Supporting Information

for

Taming a Silent Killer: Uncovering the Role of Excited States and Uncoordinated Selenium Moieties in the CO Photorelease Mechanism of Manganese(I) Carbonyl Compounds

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S1. Bonding Analysis

Upon comparing the bond order of selenium, bromide and nitrogen atoms to the manganese ion, it becomes evident that the Mn1-Br1 bond consistently exhibits the strongest bond order across all compounds (1.12 – 1.14), followed by the Mn1-Se1 bond order (0.82 – 0.85), and the Mn1-N1 bond order (0.47). These values indicate a single bond character for Mn1-N1 and a multiple bond character in Mn1-Se1 and Mn1-Br1.

The Hirshfeld analysis is entirely consistent with the bond orders observed, and it provides a clear picture of the electronic charge inflow and outflow. The values clearly indicate that electronic charge flows from the bromide ion towards to manganese(I), increasing the charge of the bromide from -1 to -0.31, while the charge of the manganese ion is reduced from +1 to +0.01. A comparable interpretation can be formulated with regard to Se1, which exhibits a visible depletion of electronic density, exhibiting a charge of +0.16, in comparison to Se2, which shows a charge close to zero. Despite the longer length of the Mn1-Br1 bond (ca. 2.53 Å) and the relatively shorter Mn1-Se1 bond distance (ca. 2.47 Å), the use of $b_{AB}^{Löwdin}$ and Hirshfeld charge analysis enabled a more nuanced understanding of these bonds due to the effective orbital overlap contributing to the manganese-ligand bond.

Examining the Mn-CO bonds, the Mn1-C3 bond (*trans* to bromide) exhibits the highest $b_{AB}^{Löwdin}$ value (1.61 – 1.64), while Mn1-C1 (*trans* to selenium) and Mn1-C2 (*trans* to nitrogen) have similar values, 1.51 – 1.52 and 1.52 – 1.54, respectively. As for the C-O bonds, the $b_{AB}^{Löwdin}$ values fall within the range of 2.96 – 3.03, with the C3-O3 showing the weakest values (2.96 – 2.98). C1-O1 and C2-O2 present closely aligned values, ranging from 3.01 to 3.03. The bond orders for the Mn-CO and C-O align with of the *trans* bonded atoms, emphasizing the role of π-backbonding. This effect is further emphasized when comparing free carbon monoxide ($b_{AB}^{Löwdin}$ of 3.46) with the carbonyl groups; the three ligands exhibit shorter bond orders (2.96 – 3.03) due to their coordination with the metallic center. $b_{AB}^{Löwdin}$ values revealed that the coordination of CO to the manganese shifts the C-O bond order from a triple to a double/triple bond character. The Hirshfeld charges determined (Table S8) indicate the differences between manganese-carbonyl bonds, stemming from the slight difference and opposite signs between them. The Hirshfeld analysis points out that Mn1 not only receives charge from Br1, Se1, and N1 atoms, but also injects part of it through π-backbonding into CO groups,

resulting in a more positive charge on manganese and a slightly more negative charge on the CO ligands.[1]

The Extended Transition State-Natural Orbitals for Chemical Valence (ETS-NOCV) method was employed to elucidate the electron density rearrangement occurring during bond formation, thereby enabling the classification of the ligand as either σ-donating and π-accepting (Table S9). Three strong interactions are observed for each Mn-CO, one for Mn-Br, and two for Mn-κ^2L. For the carbonyl ligands, the $\Delta E_{orb\text{-}tot}$ for Mn1-C1O1 and Mn1-C2O2 is close to -89 kcal mol^{-1}, and for Mn1-C3O3, it ranges from -92.5 to -97.1 kcal mol^{-1}.

The three main contributions can be separated into the following ranges: $\Delta E_{orb\text{-}1}$ falls in the range of -38.8 to -41.5 kcal mol^{-1} for the three carbonyls, while $\Delta E_{orb\text{-}2}$ and $\Delta E_{orb\text{-}3}$ vary within the range of -21.5 to -28.2 kcal mol^{-1}. Figure S1 illustrates the formation of an σ-bond between the manganese and carbonyl in the compound **Mn(*p*OCH$_3$)**. The density flow channel represents the CO density donation to the metallic center, as described by $\Delta E_{orb\text{-}1}$. The $\Delta E_{orb\text{-}2}$ and $\Delta E_{orb\text{-}3}$ contributions show a π-backbonding from the manganese to CO (Figure S1), in which the *trans* nitrogen and selenium of ligand present a similar contribution to the electron density donated to manganese, but lower than the donation of bromide, a weak field ligand of the σ-donor type, which is also in line with the previous Hirshfeld analysis. For the Mn1-Br1 and Mn1-κ^2L, the density flow channel describes the major contributions of ΔE_{orb} as a σ-bond between the two fragments.

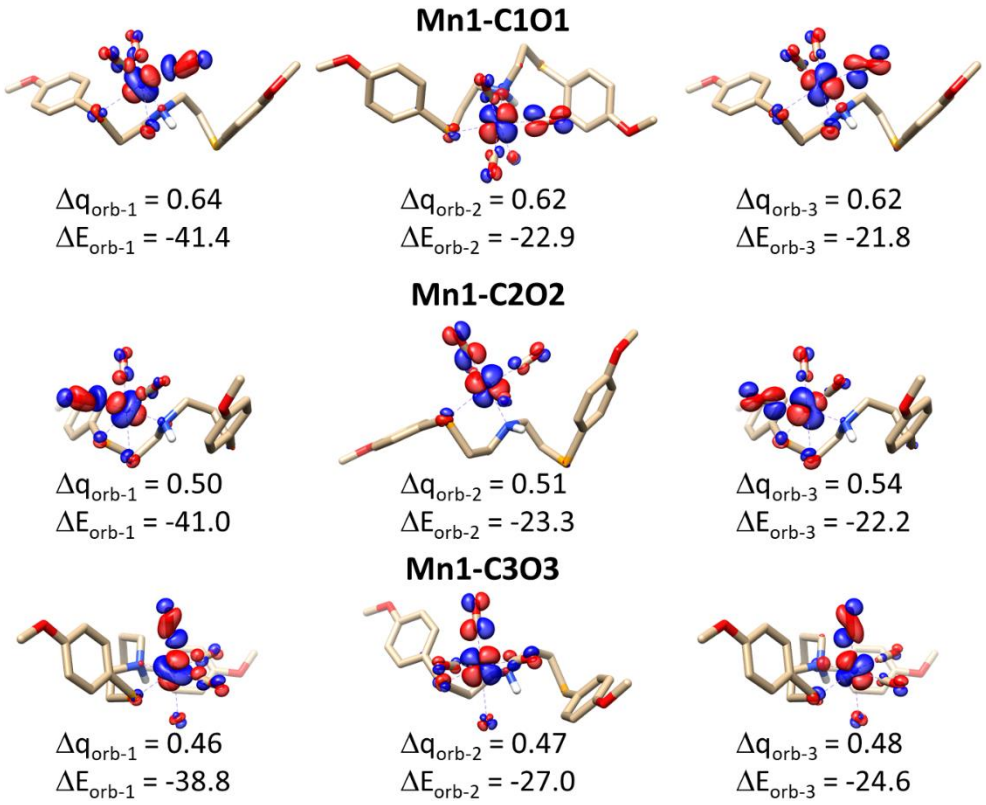

Figure S 1. Plot of the most relevant density flow channel with their respective energies (ΔE_{orb}) and charge transfer estimation (Δq_{orb}) values of compound Mn(pOCH$_3$) for the interaction Mn-CO. The charge flow direction is from blue to red, with red indicating density depletion and blue indicating density increment. Hydrogen atoms attached to carbon are omitted for clarity. C1O1 is trans to selenium, C2O2 is trans to nitrogen, and C3O3 is trans to bromide.

S2. Elemental Analysis and mass spectrometry

Elemental analysis showed a good relation between experimental and calculated percentages with the proposed molecular structure, with the largest difference observed for the carbon composition in **Mn(*m*CF$_3$)** (0.20%) and **Mn(*p*CH$_3$)** (0.14%), all other percentage differences of C, H, and N are below 0.08%.

In the positive ion mode ESI-MS (Figures S48-S52), the compounds **Mn(*m*CF$_3$)**, **Mn(*p*OCH$_3$)**, and **Mn(*p*CH$_3$)** showed the same base peak corresponding to the species without the coordinated bromide, $[Mn(L)(CO)_3]^+$. The **Mn(*o*CH$_3$)** exhibited the free ligand as the base peak $[L+H]^+$, while the specie without the coordinated bromide had an intensity close to the base peak (98.5%). The **Mn(*p*Cl)** displayed two peaks of higher intensity (38.6% and 25.3%) corresponded to the species $[Mn(L)(CO)_3]^+$ and $[L+H]^+$, respectively.

The obtained mass spectrum results support the proposed compounds structures, as four out of the five MCCs displayed the species $[Mn(L)(CO)_3]^+$ as base peak or in close proximity to it. However, the application of high potential values can lead to the rupture

of manganese-ligand and manganese-carbonyl bonds. This phenomenon leads to the emergence of species with a higher mass-to-charge ratio than expected, as illustrated in Figures S48-S52.

S3. Determination of the active species in solution

The stability of the MCCs was verified in the dark, employing both a coordinating solvent (acetonitrile) and non-coordinating solvent (dichloromethane) and using molar conductivity, UV-Vis, and IR spectroscopy measurements. Initially, solutions of the compounds were prepared with both solvents and at the same concentration (1.0×10^{-3} mol L^{-1}) to check their molar conductivity at 0 and 20 hours after incubation. The results are presented in Table S12, where it is observed that for the non-coordinating solvent, CH_2Cl_2, there is a negligible difference (maximum 0.02 variation). However, for the coordinating solvent, CH_3CN, there is an increase in the conductivity value (maximum 18.08 of increase), indicating that some species became cationic in solution. This change can be attributed to the exchange of bromide for acetonitrile or the coordination of free selenium portion.

In the electronic spectrum, a variation in the MLCT centered at ca. 387 nm was observed over the same 20 h period. Figures S53 and S54 illustrate the variations in λ_{max} for the five compounds in dichloromethane and acetonitrile, respectively. It can be observed that during the period in which the MLCT variation occurs for the non-coordinating solvent, there is a negligible change in the absorption value. However, for compounds dissolved in acetonitrile, a hypsochromic shift of the bands was evident, with variations ranging between 8 and 15 nm from the initial to the final λ_{max} value. Figure S55 shows a comparison between the electronic profile of both solvents after the incubation period.

This hypsochromic shift can be attributed to three factors: *i*) the coordinated bromide may be replaced by a solvent molecule; *ii*) the free selenium portion of the ligand may be coordinating to manganese; or *iii*) effect of the solvent on the stabilization of molecular orbitals (solvatochromism). Gonzales *et al*. reported that replacing bromide with acetonitrile results in a hypsochromic shift of approximately 100 nm.[2] A substantial shift is expected, in accordance with the spectrochemical series, whereby a weak field ligand is replaced by an intermediate field ligand. The second factor is also associated with the change from a weak field ligand to a weak-intermediate field ligand, as

previously described. The third factor is known as solvatochromism, which describes a change in the position, profile, and intensity of a band resulting from the medium in which it is occurring. This phenomenon is a consequence of the polarity of the solvent employed. Given that acetonitrile is more polar than dichloromethane, negative solvatochromism occurs, wherein increasing polarity results in an increase in the energy difference between the frontier orbitals, leading to a hypsochromic shift.

To better understand which of the three factors occurs, the variation of CO stretches in the infrared region in both solvents was monitored for a period of 20 hours. Figures S56 and S57 present a comparison between the initial and final times for all compounds in dichloromethane and acetonitrile, respectively. In dichloromethane, it is evident that there was no variation in the profile of the bands associated with carbonyls, and there was also no change in the other bands attributed to the stretching or bending vibrations of the ligands. This observation indicates the stability of the compound in the non-coordinating solvent solution, as corroborated by the electronic spectrum and molar conductivity. In contrast, in acetonitrile, a noteworthy phenomenon is appearance of a novel band at 2062 cm^{-1}, which is situated approximately 40 cm^{-1} higher than the symmetric band observed in dichloromethane. Additionally, there is an observable increase in intensity of a new, more energetic band related to the asymmetric stretching of CO, although lacking precise definition. Figure S58 illustrate this comparison for both solvents after the incubation period.

In order to facilitate the comprehension of the species present in solution, electronic structure calculations were conducted, comprising geometry optimization with consideration of the three potential species for each ligand employed: [Mn(κ^2-L)$(CO)_3$Br], [Mn(κ^2-L)$(CO)_3(CH_3CN)]^+$, and [Mn(κ^3-L)$(CO)_3]^+$. The three species can be treated as three reactions in equilibrium, as shown in Scheme S1. The values obtained for $\Delta G_{dir,n}$ and $\Delta G_{rev,n}$ are presented in Table S13. For the three reactions, the direct reaction (ΔG_{dir}) has a positive value and, consequently, is not spontaneous. For the first and third reactions in Scheme S1, the $\Delta G_{rev,1}$ is approximately -100 kcal mol^{-1} and $\Delta G_{rev,2}$ is approximately -104 kcal mol^{-1}, indicating that species [Mn(κ^2-L)$(CO)_3$Br] will be present in greater quantity. For reaction b, where there is an equilibrium between [Mn(κ^2-L)$(CO)_3(CH_3CN)]^+$ and [Mn(κ^3-L)$(CO)_3]^+$, the $\Delta G_{rev,2}$ is approximately -4 kcal mol^{-1}, and consequently, the reverse reaction is slightly favored.

a) $[Mn(\kappa^2\text{-L})(CO)_3Br] + CH_3CN \underset{\Delta G_{rev,1}}{\overset{\Delta G_{dir,1}}{\rightleftharpoons}} [Mn(\kappa^2\text{-L})(CO)_3(CH_3CN)]^+ + Br^-$

b) $[Mn(\kappa^2\text{-L})(CO)_3(CH_3CN)]^+ + Br^- \underset{\Delta G_{rev,2}}{\overset{\Delta G_{dir,2}}{\rightleftharpoons}} [Mn(\kappa^3\text{-L})(CO)_3]^+ + CH_3CN + Br^-$

c) $[Mn(\kappa^2\text{-L})(CO)_3Br] \underset{\Delta G_{rev,3}}{\overset{\Delta G_{dir,3}}{\rightleftharpoons}} [Mn(\kappa^3\text{-L})(CO)_3]^+ + Br^-$

Scheme S1. Equilibrium between the possibles species in acetonitrile solution.

Analyzing the calculated νCO values (Table S14), the exchange of bromide for acetonitrile leads to an increase in CO stretching energy, which also expected if the ligand is coordinated in the κ^3 coordination mode. Species $[Mn(\kappa^2\text{-L})(CO)_3(CH_3CN)]^+$ and $[Mn(\kappa^3\text{-L})(CO)_3]^+$ exhibit similar νCO values, with $[Mn(\kappa^2\text{-L})(CO)_3(CH_3CN)]^+$ displaying the most energetic stretches. Moreover, it is observed that the energy difference between the asymmetric stretching follows the trend $[Mn(\kappa^2\text{-L})(CO)_3Br] > [Mn(\kappa^3\text{-L})(CO)_3]^+ > [Mn(\kappa^2\text{-L})(CO)_3(CH_3CN)]^+$.

Considering the transitions of the states S_2 and S_3 from the simulated absorption spectrum (Table S15), which are assigned to the band at ca. 387 nm, a hypsochromic shift is observed for the species $[Mn(\kappa^3\text{-L})(CO)_3]^+$ and $[Mn(\kappa^2\text{-L})(CO)_3(CH_3CN)]^+$ compared to $[Mn(\kappa^2\text{-L})(CO)_3Br]$, ranging from 7 to 14 nm for S_2 and from 0 to 6 nm for S_3.

The computational results corroborate the experimentally obtained IR and UV-Vis spectra, indicating that the species coordinated with bromide is the most stable, which also justifies the slight variation in the spectra observed 20 hours after preparing the solution when the coordinating solvent was used. Nevertheless, it is not feasible to ascertain the exact form of the sample in acetonitrile solution, whether it is $[Mn(\kappa^3\text{-L})(CO)_3]^+$ or $[Mn(\kappa^2\text{-L})(CO)_3(CH_3CN)]^+$ form, as similar values were found for the energy, CO stretching frequency and the UV-Vis transition of the lower energy band. It is only possible to conclude that in a non-coordinating solvent, the $[Mn(\kappa^2\text{-L})(CO)_3Br]$ species is the most stable.

S4. References

1 B. D. Matson, E. A. McLoughlin, K. C. Armstrong, R. M. Waymouth and R. Sarangi, *Inorg. Chem.*, 2019, **58**, 7453–7465.
2 M. A. Gonzalez, S. J. Carrington, N. L. Fry, J. L. Martinez and P. K. Mascharak, *Inorg. Chem.*, 2012, **51**, 11930–11940.

S5. Figures and Tables

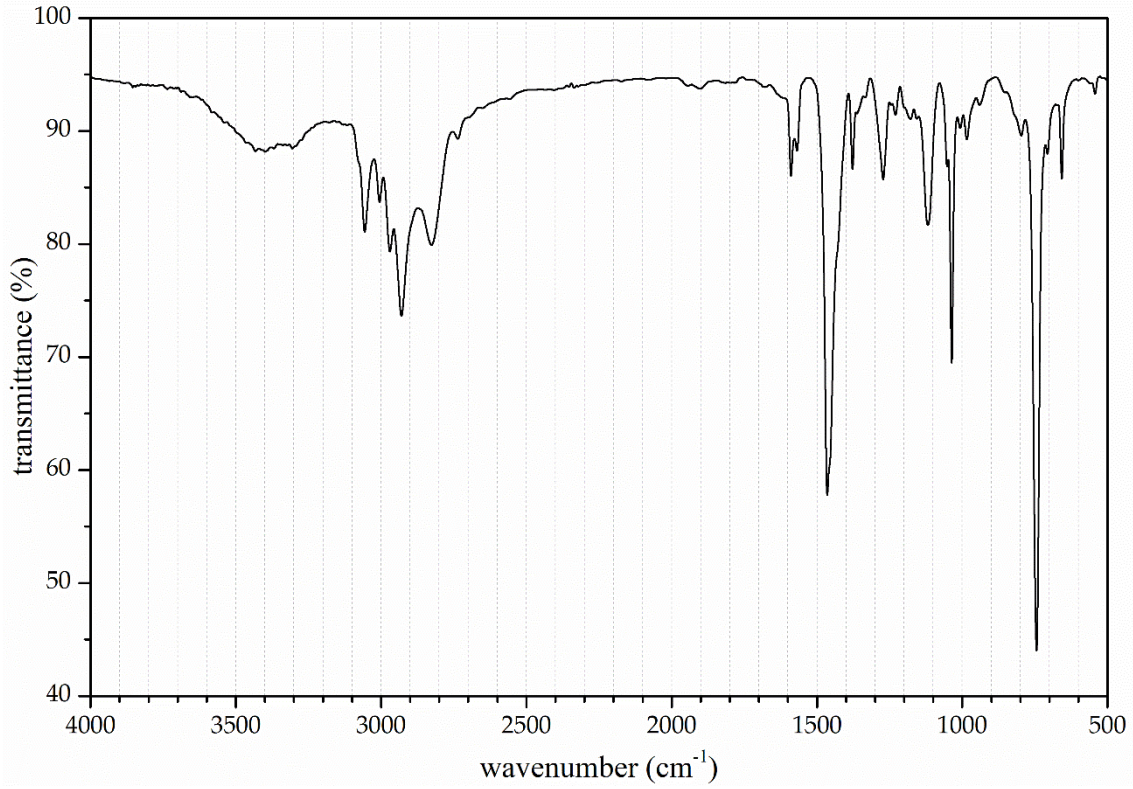

Figure S 2. Infrared spectra in KBr for ligand oCH_3.

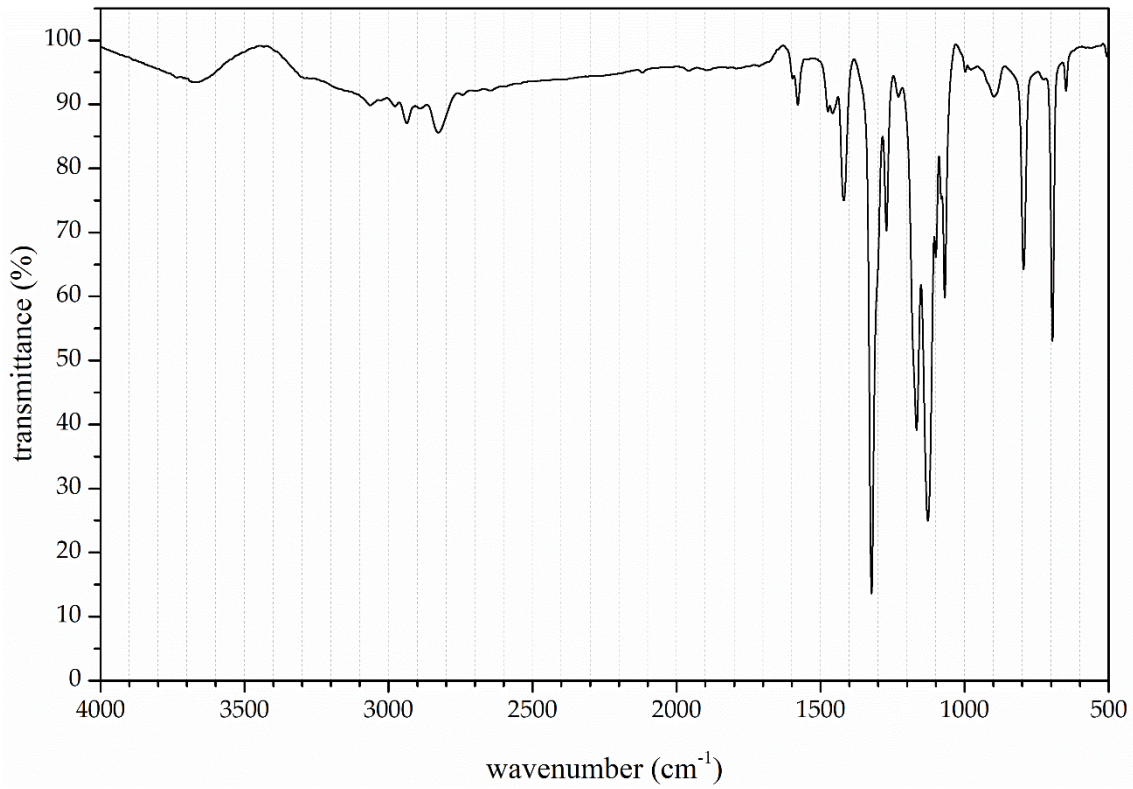

Figure S 3. Infrared spectra in KBr for ligand mCF_3.

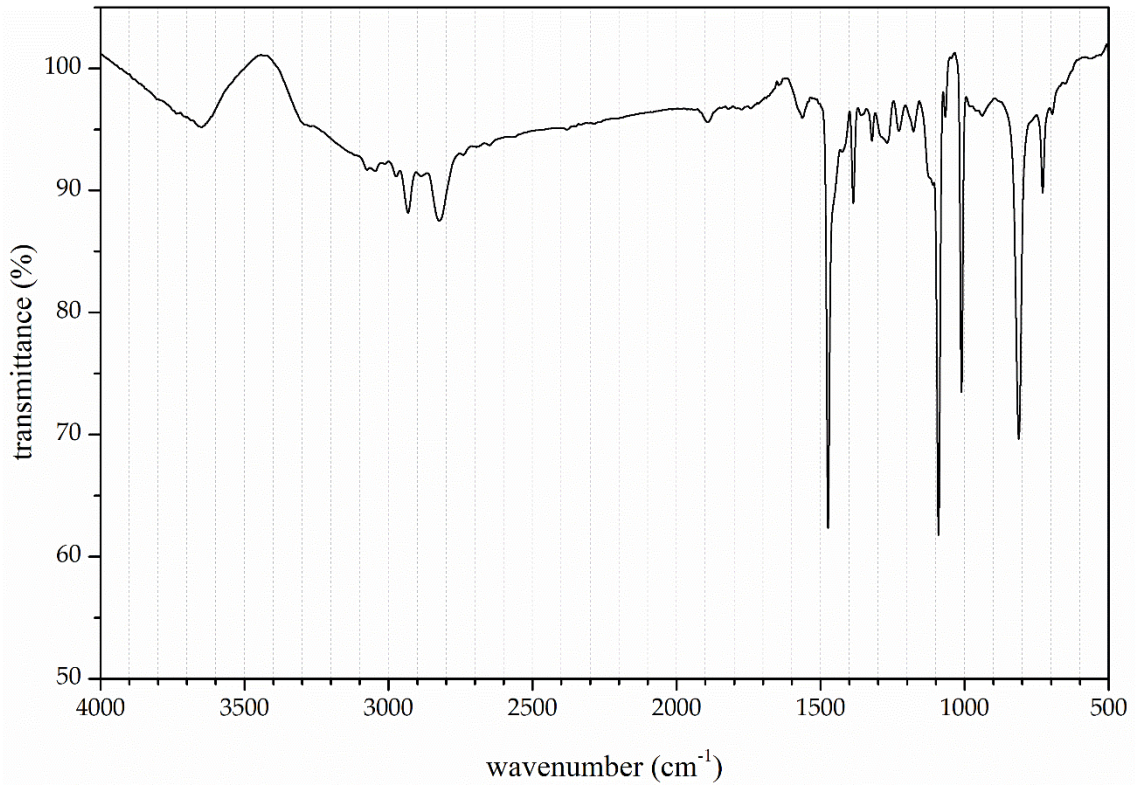

Figure S 4. Infrared spectra in KBr for ligand pCl.

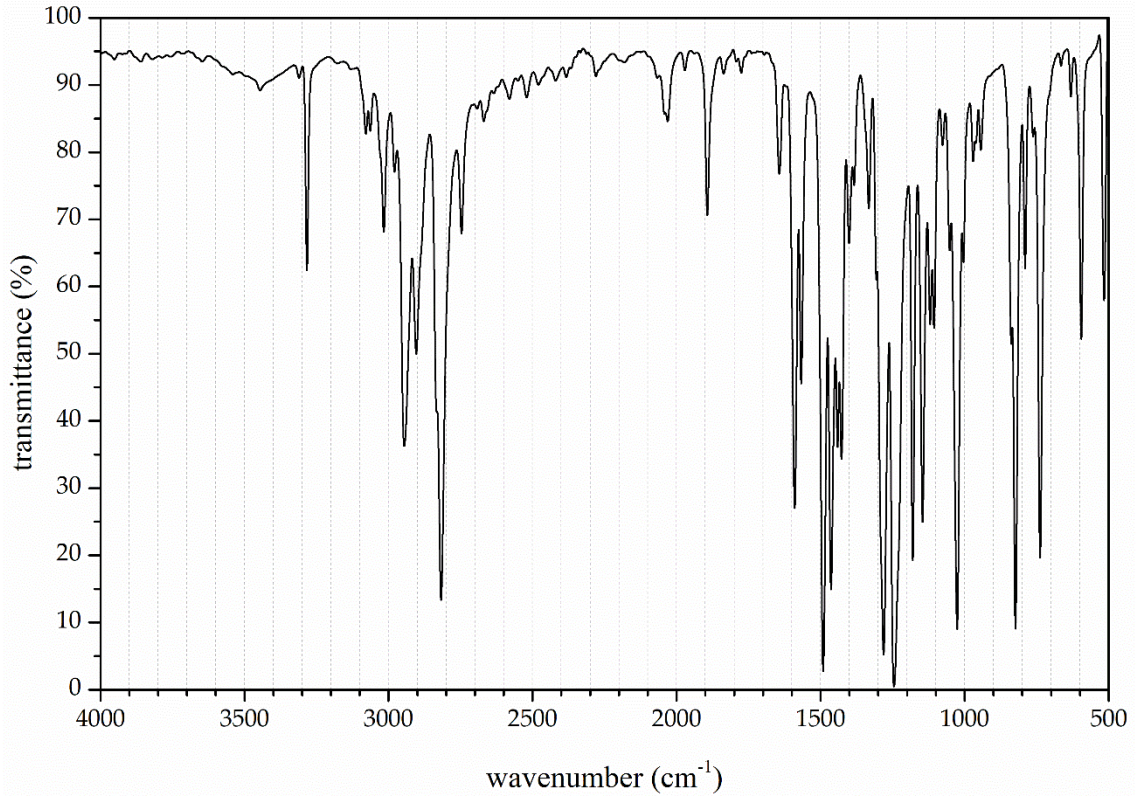

Figure S 5. Infrared spectra in KBr for ligand pOCH₃.

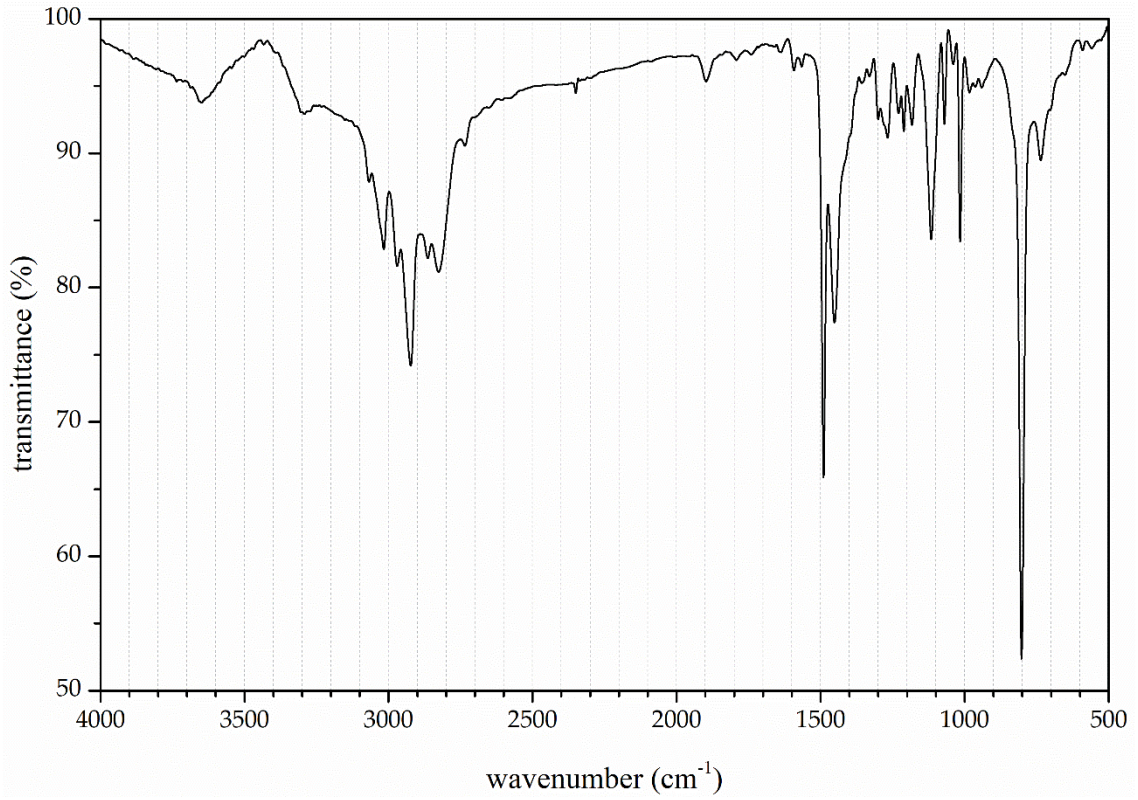

Figure S 6. Infrared spectra in KBr for ligand pCH₃.

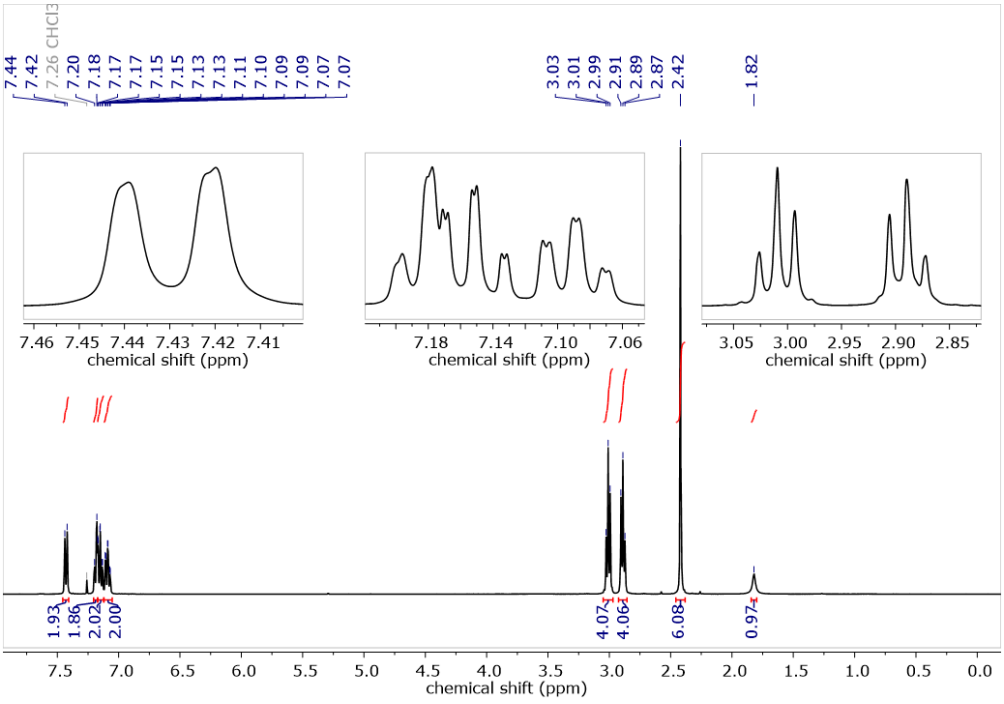

Figure S 7. ¹H NMR spectrum of ligand oCH₃.

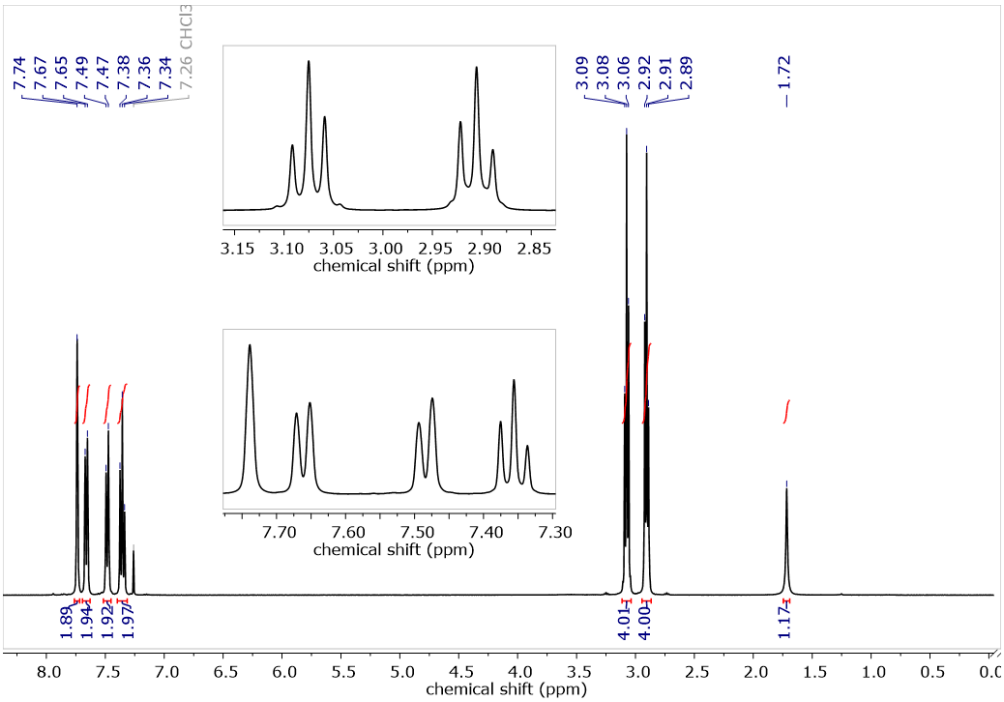

Figure S 8. ^{1}H NMR spectrum of ligand mCF_3.

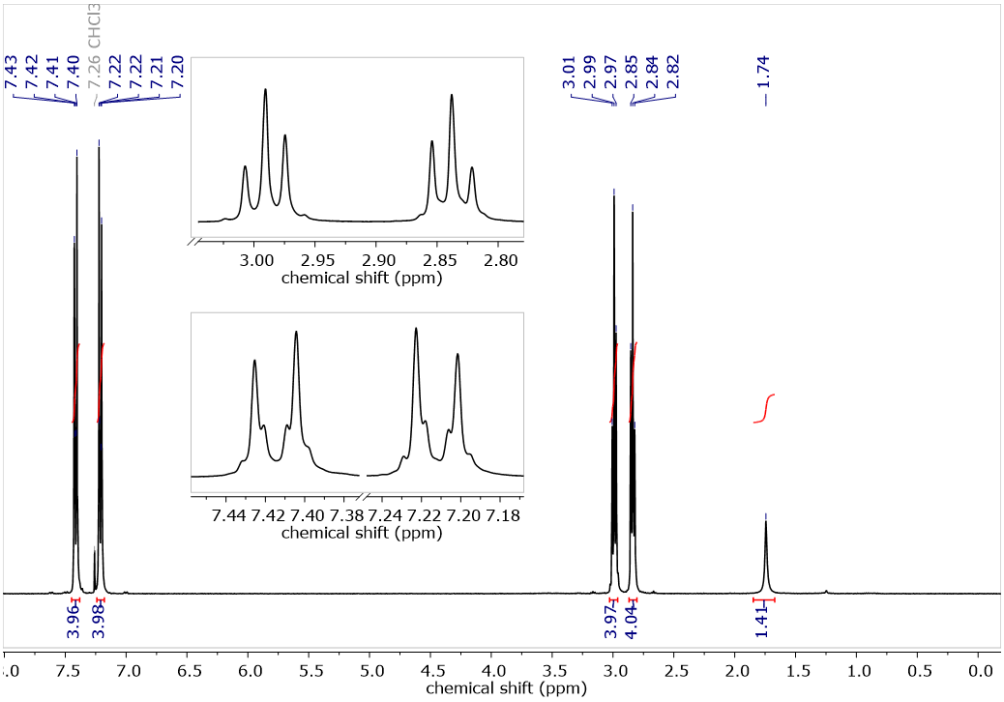

Figure S 9. ^{1}H NMR spectrum of ligand pCl.

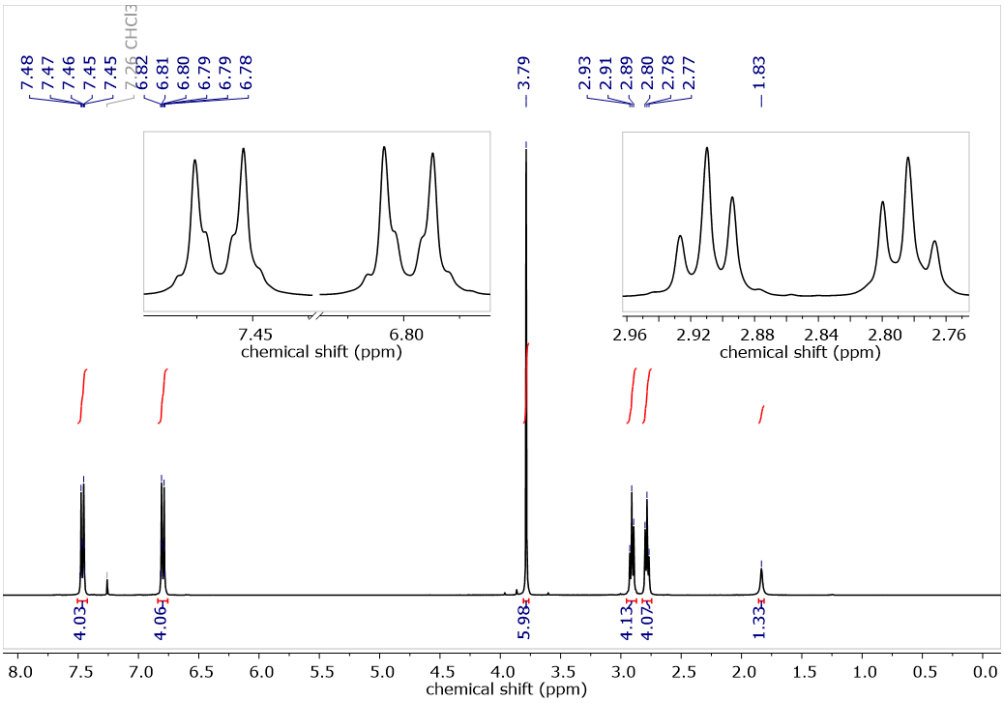

Figure S 10. ^{1}H NMR spectrum of ligand $pOCH_3$.

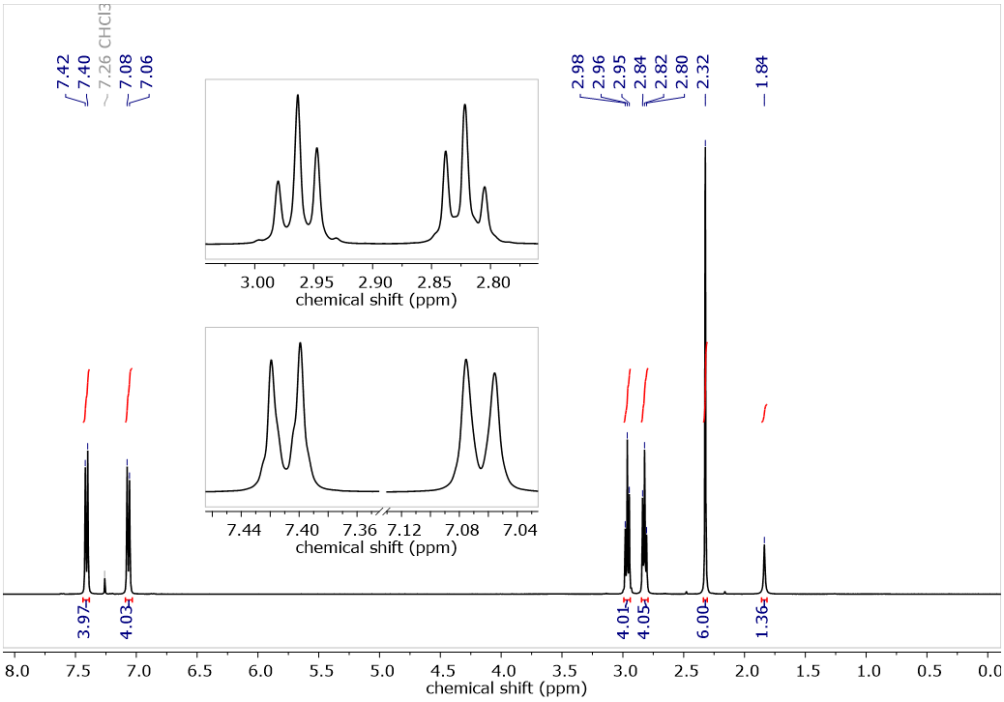

Figure S 11. ^{1}H NMR spectrum of ligand pCH_3.

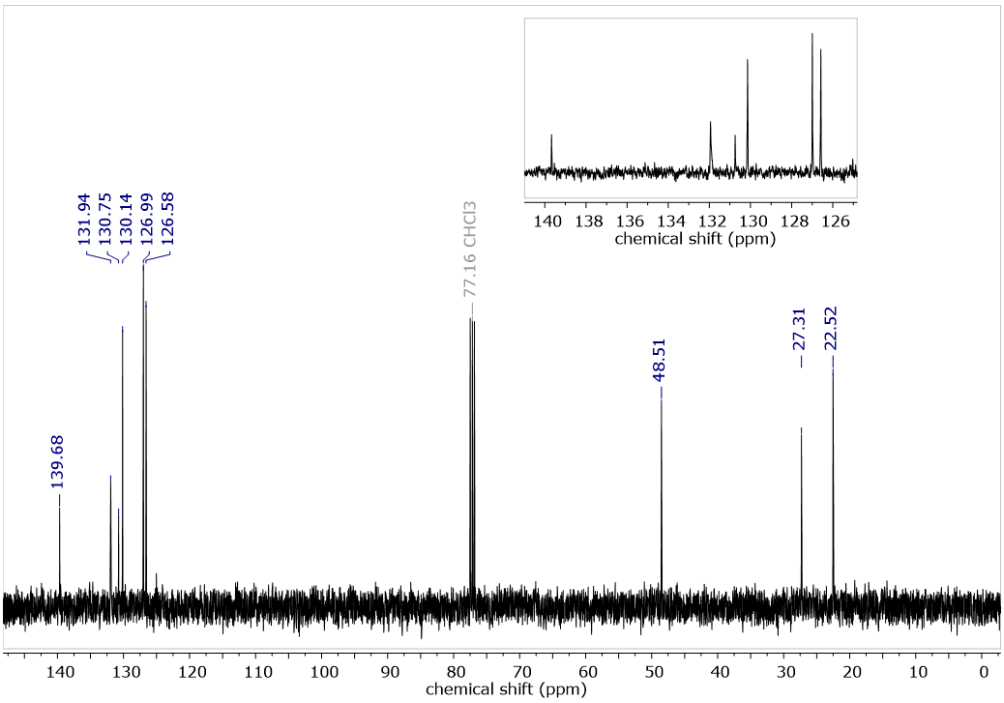

Figure S 12. ^{13}C NMR spectrum of ligand oCH_3.

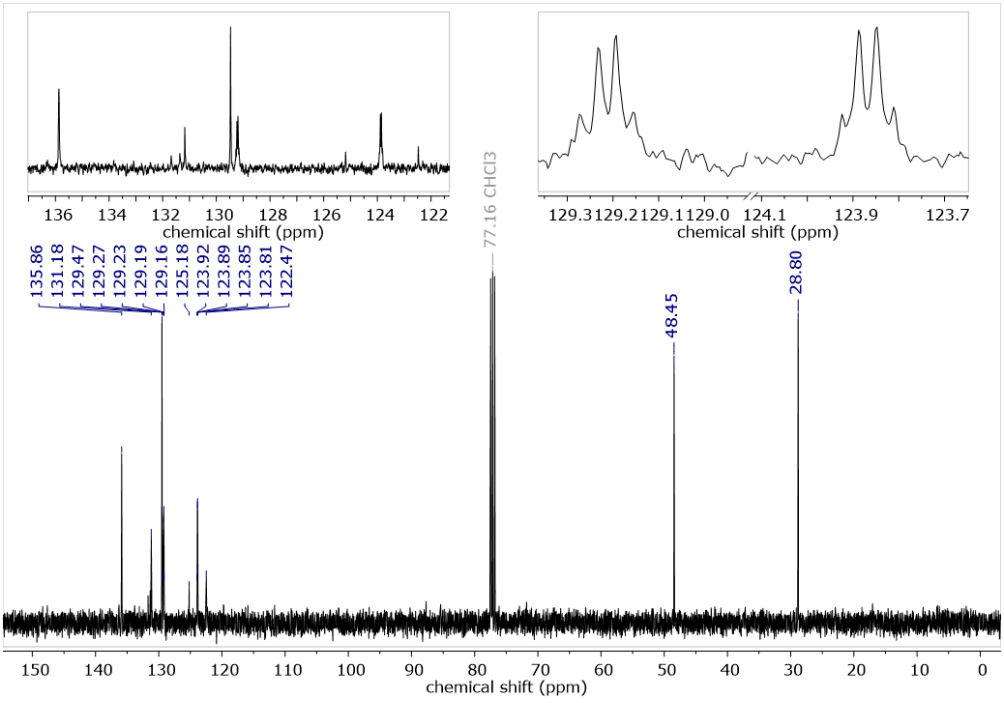

Figure S 13. ^{13}C NMR spectrum of ligand mCF_3.

