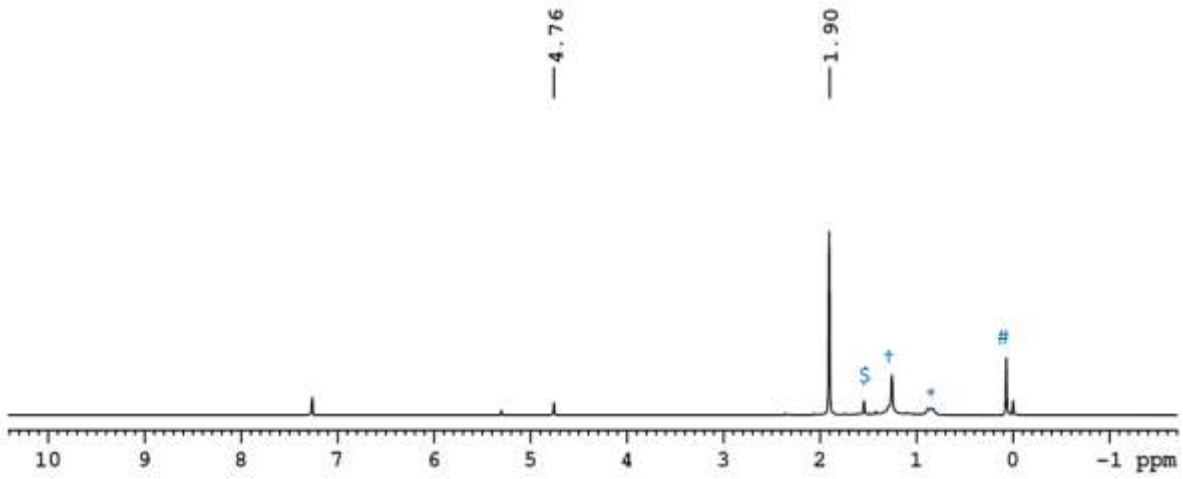

Figure S23. ^{1}H NMR spectrum of **5** in $CDCl_3$. ($H_2O, †Hexane, *H-Grease, #Silicone grease)

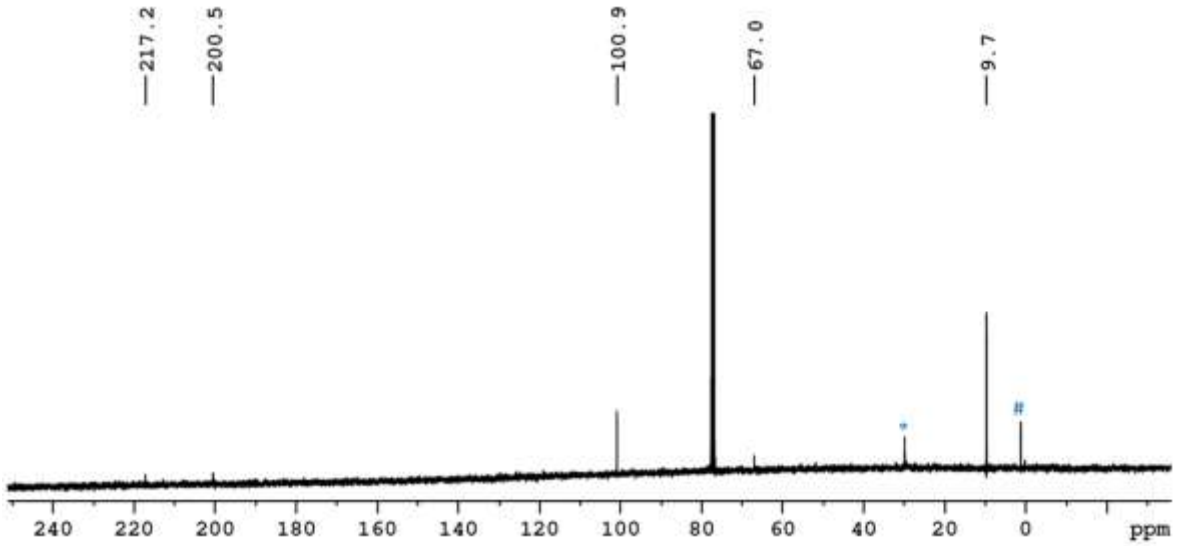

Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in $CDCl_3$. (*H-Grease, #Silicone grease)

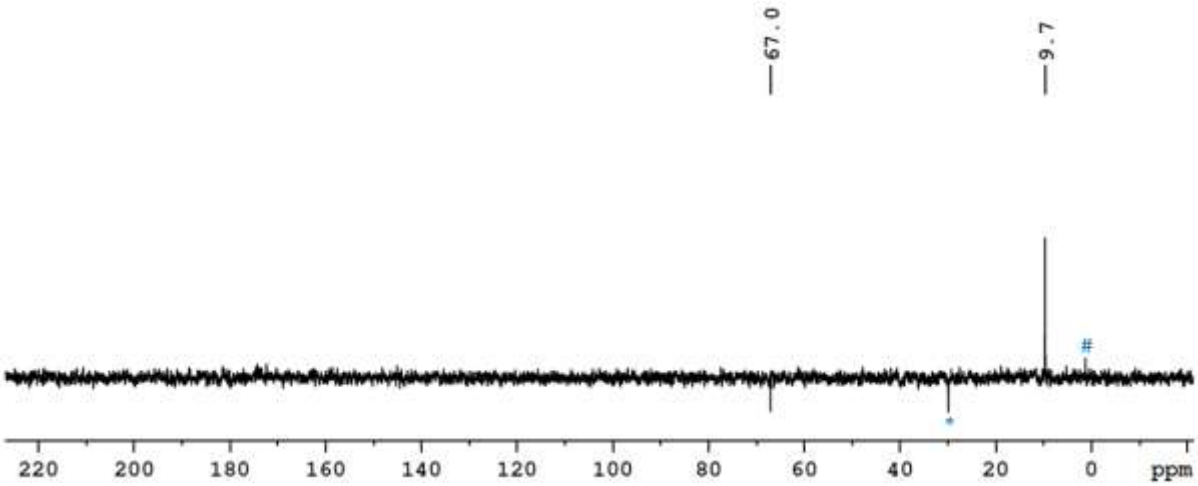

Figure S25. ^{13}C DEPT-135 NMR spectrum of compound **5** in $CDCl_3$. (*H-Grease, #Silicone grease)

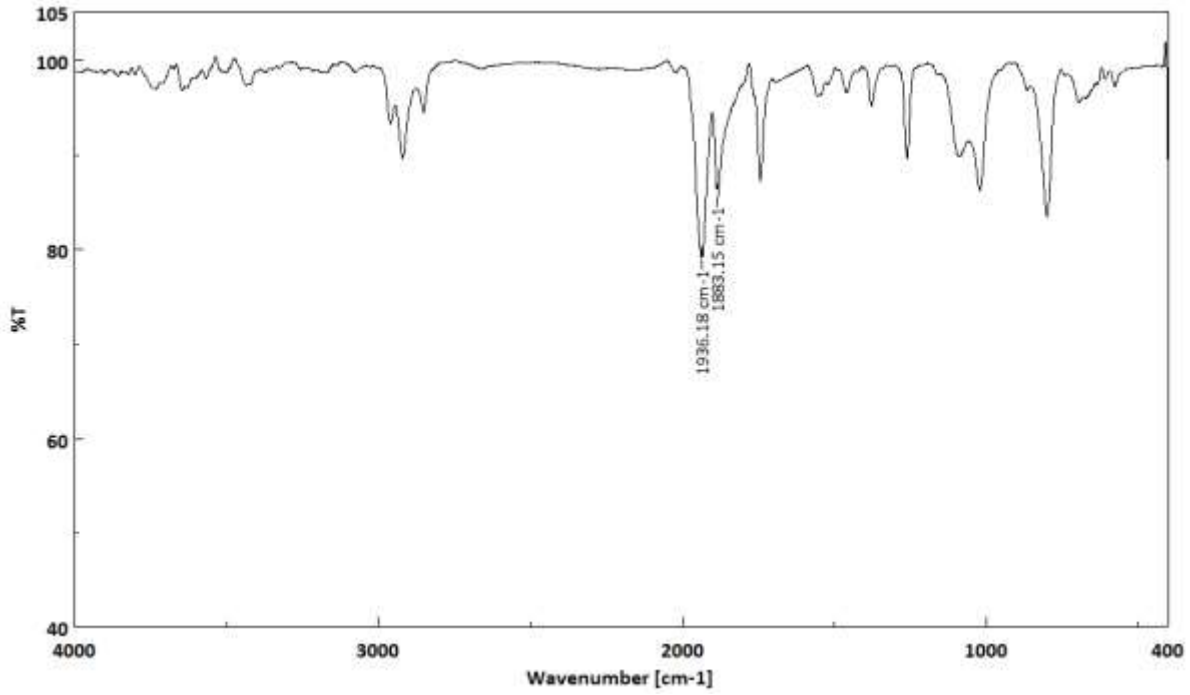

Figure S26. IR spectrum of **5** in CH_2Cl_2.

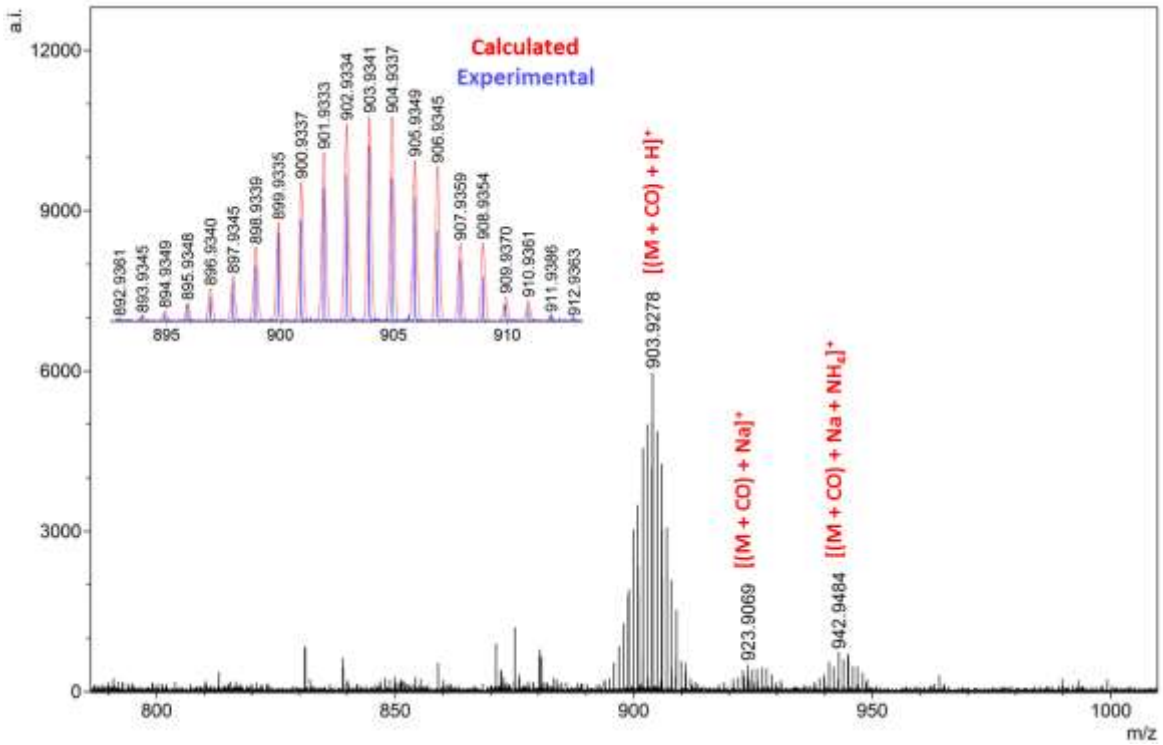

Figure S27. ESI-MS spectrum of **6** in CH_2Cl_2.

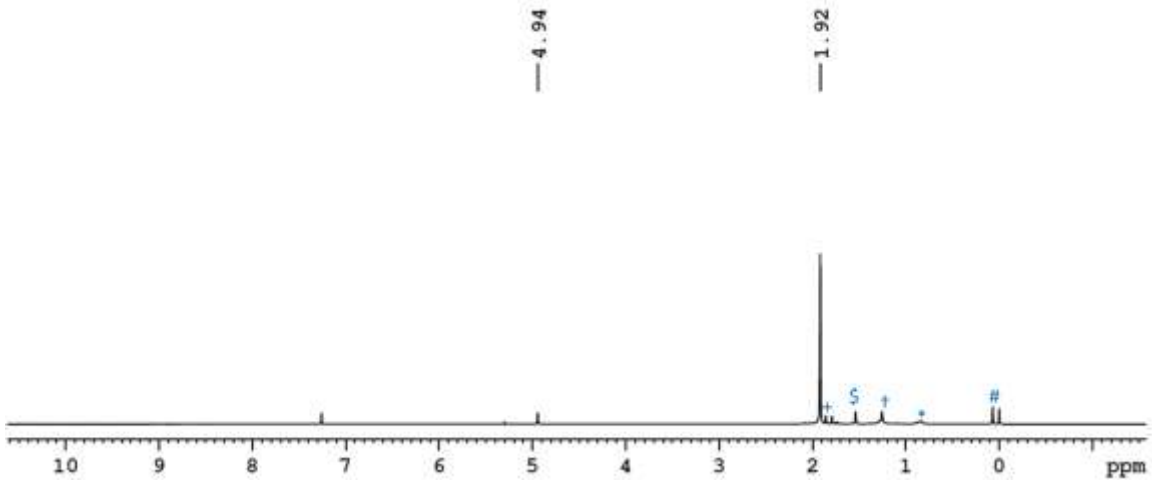

Figure S28. ^{1}H NMR spectrum of **6** in $CDCl_3$. (+inseparable impurity, $H_2O, †Hexane, *H-Grease, #Silicone grease)

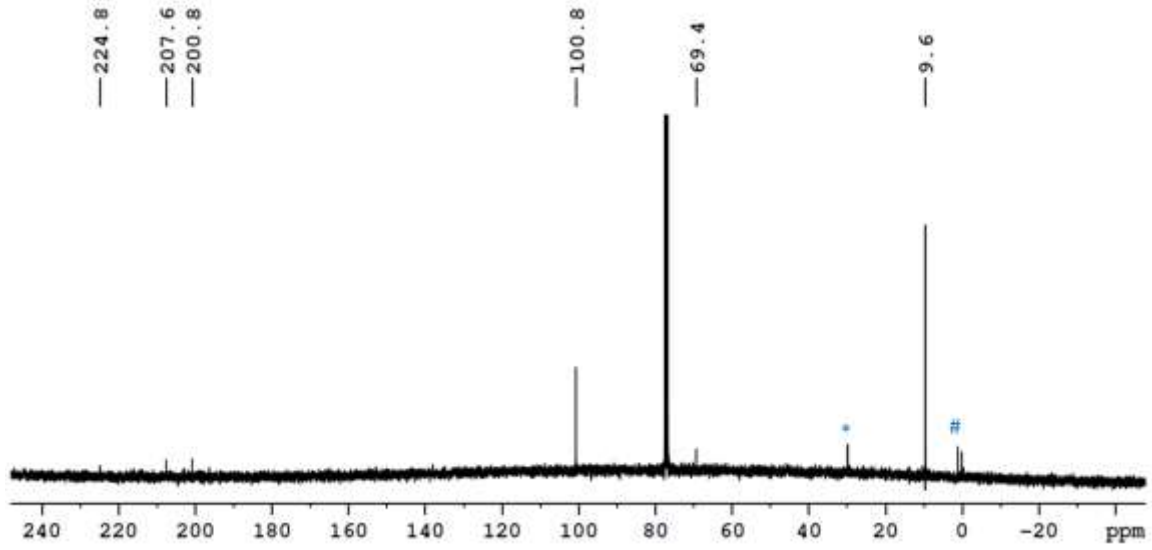

Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$. (*H-Grease, #Silicone grease)

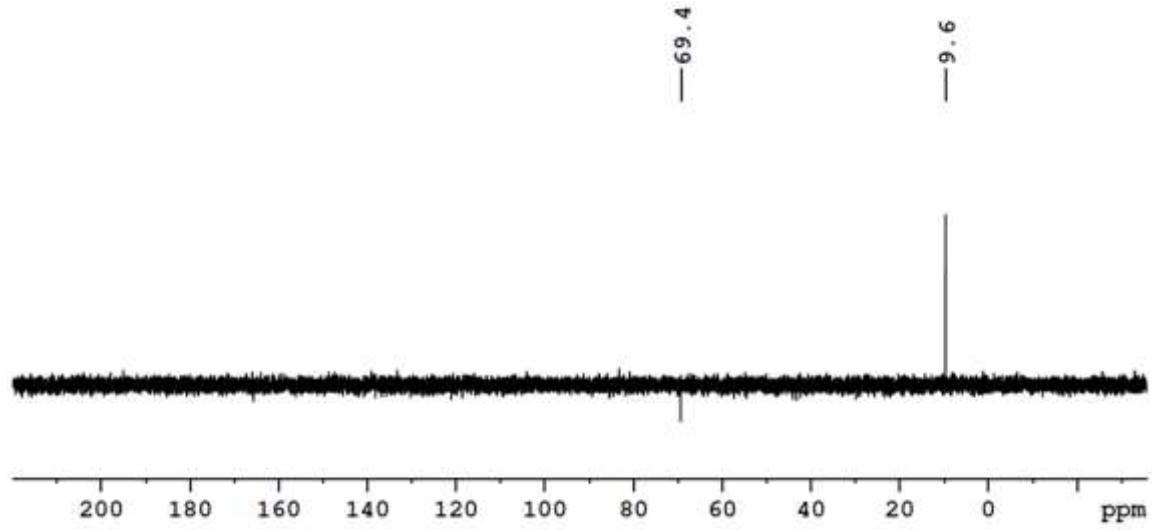

Figure S30. ^{13}C DEPT-135 NMR spectrum of compound **6** in $CDCl_3$.

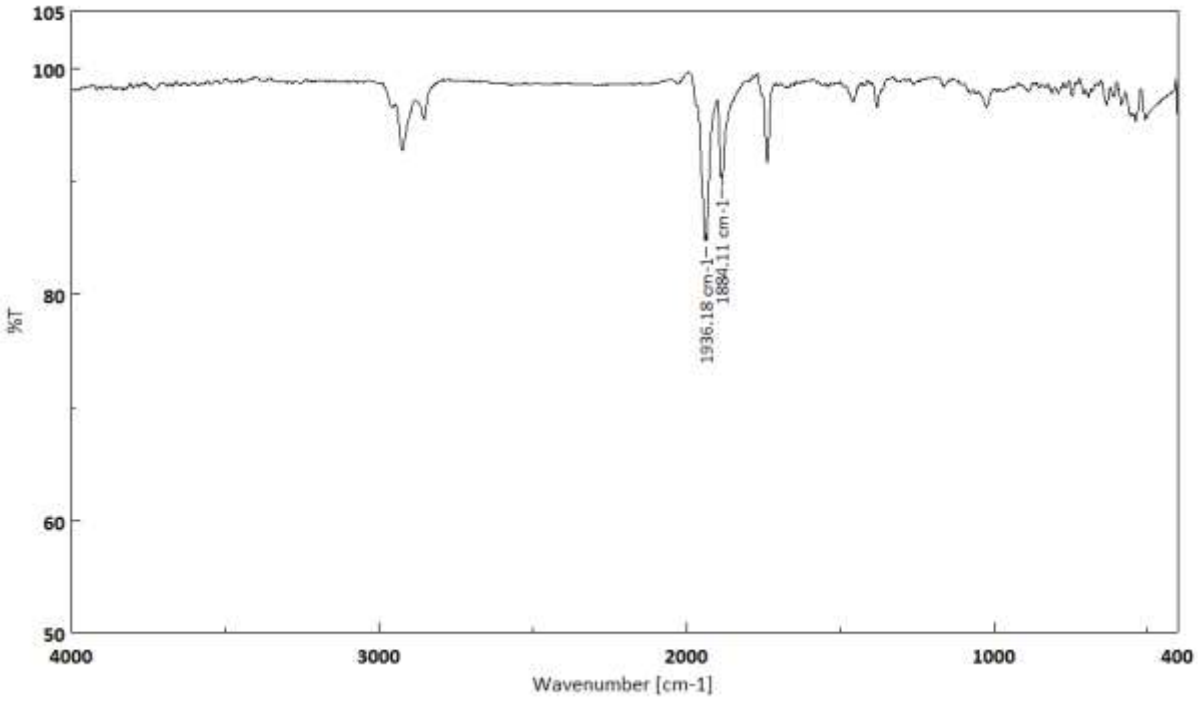

Figure S31. IR spectrum of **6** in CH_2Cl_2.