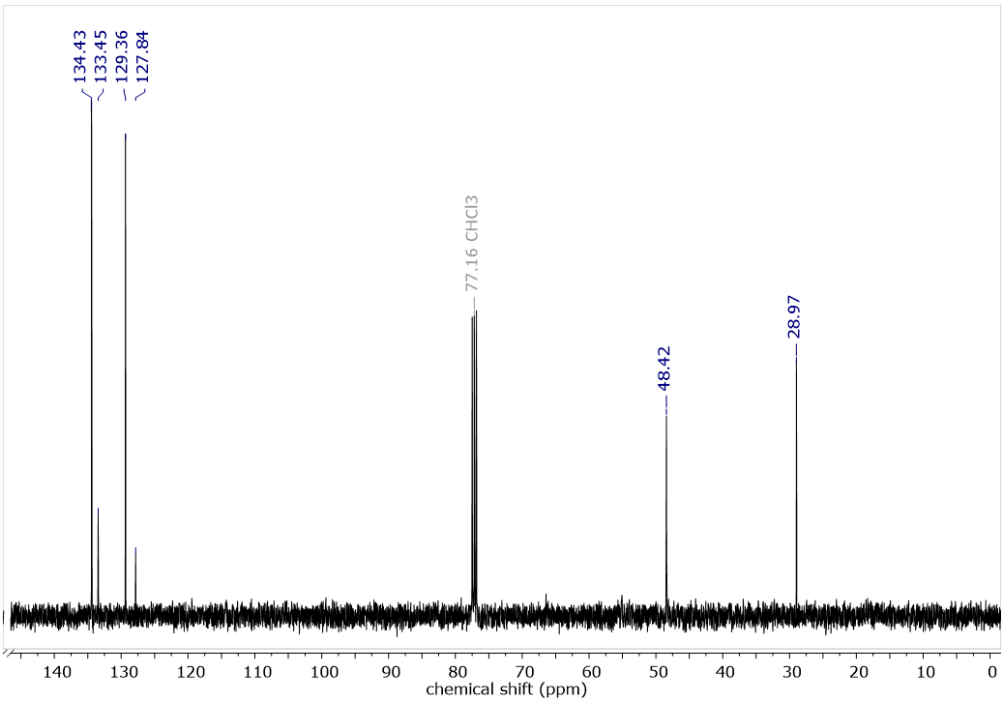

Figure S 14. ^{13}C NMR spectrum of ligand pCl.

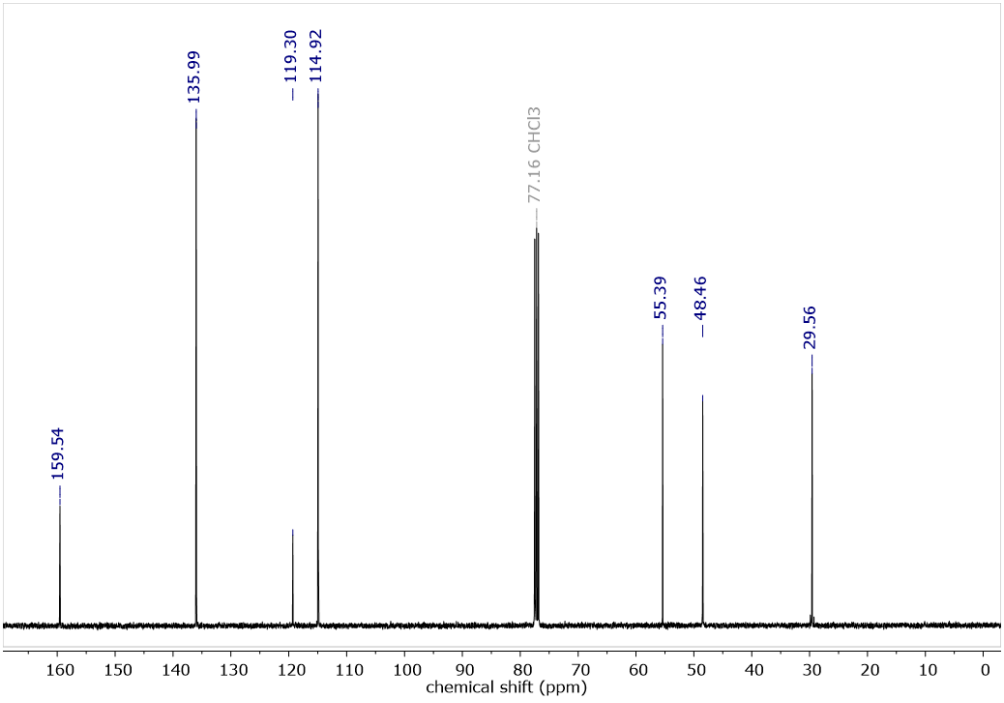

Figure S 15. ^{13}C NMR spectrum of ligand $pOCH_3$.

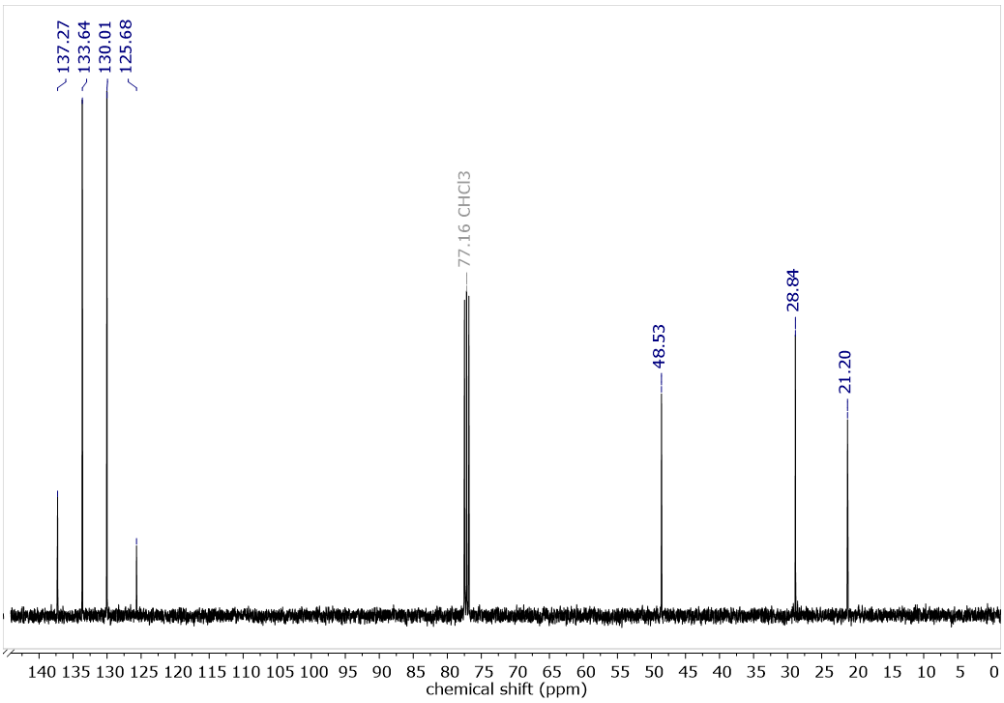

Figure S 16. ^{13}C NMR spectrum of ligand pCH_3.

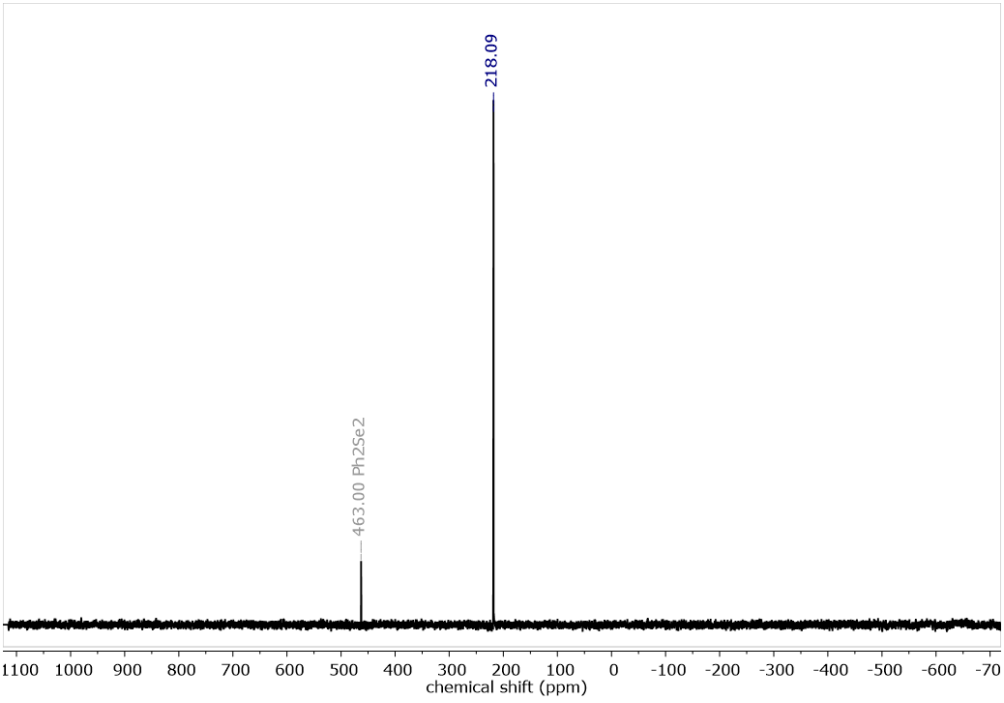

Figure S 17. ^{77}Se NMR spectrum of ligand oCH_3.

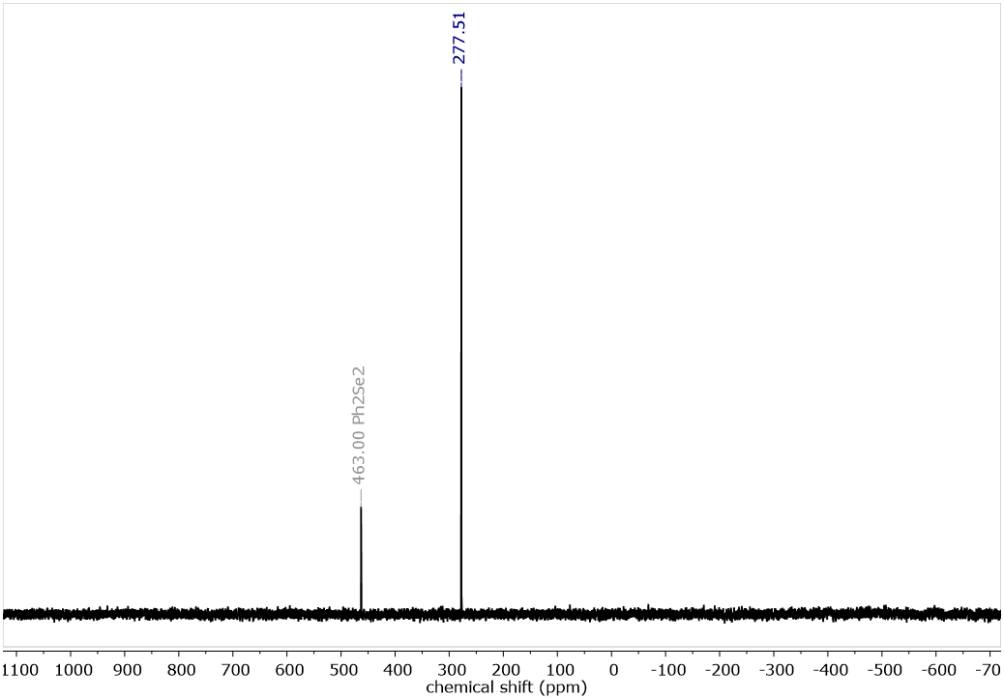

Figure S 18. ^{77}Se NMR spectrum of ligand mCF_3.

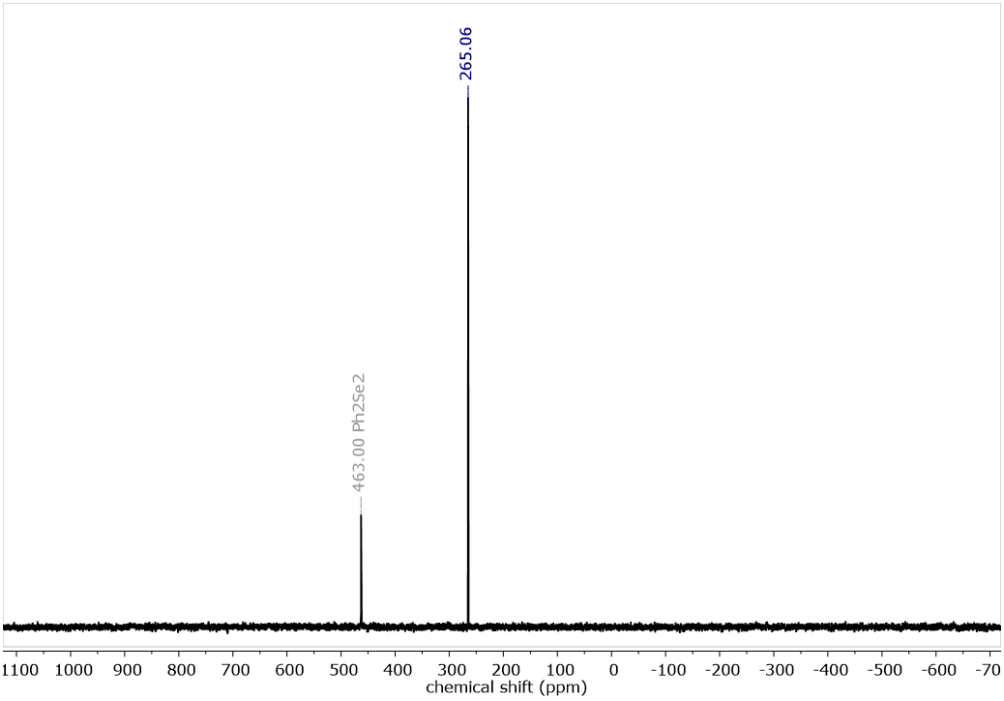

Figure S 19. ^{77}Se NMR spectrum of ligand pCl.

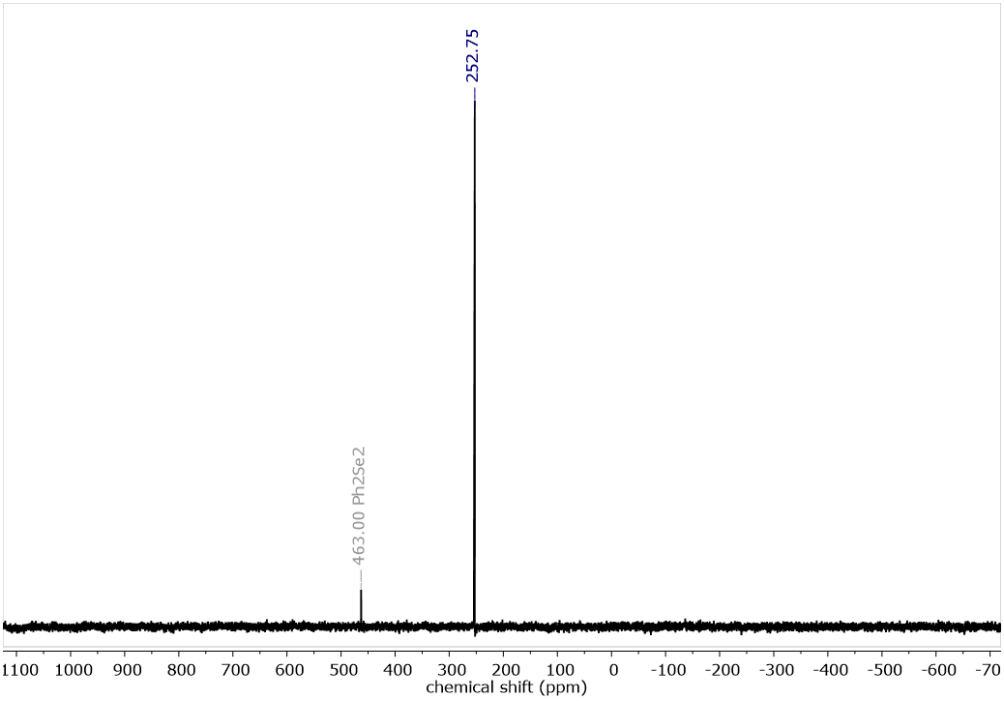

Figure S 20. ^{77}Se NMR spectrum of ligand $pOCH_3$.

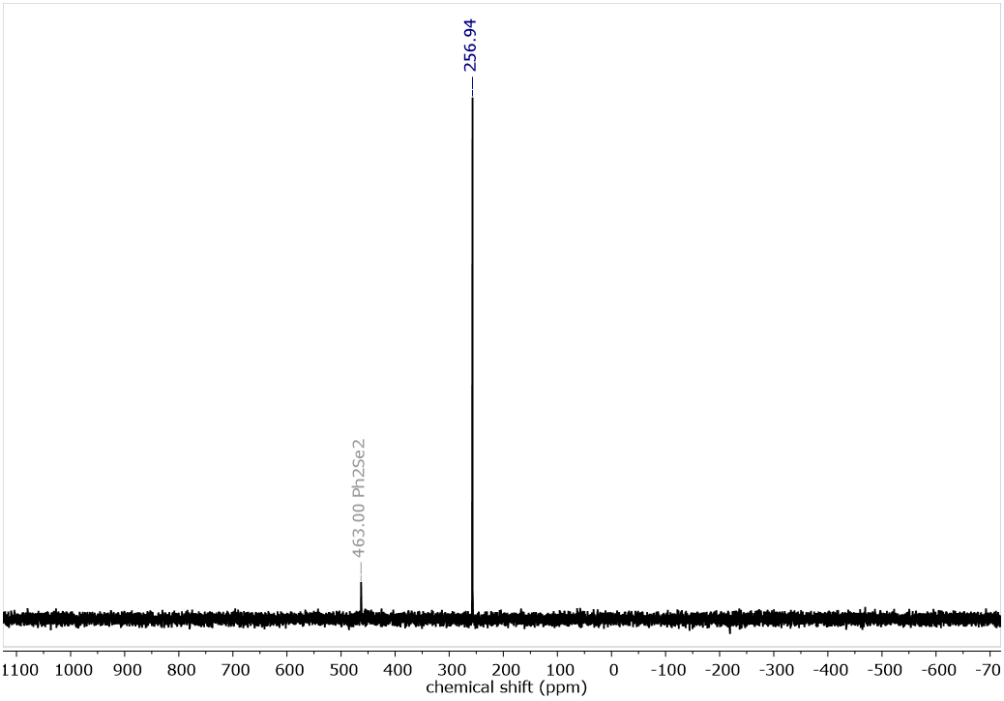

Figure S 21. ^{77}Se NMR spectrum of ligand pCH_3.

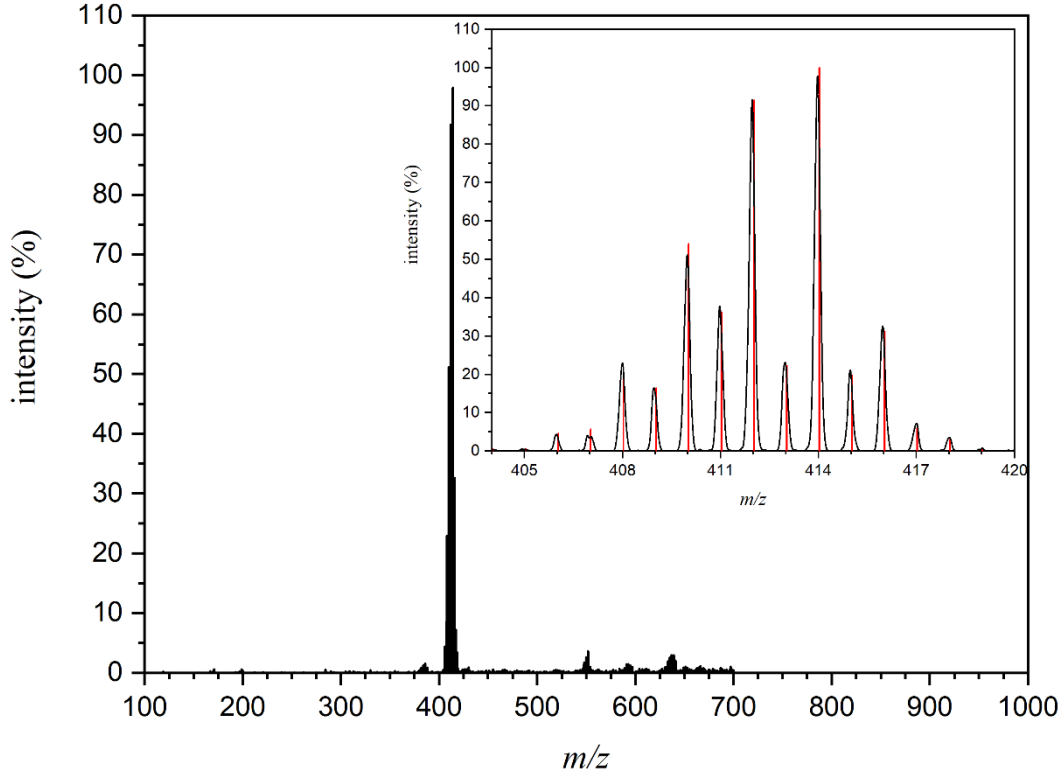

Figure S 22. ESI-MS spectrum (positive mode) in acetonitrile of ligand oCH$_3$. Insert: peak base of calculated (red) and experimental (black) isotopic distributions for the specie [M + H]$^+$.

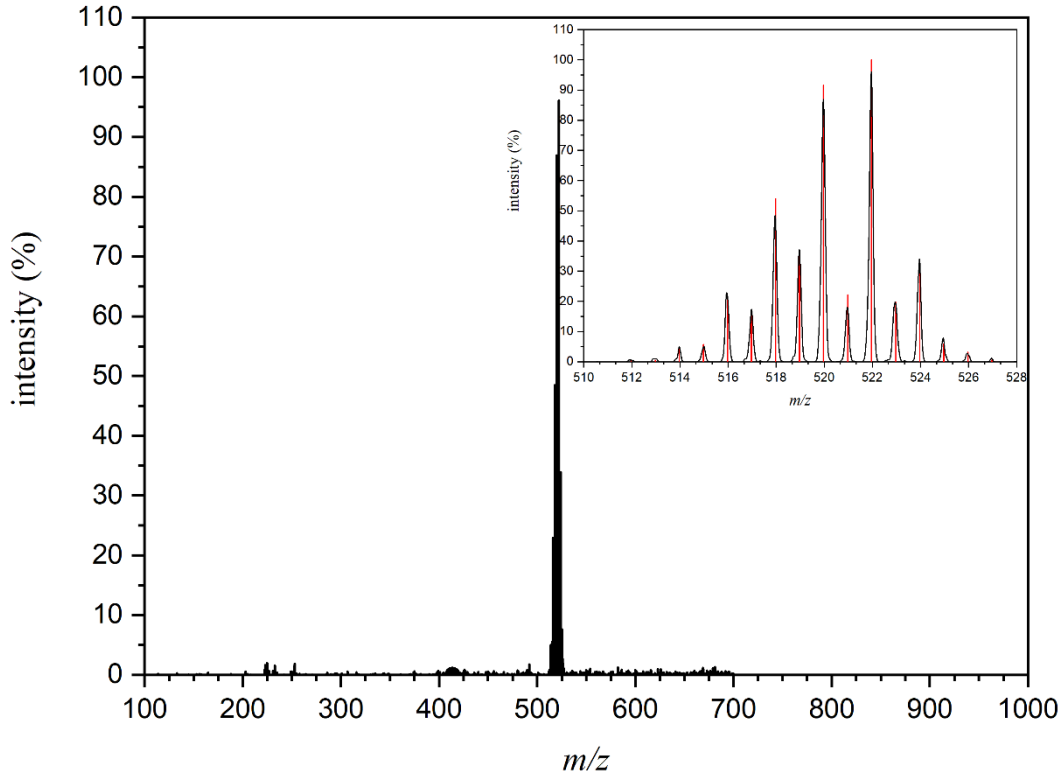

Figure S 23. ESI-MS spectrum (positive mode) in acetonitrile of ligand mCF$_3$. Insert: peak base of calculated (red) and experimental (black) isotopic distributions for the specie [M + H]$^+$.

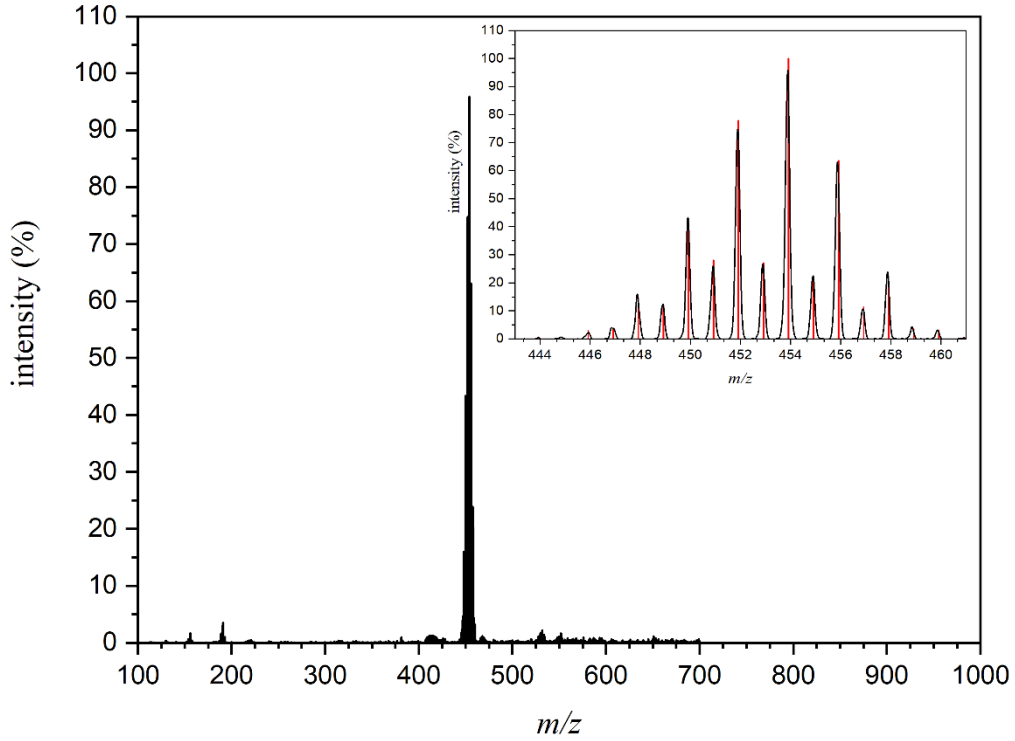

Figure S 24. ESI-MS spectrum (positive mode) in acetonitrile of ligand pCl. Insert: peak base of calculated (red) and experimental (black) isotopic distributions for the specie $[M + H]^+$.

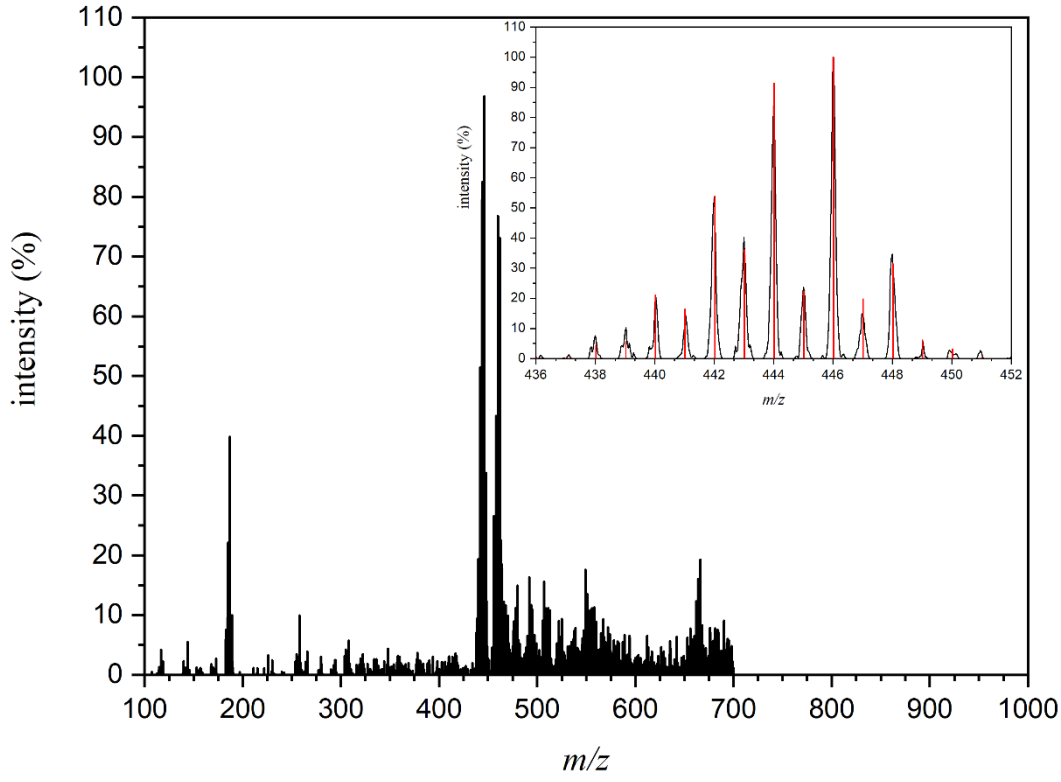

Figure S 25. ESI-MS spectrum (positive mode) in acetonitrile of ligand $pOCH_3$. Insert: peak base of calculated (red) and experimental (black) isotopic distributions for the specie $[M + H]^+$.

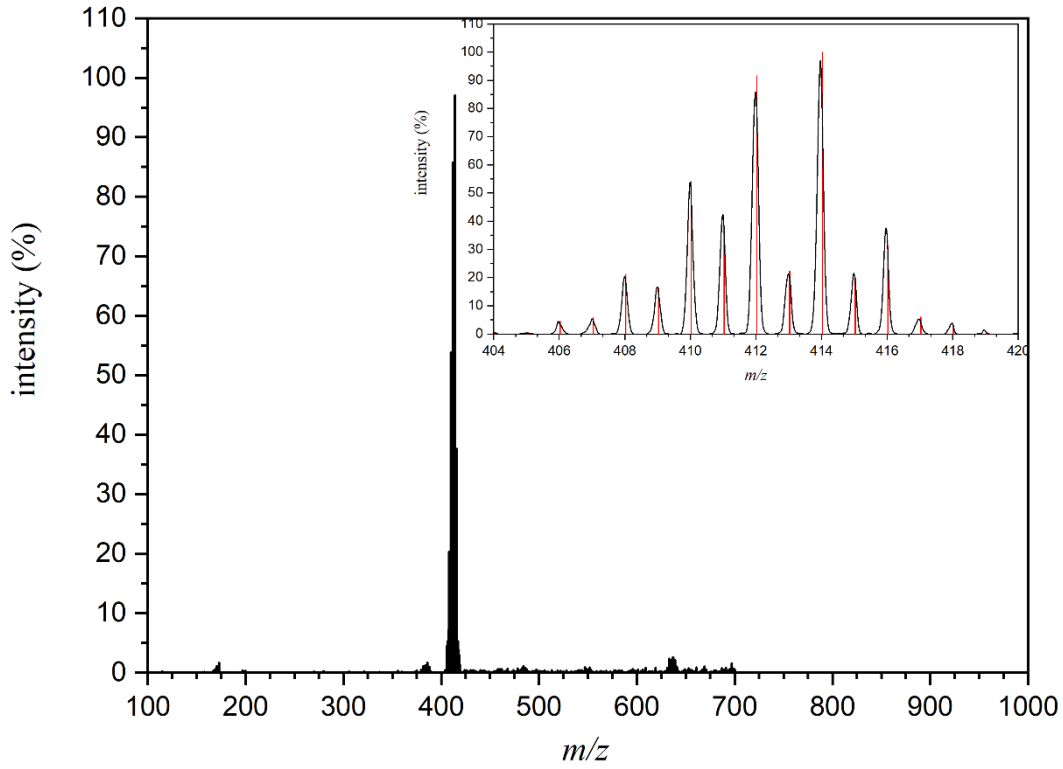

Figure S 26. ESI-MS spectrum (positive mode) in acetonitrile of ligand pCH_3. Insert: peak base of calculated (red) and experimental (black) isotopic distributions for the specie $[M + H]^+$.

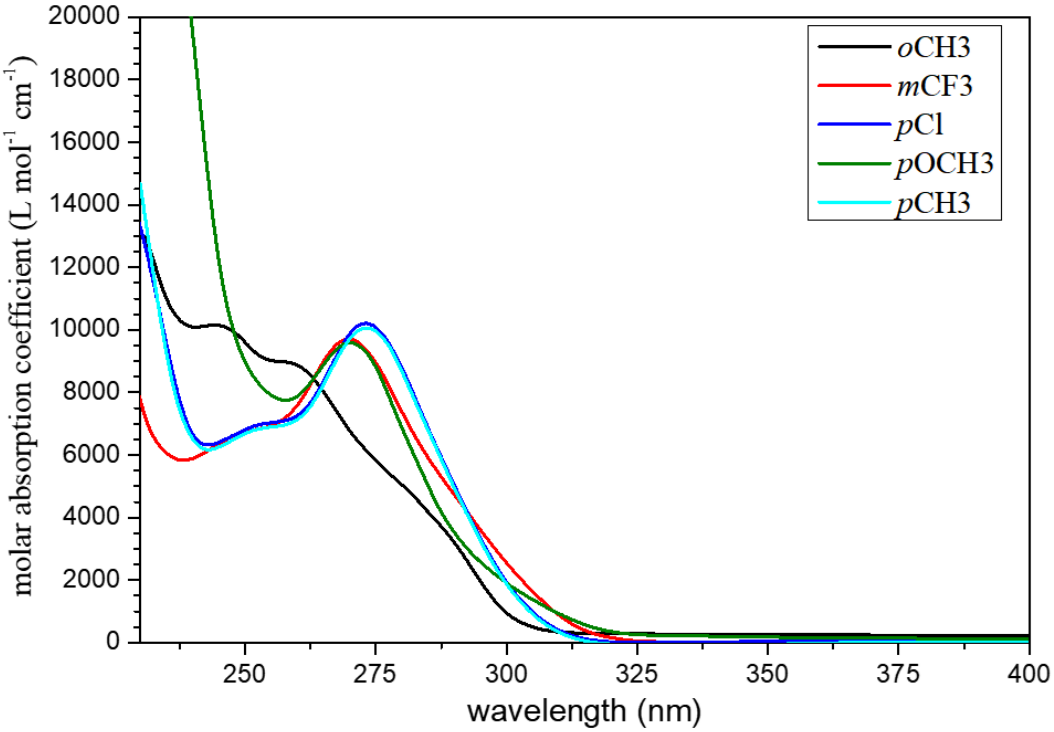

Figure S 27. Spectrum electronic of the five organochalcogen ligands in dichloromethane.

Table S 1. Selected bond lengths (Å) and angles (º) of the synthesized MCCs obtained via X-ray crystallography.

	Mn(*o*CH_3)	**Mn(*m*CF_3)**	**Mn(*p*Cl)**	**Mn(*p*OCH_3)**	**Mn(*p*CH_3)**
Bond length (Å)					
Mn1-C1	1.806(3)	1.8194(19)	1.810(2)	1.806(3)	1.810(3)
Mn1-C2	1.803(3)	1.7996(19)	1.797(2)	1.796(2)	1.796(3)
Mn1-C3	1.797(3)	1.7893(18)	1.792(2)	1.794(3)	1.789(2)
Mn1-Se1	2.4730(6)	2.4880(3)	2.4743(4)	2.4589(4)	2.4708(4)
Mn1-Br1	2.5215(6)	2.5305(3)	2.5424(4)	2.5433(4)	2.5185(4)
Mn1-N1	2.132(3)	2.1393(14)	2.1325(17)	2.1313(19)	2.1329(19)
C1-O1	1.149(4)	1.138(2)	1.148(3)	1.150(3)	1.145(3)
C2-O2	1.145(4)	1.152(2)	1.149(3)	1.152(3)	1.153(3)
C3-O3	1.146(4)	1.148(2)	1.151(3)	1.151(3)	1.151(3)
Bond angle (°)					
C3-Mn1-C1	92.51(15)	90.30(8)	91.19(10)	91.78(11)	90.85(11)
C3-Mn1-C2	91.54(15)	90.37(8)	88.45(10)	89.30(11)	92.52(11)
C1-Mn1-C2	86.12(14)	88.29(9)	90.31(10)	89.76(11)	88.44(12)
N1-Mn1-Se1	86.29(7)	85.53(4)	85.86(5)	86.94(6)	85.93(5)
Se1-Mn1-C1	172.36(11)	172.80(6)	172.37(7)	170.02(7)	170.89(8)
N1-Mn1-C2	176.66(12)	175.81(7)	172.72(8)	175.33(9)	175.39(10)
Br1-Mn1-C3	174.43(10)	179.45(6)	179.22(7)	177.55(8)	177.13(8)

Table S 2. Crystal data and structure refinement for Mn(oCH$_3$).

Empirical formula	C21 H23 Br Mn N O3 Se2	
Formula weight	630.17	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 13.1607(9) Å	α= 90°.
	b = 12.1226(8) Å	β= 103.543(2)°.
	c = 14.9077(9) Å	γ = 90°.
Volume	2312.3(3) Å^3	
Z	4	
Density (calculated)	1.810 Mg/m^3	
Absorption coefficient	5.469 mm^{-1}	
F(000)	1232	
Crystal size	0.400 x 0.200 x 0.120 mm^3	
Theta range for data collection	1.592 to 30.543°.	
Index ranges	-18<=h<=18, -14<=k<=17, -21<=l<=21	
Reflections collected	24270	
Independent reflections	7062 [R(int) = 0.0456]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.4604	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7062 / 0 / 264	
Goodness-of-fit on F^2	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.0697	
R indices (all data)	R1 = 0.0801, wR2 = 0.0774	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.3171 and -1.102 e.Å^{-3}	

Table S 3. Crystal data and structure refinement for Mn(mCF$_3$).

Empirical formula	C21 H17 Br F6 Mn N O3 Se2	
Formula weight	738.12	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 7.8186(3) Å	α= 90°.
	b = 12.1015(5) Å	β= 94.5210(10)°.
	c = 26.1675(12) Å	γ = 90°.
Volume	2468.18(18) Å^3	
Z	4	
Density (calculated)	1.986 Mg/m^3	
Absorption coefficient	5.173 mm^{-1}	
F(000)	1424	
Crystal size	0.400 x 0.140 x 0.100 mm^3	
Theta range for data collection	1.561 to 30.551°.	
Index ranges	-10<=h<=11, -17<=k<=17, -37<=l<=31	
Reflections collected	32585	
Independent reflections	7522 [R(int) = 0.0261]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.5188	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7522 / 87 / 346	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0251, wR2 = 0.0502	
R indices (all data)	R1 = 0.0352, wR2 = 0.0529	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.619 and -0.433 e.Å^{-3}	

Table S 4. Crystal data and structure refinement for Mn(pCl).

Empirical formula	C19 H17 Br Cl2 Mn N O3 Se2	
Formula weight	671.00	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 11.0199(4) Å	α= 90°.
	b = 13.2640(5) Å	β= 99.6860(10)°.
	c = 15.7873(6) Å	γ = 90°.
Volume	2274.70(15) $Å^3$	
Z	4	
Density (calculated)	1.959 Mg/m^3	
Absorption coefficient	5.793 mm^{-1}	
F(000)	1296	
Crystal size	0.400 x 0.200 x 0.120 mm^3	
Theta range for data collection	2.017 to 30.546°.	
Index ranges	-15<=h<=15, -18<=k<=18, -17<=l<=22	
Reflections collected	24113	
Independent reflections	6954 [R(int) = 0.0323]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.4604	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6954 / 0 / 263	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0310, wR2 = 0.0495	
R indices (all data)	R1 = 0.0504, wR2 = 0.0535	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.603 and -0.502 $e.Å^{-3}$	

Table S 5. Crystal data and structure refinement for Mn(pOCH$_3$).

Empirical formula	C21 H23 Br Mn N O5 Se2	
Formula weight	662.17	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 14.4793(10) Å	α= 90°.
	b = 11.6911(7) Å	β= 96.235(2)°.
	c = 14.1830(8) Å	γ = 90°.
Volume	2386.7(3) Å^3	
Z	4	
Density (calculated)	1.843 Mg/m^3	
Absorption coefficient	5.309 mm^{-1}	
F(000)	1296	
Crystal size	0.400 x 0.180 x 0.040 mm^3	
Theta range for data collection	2.244 to 30.590°.	
Index ranges	-19<=h<=20, -16<=k<=16, -20<=l<=20	
Reflections collected	28888	
Independent reflections	7309 [R(int) = 0.0431]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.5423	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7309 / 0 / 283	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0342, wR2 = 0.0547	
R indices (all data)	R1 = 0.0581, wR2 = 0.0608	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.829 and -0.663 e.Å^{-3}	

Table S 6. Crystal data and structure refinement for Mn(pCH$_3$).

Empirical formula	C21 H23 Br Mn N O3 Se2	
Formula weight	630.17	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.0773(3) Å	α= 90°.
	b = 22.5834(9) Å	β= 93.3390(10)°.
	c = 13.0086(5) Å	γ = 90°.
Volume	2368.91(16) Å^3	
Z	4	
Density (calculated)	1.767 Mg/m^3	
Absorption coefficient	5.338 mm^{-1}	
F(000)	1232	
Crystal size	0.400 x 0.120 x 0.080 mm^3	
Theta range for data collection	1.803 to 31.048°.	
Index ranges	-11<=h<=11, -27<=k<=32, -17<=l<=18	
Reflections collected	24784	
Independent reflections	7577 [R(int) = 0.0283]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7462 and 0.5045	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7577 / 0 / 265	
Goodness-of-fit on F^2	1.075	
Final R indices [I>2sigma(I)]	R1 = 0.0345, wR2 = 0.0626	
R indices (all data)	R1 = 0.0543, wR2 = 0.0673	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.676 and -0.601 e.Å^{-3}	

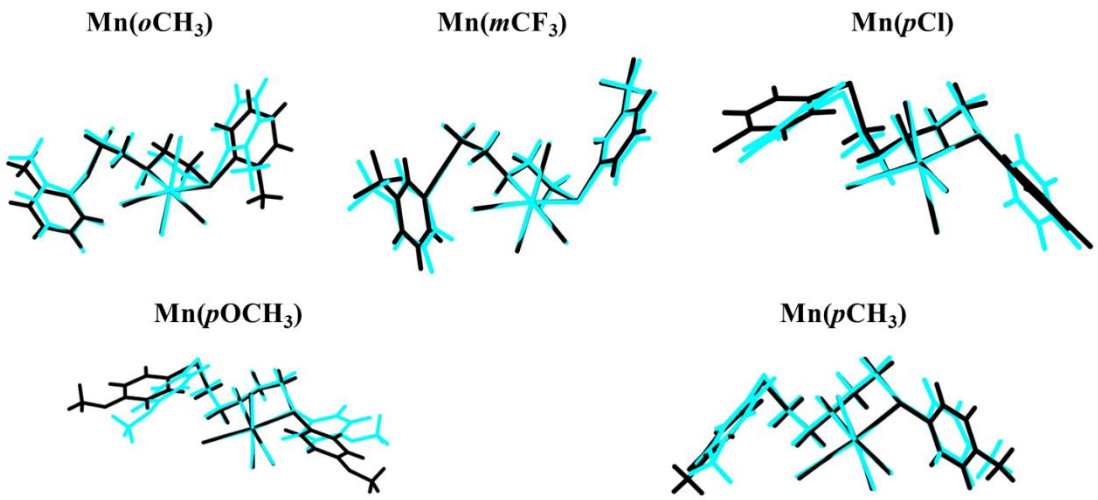

Figure S 28. Overlay between the optimized structure (blue) and ray-X structure (black).

Table S 7. Comparative between the main bond length and angle at level B3LYP/ZORA-def2-TZVP/SARC-J/D3BJ for the Mn and Br, the rest of atoms are obtained at level B3LYP/ZORA-def2-TZVP(-f)/SARC-J/D3BJ, in Orca 5.0.3 Software.

	Mn(*o*CH$_3$)		**Mn(*m*CF$_3$)**		**Mn(*p*Cl)**		**Mn(*p*OCH$_3$)**		**Mn(*p*CH$_3$)**	
	exp	calc	exp	calc	exp	calc	exp	calc	exp	calc
RMSD	0.704		0.233		0.759		1.090		0.429	
Bond length (Å)										
Mn1-C1	1.806	1.808	1.819	1.810	1.810	1.808	1.806	1.808	1.810	1.808
Mn1-C2	1.803	1.807	1.800	1.809	1.797	1.809	1.796	1.811	1.796	1.806
Mn1-C3	1.797	1.790	1.789	1.792	1.792	1.792	1.794	1.785	1.789	1.790
Mn1-Se1	2.473	2.556	2.488	2.544	2.474	2.538	2.4589	2.536	2.4708	2.542
Mn1-Br1	2.522	2.566	2.530	2.568	2.542	2.568	2.5433	2.572	2.5185	2.563
Mn1-N1	2.132	2.225	2.139	2.229	2.132	2.232	2.1313	2.230	2.1329	2.232
C1-O1	1.149	1.144	1.138	1.143	1.148	1.143	1.150	1.144	1.145	1.144
C2-O2	1.145	1.144	1.152	1.144	1.149	1.144	1.152	1.143	1.153	1.144
C3-O3	1.146	1.150	1.148	1.149	1.151	1.149	1.151	1.152	1.151	1.150
Bond angle (°)										
C3-Mn1-C1	92.51	93.71	90.30	93.13	91.19	93.29	91.78	91.86	90.85	92.84
C3-Mn1-C2	91.54	93.88	90.37	93.32	88.45	93.09	89.30	91.72	92.52	92.92
C1-Mn1-C2	86.12	90.11	88.29	90.47	90.31	90.59	89.76	90.77	88.44	90.87
N1-Mn1-Se1	86.29	84.26	85.53	84.00	85.86	84.29	86.94	84.09	85.93	84.17
Se1-Mn1-C1	172.36	171.50	172.80	170.75	172.37	170.18	170.02	167.28	170.89	169.72
N1-Mn1-C2	176.66	172.20	175.81	173.34	172.72	173.86	175.33	172.90	175.39	173.30
Br1-Mn1-C3	174.43	175.87	179.45	175.29	179.22	175.16	177.55	178.88	177.13	176.51

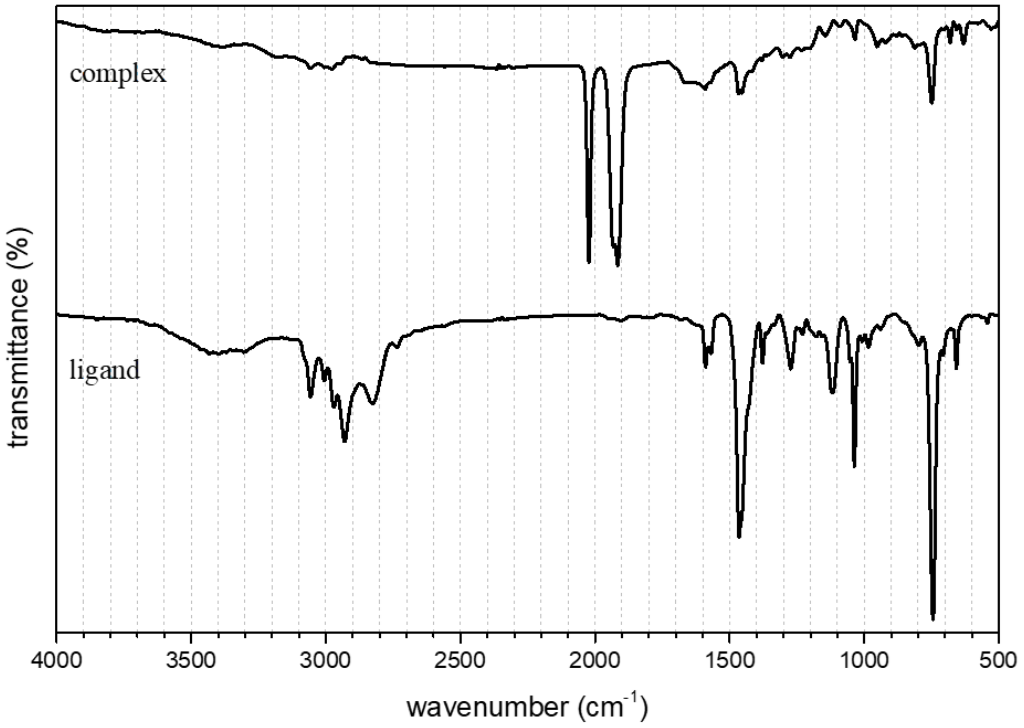

Figure S 29. Infrared spectra in KBr for Mn(oCH$_3$) and respective ligand.