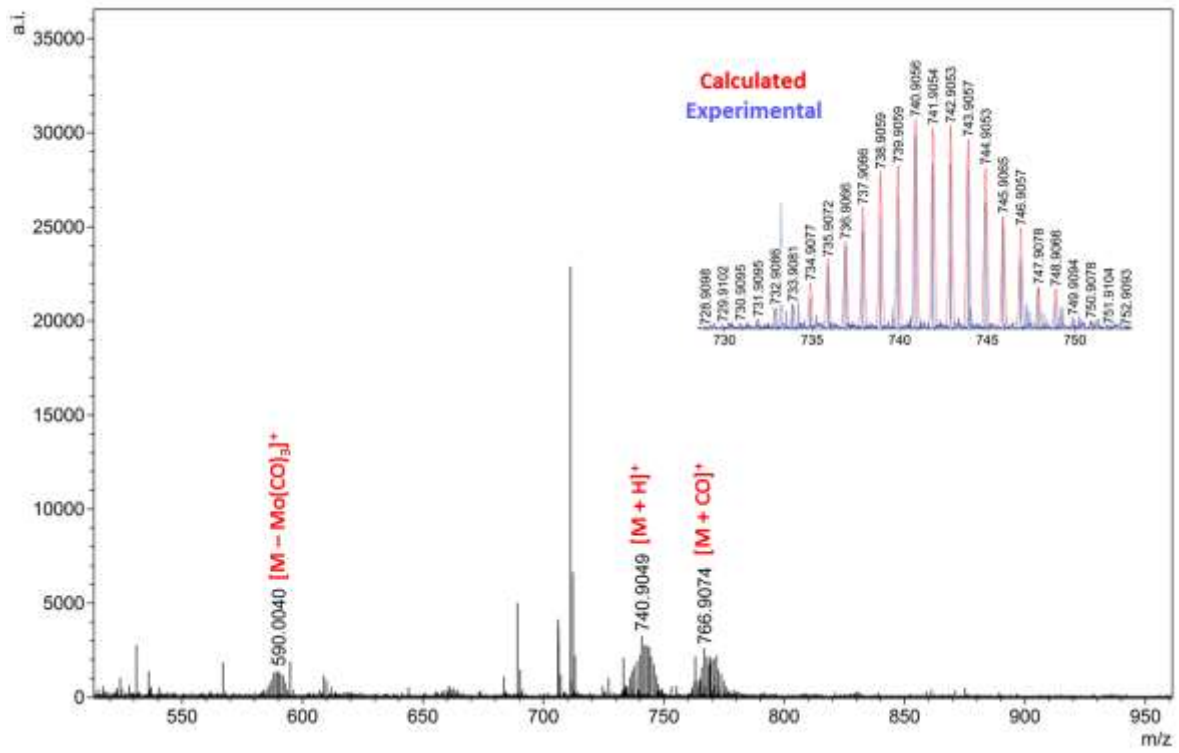

Figure S32. ESI-MS spectrum of **7** in CH_2Cl_2.

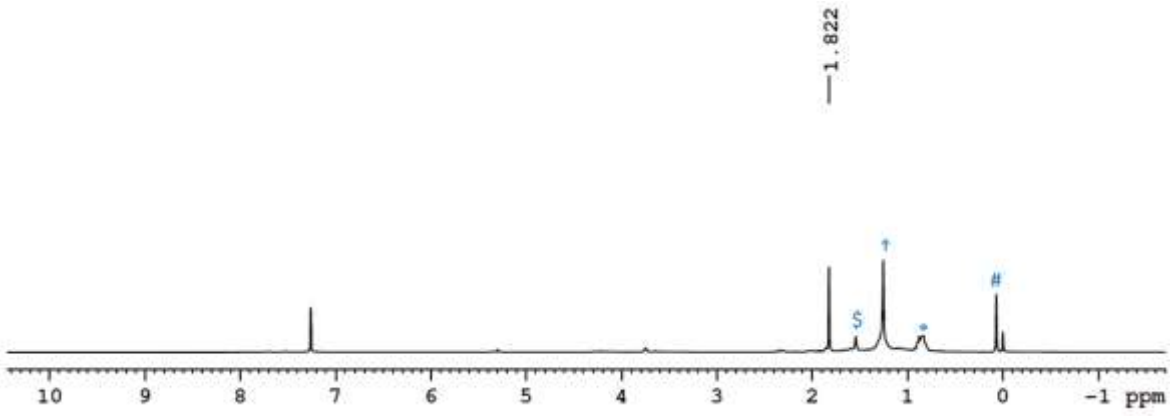

Figure S33. ^{1}H NMR spectrum of **7** in $CDCl_3$. ($H_2O, †Hexane, *H-Grease, #Silicone grease)

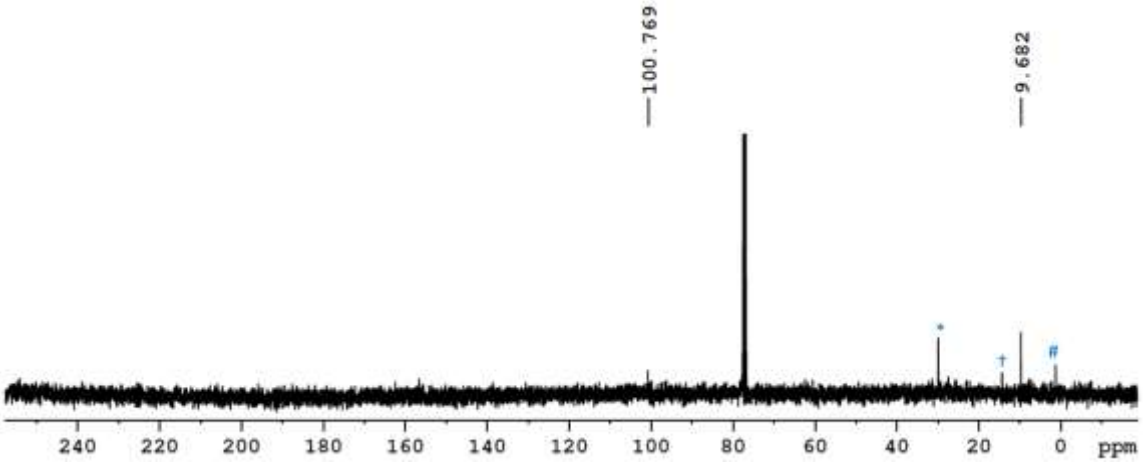

Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum of **7** in $CDCl_3$. (*H-Grease, †Hexane, #Silicone grease)

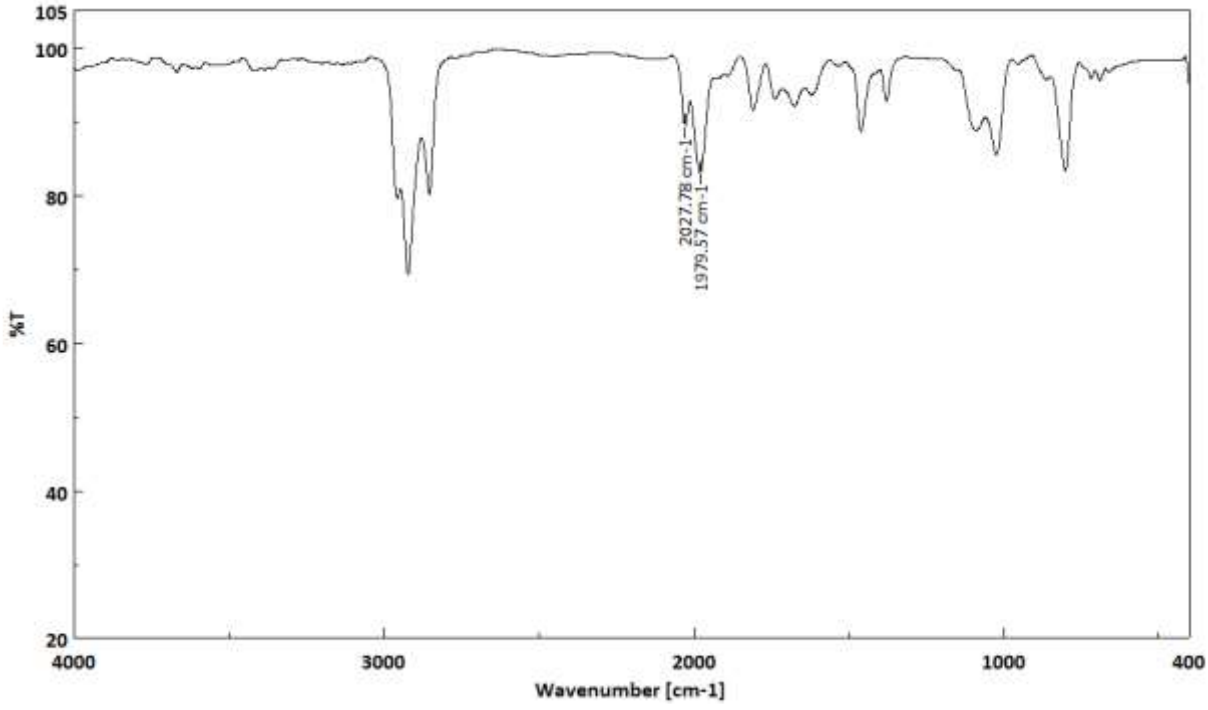

Figure S35. IR spectrum of **7** in CH_2Cl_2.

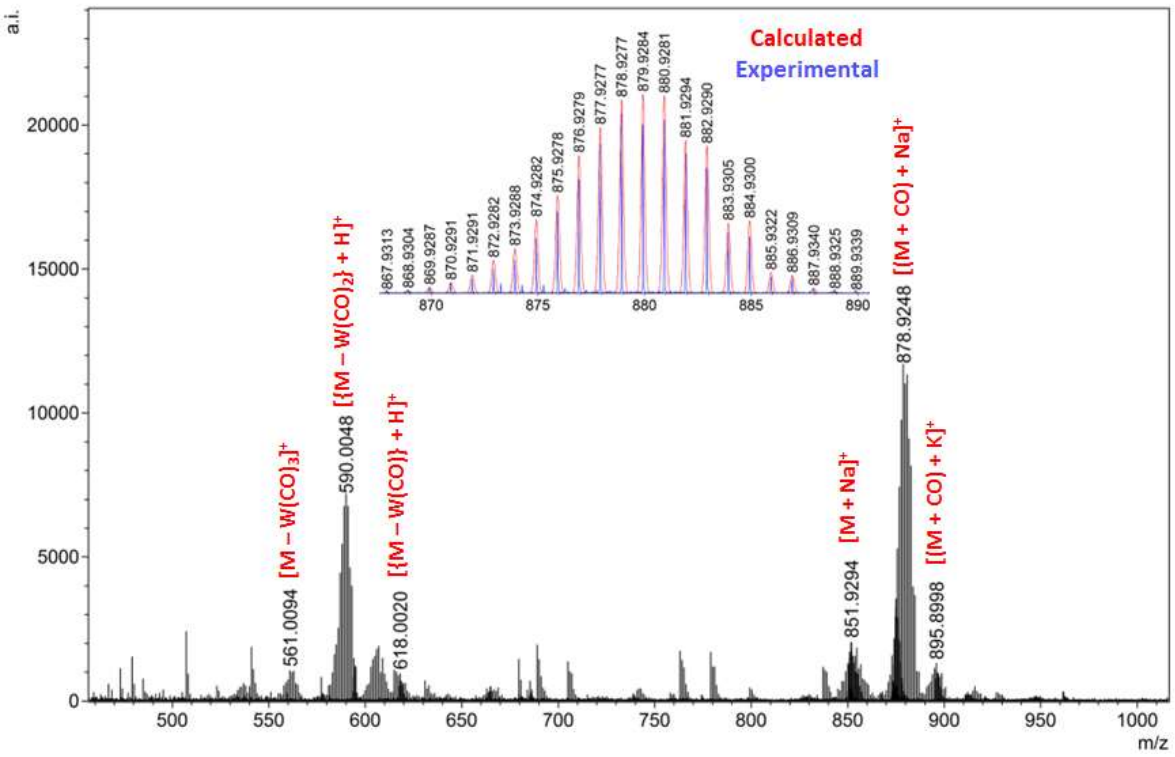

Figure S36. ESI-MS spectrum of **8** in CH_2Cl_2.

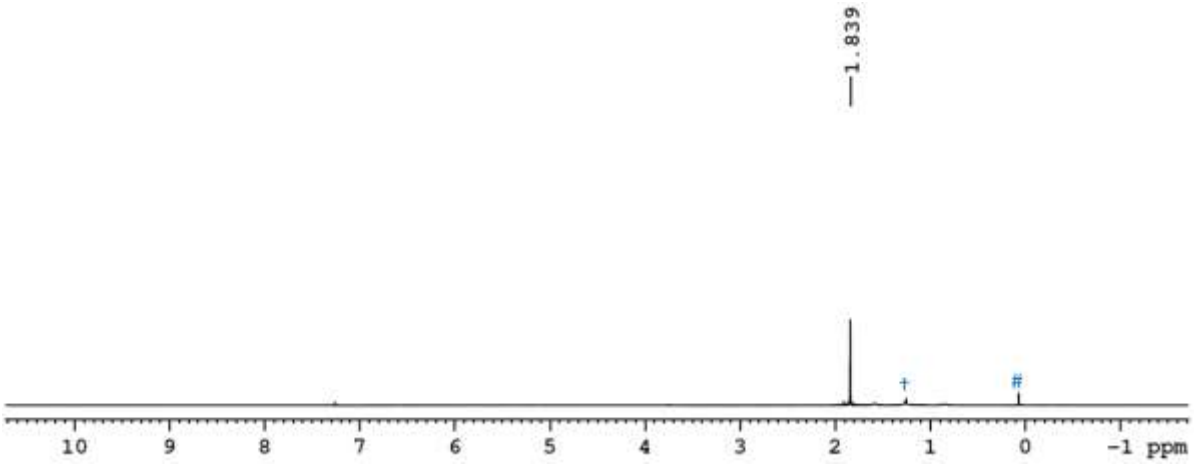

Figure S37. ^{1}H NMR spectrum of **8** in $CDCl_3$. (†Hexane, #Silicone grease)

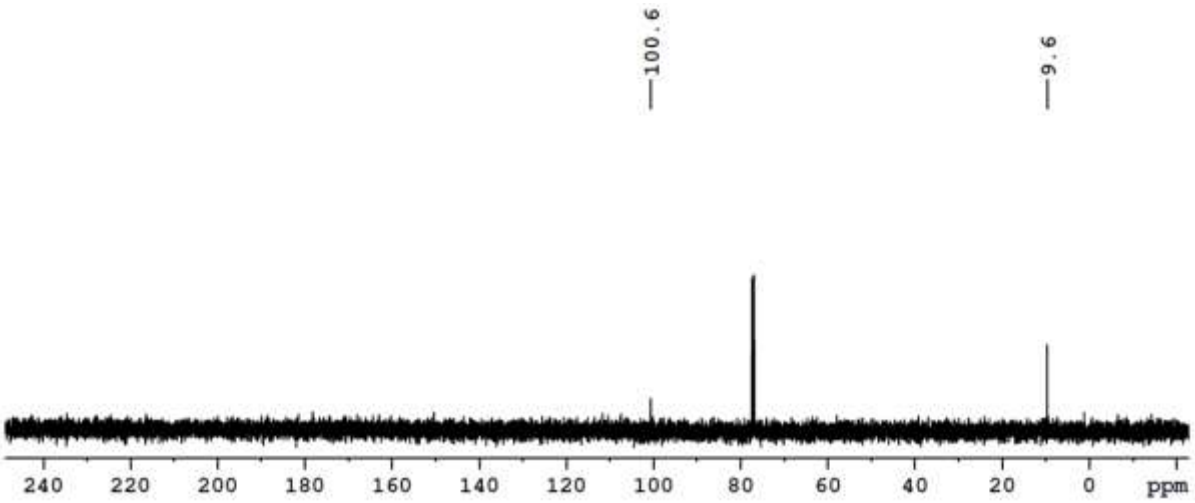

Figure S38. $^{13}C\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$.

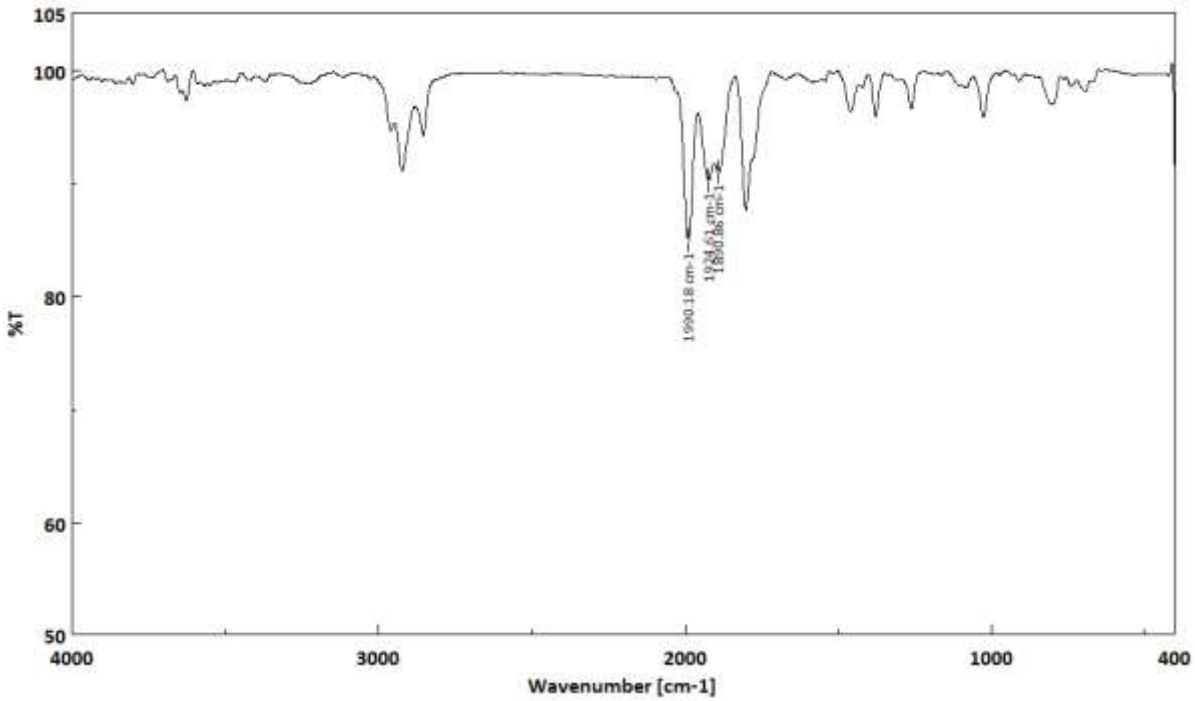

Figure S39. IR spectrum of **8** in CH_2Cl_2.

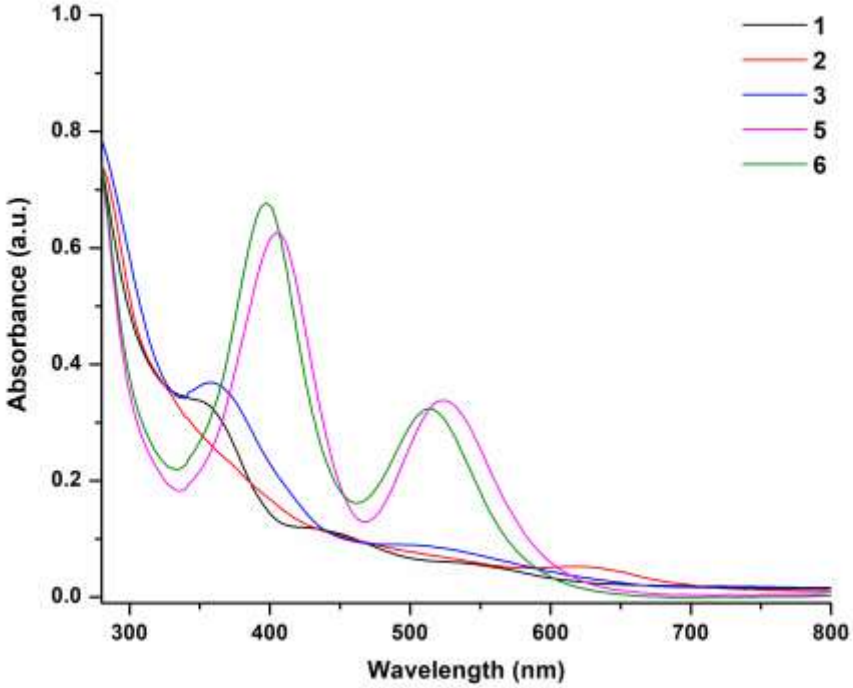

Figure S40. Combined UV−vis spectra of **1**, **2**, **3**, **5** and **6** in CH_2Cl_2.

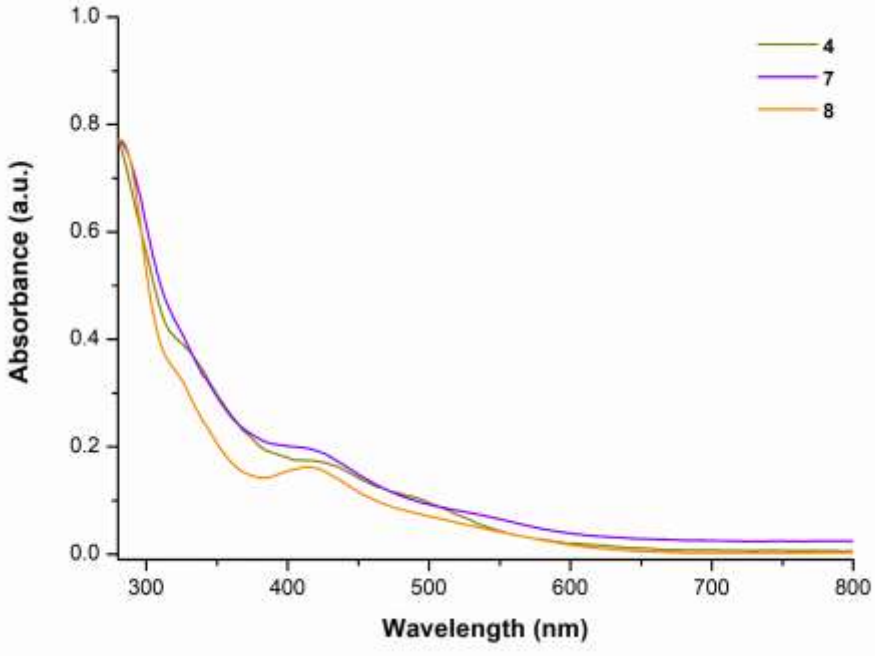

Figure S41. Combined UV−vis spectra of **4**, **7** and **8** in CH_2Cl_2.

III. Computational Details

Table.S1. Selected geometrical parameters and Wiberg bond indices (WBI) of **1**-**8**.

1				**2**			
	Expt.	Cal.	WBI		Expt.	Cal.	WBI
Ru1-Ru2	2.974	3.046	0.227	Ru1-Ru2	2.780	2.829	0.338
Ru1-B1	2.266	2.332	0.365	Ru1-Cr1	2.769	2.811	0.294
Ru2-B1	2.156	2.174	0.529	Ru2-Cr1	2.744	2.807	0.336
Ru2-B2	2.130	2.137	0.539	Ru1-S1	2.299	2.327	0.765
Ru2-B3	2.278	2.335	0.364	Ru2-S1	2.310	2.345	0.751
Ru1-S2	2.261	2.301	0.852	Cr1-S2	2.331	2.354	0.800
B1-S1	1.904	1.924	0.986	Ru2-S2	2.342	2.380	0.708
C21-S1	1.668	1.692	1.301	Ru1-B1	2.129	2.138	0.496
C21-S2	1.651	1.652	1.536	Ru2-B1	2.089	2.103	0.574
B1-B2	1.803	1.792	0.562	Cr1-B1	2.135	2.133	0.462
B2-B3	1.873	1.882	0.477				
3				**4**			
	Expt.	Cal.	WBI		Expt.	Cal.	WBI
Ru1-Ru2	2.789	2.833	0.343	Ru1-Ru2	2.749	2.828	0.295
Ru1-Cr1	2.800	2.850	0.327	Ru1-Cr1	7.760	2.810	0.285
Ru2-Cr1	2.776	2.836	0.260	Ru2-Cr1	2.772	2.968	0.219
Ru1-S1	2.278	2.296	0.783	Ru1-S1	2.289	2.309	0.792
Ru2-S1	2.307	2.340	0.743	Ru2-S1	2.295	2.342	0.743
Cr1-S2	2.454	2.541	0.575	Cr1-S1	2.250	2.270	0.889
Ru1-B1	2.086	2.073	0.604				
Ru2-B1	2.156	2.165	0.475				
Cr1-B1	2.168	2.150	0.458				
Ru1-B2	2.053	2.067	0.660				
Cr1-B2	2.213	2.229	0.380				
B2-S2	1.908	1.886	0.934				
5				**6**			
	Expt.	Cal.	WBI		Expt.	Cal.	WBI
Ru2-Mo1		2.935	0.307	Ru2-W1	2.871	2.938	0.318
Ru3-Mo1		2.935	0.307	Ru3-W1	2.868	2.938	0.318
Ru2-S4		2.395	0.721	Ru2-S4	2.374	2.400	0.709
Ru3-S5		2.395	0.721	Ru3-S5	2.371	2.400	0.709
Mo1-S4		2.549	0.712	W1-S4	2.499	2.548	0.698
Mo1-S5		2.549	0.712	W1-S5	2.503	2.548	0.698
7				**8**			
	Expt.	Cal.	WBI		Expt.	Cal.	WBI
Ru1-Ru2	2.755	2.834	0.291	Ru1-Ru2		2.830	0.291
Ru1-Mo1	2.845	2.933	0.292	Ru1-W1		2.966	0.294
Ru2-Mo1	2.875	3.042	0.221	Ru2-W1		3.012	0.233
Ru1-S1	2.306	2.315	0.795	Ru1-S1		2.312	0.795
Ru2-S1	2.319	2.348	0.744	Ru2-S1		2.346	0.741
Mo1-S1	2.390	2.422	0.839	W1-S1		2.439	0.813

Table S2. Calculated natural charges (q_M, q_B) and natural valence population (Pop) of **1**-**8**.

Compounds	q_M	q_S	Pop (M_{val})	Pop (S_{val})
1	-0.712	0.255	8.699	5.705
	-0.841	0.406	8.832	5.554
2	-0.764	0.533	8.768	5.424
	-0.768	0.529	8.757	5.437
	-2.473		8.455	
3	-0.856	0.552	8.865	5.404
	-0.750	0.349	8.755	5.616
	-2.408		8.391	
4	-0.657	0.493	8646	5.466
	-0.727		8.720	
	-2.388		8.317	
5	-0.808	0.366	8.811	5.599
	-0.808	0.366	8.811	5.599
	-1.493		7.500	
6	-0.820	0.323	8.825	5.641
	-0.820	0.323	8.825	5.641
	-1.083		7.075	
7	-0.640	0.388	8.632	5.568
	-0.721		8.717	
	-1.719		7.736	
8	-0.625	0.335	8.617	5.620
	-0.725		8.722	
	-1.378		7.379	

Table S3. Calculated HOMO–LUMO energy gap of **1**-**8**.

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
ΔE_{H-L} (eV)	3.11	2.91	3.31	3.10	3.06	3.08	3.12	3.11

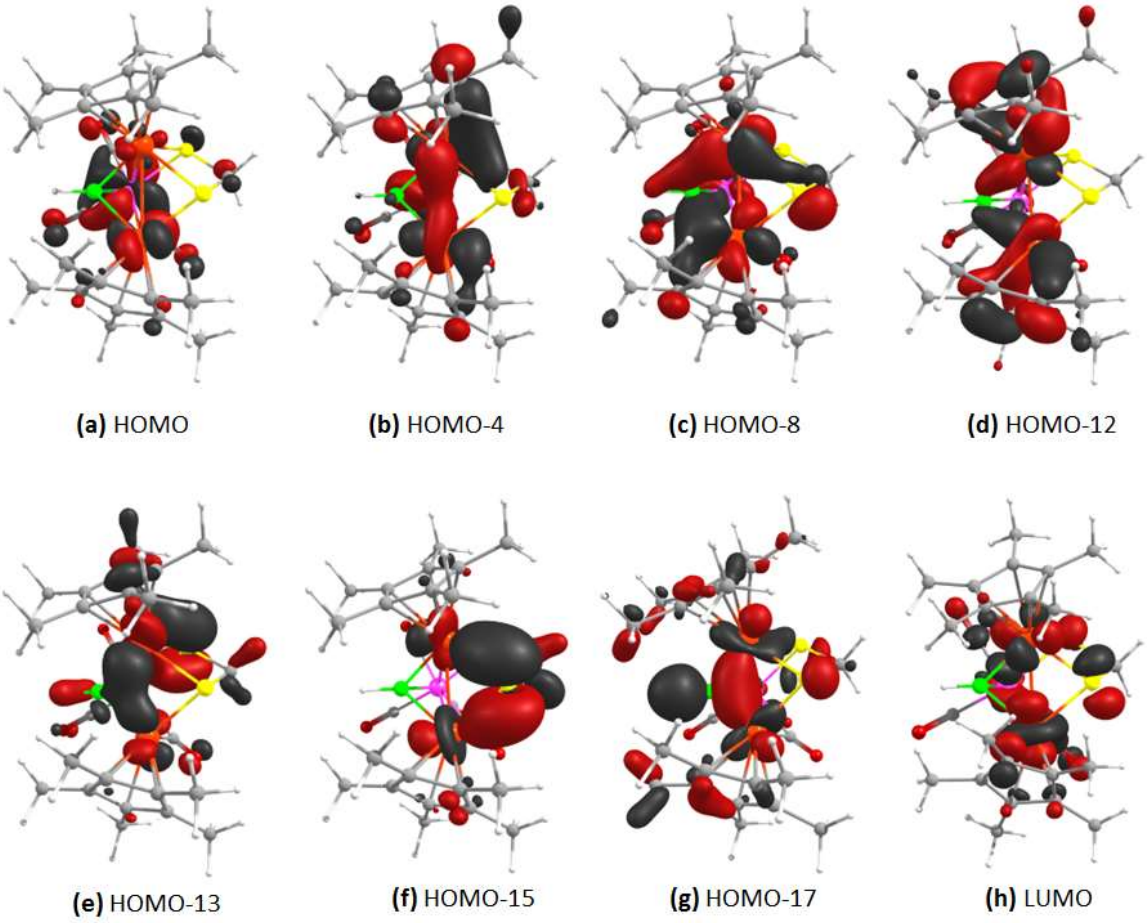

Figure S42. Selected frontier molecular orbitals of **2**. [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$]

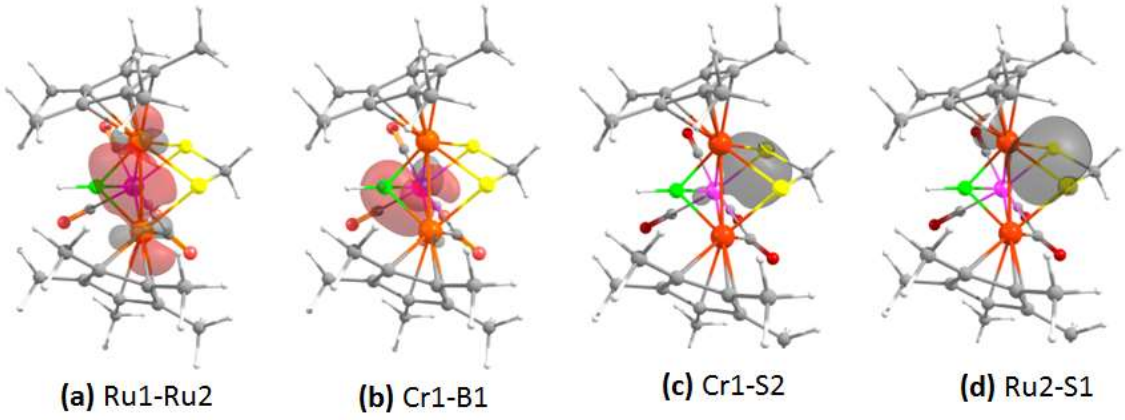

Figure S43. Selected natural bonding orbitals interaction of **2**. [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$]

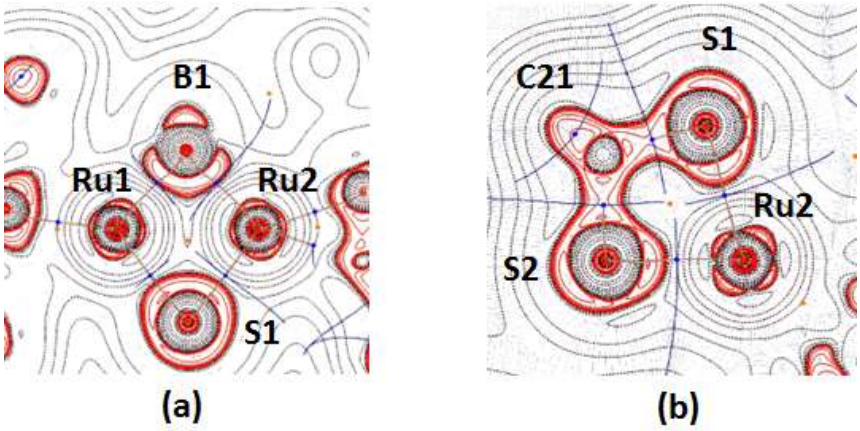

Figure S44. Contour-line diagram of the Laplacian of the electron density, $\nabla^2\rho(r)$, along the (a) Ru1-B1-Ru2 and (B) Ru1-S1-S2 plane, respectively of **2**. Dashed red lines indicate areas of charge concentration ($\nabla^2\rho(r) < 0$), while dotted black lines indicate areas of charge depletion ($\nabla^2\rho(r) > 0$). Solid brown lines connecting the atomic nuclei are the bond paths. The thick blue lines indicate the zero-flux surfaces crossing the molecular plane. Blue and orange dots indicate BCPs (bond critical points) and RCPs (ring critical points), respectively.

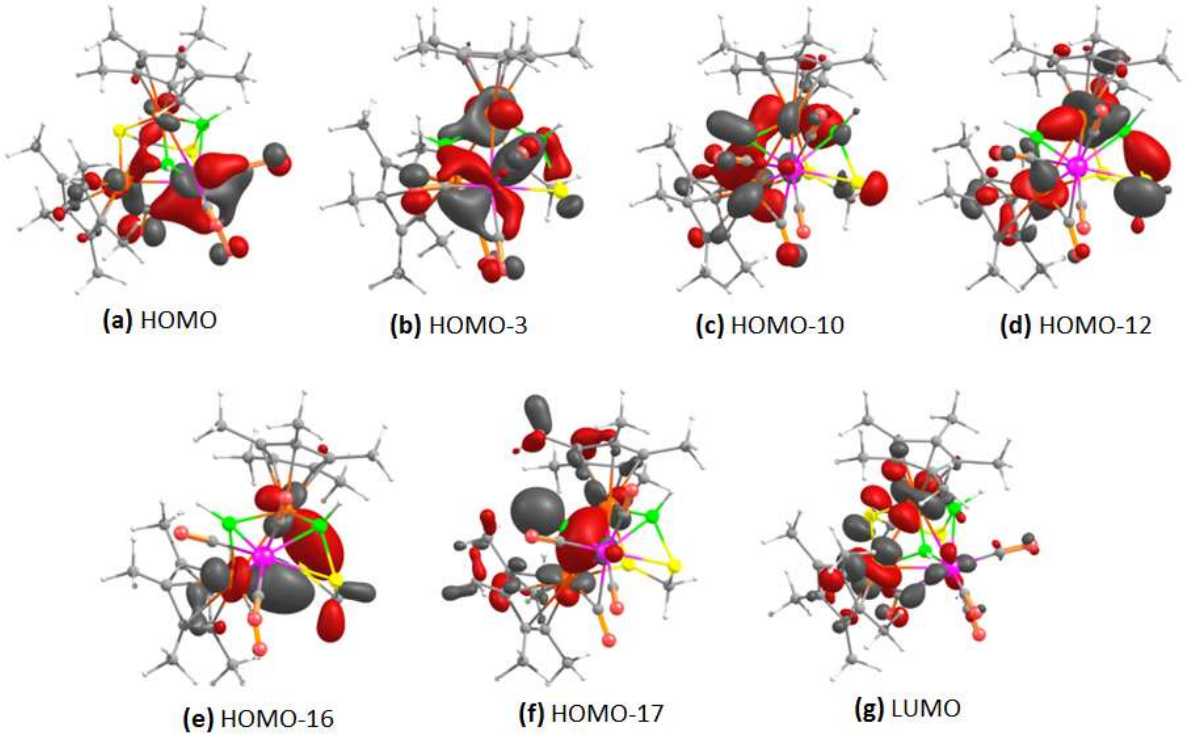

Figure S45. Selected frontier molecular orbitals of **3**. [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$]

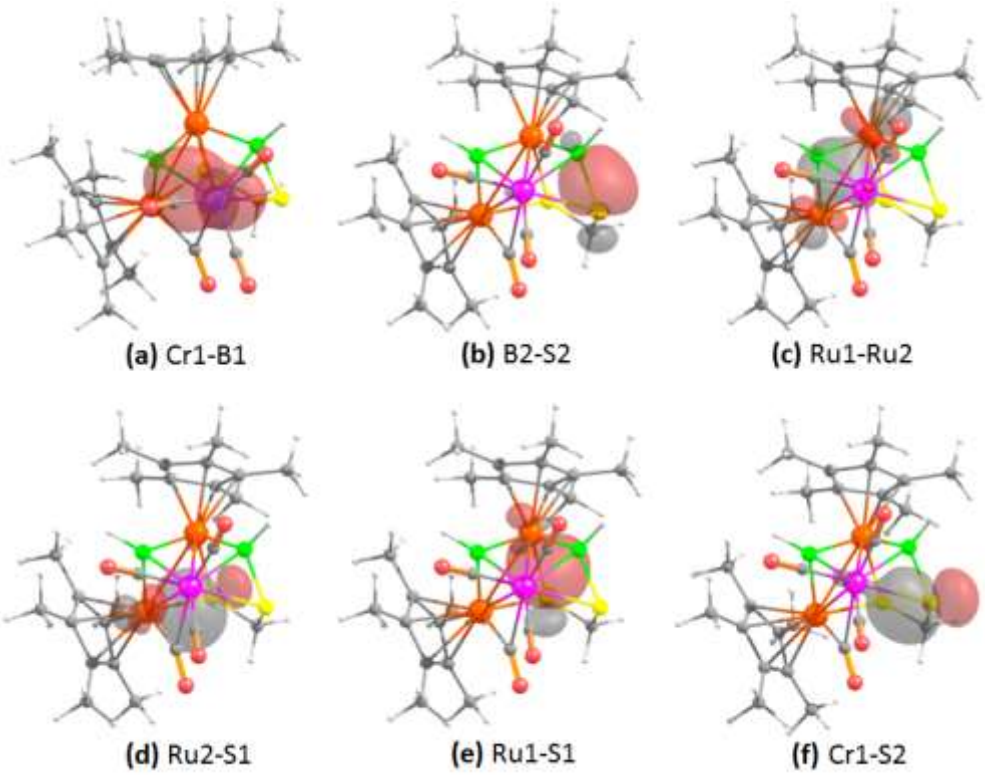

Figure S46. Selected natural bonding orbitals interaction of **3**. [isocontour values: ±0.04 (e/bohr^3)$^{1/2}$]

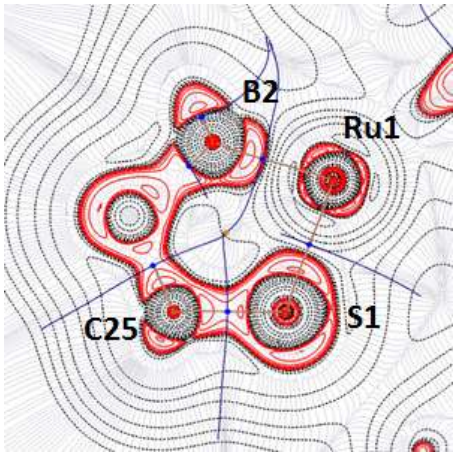

Figure S47. Contour-line diagram of the Laplacian of the electron density, $\nabla^2\rho(r)$, along the B2-Ru1-S1 plane of **3**. Dashed red lines indicate areas of charge concentration ($\nabla^2\rho(r) < 0$), while dotted black lines indicate areas of charge depletion ($\nabla^2\rho(r) > 0$). Solid brown lines connecting the atomic nuclei are the bond paths. The thick blue lines indicate the zero-flux surfaces crossing the molecular plane. Blue and orange dots indicate BCPs (bond critical points) and RCPs (ring critical points), respectively.