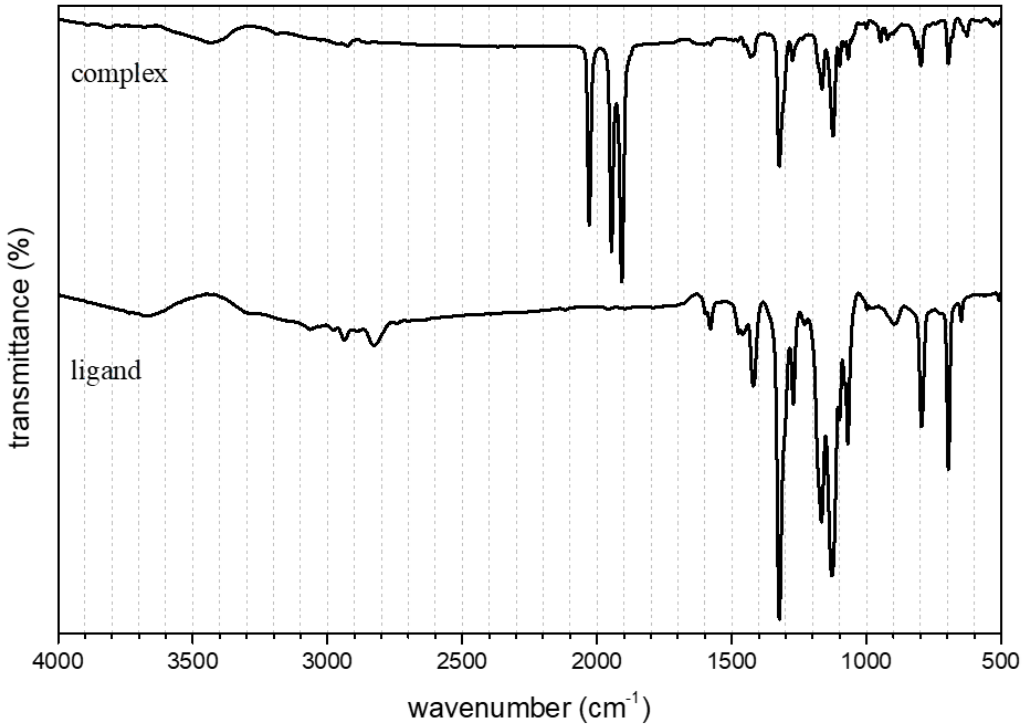

Figure S 30. Infrared spectra in KBr for Mn(mCF$_3$) and respective ligand.

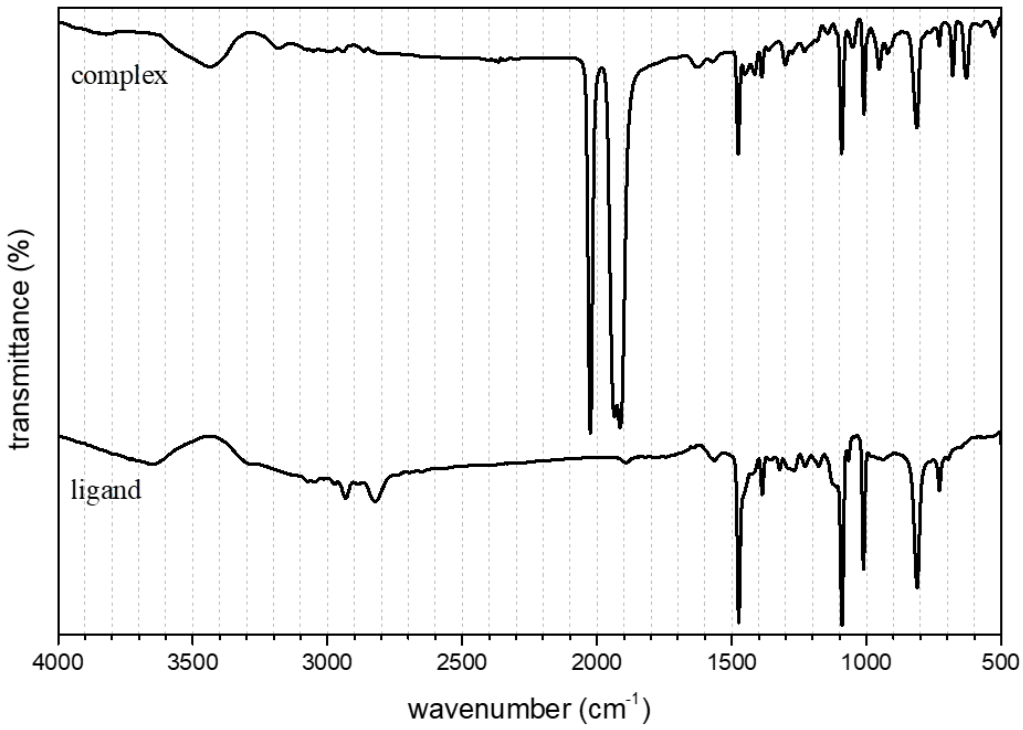

Figure S 31. Infrared spectra in KBr for Mn(pCl) and respective ligand.

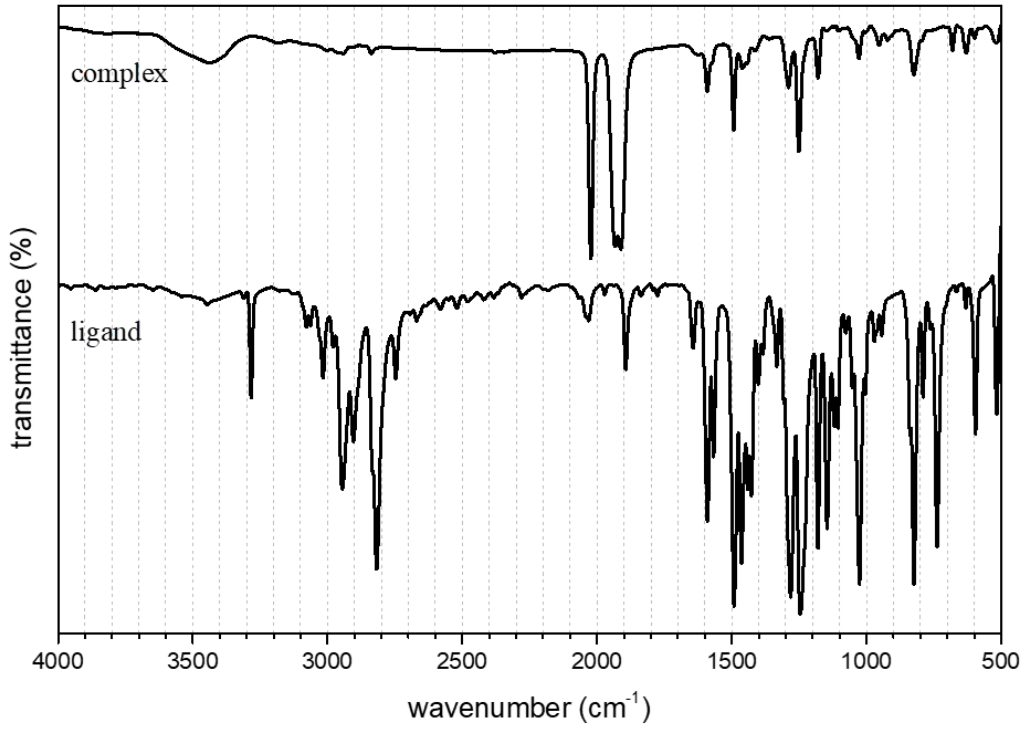

Figure S 32. Infrared spectra in KBr for Mn(pOCH$_3$) and respective ligand.

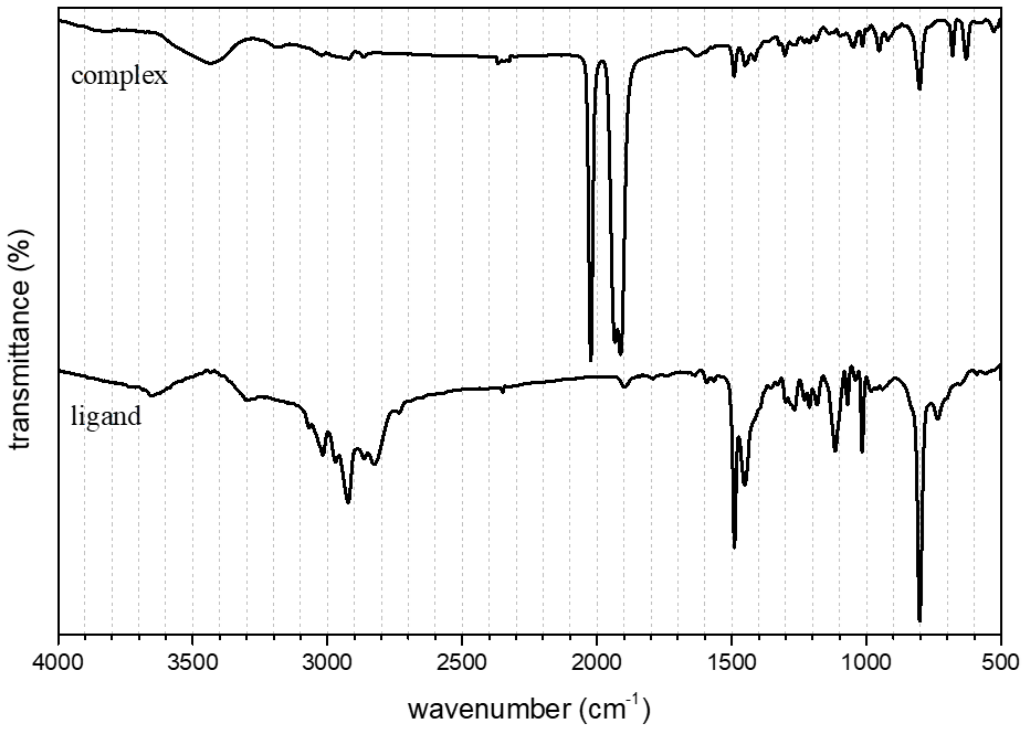

Figure S 33. Infrared spectra in KBr for Mn(pCH$_3$) and respective ligand.

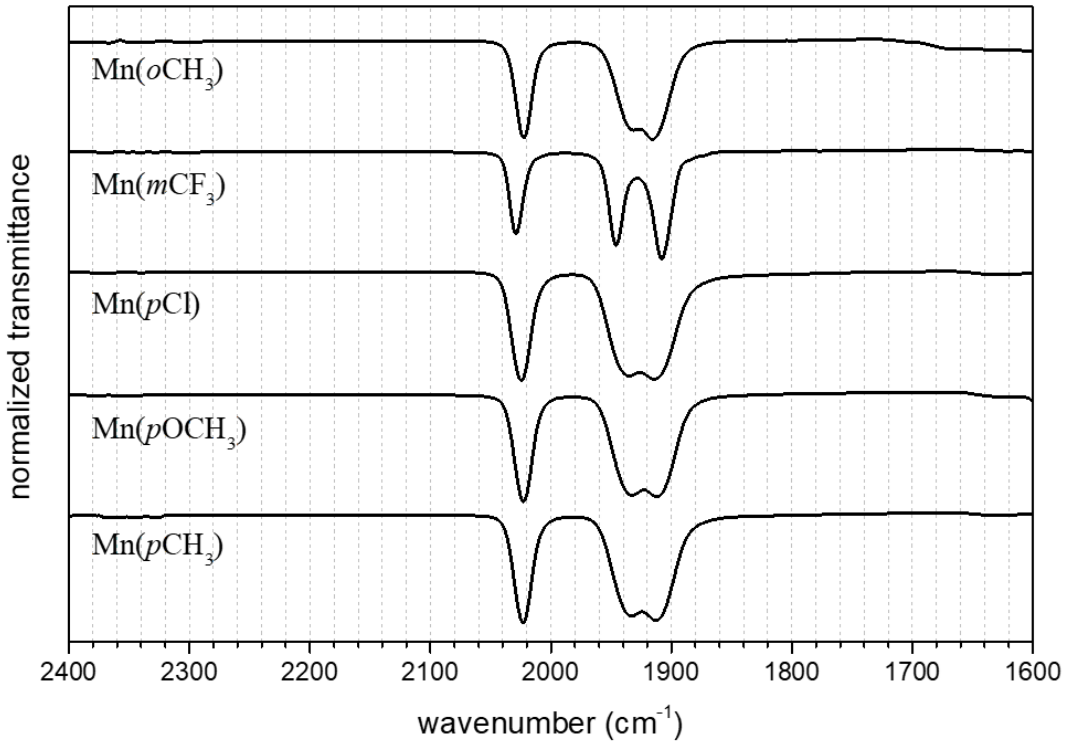

Figure S 34. Infrared spectra (KBr) for all metal carbonyl compounds in the range of carbonyl bands.

Table S 8. Experimental (exp) and calculated (calc) values referring to the stretching frequencies of the carbonyl groups at level B3LYP/ZORA-def2-TZVPP/SARC-J/D3BJ in Orca 5.0.3 Software. Vibrational scaling factor: 0.957 ± 0.007.

	νCO (A_1)		νCO (E)			
	exp	Calc	exp		calc	
Mn(*o*CH_3)	2022	2006	1932	1916	1947	1918
Mn(*m*CF_3)	2029	2009	1946	1908	1950	1922
Mn(*p*Cl)	2024	2008	1935	1914	1950	1920
Mn(*p*OCH_3)	2023	2008	1932	1912	1952	1907
Mn(*p*CH_3)	2023	2005	1933	1912	1946	1917

Table S 9. Löwdin bond order ($b_{AB}^{Löwdin}$) and atomic charges ($q^{Löwdin}$ and $q^{Hirshfeld}$) obtained for the five MCCs and carbon monoxide (CO). C1O1 is trans to selenium, C2O2 is trans to nitrogen, and C3O3 is trans to bromide.

Mn(*o*CH_3)					**Mn(*m*CF_3)**				
Bond	$b_{AB}^{Löwdin}$	Atom	$q^{Löwdin}$	$q^{Hirshfeld}$	Bond	$b_{AB}^{Löwdin}$	Atom	$q^{Löwdin}$	$q^{Hirshfeld}$
Mn1-C1	1.52	Mn1	-1.24	0.01	Mn1-C1	1.51	Mn1	-1.24	0.01
Mn1-C2	1.54	C1O1	0.14	-0.04	Mn1-C2	1.53	C1O1	0.16	-0.02
Mn1-C3	1.61	C2O2	0.15	-0.04	Mn1-C3	1.61	C2O2	0.14	-0.02
Mn1-Se1	0.82	C3O3	0.10	-0.09	Mn1-Se1	0.82	C3O3	0.11	-0.08
Mn1-Br1	1.13	L	0.86	0.46	Mn1-Br1	1.13	L	0.82	0.45
Mn1-N1	0.47	Br	-0.01	-0.31	Mn1-N1	0.47	Br	0.00	-0.31
C1-O1	3.01	Se1	0.88	0.16	C1-O1	3.01	Se1	0.89	0.17
C2-O2	3.01	Se2	0.52	0.01	C2-O2	3.02	Se2	0.52	0.01
C3-O3	2.98	-	-	-	C3-O3	2.98	-	-	-
Mn(*p*Cl)					**Mn(*p*OCH_3)**				
Bond	$b_{AB}^{Löwdin}$	Atom	$q^{Löwdin}$	$q^{Hirshfeld}$	Bond	$b_{AB}^{Löwdin}$	Atom	$q^{Löwdin}$	$q^{Hirshfeld}$
Mn1-C1	1.52	Mn1	-1.24	0.01	Mn1-C1	1.51	Mn1	-1.24	0.01
Mn1-C2	1.53	C1O1	0.16	-0.03	Mn1-C2	1.52	C1O1	0.16	-0.03
Mn1-C3	1.61	C2O2	0.14	-0.03	Mn1-C3	1.64	C2O2	0.15	-0.03
Mn1-Se1	0.83	C3O3	0.11	-0.08	Mn1-Se1	0.85	C3O3	0.08	-0.09
Mn1-Br1	1.13	L	0.84	0.45	Mn1-Br1	1.12	L	0.84	0.44
Mn1-N1	0.47	Br	0.00	-0.31	Mn1-N1	0.47	Br	0.01	-0.30
C1-O1	3.01	Se1	0.89	0.16	C1-O1	3.01	Se1	0.87	0.15
C2-O2	3.02	Se2	0.51	0.00	C2-O2	3.03	Se2	0.50	-0.01
C3-O3	2.98	-	-	-	C3-O3	2.96	-	-	-
Mn(*p*CH_3)					**CO**				
Bond	$b_{AB}^{Löwdin}$	Atom	$q^{Löwdin}$	$q^{Hirshfeld}$	Bond	$b_{AB}^{Löwdin}$	Atom	$q^{Löwdin}$	$q^{Hirshfeld}$
Mn1-C1	1.52	Mn1	-1.24	0.01	C≡O	3.46	C	-0.26	0.09
Mn1-C2	1.54	C1O1	0.15	-0.03	-	-	O	0.26	-0.09
Mn1-C3	1.61	C2O2	0.14	-0.03	-	-	-	-	
Mn1-Se1	0.83	C3O3	0.10	-0.09	-	-	-	-	
Mn1-Br1	1.14	L	0.85	0.46	-	-	-	-	
Mn1-N1	0.47	Br	0.00	-0.31	-	-	-	-	
C1-O1	3.01	Se1	0.88	0.16	-	-	-	-	
C2-O2	3.02	Se2	0.50	-0.01	-	-	-	-	
C3-O3	2.98	-	-	-	-	-	-	-	

Table S 10. Generalized Kohn-Sham energy decomposition analysis in kcal mol^{-1}. C1O1 is trans to selenium, C2O2 is trans to nitrogen, and C3O3 is trans to bromide. In parenthesis is the percentage of attractive interactions[a].

bond	ΔE^{TOT}	ΔE^{elstat}	ΔE^{exch}	ΔE^{rep}	ΔE^{pol}	ΔE^{disp}	ΔE^{corr}	$\Delta E^{Pauli\ [b]}$	$\Delta E^{orb\ [c]}$
Mn(*o*CH$_3$)									
Mn1-C1O1	-45.15	-104.49 (28.2%)	-161.45 (43.6%)	325.08	-55.14 (14.9%)	-7.80 (2.1%)	-41.36 (11.2%)	163.63	-104.30
Mn1-C2O2	-46.11	-103.57 (28.2%)	-160.09 (43.6%)	320.93	-52.51 (14.3%)	-6.99 (1.9%)	-43.89 (12.0%)	160.84	-103.39
Mn1-C3O3	-52.66	-104.05 (28.1%)	-157.78 (42.6%)	317.31	-54.60 (14.8%)	-8.37 (2.3%)	-45.17 (12.2%)	159.53	-108.14
Mn1-Br1	-133.68	-159.69 (43.5%)	-130.71 (35.6%)	233.26	-47.58 (13.0%)	-9.80 (2.7%)	-19.16 (5.2%)	102.55	-76.54
Mn1-κ^2L	-73.11	-104.62 (28.4%)	-160.47 (43.5%)	295.54	-56.77 (15.4%)	-26.30 (7.1%)	-20.50 (5.6%)	135.07	-103.57
Mn(*m*CF$_3$)									
Mn1-C1O1	-45.42	-103.08 (28.1%)	-159.56 (43.6%)	320.89	-54.20 (14.8%)	-8.26 (2.3%)	-41.22 (11.3%)	161.33	-103.68
Mn1-C2O2	-46.26	-102.21 (28.4%)	-155.94 (43.3%)	313.66	-51.82 (14.4%)	-6.38 (1.8%)	-43.57 (12.1%)	157.72	-101.77
Mn1-C3O3	-52.10	-103.78 (28.1%)	-157.53 (42.7%)	316.82	-54.13 (14.7%)	-8.21 (2.2%)	-45.28 (12.3%)	159.29	-107.62
Mn1-Br1	-140.04	-167.02 (44.2%)	-133.17 (35.3%)	237.46	-48.02 (12.7%)	-10.18 (2.7%)	-19.11 (5.1%)	104.29	-77.31
Mn1-κ^2L	-71.48	-104.77 (28.3%)	-162.00 (43.7%)	299.33	-57.34 (15.5%)	-26.21 (7.1%)	-20.50 (5.5%)	137.33	-104.05
Mn(*p*Cl)									
Mn1-C1O1	-45.30	-103.55 (28.2%)	-159.98 (43.6%)	321.97	-54.66 (14.9%)	-8.08 (2.2%)	-41.00 (11.2%)	161.99	-103.74
Mn1-C2O2	-46.32	-102.19 (28.4%)	-155.99 (43.3%)	313.74	-51.78 (14.4%)	-6.40 (1.8%)	-43.70 (12.1%)	157.75	-101.88
Mn1-C3O3	-52.04	-104.07 (28.1%)	-158.44 (42.8%)	318.39	-54.40 (14.7%)	-8.20 (2.2%)	-45.33 (12.2%)	159.95	-107.93
Mn1-Br1	-137.71	-164.12 (44.0%)	-131.99 (35.4%)	235.55	-48.24 (12.9%)	-9.98 (2.7%)	-18.92 (5.1%)	103.56	-77.14
Mn1-κ^2L	-71.79	-106.01 (28.4%)	-163.16 (43.7%)	301.62	-57.30 (15.3%)	-25.80 (6.9%)	-21.13 (5.7%)	138.46	-104.23
Mn(*p*OCH$_3$)									
Mn1-C1O1	-45.45	-104.69 (28.2%)	-162.28 (43.7%)	326.16	-55.12 (14.8%)	-8.24 (2.2%)	-41.29 (11.1%)	163.88	-104.65
Mn1-C2O2	-45.47	-102.55 (28.4%)	-156.68 (43.4%)	315.15	-51.80 (14.4%)	-6.11 (1.7%)	-43.48 (12.1%)	158.47	-101.39
Mn1-C3O3	-52.76	-107.85 (28.1%)	-164.58 (42.8%)	331.55	-57.51 (15.0%)	-7.59 (2.0%)	-46.79 (12.2%)	166.97	-111.89
Mn1-Br1	-130.71	-159.41 (42.4%)	-137.62 (36.6%)	245.50	-50.62 (13.5%)	-10.17 (2.7%)	-18.39 (4.9%)	107.88	-79.18
Mn1-κ^2L	-74.18	-108.29 (28.9%)	-162.65 (43.5%)	300.15	-55.89 (14.9%)	-24.80 (6.6%)	-22.70 (6.1%)	137.50	-103.39
Mn(*p*CH$_3$)									
Mn1-C1O1	-45.78	-104.31 (28.2%)	-160.94 (43.6%)	323.76	-55.29 (15.0%)	-8.16 (2.2%)	-40.85 (11.1%)	162.82	-104.30
Mn1-C2O2	-46.22	-103.69 (28.4%)	-158.68 (43.4%)	319.21	-52.92 (14.5%)	-6.42 (1.8%)	-43.73 (12.0%)	160.53	-103.07
Mn1-C3O3	-52.20	-105.19 (28.2%)	-159.63 (42.7%)	321.27	-55.30 (14.8%)	-8.07 (2.2%)	-45.28 (12.1%)	161.64	-108.65
Mn1-Br1	-132.46	-160.41 (43.0%)	-134.75 (36.1%)	240.36	-48.15 (12.9%)	-10.11 (2.7%)	-19.40 (5.2%)	105.61	-77.66
Mn1-κ^2L	-73.41	-106.57 (28.6%)	-162.17 (43.5%)	299.31	-57.22 (15.4%)	-25.79 (6.9%)	-20.97 (5.6%)	137.14	-103.98

[a] = $\Delta E^{elstat} + \Delta E^{exch} + \Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$; [b] = $\Delta E^{exch} + \Delta E^{rep}$; [c] = $\Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$

Table S 11. The most relevant density flow channel with their respective energies (ΔE_{orb}) in kcal mol^{-1} and charge transfer estimation (Δq_{orb}) values for each ligand bonded to manganese. C1O1 is trans to selenium, C2O2 is trans to nitrogen, and C3O3 is trans to bromide.

bond	$\Delta E_{orb\text{-}tot}$	$\Delta E_{orb\text{-}1}$	$\Delta q_{orb\text{-}1}$	$\Delta E_{orb\text{-}2}$	$\Delta q_{orb\text{-}2}$	$\Delta E_{orb\text{-}3}$	$\Delta q_{orb\text{-}3}$	$\Delta E_{orb\text{-}rest}$
Mn(*o*CH$_3$)								
Mn1-C1O1	-89.46	-41.37	0.64	-22.88	0.50	-21.78	0.46	-3.43
Mn1-C2O2	-89.48	-41.00	0.62	-23.26	0.51	-22.18	0.47	-3.05
Mn1-C3O3	-93.05	-38.85	0.62	-26.98	0.54	-24.57	0.48	-2.66
Mn1-Br1	-58.63	-32.02	0.60	-5.29	0.21	-4.64	0.18	-16.67
Mn1-k^{2}L	-68.66	-29.12	0.61	-20.14	0.44	-3.93	0.20	-15.47
Mn(*m*CF$_3$)								
Mn1-C1O1	-88.50	-40.98	0.64	-22.59	0.50	-21.53	0.46	-3.40
Mn1-C2O2	-88.65	-40.62	0.62	-23.19	0.51	-22.00	0.47	-2.84
Mn1-C3O3	-92.53	-38.98	0.62	-26.69	0.54	-24.29	0.48	-2.58
Mn1-Br1	-58.65	-31.80	0.59	-5.56	0.22	-4.72	0.18	-16.56
Mn1-k^{2}L	-68.95	-29.21	0.61	-20.17	0.45	-4.37	0.22	-15.20
Mn(*p*Cl)								
Mn1-C1O1	-88.74	-41.07	0.64	-22.66	0.50	-21.59	0.46	-3.43
Mn1-C2O2	-88.72	-40.56	0.62	-23.26	0.51	-22.07	0.47	-2.83
Mn1-C3O3	-92.75	-39.06	0.62	-26.80	0.54	-24.28	0.48	-2.61
Mn1-Br1	-58.75	-31.84	0.59	-5.54	0.21	-4.67	0.18	-16.71
Mn1-k^{2}L	-69.54	-29.67	0.62	-20.19	0.45	-4.42	0.22	-15.25
Mn(*p*OCH$_3$)								
Mn1-C1O1	-89.48	-41.46	0.64	-22.83	0.51	-21.65	0.46	-3.54
Mn1-C2O2	-88.40	-41.24	0.63	-22.72	0.50	-21.54	0.46	-2.89
Mn1-C3O3	-97.07	-40.75	0.64	-28.21	0.55	-25.22	0.48	-2.90
Mn1-Br1	-60.11	-33.05	0.61	-5.98	0.22	-4.47	0.18	-16.60
Mn1-k^{2}L	-69.62	-29.45	0.61	-19.86	0.44	-4.80	0.23	-15.52
Mn(*p*CH$_3$)								
Mn1-C1O1	-89.23	-41.00	0.64	-22.93	0.51	-21.81	0.46	-3.49
Mn1-C2O2	-89.81	-41.04	0.63	-23.52	0.51	-22.31	0.47	-2.95
Mn1-C3O3	-93.55	-39.48	0.63	-27.03	0.54	-24.43	0.48	-2.62
Mn1-Br1	-58.98	-32.29	0.60	-5.44	0.21	-4.53	0.18	-16.72
Mn1-k^{2}L	-69.36	-29.83	0.62	-20.05	0.45	-4.29	0.22	-15.19

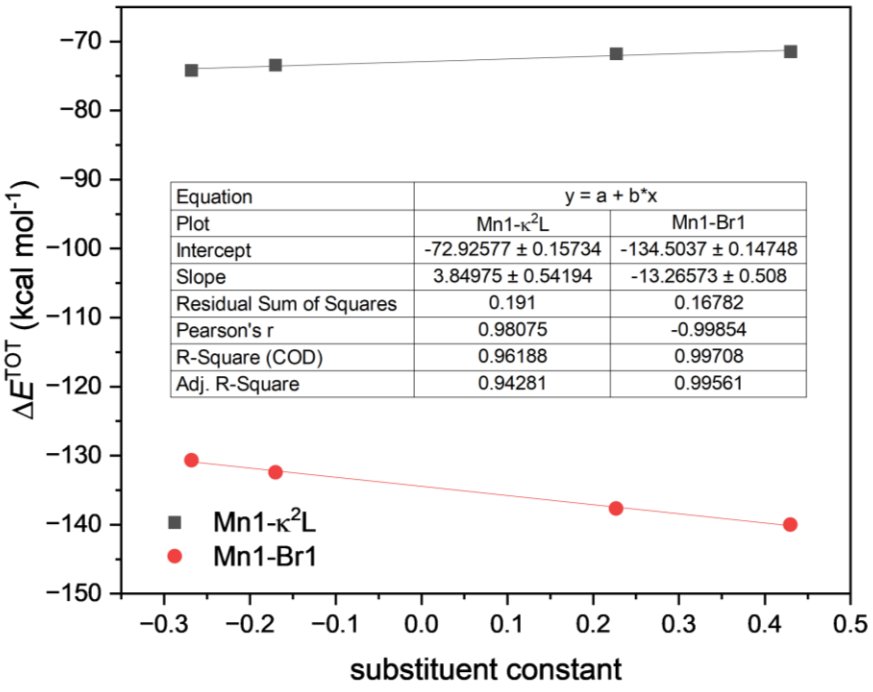

Figure S 35. Plot of para- and meta- Hammet constant versus total interaction energy value (ΔE^{TOT}).

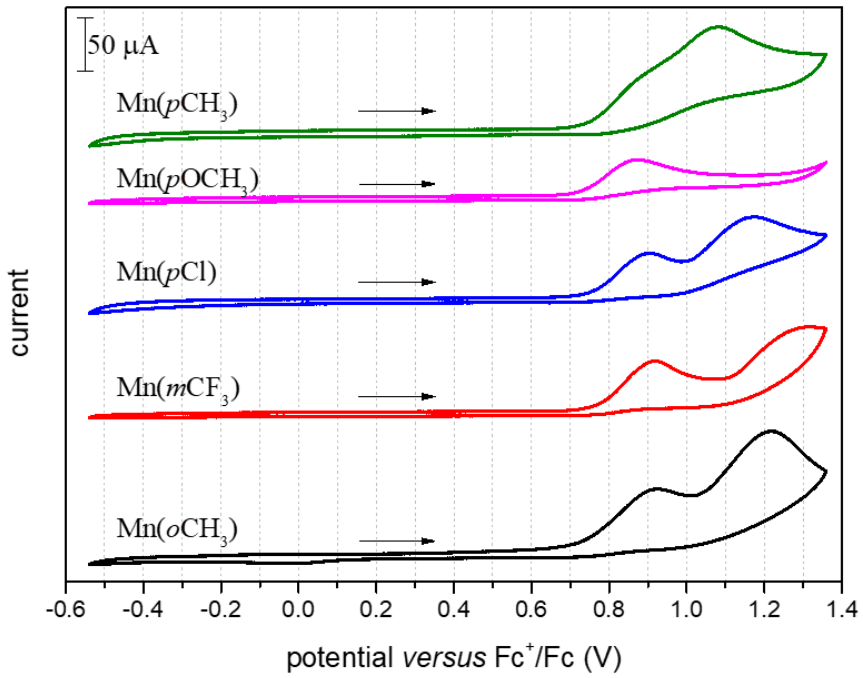

Figure S 36. Cyclic voltammetry in CH_2Cl_2 with $TBAPF_6$ (0.1 mol L^{-1}), electrodes: glass carbon (work), Ag/AgCl (reference), and platinum wire (counter) in 100 mV s^{-1}, 1x10^{-3} mol L^{-1}.

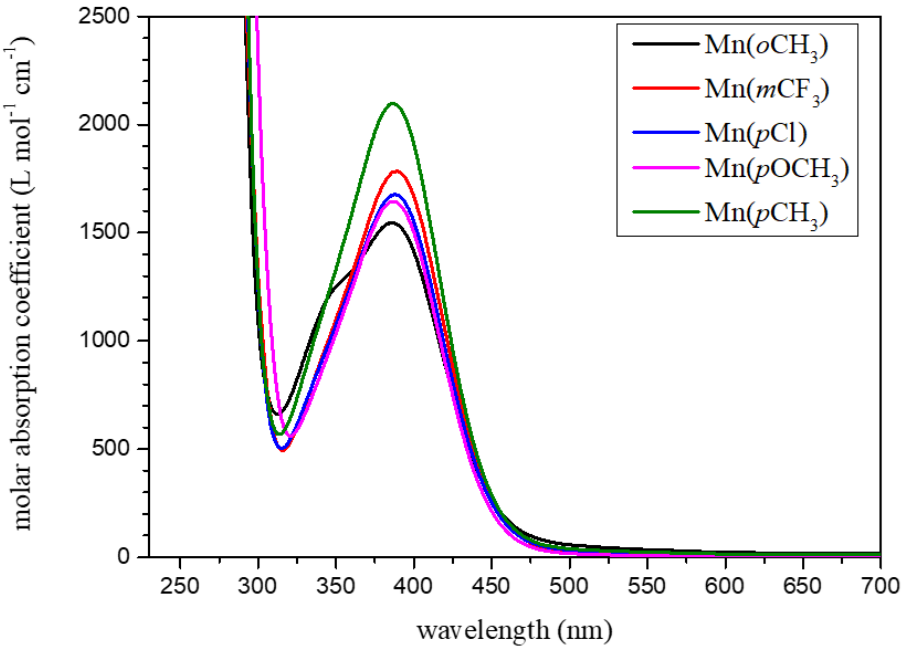

Figure S 37. Spectrum electronic for the MCC in dichloromethane.

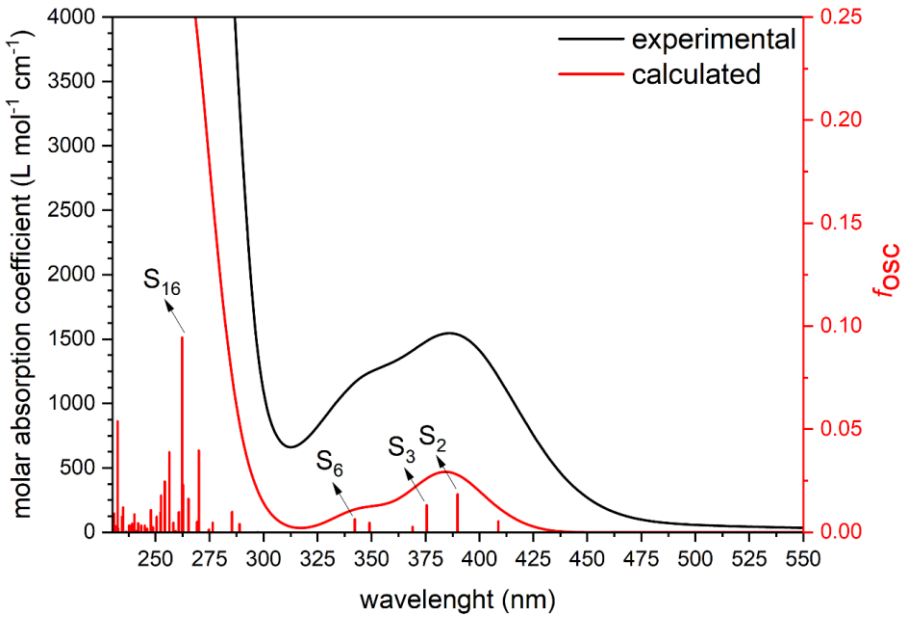

Figure S 38. Overlap between experimental and calculated spectra with key transitions highlighted for Mn(oCH$_3$).

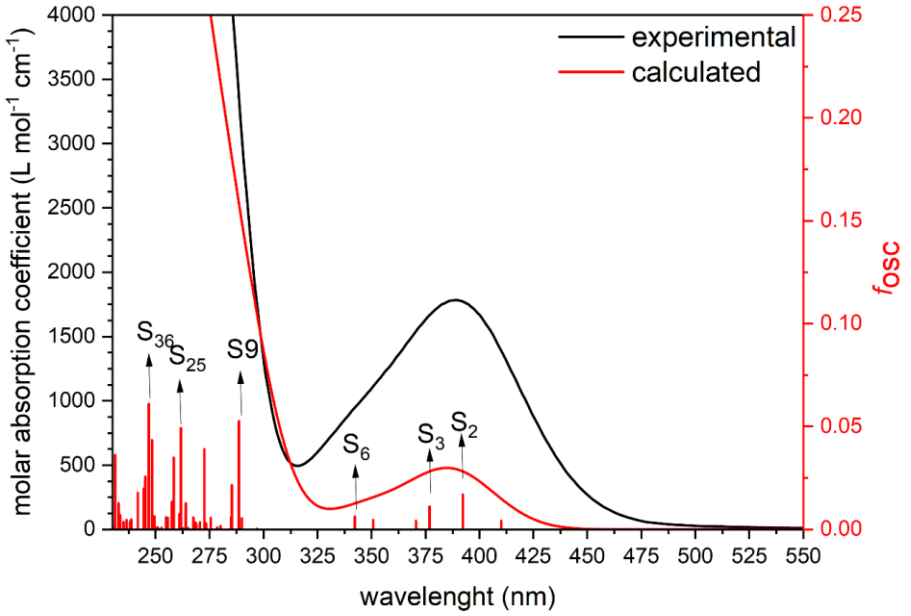

Figure S 39. Overlap between experimental and calculated spectra with key transitions highlighted for Mn(mCF$_3$).

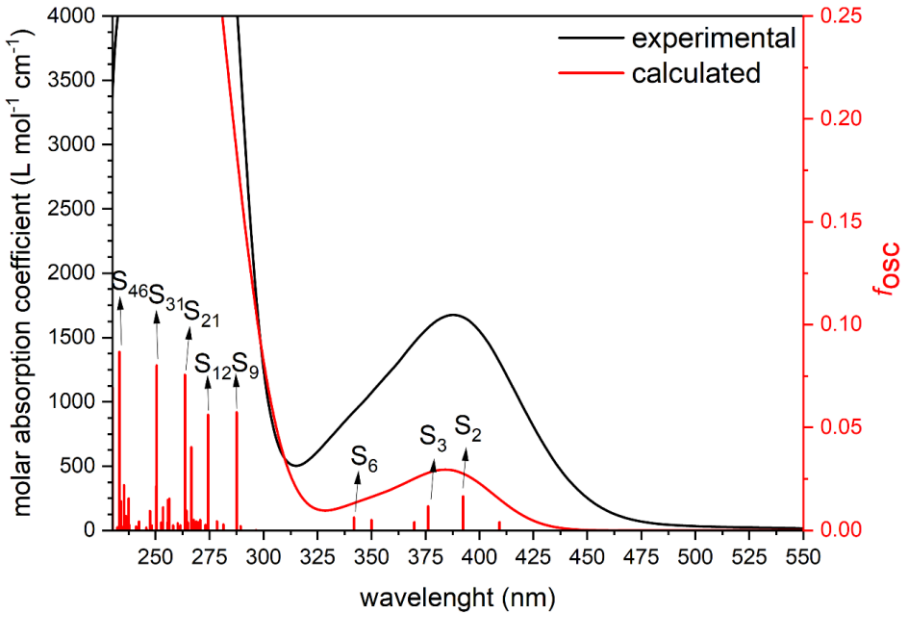

Figure S 40. Overlap between experimental and calculated spectra with key transitions highlighted for Mn(pCl).

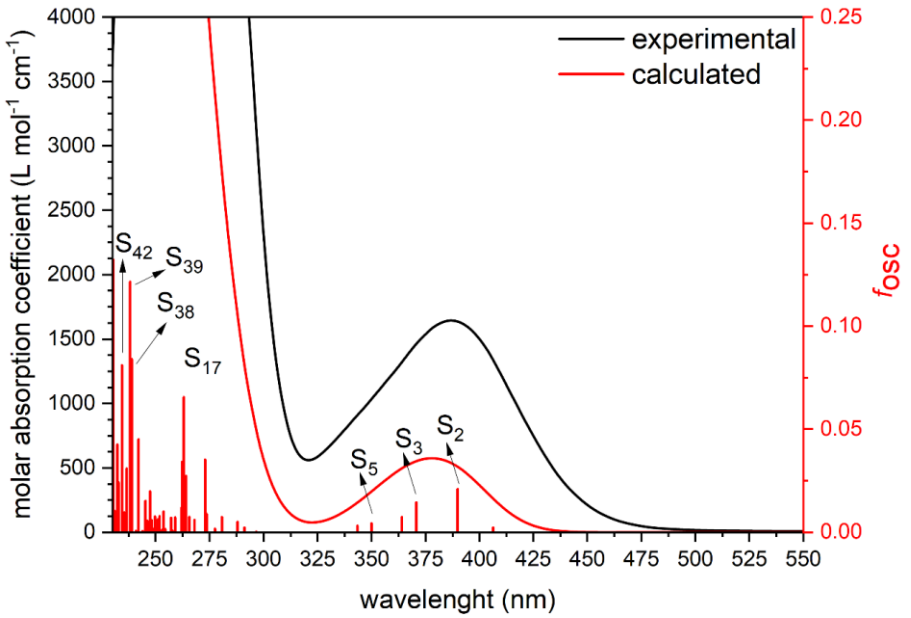

Figure S 41. Overlap between experimental and calculated spectra with key transitions highlighted for Mn(pOCH$_3$).

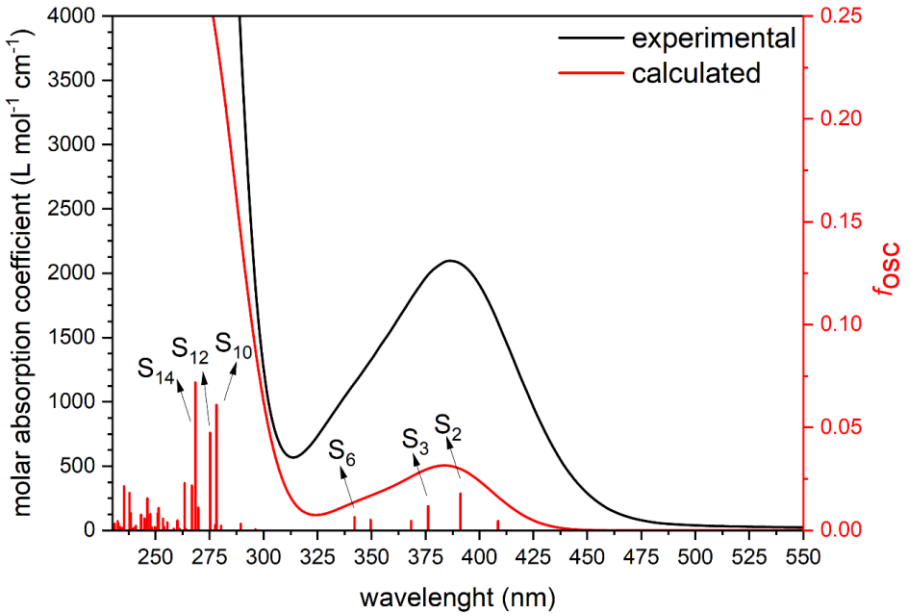

Figure S 42. Overlap between experimental and calculated spectra with key transitions highlighted for Mn(pCH$_3$).

Table S 12. Selected computed excitation energies, oscillator strengths (f) and electronic transitions.

State	Energy (nm) exp	Energy (nm) calc	Oscillator strength (f_{osc})	Transitions
			Mn(*o*CH$_3$)	
S_2	387	390	0.01847	HOMO-1 → LUMO (24.2%)
S_3		376	0.01314	HOMO-3 → LUMO (43.3%), HOMO-3 → LUMO+1 (18.2%)
S_6	357	342	0.00643	HOMO-3 → LUMO+1 (39.1%), HOMO-3 → LUMO (31.0%)
S_{16}	-	262	0.09454	HOMO-4 → LUMO+1 (47.5%)
			Mn(*m*CF$_3$)	
S_2	388	392	0.01698	HOMO-2 → LUMO+1 (17.5%)
S_3		377	0.01120	HOMO-3 → LUMO (33.3%), HOMO-3 → LUMO+5 (15.7%)
S_6	-	342	0.00623	HOMO-3 → LUMO+1 (41.3%), HOMO-3 → LUMO+2 (19.2%)
S_9	-	289	0.05271	HOMO → LUMO+2 (21.0%)
S_{25}	-	262	0.04936	HOMO-4 → LUMO (26.3%)
S_{36}	-	247	0.06101	HOMO-3 → LUMO+5 (17.1%), HOMO-4 → LUMO+3 (16.4%)
			Mn(*p*Cl)	
S_2	387	392	0.01661	HOMO-2 → LUMO+1 (18.4%)
S_3		376	0.01175	HOMO-3 → LUMO (49.0%)
S_6	-	342	0.00628	HOMO-3 → LUMO+1 (48.7%)
S_9	-	288	0.05742	HOMO → LUMO+2 (46.6%), HOMO-2 → LUMO+2 (18.7%)
S_{12}	-	274	0.05619	HOMO-4 → LUMO (28.0%)
S_{21}	-	264	0.07572	HOMO-4 → LUMO (15.7%)
S_{31}	-	250	0.08024	HOMO-4 → LUMO+3 (32.8%)
S_{46}	-	233	0.08676	HOMO-4 → LUMO+4 (33.7%), HOMO-4 → LUMO+6 (16.4%)
			Mn(*p*OCH$_3$)	
S_2	387	390	0.02099	HOMO-2 → LUMO (35.7%), HOMO-1 → LUMO (18.8%)
S_3		371	0.01453	HOMO-5 → LUMO (19.7%), HOMO-5 → LUMO+1 (17.3%)
S_5	-	350	0.00443	HOMO-1 → LUMO+1 (32.7%), HOMO-2 → LUMO+1 (15.1%)
S_{17}	-	263	0.06565	HOMO → LUMO+5 (10.5%), HOMO-3 → LUMO+1 (10.0%)
S_{38}	-	239	0.08404	HOMO-1 → LUMO+5 (28.5%), HOMO-1 → LUMO+6 (22.9%)
S_{39}	-	238	0.12158	HOMO-3 → LUMO+3 (33.1%)
S_{42}	-	234	0.08099	HOMO-5 → LUMO+3 (44.8%), HOMO-4 → LUMO+3 (15.4%)
			Mn(*p*CH$_3$)	
S_2	387	391	0.01786	HOMO-1 → LUMO (17.0%), HOMO-2 → LUMO+1 (16.1%)
S_3		376	0.01182	HOMO-4 → LUMO (46.0%)
S_6	-	342	0.00644	HOMO-4 → LUMO+1 (41.8%), HOMO-4 → LUMO (24.5%)
S_{10}	-	278	0.06112	HOMO → LUMO+2 (19.9%)
S_{12}	-	275	0.04749	HOMO-3 → LUMO (29.8%)
S_{14}	-	268	0.07199	HOMO-3 → LUMO+1 (50.5%)

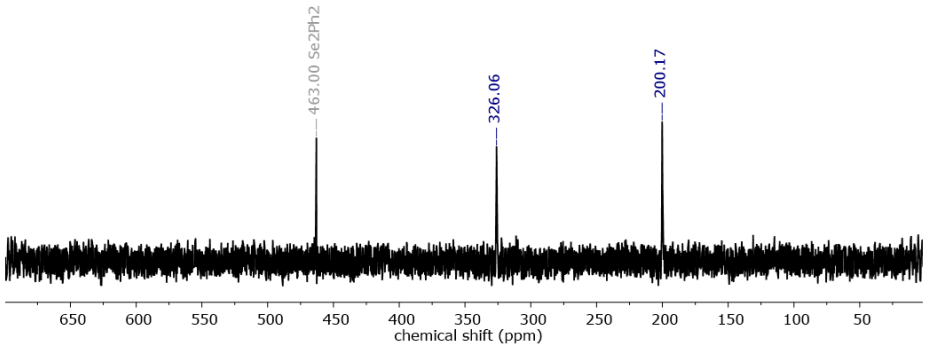

Figure S 43. ^{77}Se NMR spectrum of Mn(oCH_3).