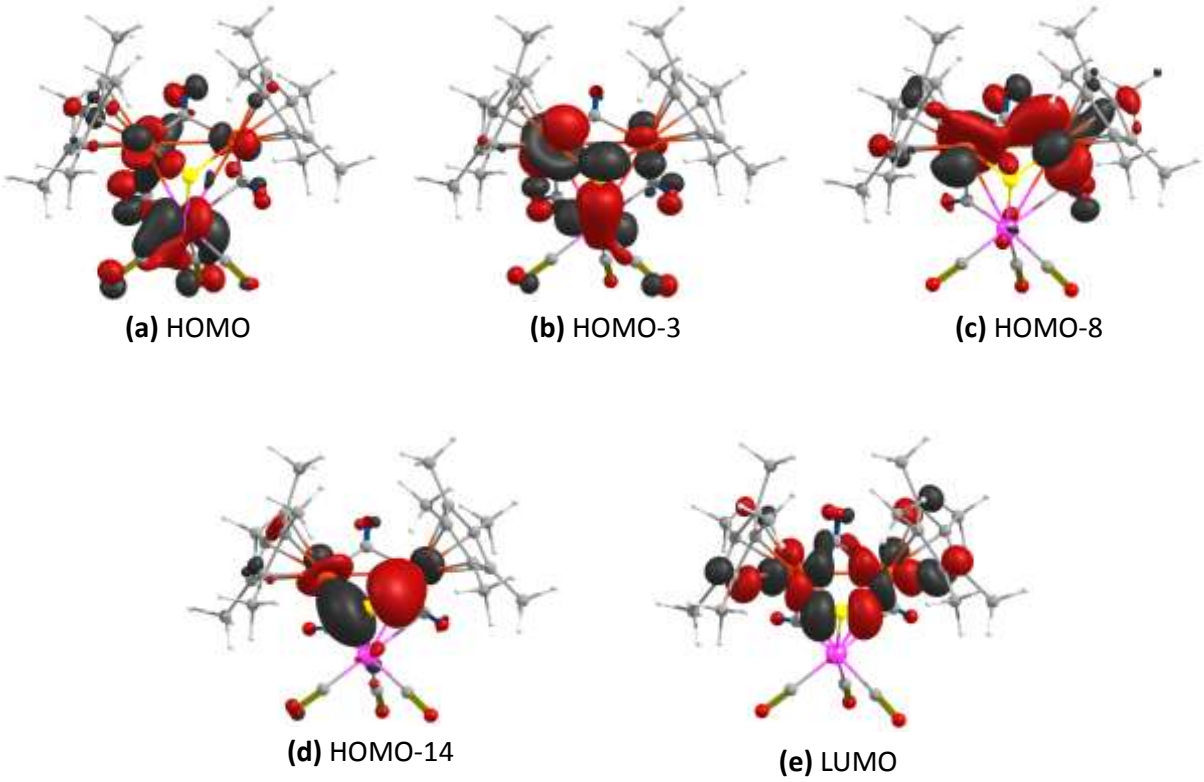

Figure S48. Selected frontier molecular orbitals of **4**. [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$]

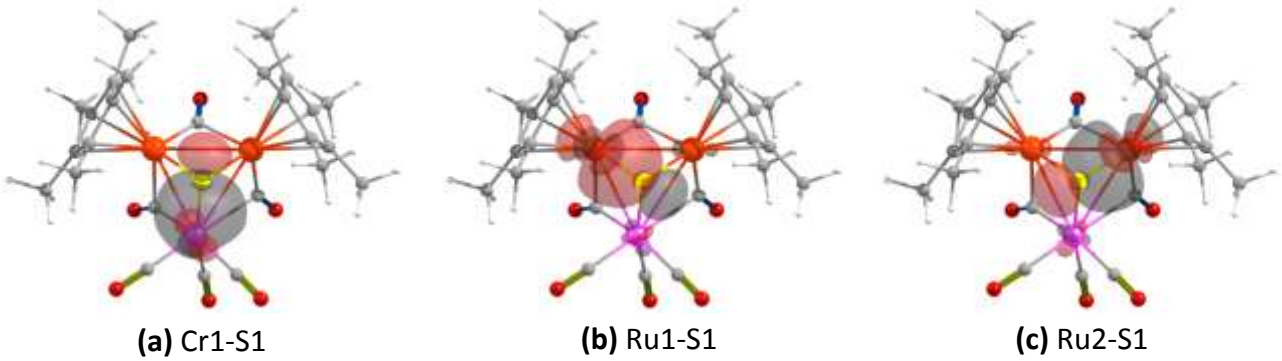

Figure S49. Selected natural bonding orbitals interaction of **4**. [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$]

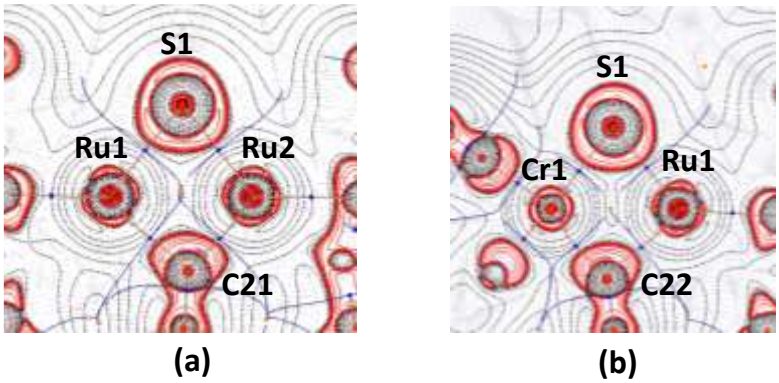

Figure S50. Contour-line diagram of the Laplacian of the electron density, $\nabla^2\rho(r)$, along the (a) Ru1-S1-Ru2 and (B) Cr1-S1-Ru1 plane, respectively of **4**. Dashed red lines indicate areas of charge concentration ($\nabla^2\rho(r) < 0$), while dotted black lines indicate areas of charge depletion ($\nabla^2\rho(r) > 0$). Solid brown lines connecting the atomic nuclei are the bond paths. The thick blue lines indicate the zero-flux surfaces crossing the molecular plane. Blue and orange dots indicate BCPs (bond critical points) and RCPs (ring critical points), respectively.

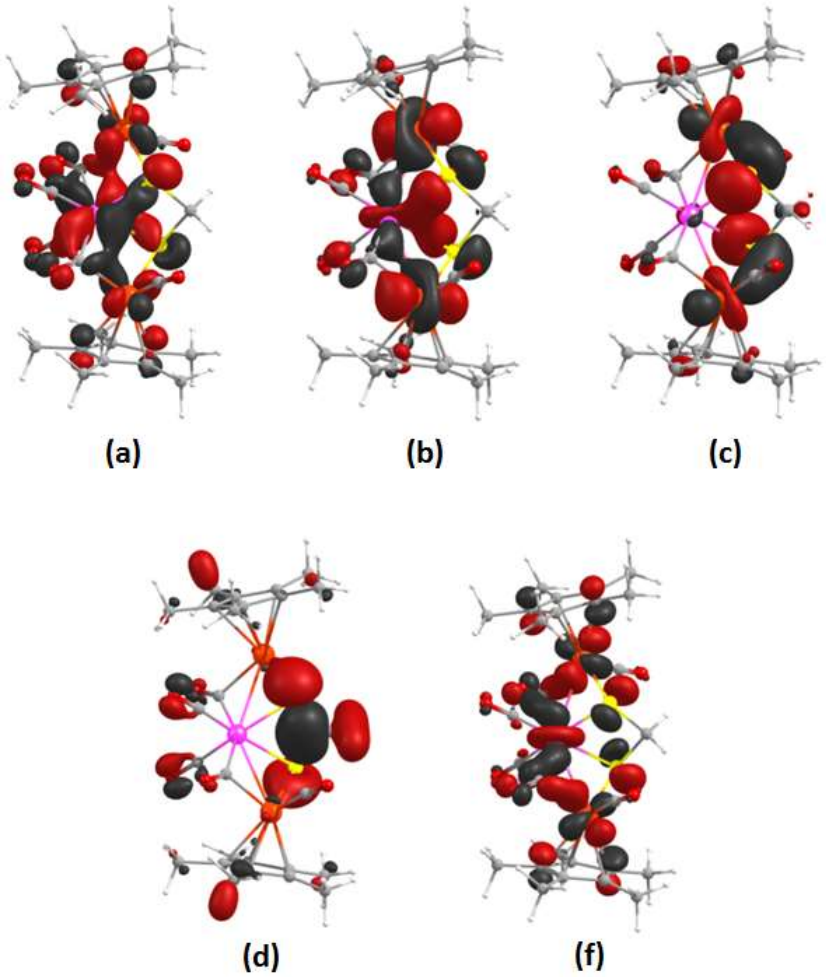

Figure S51. Selected frontier molecular orbitals of **6**. [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$]

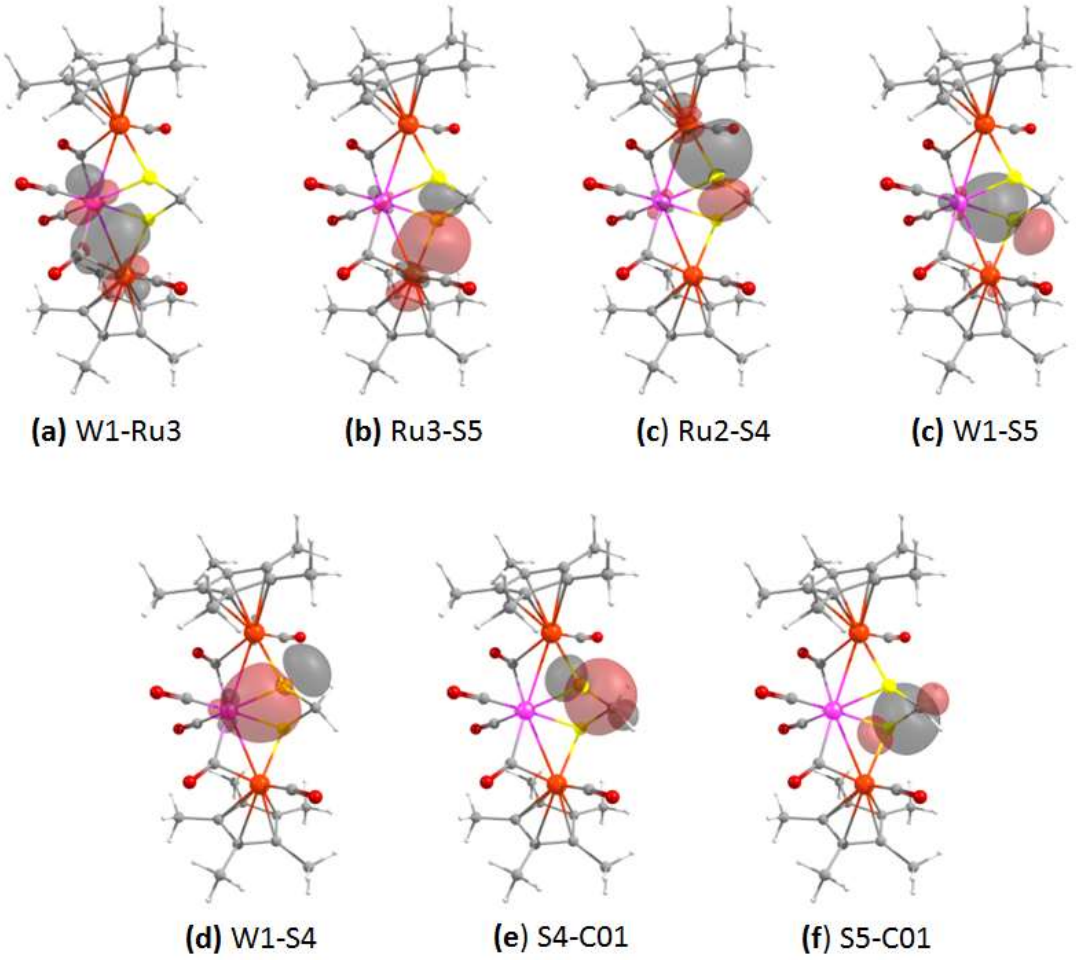

Figure S52. Selected natural bonding orbitals interaction of **6**. [isocontour values: ±0.04 (e/bohr^3)$^{1/2}$]

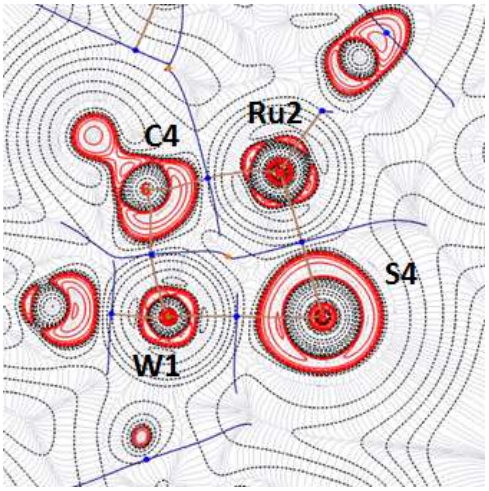

Figure S53. Contour-line diagram of the Laplacian of the electron density, $\nabla^2\rho(r)$, along the Ru2-S4-W1 plane of **6**. Dashed red lines indicate areas of charge concentration ($\nabla^2\rho(r) < 0$), while dotted black lines indicate areas of charge depletion ($\nabla^2\rho(r) > 0$). Solid brown lines connecting the atomic nuclei are the bond paths. The thick blue lines indicate the zero-flux surfaces crossing the molecular plane. Blue and orange dots indicate BCPs (bond critical points) and RCPs (ring critical points), respectively.

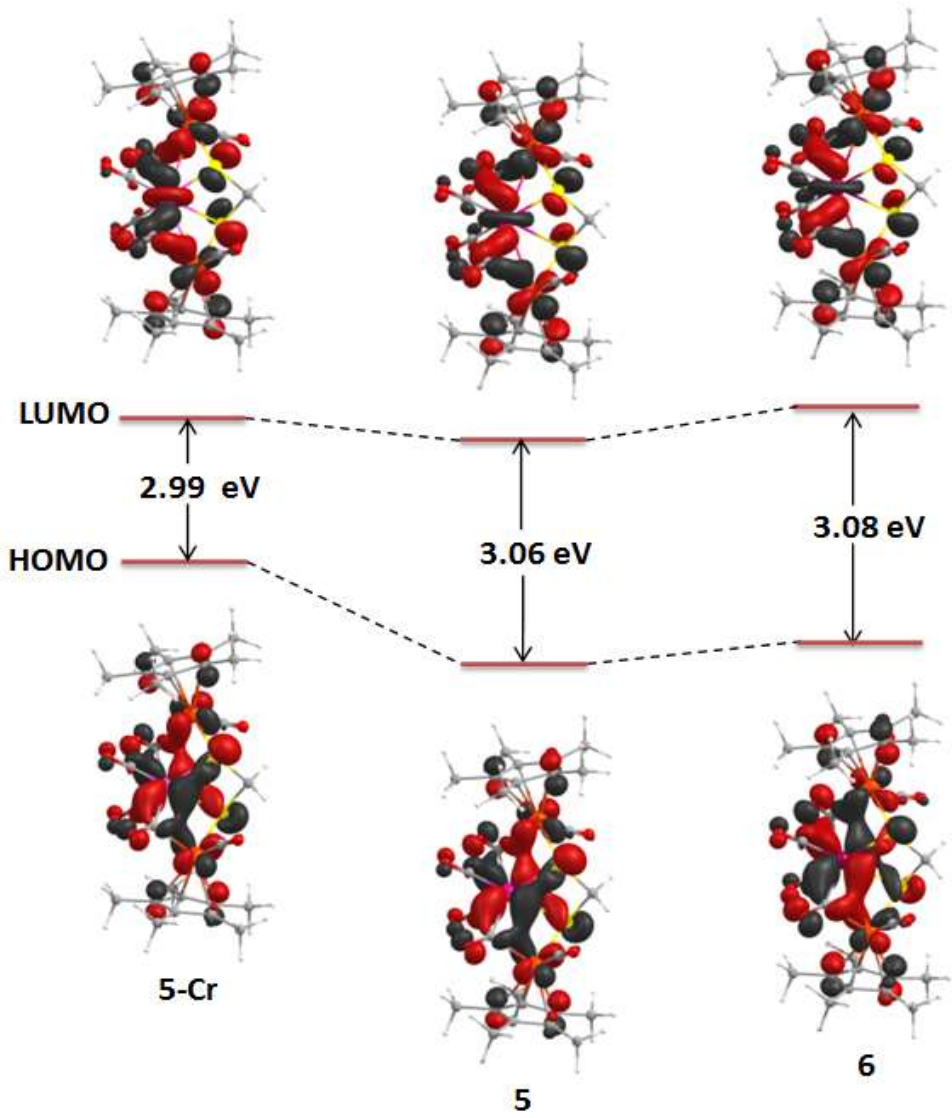

Figure S54. Comparison of frontier molecular orbitals of [{Cp*Ru(CO)}$_2$(μ-CO)$_2$(μ_3-CH$_2$S$_2$-κ^2S':κ^2S''){Cr(CO)$_2$}] (**5-Cr**), **5**, **6**, respectively. [isocontour values: ±0.04 (e/bohr^3)$^{1/2}$]

Table S4. TD-DFT calculated energies (excitation energy (eV), λ_{calc} (nm)), oscillator strength (*f*), and main composition of the first UV−vis electronic excitations for **1**. Experimental absorption wavelengths (λ_{exp}, nm) of **1** are given for comparison.