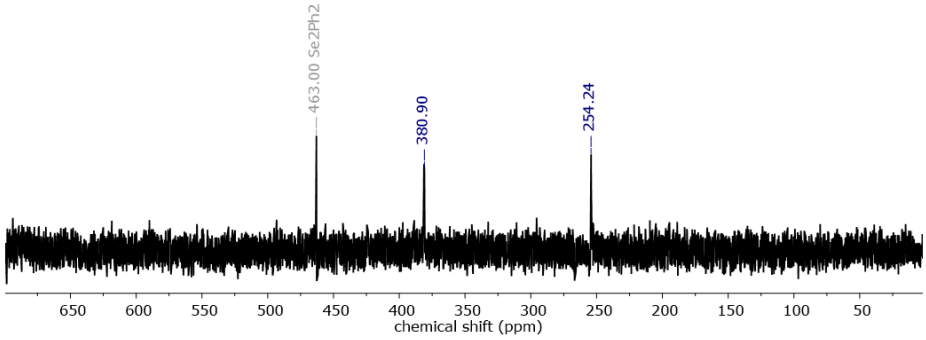

Figure S 44. ^{77}Se NMR spectrum of Mn(mCF_3).

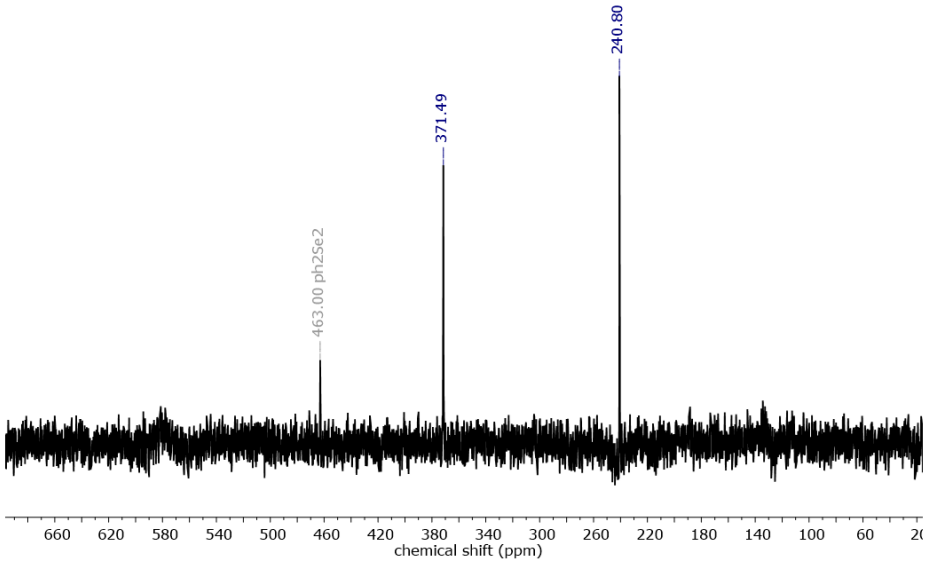

Figure S 45. ^{77}Se NMR spectrum of Mn(pCl).

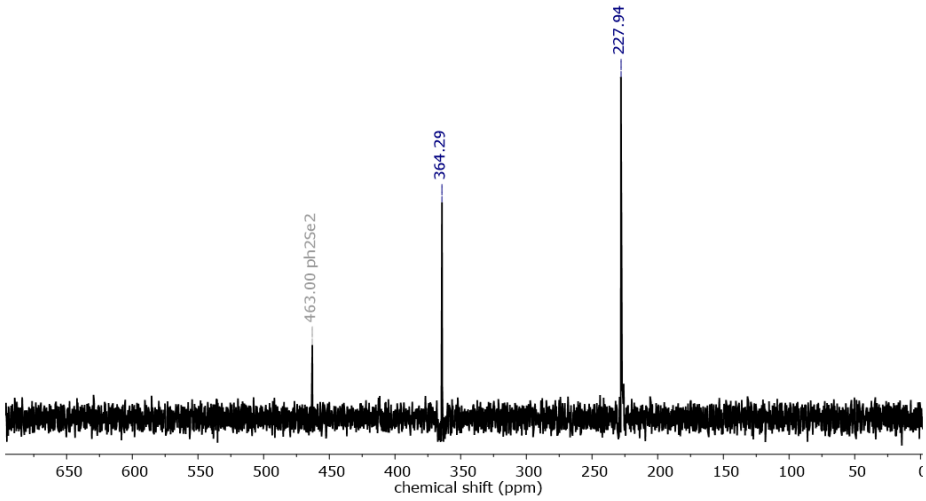

Figure S 46. ^{77}Se NMR spectrum of Mn(pOCH$_3$).

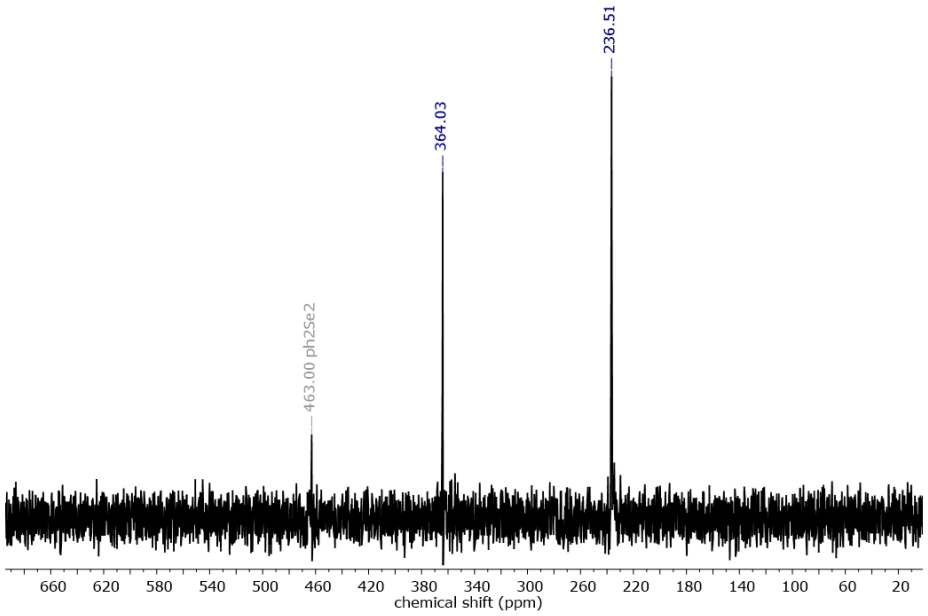

Figure S 47. ^{77}Se NMR spectrum of Mn(pCH_3).

Table S 13. Comparative chemical shifts ^{77}Se NMR in $CDCl_3$ between compounds and the free ligand.

	Mn(L)		Free ligand
Mn(*o*CH_3)	326	200	218
Mn(*m*CF_3)	381	254	278
Mn(*p*Cl)	371	241	265
Mn(*p*OCH_3)	364	228	253
Mn(*p*CH_3)	364	237	257

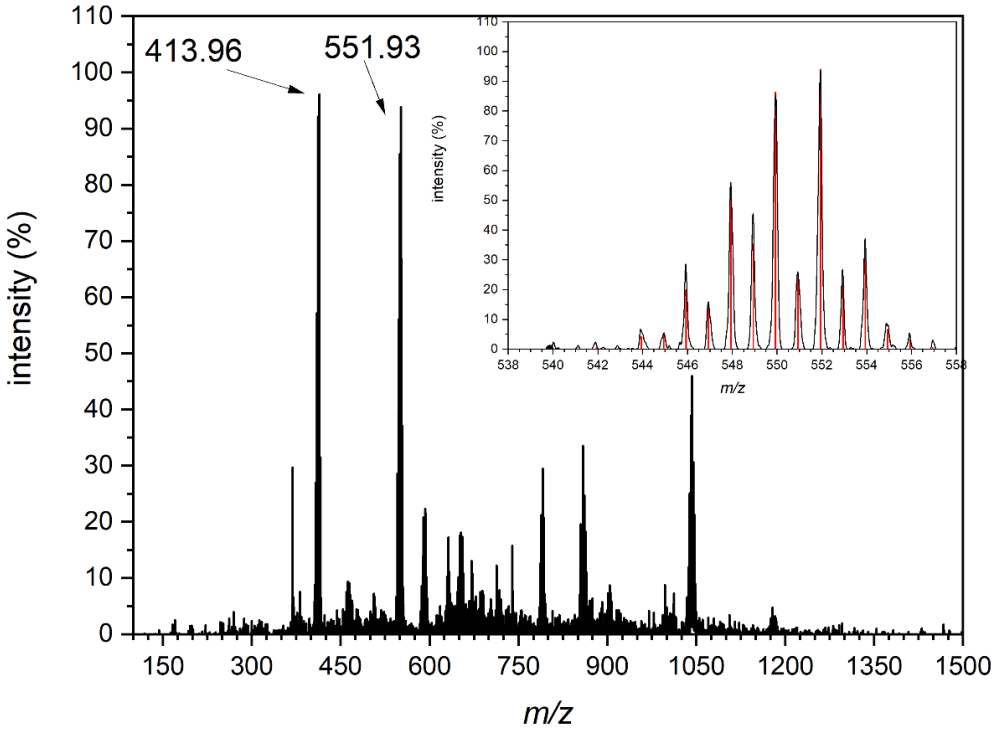

Figure S 48. ESI-MS spectrum (positive mode) in acetonitrile of Mn(oCH$_3$). Insert: calculated (red) and experimental (black) isotopic distributions for the specie [Mn(L)(CO)$_3$]$^+$.

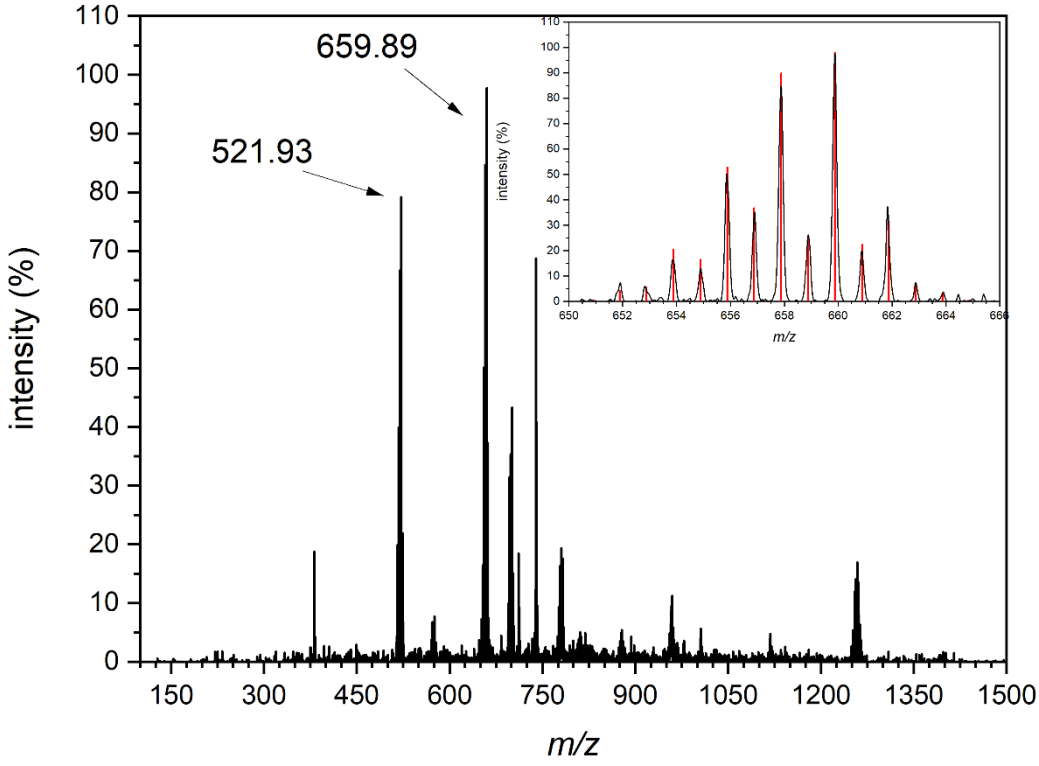

Figure S 49. ESI-MS spectrum (positive mode) in acetonitrile of Mn(mCF$_3$). Insert: calculated (red) and experimental (black) isotopic distributions for the specie [Mn(L)(CO)$_3$]$^+$.

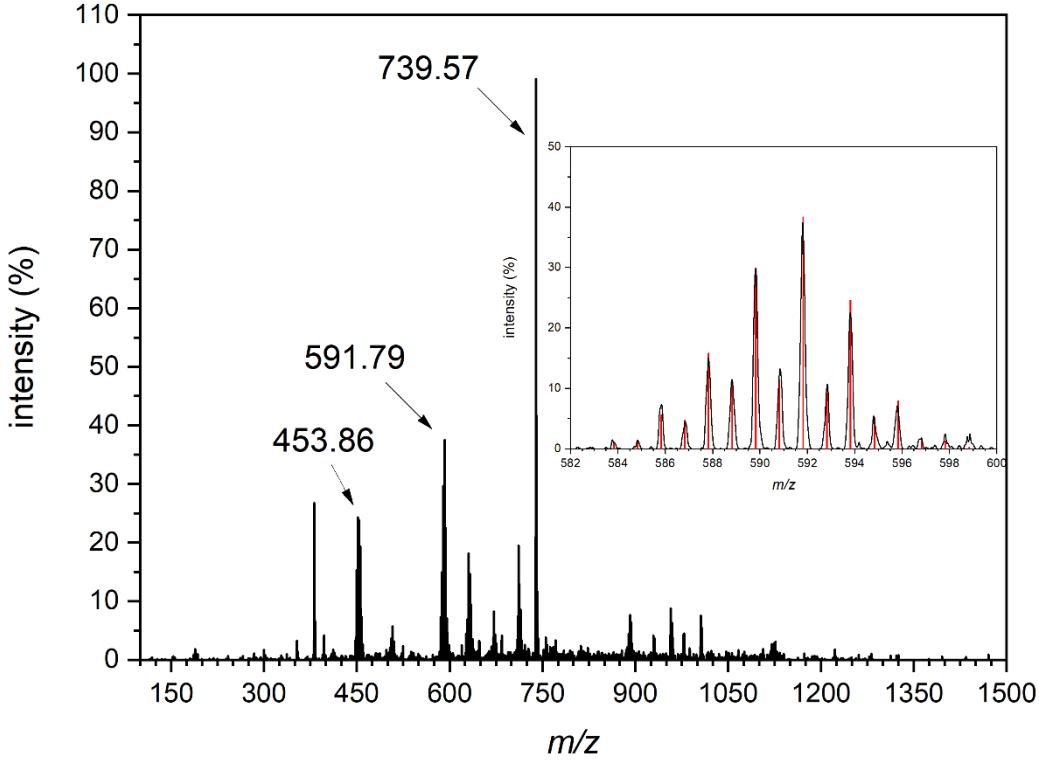

Figure S 50. ESI-MS spectrum (positive mode) in acetonitrile of Mn(pCl). Insert: calculated (red) and experimental (black) isotopic distributions for the specie $[Mn(L)(CO)_3]^+$.

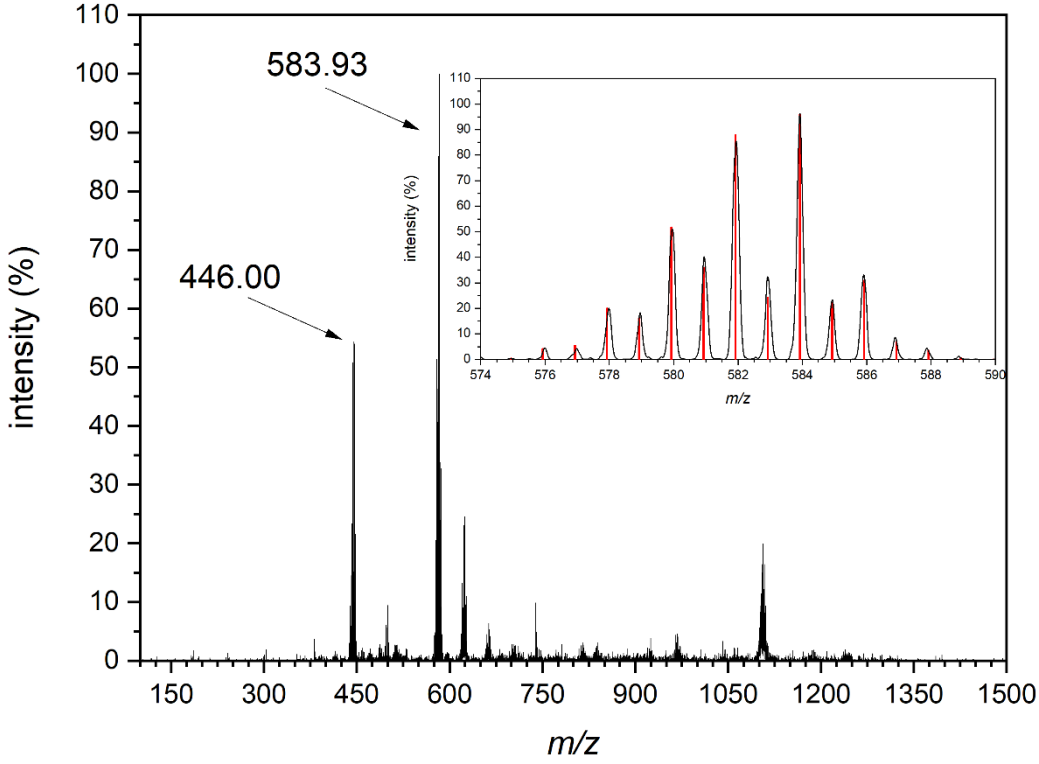

Figure S 51. ESI-MS spectrum (positive mode) in acetonitrile of $Mn(pOCH_3)$. Insert: calculated (red) and experimental (black) isotopic distributions for the specie $[Mn(L)(CO)_3]^+$.

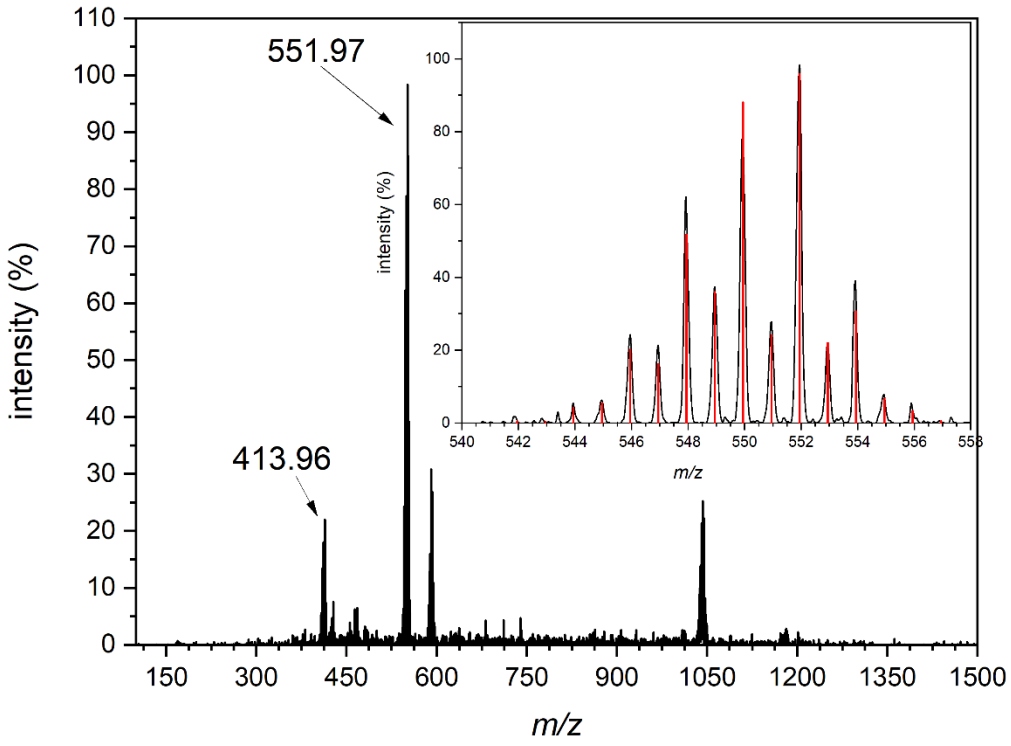

Figure S 52. ESI-MS spectrum (positive mode) in acetonitrile of Mn(mCH$_3$). Insert: calculated (red) and experimental (black) isotopic distributions for the specie [Mn(L)(CO)$_3$]$^+$.

Table S 14. Molar conductivity values obtained for manganese compounds incubated in CH_2Cl_2 and CH_3CN.

Solvent	Time	Molar conductivity (Ω^{-1} mol^{-1} cm^2)				
		Mn(*o*CH$_3$)	**Mn(*m*CF$_3$)**	**Mn(*p*Cl)**	**Mn(*p*OCH$_3$)**	**Mn(*p*CH$_3$)**
Dichloromethane	0 h	0.06	0.09	0.09	0.10	0.08
	20 h	0.08	0.07	0.08	0.09	0.08
Acetonitrile	0 h	1.62	1.31	1.08	1.67	1.81
	20 h	18.60	15.51	16.90	18.55	19.89

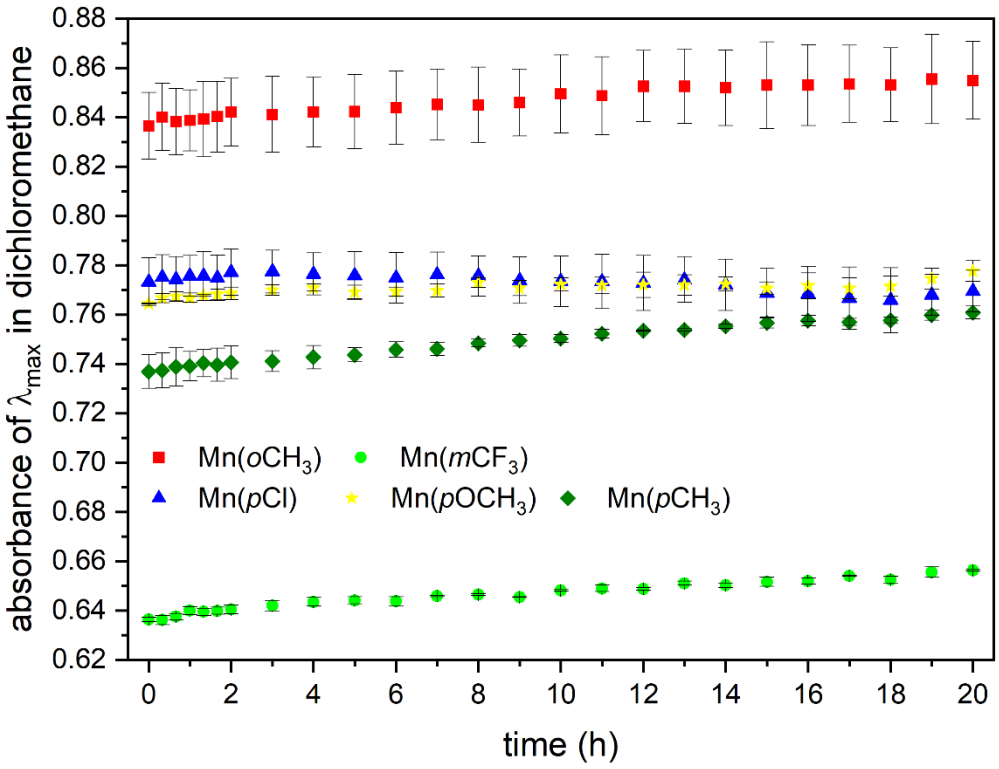

Figure S 53. Variation in the absorption of MLCT in CH_2Cl_2 solution over a period of 20 hours.

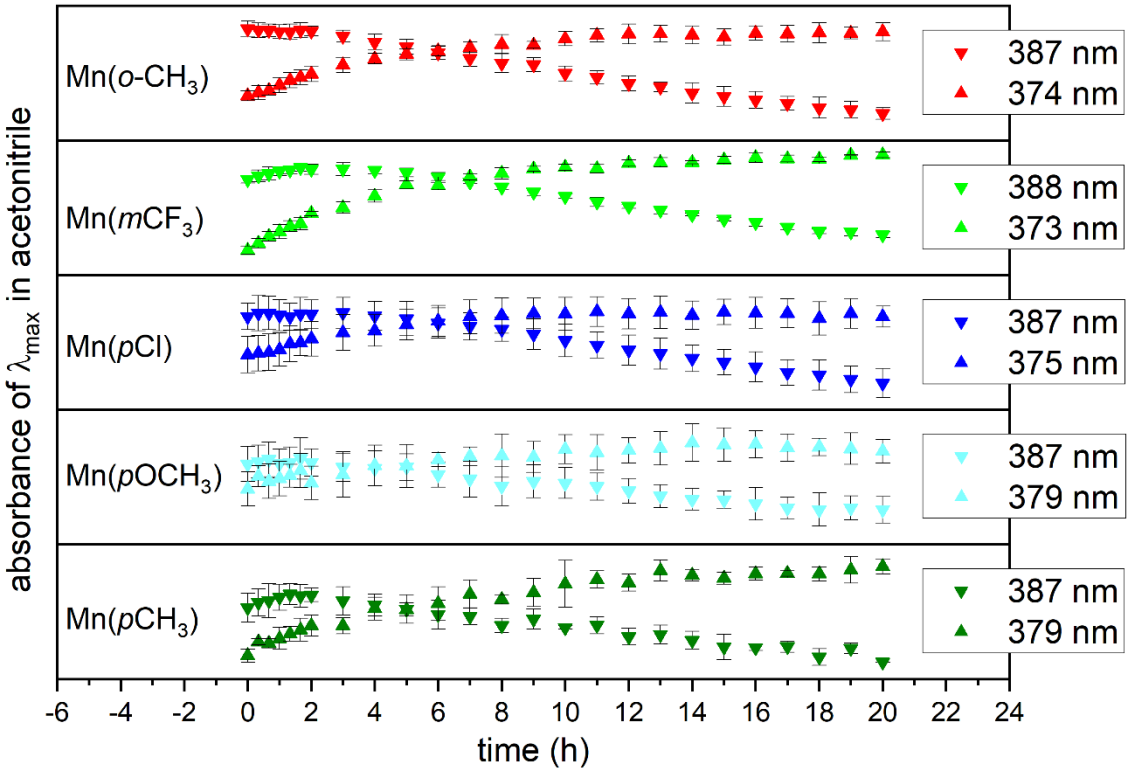

Figure S 54. Variation in the absorption of MLCT in CH_3CN solution over a period of 20 hours.

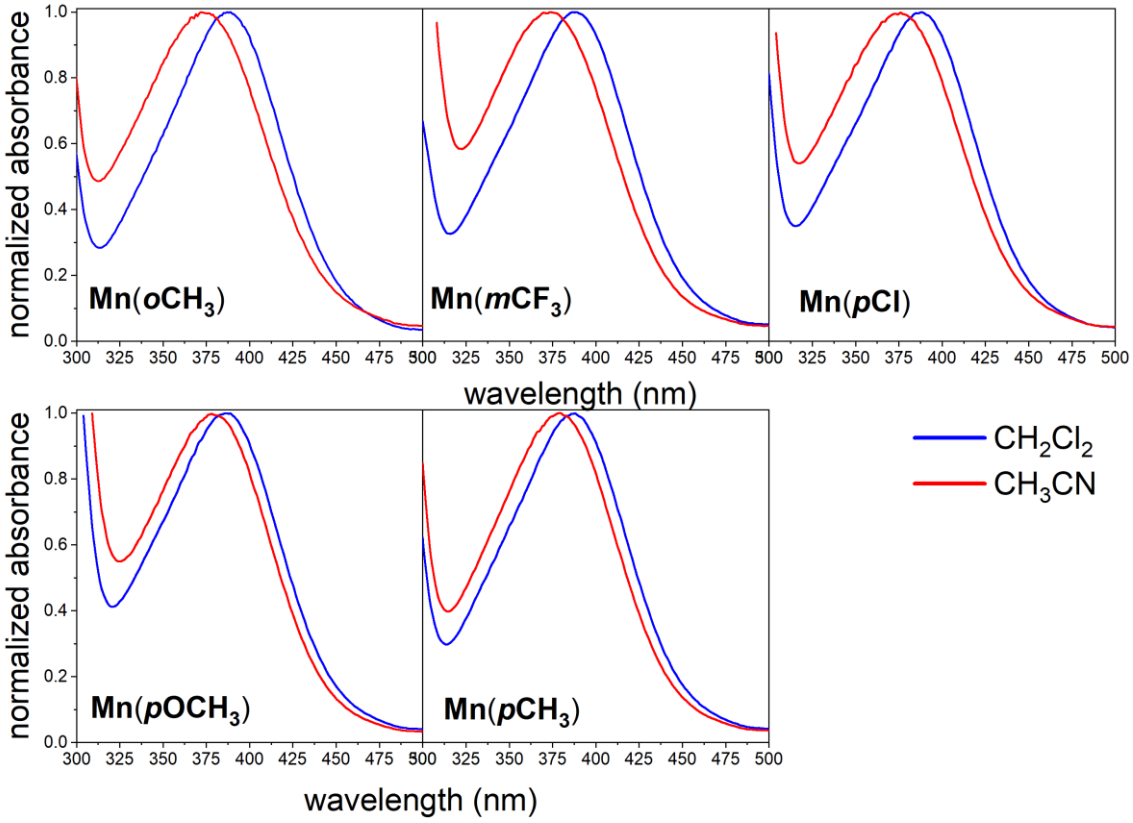

Figure S 55. Electronic spectra of the five compounds after 20 hours of incubation in CH_2Cl_2 and CH_3CN.

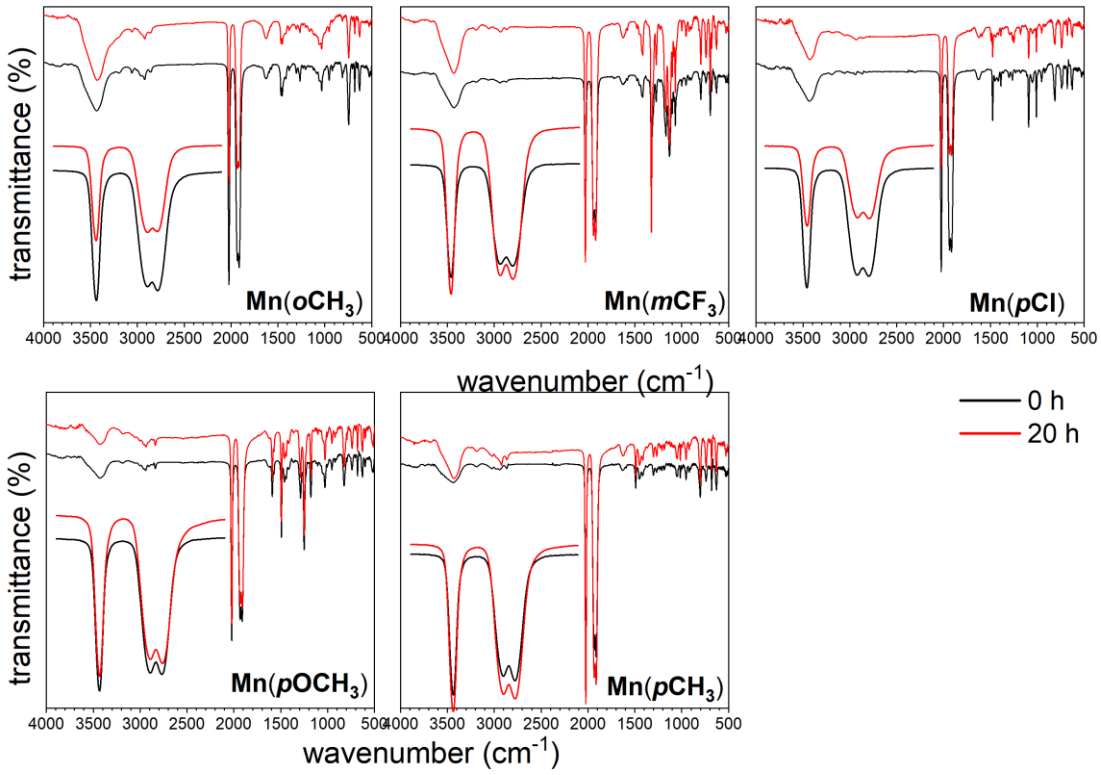

Figure S 56. Infrared spectra (KBr) of the five compounds after 20 hours of incubation in CH_2Cl_2.

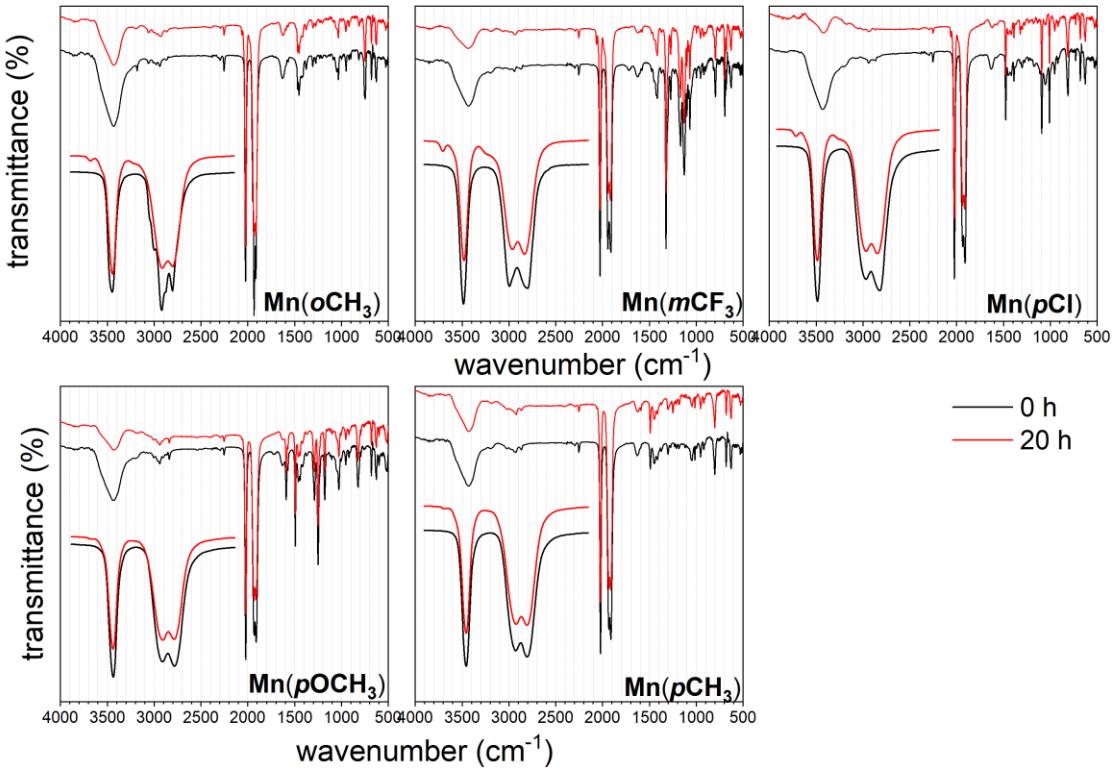

Figure S 57. Infrared spectra (KBr) of the five compounds after 20 hours of incubation in CH_3CN.

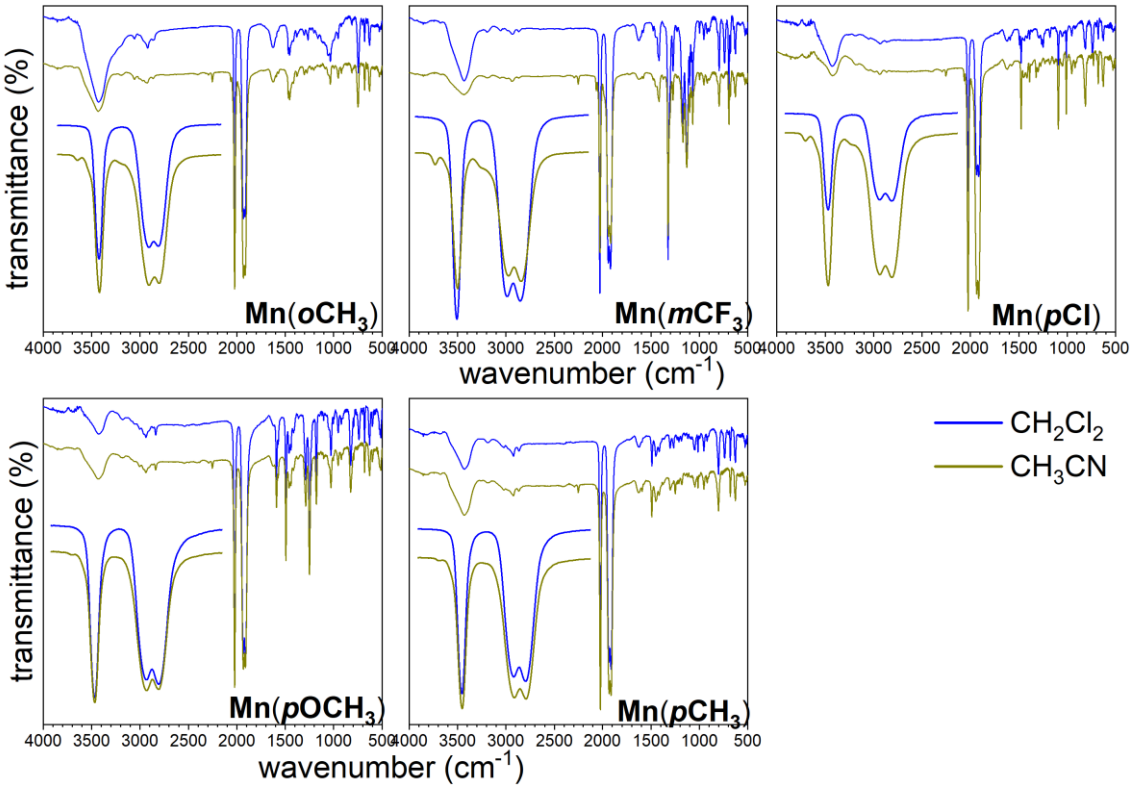

Figure S 58. Comparative infrared spectrum (KBr) of the five compounds after 20 hours of incubation in CH_2Cl_2 and CH_3CN.

Table S 15. Change in Gibbs free energy (kcal mol^{-1}) for the three reactions shown in Scheme S1.

L	$\Delta G_{dir,1}$	$\Delta G_{rev,1}$	$\Delta G_{dir,2}$	$\Delta G_{rev,2}$	$\Delta G_{dir,3}$	$\Delta G_{rev,}$
(*o*CH$_3$)	98	-98	11	-11	109	-109
(*m*CF$_3$)	104	-104	3	-3	107	-107
(*p*Cl)	102	-102	3	-3	105	-105
(*p*OCH$_3$)	97	-97	1	-1	98	-98
(*p*CH$_3$)	99	-99	2	-2	101	-101

Table S 16. Stretching frequencies for CO and CN of [Mn(κ²-L)(CO)$_3$Br], [Mn(κ²-L)(CO)$_3$(CH$_3$CN)]$^+$ and [Mn(κ³-L)(CO)$_3$]$^+$ at level B3LYP/ZORA-def2-TZVPP/SARC-J/D3BJ in Orca 5.0.3 Software. Vibrational scaling factor: 0.957 ± 0.007.

L	[Mn(κ²-L)(CO)$_3$Br]			[Mn(κ²-L)(CO)$_3$(CH$_3$CN)]$^+$				[Mn(κ³-L)(CO)$_3$]$^+$		
	νCO			νCO			νCN	νCO		
(*o*CH$_3$)	2006	1947	1918	2034	1974	1972	2282	2024	1969	1961
(*m*CF$_3$)	2009	1950	1922	2036	1978	1975	2281	2030	1973	1968
(*p*Cl)	2008	1950	1920	2034	1973	1971	2281	2028	1972	1967
(*p*OCH$_3$)	2008	1952	1907	2035	1977	1966	2284	2025	1968	1962
(*p*CH$_3$)	2005	1946	1917	2033	1973	1970	2283	2026	1969	1964

Table S 17. Calculated absorption spectrum of [Mn(κ²-L)(CO)$_3$Br], [Mn(κ²-L)(CO)$_3$(CH$_3$CN)]$^+$ and [Mn(κ³-L)(CO)$_3$]$^+$ at level B3LYP/ZORA-def2-TZVPP/SARC-J/D3BJ in Orca 5.0.3 Software.

L	[Mn(κ²-L)(CO)$_3$Br]			[Mn(κ²-L)(CO)$_3$(CH$_3$CN)]$^+$			[Mn(κ³-L)(CO)$_3$]$^+$		
	State	Energy (nm)	$f_{oscillator}$	State	Energy (nm)	$f_{oscillator}$	State	Energy (nm)	$f_{oscillator}$
(*o*CH$_3$)	S_2	390	0.01847	S_2	383	0.01742	S_2	376	0.01983
	S_3	376	0.01314	S_3	370	0.00740	S_3	374	0.01883
(*m*CF$_3$)	S_2	392	0.01698	S_2	382	0.01512	S_2	383	0.02223
	S_3	377	0.01120	S_3	372	0.00817	S_3	377	0.00727
(*p*Cl)	S_2	392	0.01661	S_2	381	0.01504	S_2	382	0.02258
	S_3	376	0.01175	S_3	370	0.00941	S_3	377	0.00720
(*p*OCH$_3$)	S_2	390	0.02099	S_2	378	0.01408	S_2	379	0.02201
	S_3	371	0.01453	S_3	368	0.01119	S_3	375	0.00699
(*p*CH$_3$)	S_2	391	0.01786	S_2	380	0.01481	S_2	380	0.02232
	S_3	376	0.01182	S_3	370	0.00936	S_3	376	0.00704

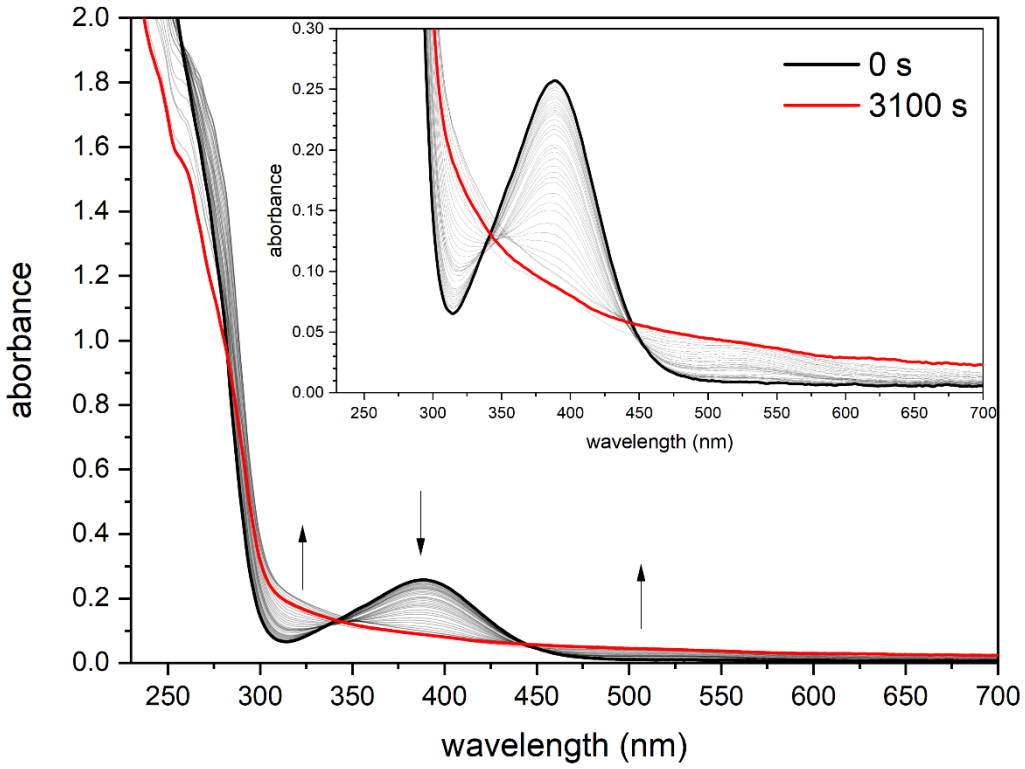

Figure S 59. Variation in the electronic spectrum in CH_2Cl_2 using violet LEDs (395 ± 5nm) for $Mn(oCH_3)$.

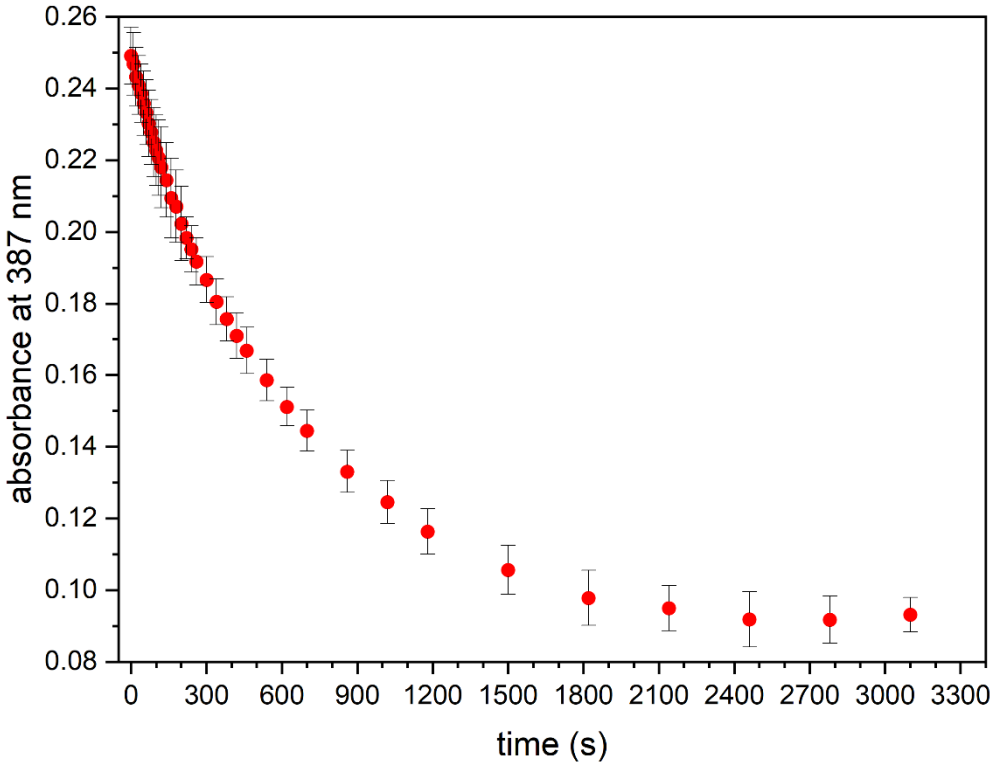

Figure S 60. Variation in absorption at the maximum MLCT wavelength for $Mn(oCH_3)$.

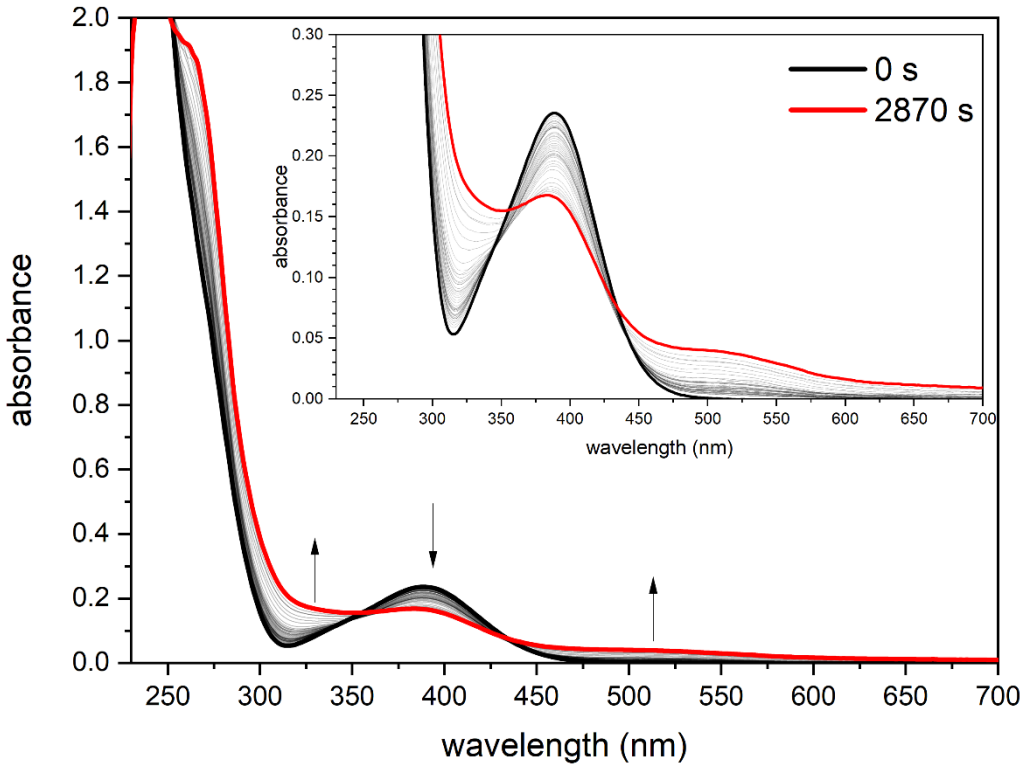

Figure S 61. Variation in the electronic spectrum in CH_2Cl_2 using violet LEDs (395 ± 5nm) for $Mn(mCF_3)$.

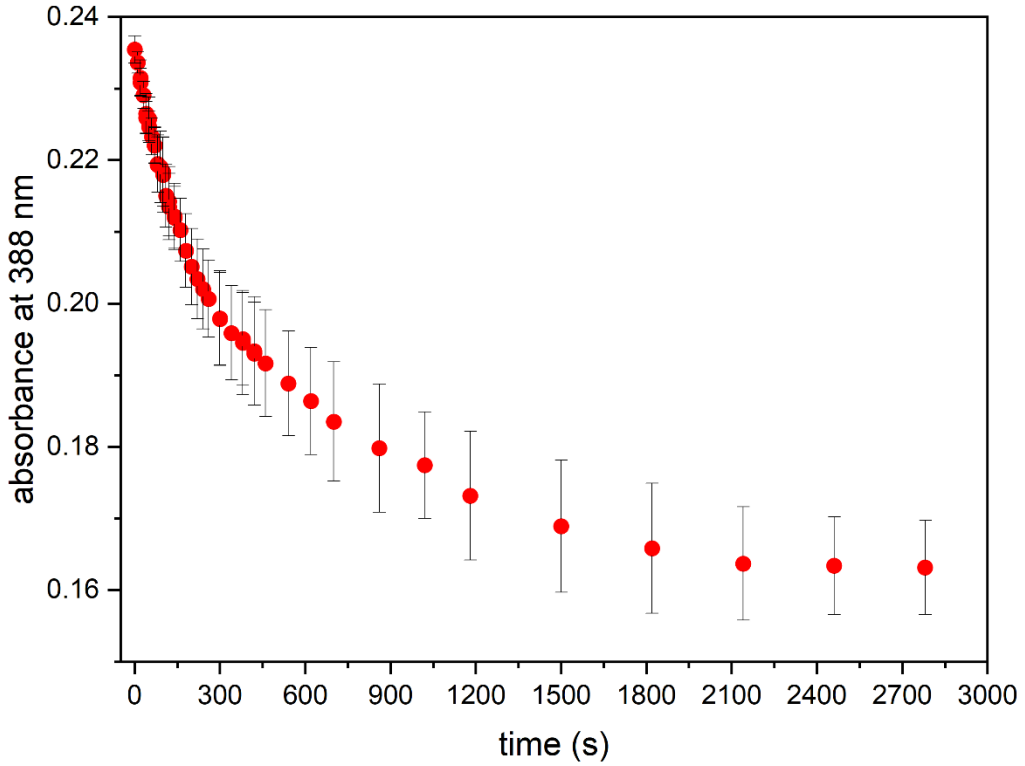

Figure S 62. Variation in absorption at the maximum MLCT wavelength for $Mn(mCF_3)$.

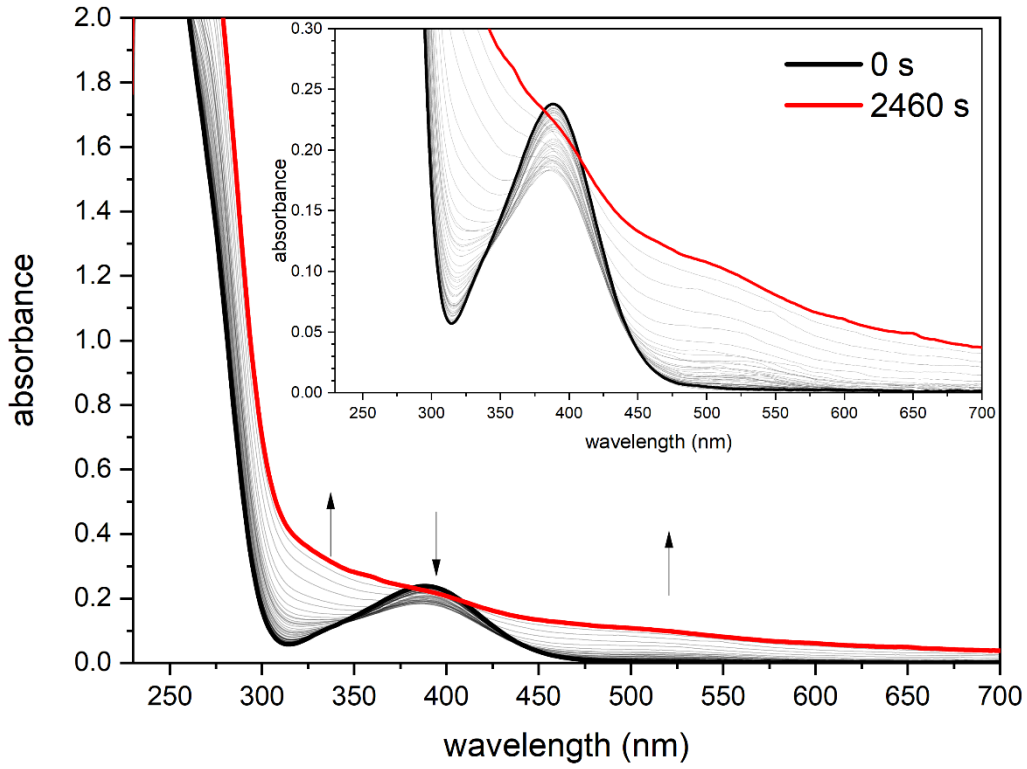

Figure S 63. Variation in the electronic spectrum in CH_2Cl_2 using violet LEDs (395 ± 5nm) for Mn(pCl).

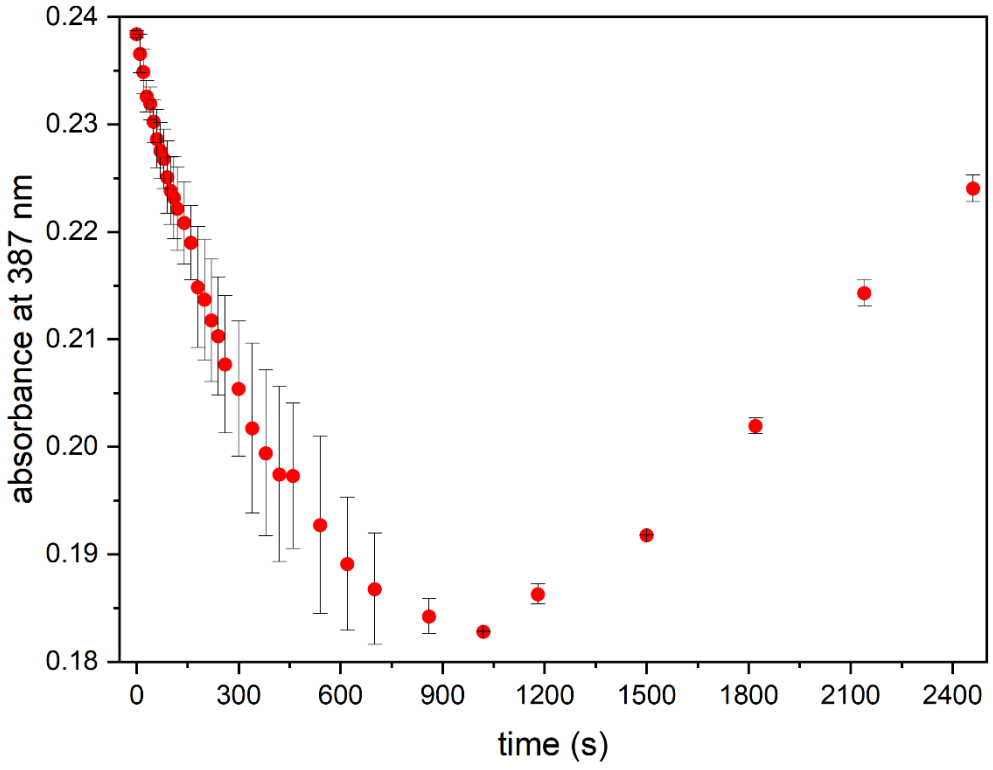

Figure S 64. Variation in absorption at the maximum MLCT wavelength for Mn(pCl).

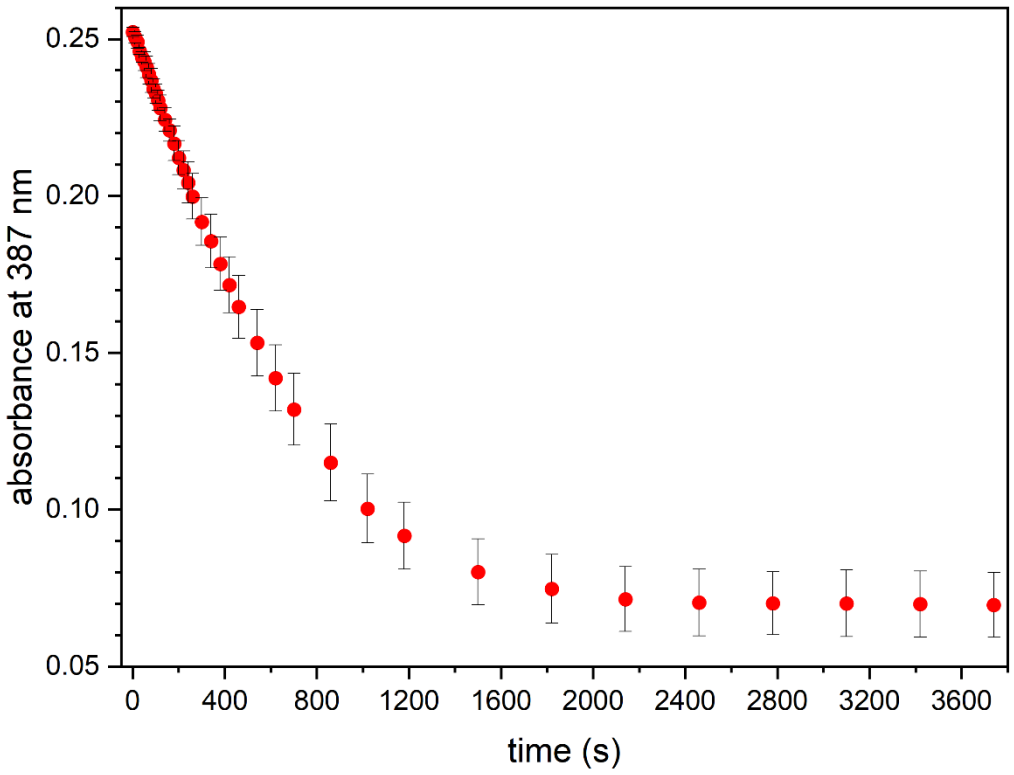

Figure S 65 Variation in absorption at the maximum MLCT wavelength for Mn(pOCH₃).

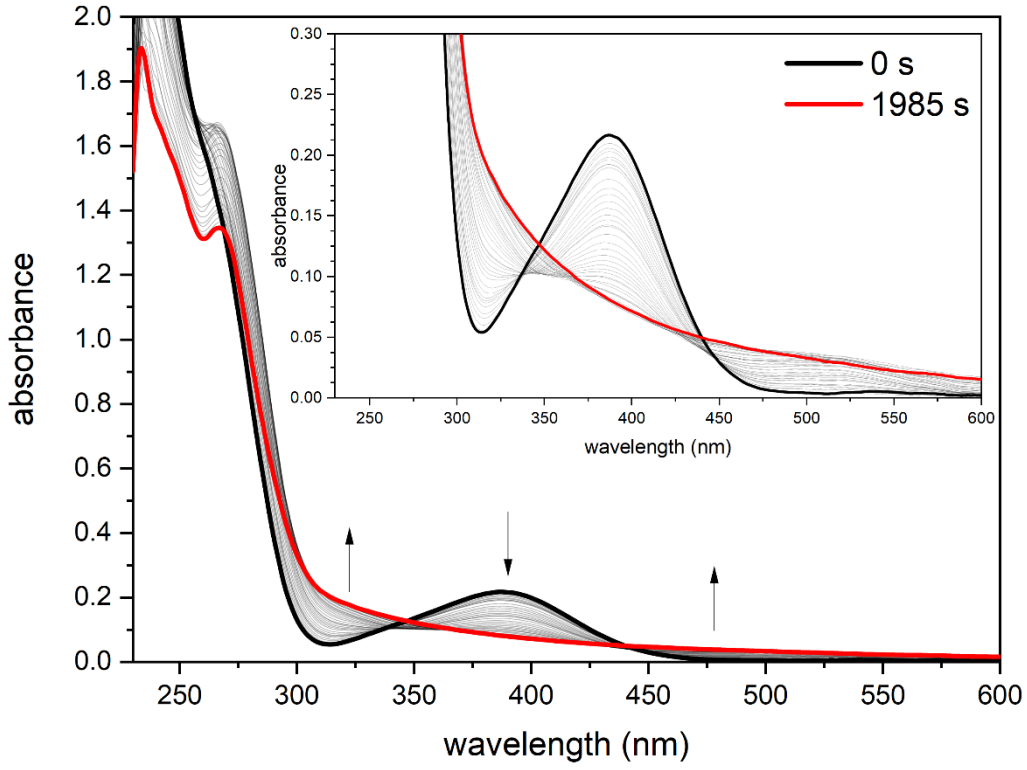

Figure S 66. Variation in the electronic spectrum in CH_2Cl_2 using violet LEDs (395 ± 5nm) for Mn(pCH₃).

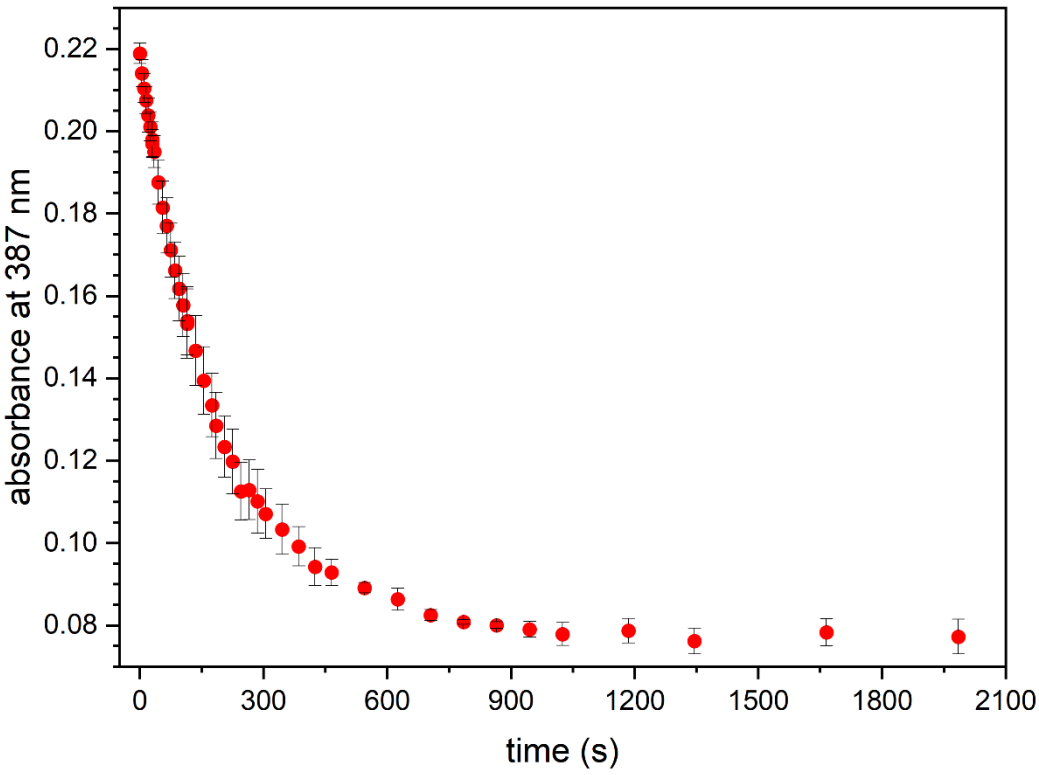

Figure S 67. Variation in absorption at the maximum MLCT wavelength for Mn(pCH₃).

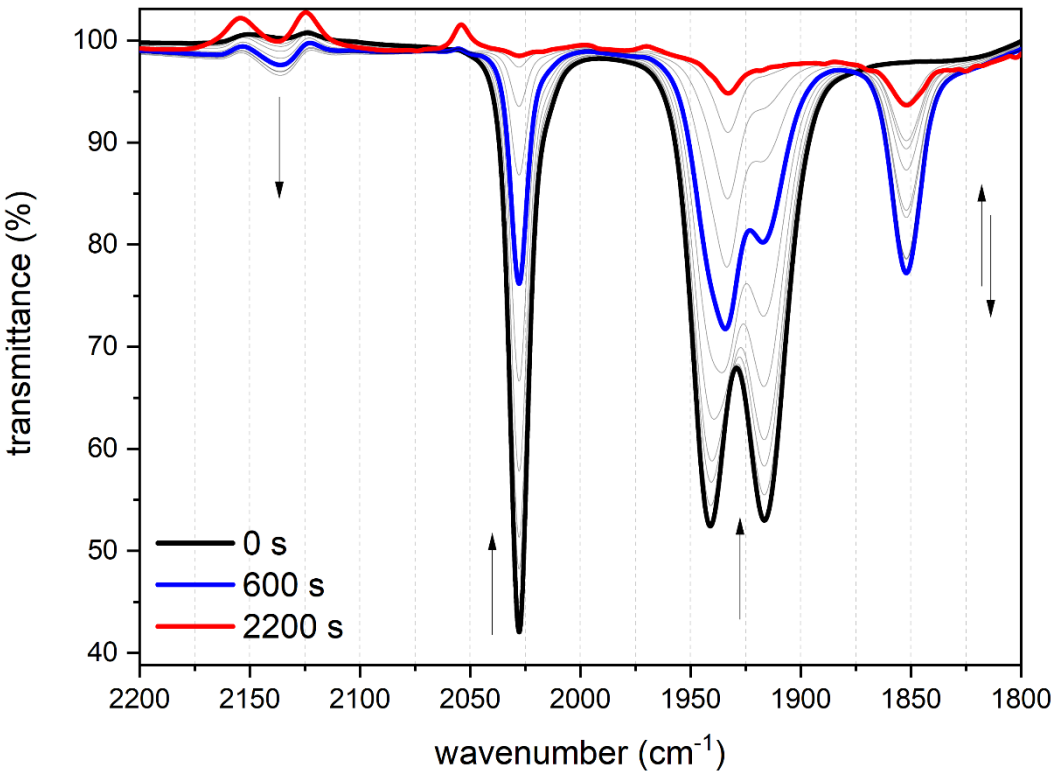

Figure S 68. Photorelease using violet LEDs (395 ± 5 nm) in CH_2Cl_2 following the variation in the region related to carbonyl stretching in the infrared for Mn(oCH₃).

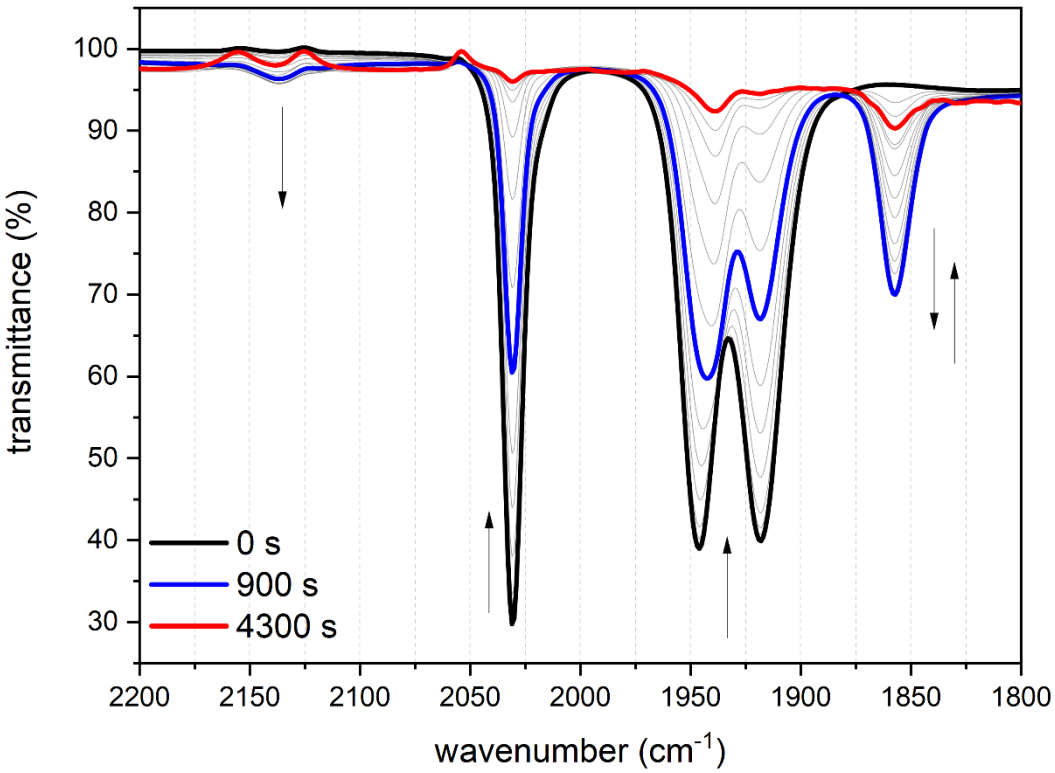

Figure S 69. Photorelease using violet LEDs (395 ± 5 nm) in CH_2Cl_2 following the variation in the region related to carbonyl stretching in the infrared for Mn(mCF_3).

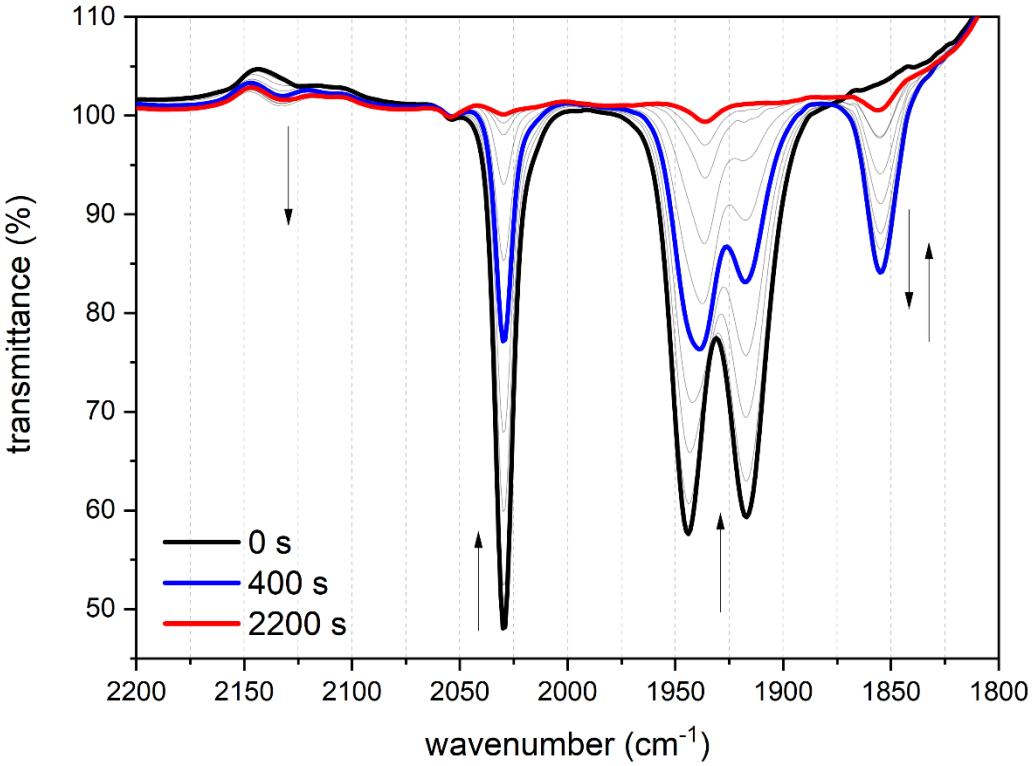

Figure S 70. Photorelease using violet LEDs (395 ± 5 nm) in CH_2Cl_2 following the variation in the region related to carbonyl stretching in the infrared for Mn(pCl).

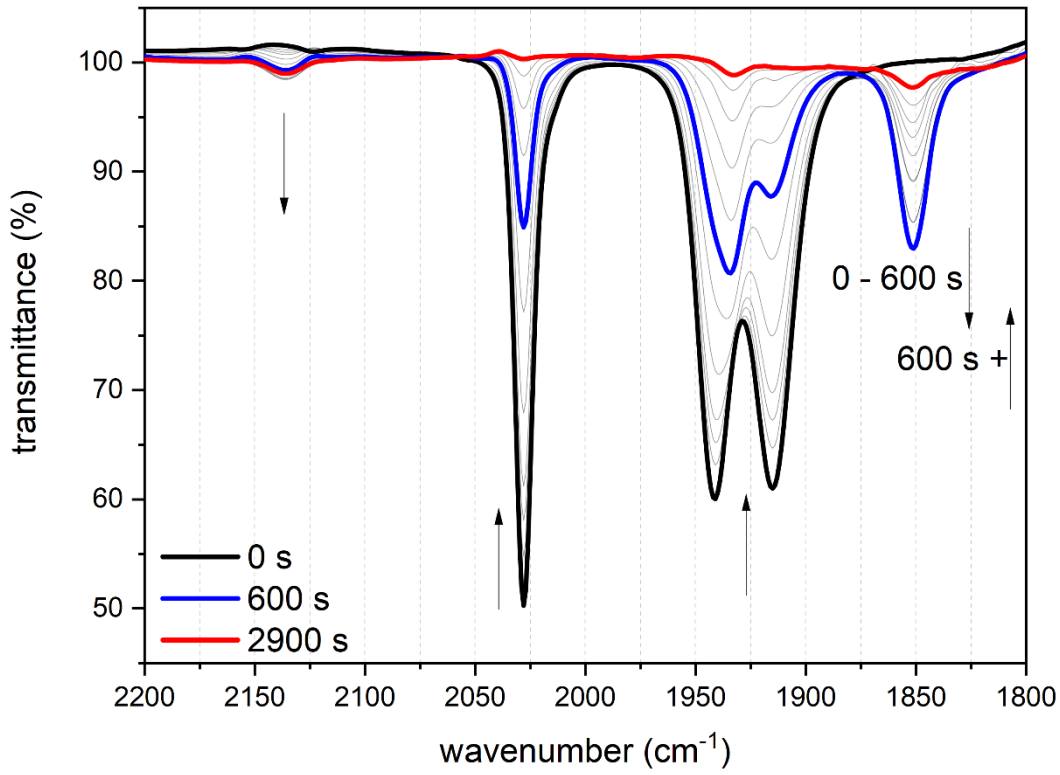

Figure S 71. Photorelease using violet LEDs (395 ± 5 nm) in CH_2Cl_2 following the variation in the region related to carbonyl stretching in the infrared for Mn(pCH_3).

Table S 18. Main bond lengths and angles for the S_0, S_1 and S_2 states of MCCs.

	Mn(*o*CH_3)			**Mn(*m*CF_3)**			**Mn(*p*Cl)**		
	Bond length (Å)								
	S_0	S_1	S_2	S_0	S_1	S_2	S_0	S_1	S_2
Mn1-C1	1.808	1.911	1.842	1.810	1.903	1.822	1,809	1,905	1,823
Mn1-C2	1.807	1.816	1.861	1.809	1.820	1.869	1,808	1,820	1,869
Mn1-C3	1.790	1.856	1.924	1.792	1.854	1.971	1,792	1,853	1,971
Mn1-Se1	2.556	3.137	2.600	2.544	3.211	2.665	2,538	3,213	2,662
Mn1-Br1	2.566	2.525	2.835	2.568	2.510	2.649	2,568	2,507	2,653
Mn1-N1	2.225	2.123	2.171	2.229	2.124	2.150	2,232	2,124	2,153
C1-O1	1.144	1.140	1.142	1.143	1.140	1.144	1,144	1,140	1,144
C2-O2	1.144	1.144	1.140	1.144	1.143	1.139	1,143	1,143	1,139
C3-O3	1.150	1.144	1.142	1.149	1.144	1.147	1,149	1,144	1,147
	angle (°)								
Mn1-C1-O1	178.34	168.82	178.53	179.00	170.93	178.72	178,97	170,83	178,72
Mn1-C2-O2	179.37	178.61	178.22	179.69	179.33	176.50	179,41	178,90	176,58
Mn1-C3-O3	179.84	174.86	168.00	179.52	174.68	153.31	178,91	174,89	153,25
N1-Mn1-Se1	84.26	80.38	84.94	84.00	79.25	84.74	84,29	79,32	84,88
Se1-Mn1-C1	171.50	169.59	162.03	170.75	169.02	168.26	170,18	169,26	168,56
N1-Mn1-C2	172.20	172.48	161.60	173.34	173.43	170.69	173,86	144,68	170,39
Br1-Mn1-C3	175.87	148.32	167.97	175.29	144.17	170.44	175,16	172,70	169,41

	Mn(*p*OCH_3)			**Mn(*p*CH_3)**		
	Bond length (Å)					
	S_0	S_1	S_2	S_0	S_1	S_2
Mn1-C1	1,808	1,888	1,850	1,808	1,903	1,824
Mn1-C2	1,811	1,825	1,859	1,806	1,817	1,867
Mn1-C3	1,785	1,841	1,924	1,790	1,854	1,972
Mn1-Se1	2,537	3,392	2,557	2,542	3,181	2,665
Mn1-Br1	2,572	2,479	2,865	2,563	2,513	2,646
Mn1-N1	2,230	2,119	2,173	2,232	2,126	2,156
C1-O1	1,144	1,142	1,142	1,144	1,141	1,145
C2-O2	1,143	1,142	1,140	1,144	1,144	1,140
C3-O3	1,152	1,147	1,143	1,150	1,145	1,48
	angle (°)					
Mn1-C1-O1	178,66	169,86	177,85	178,54	171,53	179,34
Mn1-C2-O2	179,90	179,67	177,05	179,29	178,76	176,34
Mn1-C3-O3	177,02	173,47	165,08	178,75	174,67	152,73
N1-Mn1-Se1	84,09	77,39	84,87	84,17	79,59	84,74
Se1-Mn1-C1	167,28	171,76	158,01	169,72	166,70	167,38
N1-Mn1-C2	172,90	173,82	162,89	173,30	173,63	170,38
Br1-Mn1-C3	178,88	141,08	172,07	176,51	144,63	171,05

Table S 19. Generalized Kohn-Sham energy decomposition analysis in kcal mol^{-1}. C1O1 is trans to selenium, C2O2 is trans to nitrogen, and C3O3 is trans to bromide. In parenthesis is the percentage of attractive interactions[a]. Data referring to the structure of the S_1 state.

bond	ΔE^{TOT}	ΔE^{elstat}	ΔE^{exch}	ΔE^{rep}	ΔE^{pol}	ΔE^{disp}	ΔE^{corr}	$\Delta E^{Pauli\ [b]}$	$\Delta E^{orb\ [c]}$
				Mn(*o*CH$_3$)					
Mn1-C1O1	-44.14	-81.23 (27.8%)	-124.16 (42.5%)	247.75	-33.50 (11.5%)	-7.57 (2.6%)	-45.43 (15.6%)	123.59	-86.50
Mn1-C2O2	-43.34	-104.96 (28.3%)	-163.00 (43.9%)	328.15	-52.34 (14.1%)	-6.23 (1.7%)	-44.96 (12.1%)	165.15	-103.53
Mn1-C3O3	-40.45	-101.93 (28.6%)	-154.74 (43.4%)	315.88	-46.67 (13.1%)	-8.33 (2.3%)	-44.67 (12.5%)	161.14	-99.67
Mn1-Br1	-130.04	-165.79 (42.6%)	-143.50 (36.9%)	258.82	-48.93 (12.6%)	-10.00 (2.6%)	-20.65 (5.3%)	115.32	-79.58
Mn1-k^{2}L	-59.50	-92.25 (29.0%)	-139.63 (44.0%)	258.12	-40.40 (12.7%)	-25.58 (8.1%)	-19.76 (6.2%)	118.49	-85.74
				Mn(*m*CF$_3$)					
Mn1-C1O1	-42.46	-89.28 (28.1%)	-135.68 (42.7%)	275.45	-39.47 (12.4%)	-7.49 (2.4%)	-45.98 (14.5%)	139.77	-92.94
Mn1-C2O2	-42.03	-105.15 (28.3%)	-163.87 (44.0%)	330.16	-52.40 (14.1%)	-5.77 (1.6%)	-45.00 (12.1%)	166.29	-103.17
Mn1-C3O3	-37.47	-105.16 (28.9%)	-158.02 (43.5%)	325.85	-48.07 (13.2%)	-7.79 (2.1%)	-44.27 (12.2%)	167.83	-100.13
Mn1-Br1	-137.47	-176.40 (43.5%)	-147.49 (36.4%)	267.99	-51.59 (12.7%)	-9.93 (2.4%)	-20.05 (4.9%)	120.50	-81.57
Mn1-k^{2}L	-56.34	-89.12 (29.4%)	-133.07 (43.9%)	246.82	-39.14 (12.9%)	-23.89 (7.9%)	-17.95 (5.9%)	113.75	-80.98
				Mn(*p*Cl)					
Mn1-C1O1	-42.83	-87.27 (28.0%)	-132.82 (42.7%)	268.54	-37.61 (12.1%)	-7.64 (2.5%)	-46.03 (14.8%)	135.72	-91.28
Mn1-C2O2	-42.30	-104.75 (28.3%)	-162.99 (44.0%)	328.35	-52.03 (14.0%)	-5.79 (1.6%)	-45.08 (12.2%)	165.36	-102.90
Mn1-C3O3	-37.77	-105.22 (28.9%)	-158.32 (43.5%)	326.20	-48.02 (13.2%)	-7.81 (2.1%)	-44.60 (12.3%)	167.88	-100.43
Mn1-Br1	-134.67	-174.05 (42.9%)	-149.32 (36.8%)	270.87	-52.55 (13.0%)	-10.06 (2.5%)	-19.57 (4.8%)	121.55	-82.18
Mn1-k^{2}L	-56.63	-89.66 (29.2%)	-134.96 (44.0%)	250.00	-38.92 (12.7%)	-24.25 (7.9%)	-18.84 (6.1%)	115.04	-82.01
				Mn(*p*OCH$_3$)					
Mn1-C1O1	-41.55	-96.64 (28.2%)	-147.27 (42.9%)	301.64	-44.75 (13.0%)	-7.83 (2.3%)	-46.69 (13.6%)	154.37	-99.27
Mn1-C2O2	-40.18	-107.03 (28.2%)	-168.81 (44.4%)	339.99	-54.29 (14.3%)	-5.62 (1.5%)	-44.42 (11.7%)	171.18	-104.33
Mn1-C3O3	-36.94	-111.35 (29.1%)	-166.72 (43.5%)	346.14	-52.90 (13.8%)	-7.20 (1.9%)	-44.90 (11.7%)	179.42	-105.00
Mn1-Br1	-130.78	-172.20 (42.3%)	-150.92 (37.0%)	276.74	-54.82 (13.5%)	-9.82 (2.4%)	-19.76 (4.8%)	125.82	-84.40
Mn1-k^{2}L	-54.46	-88.31 (30.0%)	-129.15 (43.9%)	239.53	-35.09 (11.9%)	-23.04 (7.8%)	-18.40 (6.3%)	110.38	-76.53
				Mn(*p*CH$_3$)					
Mn1-C1O1	-42.85	-89.43 (28.2%)	-135.59 (42.7%)	274.69	-38.67 (12.2%)	-7.58 (2.4%)	-46.28 (14.6%)	139.10	-92.53
Mn1-C2O2	-42.55	-106.02 (28.3%)	-165.05 (44.0%)	332.62	-52.98 (14.1%)	-5.80 (1.5%)	-45.32 (12.1%)	167.57	-104.10
Mn1-C3O3	-36.95	-106.07 (28.9%)	-159.92 (43.6%)	329.85	-48.23 (13.1%)	-7.80 (2.1%)	-44.78 (12.2%)	169.93	-100.81
Mn1-Br1	-129.87	-168.25 (42.3%)	-147.68 (37.2%)	267.51	-51.53 (13.0%)	-9.95 (2.5%)	-19.97 (5.0%)	119.83	-81.45
Mn1-k^{2}L	-58.74	-91.00 (29.4%)	-135.52 (43.8%)	250.80	-39.43 (12.7%)	-24.01 (7.8%)	-19.57 (6.3%)	115.28	-83.01

[a] = $\Delta E^{elstat} + \Delta E^{exch} + \Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$; [b] = $\Delta E^{exch} + \Delta E^{rep}$; [c] = $\Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$

Table S 20. Generalized Kohn-Sham energy decomposition analysis in kcal mol^{-1}. C1O1 is trans to selenium, C2O2 is trans to nitrogen, and C3O3 is trans to bromide. In parenthesis is the percentage of attractive interactions[a]. Data referring to the structure of the S_2 state.

bond	ΔE^{TOT}	ΔE^{elstat}	ΔE^{exch}	ΔE^{rep}	ΔE^{pol}	ΔE^{disp}	ΔE^{corr}	$\Delta E^{Pauli\ [b]}$	$\Delta E^{orb\ [c]}$
				Mn(*o*CH$_3$)					
Mn1-C1O1	-46.27	-90.26 (28.4%)	-135.65 (42.6%)	272.04	-41.74 (13.1%)	-7.79 (2.4%)	-42.86 (13.5%)	136.39	-92.39
Mn1-C2O2	-44.83	-87.84 (28.4%)	-133.43 (43.1%)	264.55	-38.87 (12.6%)	-6.78 (2.2%)	-42.47 (13.7%)	131.12	-88.12
Mn1-C3O3	-48.57	-66.77 (27.6%)	-100.18 (414%)	193.45	-25.75 (10.6%)	-7.68 (3.2%)	-41.64 (17.2%)	93.27	-75.07
Mn1-Br1	-129.13	-139.88 (44.1%)	-108.77 (34.3%)	187.87	-35.63 (11.2%)	-9.89 (3.1%)	-22.82 (7.2%)	79.10	-68.34
Mn1-k^{2}L	-77.33	-109.26 (28.6%)	-165.52 (43.3%)	304.65	-54.39 (14.2%)	-26.96 (7.1%)	-25.85 (6.8%)	139.13	-107.20
				Mn(*m*CF$_3$)					
Mn1-C1O1	-49.06	-93.60 (28.2%)	-140.98 (42.5%)	282.96	-44.40 (13.4%)	-8.05 (2.4%)	-44.98 (13.5%)	141.98	-97.43
Mn1-C2O2	-45.18	-84.11 (28.3%)	-127.60 (43.0%)	251.80	-38.41 (12.9%)	-6.18 (2.1%)	-40.68 (13.7%)	124.20	-85.27
Mn1-C3O3	-41.51	-55.76 (25.7%)	-93.54 (43.1%)	175.64	-21.73 (10.0%)	-7.68 (3.5%)	-38.44 (17.7%)	82.10	-67.85
Mn1-Br1	-137.69	-157.50 (44.6%)	-122.44 (34.7%)	215.54	-39.28 (11.1%)	-9.92 (2.8%)	-24.09 (6.8%)	93.10	-73.29
Mn1-k^{2}L	-70.19	-106.61 (28.7%)	-163.02 (43.9%)	300.75	-51.75 (14.0%)	-26.04 (7.0%)	-23.53 (6.3%)	137.73	-101.32
				Mn(*p*Cl)					
Mn1-C1O1	-49.30	-93.28 (28.2%)	-140.40 (42.4%)	281.59	-44.20 (13.4%)	-8.05 (2.4%)	-44.96 (13.6%)	141.19	-97.21
Mn1-C2O2	-45.31	-84.01 (28.3%)	-127.35 (42.9%)	251.27	-38.24 (12.9%)	-6.18 (2.1%)	-40.80 (13.8%)	123.92	-85.22
Mn1-C3O3	-41.40	-55.85 (25.6%)	-94.01 (43.2%)	176.39	-21.71 (10.0%)	-7.71 (3.5%)	-38.52 (17.7%)	82.38	-67.94
Mn1-Br1	-134.95	-154.45 (44.2%)	-121.69 (34.8%)	214.26	-39.26 (11.2%)	-9.79 (2.8%)	-24.01 (6.9%)	92.57	-73.06
Mn1-k^{2}L	-70.46	-107.69 (28.7%)	-165.00 (44.0%)	304.27	-51.81 (13.8%)	-25.96 (6.9%)	-24.27 (6.5%)	139.27	-102.04
				Mn(*p*OCH$_3$)					
Mn1-C1O1	-45.71	-88.54 (28.3%)	-133.59 (42.7%)	266.93	-41.11 (13.1%)	-7.89 (2.5%)	-41.52 (13.3%)	133.34	-90.52
Mn1-C2O2	-45.49	-86.20 (28.7%)	-128.12 (42.6%)	255.25	-38.24 (12.7%)	-5.95 (2.0%)	-42.24 (14.0%)	127.13	-86.43
Mn1-C3O3	-49.46	-65.46 (27.3%)	-99.12 (41.3%)	190.37	-25.51 (10.6%)	-6.86 (2.9%)	-42.88 (17.9%)	91.25	-75.25
Mn1-Br1	-125.91	-136.14 (43.5%)	-108.20 (34.6%)	186.88	-37.01 (11.8%)	-9.80 (3.1%)	-21.64 (6.9%)	78.68	-68.45
Mn1-k^{2}L	-78.40	-115.16 (29.2%)	-170.83 (43.3%)	316.49	-55.74 (14.1%)	-24.67 (6.2%)	-28.49 (7.2%)	145.66	-108.90
				Mn(*p*CH$_3$)					
Mn1-C1O1	-49.61	-93.50 (28.2%)	-140.42 (42.4%)	281.41	-44.48 (13.4%)	-8.10 (2.4%)	-44.51 (13.4%)	140.99	-97.09
Mn1-C2O2	-45.29	-84.92 (28.3%)	-129.03 (43.0%)	254.62	-38.87 (13.0%)	-6.18 (2.1%)	-40.92 (13.6%)	125.59	-85.97
Mn1-C3O3	-41.34	-55.36 (25.6%)	-93.34 (43.1%)	175.02	-21.58 (10.0%)	-7.58 (3.5%)	-38.50 (17.8%)	81.68	-67.66
Mn1-Br1	-129.97	-150.10 (43.3%)	-123.40 (35.6%)	216.93	-38.82 (11.2%)	-9.98 (2.9%)	-24.61 (7.1%)	93.53	-73.41
Mn1-k^{2}L	-72.00	-107.21 (28.9%)	-162.29 (43.8%)	298.70	-51.15 (13.8%)	-25.95 (7.0%)	-24.11 (6.5%)	136.41	-101.21

[a] = $\Delta E^{elstat} + \Delta E^{exch} + \Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$; [b] = $\Delta E^{exch} + \Delta E^{rep}$; [c] = $\Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$

Table S 21. Stretching frequencies for CO of [Mn(κ^3-L)$(CO)_2$Br] at level B3LYP/ZORA-def2-TZVPP/SARC-J/D3BJ in Orca 5.0.3 Software. Vibrational scaling factor: 0.957 ± 0.007.

L	Experimental		*Geometries*							
			a		b		c		d	
(*o*CH_3)	1852	1934	1878	1934	1887	1940	1877	1946	1892	1962
(*m*CF_3)	1857	1942	1886	1943	1895	1946	1878	1949	1897	1970
(*p*Cl)	1855	1939	1884	1941	1893	1944	1876	1945	1894	1964
(*p*OCH_3)	1850	1935	1878	1936	1880	1936	1874	1946	1889	1962
(*p*CH_3)	1851	1934	1879	1937	1888	1940	1874	1943	1891	1962

Table S 22. Calculated absorption spectrum of [Mn(κ^3-L)$(CO)_3$B] at level B3LYP/ZORA-def2-TZVPP/SARC-J/D3BJ in Orca 5.0.3 Software considering dichloromethane as solvent.

L	State	a		b		c		d	
		Energy (nm)	$f_{oscillator}$	Energy (nm)	$f_{oscillator}$	Energy (nm)	$f_{oscillator}$	Energy (nm)	$f_{oscillator}$
(*o*CH_3)	S_1	566	0.00168	576	0.00185	557	0.01940	890	0.00138
	S_2	532	0.00508	527	0.00546	518	0.00252	478	0.00014
	S_3	460	0.00304	416	0.00353	408	0.00205	452	0.00755
	S_4	432	0.00160	389	0.00043	395	0.00494	436	0.00563
	S_5	378	0.01726	380	0.00115	376	0.00051	432	0.00419
(*m*CF_3)	S_1	572	0.00038	585	0.00114	538	0.01497	906	0.00163
	S_2	539	0.00436	544	0.00458	507	0.00158	476	0.00043
	S_3	444	0.00275	418	0.00354	403	0.00096	454	0.00427
	S_4	424	0.00123	395	0.00112	394	0.00559	442	0.00201
	S_5	372	0.01373	386	0.00146	378	0.00270	434	0.00502
(*p*Cl)	S_1	572	0.00038	583	0.00129	536	0.01631	891	0.00134
	S_2	539	0.00438	543	0.00436	506	0.00140	478	0.00033
	S_3	442	0.00269	416	0.00312	401	0.00105	455	0.00346
	S_4	421	0.00141	393	0.00146	394	0.00585	440	0.00758
	S_5	372	0.00819	386	0.00134	377	0.00161	428	0.00417
(*p*OCH_3)	S_1	568	0.00035	578	0.00153	546	0.01646	875	0.00094
	S_2	539	0.00429	538	0.00507	509	0.00476	472	0.00010
	S_3	437	0.00283	412	0.00340	404	0.00193	444	0.00330
	S_4	417	0.00146	388	0.00147	394	0.00456	437	0.00489
	S_5	371	0.00255	382	0.00116	373	0.00155	424	0.00370
(*p*CH_3)	S_1	570	0.00033	580	0.00140	534	0.01636	888	0.00119
	S_2	538	0.00442	540	0.00490	502	0.00166	475	0.00016
	S_3	439	0.00266	412	0.00332	398	0.00137	449	0.00377
	S_4	418	0.00140	389	0.00146	394	0.00556	440	0.00618
	S_5	371	0.00466	383	0.00114	376	0.00158	426	0.00389

Table S 23. Main bond lengths and angles for the S_0, S_1 and S_4 states of biscarbonyl geometries b.