No	Excitation Energy (eV)	Wavelength λ (nm)		Main electronic transition (% weight) [b]
		Calc. (*f*) [a]	Expt.	
1	2.424	511 (0.055)	548	HOMO→LUMO (91)
2	2.525	491 (0.010)		HOMO→LUMO+1 (90)
3	2.890	429 (0.010)	444	HOMO-1→LUMO+1 (56)
				HOMO-2→LUMO (11)
				HOMO→LUMO+2 (19)
4	2.949	420 (0.030)		HOMO-2→LUMO (68)
				HOMO→LUMO+4 (16)
5	3.442	360 (0.031)	354	HOMO-3→LUMO (58)

6	3.664	338 (0.011)	HOMO-5→LUMO (21)
			HOMO-2→LUMO+2 (18)
			HOMO-1→LUMO+2 (21)
7	3.750	331 (0.032)	HOMO-5→LUMO (47)
			HOMO-2→LUMO+2 (13)
			HOMO-1→LUMO+2 (15)
8	4.022	308 (0.021)	HOMO-4→LUMO+1 (12)
			HOMO-3→LUMO+1 (22)
			HOMO→LUMO+4 (27)
9	4.212	294 (0.011)	HOMO-5→LUMO+1 (47)
			HOMO-4→LUMO+1 (14)
10	4.279	290 (0.010)	HOMO-3→LUMO+3 (21)
			HOMO-2→LUMO+3 (28)
			HOMO-1→LUMO+3 (15)

[a]Oscillator strength greater than 0.010 and [b]Components with greater than 10% contribution shown.

Table S5. TD-DFT calculated energies (excitation energy (eV), λ_{calc} (nm)), oscillator strength (*f*), and main composition of the first UV−vis electronic excitations for **2**. Experimental absorption wavelengths (λ_{exp}, nm) of **2** are given for comparison.

No	Excitation Energy (eV)	Wavelength λ (nm)		Main electronic transition (% weight) [b]
		Calc. (*f*) [a]	Expt.	
1	1.888	657 (0.002)		HOMO→LUMO (79)
				HOMO-1→LUMO (14)
2	2.136	580 (0.021)	630	HOMO-1→LUMO (67)
				HOMO-2→LUMO (12)
3	2.302	539 (0.013)		HOMO-2→LUMO (75)
4	2.567	483 (0.012)		HOMO→LUMO+1 (65))
5	2.723	455 (0.018)		HOMO→LUMO+2 (21)
				HOMO-1→LUMO+1 (17)
				HOMO-4→LUMO+1 (16)
				HOMO-3→LUMO (14)
6	2.840	437 (0.021)		HOMO-1→LUMO+2 (23)
				HOMO-4→LUMO (21)
7	3.121	397 (0.048)		HOMO-2→LUMO+1 (18)
				HOMO-4→LUMO+1 (14)
				HOMO-2→LUMO+2 (13)
				HOMO-5→LUMO (11)
8	3.223	385 (0.024)		HOMO-6→LUMO (25)
				HOMO→LUMO+3 (17)
9	3.373	368 (0.040)		HOMO-4→LUMO+1 (24)
				HOMO-3→LUMO+2 (20)
10	3.432	361 (0.025)		HOMO-4→LUMO+1 (35)
				HOMO-7→LUMO (13)

[a]Oscillator strength greater than 0.010 and [b]Components with greater than 10% contribution shown.

Table S6. TD-DFT calculated energies (excitation energy (eV), λ_{calc} (nm)), oscillator strength (*f*), and main composition of the first UV−vis electronic excitations for **3**. Experimental absorption wavelengths (λ_{exp}, nm) of **3** are given for comparison.

No	Excitation Energy (eV)	Wavelength λ (nm)		Main electronic transition (% weight) [b]
		Calc. (*f*) [a]	Expt.	
1	2.317	535 (0.013)		HOMO-2→LUMO (43)
				HOMO-1→LUMO (36)
				HOMO→LUMO (15)
2	2.512	494 (0.050)	512	HOMO→LUMO (48)
				HOMO-2→LUMO (30)
3	2.873	432 (0.16)		HOMO-1→LUMO+2 (45)
				HOMO-2→LUMO+2 (24)
				HOMO→LUMO+1 (17)
4	2.953	420 (0.012)		HOMO-3→LUMO (78)
5	3.216	385 (0.025)		HOMO→LUMO+2 (54)
				HOMO-2→LUMO+2 (12)
6	3.365	368 (0.019)		HOMO-6→LUMO (34)
				HOMO-7→LUMO (14)
				HOMO-5→LUMO (11)
7	3.397	365 (0.013)		HOMO-3→LUMO+1 (31)
				HOMO-3→LUMO+2 (14)
8	3.530	351 (0.030)		HOMO-4→LUMO+1 (27)
				HOMO-8→LUMO (15)
				HOMO-1→LUMO+3 (11)
9	3.573	347 (0.034)	360	HOMO-2→LUMO+3 (32)
				HOMO-3→LUMO+1 (14)
10	3.618	343 (0.023)		HOMO-6→LUMO (44)
				HOMO-8→LUMO (14)
				HOMO-7→LUMO (12)

[a]Oscillator strength greater than 0.010 and [b]Components with greater than 10% contribution shown.

Table S7. TD-DFT calculated energies (excitation energy (eV), λ_{calc} (nm)), oscillator strength (*f*), and main composition of the first UV−vis electronic excitations for **4**. Experimental absorption wavelengths (λ_{exp}, nm) of **4** are given for comparison.

No	Excitation Energy (eV)	Wavelength λ (nm)		Main electronic transition (% weight) [b]
		Calc. (*f*) [a]	Expt.	
1	2.621	473 (0.026)		HOMO→LUMO+2 (65)
2	2.704	459 (0.019)		HOMO-2→LUMO (35)
				HOMO-1→LUMO+2 (32)
				HOMO-2→LUMO+1 (15)
3	2.717	456 (0.015)		HOMO-2→LUMO+1 (28)
				HOMO-2→LUMO+2 (23)
				HOMO→LUMO+1 (17)
				HOMO-2→LUMO (16)
4	3.012	412 (0.046)	424	HOMO-2→LUMO+2 (31)
				HOMO-2→LUMO+1 (15)

				HOMO-4→LUMO (15)
5	3.120	397 (0.011)		HOMO-5→LUMO (60) HOMO-4→LUMO (16)
6	3.447	360 (0.012)		HOMO-5→LUMO+2 (27) HOMO-4→LUMO+2 (26) HOMO-6→LUMO (11)
7	3.495	355 (0.041)		HOMO-5→LUMO+2 (15) HOMO-4→LUMO+1 (14) HOMO-3→LUMO+2 (13)
8	3.607	344 (0.028)		HOMO→LUMO+3 (27) HOMO-5→LUMO+1 (17) HOMO-1→LUMO+3 (14)
9	3.733	332 (0.033)		HOMO-7→LUMO (42) HOMO-6→LUMO (12) HOMO-2→LUMO+3 (12)
10	3.755	330 (0.025)		HOMO-6→LUMO+1 (28) HOMO→LUMO+4 (21) HOMO-1→LUMO+4 (12)

[a]Oscillator strength greater than 0.010 and [b]Components with greater than 10% contribution shown.

Table S8. TD-DFT calculated energies (excitation energy (eV), λ_{calc} (nm)), oscillator strength (*f*), and main composition of the first UV−vis electronic excitations for **5**. Experimental absorption wavelengths (λ_{exp}, nm) of **5** are given for comparison.

No	Excitation Energy (eV)	Wavelength λ (nm)		Main electronic transition (% weight) [b]
		Calc. (*f*) [a]	Expt.	
1	2.311	536 (0.187)	524	HOMO→LUMO (73) HOMO-2→LUMO (12)
2	2.462	504 (0.048)		HOMO-2→LUMO (51) HOMO-3→LUMO (23) HOMO→LUMO (16)
3	2.725	455 (0.013)		HOMO-4→LUMO (75)
4	3.088	401 (0.209)	406	HOMO-1→LUMO+1 (39) HOMO-5→LUMO (20) HOMO-3→LUMO+1 (17)
5	3.115	398 (0.091)		HOMO-3→LUMO+1 (49) HOMO-2→LUMO+1 (22) HOMO-1→LUMO+1 (13)
6	3.232	384 (0.153)		HOMO-5→LUMO (61) HOMO-1→LUMO+1 (19)
7	3.314	374 (0.017)		HOMO-6→LUMO (50) HOMO→LUMO+2 (26)
8	3.381	367 (0.042)		HOMO-7→LUMO (69)
9	3.513	353 (0.043)		HOMO-4→LUMO+1 (31) HOMO-1→LUMO+2 (27) HOMO→LUMO+2 (19)
10	4.077	304 (0.016)		HOMO-9→LUMO (26)

				HOMO-3→LUMO+3 (21)
				HOMO-7→LUMO+1 (12)

[a]Oscillator strength greater than 0.010 and [b]Components with greater than 10% contribution shown.

Table S9. TD-DFT calculated energies (excitation energy (eV), λ_{calc} (nm)), oscillator strength (*f*), and main composition of the first UV−vis electronic excitations for **6**. Experimental absorption wavelengths (λ_{exp}, nm) of **6** are given for comparison.

No	Excitation Energy (eV)	Wavelength λ (nm)		Main electronic transition (% weight) [b]
		Calc. (*f*) [a]	Expt.	
1	2.377	524 (0.179)	514	HOMO→LUMO (64)
				HOMO-2→LUMO (23)
2	2.476	501 (0.046)		HOMO-3→LUMO (68)
				HOMO→LUMO (21)
3	3.042	408 (0.041)		HOMO-2→LUMO+1 (84)
4	3.111	399 (0.351)	398	HOMO-1→LUMO+1 (52)
				HOMO-2→LUMO+1 (12)
5	3.251	381 (0.079)		HOMO-5→LUMO (64)
				HOMO-1→LUMO+1 (11)
6	3.398	365 (0.037)		HOMO-6→LUMO (30)
				HOMO-4→LUMO+1 (25)
				HOMO→LUMO+2 (20)
7	3.505	354 (0.075)		HOMO-4→LUMO+1 (35)
				HOMO→LUMO+2 (28)
8	3.633	341 (0.019)		HOMO-3→LUMO+2 (49)
				HOMO-4→LUMO+1 (16)
				HOMO-1→LUMO+4 (12)
9	4.069	305 (0.031)		HOMO-7→LUMO+1 (29)
				HOMO-6→LUMO+2 (15)
				HOMO-2→LUMO+4 (14)
10	4.088	303 (0.016)		HOMO-2→LUMO+4 (28)
				HOMO-9→LUMO (22)
				HOMO-1→LUMO+5 (14)
				HOMO-7→LUMO+1 (11)

[a]Oscillator strength greater than 0.010 and [b]Components with greater than 10% contribution shown.

Table S10. TD-DFT calculated energies (excitation energy (eV), λ_{calc} (nm)), oscillator strength (*f*), and main composition of the first UV−vis electronic excitations for **7**. Experimental absorption wavelengths (λ_{exp}, nm) of **7** are given for comparison.

No	Excitation Energy (eV)	Wavelength λ (nm)		Main electronic transition (% weight) [b]
		Calc. (*f*) [a]	Expt.	
1	2.482	500 (0.010)		HOMO-1→LUMO (43)
				HOMO-3→LUMO (25)
2	2.592	478 (0.011)		HOMO-1→LUMO (33)
				HOMO-3→LUMO (23)
				HOMO-3→LUMO+1 (21)

3	2.687	462 (0.024)		HOMO→LUMO+2 (70)
4	2.751	451 (0.021)		HOMO-2→LUMO (51))
5	2.878	430 (0.026)		HOMO-3→LUMO+1 (25) HOMO-4→LUMO (13) HOMO-2→LUMO+1 (12) HOMO-2→LUMO (11)
6	3.076	403 (0.044)	418	HOMO-2→LUMO+2 (62)
7	3.232	384 (0.014)		HOMO-3→LUMO+2 (76)
8	3.431	361 (0.046)		HOMO-6→LUMO (13) HOMO-1→LUMO+3 (12)
9	3.687	336 (0.015)		HOMO-1→LUMO+3 (33) HOMO-8→LUMO (13)
10	3.736	332 (0.016)		HOMO-2→LUMO+3 (36) HOMO-7→LUMO (15) HOMO→LUMO+5 (12)

[a]Oscillator strength greater than 0.010 and [b]Components with greater than 10% contribution shown.

Table S11. TD-DFT calculated energies (excitation energy (eV), λ_{calc} (nm)), oscillator strength (*f*), and main composition of the first UV−vis electronic excitations for **8**. Experimental absorption wavelengths (λ_{exp}, nm) of **8** are given for comparison.

No	Excitation Energy (eV)	Wavelength λ (nm)		Main electronic transition (% weight) [b]
		Calc. (*f*) [a]	Expt.	
1	2.541	488 (0.014)		HOMO-3→LUMO (35) HOMO-1→LUMO+1 (22) HOMO-1→LUMO (16)
2	2.607	476 (0.013)		HOMO→LUMO+2 (50) HOMO-2→LUMO (23)
3	2.686	462 (0.024)		HOMO-1→LUMO+2 (43) HOMO→LUMO+2 (22) HOMO-2→LUMO (11)
4	2.744	452 (0.024)		HOMO-2→LUMO (39) HOMO-1→LUMO+2 (22)
5	2.868	433 (0.012)		HOMO-3→LUMO+1 (48)
6	3.056	406 (0.047)	416	HOMO-2→LUMO+2 (51)
7	3.224	385 (0.016)		HOMO→LUMO+3 (53) HOMO+5→LUMO+1 (13)

8	3.278	378 (0.018)	HOMO-4→LUMO+2 (52) HOMO-5→LUMO (19)
9	3.348	370 (0.025)	HOMO-1→LUMO+3 (28) HOMO-5→LUMO (18)
10	3.636	341 (0.039)	HOMO-1→LUMO+3 (23) HOMO-8→LUMO+1 (21)

[a]Oscillator strength greater than 0.010 and [b]Components with greater than 10% contribution shown.

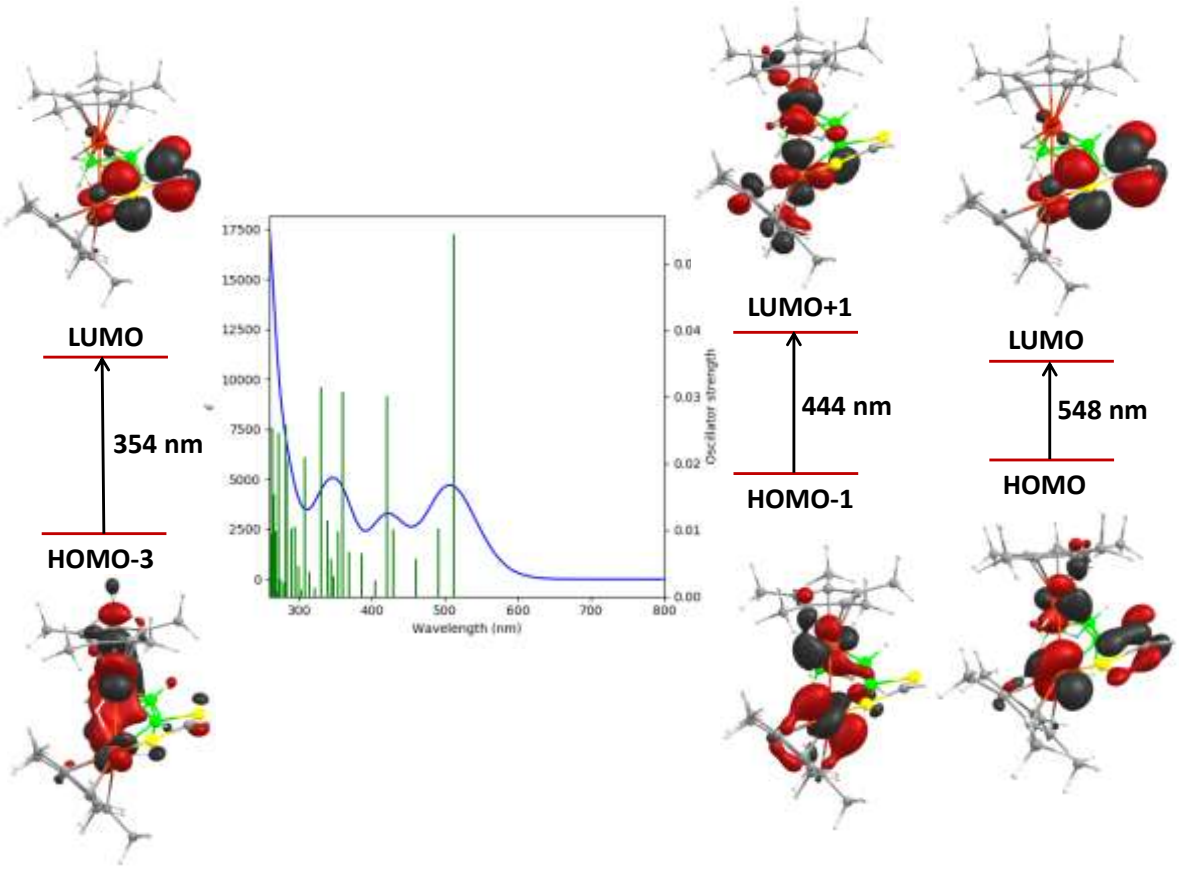

Figure S55. Absorption spectrum of **1** computed at TD-DFT-B3LYP/Def2-TZVP level of theory (ε in $LM^{-1}cm^{-1}$) and selected molecular orbitals of **1** related to most intense electronic transitions [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$].

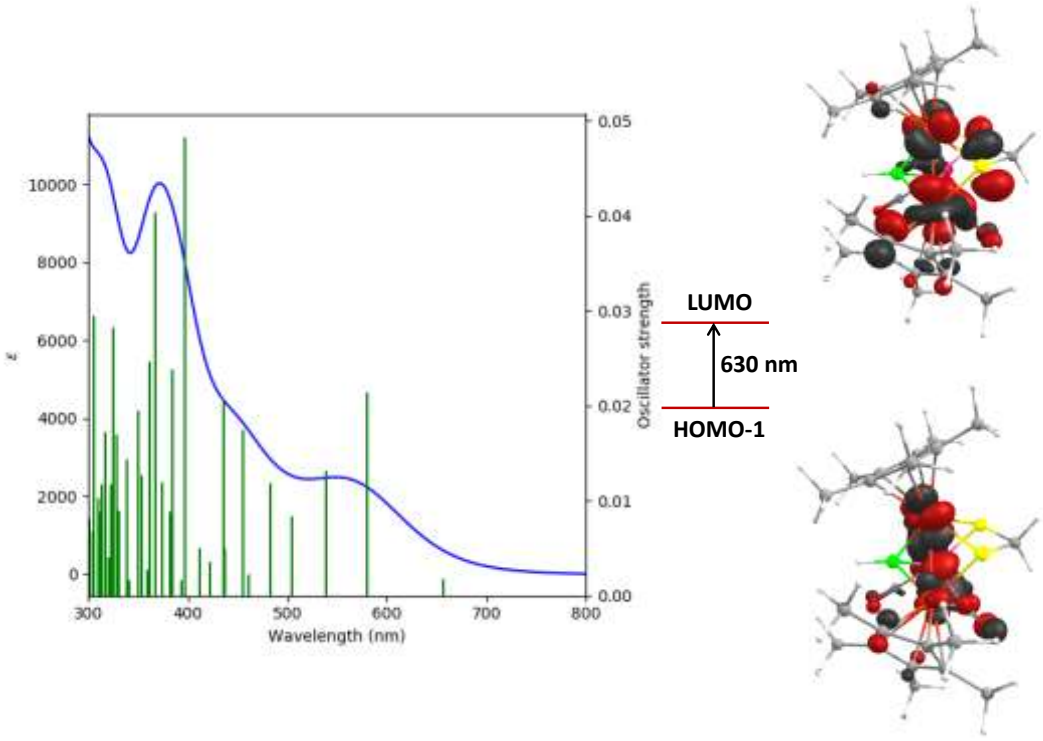

Figure S56. Absorption spectrum of **2** computed at the TD-DFT-B3LYP/Def2-TZVP level of theory (ε in $LM^{-1}cm^{-1}$) and selected molecular orbitals of **2** related to most intense electronic transitions [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$].