	Mn(*o*CH_3)			**Mn(*m*CF_3)**			**Mn(*p*Cl)**		
	Bond length (Å)								
	S_0	S_1	S_4	S_0	S_1	S_4	S_0	S_1	S_4
Mn-C4	1.783	1.846	1.829	1.785	1.850	1.824	1.786	1.849	1.826
Mn-C5	1.777	1.797	1.834	1.786	1.790	1.827	1.784	1.790	1.846
Mn-Se1	2.564	2.556	2.712	2.533	2.509	2.567	2.533	2.505	2.646
Mn-Se2	2.421	3.273	2.529	2.443	3.276	2.593	2.438	3.259	2.546
Mn-Br	2.555	2.485	2.472	2.558	2.528	2.412	2.557	2.525	2.470
Mn-N	2.210	2.157	2.318	2.215	2.195	2.176	2.216	2.198	2.310
C4-O4	1.153	1.149	1.153	1.153	1.146	1.139	1.153	1.147	1.152
C5-O5	1.153	1.147	1.152	1.151	1.150	1.140	1.151	1.150	1.150
	angle (°)								
Mn-C4-O4	179.10	179.58	169.23	178.00	176.31	179.46	178.13	176.50	171.85
Mn-C5-O5	178.21	172.29	167.51	177.79	178.80	178.32	177.45	178.69	168.08
N-Mn-C4	176.70	176.28	171.21	174.58	152.35	173.34	174.59	151.56	168.92
Se1-Mn-C5	170.01	158.31	172.47	168.16	174.29	174.21	167.67	174.45	170.40
Se2-Mn-Br	166.71	154.27	164.40	165.37	158.75	174.47	166.33	158.71	165.11

	Mn(*p*OCH_3)			**Mn(*p*CH_3)**		
	Bond length (Å)					
	S_0	S_1	S_4	S_0	S_1	S_4
Mn-C4	1.783	1.852	1.826	1.785	1.850	1.825
Mn-C5	1.775	1.783	1.846	1.783	1.788	1.852
Mn-Se1	2.548	2.511	2.653	2.533	2.505	2.654
Mn-Se2	2.433	3.179	2.553	2.440	3.218	2.581
Mn-Br	2.564	2.542	2.480	2.564	2.534	2.477
Mn-N	2.209	2.196	2.313	2.213	2.198	2.313
C4-O4	1.153	1.147	1.153	1.153	1.147	1.154
C5-O5	1.155	1.153	1.152	1.152	1.151	1.150
	angle (°)					
Mn-C4-O4	178.59	175.11	171.75	177.80	176.27	170.92
Mn-C5-O5	177.28	178.36	167.20	177.06	178.69	168.01
N-Mn-C4	175.54	147.92	169.46	174.22	151.34	169.36
Se1-Mn-C5	168.09	172.88	169.81	167.52	174.47	170.04
Se2-Mn-Br	163.59	156.72	166.29	165.67	158.09	168.48

Table S 24. Main bond lengths and angles for the S_0, S_1 and S_4 states of biscarbonyl geometries c.

	Mn(*o*CH_3)			**Mn(*m*CF_3)**			**Mn(*p*Cl)**		
	Bond length (Å)								
	S_0	S_1	S_4	S_0	S_1	S_4	S_0	S_1	S_4
Mn-C6	1.771	1.854	1.794	1.770	1.808	1.791	1.771	1.844	1.767
Mn-C7	1.793	1.800	1.809	1.793	1.832	1.810	1.791	1.807	1.836
Mn-Se1	2.482	2.789	2.511	2.460	2.654	2.476	2.467	2.726	2.620
Mn-Se2	2.484	2.819	2.589	2.466	2.916	2.563	2.460	2.866	2.542
Mn-Br	2.631	2.501	2.467	2.608	2.524	2.469	2.614	2.505	2.512
Mn-N	2.196	2.171	2.184	2.216	2.149	2.204	2.214	2.171	2.141
C6-O6	1.157	1.148	1.165	1.157	1.153	1.165	1.157	1.148	1.167
C7-O7	1.150	1.150	1.159	1.149	1.144	1.156	1.150	1.148	1.152
	angle (°)								
Mn-C6-O6	178.51	174.17	176.30	179.26	176.19	178.91	179.00	174.59	175.34
Mn-C7-O7	178.78	178.95	178.15	179.45	177.66	179.03	179.73	178.09	179.36
Br-Mn-C6	170.58	170.36	172.36	173.54	176.51	177.11	172.37	175.71	173.87
N-Mn-C7	169.60	173.10	172.77	172.66	171.46	174.38	171.84	175.66	174.04
Se1-Mn-Se2	166.75	158.47	168.27	168.04	158.00	161.71	168.04	161.15	171.26

	Mn(*p*OCH_3)			**Mn(*p*CH_3)**		
	Bond length (Å)					
	S_0	S_1	S_4	S_0	S_1	S_4
Mn-C6	1.769	1.848	1.796	1.770	1.846	1.800
Mn-C7	1.793	1.802	1.796	1.791	1.804	1.796
Mn-Se1	2.468	2.722	2.513	2.465	2.713	2.513
Mn-Se2	2.488	2.893	2.591	2.471	2.893	2.581
Mn-Br	2.625	2.501	2.462	2.618	2.502	2.460
Mn-N	2.201	2.167	2.188	2.210	2.170	2.192
C6-O6	1.157	1.149	1.161	1.157	1.148	1.159
C7-O7	1.150	1.149	1.159	1.151	1.149	1.159
	angle (°)					
Mn-C6-O6	178.95	174.39	177.63	179.12	174.52	177.39
Mn-C7-O7	178.81	178.16	179.56	179.46	178.13	179.33
Br-Mn-C6	171.46	176.57	170.81	172.53	176.44	171.77
N-Mn-C7	172.59	175.47	172.76	172.27	175.73	172.77
Se1-Mn-Se2	167.75	160.22	163.34	168.02	160.66	162.86

Table S 25. Generalized Kohn-Sham energy decomposition analysis in kcal mol^{-1}. C4O4 is trans to nitrogen, C5O5 is trans to selenium. In parenthesis is the percentage of attractive interactions[a]. Data referring to the geometries b of the S_0 state.

Bond	ΔE^{TOT}	ΔE^{elstat}	ΔE^{exch}	ΔE^{rep}	ΔE^{pol}	ΔE^{disp}	ΔE^{corr}	$\Delta E^{Pauli\ [b]}$	$\Delta E^{orb\ [c]}$
Structure B: Mn(*o*CH_3)									
Mn-C4O4	-53.65	-109.80 (28.1%)	-166.51 (42.7%)	336.69	-55.34 (14.2%)	-8.10 (2.1%)	-50.59 (13.0%)	170.18	-114.03
Mn-C5O5	-50.52	-113.49 (28.0%)	-176.13 (43.4%)	355.43	-56.69 (14.0%)	-8.68 (2.1%)	-50.97 (12.6%)	179.30	-116.34
Mn-Br	-123.00	-151.94 (43.5%)	-126.32 (36.1%)	226.50	-44.95 (12.9%)	-8.47 (2.4%)	-17.81 (5.1%)	100.18	-71.23
Mn-k^{3}L	-97.81	-138.50 (28.6%)	-207.75 (42.9%)	386.72	-76.40 (15.8%)	-27.08 (5.6%)	-34.81 (7.2%)	178.97	-138.29
Structure B: Mn(*m*CF_3)									
Mn-C4O4	-54.03	-109.44 (28.3%)	-163.65 (42.4%)	332.38	-56.01 (14.5%)	-7.58 (2.0%)	-49.73 (12.9%)	168.73	-113.32
Mn-C5O5	-49.22	-109.93 (28.1%)	-169.68 (43.3%)	342.41	-54.02 (13.8%)	-8.56 (2.2%)	-49.44 (12.6%)	172.73	-112.02
Mn-Br	-128.77	-157.93 (44.2%)	-126.71 (35.5%)	228.32	-44.98 (12.6%)	-8.39 (2.3%)	-19.08 (5.3%)	101.61	-72.45
Mn-k^{3}L	-94.23	-137.82 (28.5%)	-207.97 (43.0%)	388.86	-75.62 (15.7%)	-26.10 (5.4%)	-35.58 (7.4%)	180.89	-137.30
Structure B: Mn(*p*Cl)									
Mn-C4O4	-53.78	-109.36 (28.4%)	-163.21 (42.3%)	331.66	-55.85 (14.5%)	-7.22 (1.9%)	-49.80 (12.9%)	168.45	-112.87
Mn-C5O5	-49.41	-110.61 (28.1%)	-170.74 (43.3%)	344.48	-54.88 (13.9%)	-8.34 (2.1%)	-49.32 (12.5%)	173.74	-112.54
Mn-Br	-126.88	-156.91 (43.8%)	-128.76 (35.9%)	231.68	-46.39 (12.9%)	-8.43 (2.4%)	-18.07 (5.0%)	102.92	-72.89
Mn-k^{3}L	-95.50	-138.82 (28.7%)	-207.40 (42.9%)	387.48	-75.71 (15.7%)	-25.22 (5.2%)	-35.83 (7.4%)	180.08	-136.76
Structure B: Mn(*p*OCH_3)									
Mn-C4O4	-54.17	-109.18 (28.4%)	-162.35 (42.3%)	329.97	-55.14 (14.4%)	-7.28 (1.9%)	-50.20 (13.1%)	167.62	-112.62
Mn-C5O5	-51.02	-113.73 (27.9%)	-176.37 (43.3%)	355.94	-57.71 (14.2%)	-8.13 (2.0%)	-51.01 (12.5%)	179.57	-116.85
Mn-Br	-121.15	-149.65 (43.3%)	-125.17 (36.2%)	224.68	-46.26 (13.4%)	-8.31 (2.4%)	-16.45 (4.8%)	99.51	-71.02
Mn-k^{3}L	-99.27	-141.22 (29.1%)	-207.13 (42.6%)	386.40	-76.31 (15.7%)	-24.94 (5.1%)	-36.09 (7.4%)	179.27	-137.34
Structure B: Mn(*p*CH_3)									
Mn-C4O4	-54.23	-109.59 (28.4%)	-163.31 (42.3%)	331.94	-55.96 (14.5%)	-7.22 (1.9%)	-50.10 (13.0%)	168.63	-113.28
Mn-C5O5	-49.83	-110.70 (28.1%)	-170.51 (43.3%)	344.04	-54.82 (13.9%)	-8.24 (2.1%)	-49.60 (12.6%)	173.53	-112.66
Mn-Br	-121.50	-151.45 (43.2%)	-127.59 (36.4%)	229.05	-45.11 (12.9%)	-8.39 (2.4%)	-18.02 (5.1%)	101.46	-71.52
Mn-k^{3}L	-97.85	-140.57 (28.9%)	-207.75 (42.8%)	387.73	-76.72 (15.8%)	-25.06 (5.2%)	-35.48 (7.3%)	179.98	-137.26

[a] = $\Delta E^{elstat} + \Delta E^{exch} + \Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$; [b] = $\Delta E^{exch} + \Delta E^{rep}$; [c] = $\Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$

Table S 26. Generalized Kohn-Sham energy decomposition analysis in kcal mol^{-1}. C6O6 is trans to bromide, C7O7 is trans to nitrogen. In parenthesis is the percentage of attractive interactions[a]. Data referring to the geometries c of the S_0 state.

Bond	ΔE^{TOT}	ΔE^{elstat}	ΔE^{exch}	ΔE^{rep}	ΔE^{pol}	ΔE^{disp}	ΔE^{corr}	$\Delta E^{Pauli\ [b]}$	$\Delta E^{orb\ [c]}$
Structure C: Mn(*o*CH$_3$)									
Mn-C6O6	-56.92	-113.91 (27.6%)	-177.42 (43.0%)	356.06	-56.32 (13.6%)	-9.48 (2.3%)	-55.85 (13.5%)	178.64	-121.65
Mn-C7O7	-50.58	-103.91 (28.3%)	-156.52 (42.7%)	316.17	-47.84 (13.0%)	-7.29 (2.0%)	-51.19 (14.0%)	159.65	-106.32
Mn-Br	-124.21	-154.29 (43.0%)	-133.06 (37.1%)	234.76	-42.42 (11.8%)	-9.66 (2.7%)	-19.54 (5.4%)	101.70	-71.62
Mn-k^{3}L	-101.79	-156.62 (28.0%)	-244.32 (43.6%)	458.27	-71.91 (12.8%)	-29.48 (5.3%)	-57.73 (10.3%)	213.95	-159.12
Structure C: Mn(*m*CF$_3$)									
Mn-C6O6	-57.40	-112.50 (27.6%)	-174.41 (42.8%)	350.18	-56.61 (13.9%)	-9.41 (2.3%)	-54.65 (13.4%)	175.77	-120.67
Mn-C7O7	-50.89	-104.01 (28.4%)	-155.45 (42.5%)	314.82	-48.30 (13.2%)	-7.05 (1.9%)	-50.89 (13.9%)	159.37	-106.24
Mn-Br	-131.52	-163.11 (43.8%)	-136.01 (36.5%)	240.85	-43.05 (11.6%)	-10.59 (2.8%)	-19.61 (5.3%)	104.84	-73.25
Mn-k^{3}L	-99.81	-153.17 (27.7%)	-241.26 (43.6%)	453.29	-70.82 (12.8%)	-30.02 (5.4%)	-57.83 (10.5%)	212.03	-158.67
Structure C: Mn(*p*Cl)									
Mn-C6O6	-57.02	-112.75 (27.6%)	-175.63 (42.9%)	352.12	-56.14 (13.7%)	-9.44 (2.3%)	-55.17 (13.5%)	176.49	-120.75
Mn-C7O7	-51.65	-103.89 (28.4%)	-154.98 (42.4%)	313.72	-48.75 (13.3%)	-7.12 (1.9%)	-50.63 (13.9%)	158.74	-106.50
Mn-Br	-128.27	-157.93 (43.7%)	-131.55 (36.4%)	232.90	-42.05 (11.6%)	-10.13 (2.8%)	-19.51 (5.4%)	101.35	-71.69
Mn-k^{3}L	-100.15	-155.46 (27.8%)	-243.54 (43.6%)	458.16	-70.85 (12.7%)	-29.65 (5.3%)	-58.82 (10.5%)	214.62	-159.32
Structure C: Mn(*p*OCH$_3$)									
Mn-C6O6	-57.01	-114.81 (27.6%)	-179.39 (43.0%)	359.71	-56.98 (13.7%)	-9.48 (2.3%)	-56.06 (13.5%)	180.32	-122.52
Mn-C7O7	-50.98	-104.25 (28.5%)	-155.29 (42.5%)	314.69	-48.33 (13.2%)	-6.82 (1.9%)	-50.98 (13.9%)	159.40	-106.13
Mn-Br	-122.26	-151.86 (42.8%)	-131.54 (37.1%)	232.23	-43.13 (12.2%)	-9.57 (2.7%)	-18.38 (5.2%)	100.69	-71.08
Mn-k^{3}L	-102.82	-157.34 (28.2%)	-242.69 (43.5%)	455.51	-71.44 (12.8%)	-28.53 (5.1%)	-58.32 (10.4%)	212.82	-158.29
Structure C: Mn(*p*CH$_3$)									
Mn-C6O6	-57.17	-113.25 (27.6%)	-176.53 (42.9%)	353.87	-56.27 (13.7%)	-9.44 (2.3%)	-55.56 (13.5%)	177.34	-121.27
Mn-C7O7	-51.87	-104.35 (28.4%)	-155.52 (42.4%)	314.96	-49.06 (13.4%)	-7.07 (1.9%)	-50.84 (13.9%)	159.44	-106.97
Mn-Br	-122.52	-151.88 (43.1%)	-130.18 (36.9%)	229.96	-40.49 (11.5%)	-10.04 (2.8%)	-19.88 (5.6%)	99.78	-70.41
Mn-k^{3}L	-101.53	-155.96 (28.0%)	-242.77 (43.5%)	456.21	-71.20 (12.8%)	-29.46 (5.3%)	-58.35 (10.5%)	213.44	-159.01

[a] = $\Delta E^{elstat} + \Delta E^{exch} + \Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$; [b] = $\Delta E^{exch} + \Delta E^{rep}$; [c] = $\Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$

Table S 27. Generalized Kohn-Sham energy decomposition analysis in kcal mol^{-1}. C4O4 is trans to nitrogen, C5O5 is trans to selenium. In parenthesis is the percentage of attractive interactions[a]. Data referring to the geometries b of the S_4 state.

Bond	ΔE^{TOT}	ΔE^{elstat}	ΔE^{exch}	ΔE^{rep}	ΔE^{pol}	ΔE^{disp}	ΔE^{corr}	$\Delta E^{Pauli\ [b]}$	$\Delta E^{orb\ [c]}$
Structure B: Mn(*o*CH$_3$)									
Mn-C4O4	-51.90	-96.56 (28.0%)	-145.69 (42.3%)	292.84	-44.98 (13.0%)	-7.37 (2.1%)	-50.15 (14.5%)	147.15	-102.50
Mn-C5O5	-50.31	-95.09 (27.6%)	-148.33 (43.1%)	294.11	-42.28 (12.3%)	-8.02 (2.3%)	-50.70 (14.7%)	145.78	-101.00
Mn-Br	-123.60	-155.83 (43.7%)	-128.37 (36.0%)	232.60	-44.57 (12.5%)	-8.22 (2.3%)	-19.21 (5.4%)	104.23	-72.00
Mn-k^{3}L	-86.58	-107.24 (28.0%)	-163.48 (42.6%)	296.98	-56.59 (14.8%)	-24.85 (6.5%)	-31.40 (8.2%)	133.50	-112.84
Structure B: Mn(*m*CF$_3$)									
Mn-C4O4	-48.27	-105.97 (28.5%)	-160.91 (43.2%)	324.12	-51.57 (13.8%)	-7.13 (1.9%)	-46.81 (12.6%)	163.21	-105.51
Mn-C5O5	-45.38	-106.54 (27.8%)	-168.84 (44.1%)	337.40	-52.56 (13.7%)	-8.80 (2.3%)	-46.04 (12.0%)	168.56	-107.40
Mn-Br	-123.83	-169.39 (43.1%)	-145.93 (37.1%)	269.02	-47.70 (12.1%)	-8.34 (2.1%)	-21.50 (5.5%)	123.09	-77.54
Mn-k^{3}L	-84.69	-125.39 (28.7%)	-189.13 (43.4%)	351.50	-64.80 (14.9%)	-25.34 (5.8%)	-31.52 (7.2%)	162.37	-121.66
Structure B: Mn(*p*Cl)									
Mn-C4O4	-52.38	-100.32 (28.3%)	-148.85 (42.0%)	301.72	-48.27 (13.6%)	-7.05 (2.0%)	-49.62 (14.0%)	152.87	-104.94
Mn-C5O5	-49.17	-91.17 (27.6%)	-142.23 (43.1%)	280.64	-40.04 (12.1%)	-8.01 (2.4%)	-48.35 (14.7%)	138.41	-96.40
Mn-Br	-126.56	-160.72 (44.0%)	-130.92 (35.9%)	238.31	-45.45 (12.5%)	-8.16 (2.2%)	-19.62 (5.4%)	107.39	-73.23
Mn-k^{3}L	-85.52	-111.94 (28.1%)	-170.93 (42.9%)	312.95	-58.18 (14.6%)	-24.29 (6.1%)	-33.14 (8.3%)	142.02	-115.61
Structure B: Mn(*p*OCH$_3$)									
Mn-C4O4	-52.65	-98.64 (28.3%)	-146.72 (42.0%)	296.40	-46.45 (13.3%)	-6.97 (2.0%)	-50.26 (14.4%)	149.68	-103.68
Mn-C5O5	-49.71	-90.62 (27.6%)	-141.38 (43.1%)	278.54	-39.52 (12.0%)	-7.98 (2.4%)	-48.75 (14.9%)	137.16	-96.25
Mn-Br	-120.50	-153.36 (43.3%)	-128.81 (36.4%)	233.49	-45.97 (13.0%)	-8.10 (2.3%)	-17.76 (5.0%)	104.68	-71.83
Mn-k^{3}L	-88.56	-112.58 (28.5%)	-167.75 (42.5%)	306.47	-57.55 (14.6%)	-24.00 (6.1%)	-33.14 (8.4%)	138.72	-114.69
Structure B: Mn(*p*CH$_3$)									
Mn-C4O4	-52.36	-102.51 (28.4%)	-152.22 (42.1%)	309.04	-49.03 (13.6%)	-7.07 (2.0%)	-50.58 (14.0%)	156.82	-106.68
Mn-C5O5	-48.63	-90.49 (27.7%)	-141.12 (43.1%)	278.63	-39.41 (12.0%)	-8.27 (2.5%)	-47.96 (14.7%)	137.51	-95.64
Mn-Br	-121.35	-154.62 (43.5%)	-129.08 (36.3%)	233.85	-43.74 (12.3%)	-8.14 (2.3%)	-19.62 (5.5%)	104.77	-71.50
Mn-k^{3}L	-86.59	-111.07 (28.2%)	-168.21 (42.8%)	306.68	-58.05 (14.8%)	-24.62 (6.3%)	-31.33 (8.0%)	138.47	-114.00

[a] = $\Delta E^{elstat} + \Delta E^{exch} + \Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$; [b] = $\Delta E^{exch} + \Delta E^{rep}$; [c] = $\Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$

Table S 28. Generalized Kohn-Sham energy decomposition analysis in kcal mol^{-1}. C6O6 is trans to bromide, C7O7 is trans to nitrogen. In parenthesis is the percentage of attractive interactions[a]. Data referring to the geometries c of the S_4 state.

Bond	ΔE^{TOT}	ΔE^{elstat}	ΔE^{exch}	ΔE^{rep}	ΔE^{pol}	ΔE^{disp}	ΔE^{corr}	$\Delta E^{Pauli\ [b]}$	$\Delta E^{orb\ [c]}$
Structure C: Mn(*o*CH_3)									
Mn-C6O6	-57.49	-110.90 (27.6%)	-171.87 (42.8%)	344.34	-56.65 (14.1%)	-9.22 (2.3%)	-53.18 (13.2%)	172.47	-119.05
Mn-C7O7	-47.18	-107.21 (28.0%)	-167.03 (43.6%)	335.72	-49.74 (13.0%)	-7.22 (1.9%)	-51.70 (13.5%)	168.69	-108.66
Mn-Br	-121.91	-169.44 (41.5%)	-158.20 (38.7%)	286.35	-49.76 (12.2%)	-10.08 (2.5%)	-20.78 (5.1%)	128.15	-80.62
Mn-k^{3}L	-96.46	-139.50 (28.0%)	-215.91 (43.4%)	401.24	-60.13 (12.1%)	-29.05 (5.8%)	-53.11 (10.7%)	185.33	-142.29
Structure C: Mn(*m*CF_3)									
Mn-C6O6	-59.47	-105.27 (27.6%)	-161.35 (42.3%)	322.34	-54.20 (14.2%)	-9.06 (2.4%)	-51.94 (13.6%)	160.99	-115.20
Mn-C7O7	-48.36	-103.43 (28.3%)	-157.20 (43.1%)	316.77	-47.82 (13.1%)	-6.64 (1.8%)	-50.05 (13.7%)	159.57	-104.51
Mn-Br	-127.65	-179.09 (42.0%)	-164.76 (38.6%)	298.76	-49.85 (11.7%)	-11.24 (2.6%)	-21.47 (5.0%)	134.00	-82.56
Mn-k^{3}L	-94.76	-140.56 (27.9%)	-218.71 (43.4%)	409.04	-61.67 (12.2%)	-29.46 (5.8%)	-53.40 (10.6%)	190.33	-144.53
Structure C: Mn(*p*Cl)									
Mn-C6O6	-57.90	-112.16 (27.4%)	-174.65 (42.7%)	351.12	-57.65 (14.1%)	-8.50 (2.1%)	-56.07 (13.7%)	176.47	-122.22
Mn-C7O7	-48.12	-93.80 (28.3%)	-141.56 (42.7%)	283.20	-41.22 (12.4%)	-6.64 (2.0%)	-48.10 (14.5%)	141.64	-95.96
Mn-Br	-128.09	-167.87 (42.8%)	-148.13 (37.8%)	263.88	-46.23 (11.8%)	-10.71 (2.7%)	-19.02 (4.9%)	115.75	-75.96
Mn-k^{3}L	-95.49	-146.08 (28.0%)	-228.79 (43.8%)	426.34	-62.15 (11.9%)	-28.22 (5.4%)	-56.59 (10.8%)	197.55	-146.96
Structure C: Mn(*p*OCH_3)									
Mn-C6O6	-54.78	-111.56 (27.3%)	-177.92 (43.5%)	354.05	-54.45 (13.3%)	-9.41 (2.3%)	-55.49 (13.6%)	176.13	-119.35
Mn-C7O7	-49.63	-106.63 (28.3%)	-161.44 (42.9%)	327.11	-50.97 (13.5%)	-6.64 (1.8%)	-51.07 (13.6%)	165.67	-108.68
Mn-Br	-121.35	-167.61 (42.0%)	-153.76 (38.5%)	277.98	-49.14 (12.3%)	-9.65 (2.4%)	-19.17 (4.8%)	124.22	-77.96
Mn-k^{3}L	-93.93	-148.03 (28.2%)	-230.02 (43.9%)	430.16	-64.18 (12.2%)	-27.79 (5.3%)	-54.08 (10.3%)	200.14	-146.05
Structure C: Mn(*p*CH_3)									
Mn-C6O6	-54.42	-110.56 (27.3%)	-176.67 (43.6%)	351.15	-53.82 (13.3%)	-9.32 (2.3%)	-55.20 (13.6%)	174.48	-118.34
Mn-C7O7	-49.53	-106.64 (28.3%)	-161.47 (42.9%)	327.22	-51.15 (13.6%)	-6.63 (1.8%)	-50.85 (13.5%)	165.75	-108.63
Mn-Br	-122.17	-168.17 (42.1%)	-153.57 (38.4%)	277.36	-47.81 (12.0%)	-9.68 (2.4%)	-20.31 (5.1%)	123.79	-77.80
Mn-k^{3}L	-93.28	-147.30 (28.2%)	-229.38 (43.9%)	428.74	-63.72 (12.2%)	-27.68 (5.3%)	-53.93 (10.3%)	199.36	-145.33

[a] = $\Delta E^{elstat} + \Delta E^{exch} + \Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$; [b] = $\Delta E^{exch} + \Delta E^{rep}$; [c] = $\Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$

Table S 29. Generalized Kohn-Sham energy decomposition analysis in kcal mol^{-1}. C4O4 is trans to nitrogen, C5O5 is trans to selenium. In parenthesis is the percentage of attractive interactions[a]. Data referring to the geometries b of the S_1 state.

Bond	ΔE^{TOT}	ΔE^{elstat}	ΔE^{exch}	ΔE^{rep}	ΔE^{pol}	ΔE^{disp}	ΔE^{corr}	$\Delta E^{Pauli\ [b]}$	$\Delta E^{orb\ [c]}$
Structure B: Mn(*o*CH_3)									
Mn-C4O4	-48.84	-105.99 (28.5%)	-158.57 (42.7%)	322.72	-48.33 (13.0%)	-6.59 (1.8%)	-52.08 (14.0%)	164.15	-107.00
Mn-C5O5	-53.69	-95.70 (27.4%)	-150.26 (43.1%)	295.23	-40.70 (11.7%)	-9.02 (2.6%)	-53.24 (15.3%)	144.97	-102.96
Mn-Br	-125.87	-158.38 (43.6%)	-132.21 (36.4%)	237.24	-44.03 (12.1%)	-9.07 (2.5%)	-19.42 (5.3%)	105.03	-72.52
Mn-k^{3}L	-85.26	-112.58 (28.6%)	-168.35 (42.8%)	308.51	-44.89 (11.4%)	-26.82 (6.8%)	-41.13 (10.4%)	140.16	-112.84
Structure B: Mn(*m*CF_3)									
Mn-C4O4	-48.78	-104.90 (28.6%)	-156.35 (42.6%)	318.36	-48.11 (13.1%)	-6.61 (1.8%)	-51.18 (13.9%)	162.01	-105.90
Mn-C5O5	-54.12	-94.32 (27.3%)	-148.75 (43.1%)	291.38	-40.55 (11.7%)	-9.12 (2.6%)	-52.76 (15.3%)	142.63	-102.43
Mn-Br	-131.43	-162.97 (44.6%)	-130.21 (35.6%)	234.26	-43.04 (11.8%)	-9.62 (2.6%)	-19.85 (5.4%)	104.05	-72.51
Mn-k^{3}L	-83.06	-109.50 (28.3%)	-165.36 (42.8%)	303.56	-42.34 (11.0%)	-27.59 (7.1%)	-41.82 (10.8%)	138.20	-111.75
Structure B: Mn(*p*Cl)									
Mn-C4O4	-48.08	-104.67 (28.6%)	-156.05 (42.7%)	317.66	-47.41 (13.0%)	-6.29 (1.7%)	-51.31 (14.0%)	161.61	-105.01
Mn-C5O5	-54.44	-97.69 (27.5%)	-152.78 (43.0%)	301.08	-42.78 (12.0%)	-8.87 (2.5%)	-53.40 (15.0%)	148.30	-105.05
Mn-Br	-129.91	-160.22 (44.4%)	-128.74 (35.7%)	230.74	-43.85 (12.2%)	-8.98 (2.5%)	-18.85 (5.2%)	102.00	-71.68
Mn-k^{3}L	-85.15	-110.90 (28.7%)	-164.17 (42.5%)	301.20	-43.12 (11.2%)	-25.95 (6.7%)	-42.20 (10.9%)	137.03	-111.27
Structure B: Mn(*p*OCH_3)									
Mn-C4O4	-48.76	-106.09 (28.6%)	-157.98 (42.6%)	321.94	-48.50 (13.1%)	-6.32 (1.7%)	-51.81 (14.0%)	163.96	-106.63
Mn-C5O5	-54.30	-97.23 (27.5%)	-152.27 (43.0%)	299.65	-42.02 (11.9%)	-8.89 (2.5%)	-53.55 (15.1%)	147.38	-104.46
Mn-Br	-123.38	-153.75 (43.5%)	-128.43 (36.3%)	230.00	-44.14 (12.5%)	-8.91 (2.5%)	-18.15 (5.1%)	101.57	-71.20
Mn-k^{3}L	-86.41	-111.97 (28.9%)	-164.17 (42.4%)	301.05	-43.01 (11.1%)	-25.92 (6.7%)	-42.38 (10.9%)	136.88	-111.31
Structure B: Mn(*p*CH_3)									
Mn-C4O4	-48.51	-105.74 (28.6%)	-157.48 (42.6%)	320.87	-48.31 (13.1%)	-6.30 (1.7%)	-51.55 (14.0%)	163.39	-106.16
Mn-C5O5	-54.41	-97.27 (27.5%)	-152.16 (43.0%)	299.59	-42.27 (11.9%)	-8.85 (2.5%)	-53.44 (15.1%)	147.43	-104.56
Mn-Br	-124.40	-154.84 (43.8%)	-128.14 (36.2%)	229.51	-42.74 (12.1%)	-8.92 (2.5%)	-19.26 (5.4%)	101.37	-70.92
Mn-k^{3}L	-86.03	-111.50 (28.9%)	-163.70 (42.4%)	300.20	-43.30 (11.2%)	-25.86 (6.7%)	-41.86 (10.8%)	136.50	-111.02

[a] = $\Delta E^{elstat} + \Delta E^{exch} + \Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$; [b] = $\Delta E^{exch} + \Delta E^{rep}$; [c] = $\Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$

Table S 30. Generalized Kohn-Sham energy decomposition analysis in kcal mol^{-1}. C6O6 is trans to bromide, C7O7 is trans to nitrogen. In parenthesis is the percentage of attractive interactions[a]. Data referring to the geometries c of the S_1 state.

Bond	ΔE^{TOT}	ΔE^{elstat}	ΔE^{exch}	ΔE^{rep}	ΔE^{pol}	ΔE^{disp}	ΔE^{corr}	$\Delta E^{Pauli\ [b]}$	$\Delta E^{orb\ [c]}$
Structure C: Mn(*o*CH_3)									
Mn-C6O6	-53.71	-95.42 (27.4%)	-149.94 (43.1%)	294.41	-40.47 (11.6%)	-9.03 (2.6%)	-53.26 (15.3%)	144.47	-102.76
Mn-C7O7	-48.80	-105.77 (28.5%)	-158.28 (42.7%)	322.05	-48.15 (13.0%)	-6.58 (1.8%)	-52.06 (14.0%)	163.77	-106.79
Mn-Br	-125.89	-158.41 (43.6%)	-132.17 (36.4%)	237.22	-44.03 (12.1%)	-9.07 (2.5%)	-19.42 (5.3%)	105.05	-72.52
Mn-k^{3}L	-85.19	-112.42 (28.6%)	-168.18 (42.8%)	308.17	-44.90 (11.4%)	-26.81 (6.8%)	-41.05 (10.4%)	139.99	-112.76
Structure C: Mn(*m*CF_3)									
Mn-C6O6	-57.34	-105.03 (27.9%)	-159.15 (42.2%)	319.38	-49.70 (13.2%)	-8.36 (2.2%)	-54.48 (14.5%)	160.23	-112.54
Mn-C7O7	-46.11	-100.06 (28.6%)	-149.66 (42.9%)	303.15	-43.66 (12.5%)	-6.02 (1.7%)	-49.86 (14.3%)	153.49	-99.54
Mn-Br	-130.61	-165.85 (43.7%)	-140.06 (36.9%)	249.21	-43.99 (11.6%)	-10.49 (2.8%)	-19.43 (5.1%)	109.15	-73.91
Mn-k^{3}L	-85.66	-114.34 (28.6%)	-170.66 (42.7%)	314.34	-45.80 (11.5%)	-26.86 (6.7%)	-42.34 (10.6%)	143.68	-115.00
Structure C: Mn(*p*Cl)									
Mn-C6O6	-54.46	-97.65 (27.5%)	-152.71 (43.0%)	300.94	-42.76 (12.0%)	-8.86 (2.5%)	-53.41 (15.0%)	148.23	-105.03
Mn-C7O7	-48.07	-104.52 (28.6%)	-155.78 (42.7%)	317.09	-47.26 (12.9%)	-6.27 (1.7%)	-51.34 (14.1%)	161.31	-104.87
Mn-Br	-129.94	-159.98 (44.5%)	-128.33 (35.7%)	229.95	-43.81 (12.2%)	-8.97 (2.5%)	-18.80 (5.2%)	101.62	-71.58
Mn-k^{3}L	-85.23	-110.84 (28.7%)	-163.92 (42.5%)	300.70	-43.02 (11.1%)	-25.92 (6.7%)	-42.22 (10.9%)	136.78	-111.16
Structure C: Mn(*p*OCH_3)									
Mn-C6O6	-54.30	-97.26 (27.5%)	-152.30 (43.0%)	299.74	-42.04 (11.9%)	-8.88 (2.5%)	-53.56 (15.1%)	147.44	-104.48
Mn-C7O7	-48.76	-106.10 (28.6%)	-158.02 (42.6%)	322.02	-48.53 (13.1%)	-6.32 (1.7%)	-51.80 (14.0%)	164.00	-106.65
Mn-Br	-123.39	-153.69 (43.5%)	-128.43 (36.3%)	229.98	-44.20 (12.5%)	-8.91 (2.5%)	-18.14 (5.1%)	101.55	-71.25
Mn-k^{3}L	-86.41	-112.04 (28.9%)	-164.24 (42.4%)	301.14	-43.00 (11.1%)	-25.92 (6.7%)	-42.35 (10.9%)	136.90	-111.27
Structure C: Mn(*p*CH_3)									
Mn-C6O6	-54.38	-97.41 (43.0%)	-152.41 (43.0%)	300.12	-42.34 (11.9%)	-8.86 (2.5%)	-53.49 (15.1%)	147.71	-104.69
Mn-C7O7	-48.48	-105.56 (42.6%)	-157.22 (42.6%)	320.29	-48.12 (13.0%)	-6.29 (1.7%)	-51.57 (14.0%)	163.07	-105.98
Mn-Br	-124.43	-154.70 (36.2%)	-127.88 (36.2%)	228.99	-42.67 (12.1%)	-8.92 (2.5%)	-19.25 (5.4%)	101.11	-70.84
Mn-k^{3}L	-86.06	-111.47 (42.4%)	-163.76 (42.4%)	300.29	-43.36 (11.2%)	-25.86 (6.7%)	-41.89 (10.8%)	136.53	-111.11

[a] = $\Delta E^{elstat} + \Delta E^{exch} + \Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$; [b] = $\Delta E^{exch} + \Delta E^{rep}$; [c] = $\Delta E^{pol} + \Delta E^{disp} + \Delta E^{corr}$

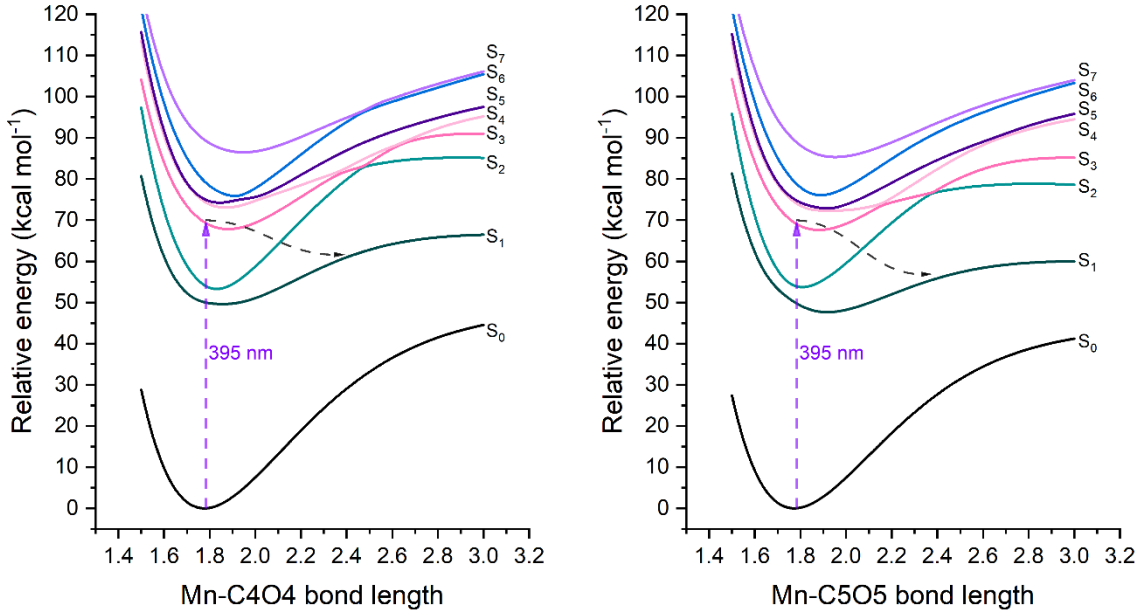

Figure S 72. Potential Energy Curves along photoinduced CO dissociation for specie b: Mn(κ³-oCH₃).

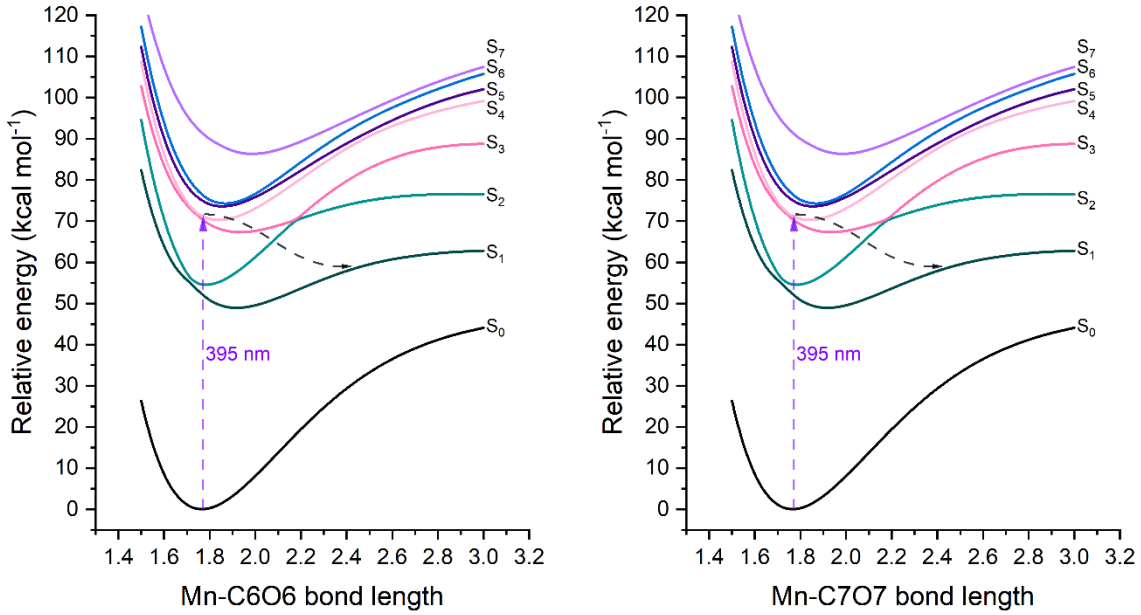

Figure S 73. Potential Energy Curves along photoinduced CO dissociation for specie c: Mn(κ³-oCH₃).

S6. Coordinates system obtained for all structures

Table S 31. Coordinates of the optimized structure of compound Mn(oCH₃).

Mn	7.55408685963833	7.78743842569220	3.88259952763089
Br	7.16986876197493	9.94096059676971	2.54552406086969
C	9.06886746668267	7.53219868576191	2.92365538819987
O	10.01694680282235	7.37503086408496	2.30174678183421
C	6.63115264414565	6.81084412603314	2.66816646279758
O	6.08000118930709	6.16930239343794	1.89729447638299
C	7.84541654707458	6.36786282757832	4.94116165586409
O	8.04263766721068	5.45643275717617	5.61438782892639
Se	8.69340638719910	9.45289904997699	5.44712524372195
C	6.97390535766646	10.18556589924478	6.07171029710368
H	7.13680955088379	10.73022731151306	6.99813387146451
H	6.71866055743764	10.89159865590215	5.28446770823104
C	5.92031182537411	9.11278649211901	6.21808429027907
H	6.20813818859413	8.38309573777261	6.97542388483679
H	4.99401335582265	9.59391127715015	6.54931800990775
N	5.69713025902496	8.38021918510839	4.95762736433319
H	5.33652971710068	9.04366779547472	4.27145647186880
C	4.70037310038100	7.30208889632850	5.12007283812668
H	5.10489387012044	6.58108944987128	5.83474202225939
H	4.61287236079314	6.79270499883616	4.16408364100543
C	3.31440190012034	7.73746675073584	5.56905947475068
H	3.30853943794224	8.18599659887686	6.56140310596566
H	2.65486861036703	6.87342883894334	5.59031368054173
Se	2.50855847693964	9.13165598107070	4.40795167035062
C	9.30243893482753	8.54925507740637	7.06938999543858
C	10.47547468421676	7.78903599960226	6.97119639306342
C	10.95189164981246	7.17378897985580	8.12794560271486
H	11.85917624427588	6.58533442207315	8.06490988863314
C	10.29866278894156	7.30033057782509	9.34535889453100
H	10.69424905847920	6.81078591458609	10.22566153844577
C	9.14456927721983	8.06493567215811	9.42629046858798
H	8.62727254144774	8.18242616103816	10.36971020369729
C	8.65037354742649	8.69022694249929	8.28853271261755
H	7.75919912141802	9.29279463239676	8.37549488473417
C	11.21400375181879	7.61381961738657	5.67514762209010
H	10.69088695744055	6.92145800852365	5.01422562383417
H	12.21054367302153	7.21190539394083	5.85242647760194
H	11.32567118197637	8.55633908101686	5.13462881344757
C	2.89628088765241	8.36635047743975	2.66643654111389
C	2.34503479050608	7.15218469503720	2.23169709331388
C	2.67665748796418	6.71656826405487	0.94847340274177
H	2.26841809635374	5.77669811077434	0.59640181942652
C	3.50905368235887	7.45423820115080	0.11788749736917
H	3.75262698049478	7.08105294674016	-0.86847088638921
C	4.03588817713156	8.65817363665372	0.55920097888103
H	4.70745359214058	9.23395091212724	-0.06307689011195
C	3.72874371565357	9.11009556316207	1.83447034881209
H	4.16430054211259	10.03171305369153	2.19149246606367
C	1.43813395378032	6.31308415130425	3.08677925616763
H	2.01031619182841	5.66944381323673	3.76128332121930
H	0.82127709194496	5.66194826894931	2.46797879502075
H	0.78583250313065	6.93436682990900	3.70108137968058

Table S 32. Coordinates of the optimized structure of compound Mn(mCF₃).

Mn	5.32294447182289	8.93876049026614	17.97495017597381
Br	6.37539936232485	11.05488698388454	16.96330570303039
C	5.81349353382655	7.98990100004141	16.50940381519559
O	6.14090822981340	7.38253998771132	15.59701443802226
C	6.88868081319016	8.52795687088769	18.79114478544175
O	7.86966011196902	8.26864178636913	19.32050376617115

C	4.45864761169581	7.54468961280404	18.70554326493891
O	3.89823676063787	6.65091067308036	19.16195625625587
Se	4.73911946995507	10.59586289284854	19.81506773420966
C	3.28453699333974	11.42343327608252	18.77108819429005
H	2.62364426330522	11.96048086206687	19.44633212712382
H	3.81657167951479	12.14260103505769	18.15158063099842
C	2.54642431260071	10.40395825679971	17.93733606350260
H	2.05323913321764	9.66421775065209	18.56973447594565
H	1.76968253389096	10.93060021430483	17.37315781899882
N	3.45567736946970	9.68806365744561	17.02291978587960
H	3.87199843364967	10.38139765102235	16.39935929557689
C	2.73650012876958	8.70377835435115	16.18972119549510
H	2.27989082499658	7.96865912838624	16.85684856871777
H	3.47596254882744	8.17807214210619	15.59183972680089
C	1.67556949690360	9.27366289734495	15.25891446682670
H	0.82585871126362	9.70463446755560	15.78617421433323
H	1.29944558833049	8.48492709509340	14.61089525204495
Se	2.34837658881958	10.75222276072055	14.11691451777466
C	3.70137627635237	9.61264223371848	21.13741728702774
C	2.37771560771048	9.89114812525916	21.43695795073085
H	1.83698788936625	10.67379850119747	20.92655569864496
C	1.72217888303424	9.14567070912361	22.41458014668828
C	2.38450717730724	8.13794288870462	23.10066845600575
H	1.86587182617097	7.56197454364526	23.85322211126560
C	3.71605809670810	7.87477141987466	22.80217888915409
H	4.24077389097261	7.08766895054181	23.32678986267681
C	4.37365543787596	8.60484428110656	21.82510405519959
H	5.40539442812805	8.37791884537542	21.58882786612270
C	0.29694984595593	9.48835088712495	22.74835358287151
C	3.85685513763732	9.80472478783125	13.35543304854658
C	3.65299239207844	8.67023135082396	12.57668141968239
H	2.65271703484406	8.31627159460088	12.37185157070928
C	4.74765036355627	7.99823315058174	12.04822340423424
C	6.04050923400854	8.46249973333886	12.27657997663054
H	6.88577303501726	7.93216728081832	11.86081816282110
C	6.23262828807419	9.60186242386938	13.04101610759521
H	7.23303042811844	9.96074098308698	13.24166844533416
C	5.14467094227029	10.27254947177413	13.58822338765925
H	5.30859274690523	11.13421549549241	14.21908384104880
C	4.54132149176677	6.73493944576416	11.26127533931381
F	-0.42282295513333	9.78205632518465	21.63927359809509
F	-0.33971211419934	8.48589221009161	23.38380339214952
F	0.22289272784503	10.57557891528682	23.55226983380557
F	4.67154983356041	5.63382788070116	12.04117346285829
F	3.31134923782826	6.67043749760055	10.70620282497634
F	5.43868384410474	6.60749022059737	10.26067000460190

Table S 33. Coordinates of the optimized structure of compound Mn(pCl).

Mn	4.38144592611025	4.48167960875667	10.55809454585036
Br	4.84354329618527	3.72831120301035	12.96927260620276
C	2.60969396421317	4.19242914185647	10.80984419245921
O	1.49429490651120	3.98772537147132	10.96052391720444
C	4.59378999606676	2.78291322726357	9.96105087161473
O	4.73793742029443	1.71560371010190	9.57350344331385
C	4.14406375577082	5.14236317277333	8.90481856644729
O	3.98300772054738	5.58140284132416	7.85474858231470
Se	6.89366388968982	4.82626921435624	10.61391485700478
C	6.76158220547916	6.47708975806248	11.68356371765596
H	6.68484580008701	6.09629245304550	12.69993990725113
H	7.68740406263686	7.03816898177018	11.58459736989731
C	5.55234766625223	7.29744985499792	11.30312101754853
H	5.53012769640546	8.18199943707429	11.94801740536656
H	5.62050723207745	7.63862011151610	10.26918054453832

N	4.30229281658828	6.52794665652373	11.44278912321545
H	4.20780919336338	6.27058260449144	12.42529926513256
C	3.11859687796479	7.32601552911814	11.06352818807261
H	2.24519103011060	6.69227538410922	11.19327179661807
H	3.19675565540556	7.55441713911675	9.99789549494715
C	2.90549214152038	8.61768682386007	11.83987203857649
H	1.94861651386935	9.05273207178448	11.55868791363821
H	3.67798029006576	9.36281452872254	11.65502080633262
Se	2.91417802062761	8.36656488647230	13.81153978687373
C	7.38543125416846	5.56589274663115	8.88239916433291
C	7.26745281217820	4.70504050862372	7.79514930164525
H	6.89117989880179	3.69889046442551	7.93033872179390
C	7.61678935315216	5.13006088804802	6.52297389927311
H	7.52251379376437	4.46520645823678	5.67628661888326
C	8.08047709533101	6.42607008432763	6.34311166035090
C	8.20553718407279	7.29282339859439	7.41708690566416
H	8.56973675192466	8.29869132470359	7.26247578472679
C	7.86029562718605	6.85632334464238	8.69125819027781
H	7.97285263503308	7.54121753882519	9.51901312879725
C	1.57801545297999	6.96743604034184	13.86638241000006
C	1.95382733190751	5.67055780960852	14.19663972373859
H	2.98428334305803	5.43210041590884	14.41842678871608
C	1.01195775071253	4.64974963074652	14.20325709373758
H	1.30998789817218	3.63685018477951	14.43241355506360
C	-0.30179260641925	4.94037931951426	13.87403088058467
C	-0.69462022803091	6.23300809449606	13.54973469086336
H	-1.72631365244627	6.43946800017216	13.30209158125095
C	0.25037506014293	7.24880162926255	13.55419966071448
H	-0.05061610648188	8.26034374665316	13.31549373744352
Cl	8.51036295012810	6.97259309940909	4.73865664126659
Cl	-1.48901367717887	3.65683756046952	13.85428290279756

Table S 34. Coordinates of the optimized structure of compound Mn(pOCH$_3$).

Mn	4.53688437294598	4.39711793115422	10.26944474277409
Br	5.02407594114896	2.33500685671232	11.72937444931572
C	5.98267717712623	5.19298935874291	11.01595587061051
O	6.87468527414980	5.70941512018948	11.51322151449547
C	3.47527346647909	5.07385170953135	11.57623838691273
O	2.80243266061972	5.49753102946606	12.39829680535841
C	4.24374225332216	5.80480884705813	9.20214201470456
O	4.09094861448132	6.73900157160950	8.54562072336086
Se	2.65947225383971	2.86015000726173	9.52158290429782
C	3.85460865639643	1.72997594448051	8.41409042547807
H	4.26640836755685	1.00892380867234	9.11666161574325
H	3.23033892276183	1.22553257651412	7.68084433077391
C	4.93716791782076	2.55036888357897	7.75907352661027
H	5.57783415911079	1.86863515772625	7.19087123710824
H	4.51325313351069	3.26826948755022	7.05598179076618
N	5.73502794990024	3.29206802457917	8.75490642418050
H	6.15008944738114	2.59617132266179	9.37583662262272
C	6.84258688095068	4.04940512017789	8.13686590944861
H	7.39712258007975	4.52204868524467	8.94423030344352
H	6.40796567832826	4.84862335929325	7.53093242171954
C	7.80913141978382	3.23703319503482	7.28477155918604
H	8.66567769927729	3.85332513736824	7.01924524551016
H	7.35966207510069	2.87089839289927	6.36269358671557
Se	8.49756704882232	1.60807612549243	8.19063666300547
C	1.53262148393728	3.51176565860183	8.07855775711127
C	0.26067912186727	2.96257583580377	7.98506920647186
H	-0.06447476663396	2.22900803722784	8.71157611877145
C	-0.60775111033508	3.33839180480522	6.96559779194562
H	-1.59072577813465	2.89440038690063	6.91945828372749
C	-0.19482038918677	4.27783158748775	6.02238341752228

C	1.08080022310903	4.84008585400943	6.12148733748598
H	1.38098988536218	5.57904470079431	5.39067707176762
C	1.93377909989978	4.46311045840853	7.14184962232108
H	2.90556766289144	4.92540779132666	7.20789995227054
O	-0.95397757636093	4.70928559557696	4.98312462394539
C	-2.25936531644260	4.16474797592182	4.83390373516487
H	-2.22213401733029	3.08238317058935	4.68319222671197
H	-2.67941462297952	4.63924533418221	3.95083255246152
H	-2.88511865951727	4.39185000716238	5.70115073136722
C	9.41734351129894	2.49011915485484	9.64301208295156
C	8.80037436788574	2.64902552851182	10.88458866425029
H	7.79495391825412	2.28636438705941	11.05500982375191
C	9.46892436261979	3.27879857030239	11.91786202467654
H	8.99329767508298	3.41736487535004	12.87919193561167
C	10.76958301063772	3.75140823075464	11.73037437089664
C	11.39297416963796	3.58909442815395	10.49278307150395
H	12.39982450262393	3.94066040218430	10.32406087827364
C	10.71206021870814	2.95682165663462	9.45815689717297
H	11.20162426929896	2.82438402410221	8.50222456443941
O	11.34672442588108	4.34956557313531	12.80578659197719
C	12.68166228820910	4.81704911683561	12.67554617664205
H	13.36673396710458	3.99939583886306	12.43392340192708
H	12.94586188376122	5.23622674390630	13.64318718070397
H	12.75805423795501	5.59417661755285	11.90969083203213

Table S 35. Coordinates of the optimized structure of compound Mn(pCH$_3$).

Mn	3.50239195675854	6.58924559123558	4.72059285502972
Br	4.44826465796178	4.89157326274250	3.04711220138819
C	1.87507755651414	5.81319212551017	4.54666614118037
O	0.83764162932772	5.34773675349106	4.41430816065817
C	3.13247353715322	7.71481128129014	3.34946719491852
O	2.90535736332631	8.42857496067246	2.48394010961420
C	2.90859168901641	7.73929141753490	5.96283342348385
O	2.49873355418022	8.45992748144473	6.76042549655060
Se	5.94128319257016	7.33058991496114	4.72272349926397
C	6.50801375528104	5.78304171783184	5.80822836426920
H	6.59769635269968	4.98558889697919	5.07373803028988
H	7.48637580418181	5.98840426742477	6.23310519215104
C	5.48653817175313	5.45804446143271	6.86889013887407
H	5.85665586909702	4.60667837623260	7.44907578995726
H	5.35605622414186	6.30000263297674	7.55111166246613
N	4.17463062373203	5.14128149863599	6.27404136380211
H	4.29654662866259	4.31830985024913	5.68437272215879
C	3.16289951713676	4.81895668589747	7.30055665525927
H	2.24065720441301	4.57508651003618	6.77930466818284
H	2.97683967704752	5.72454307128038	7.88292098306518
C	3.50647733062559	3.67816787733272	8.24857042447116
H	2.64061401531944	3.45700521659528	8.86941441896774
H	4.34153325225924	3.90753995355375	8.90902402592198
Se	4.04237443060308	2.00384511388118	7.32136989186109
C	6.17720999419919	8.74006525145158	6.04655091586656
C	5.37468593548049	9.87071259585916	5.93817147156662
H	4.60383584563338	9.92371451738346	5.18089227641865
C	5.55394792188938	10.93551673358842	6.80787551018151
H	4.91806486172375	11.80750965772070	6.71235639225126
C	6.52677133752594	10.89834020826560	7.80724120552854
C	7.32801014004782	9.76276662513502	7.89471614708107
H	8.10008667963086	9.71054346090706	8.65324321153780
C	7.16488346561271	8.69416876699843	7.02099970454669
H	7.82240162037372	7.84095435182675	7.11013655893814
C	6.68846711474668	12.04165461079584	8.77017159912123
H	5.90397565662615	12.02388570281695	9.53177534710365
H	6.62159989265626	13.00300291272618	8.25819507569306

H	7.64928522574141	11.99462337845801	9.28296547093294
C	2.52824193997412	1.92375464583656	6.11889535837584
C	2.72037900829576	2.13386612744509	4.75872076615189
H	3.70824188728803	2.32714288364046	4.36563948603323
C	1.63202457376704	2.13764217577178	3.89750397749633
H	1.79869348732865	2.33319115475705	2.84544861667777
C	0.33727116668004	1.94326895644598	4.37280715616763
C	0.16336514119021	1.71579742084562	5.73869280816248
H	-0.83404811747199	1.55001864969306	6.12865763481253
C	1.24519352991668	1.69787995403065	6.60802981899540
H	1.09005620699750	1.51044499264093	7.66271857205187
C	-0.84279450993537	2.02734102347161	3.44646934154634
H	-1.13081572533577	3.07130450084659	3.29423377435196
H	-1.70660896937423	1.49944685530015	3.85192909832593
H	-0.61084430497125	1.60651696611802	2.46725429029695

Table S 36. Coordinates of the optimized structure of geometry a with ligand oCH_3.

Mn	7.47251054631803	7.78902897032336	4.12026136066435
Br	9.56000463123146	7.33508535801068	2.78374760884661
C	7.03699821330790	9.17650164539931	3.09518556532776
O	6.73875761156828	10.05943042388117	2.41389293388562
C	6.52300494103773	6.74286687124720	3.04983103614443
O	5.91284683820563	6.07861737857273	2.32969743595637
Se	8.74369844148239	9.51933257383769	5.59429214579742
C	7.01009894529080	10.21894937738536	6.21648653702536
H	7.16598388108939	10.91978646485310	7.03348466393345
H	6.64531694511320	10.77718463760410	5.35664846737309
C	6.05956407978424	9.10948363116887	6.61922468366571
H	6.44308960547021	8.61297970175637	7.50507682272398
H	5.08836285027988	9.53798880150449	6.88959041736412
N	5.87864690894722	8.07317835264842	5.57411381968036
H	5.15444696300632	8.38815648490048	4.94169520126069
C	5.42247299476597	6.79083237242456	6.16288210637697
H	4.63778459502014	6.97252845283945	6.90781893684628
H	4.98533145783099	6.20779695805066	5.35933878887102
C	6.55826559507508	6.01970046791672	6.81298976904318
H	6.93628467829916	6.52507586171116	7.69999242710882
H	6.25136681950344	5.02216781884552	7.10587656070258
Se	8.16048303537556	5.92956702017276	5.65428715305150
C	9.43574952100563	8.79106766083524	7.26633079052945
C	10.63269794483911	8.06233689651445	7.19817541478475
C	11.12379345340412	7.51027304626332	8.38123524065851
H	12.03982327037629	6.93505506148791	8.33803620197519
C	10.47751179231734	7.68334522458408	9.59737854311332
H	10.88330790601148	7.23748709896868	10.49536913265113
C	9.32213925516070	8.44841244230508	9.65391383680396
H	8.82087841363296	8.62159284632188	10.59684393108406
C	8.80758383172554	9.00526540478304	8.48890732089418
H	7.92419057532482	9.61996243330145	8.55966248436790
C	11.39407627219620	7.90309363049120	5.91737531385898
H	10.77954834442819	7.51386429271737	5.10378837118570
H	12.24287333276684	7.23508699182917	6.05296579670134
H	11.77921701023280	8.86700999714716	5.57369412164741
C	8.19343216748823	4.22277250254279	4.71442364051503
C	7.13463024711008	3.38451898886906	4.34760024701844
C	7.45367081575655	2.24275393608678	3.60700098510092
H	6.64823566105295	1.58112456581581	3.31431149521064
C	8.75239261425492	1.94534454903946	3.22304196651019
H	8.95238685722626	1.05754117175340	2.63835692861088
C	9.78520346537378	2.79613962898405	3.58716038168811
H	10.80404999577707	2.59103914775839	3.28880213348458
C	9.50318476684062	3.92518041850785	4.33980581169647
H	10.30429198191268	4.59541813533674	4.61757555910047

C	5.68968126046876	3.63718885804760	4.67229362051104
H	5.49861822165463	3.64558394134887	5.74505223310295
H	5.06862500178104	2.85566362033923	4.23881110116229
H	5.35502544187671	4.58283788296509	4.25278295438201

Table S 37. Coordinates of the optimized structure of geometry a with ligand mCF_3.

Mn	7.89431758320798	7.71631833876455	4.20999198144344
Br	10.30299341513679	7.58183668497451	3.43894730517447
C	7.42531314710388	8.98547365460947	3.05923333503488
O	7.09892048894193	9.78596276841318	2.29431235567518
C	7.27686799545336	6.53512214297721	3.02501713078356
O	6.86609375444407	5.81122583916429	2.22881743718497
Se	8.65673458295452	9.62292085608679	5.69162936015263
C	6.79542064950544	10.03862130803569	6.19478263908742
H	6.77140323576443	10.73829026306099	7.02662356955249
H	6.40923539130057	10.54844412753392	5.31355651352468
C	6.02414631982156	8.77584172847563	6.51014531819250
H	6.44460410928165	8.31964617163277	7.40281027233869
H	4.98083522909864	9.02064825078351	6.73757034299390
N	6.08035005081615	7.77272529162856	5.41780890160808
H	5.40634245264259	8.04260575654570	4.71187347475070
C	5.69163379379935	6.42700111418566	5.90392371130762
H	4.76802450891113	6.48495425941832	6.49275248913147
H	5.48976855892307	5.81557058366869	5.02773904873239
C	6.78265632212229	5.79046286547014	6.74793600679669
H	6.95869718410111	6.33169763855442	7.67500223863063
H	6.53377979432715	4.76770523118347	7.01649433727695
Se	8.53305985895768	5.83133568752789	5.84182158082025
C	9.32318656529393	8.93162409061866	7.37632292215867
C	10.46744615917975	8.13837809232677	7.30925858611748
C	11.00959220011856	7.63045131392162	8.48242290410733
C	10.42423943898971	7.90130620118029	9.71608296718446
H	10.85116214308823	7.49119245282069	10.61969354802697
C	9.29086532371327	8.69704316096430	9.77138712645604
H	8.83328361345358	8.91955585849234	10.72575527818671
C	8.74181184327349	9.22033844480375	8.60538874273709
H	7.87138276024345	9.85632608128362	8.67396070334394
C	8.38594053223766	4.27855120510107	4.69540460141744
C	7.26906645932975	3.46437489091076	4.65153453601251
C	7.22224099532123	2.41487654836680	3.73634751350540
C	8.28636385254564	2.17356738312949	2.88149598439503
H	8.23760168212024	1.36354232977135	2.16964739138601
C	9.40845611405167	2.99308639865701	2.94559870728314
H	10.24025455932652	2.82021019241237	2.27703672347252
C	9.46580188414770	4.04503549903505	3.84541790214981
H	10.31938697191334	4.70824119933830	3.85762301123706
H	10.91412018147813	7.90806036602484	6.35018895052754
H	6.41871813345936	3.63005770766505	5.29425291896540
C	12.26477477362988	6.79886896201366	8.43982276516408
F	13.35752365766947	7.54082164912835	8.73172443806167
F	12.22547995071762	5.79856389930693	9.34773238675854
F	12.47218518929597	6.24209702913596	7.23677007234880
C	5.97385334383306	1.58140994118471	3.68695262357603
F	4.88968719179539	2.32535149717525	3.36131806092097
F	6.05073066169991	0.58167209130068	2.79285584859552
F	5.69739470345746	1.02261267023429	4.89015143970984

Table S 38. Coordinates of the optimized structure of geometry a with ligand pCl.

Mn	7.88746400265512	7.77414525699655	4.22648155150758
Br	10.29199879631616	7.62491849932469	3.43164531072692
C	7.42803766679674	9.05143759035588	3.08104646891143
O	7.10860336861839	9.85703826232500	2.31826433311476
C	7.24171181010011	6.60126765504365	3.04939740041155

O	6.80523044427255	5.88331443294992	2.26098913899531
Se	8.67467461307740	9.67011919497096	5.71390493082551
C	6.81744884576764	10.12345102672787	6.19556436554049
H	6.79993739997363	10.82823924668623	7.02354149518089
H	6.44884189749654	10.63496044423326	5.30797759885894
C	6.01862906469330	8.87875178837238	6.51441893229359
H	6.41185690244336	8.43352042547226	7.42435661238232
H	4.97482875751556	9.14430917474910	6.71412835118488
N	6.08083737545153	7.85144415111698	5.44346883025869
H	5.40392202041522	8.10066131717142	4.73302576761898
C	5.70284004057920	6.51539068788397	5.96437025970926
H	4.78529181220666	6.58443199332653	6.56172033729820
H	5.49675612708142	5.87875534035103	5.10673501680023
C	6.80907583659306	5.90794239858777	6.80837082702580
H	7.02694805414581	6.49760472017118	7.69640750403752
H	6.55381853667580	4.90660402249349	7.14167806047256
Se	8.52377378411977	5.87799326010978	5.84063772026884
C	9.31015480371981	8.95993670875345	7.40099066325565
C	10.44386282474751	8.15125076332434	7.34282567933691
C	10.97835071787457	7.61893273132743	8.50776176666461
C	10.37311380762022	7.89321378921683	9.72758274104362
C	9.24958203830668	8.70479357617632	9.79692016831254
H	8.79653547010239	8.92069839615588	10.75373962837878
C	8.72356887981818	9.24502854526615	8.62898810172958
H	7.86382544545844	9.89527620742279	8.70154562802185
C	8.30185349606676	4.29268081824499	4.74776994040094
C	7.26461072206154	3.38434538695080	4.90191597222176
C	7.18169805326930	2.27504588294320	4.06750430482354
C	8.14325701773678	2.08616028443875	3.08722518660541
C	9.18429914124532	2.99162223008847	2.92740151395642
H	9.91957025427410	2.84124256556947	2.15053247673761
C	9.26364503278356	4.09719599055984	3.76003340775112
H	10.04834287271736	4.82739505069725	3.61179766044893
H	10.90000648449521	7.92658292329899	6.38656739721842
H	6.50319875448065	3.51487782840150	5.65599105037199
H	11.85317391340338	6.98656984641384	8.46665046849555
H	6.37344021206280	1.56685039580993	4.17790811181823
Cl	11.03032134261017	7.21509561943924	11.19273596416132
Cl	8.03994049215000	0.69491523208036	2.04154816982074

Table S 39. Coordinates of the optimized structure of geometry a with ligand $pOCH_3$.

Mn	7.99770827428778	7.63452945953412	4.24512018621034
Br	10.44295260183283	7.56488370556187	3.55917216443663
C	7.54222077427405	8.88501189823802	3.07099719264290
O	7.22326337503882	9.67768402289830	2.29318703633814
C	7.44090415139894	6.42316956403510	3.06316780516416
O	7.04776186561915	5.67906120091377	2.27516819447813
Se	8.63351644361946	9.56860857314435	5.75894399490604
C	6.73497847799286	9.95725579630367	6.12202598137902
H	6.64491003195255	10.66874618534149	6.93968829380495
H	6.40227831328035	10.44619897781821	5.20807808344495
C	5.95960625978250	8.69049249947830	6.41068553746339
H	6.30464288790232	8.27705941914418	7.35413126680236
H	4.89586190844178	8.92184172268836	6.53316659314953
N	6.13049247509972	7.64534648964101	5.36941086659186
H	5.48159215386288	7.84233544958334	4.61793048756476
C	5.79641457148099	6.30260562293887	5.90273860224993
H	4.84745368082722	6.33577184612504	6.45268811643178
H	5.66730675661970	5.63738677986774	5.05179698207309
C	6.89114580078450	5.77358261315208	6.81220683460202
H	7.04293298370424	6.39990357846397	7.68875601466709
H	6.66733082662793	4.77112590595524	7.16486508441425
Se	8.64260239490514	5.79162979452874	5.91254992675637

C	9.18542722802877	8.87688707082949	7.48344123669093
C	10.35296373219150	8.12345067364605	7.50284592299654
C	10.83338735944616	7.59696723764538	8.69686569480849
C	10.13712618708315	7.81624519473744	9.88448766291309
C	8.97005067790350	8.58305345680618	9.86468604130858
H	8.44737770355544	8.75869190087917	10.79487096502967
C	8.50438691135193	9.11729297640570	8.67477508128578
H	7.61246427920063	9.72716444339761	8.69480962324262
C	8.51575135648450	4.17682749034148	4.84800792834081
C	7.50524112170205	3.24072182763809	4.96938798427069
C	7.48193113814984	2.11494835997475	4.14638259482595
C	8.48398301556485	1.93112493551533	3.19872715016422
C	9.50731596613359	2.87600596116656	3.08674381032134
H	10.27393395383261	2.72702356941962	2.33926519301600
C	9.52479562154185	3.98979082150983	3.90129860377020
H	10.29684218421892	4.73739801094005	3.77592819531862
H	10.88531893648410	7.92941690578683	6.57996929021788
H	6.70969725308237	3.35851501042493	5.69011933582578
H	11.73829127645606	7.00956797092543	8.68039317458673
H	6.67696275940882	1.40448434789310	4.25456934160866
O	10.51045232516985	7.33358854279892	11.09861452692787
C	11.69204932409604	6.55016047954273	11.17507927414038
H	11.60747988348794	5.64407205614249	10.56977707337156
H	12.56771174384894	7.11947855091427	10.85396421386574
H	11.80198333244867	6.27721927103555	12.22092400296735
O	8.54996797219618	0.87715364525614	2.34230412155145
C	7.52222646018221	-0.09630463645332	2.39876926369486
H	7.49025164165398	-0.58645644484401	3.37591948387308
H	6.54497912066515	0.34428026342106	2.18329210844166
H	7.76244503009417	-0.83141562905300	1.63548589405138

Table S 40. Coordinates of the optimized structure of geometry a with ligand pCH_3.

Mn	7.93298231203519	7.75727484279784	4.21922305399433
Br	10.34095005357802	7.67739841564829	3.42226793065234
C	7.43271161707377	9.01477865130506	3.07082634341978
O	7.08139392516877	9.80880401766321	2.30856291377507
C	7.32813518903990	6.55684528168429	3.04884979218041
O	6.91382808799511	5.82204527583500	2.26335682533117
Se	8.65850536763122	9.67362020990179	5.71591862002792
C	6.78564016321490	10.08138994775775	6.17503797141168
H	6.74369638176834	10.78259005504258	7.00543901674229
H	6.41712696081665	10.58727086933087	5.28424594787315
C	6.00704706206184	8.82072620630533	6.48267436794718
H	6.38669690433717	8.39199490374750	7.40569434810173
H	4.95285175201801	9.06459106529284	6.65362629742481
N	6.11781100467667	7.78417901063683	5.42449338710844
H	5.43913285613856	7.99806161009206	4.70458425024968
C	5.78798794840262	6.44121886150285	5.95980909775382
H	4.86366289695238	6.48219130562294	6.54970963668045
H	5.61394959983272	5.78576270575815	5.10940590130375
C	6.91234828533230	5.88881312502814	6.81793262314820
H	7.10674408208395	6.50183651481006	7.69540129114022
H	6.69182163009482	4.88406187456829	7.16592426271576
Se	8.62753486102783	5.89895659711966	5.85127047421291
C	9.29436380930400	8.96279551368830	7.40327092289631
C	10.46794629471433	8.21337735153764	7.34969343061506
C	10.99009320379367	7.66973951609697	8.51374699929501
C	10.36328013006505	7.85016213093647	9.74755232998808
C	9.19528891960108	8.60910089214895	9.78085629289342
H	8.69057381032997	8.77162951157695	10.72546255270201
C	8.66520361499484	9.17185376656472	8.62399398624629
H	7.76945126618442	9.77213445358935	8.69640813113816
C	8.45024801154593	4.29181911955501	4.78250440602396

C	7.42527307140443	3.37068635882481	4.92558288094786
C	7.38260421954647	2.25299676339385	4.09646808201584
C	8.35153822009372	2.03737919997337	3.12242239347152
C	9.37850077386357	2.97648904116856	3.00267475779880
H	10.14271564039909	2.83997919559670	2.24740893592417
C	9.43579939935213	4.09408031053922	3.81828844435834
H	10.21647931863249	4.83030126223434	3.68020605547508
H	10.95469712215881	8.03861750280110	6.39826815412214
H	6.64654329140574	3.49931048304188	5.66261695988358
H	11.89617380076561	7.07953500843654	8.45621872900657
H	6.57253699675505	1.54346388808246	4.21183787556447
C	10.94825848335491	7.26555652756318	11.00380044727859
H	10.19163985132144	7.15095112911522	11.77981355980438
H	11.39444961186248	6.28872206885819	10.81538391416447
H	11.73491643832821	7.91002061696283	11.40433289841947
C	8.29219509723483	0.84349237496656	2.21003261130565
H	9.22916220433414	0.28387446341352	2.22982112928046
H	7.48787767162296	0.16601761393698	2.49467950211372
H	8.12081514274930	1.15077397294460	1.17598681907107

Table S 41. Coordinates of the optimized structure of geometry b with ligand oCH₃.

Mn	7.47472174542806	7.75861920647152	4.25624985769544
Br	6.62460171521080	9.81337290664054	2.99874871801152
C	8.89553716866618	7.48597453706135	3.21369955654150
O	9.81256906143100	7.29188670869032	2.54274287160303
C	6.51411076358254	6.74302194737920	3.15856437019092
O	5.90318941536966	6.10371573188230	2.41881440080627
Se	8.65185518469770	9.56587640988592	5.64294731315294
C	6.96079776528305	10.22143282794720	6.41030366309849
H	7.17445038946753	10.84411368397346	7.27539549020177
H	6.56992612367919	10.84031380556228	5.60742605436147
C	6.02169240779525	9.08641401408524	6.75565234035422
H	6.43679165078177	8.50607879387864	7.57576907030667
H	5.06773765479069	9.49926425698215	7.10428771457749
N	5.78890331334114	8.16343856316227	5.62637586195759
H	5.20049144140204	8.62771153881331	4.93940570284315
C	5.16719573130932	6.90192580921812	6.06875954067894
H	4.32986817716426	7.09403000062022	6.75145673944160
H	4.76402576442398	6.41436277443653	5.18628830238657
C	6.16863116151095	5.99339772165529	6.76806146662166
H	6.41272319938356	6.34800386428244	7.76684904624308
H	5.80466815271635	4.97708743667496	6.85557026341545
Se	7.93666182979076	5.99564734312391	5.85023771208798
C	9.46855820138772	8.77566547829592	7.22855640286198
C	10.66203955232286	8.06171068974987	7.04375503717898
C	11.25025074903388	7.46763602650640	8.15916258471526
H	12.17012048861970	6.91238063269770	8.02492495161317
C	10.69086679185236	7.57329820127409	9.42514941940733
H	11.16875014516147	7.09759706936971	10.27078905725418
C	9.52600564464561	8.30598043925883	9.59725514813568
H	9.08714218715264	8.41829931008847	10.57978529048587
C	8.92101746845486	8.90860221145560	8.50061633862902
H	8.02701141176066	9.49101510354359	8.65964774666137
C	11.30469506483350	7.91960690004011	5.69480223129196
H	10.73226899295346	7.25573967184953	5.04719501177583
H	12.30996719287096	7.51229587644560	5.78662065250421
H	11.37681563755262	8.87687272618259	5.17512201686876
C	8.15268043264649	4.31839635600199	4.87483284246159
C	7.17886921514793	3.45307929559342	4.36577563795870
C	7.62587913158138	2.36292295528838	3.61229873990646
H	6.88575060117566	1.68581497827920	3.20505358844148
C	8.96953247225490	2.13487271348039	3.35977005408840
H	9.27026922244505	1.28637267122654	2.76034312211177

C	9.92030168151183	3.00360805635673	3.87700769004615
H	10.97386157804075	2.84662662982411	3.69063084517834
C	9.50749934666017	4.08357994318599	4.64077529190779
H	10.24690309258234	4.75866187153277	5.05220347064492
C	5.70008639058248	3.60677470504159	4.58285866143042
H	5.40899451663163	3.30212432883374	5.59036604293000
H	5.15311838142472	2.97723752108771	3.88371791619319
H	5.36998459148605	4.62749775508179	4.42215815073902

Table S 42. Coordinates of the optimized structure of geometry b with ligand mCF_3.

Mn	7.69928954923490	7.79752984969570	4.33501479449186
Br	6.72302091486501	9.75833116581262	3.01340805119687
C	9.27482162377193	7.69197674621397	3.50334170454219
O	10.30801084090051	7.60741622340230	2.99932734837980
C	6.98928485646073	6.69513049850321	3.12267745337867
O	6.54660658683439	6.01192396859940	2.30956636831337
Se	8.50116789637942	9.73648987760360	5.75431363392198
C	6.71176301119550	10.12595300286200	6.48337891951633
H	6.81015439572782	10.72190063952659	7.38701975177679
H	6.27433016608005	10.73531120443637	5.69682564726074
C	5.92050089955764	8.86062112552298	6.72846373382387
H	6.38656750643611	8.29299669669900	7.53178503341953
H	4.91098534477920	9.12432701474233	7.06577926942705
N	5.84855519767409	7.99187201823527	5.53712200963635
H	5.28739285239616	8.45078000419539	4.82319350539982
C	5.29653264556235	6.66127188307855	5.84868834955245
H	4.36022853896409	6.74319275767341	6.41438820372686
H	5.06959108579522	6.17694175566855	4.90241171639339
C	6.28454230918565	5.82635697547037	6.64993622032920
H	6.34397829412962	6.14059013141544	7.68875200054455
H	6.03290283507684	4.77013285096477	6.63727253847310
Se	8.14205457098276	6.03328102625816	5.96565920016227
C	9.36251948424447	8.94232790844862	7.30416392149040
C	10.49626507558997	8.18579635590955	7.02790000891536
C	11.15610334724232	7.52232299164579	8.05341826537954
C	10.70340353150908	7.61784490221824	9.36446054704434
H	11.21291371477399	7.08985610217312	10.15641617828018
C	9.58309618406417	8.39138618427085	9.63778630990151
H	9.22517034645286	8.47769568124202	10.65484417508352
C	8.91201999447426	9.05353453718999	8.61498024183754
H	8.04292379322201	9.64939648630499	8.85353950748759
C	8.34996570149395	4.39297683498610	4.96281706490488
C	7.28119719427893	3.68345275348246	4.43802962729883
C	7.52638895236687	2.53349909644319	3.69800080873065
C	8.82789550583732	2.10205455906491	3.46775161568059
H	9.00705893711124	1.21203419543322	2.88231849665160
C	9.89025525340079	2.82816714053226	3.98843532152562
H	10.90564022147928	2.50203190307937	3.81087180963594
C	9.65662413027716	3.97001851327698	4.74396655760173
H	10.48689428793460	4.52684568210553	5.15684872838557
H	6.26461285424922	4.01821649425498	4.56744866324904
H	10.84599228511885	8.08009572495400	6.00963830805755
C	6.36782986348992	1.72470359713812	3.18323911825970
F	5.25444391997884	2.46677879633882	3.02565053684601
F	6.63808076419196	1.14473822422372	1.99935770293499
F	6.04886343320347	0.72569410483781	4.04281223764412
C	12.35829596812323	6.68788829664140	7.70239971978520
F	13.43000898097581	7.44997175444817	7.40066826715304
F	12.72464148040470	5.86327368335761	8.69948392263134
F	12.11909799951492	5.91390850141400	6.61555731293277

Table S 43. Coordinates of the optimized structure of geometry b with ligand pCl.

Mn	7.65068842207444	7.84182655214595	4.29903369821492

Br	6.61997659898637	9.82411471753147	3.05504669465220
C	9.18661860739560	7.77490461895018	3.39096567674861
O	10.19586539452681	7.72206987639426	2.83660629793600
C	6.87833420622340	6.78225187660628	3.08913600437246
O	6.38306802803680	6.13685354602168	2.27443978466902
Se	8.50709803369812	9.74471666143012	5.73489263649229
C	6.73453861626894	10.15469201577762	6.48921191951686
H	6.85481296991881	10.75807606275187	7.38542672814483
H	6.28506268758376	10.75798721419705	5.70535204140121
C	5.94250854977698	8.89575494602140	6.76125078406742
H	6.41521869630243	8.33680456923742	7.56593081411483
H	4.93731036625198	9.16618392234686	7.10550022166411
N	5.85344438624416	8.00782296446881	5.58421000722168
H	5.25165783974140	8.44164621776160	4.88855345127183
C	5.34713270988064	6.67054059609327	5.94041945548246
H	4.44463966245508	6.74153544776505	6.56037544383914
H	5.07328167882899	6.17270986272217	5.01383660041316
C	6.39654154412360	5.86126572894940	6.68750486258778
H	6.53393442277018	6.20542232096650	7.70943744028661
H	6.14990628487423	4.80399508689715	6.71908307392453
Se	8.19373443283646	6.04286177905128	5.85264519961398
C	9.37781777968693	8.96512324810717	7.28493379192360
C	10.56683190346693	8.28218164937625	7.03439502313340
C	11.26033476216618	7.67245248894615	8.06797857338153
C	10.75551354402292	7.74058032191737	9.36062210827621
C	9.58092799929574	8.42698932124537	9.62781077342298
H	9.20563634091233	8.48276951574643	10.63947439695927
C	8.89635112410424	9.04414902724241	8.58597965143232
H	7.99108145624448	9.58697854902870	8.81434301177232
C	8.27146239869051	4.37976634123625	4.86403861353217
C	7.15454815835129	3.75546926025980	4.32338720768459
C	7.29551481734415	2.57479421666478	3.60755976979629
C	8.56137115115972	2.03530789093367	3.42327018662141
C	9.68568909409381	2.65792630603914	3.94786574038416
H	10.66432718529643	2.22707921559861	3.79510526134265
C	9.53473357368456	3.82967055796343	4.67704146387685
H	10.40714456527086	4.30952555604264	5.10011339656321
H	6.16942640279185	4.18301073362097	4.42977950216612
H	10.94970474082718	8.20988313266515	6.02451955177259
H	6.43153596004989	2.08583876221564	3.18188918760660
H	12.17951253640068	7.13914735738837	7.87376459649195
Cl	8.73977195034245	0.55724122955454	2.51977553409193
Cl	11.60542504399729	6.95167908711953	10.66104771813165

Table S 44. Coordinates of the optimized structure of geometry b with ligand pOCH₃.

Mn	7.47321117577101	7.76004661932973	4.29828546206224
Br	6.70672147313889	9.83240361467680	2.99747981265756
C	9.00717077125830	7.48233260497400	3.43226952154697
O	10.00277808402926	7.27927079386641	2.88763611157961
C	6.62787744005190	6.75698554659146	3.10240419600164
O	6.07978579802804	6.14663978924356	2.28958266882792
Se	8.48590517404262	9.60242687931968	5.73739997216733
C	6.74806206302927	10.11164460936097	6.51685500809587
H	6.91501796403478	10.67024659472806	7.43426013536246
H	6.34097723444401	10.77873311358197	5.76113306087887
C	5.85876516649444	8.90907618280027	6.74489902245599
H	6.30666052616420	8.26011504954573	7.49648135961738
H	4.89057159002455	9.24027117383142	7.14064827406203
N	5.66492963236062	8.11889437309939	5.51549323228619
H	5.15861856436103	8.67893500684272	4.83311303093266
C	4.95971800628012	6.84764925608953	5.76227796353430
H	4.04189096532229	7.01413594618154	6.33936544189875
H	4.67459920863541	6.44892206430890	4.79288362860671

C	5.83650854140553	5.84395020581472	6.50576431277474
H	5.80307329736451	5.98217765709184	7.58341891082886
H	5.55200275573340	4.82018598293041	6.28186450542732
Se	7.76151219912252	6.05028444081903	6.00531061065389
C	9.33212988858906	8.75283168109050	7.26524798132203
C	10.46736485943951	8.00151540265797	6.98858557931242
C	11.13899246686261	7.32291554117265	7.99847280999994
C	10.66599729937336	7.38830768722652	9.30896809477504
C	9.53092834217953	8.14908881338988	9.58995697873886
H	9.17903604783157	8.19832070849589	10.61125276374216
C	8.87364415298575	8.82881406125492	8.57696016628421
H	8.00224443476925	9.41547274937988	8.82963202978124
C	8.15682756138082	4.31673095376388	5.25597342538324
C	7.43026012785995	3.73516923212698	4.22826538817414
C	7.83145981612523	2.51915191243847	3.68606110612415
C	8.98185046089128	1.88993837641542	4.16433107693933
C	9.70909047131142	2.47570334034787	5.20303711609617
H	10.59530367050857	1.97335026979994	5.56494546668391
C	9.29472272962311	3.67758235329073	5.74680982027574
H	9.85997287551073	4.12794588643227	6.55191760484353
H	6.56006537916993	4.22504220482135	3.82013720595388
H	10.83137138848635	7.92137600812003	5.97204128239338
H	7.25474996924891	2.08905583228686	2.88190389434927
H	12.01635336503974	6.74595163752085	7.74963161617464
O	9.47010231415694	0.71818654215062	3.68619425850694
C	8.80447966279954	0.10489232504995	2.59212076663515
H	7.77994130672484	-0.17141197862121	2.85383045946625
H	8.79201126275641	0.76108695681814	1.71856353558399
H	9.37242602520713	-0.79228770592543	2.36260211576848
O	11.23610447188633	6.75309773585144	10.36721805116867
C	12.39890668601049	5.97455250198019	10.13634394871373
H	12.19639782309929	5.15110331045581	9.44616010070563
H	13.21485857969848	6.58507982400790	9.74125568156447
H	12.68590961537637	5.57101568217087	11.10339741227946

Table S 45. Coordinates of the optimized structure of geometry b with ligand pCH_3.

Mn	7.64923163168644	7.88940710856213	4.30383274049797
Br	6.62375762916496	9.90472383045217	3.09613010608628
C	9.21197018226047	7.84861383735550	3.44292626810636
O	10.24131593558259	7.80940170066251	2.92422122692344
C	6.91252398550363	6.86563748416648	3.04315951997142
O	6.43876223536423	6.25058759458549	2.19202283149707
Se	8.46497323923612	9.75537141381523	5.81064298885549
C	6.68017501703597	10.11652772782200	6.55961635611573
H	6.78442520757720	10.68179340610537	7.48231355946051
H	6.23207962000634	10.74806811589263	5.79728365251347
C	5.89864493302831	8.83940063875618	6.76936958002726
H	6.37572880108922	8.24899779411958	7.54849468562499
H	4.88871645599661	9.08235302321134	7.12112839461891
N	5.82502174475269	8.00785772244882	5.55129707845085
H	5.23812137820045	8.47620035801747	4.86514036947260
C	5.30821280395035	6.65772113942780	5.83598352973434
H	4.38403383480512	6.70441152378457	6.42600393208226
H	5.06864398736796	6.19689004191315	4.88121179275945
C	6.33279238664265	5.82000034192581	6.58591264360009
H	6.41689560672874	6.10713318563135	7.63083531243827
H	6.09987195680009	4.76015983819448	6.54448631742621
Se	8.16325766407866	6.06398919624845	5.83853729773012
C	9.34465093375461	8.94617638036888	7.34005323730692
C	10.55631395773080	8.31055818625060	7.07415801191714
C	11.26130064256445	7.69957266601466	8.09797900403494
C	10.78041630760513	7.69789605113872	9.40922631492840
C	9.57034802863239	8.33847227460634	9.65844153908796

H	9.17381146949575	8.35587002971569	10.66628212140552
C	8.85697218567410	8.96344248992049	8.63902537579308
H	7.92835414236714	9.46041551154565	8.87999051744207
C	8.32859006731239	4.41156515248715	4.84387324386030
C	7.26489300447898	3.79615506426512	4.19770131357100
C	7.47376716423392	2.61263994078472	3.50280922265327
C	8.73960106992743	2.03302510807091	3.42129055270330
C	9.79661297387051	2.67254809762205	4.06794054033035
H	10.78894535496305	2.24114164614864	4.02430249518743
C	9.59717791209238	3.84714175781307	4.78090149119009
H	10.42726714597481	4.31712342885430	5.29178278975631
H	6.27769368314773	4.23273235805008	4.21149515415731
H	10.94214782598732	8.27881210335866	6.06303183667334
H	6.63704398839775	2.13941300939541	3.00432101584121
H	12.19908883293963	7.20652881380009	7.87278679619398
C	8.96496051477134	0.77103547981873	2.63514525646739
H	9.76722787081285	0.17287276046764	3.06732127609143
H	8.06400054438992	0.15884522161264	2.59862125040375
H	9.24700575232240	1.00122911241667	1.60463244571087
C	11.56106909697810	7.04406976947572	10.51596421561072
H	10.93526421997737	6.86072821103161	11.38881151071892
H	11.98334852263086	6.09136032723209	10.19399444267288
H	12.39384037310750	7.67663518563470	10.83354521529662

Table S 46. Coordinates of the optimized structure of geometry c with ligand oCH₃.

Mn	7.21792954615910	7.96848098119665	4.30519979893642
Br	7.04453709393560	10.09832231003634	2.77065318843030
C	7.49716115396862	6.70241876551437	5.51171344377869
O	7.70370165905539	5.89069599134183	6.30935581890481
C	8.45786426651462	7.29413360556536	3.19886501790313
O	9.23536126995290	6.85791007362860	2.47272255387943
Se	8.71100830469249	9.52323206213083	5.53547811807637
C	7.24114239263192	10.42478823850443	6.49912270301909
H	7.61766698162761	10.79396562020651	7.44831211090593
H	7.01830759807449	11.27590710787717	5.85821841742498
C	6.02104427644025	9.53901834052074	6.66097765408736
H	6.22692946396307	8.69354875412373	7.31690210522240
H	5.21834599837475	10.13041930645768	7.11874496975208
N	5.59957562756952	9.02233002286944	5.34950865015749
H	5.57860163239696	9.80369359237189	4.69480756237944
C	4.26313440137573	8.38051890851089	5.33101414915214
H	3.72007641271465	8.62220416434194	6.24956204628273
H	3.69910983889642	8.80712730707407	4.50170551293688
C	4.32713719555827	6.87872581761874	5.15557733010140
H	4.82845669751576	6.37950036567127	5.98167845824791
H	3.33423100070799	6.45400888354708	5.02961088113411
Se	5.41165654237377	6.43746246997083	3.55406693924700
C	9.54891920160344	8.56065446688509	7.00937227468963
C	10.73104239113388	7.86902875930557	6.71089766642544
C	11.35820140477131	7.17593620941515	7.74533559263033
H	12.27263943881489	6.63822567156870	7.52834675654915
C	10.84090786231055	7.16041199857111	9.03328409922160
H	11.34959326391739	6.61136206085113	9.81405910147171
C	9.67129200986627	7.85223883891451	9.31040838955805
H	9.25408969524936	7.85033274303910	10.30848384335028
C	9.02695256959878	8.54987016517117	8.29653401135614
H	8.11455939421952	9.07591990467906	8.53040374555915
C	11.31507987754222	7.84246529382660	5.32659659411414
H	10.71097984425452	7.23484228718409	4.65234024351672
H	12.31887424715771	7.42178018765445	5.34080057049430
H	11.37492221027604	8.84172900962141	4.89072351611643
C	4.09041950670338	6.98939210686837	2.23103106627911
C	3.05178071135920	6.10451980016134	1.90030063244597

C	2.12900164122094	6.52814385545541	0.94405853518885
H	1.31763851661645	5.86385549052576	0.67366899467110
C	2.23594209223160	7.76888757397969	0.32687171598133
H	1.50581747220553	8.06315827288653	-0.41566091967184
C	3.28212745981647	8.61800758708636	0.65577734575590
H	3.38460357914814	9.58102865805651	0.17397356152196
C	4.21326233408559	8.22550305333582	1.61104608595730
H	5.03725005819775	8.87611938951594	1.86753082323739
C	2.90875261685122	4.74040055112666	2.51979914784115
H	3.82231836129830	4.15547745888302	2.41042365671170
H	2.09240573164096	4.19378851492305	2.05057370672683
H	2.69763715340820	4.79590740142737	3.58948181233973

Table S 47. Coordinates of the optimized structure of geometry c with ligand mCF_3.

Mn	7.25286907029979	7.73888045775467	4.27542268128032
Br	6.52839954901579	9.71128139464615	2.73042749779231
C	7.75034279982590	6.53343393841866	5.47252829761554
O	8.07552892784423	5.75629727763431	6.26536502496519
C	8.66796323106356	7.37722725687608	3.23544354050431
O	9.58048742214597	7.14141254124433	2.57751891158470
Se	8.31860001612802	9.61515143729908	5.45615551843769
C	6.66477515681860	10.21778771569686	6.35093117111154
H	6.92214571489201	10.75057296909709	7.26141960668888
H	6.25329100138285	10.92881618009103	5.63743916791951
C	5.70595535279799	9.07374004985654	6.60462697578144
H	6.12356701333015	8.36290277462206	7.31867492201333
H	4.78481213942304	9.48153013703486	7.03868745029250
N	5.41725769039085	8.35633349138326	5.35139309391479
H	5.16938383239644	9.04640011765025	4.64228242605894
C	4.30154241898378	7.38299195622912	5.45909389047315
H	3.98399824020417	7.31440063913557	6.50134803772354
H	3.45248015169781	7.76449810344384	4.89343094246625
C	4.65666293423762	5.98684514860440	4.97223005136528
H	5.29777960098919	5.46297767917302	5.67716629438438
H	3.76912654244972	5.38058716092836	4.80669121111188
Se	5.76097591934781	6.01290396393188	3.33818036878167
C	9.26625822174560	8.84365856260178	6.97037362280453
C	10.36679611140878	8.05733685321784	6.64406776082436
C	11.10917881112575	7.45764092962145	7.65013417484163
C	10.76907623299795	7.64270582922295	8.98726163632574
H	11.34528692393965	7.16426033344606	9.76564803240756
C	9.67630241494544	8.43381942202387	9.30508610813830
H	9.40045005114034	8.58108815922173	10.34050865249206
C	8.92330384307055	9.03642467055403	8.30152061340710
H	8.07464749132792	9.64420567755399	8.57788010455866
C	4.50123664830724	6.76824354579661	2.07474731612219
C	3.13032045334097	6.73182114844037	2.27957736460706
C	2.28059999641171	7.28623818227258	1.32796666644714
C	2.79419812360426	7.84871972729007	0.16496557338089
H	2.12887174084483	8.28406633806460	-0.56663546067445
C	4.16723061307748	7.85943460170542	-0.03830323689344
H	4.57701041691752	8.30761875768005	-0.93258278649328
C	5.02515691763816	7.33066352250525	0.91596413805028
H	6.09383959188568	7.38441952031520	0.77029884356724
H	2.70559280442874	6.28699292349125	3.16507895917677
H	10.63024662285985	7.88510565412415	5.60995948946485
C	0.79416655523875	7.24429607753148	1.54492236262316
F	0.18780779105634	8.36774302979283	1.11217020773050
F	0.21378281846108	6.21294026859393	0.88880347022350
F	0.47462668067731	7.09888382734734	2.85097302875991
C	12.30943689800346	6.62241140366580	7.29069725482545
F	13.44981529206020	7.35130537801135	7.33416119253921
F	12.47784465180667	5.58888240738291	8.14005409875003

F	12.21956194900983	6.11099336977064	6.04971741972383

Table S 48. Coordinates of the optimized structure of geometry c with ligand pCl.