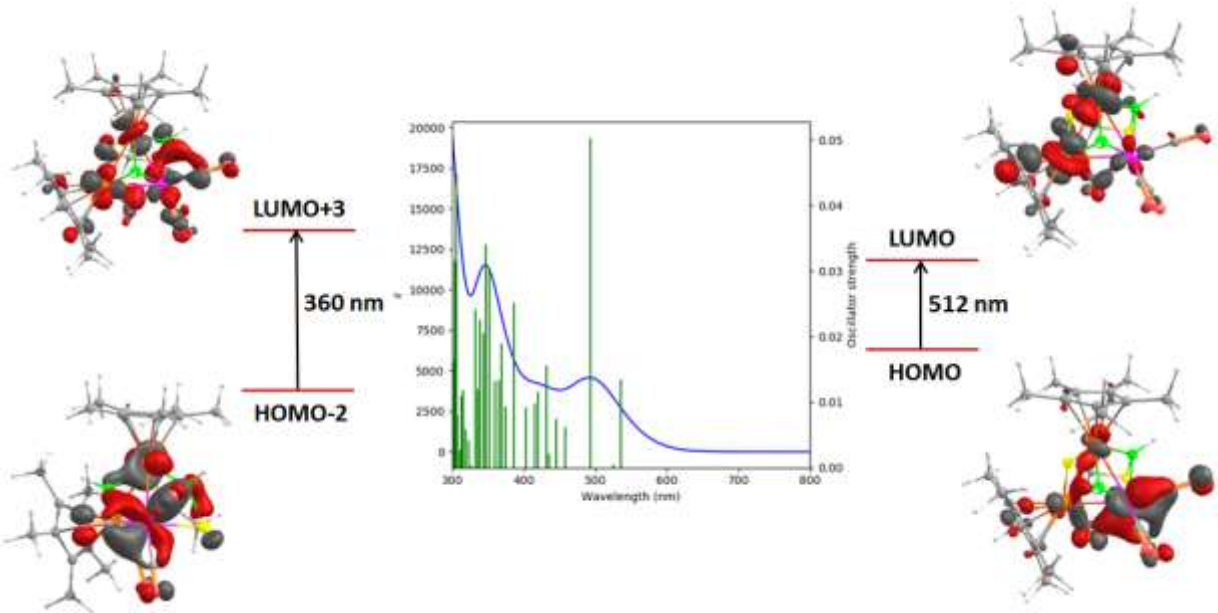

Figure S57. Absorption spectrum of **3** computed at TD-DFT-B3LYP/Def2-TZVP level of theory (ε in $LM^{-1}cm^{-1}$) and selected molecular orbitals of **3** related to most intense electronic transitions [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$].

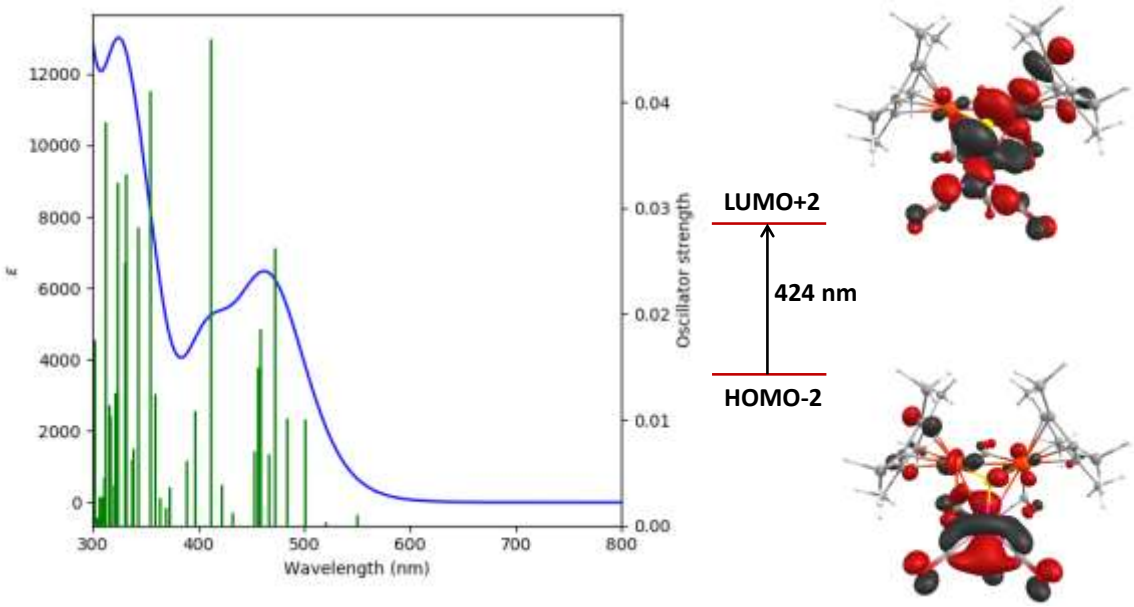

Figure S58. Absorption spectrum of **4** computed at TD-DFT-B3LYP/Def2-TZVP level of theory (ε in $LM^{-1}cm^{-1}$) and selected molecular orbitals of **4** related to most intense electronic transitions [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$].

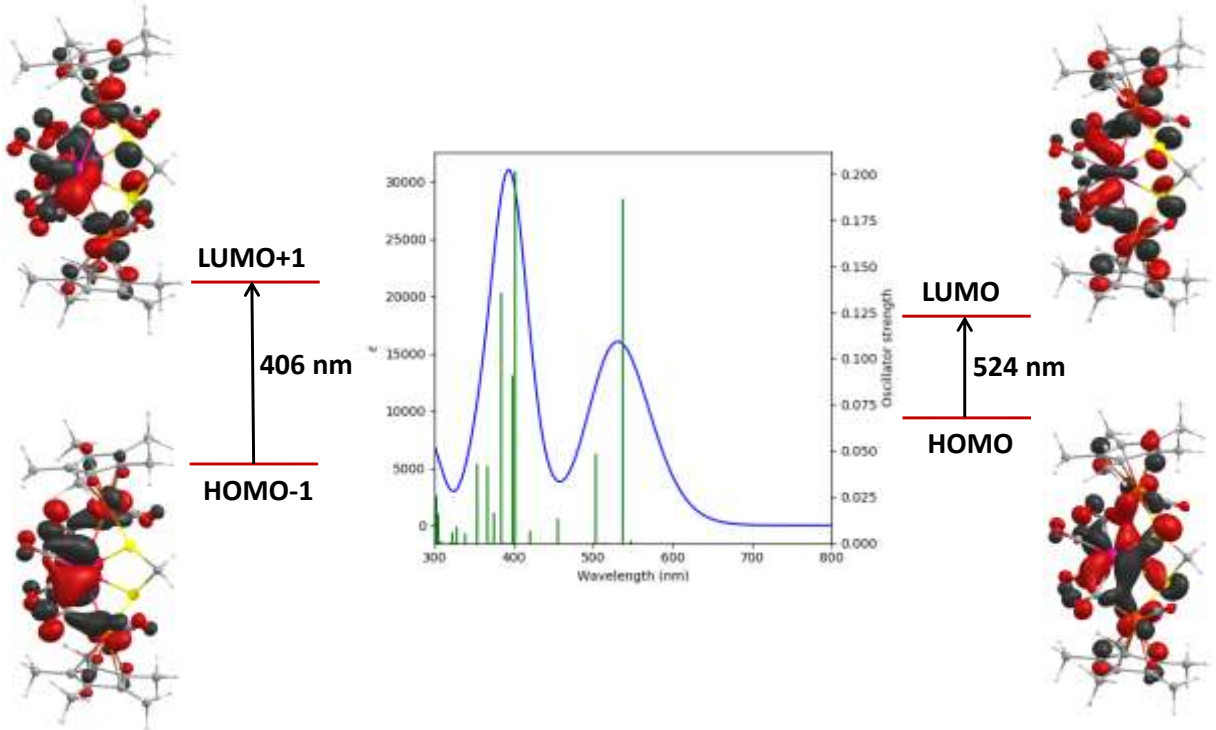

Figure S59. Absorption spectrum of **5** computed at TD-DFT-B3LYP/Def2-TZVP level of theory (ε in $LM^{-1}cm^{-1}$) and selected molecular orbitals of **5** related to most intense electronic transitions [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$].

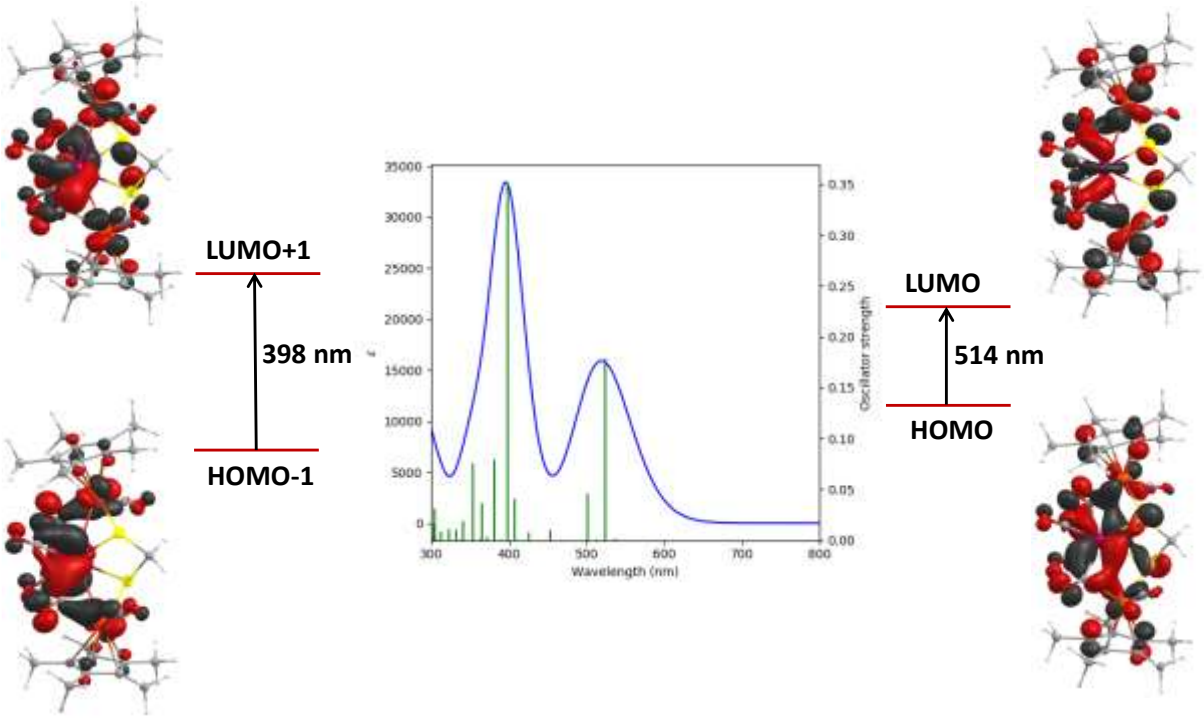

Figure S60. Absorption spectrum of **6** computed at TD-DFT-B3LYP/Def2-TZVP level of theory (ε in $LM^{-1}cm^{-1}$) and selected molecular orbitals of **6** related to most intense electronic transitions [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$]

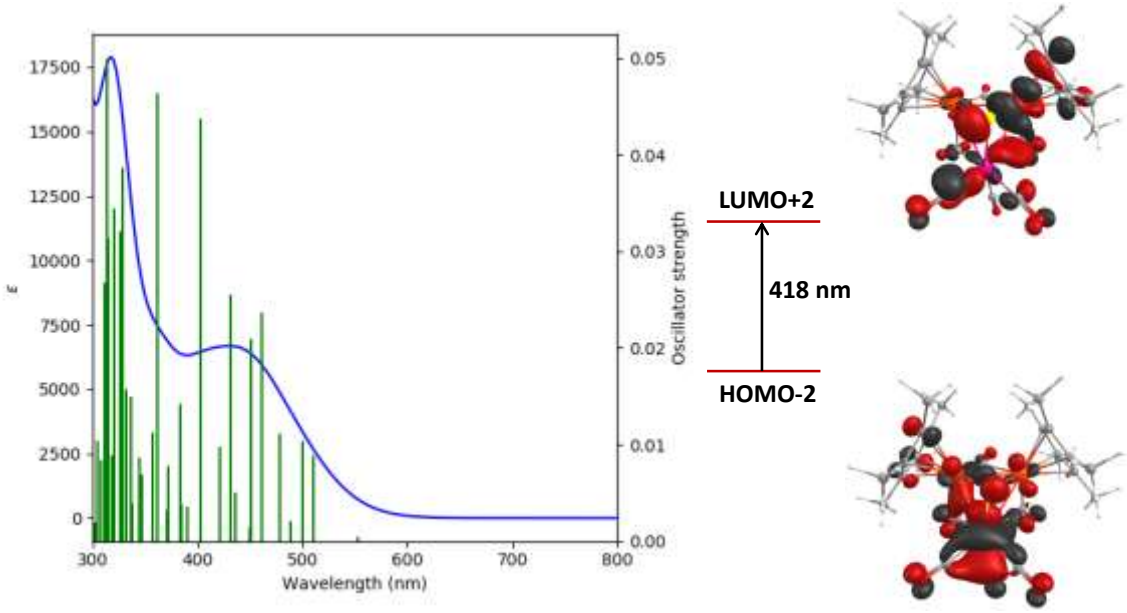

Figure S61. Absorption spectrum of **7** computed at TD-DFT-B3LYP/Def2-TZVP level of theory (ε in $LM^{-1}cm^{-1}$) and selected molecular orbitals of **7** related to most intense electronic transitions [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$].

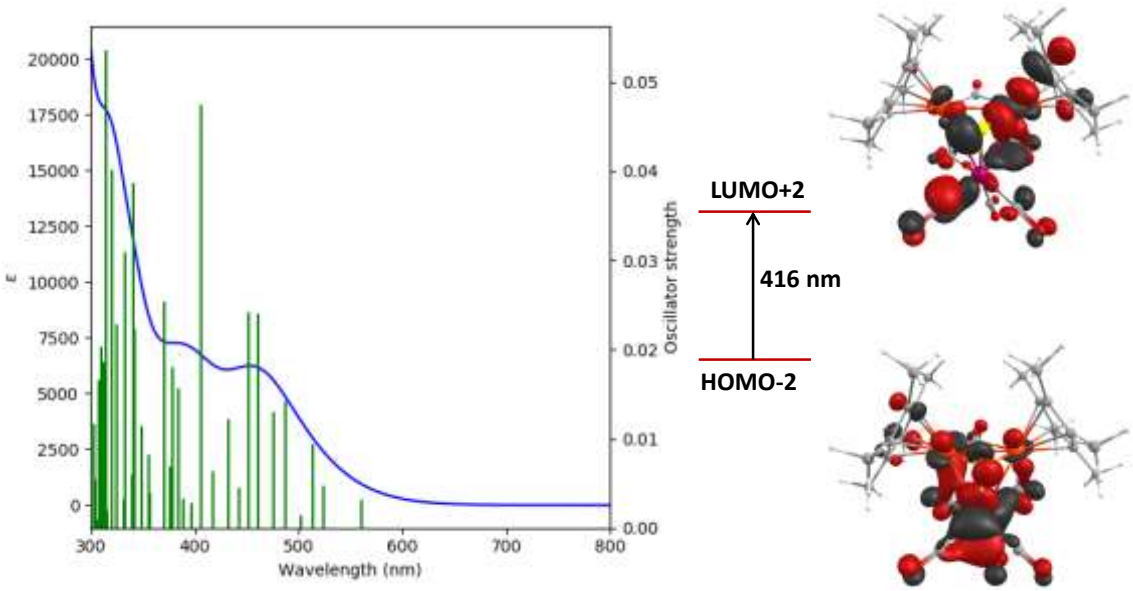

Figure S62. Absorption spectrum of **8** computed at TD-DFT-B3LYP/Def2-TZVP level of theory (ε in $LM^{-1}cm^{-1}$) and selected molecular orbitals of **8** related to most intense electronic transitions [isocontour values: ±0.04 $(e/bohr^3)^{1/2}$].

IV Cartesian coordinate of all optimized structures

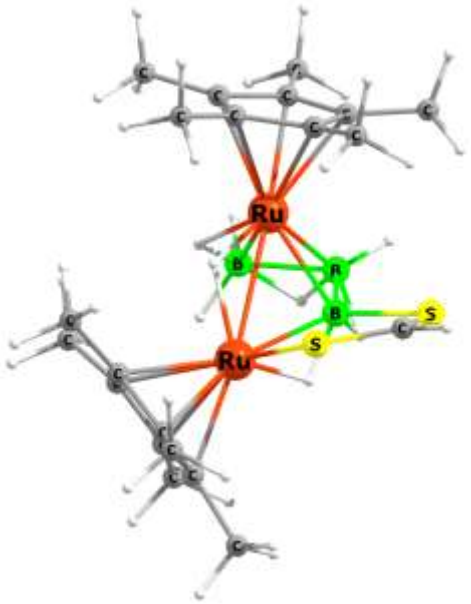

Figure S63. Optimized geometry of **1**.

Total energy = -1885.08784903 a.u.

Cartesian coordinates for the calculated structure **1** (in Å)

C	4.590947000	0.884659000	-1.195002000
H	4.679504000	1.809032000	-0.625415000
H	4.245782000	1.146977000	-2.194562000
H	5.595653000	0.458904000	-1.294941000
C	3.665036000	-0.086480000	-0.529658000
C	3.493709000	-0.257087000	0.883605000
C	2.632304000	-1.376309000	1.098945000
C	2.329663000	-1.955695000	-0.193192000
C	2.952826000	-1.162450000	-1.187502000
C	4.182722000	0.534847000	1.949449000
H	3.596527000	0.577379000	2.866966000
H	4.374888000	1.559686000	1.634240000
H	5.145887000	0.075403000	2.192626000
C	2.292214000	-1.986813000	2.423075000
H	3.034395000	-2.742144000	2.704406000
H	1.319576000	-2.476359000	2.399058000
H	2.266497000	-1.239928000	3.215713000
C	1.617923000	-3.253994000	-0.402240000
H	1.194673000	-3.328571000	-1.401211000
H	0.806537000	-3.388348000	0.311866000
H	2.315965000	-4.087639000	-0.269487000
C	2.995867000	-1.447902000	-2.656402000
H	3.883394000	-2.041167000	-2.900776000
H	3.046397000	-0.530559000	-3.242585000
H	2.119781000	-2.003480000	-2.984751000
C	-1.719317000	-0.994158000	2.989386000
H	-2.418499000	-0.935453000	3.830371000
H	-0.878029000	-0.339900000	3.214034000
H	-1.345083000	-2.016361000	2.946453000
C	-2.401240000	-0.597950000	1.716220000
C	-2.622557000	0.758254000	1.286273000
C	-3.426692000	0.711750000	0.106725000
C	-3.680577000	-0.665434000	-0.208028000
C	-3.058240000	-1.469466000	0.809078000
C	-2.316071000	1.981029000	2.093208000
H	-3.124337000	2.176878000	2.807080000
H	-2.214688000	2.863711000	1.464548000
H	-1.393994000	1.872548000	2.661434000
C	-4.047394000	1.892677000	-0.570524000
H	-4.270352000	1.687020000	-1.616172000
H	-3.395957000	2.764972000	-0.536094000
H	-4.987957000	2.159695000	-0.077099000
C	-4.608310000	-1.169124000	-1.268963000
H	-5.630369000	-1.244532000	-0.882683000
H	-4.314804000	-2.155541000	-1.625238000
H	-4.629021000	-0.505110000	-2.132252000
C	-3.183429000	-2.957252000	0.935441000
H	-2.344923000	-3.388279000	1.481487000
H	-3.228471000	-3.440863000	-0.039671000
H	-4.098671000	-3.221173000	1.475863000
C	0.484960000	3.278597000	0.333146000
B	-0.173564000	1.142567000	-1.318864000
B	-1.380236000	0.359357000	-2.387455000
B	-1.148784000	-1.508067000	-2.354228000
S	-0.415806000	3.035706000	-1.077925000
S	1.377887000	2.133295000	1.121455000
Ru	1.528350000	0.164928000	-0.060416000
Ru	-1.462003000	-0.326283000	-0.364880000
H	1.119970000	0.993447000	-1.510635000
H	-0.337085000	1.112841000	-2.664290000
H	-2.306954000	0.935419000	-2.864536000
H	-0.993934000	-0.500354000	-3.249107000
H	-0.139693000	-2.045912000	-2.728498000
H	-2.143839000	-2.058794000	-2.723670000
H	-0.002809000	-0.607268000	0.481285000
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H	-0.864429000	-1.726612000	-1.016879000

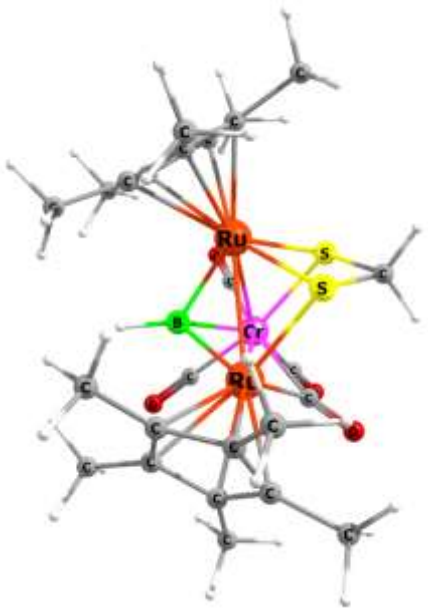

Figure S64. Optimized geometry of **2**.

Total energy = -3329.89568954 a.u.

Cartesian coordinates for the calculated structure **2** (in Å)

C	-2.725241000	-2.216813000	-0.310212000	C	3.060496000	-0.396858000	1.419072000
C	-2.267969000	-2.135395000	1.040748000	C	2.432870000	-1.690126000	1.396219000
C	-2.763463000	-0.916131000	1.607912000	C	1.903689000	-2.392169000	2.604544000
C	-3.527299000	-0.247455000	0.600893000	H	2.736483000	-2.727070000	3.231894000
C	-3.514379000	-1.054481000	-0.588101000	H	1.320274000	-3.271371000	2.341328000
C	-2.541889000	-3.390759000	-1.219966000	H	1.281431000	-1.737548000	3.213841000
H	-1.589083000	-3.891116000	-1.049395000	C	2.240786000	-3.632390000	-0.333503000
H	-2.577306000	-3.099419000	-2.268349000	H	1.405245000	-4.020857000	0.247034000
H	-3.335665000	-4.125584000	-1.051842000	H	3.081641000	-4.321017000	-0.201874000
C	-1.585149000	-3.229397000	1.795529000	H	1.955322000	-3.658924000	-1.384819000
H	-2.328492000	-3.909796000	2.225428000	C	3.944632000	-1.561836000	-2.050362000
H	-0.987228000	-2.840187000	2.616174000	H	4.054042000	-0.634427000	-2.611673000
H	-0.936904000	-3.823344000	1.152623000	H	3.310882000	-2.231224000	-2.631348000
C	-2.707285000	-0.538761000	3.054089000	H	4.935800000	-2.023411000	-1.984244000
H	-3.568702000	-0.963371000	3.581014000	C	4.538311000	0.975074000	-0.230916000
H	-2.727702000	0.539464000	3.196557000	H	4.440002000	1.231082000	-1.284993000
H	-1.807287000	-0.915380000	3.536566000	H	5.586450000	0.717912000	-0.046487000
C	-4.350619000	0.984858000	0.810683000	H	4.309094000	1.866870000	0.348980000
H	-4.484735000	1.544432000	-0.113122000	C	3.241610000	0.447231000	2.641139000
H	-3.901199000	1.650771000	1.545759000	H	4.094751000	0.082632000	3.223630000
H	-5.344073000	0.707888000	1.178171000	H	2.364823000	0.415500000	3.286285000
C	-4.321700000	-0.807705000	-1.824796000	H	3.433464000	1.488657000	2.392520000
H	-3.908859000	-1.334921000	-2.684193000	H	0.072750000	0.040951000	2.415501000
H	-4.362184000	0.250092000	-2.076287000	C	0.430103000	0.379446000	-2.962300000
H	-5.349104000	-1.159639000	-1.684450000	H	-0.424993000	0.858022000	-3.436630000
C	2.620828000	-2.251217000	0.100417000	H	1.130554000	0.032640000	-3.720433000
C	3.384499000	-1.315940000	-0.682673000	C	-1.684355000	1.404575000	-1.085579000
C	3.658547000	-0.175562000	0.142856000	C	1.469132000	3.009817000	0.695791000

C	-0.747769000	3.691542000	-0.454159000	O	-1.266457000	2.616265000	2.722929000
C	-0.782989000	2.358213000	1.701769000	Ru	-1.403915000	-0.370103000	-0.179911000
Cr	-0.001731000	2.053604000	0.066167000	Ru	1.425050000	-0.348207000	-0.210449000
O	-2.432662000	1.853208000	-1.866926000	S	-0.017306000	-1.055513000	-1.918762000
O	2.353125000	3.611909000	1.122851000	S	1.331125000	1.442844000	-1.774957000
O	-1.211202000	4.693370000	-0.763460000	B	0.047247000	0.279797000	1.249294000

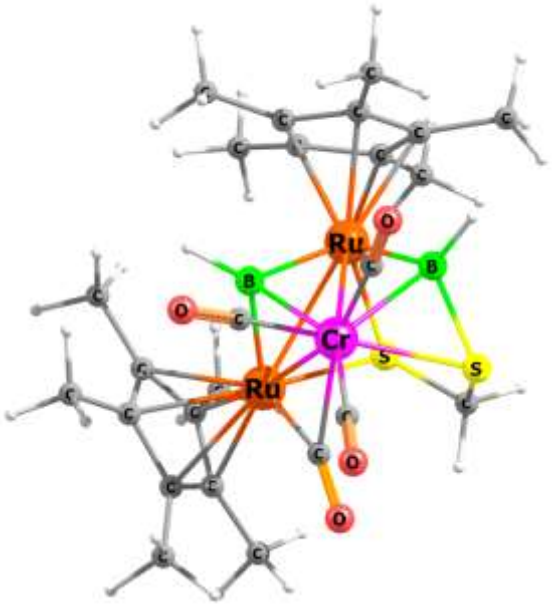

Figure S65. Optimized geometry of **3**.

Total energy = -3355.35413737 a.u.

Cartesian coordinates for the calculated structure **3** (in Å)

Cr	0.132598000	2.071927000	0.241743000	C	-4.103579000	1.002446000	1.526205000
Ru	-1.435987000	-0.272771000	-0.162326000	H	-3.531817000	1.336537000	2.390433000
Ru	1.392082000	-0.436553000	-0.164788000	H	-4.204644000	1.850797000	0.852816000
C	-2.520686000	-2.270646000	0.578372000	H	-5.106550000	0.734045000	1.875344000
C	-2.749719000	-1.221054000	1.520372000	C	-2.045928000	-3.654613000	0.889237000
C	-2.523856000	-1.304321000	2.996873000	H	-1.483167000	-3.691243000	1.818355000
H	-1.667752000	-1.929829000	3.244816000	H	-2.903539000	-4.326783000	1.004880000
H	-2.349763000	-0.323271000	3.435118000	H	-1.424753000	-4.067821000	0.094554000
H	-3.402334000	-1.736222000	3.487975000	C	3.234217000	-1.615498000	-0.740562000
C	-3.462472000	-0.171685000	0.855252000	C	3.604196000	-0.742315000	0.327862000
C	-3.663344000	-0.573976000	-0.509990000	C	2.854487000	-1.107661000	1.493027000
C	-3.054487000	-1.857872000	-0.675348000	C	2.055212000	-2.243096000	1.156049000
C	-3.117226000	-2.703206000	-1.909472000	C	2.258530000	-2.540109000	-0.227354000
H	-2.242139000	-3.345396000	-2.005422000	C	1.714288000	-3.716151000	-0.976183000
H	-4.000712000	-3.349875000	-1.883884000	H	0.801520000	-4.095814000	-0.520832000
H	-3.181309000	-2.096661000	-2.811690000	H	1.487030000	-3.462494000	-2.011313000
C	-4.568606000	0.089558000	-1.501789000	H	2.443014000	-4.532736000	-0.987351000
H	-4.254650000	-0.098032000	-2.528413000	C	1.316009000	-3.072047000	2.154430000
H	-5.587973000	-0.296621000	-1.394110000	H	0.674410000	-3.806393000	1.676205000
H	-4.607816000	1.167147000	-1.359596000	H	2.032031000	-3.617956000	2.777523000

H	0.708155000	-2.460514000	2.820496000
C	3.057776000	-0.565562000	2.872565000
H	3.365220000	0.478476000	2.858497000
H	2.149078000	-0.628749000	3.468433000
H	3.837951000	-1.133646000	3.391151000
C	4.717868000	0.256710000	0.302169000
H	4.885781000	0.658193000	-0.694133000
H	4.529010000	1.094899000	0.971368000
H	5.642924000	-0.226752000	0.631871000
C	3.858847000	-1.655614000	-2.101231000
H	4.128273000	-0.658575000	-2.448286000
H	4.772428000	-2.259338000	-2.089238000
H	3.185845000	-2.093945000	-2.837307000
C	1.956669000	1.269248000	-0.866312000
C	0.636723000	2.106627000	2.009394000
C	1.228734000	3.593856000	0.080694000
C	-1.206359000	3.205297000	0.836208000
O	2.755044000	1.803922000	-1.532033000
O	0.975428000	2.285106000	3.102358000
O	1.874776000	4.536059000	0.017749000
O	-1.977069000	3.925596000	1.298704000
S	-0.077920000	-0.664399000	-1.971427000
B	-0.056830000	0.213460000	1.306986000
S	-0.566332000	2.345782000	-2.186506000
C	-0.009964000	0.843307000	-3.028247000
H	1.002372000	0.973716000	-3.406889000
H	-0.684925000	0.666987000	-3.864977000
B	-1.738401000	1.638836000	-0.889389000
H	-2.763377000	2.239702000	-0.832036000
H	-0.043571000	-0.156636000	2.438224000

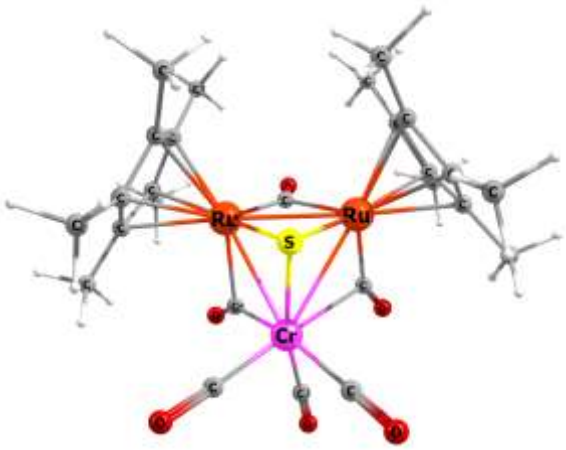

Figure S66. Optimized geometry of **4**.

Total energy = -3093.66952795 a.u.

Cartesian coordinates for the calculated structure **4** (in Å)

C	3.076968000	-1.521704000	-1.006065000
C	2.337516000	-2.467526000	-0.214681000
C	2.398673000	-2.058011000	1.155460000
C	3.177496000	-0.852974000	1.214159000
C	3.601951000	-0.533589000	-0.116089000
C	4.557261000	0.556915000	-0.482268000
H	4.471747000	1.415112000	0.182310000
H	4.403694000	0.903627000	-1.501430000
H	5.582660000	0.180767000	-0.406542000
C	3.363351000	-1.632687000	-2.470350000
H	4.277487000	-2.210508000	-2.641115000
H	3.496305000	-0.651563000	-2.923066000
H	2.550419000	-2.129107000	-2.998406000
C	1.773015000	-3.756241000	-0.722400000
H	2.568350000	-4.504937000	-0.792663000
H	1.335829000	-3.644298000	-1.712724000
H	1.008441000	-4.153757000	-0.056856000
C	1.908751000	-2.830386000	2.339464000
H	1.092221000	-3.500117000	2.075492000
H	1.556338000	-2.171470000	3.131913000
H	2.715491000	-3.444363000	2.753480000
C	3.602477000	-0.144714000	2.462996000
H	4.543608000	-0.565650000	2.832579000
H	2.862037000	-0.245639000	3.255201000
H	3.762442000	0.918468000	2.292548000
C	-3.368435000	-1.155945000	-0.909519000
C	-3.741358000	-0.137354000	0.042733000
C	-3.259579000	-0.531233000	1.327528000
C	-2.583365000	-1.791393000	1.178817000
C	-2.672062000	-2.178193000	-0.196583000
C	-3.778639000	-1.214688000	-2.347810000
H	-3.038568000	-1.740416000	-2.950002000

H	-3.900529000	-0.219437000	-2.771954000
H	-4.732666000	-1.741111000	-2.453713000
C	-4.634469000	1.031701000	-0.233157000
H	-4.512974000	1.406860000	-1.247145000
H	-4.445664000	1.855914000	0.453097000
H	-5.680242000	0.732206000	-0.112193000
C	-3.532876000	0.165662000	2.623152000
H	-4.463981000	-0.208016000	3.062144000
H	-3.639947000	1.240888000	2.489490000
H	-2.735088000	-0.000791000	3.345058000
C	-2.049520000	-2.617892000	2.305938000
H	-1.533108000	-2.004846000	3.043943000
H	-1.350585000	-3.374528000	1.954260000
H	-2.865389000	-3.137865000	2.818217000
C	-2.239196000	-3.486028000	-0.776873000
H	-3.092898000	-4.169514000	-0.820757000
H	-1.468909000	-3.963179000	-0.173859000
H	-1.853130000	-3.369892000	-1.787782000
C	0.010831000	-1.004413000	-1.400119000
C	1.444751000	1.375073000	-1.282928000
C	1.771705000	2.963818000	0.874455000
C	0.156648000	3.470036000	-1.180919000
C	-0.813833000	3.293215000	1.176620000
C	-1.561240000	1.244064000	-1.312359000
Cr	0.292120000	2.155354000	0.140971000
O	-0.101272000	-1.587414000	-2.413241000
O	2.053878000	1.498015000	-2.271583000
O	2.707425000	3.437136000	1.355840000
O	0.092076000	4.274288000	-1.995351000
O	-1.458526000	3.997154000	1.810326000
O	-2.042251000	1.796285000	-2.210087000
Ru	1.323287000	-0.452918000	-0.030872000
Ru	-1.493513000	-0.206810000	-0.063231000
S	-0.007866000	0.459996000	1.619702000

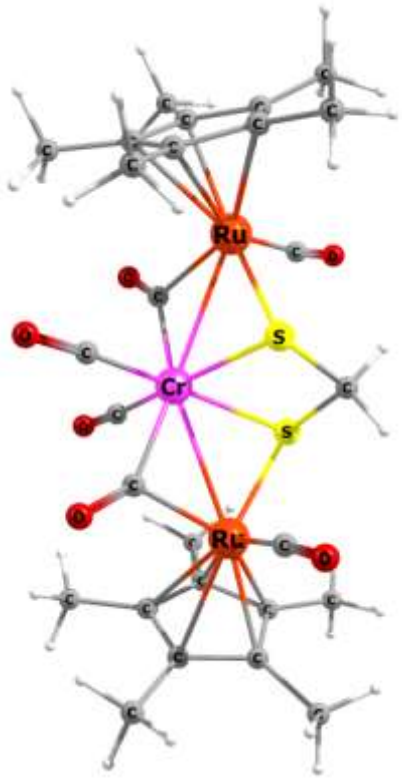

Figure S67. Optimized geometry of [{Cp*Ru(CO)}$_2$(μ-CO)$_2$(μ_3-CH$_2$S$_2$-κ^2S':κ^2S''){Cr(CO)$_2$}].

Total energy = -3531.21372068 a.u.

Cartesian coordinates for the calculated structure [{Cp*Ru(CO)}$_2$(μ-CO)$_2$(μ_3-CH$_2$S$_2$-κ^2S':κ^2S''){Cr(CO)$_2$}] (in Å)

O	1.931147000	1.888179000	-2.064738000
O	-1.930618000	1.885465000	2.067362000
C	-1.565288000	1.153194000	1.230026000
O	1.007320000	2.788930000	1.864700000
O	-1.007850000	2.788108000	-1.864803000
O	-2.344545000	-2.096982000	2.640046000
C	0.000176000	-2.393056000	-0.001199000
O	2.344773000	-2.093800000	-2.642420000

C	-2.401176000	-1.419780000	1.711846000
C	2.401321000	-1.417636000	-1.713475000
C	-4.393880000	-0.933335000	-1.145600000
C	4.750306000	0.510714000	-0.636726000
C	0.668658000	1.955311000	1.146732000
C	4.393029000	-0.933358000	1.146744000
C	1.565821000	1.154688000	-1.228454000
C	-0.669061000	1.954983000	-1.146337000
C	3.997197000	0.391825000	1.554887000
C	-4.242071000	1.275069000	-0.464468000
C	4.242879000	1.274592000	0.463777000
C	4.868858000	-0.855649000	-0.197381000
C	-4.869204000	-0.854195000	0.198674000
C	-4.749475000	0.512334000	0.636912000
C	-3.997526000	0.391361000	-1.554991000
C	-3.589219000	0.765477000	-2.946457000
H	-2.925046000	0.020238000	-3.385016000
H	-4.470458000	0.836924000	-3.592271000
H	-3.076822000	1.723983000	-2.977142000
C	-4.441918000	-2.132815000	-2.038338000
H	-3.581389000	-2.171029000	-2.705107000
H	-4.460249000	-3.059893000	-1.467168000
H	-5.343633000	-2.107710000	-2.659241000
C	-5.252126000	1.082048000	1.927212000
H	-5.347869000	0.313878000	2.693530000
H	-4.580726000	1.848694000	2.311905000
H	-6.238665000	1.537044000	1.790586000
C	-5.533492000	-1.959997000	0.960155000
H	-5.396518000	-1.854707000	2.035181000
H	-6.609829000	-1.952020000	0.762644000
H	-5.152332000	-2.938133000	0.670467000
C	-4.119964000	2.765386000	-0.473989000
H	-3.463309000	3.120079000	-1.264107000
H	-5.107884000	3.209035000	-0.635007000
H	-3.744226000	3.144396000	0.475864000
C	4.121384000	2.764968000	0.472328000
H	3.747928000	3.143657000	-0.478532000
H	3.463050000	3.120241000	1.260807000
H	5.109084000	3.208318000	0.635483000
C	5.253704000	1.079006000	-1.927375000
H	5.348417000	0.310270000	-2.693253000
H	4.583296000	1.846327000	-2.312457000
H	6.240847000	1.532787000	-1.791065000
C	5.532677000	-1.962475000	-0.957782000
H	5.396135000	-1.857917000	-2.032936000
H	6.608960000	-1.955075000	-0.759944000
H	5.150765000	-2.940133000	-0.667479000
C	3.588556000	0.767277000	2.945908000
H	2.923998000	0.022635000	3.384888000
H	4.469600000	0.838992000	3.591964000
H	3.076486000	1.725983000	2.975620000
C	4.439822000	-2.132198000	2.040390000
H	3.578740000	-2.169591000	2.706496000
H	4.458262000	-3.059698000	1.469919000
H	5.341043000	-2.106951000	2.662001000
H	-0.661625000	-3.026486000	0.584624000
H	0.662279000	-3.025634000	-0.587631000
Ru	-2.686259000	-0.342921000	0.222812000
Ru	2.686263000	-0.342507000	-0.223066000
S	-0.952767000	-1.285218000	-1.102364000
S	0.952837000	-1.286086000	1.101150000
Cr	-0.000058000	0.663315000	0.000319000

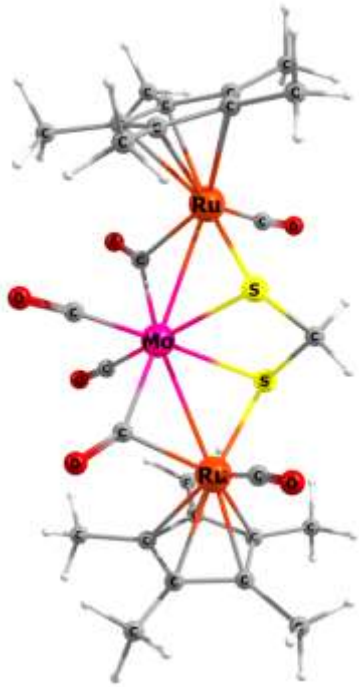

Figure S68. Optimized geometry of **5**.

Total energy = -2555.01057924 a.u.

Cartesian coordinates for the calculated structure **5** (in Å)

O	2.096857000	1.967688000	-2.032365000	H	-4.472600000	0.680460000	-3.625381000
O	-2.096754000	1.967453000	2.032736000	H	-3.098464000	1.594400000	-3.007505000
C	-1.664073000	1.231107000	1.231493000	C	-4.431510000	-2.258124000	-1.995659000
O	0.999279000	2.898812000	1.991723000	H	-3.563941000	-2.300544000	-2.652922000
O	-0.999029000	2.898146000	-1.992431000	H	-4.443136000	-3.171239000	-1.402259000
O	-2.321011000	-2.040676000	2.703870000	H	-5.327325000	-2.259946000	-2.625410000
C	0.000006000	-2.466816000	-0.000236000	C	-5.337870000	1.039133000	1.877520000
O	2.321205000	-2.040010000	-2.704253000	H	-5.427516000	0.289256000	2.662503000
C	-2.406178000	-1.391699000	1.758036000	H	-4.688100000	1.829873000	2.249867000
C	2.406202000	-1.391160000	-1.758328000	H	-6.332068000	1.468484000	1.715882000
C	-4.409862000	-1.036753000	-1.132411000	C	-5.548591000	-2.030577000	0.989165000
C	4.807230000	0.445352000	-0.609483000	H	-5.418016000	-1.896472000	2.061824000
C	0.682486000	2.082766000	1.243891000	H	-6.624135000	-2.046550000	0.787617000
C	4.409397000	-1.036262000	1.133477000	H	-5.148930000	-3.008517000	0.724934000
C	1.664307000	1.231137000	-1.231234000	C	-4.202315000	2.681435000	-0.556386000
C	-0.682480000	2.082449000	-1.244120000	H	-3.528213000	3.024449000	-1.337384000
C	4.027030000	0.284468000	1.570321000	H	-5.191945000	3.102368000	-0.761944000
C	-4.299753000	1.190334000	-0.505998000	H	-3.862787000	3.095345000	0.392165000
C	4.300273000	1.190262000	0.504909000	C	4.203350000	2.681435000	0.554105000
C	4.899260000	-0.933490000	-0.203086000	H	3.865482000	3.094806000	-0.395263000
C	-4.899597000	-0.932463000	0.204111000	H	3.528121000	3.025230000	1.333799000
C	-4.806869000	0.446661000	0.609198000	H	5.192799000	3.102134000	0.761018000
C	-4.027080000	0.283461000	-1.570574000	C	5.338574000	1.036355000	-1.878354000
C	-3.601566000	0.631039000	-2.963852000	H	5.427385000	0.285803000	-2.662786000
H	-2.922875000	-0.116299000	-3.375645000	H	4.689465000	1.827417000	-2.251180000

H	6.333197000	1.464913000	-1.717233000	H	3.562424000	-2.298515000	2.654703000
C	5.547841000	-2.032636000	-0.987040000	H	4.442023000	-3.170507000	1.405234000
H	5.417709000	-1.899296000	-2.059849000	H	5.325830000	-2.258316000	2.627993000
H	6.623311000	-2.049130000	-0.785132000	H	-0.640132000	-3.099312000	0.611070000
H	5.147477000	-3.010117000	-0.722177000	H	0.640192000	-3.099152000	-0.611656000
C	3.601774000	0.633642000	2.963278000	Ru	-2.724672000	-0.373650000	0.232068000
H	2.923767000	-0.113618000	3.376322000	Ru	2.724602000	-0.373486000	-0.232051000
H	4.473025000	0.684563000	3.624415000	S	-1.000782000	-1.382294000	-1.089261000
H	3.098025000	1.596709000	3.005844000	S	1.000735000	-1.382472000	1.089026000
C	4.430316000	-2.256866000	1.997818000	Mo	-0.000057000	0.692979000	0.000094000

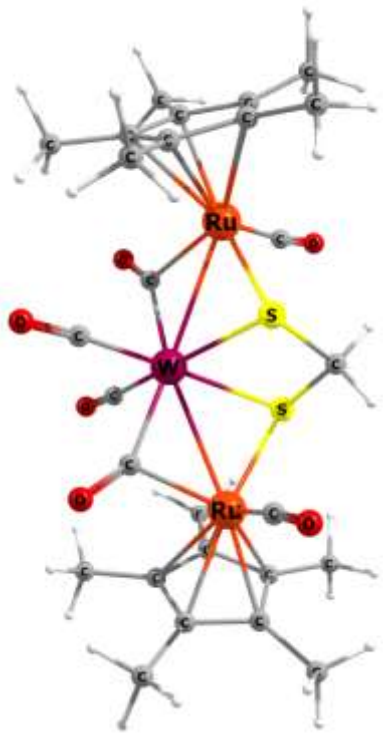

Figure S69. Optimized geometry of **6**.

Total energy = -2553.89283014 a.u.

Cartesian coordinates for the calculated structure **6** (in Å)

O	-2.103915000	1.914185000	2.046053000	C	-0.702869000	2.039195000	-1.250961000
O	2.104053000	1.914405000	-2.046076000	C	-4.413643000	-1.085586000	-1.138699000
C	1.649920000	1.194285000	-1.239467000	C	-1.650153000	1.194048000	1.239236000
O	-1.021793000	2.851152000	-2.004401000	C	0.702824000	2.038589000	1.251324000
O	1.021694000	2.850147000	2.005214000	C	-4.032914000	0.238983000	-1.566084000
O	2.326349000	-2.080757000	-2.710733000	C	4.305286000	1.137014000	0.495452000
C	-0.000063000	-2.525171000	-0.000170000	C	-4.306027000	1.136982000	-0.493764000
O	-2.325422000	-2.079899000	2.711114000	C	-4.901297000	-0.993892000	0.198438000
C	2.408784000	-1.434994000	-1.762132000	C	4.901617000	-0.992658000	-0.199479000
C	-2.408672000	-1.434733000	1.762194000	C	4.808137000	0.384146000	-0.615251000
C	4.413959000	-1.086325000	1.137557000	C	4.032696000	0.237580000	1.566647000
C	-4.808554000	0.382499000	0.615946000	C	3.613348000	0.595651000	2.959252000

H	2.939390000	-0.150249000	3.381280000
H	4.487850000	0.653109000	3.615577000
H	3.107646000	1.557806000	2.997989000
C	4.433678000	-2.301667000	2.009412000
H	3.566842000	-2.337673000	2.668112000
H	4.442929000	-3.218985000	1.422450000
H	5.329793000	-2.301310000	2.638724000
C	5.337683000	0.966581000	-1.888815000
H	5.424749000	0.210970000	-2.668585000
H	4.687987000	1.755410000	-2.265245000
H	6.332856000	1.395488000	-1.732014000
C	5.547678000	-2.096858000	-0.978326000
H	5.412520000	-1.971579000	-2.051488000
H	6.624140000	-2.110966000	-0.781444000
H	5.149473000	-3.072765000	-0.704453000
C	4.211250000	2.628617000	0.535219000
H	3.543581000	2.978913000	1.318558000
H	5.203085000	3.049380000	0.730306000
H	3.865605000	3.035787000	-0.414101000
C	-4.212513000	2.628663000	-0.531874000
H	-3.868392000	3.034981000	0.418346000
H	-3.543817000	2.979961000	-1.313907000
H	-5.204196000	3.049270000	-0.728069000
C	-5.338297000	0.963032000	1.890304000
H	-5.424310000	0.206519000	2.669317000
H	-4.689291000	1.752153000	2.267321000
H	-6.333971000	1.391070000	1.734312000
C	-5.546789000	-2.099382000	0.975925000
H	-5.411847000	-1.975249000	2.049248000
H	-6.623220000	-2.113930000	0.778903000
H	-5.147954000	-3.074733000	0.700992000
C	-3.613952000	0.599066000	-2.958291000
H	-2.940679000	-0.146586000	-3.381826000
H	-4.488721000	0.658158000	-3.614119000
H	-3.107662000	1.560958000	-2.995723000
C	-4.432629000	-2.299889000	-2.012004000
H	-3.565500000	-2.334895000	-2.670374000
H	-4.441896000	-3.217901000	-1.426136000
H	-5.328472000	-2.299004000	-2.641700000
H	0.644051000	-3.156280000	-0.608624000
H	-0.644224000	-3.156343000	0.608180000
W	0.000047000	0.644489000	-0.000193000
Ru	2.726795000	-0.426082000	-0.229709000
Ru	-2.726755000	-0.425930000	0.229653000
S	0.993725000	-1.433551000	1.089962000
S	-0.993862000	-1.433428000	-1.090211000

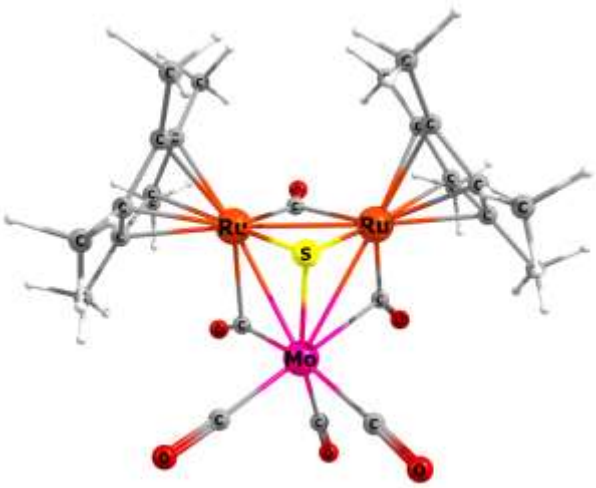

Figure S70. Optimized geometry of **7**.

Total energy = -2117.45397394 a.u.

Cartesian coordinates for the calculated structure **7** (in Å)

C	3.026993000	-1.730907000	-1.004668000
C	2.274675000	-2.651721000	-0.194920000
C	2.356100000	-2.224902000	1.170366000
C	3.160918000	-1.034500000	1.205091000
C	3.579138000	-0.742574000	-0.133366000
C	4.550444000	0.325894000	-0.520808000
H	4.470921000	1.202694000	0.119855000
H	4.411480000	0.646566000	-1.550379000
H	5.570392000	-0.060746000	-0.425336000
C	3.298206000	-1.869337000	-2.469386000
H	4.190306000	-2.481214000	-2.638211000
H	3.462994000	-0.899865000	-2.936080000

H	2.464870000	-2.343531000	-2.985832000
C	1.682267000	-3.936384000	-0.680240000
H	2.463642000	-4.699665000	-0.751505000
H	1.234779000	-3.828784000	-1.666550000
H	0.919653000	-4.312675000	-0.000240000
C	1.864146000	-2.974506000	2.367839000
H	1.022942000	-3.620355000	2.122211000
H	1.544804000	-2.299802000	3.160851000
H	2.659403000	-3.609748000	2.771864000
C	3.609715000	-0.313473000	2.438361000
H	4.552616000	-0.736381000	2.801098000
H	2.879291000	-0.396692000	3.241746000
H	3.775849000	0.746116000	2.250823000
C	-3.394914000	-1.220629000	-0.925108000
C	-3.760899000	-0.197149000	0.023945000
C	-3.298936000	-0.598870000	1.313954000
C	-2.642323000	-1.870415000	1.170720000
C	-2.722300000	-2.254097000	-0.206374000
C	-3.790408000	-1.272041000	-2.367488000
H	-3.056720000	-1.817210000	-2.960069000
H	-3.882153000	-0.275124000	-2.794781000
H	-4.755847000	-1.775244000	-2.482510000
C	-4.632202000	0.985896000	-0.260564000
H	-4.493613000	1.359409000	-1.272863000
H	-4.438284000	1.806397000	0.428750000
H	-5.683706000	0.702403000	-0.151054000
C	-3.576757000	0.099720000	2.607689000
H	-4.514762000	-0.265367000	3.039174000
H	-3.673424000	1.175827000	2.473210000
H	-2.786212000	-0.073895000	3.335889000
C	-2.132416000	-2.707666000	2.300818000
H	-1.623410000	-2.103103000	3.050699000
H	-1.432947000	-3.466608000	1.955079000
H	-2.960335000	-3.225264000	2.795947000
C	-2.305961000	-3.569112000	-0.782032000
H	-3.170459000	-4.238589000	-0.831189000
H	-1.547981000	-4.057713000	-0.172722000
H	-1.910957000	-3.460328000	-1.790196000
C	-0.000605000	-1.138863000	-1.392276000
C	1.484745000	1.301382000	-1.396698000
C	1.926205000	2.995626000	0.816958000
C	0.105532000	3.555298000	-1.290114000
C	-0.806824000	3.378252000	1.299179000
C	-1.552716000	1.143943000	-1.324010000
O	-0.138526000	-1.711781000	-2.407636000
O	2.098787000	1.305716000	-2.383935000
O	2.892725000	3.463480000	1.242282000
O	-0.025275000	4.347300000	-2.107233000
O	-1.391787000	4.118621000	1.946071000
O	-2.053844000	1.635392000	-2.249341000
Ru	1.301860000	-0.634177000	-0.010375000
Ru	-1.513187000	-0.307744000	-0.046321000
S	-0.012486000	0.284367000	1.659470000
Mo	0.308035000	2.122859000	0.116251000

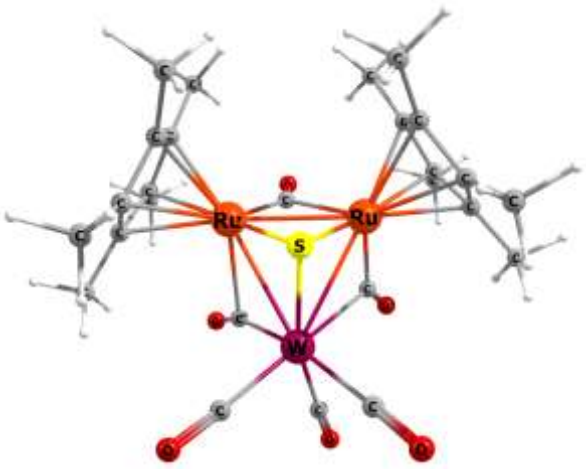

Figure S71. Optimized geometry of **8**.

Total energy = -2116.33528952 a.u.

Cartesian coordinates for the calculated structure **8** (in Å)

C	3.041401000	-1.854727000	-1.013727000
C	2.312205000	-2.798052000	-0.208719000
C	2.389891000	-2.380556000	1.160580000
C	3.171497000	-1.174370000	1.201049000
C	3.575621000	-0.861357000	-0.136988000
C	4.516724000	0.234667000	-0.521748000

H	4.420908000	1.102651000	0.128711000
H	4.360417000	0.562027000	-1.546818000
H	5.547294000	-0.126214000	-0.439851000
C	3.307787000	-1.974583000	-2.480933000
H	4.211217000	-2.566836000	-2.659387000
H	3.450641000	-0.998088000	-2.940171000
H	2.481667000	-2.461219000	-2.997353000
C	1.743872000	-4.090479000	-0.702067000
H	2.539556000	-4.838179000	-0.780450000
H	1.291977000	-3.984265000	-1.686510000
H	0.989766000	-4.486098000	-0.023513000
C	1.917761000	-3.151538000	2.352566000
H	1.080143000	-3.801965000	2.105848000
H	1.599715000	-2.491182000	3.158111000
H	2.722557000	-3.784983000	2.740362000
C	3.609958000	-0.452024000	2.437474000
H	4.567212000	-0.851249000	2.789198000
H	2.888819000	-0.562515000	3.245953000
H	3.745248000	0.613511000	2.258151000
C	-3.368695000	-1.432113000	-0.937749000
C	-3.762896000	-0.391351000	-0.021025000
C	-3.322041000	-0.756640000	1.287664000
C	-2.653353000	-2.026238000	1.188175000
C	-2.700202000	-2.442079000	-0.180964000
C	-3.732422000	-1.519711000	-2.386519000
H	-2.981935000	-2.072384000	-2.950304000
H	-3.820730000	-0.533232000	-2.837892000
H	-4.691663000	-2.032507000	-2.510714000
C	-4.637554000	0.777096000	-0.350549000
H	-4.481982000	1.127100000	-1.368655000
H	-4.463929000	1.615388000	0.322667000
H	-5.688570000	0.487077000	-0.254174000
C	-3.631660000	-0.028578000	2.557919000
H	-4.577619000	-0.386853000	2.977568000
H	-3.729465000	1.043678000	2.395882000
H	-2.857167000	-0.181226000	3.307815000
C	-2.155489000	-2.833157000	2.345492000
H	-1.697690000	-2.203451000	3.107393000
H	-1.415284000	-3.568182000	2.034503000
H	-2.981877000	-3.376637000	2.814922000
C	-2.258714000	-3.766444000	-0.714876000
H	-3.111919000	-4.451159000	-0.750332000
H	-1.497553000	-4.224245000	-0.085782000
H	-1.858158000	-3.680787000	-1.723014000
C	0.009383000	-1.320323000	-1.383404000
C	1.430161000	1.217522000	-1.455214000
C	1.847891000	2.885969000	0.791117000
C	-0.054648000	3.435101000	-1.279194000
C	-0.927508000	3.138344000	1.314409000
C	-1.535780000	0.965920000	-1.342951000
O	-0.127298000	-1.896158000	-2.397527000
O	2.052721000	1.187796000	-2.434912000
O	2.802619000	3.378779000	1.216738000
O	-0.249503000	4.241648000	-2.070381000
O	-1.546769000	3.833147000	1.981381000
O	-2.058546000	1.390205000	-2.293116000
Ru	1.300518000	-0.809959000	0.002784000
Ru	-1.511403000	-0.490053000	-0.039764000
S	-0.014732000	0.118273000	1.661879000
W	0.239029000	1.958582000	0.082007000