Mn	7.05887803076851	7.97352703070559	4.46471592076993
Br	6.56449083532501	10.01404465055550	2.90796540039460
C	7.42635441283873	6.74971442758480	5.69060612838009
O	7.66198864777120	5.96356296048292	6.50587568244946
C	8.37689741968167	7.40487968850038	3.39295822157218
O	9.21950666675175	7.03863243690292	2.70108081903801
Se	8.39908675181889	9.69224683901673	5.62069273829589
C	6.91041979895061	10.37806784932327	6.72957314723288
H	7.30666222866075	10.71595907762837	7.68244209714845
H	6.57107811257035	11.24834907298376	6.17047231654612
C	5.78910140206868	9.36779235626565	6.88862681001208
H	6.10761040556207	8.51640851371332	7.49028372313128
H	4.95498251938811	9.85327118217150	7.41007675341399
N	5.36833272359522	8.88750781462603	5.56352304031996
H	5.29640790119024	9.68879586760047	4.93660978214329
C	4.07550754917547	8.16783447031856	5.51424393099113
H	3.52494077302940	8.32004266524418	6.44710031011978
H	3.48267412054311	8.60744883953787	4.71241059126047
C	4.22824853475428	6.68335472537964	5.25282328422226
H	4.75495907031075	6.16969314241486	6.05442991212452
H	3.26573076628992	6.19937878957097	5.10845812954506
Se	5.37447208738038	6.36506354152975	3.67296933153701
C	9.43303335773260	8.72485497518608	6.94817390666784
C	10.54403459407478	8.05059975605095	6.44772135861126
C	11.34566653625946	7.29735950026553	7.29032891348670
C	11.03058938436692	7.22279113765850	8.64134666753618
C	9.93058257011464	7.89369320093388	9.15230833525188
H	9.69565642686424	7.82393911843018	10.20448171261439
C	9.12965025303522	8.64592927370898	8.29945522754004
H	8.26935729360492	9.15039390561973	8.71328964896705
C	4.22332525422928	7.04404931787980	2.26866838753348
C	2.84918989152263	6.83418028511741	2.27886294700836
C	2.07338202437430	7.24854058503816	1.20331242418900
C	2.68895360059866	7.85407844520362	0.11583639100762
C	4.06134903936468	8.05798904330266	0.09327890395645
H	4.52478674922248	8.54068336250645	-0.75449145521034
C	4.82929436884207	7.65477014121416	1.17687146577157
H	5.89160801019505	7.84387965138704	1.17691858299616
H	2.36618174595837	6.33721699962469	3.10842069502931
H	10.78183921881030	8.09538501373335	5.39269257720697
H	1.00455360638562	7.09171149966914	1.20304407166588
H	12.20406320273848	6.76764856374558	6.90387326999135
Cl	1.72213715410487	8.36001123042558	-1.24425889473687
Cl	12.02777809417489	6.26672578124093	9.70324208626698

Table S 49. Coordinates of the optimized structure of geometry c with ligand pOCH$_3$.

Mn	7.24543658335562	7.86485365691792	4.34150846752715
Br	7.21886825619558	9.90667722113491	2.69158890045725
C	7.38129845048203	6.65256196666328	5.62270983728836
O	7.48673166783137	5.87023734910411	6.46879950873134
C	8.58059023342184	7.09546376487057	3.42420364946324
O	9.44682367182990	6.59541006228803	2.85650683469374
Se	8.70272056527404	9.44023910417087	5.56073775189265
C	7.21360921377426	10.42174593116394	6.40740784530715
H	7.55299252461916	10.83378408385051	7.35306240828287
H	7.03671158469724	11.24257008511959	5.71471459939900
C	5.97484895279364	9.56209158844026	6.55898001672954
H	6.14803271729238	8.74204376927569	7.25593903295773
H	5.16497516886398	10.18170200073213	6.96370202213787
N	5.59314487566782	8.99710101932533	5.25420882613086

H	5.61216224068133	9.74890210548683	4.56653053288975
C	4.24598063368532	8.37550972769172	5.21448251630239
H	3.69240409875580	8.63059896058173	6.12267444426036
H	3.70118118863524	8.80718720894109	4.37511272275691
C	4.28714554119955	6.87097852799825	5.04792611011776
H	4.73815645184580	6.36649798179080	5.89923796619223
H	3.29342088375736	6.46472522855597	4.87294813768094
Se	5.42824814367057	6.38934008190604	3.49733409803097
C	9.40188836234847	8.47714977067374	7.09443977184426
C	10.42001449213192	7.57442266397767	6.81960852205481
C	10.98866770820262	6.81184516191047	7.83187085208950
C	10.53157079318022	6.95149643083056	9.14182284284971
C	9.51302897045956	7.86312887541375	9.41919351963118
H	9.16732560156134	7.96142979082982	10.43892061411829
C	8.95265384937541	8.61878185168204	8.40294768881227
H	8.16152967885135	9.31002584207108	8.65260736596111
C	4.18563836140042	6.99777122212661	2.13506900299226
C	3.19255598784822	6.11085184717061	1.73846089996218
C	2.24185953047117	6.48656940093890	0.79488763707948
C	2.29609406562410	7.76395134630045	0.23544409698337
C	3.30844727337860	8.64545416032130	0.62125488057671
H	3.34709658749295	9.62513813874987	0.16513488462317
C	4.24842939575881	8.26690618722688	1.56379166042239
H	5.03947597951309	8.94894587149195	1.84179567277577
H	3.15226774750751	5.11595603375087	2.16272084017648
H	10.77168473947148	7.44204124141388	5.80414871954126
H	1.47871110266587	5.78108064752116	0.50417354270862
H	11.77255852463349	6.11264647264550	7.58539453839824
O	1.41724854446779	8.23329268567068	-0.68748425419830
C	0.38803613323644	7.36913848113266	-1.14114689462294
H	0.79981846277512	6.47556998420421	-1.61728694328996
H	-0.27211015097932	7.07166325918672	-0.32209882059843
H	-0.17937106726218	7.93815213440222	-1.87240390604178
O	11.00945935321553	6.24942627253930	10.20275433212095
C	12.03728467809761	5.29975694610797	9.96878322005700
H	11.70653747876320	4.51861568388801	9.27962068102837
H	12.93638834401440	5.77716779748180	9.57031474915383
H	12.26209243946433	4.85764300432906	10.93540394155965

Table S 50. Coordinates of the optimized structure of geometry c with ligand pCH_3.

Mn	7.03603710066534	7.94103579347752	4.49212243138995
Br	6.59372215868814	9.95939029903991	2.88527844500252
C	7.36570567400263	6.73408126134188	5.74413027939737
O	7.57473445262598	5.95614116210753	6.57492202613754
C	8.37053547584387	7.33356244442833	3.46422653805863
O	9.23512166685594	6.94541336405772	2.81163377297086
Se	8.39666590329251	9.65393418065330	5.62808972843837
C	6.90713580228039	10.39560716106918	6.69698008692779
H	7.29762437505772	10.75022768439862	7.64620028791334
H	6.58936958534420	11.25624232255501	6.11089649487631
C	5.76688905510603	9.40946134465600	6.86865243958408
H	6.06463103314496	8.56887377167163	7.49561227583223
H	4.93501661796764	9.92188699451808	7.36788118160571
N	5.35092606037325	8.90071753633926	5.55283702271131
H	5.29117002839783	9.68653257747609	4.90542129931226
C	4.05184527910577	8.19180889294489	5.51748441986656
H	3.49798667371199	8.37618819103027	6.44278518634370
H	3.46684191351126	8.61162684265829	4.69943959394340
C	4.19446473505122	6.69961626844078	5.29917714626980
H	4.72296953618269	6.20638832764347	6.11200344013735
H	3.22789814844051	6.21873353790462	5.17350988292124
Se	5.32302392750366	6.33856189531334	3.71539634452008
C	9.39571804758404	8.70325850372003	6.99396295973481

C	10.50394703522436	8.00052902016266	6.52900133856846
C	11.27605049290119	7.26099144840130	7.40995535674300
C	10.96802514983134	7.20501970433123	8.77033744608476
C	9.85640825347000	7.91411239441384	9.21626300648726
H	9.58745630099225	7.87950462036361	10.26486876877565
C	9.07170092119488	8.65872244237226	8.34097825569867
H	8.20896993275125	9.18049814026448	8.72851119380090
C	4.14603913976439	7.00613891540393	2.32566872631990
C	2.77509760524247	6.77930480033775	2.36121271764598
C	1.97914268564390	7.19783513418778	1.30247164318502
C	2.53328350702529	7.82856803072224	0.18863725929197
C	3.91298815459543	8.02614776393823	0.16552496364291
H	4.36913722652414	8.51464197126597	-0.68635199665021
C	4.71901824639701	7.62638876793671	1.22280538030577
H	5.77962139727736	7.82363448775212	1.19873945050363
H	2.31652438653309	6.26653413819946	3.19539973685772
H	10.75563349939334	8.01244461332449	5.47603690216086
H	0.91156742930160	7.01856597104739	1.33949810012827
H	12.12872133942257	6.71067364610222	7.03190967709364
C	1.66383407681612	8.30438010180760	-0.94268969827532
H	2.19944101740947	8.27970117730920	-1.89162681388731
H	0.76761022040270	7.69146121460356	-1.03997426228390
H	1.34018387024924	9.33541574161776	-0.77778628126226
C	11.82389340450406	6.41553252648837	9.72199614449410
H	11.26433712023729	6.12223922006992	10.60997362018195
H	12.20960144041830	5.51192566074582	9.24934263556183
H	12.68438193973847	7.00263655538325	10.05354304593081

Table S 51. Coordinates of the optimized structure of geometry d with ligand oCH_3.

Mn	7.03686746450125	7.87349673057577	4.41127574289588
Br	8.77752804453529	6.28988437680831	3.36145515323618
C	7.19797418498309	6.73105374044325	5.84673060130058
O	7.34931846942473	5.99569030391558	6.71540377058211
C	7.27272863160349	8.85060749390422	2.86626150291828
O	7.52450962411150	9.44107113297523	1.91333289924313
Se	8.58521232314985	9.45574603058625	5.52124978752555
C	7.17421042002852	10.36548703333407	6.57974156871188
H	7.57550883975458	10.60600257727437	7.55985901798455
H	7.00766503328215	11.30167528670285	6.04615933089628
C	5.88852480119780	9.56465598798260	6.66521534373594
H	6.02139740706697	8.67057478497902	7.27147325535843
H	5.11727927162169	10.18326342001652	7.14153295042916
N	5.45771532757579	9.14164214845835	5.31867531926632
H	5.45157563765922	9.96969215868142	4.73574581400049
C	4.08583563658459	8.57093223807525	5.26544797335428
H	3.49954645472581	8.93155451584082	6.11708741351100
H	3.60815789074524	8.94963336263915	4.36304785318774
C	4.05816401198394	7.05647331035086	5.22541510049155
H	4.46519403536691	6.60273887605105	6.12635574817517
H	3.04324543378283	6.69529100970425	5.07295586587777
Se	5.21173852226980	6.38611107719491	3.75289338868520
C	9.56471989432749	8.54056795702527	6.92815227675953
C	10.83860944408959	8.06674554783233	6.58930605725253
C	11.55197750538843	7.38838264252788	7.57719815005248
H	12.53702061597703	7.01030372666401	7.33496220381818
C	11.03139767631688	7.18751678689141	8.84867102138324
H	11.61012763893039	6.65375845864390	9.59042396884494
C	9.76678781514232	7.66532766713757	9.15980933738066
H	9.34382234468013	7.50459670775370	10.14224359223495
C	9.03158771854035	8.34008976872001	8.19370152041367
H	8.03786435367178	8.68355144539936	8.43862287019326
C	11.42161477948784	8.25629622778887	5.21848599234297
H	10.82393655882356	7.73386805871756	4.46693886439582

H	12.43621204697713	7.86433216131446	5.17502809436900
H	11.45361941323002	9.31325779844536	4.94344284862863
C	4.03459672893531	6.98385469160979	2.31294036320570
C	3.04614968838373	6.10638921814057	1.84201337500198
C	2.21406426503707	6.56000599534358	0.81773051361787
H	1.44633853126084	5.89758236862489	0.43789652924815
C	2.35354564690855	7.82975070605310	0.27191079236811
H	1.69503911146940	8.14776574837534	-0.52546343274063
C	3.34307686656127	8.68024920522489	0.74321130537601
H	3.47151807726487	9.66620594306243	0.31731348185961
C	4.18343550732252	8.25011817558994	1.76310439829658
H	4.96874111883093	8.89723965597004	2.11980787055177
C	2.86384529639973	4.71726997046996	2.39108518331224
H	3.77667496364185	4.12897771295107	2.29480221781258
H	2.06456447150710	4.20078817906360	1.86211757913334
H	2.61037445493851	4.73088987816442	3.45261762351905

Table S 52. Coordinates of the optimized structure of geometry d with ligand mCF$_3$.

Mn	6.88401815000630	7.83507395234387	4.53226074119153
Br	8.92338030381178	7.12701574284037	3.12234279549980
C	7.44459636671477	6.60666018207343	5.77973649152331
O	7.82816840102655	5.82662360859154	6.53135110407176
C	6.58652841975269	8.98816783369176	3.11400145544042
O	6.44392595133634	9.68160513920698	2.21268327865246
Se	7.94450582528378	9.65539331636793	5.81262721247142
C	6.44392852635385	9.86819591409318	7.11655483489220
H	6.86421590948901	9.94267836872075	8.11381272678215
H	5.99241166969123	10.82722689357044	6.86393441111703
C	5.42376828218644	8.74746435431480	7.02821711795426
H	5.81917785788850	7.82607140164565	7.45087719419578
H	4.53776171929150	9.03481530492792	7.60855530345681
N	5.06875719429781	8.50395957699653	5.61736306935955
H	4.87886803662799	9.40808802856403	5.20231015847071
C	3.85683801388866	7.68117732487821	5.39057859638761
H	3.18258686956385	7.75704097913082	6.25014563578143
H	3.33665133781700	8.10894304985698	4.53532923446784
C	4.15424065669164	6.22077741511378	5.10917743715783
H	4.62173461291195	5.72359017922803	5.95755997087638
H	3.24730274733691	5.67511311268160	4.85806888368217
Se	5.49802756243614	6.00099865766084	3.67627922244182
C	9.33047242657775	8.97939169237977	6.99986535313134
C	10.21327697624794	8.02773568747580	6.50009951658508
C	11.26569859447999	7.60474696378684	7.30148233124847
C	11.43533584766113	8.11105860178444	8.58715450078962
H	12.25598381763330	7.76637031729470	9.20047862838640
C	10.55492568019501	9.06793379863533	9.06669216034656
H	10.68793325625080	9.47902668709873	10.05813553631296
C	9.50967621050814	9.51747864572669	8.26747595718873
H	8.85722607919116	10.29490108227024	8.64022307789986
C	4.51464985226031	6.63902112204509	2.13297806181342
C	3.13670015937886	6.79998696180441	2.10168915889918
C	2.53343448980451	7.29500799330808	0.94855977422173
C	3.29449702216876	7.59677038468635	-0.17453170337188
H	2.81819473302711	7.98632738096748	-1.06258363204631
C	4.67002056583634	7.40786025128110	-0.13812168309604
H	5.27076218249669	7.64784914510058	-1.00423244720552
C	5.28569330512718	6.93703253952118	1.01223118461831
H	6.36255593233693	6.82890571165322	1.05048270450742
H	2.52147989583529	6.55764784988931	2.95399381222984
H	10.08145136632248	7.62275112668589	5.50431645389693
C	1.04166208581715	7.47857009196619	0.90101762743396
F	0.69229898801602	8.58882861299667	0.21987621601993
F	0.42217161853133	6.44097851556229	0.29394623968185

F	0.50090213701357	7.58470679651137	2.13558928256396
C	12.24864152195870	6.57899957960037	6.80067689459410
F	13.52061551920395	7.03545324651713	6.90149588881571
F	12.19532356291373	5.44318752510634	7.53579403807369
F	12.04347161579935	6.24125454884279	5.52298449858508

Table S 53. Coordinates of the optimized structure of geometry d with ligand pCl.

Mn	7.10906437042869	7.97274716415919	4.37052139667624
Br	9.03762235724225	6.70637163344392	3.23395247740884
C	7.32792501099603	6.74119050829677	5.72331645357444
O	7.49644847062540	5.94445191307516	6.53283968470910
C	7.23566924524342	9.04527051030383	2.87404589985508
O	7.40069780721922	9.68836464862074	1.93696271940785
Se	8.58641708112931	9.55891749169386	5.57234905043753
C	7.10348023461368	10.41776176658206	6.56652739392104
H	7.45980274674911	10.75939754458797	7.53277242493358
H	6.87303535737249	11.30232415346353	5.97111263729880
C	5.88848968481166	9.51940543445521	6.69055657643155
H	6.11535150098499	8.63740849920023	7.28817770851604
H	5.08741539144886	10.07365122556247	7.19568553391362
N	5.45111354775354	9.07648495287055	5.35261934919072
H	5.36531604104559	9.90877947231673	4.78285677128589
C	4.12595931804431	8.40000671575080	5.32086830808911
H	3.56402417382546	8.63983710511862	6.22869179033353
H	3.56707836216858	8.81186424060829	4.48144506979315
C	4.20739494246561	6.89547458994215	5.15389875679078
H	4.66009834100233	6.39987045469623	6.00960890455554
H	3.22018578351809	6.47296578906270	4.97965983666593
Se	5.38130313156882	6.42075163684203	3.62139473830341
C	9.47902356552165	8.58324015736957	6.99604681174857
C	10.33828832858634	7.56641623040910	6.58867609784219
C	11.04634928141109	6.84050437668323	7.53494578564473
C	10.88793601570929	7.13409915799349	8.88318876467863
C	10.03319393641176	8.14505253954273	9.29574929717783
H	9.91829811707566	8.36147605207816	10.34784215415333
C	9.33032295266385	8.87577195380326	8.34432416786216
H	8.67629325950172	9.66464047248439	8.68468828576519
C	4.15757608676494	7.05232243784936	2.24498694019813
C	3.24283892310961	6.13725338733970	1.73022790888802
C	2.32982592245389	6.52788339159131	0.75976977814092
C	2.34569893089727	7.83988747681622	0.30390518148020
C	3.26186469127727	8.75834154586476	0.79771289709507
H	3.27022691157139	9.77052712234925	0.42030415050256
C	4.16882331364717	8.35747086452411	1.77090823292500
H	4.89258067701737	9.06522065703706	2.14168441641221
H	3.24381660424944	5.11423741779219	2.08199048315958
H	10.42428081833077	7.31032327577773	5.53958234678863
H	1.61758080342387	5.82303355141058	0.35592358505607
H	11.70486784656288	6.04181779986867	7.22607552572945
Cl	1.20262291454285	8.34039352263819	-0.91065007724589
Cl	11.76778953301215	6.21849253612342	10.07850017490534

Table S 54. Coordinates of the optimized structure of geometry d with ligand pOCH$_3$.

Mn	6.99032990861493	7.78171236192328	4.42651759622630
Br	8.86510872007391	6.35850228749434	3.37041860089034
C	7.08034549753552	6.55547804850316	5.79247738411893
O	7.15812957264393	5.75054974608748	6.60951331664374
C	7.23657427949127	8.82530415912416	2.92334944800869
O	7.48015077325852	9.44687293607666	1.98915217580852
Se	8.45904103708243	9.35824028964373	5.65218156321959
C	6.98148695499170	10.17328109702352	6.70934648225569
H	7.34179154075240	10.36221575593712	7.71542249486148
H	6.79297083486336	11.13414794478425	6.22958156449114

C	5.73160479294733	9.31781460704972	6.71964572306591
H	5.89606790434036	8.40024476840672	7.28206889386011
H	4.92415011230994	9.87551444283895	7.21148199527066
N	5.34839929510293	8.95909845763968	5.34007137869456
H	5.34261708138109	9.81862745846968	4.80459388325464
C	3.99092912119392	8.36619425643178	5.21163084887746
H	3.37781160821934	8.65109454381434	6.07276153406270
H	3.52391187126687	8.80052207285879	4.32881543281021
C	3.99708320870086	6.85855792911389	5.06137950681394
H	4.37925464114923	6.35025540382304	5.94383106864822
H	2.99866082099527	6.48782986194125	4.83972492947949
Se	5.21879382449358	6.31337589184665	3.59104831933403
C	9.43187557923725	8.46906483986138	7.07724451105323
C	9.98076297942631	7.22071349178788	6.83021243706549
C	10.75572651725543	6.59403460677126	7.80098220315920
C	10.98029960063317	7.21945134093430	9.02527384553014
C	10.44489028054096	8.48885780740358	9.26030622894799
H	10.64375151852123	8.97146232399923	10.20720155701476
C	9.68875391040838	9.11415128606328	8.28576786537466
H	9.31310370406741	10.11055768006496	8.47627052370455
C	4.12080735339331	7.01106142611511	2.14897475159977
C	3.22231122710008	6.14138198022938	1.54485962227280
C	2.38773940785222	6.57560009060337	0.51965259521881
C	2.45886098202973	7.90015449687851	0.08840215814615
C	3.36819023453250	8.77451628966760	0.68944629068051
H	3.42010337612244	9.79441577979183	0.33444145218202
C	4.19125268852618	8.33097029344104	1.70831185908635
H	4.90155734208427	9.01220645386623	2.14883063954274
H	3.17035308644294	5.11025718483442	1.86861420993190
H	9.81245159393457	6.72681973223298	5.88151936053227
H	1.70161066265312	5.87727901355854	0.06570442032231
H	11.16565710115196	5.61922069472950	7.58680628449219
O	1.69819645943514	8.42670089305330	-0.90388797029356
C	0.75287282860697	7.58672395640183	-1.54851966239315
H	1.24238599017671	6.74593151864066	-2.04613428676955
H	0.01120749327020	7.20792999438665	-0.84047361286720
H	0.25912612709996	8.20751176432353	-2.29081101850556
O	11.70548519822785	6.68419311235796	10.04241925914891
C	12.28403364076490	5.40262446819671	9.84900749113224
H	11.51826047294835	4.64481342099539	9.66565638944737
H	12.99251251288841	5.40854610897343	9.01687264680514
H	12.81032705025880	5.17004171700327	10.77067049574078

Table S 55. Coordinates of the optimized structure of geometry d with ligand pCH_3.

Mn	7.10960760998020	8.06178078066132	4.40552640339249
Br	9.04101463622966	6.81715809050679	3.24359806066538
C	7.35103541244006	6.82585105056194	5.75121992091693
O	7.53108666138653	6.02393609650857	6.55337857227723
C	7.20793088557141	9.14033109772523	2.91218055657222
O	7.35464450427287	9.78693251015971	1.97393592985480
Se	8.57570951993019	9.65437779457943	5.61689001627013
C	7.09451802508942	10.47467497012299	6.64462636647733
H	7.45678188680024	10.78394391802988	7.61984055327341
H	6.85742598500411	11.37797070927509	6.08084190253793
C	5.88193164512538	9.56948871127730	6.74540700922571
H	6.10951714004042	8.67625736027605	7.32558615222906
H	5.07647664458605	10.11047355517494	7.25850183432453
N	5.45142172300605	9.15250631724427	5.39714430018956
H	5.37181653377752	9.99443407543444	4.84071762013578
C	4.12726992844152	8.47821771618726	5.34195504405037
H	3.54282955512569	8.73049989007071	6.23263368446919
H	3.59154424921382	8.87935944493051	4.48238167658985
C	4.21323101101821	6.97231748150587	5.19422031155007

H	4.66232282612599	6.48940273041444	6.05931738489818
H	3.22823173722778	6.54512005049201	5.01888815059302
Se	5.39504052019234	6.48404697989940	3.67253783400550
C	9.49087634788613	8.64659304190402	7.00206600349235
C	10.41584015058702	7.71005191843440	6.54671103812777
C	11.12065105236920	6.94704005249726	7.46233169424771
C	10.92366010795852	7.09176314019031	8.83749363777230
C	9.99690234358874	8.03573459550579	9.26783790381884
H	9.82143229109945	8.16774478608700	10.32837495277511
C	9.28237085490270	8.81499153122022	8.36122793090389
H	8.57151516434817	9.53400091030572	8.74122388795493
C	4.17452482202782	7.06233058782446	2.27269545219991
C	3.29446194121419	6.11481372352458	1.75845510443296
C	2.39792072560409	6.46893622721067	0.75894585800163
C	2.36633365624746	7.76582240186170	0.24634245818382
C	3.25804136162609	8.70159164155654	0.77038901006021
H	3.25783543315225	9.71345132443212	0.38407150562236
C	4.15706669382813	8.35743530985383	1.77202745108789
H	4.85106917483999	9.09382188878089	2.14496015884935
H	3.31327193146426	5.10032583296916	2.13445951570591
H	10.54752320206985	7.54436559404152	5.48512805076090
H	1.71785264643780	5.72300607047622	0.36647138425147
H	11.82632195537803	6.21118700614306	7.09688733751715
C	1.42510222603806	8.13546871016703	-0.86655912080853
H	1.91692691310490	8.03603751805331	-1.83756959769870
H	0.54732831821586	7.48973326187368	-0.87657838541431
H	1.08949065428509	9.16877616323273	-0.77703133154652
C	11.68323990303946	6.23679331352398	9.81419948640623
H	11.44955299828412	6.50557423163469	10.84380192643762
H	11.44097933174949	5.18039428279352	9.67942034270769
H	12.76101021806725	6.34054352686298	9.67433472265106

Table S 56. Coordinates of the optimized structure of compound Mn(oCH$_3$) in S$_2$ state.

Mn	7.67156823296390	7.65248830236069	3.96566996017257
Br	7.20041258249021	10.05057724020106	2.52801089020525
C	9.23312650720767	7.68209935192689	2.95356314435395
O	10.20420480804340	7.72187489637691	2.35746884331785
C	6.74968646162676	6.81408034838398	2.60949474558727
O	6.17968042558601	6.26879636275100	1.78301186467791
C	7.98880537544442	6.26765166697037	5.26357947732271
O	8.22692676214136	5.31240627543027	5.84223587952010
Se	8.74532477798603	9.49137021528300	5.45817284798340
C	6.97628648686286	10.12787856927429	6.02824222466769
H	7.08308990291433	10.68271707321341	6.95608438077258
H	6.70257637753224	10.81473094766358	5.23138189434634
C	5.97705618041971	9.00235738481654	6.15631895596305
H	6.28734491318149	8.28509542872087	6.91663333818409
H	5.02485069689090	9.43699527534773	6.47260373665736
N	5.80456141502950	8.26192943466355	4.89145142797929
H	5.48720385270313	8.92592150590322	4.18437988133499
C	4.79260046268721	7.19194965808514	5.01881470309701
H	5.19020444067648	6.43889311902774	5.70315772095569
H	4.69307808998576	6.72131015005188	4.04492622318912
C	3.41282664439618	7.62357259127713	5.49568468087257
H	3.41357189050002	7.99887461365288	6.51713875191866
H	2.74111463928894	6.76979003343874	5.46066053176837
Se	2.63180355993430	9.09709723627818	4.43151226274752
C	9.33582790864122	8.61811651554950	7.09769614531328
C	10.52482228692737	7.87699756361267	7.03208572910322
C	10.96864459834779	7.24793639634050	8.19447038637751
H	11.88544959791324	6.67342355969631	8.15405344579646
C	10.26929053987376	7.34220504798058	9.38958869988578
H	10.63756007227781	6.84008085589812	10.27379565229968

C	9.10273509102873	8.09071838678068	9.44156965983049
H	8.55069179775108	8.18534643211331	10.36705085135235
C	8.64052959485960	8.72909938512332	8.29735976552940
H	7.73870331378638	9.31723758502395	8.36325183654291
C	11.31129720044889	7.73509340972556	5.76007155048023
H	10.81733736070415	7.05408636243431	5.06583163223470
H	12.30359790986152	7.33692854981075	5.96335767295222
H	11.43272749965031	8.68879951526360	5.24338324226165
C	2.86697018540184	8.34166567772083	2.66363223721540
C	2.15899461608563	7.20987161171357	2.23098883915149
C	2.39385186476889	6.76137234484492	0.93031585536963
H	1.85984442857980	5.88747742115570	0.57786581931158
C	3.28464257039660	7.40745774475597	0.08318226393953
H	3.44685444300938	7.02761873911363	-0.91672452090699
C	3.96695071553743	8.53171364057517	0.52375097075195
H	4.67986058594387	9.03693358096709	-0.11268578121096
C	3.75583956320846	8.99635983382485	1.81432179936829
H	4.31099763413751	9.85353033912796	2.16548609288618
C	1.18207310167413	6.47175842936477	3.10268293535852
H	1.69001124974094	5.75114016498060	3.74911496123466
H	0.47232599211958	5.91241560093398	2.49470234148023
H	0.63048479082435	7.15493662446011	3.74766554848963

Table S 57. Coordinates of the optimized structure of compound Mn(mCF$_3$) in S$_2$ state.

Mn	5.29905464096725	8.82787160656309	17.95362165802887
Br	6.39843044742096	11.02392697937291	16.96108856121668
C	5.74589635908900	7.88601714527002	16.45906542583582
O	6.00168767294545	7.28982602772983	15.51695427152174
C	6.92549782479107	8.50781232851302	18.81779249436728
O	7.89295473156626	8.35045136527898	19.39785959825611
C	4.28336867905026	7.39923658366901	18.85528370392448
O	3.75996516172188	6.37917760681804	18.88981717727496
Se	4.76866163771930	10.63993411862270	19.83416185612258
C	3.31227408403071	11.35129953398322	18.71916621821347
H	2.63459621563076	11.92443058363050	19.34507847086488
H	3.82788134632898	12.03304832797735	18.04688881414580
C	2.58549319242135	10.26383866232334	17.96388384538378
H	2.14202425995805	9.53974477500026	18.64824421148512
H	1.77236719789747	10.73183352126932	17.40272087186110
N	3.48187079769934	9.53035249729427	17.04379505143509
H	3.89319446428233	10.22003625035815	16.41322830126737
C	2.73295285559544	8.56373333716023	16.21113131578074
H	2.27150941835908	7.83107668131244	16.87533100779543
H	3.45358339396781	8.03166294294094	15.59867208436379
C	1.67097133746358	9.16432970854988	15.29834404141651
H	0.81422367270468	9.56379446619204	15.83733489364291
H	1.30505626876726	8.39726181628843	14.62006999907946
Se	2.32736013720809	10.69318009523849	14.22433082222852
C	3.72405787604167	9.68815320232323	21.15426993777474
C	2.41596957432206	10.01339006413050	21.47666092039232
H	1.90797273343747	10.83530954697237	20.99582600984352
C	1.73544762440748	9.26759926800077	22.43630389112886
C	2.35951342645747	8.21308872365747	23.08926220458300
H	1.82283364500108	7.63997299081812	23.83031373559941
C	3.67535327219123	7.90044498681205	22.77021216497759
H	4.16920562211903	7.07766836606902	23.26832289622728
C	4.35390978728624	8.62463595391634	21.80121699471098
H	5.37150872121821	8.36108586232173	21.54744826502920
C	0.32534509502922	9.65793974095998	22.78070236154230
C	3.84539758962196	9.80967765294796	13.41800483318763
C	3.66230817109876	8.70005443733256	12.59739805558707
H	2.66999054226564	8.32814492894176	12.38954861375565
C	4.76799487851185	8.07988937235042	12.03127968836885

C	6.05160129809258	8.56790722260705	12.26659284690451
H	6.90541005796581	8.07599129038059	11.82308852974159
C	6.22275946889578	9.68149638635126	13.07206799983924
H	7.21463587785918	10.05898255148719	13.27716541378341
C	5.12305737892323	10.30368965355282	13.65322747691653
H	5.27281329212021	11.14600832666229	14.31175791836999
C	4.59319084133255	6.84922275783011	11.18581520330258
F	-0.39233005327525	9.96568217806349	21.67554925285514
F	-0.33610909738555	8.68048973634347	23.42501381739885
F	0.28971046927744	10.75175664323111	23.57545117866518
F	4.87109412820883	5.72332744170703	11.88303546569174
F	3.33350361592930	6.71832280074141	10.72229411144286
F	5.41359836545756	6.85150095212529	10.11491551685616

Table S 58. Coordinates of the optimized structure of compound Mn(pCl) in S_2 state.

Mn	4.34213776471903	4.52136710709326	10.54759140961943
Br	4.94804509162166	3.80288848738597	13.02816836518070
C	2.56257550423469	4.25928204541016	10.84545739364920
O	1.44072529316849	4.11356203741135	11.01562028902929
C	4.65723282139112	2.74647183383583	10.05415339178935
O	4.91565081330179	1.67955601226396	9.75044274212188
C	4.18316010449811	5.27157303647463	8.73235099503682
O	3.59177999773771	5.71820785400555	7.85665260090967
Se	6.98243828348301	4.85159224338767	10.63932918326611
C	6.72185311326615	6.53309486654549	11.62644995078588
H	6.61462904415039	6.20220181614943	12.65670083836013
H	7.62291501175874	7.13344092072521	11.54269836619595
C	5.50606261029917	7.29332749822998	11.15339258669569
H	5.45551864508671	8.22979535146308	11.71536559116990
H	5.59080358900516	7.54437117514577	10.09517185306776
N	4.25835988650107	6.52122981495699	11.33982143252516
H	4.19699667201843	6.28382256149337	12.33096847268823
C	3.06439968173866	7.32729494113788	11.00413943329557
H	2.19443268457925	6.68911738745391	11.12286561197264
H	3.12504246947907	7.59778739695825	9.94863383038374
C	2.86085818024879	8.58310163323759	11.84191080560803
H	1.88871867262612	9.01303237139886	11.61235662931532
H	3.61212912954869	9.34938212757856	11.66142407780368
Se	2.94779060078914	8.24852358795610	13.79236497334779
C	7.47717787567120	5.56941187105505	8.91194040914417
C	7.16327423896767	4.79320577950472	7.79809332827184
H	6.64010677752665	3.85465372716389	7.91732126317375
C	7.51769539675834	5.21412842389210	6.52409929866032
H	7.27579483849962	4.61281263786425	5.65996184843302
C	8.17426863882501	6.42710150553687	6.36683706590740
C	8.49093379740538	7.21226688833307	7.46677448217757
H	9.00863993449312	8.15055377104219	7.33012803068017
C	8.14623963486111	6.77543304409361	8.74039809641808
H	8.41657994665380	7.38811777400194	9.58806112349952
C	1.58426484474336	6.88256962289062	13.86336146721735
C	1.93135988748599	5.58406169413774	14.22007039349781
H	2.95896217750159	5.32400310482617	14.42873371602857
C	0.96140789712636	4.59040575348632	14.26812272710666
H	1.23410193060766	3.57717376884540	14.52368386882639
C	-0.34994978364747	4.90543946777538	13.94783334335863
C	-0.71123679896535	6.20005515784528	13.59230524770851
H	-1.73957414907951	6.42719403022900	13.35139229356121
C	0.25955244326915	7.19062415133257	13.56078247672097
H	-0.02001054813710	8.20347040459893	13.30444647655431
Cl	8.60705482844705	6.97115533576221	4.76959668374473
Cl	-1.56701147426825	3.65983397807924	13.97982453548268

Table S 59. Coordinates of the optimized structure of compound Mn(pOCH$_3$) in S_2 state.

Mn	4.81116835737479	4.39476399191643	9.94799991143219
Br	5.24828144249610	2.07960523303415	11.57786899369667
C	6.37310904523728	4.99275693161565	10.73793611341612
O	7.34309900480644	5.38822104241187	11.19226323952587
C	3.73972632189722	4.96962437665948	11.35368351481247
O	3.03583161460656	5.30187775918281	12.18663353268052
C	4.47058894573928	5.77830399628075	8.65535408110263
O	4.36345765924159	6.77611248646572	8.10786696020716
Se	2.88200763996772	2.80296955546210	9.41512637528201
C	4.01422789054169	1.63433079397337	8.29187866545364
H	4.39584739439436	0.89637881107222	8.99265387565749
H	3.36274872805573	1.15884779718388	7.56341931637177
C	5.13346353398513	2.39194309044626	7.62046324761619
H	5.75219596841080	1.66668978460193	7.08437094588487
H	4.74422410127595	3.09735458374769	6.88630096524462
N	5.95720754813625	3.14992634204577	8.58412818833724
H	6.32610048349778	2.48146896547041	9.26302229022393
C	7.09516149284266	3.82353158867829	7.92608889933830
H	7.66497531259943	4.32948764787255	8.69978647528733
H	6.68958638226396	4.59521690389133	7.26710429888044
C	8.04226661732818	2.93271528517834	7.13348238871629
H	8.89594369534492	3.52422265387849	6.80984163152853
H	7.58295191687062	2.50226996165000	6.24544468491690
Se	8.71908732208573	1.37568187417653	8.15254244076939
C	1.68553584725374	3.47555691568493	8.04195099436550
C	0.33851045509651	3.16952012213419	8.18683350199526
H	0.01032577480635	2.57020326463006	9.02568199743133
C	-0.60227199908712	3.62118979445542	7.26606246155723
H	-1.64195301115255	3.37011619758459	7.40855866001768
C	-0.18747708878948	4.38444274173794	6.17601176887448
C	1.16776051040512	4.69423932222587	6.02656919700267
H	1.47244336584621	5.29561478466825	5.18128941418422
C	2.09039023114320	4.25059533737586	6.95485750475144
H	3.12678504442225	4.52313182490905	6.83212699386909
O	-1.01574528303957	4.87010626803069	5.21840117898204
C	-2.40621709186198	4.60579854588442	5.33112571768254
H	-2.61003084985220	3.53260334811052	5.29914551374407
H	-2.87173069384527	5.08745051882866	4.47599680407719
H	-2.81585986439834	5.02604476841933	6.25291392278141
C	9.42367922175152	2.34042394870777	9.66684359085197
C	8.85133180147544	2.15993433989828	10.92613411797881
H	7.99726051794068	1.51110595944937	11.05369562753860
C	9.34377325207431	2.84672306611340	12.02022341001942
H	8.88817865253057	2.72954826699774	12.99322921454876
C	10.40864301756236	3.73578357685998	11.87158394382158
C	10.98701485032068	3.91885524116520	10.61416344059672
H	11.81570774205512	4.59597366119716	10.47493109188667
C	10.49698561231133	3.21058977610232	9.52191669044247
H	10.96345222968486	3.34144715159722	8.55453922473339
O	10.81020887059355	4.37832394409164	12.99853716244825
C	11.86103150191233	5.32394615561272	12.89756845028644
H	12.78931321001585	4.85477587419436	12.56052910354577
H	12.00228124904167	5.72259290159107	13.89843658647420
H	11.59870050478089	6.13787792484494	12.21655967712536

Table S 60. Coordinates of the optimized structure of compound Mn(pCH$_3$) in S$_2$ state.

Mn	3.40463817770166	6.61053747533615	4.84471536389133
Br	4.34866292416741	4.91215671107250	3.04959446606642
C	1.76777496067863	5.81055104731420	4.74550623171357
O	0.74183854224465	5.30568327887898	4.69629809556497
C	3.08932974849299	7.78321941111695	3.42642814071814
O	2.96506005157043	8.52194908823345	2.56751563106033
C	2.98864854273845	7.88809029303542	6.28925049373236

O	2.31886572312859	8.29653923011532	7.12723664955874
Se	5.97157920401361	7.30969342545627	4.69172749133894
C	6.44110896279416	5.75811788622408	5.80462322719163
H	6.48928779753465	4.93960386404059	5.09031534921507
H	7.42934167513905	5.91480443870662	6.22664114827125
C	5.41587625404617	5.50167214245454	6.88230212752925
H	5.76748510613945	4.66416066768014	7.49027957137142
H	5.31195947723244	6.37045778924248	7.53391727716314
N	4.08412700908425	5.19189728248621	6.31878949934637
H	4.19398772084354	4.38108958416750	5.70997368091540
C	3.11333242660682	4.82849768758816	7.37427807954313
H	2.17568296013543	4.59102099554730	6.88164294061314
H	2.94076101171440	5.71171223563805	7.99132143609789
C	3.50062527556932	3.65942136794148	8.27076577189885
H	2.64986465369419	3.39978719557746	8.89659053854218
H	4.33860987033562	3.88237326516252	8.92843919420089
Se	4.06250564224038	2.03797109350914	7.27965397757085
C	6.23327857835443	8.71892388024983	5.99188590691165
C	5.46305065298510	9.86901638335251	5.83768643655048
H	4.72880110365022	9.92957616373828	5.04613368089551
C	5.63898756139366	10.94502758110406	6.69573826496224
H	5.03681218285617	11.83451336480459	6.55811500979403
C	6.56776876270367	10.89674547157091	7.73533251553981
C	7.32948874455664	9.73816022286283	7.87670097547933
H	8.06701798160623	9.67801383804145	8.66755400790673
C	7.17344756325971	8.66009142376790	7.01280386746595
H	7.80083856615269	7.78982729298673	7.14234905173802
C	6.72420563583293	12.05096886311434	8.68639178068985
H	5.97228652702373	12.00854193247532	9.47854482847565
H	6.60240375131143	13.00565242921937	8.17417994843399
H	7.70416053623449	12.04248855932604	9.16291389127556
C	2.55600484101193	1.95384631752684	6.07497475507683
C	2.76416803434054	2.11924312062331	4.71100158983835
H	3.75624808881856	2.29750157034945	4.32366062885064
C	1.68465781499123	2.09935134400335	3.83771523664672
H	1.86417100080997	2.25897366936384	2.78246929648783
C	0.38430393357304	1.92632799290248	4.30396556672395
C	0.19348234707305	1.74568800763971	5.67556138398512
H	-0.80861088727020	1.59812491354051	6.05910117986848
C	1.26519612221229	1.75013382079804	6.55682734344720
H	1.09710161593249	1.59483730612917	7.61418520050217
C	-0.78508500404491	1.98250036648572	3.36190645862648
H	-1.12468621609142	3.01419229926270	3.23951725623583
H	-1.62743661756304	1.39985085293953	3.73484582189415
H	-0.51771193956252	1.60738755529287	2.37421673257939

Table S 61. Coordinates of the optimized structure of compound Mn(oCH$_3$) in S$_1$ state.

Mn	7.35802911796539	7.57627464939264	3.65773963249380
Br	7.29444444696540	9.83440972441133	2.53036193990267
C	8.85472109957692	7.22277522009406	2.69188151625354
O	9.81251458264589	7.01388529470078	2.10224357320524
C	6.37155543659519	6.65299057703972	2.30690309360332
O	5.96072182501208	5.96926471175370	1.49226134329879
C	8.06857479863086	6.49457692661945	4.98749576688406
O	8.51722173887171	5.75456230453311	5.73608185242461
Se	8.86252375374493	9.55744987860350	5.56886467725094
C	7.01580054477898	10.04330246301637	6.02266201857969
H	7.03164291549193	10.60984133230546	6.94988351131439
H	6.73293950379305	10.71620401458330	5.21708177024582
C	6.04793113938445	8.88157317066023	6.13442568863595
H	6.43921174479656	8.11075250620439	6.79803177274129
H	5.13024717022142	9.27011314271389	6.58493954690711
N	5.72426790393873	8.23698793832871	4.84103780091371

H	5.32534668775393	8.95469059921145	4.23659369107515
C	4.69793317930619	7.18487274977610	5.02056297371408
H	5.10657695713774	6.43504225332858	5.70152194698735
H	4.55450274411570	6.70280785611808	4.05755560616839
C	3.34364729242492	7.65656731556687	5.53063168820853
H	3.38178100596360	8.06208822957701	6.53944386396933
H	2.65099692417090	6.81926938362400	5.53664713788192
Se	2.57557112621454	9.12405392887590	4.44560032258974
C	9.41099961931399	8.69445728970915	7.20531976431810
C	10.61392304206975	7.97018364632980	7.15524616005903
C	11.03890160174037	7.32235952288994	8.31253135361574
H	11.96389680323969	6.76026489056911	8.28215343750831
C	10.30636112418206	7.37712212153829	9.49153081514134
H	10.65945476600434	6.86035031233578	10.37353294293563
C	9.12285608619919	8.10032180806590	9.52767832674096
H	8.54368569411681	8.15981944781493	10.43964389582117
C	8.67829113660692	8.75762544401428	8.38721585012233
H	7.76205731070213	9.32631879033166	8.43858192280593
C	11.43151909861913	7.89097002052433	5.89695592270285
H	10.86257004590823	7.45267141625053	5.07485103455807
H	12.32071371982905	7.28239213675203	6.05045204037090
H	11.75566625875624	8.88085865551644	5.56635432290692
C	2.86411728779754	8.38653968069099	2.67743868050359
C	2.20785718917701	7.23153620948358	2.22527820165391
C	2.46894929185703	6.80957388931152	0.92072162686070
H	1.97653799779856	5.91707359666816	0.55508260100074
C	3.33499171145968	7.50372053763512	0.08651924118333
H	3.51972901989117	7.14276864039927	-0.91627692949557
C	3.96970075489401	8.64799515252381	0.54623790422600
H	4.66529651740009	9.18832415853534	-0.08040653907065
C	3.73416257256288	9.08479949737930	1.84227529652284
H	4.25051887613236	9.95907675764411	2.21016821229144
C	1.26090140601115	6.44138215203781	3.08363217168787
H	1.79909798496189	5.74595390851691	3.73311542161172
H	0.58700487922418	5.84841596312518	2.46714070722742
H	0.66835656404269	7.09354718236675	3.72463687893903

Table S 62. Coordinates of the optimized structure of compound Mn(mCF$_3$) in S$_1$ state.

Mn	5.39645097983871	8.49869755335174	17.59200822134514
Br	6.55353983891660	10.66093579937860	17.05552235087579
C	5.82815958092617	7.59399015653382	15.97493006142859
O	6.18839505080346	6.94493357456918	15.10966152065439
C	6.99917006488942	7.91391341162302	18.22522271133561
O	8.00505591348608	7.55608148239977	18.63231956879847
C	4.62390011658403	7.50442082198502	18.95305260472273
O	4.21400738509429	6.81257087366839	19.76696694591193
Se	4.84637702415540	10.52930875647349	20.01798385239405
C	3.48859134636546	11.15332095169934	18.74342881663457
H	2.78265651777062	11.77523714842227	19.28766778974240
H	4.05260872928712	11.79369019800776	18.06999794136456
C	2.75418500113737	10.06607870064102	17.98320944936475
H	2.37467664367657	9.29797028507446	18.65649720929773
H	1.89155874770739	10.53849762869073	17.50541059455595
N	3.58006767207995	9.39616391621066	16.95334476460724
H	3.93519329824655	10.12676620725976	16.33728705492335
C	2.75723945031616	8.48377525248186	16.12702407163786
H	2.34251124697687	7.71735102386767	16.78502825284090
H	3.42531571515885	7.98311800821782	15.43292478418802
C	1.63311286559382	9.13427886400209	15.32894009402201
H	0.81901677320485	9.50435335211368	15.94857463044034
H	1.21780508118772	8.40531709112527	14.63714159747693
Se	2.22206520044663	10.72057449408597	14.29795553241668
C	3.71115150538199	9.77141079840301	21.37288169738015

C	2.33121655053737	9.92721589829155	21.42581926733081
H	1.80518778017636	10.52029296757766	20.69489673741954
C	1.60291219943927	9.30884148312458	22.43776483240660
C	2.23737372205041	8.54608262725995	23.40934773577662
H	1.66188972038204	8.06631935092344	24.18689155931916
C	3.61855230351599	8.39897029815573	23.35647864399569
H	4.12539516379232	7.80156345992933	24.10173953515055
C	4.35080377372078	8.99898369410138	22.34466879151434
H	5.42329765595808	8.85841165211427	22.30255836524656
C	0.11587003983952	9.52016974227100	22.49844199293718
C	3.75139404285871	9.90625432812689	13.44228850490645
C	3.58593889864889	8.82984924740272	12.57509587792176
H	2.59908658230486	8.45121609626089	12.35322358158301
C	4.70082113019060	8.24975596351635	11.98465557526722
C	5.97670751127698	8.74771095753651	12.23892074870286
H	6.83750488591204	8.28755435187693	11.77575261977502
C	6.13204154144700	9.82814170336223	13.09216278532551
H	7.11829369655755	10.21097082523165	13.31312408790068
C	5.02319501402409	10.40605255672703	13.70073317214205
H	5.15975086477163	11.22373430758459	14.39297052563698
C	4.54259035847786	7.04386205036520	11.09995094162883
F	-0.42725109319710	9.65772549108387	21.26710622726197
F	-0.52173960146378	8.49939543911139	23.10146346326590
F	-0.20338489461342	10.64100139192266	23.18550038893708
F	4.79997332942286	5.89948234363438	11.77464425059582
F	3.29319241022948	6.93077425587600	10.60575795160778
F	5.38719466450679	7.07222116634398	10.04966971808081

Table S 63. Coordinates of the optimized structure of compound Mn(pCl) in S_1 state.

Mn	3.79275001676736	4.52060998771807	10.54749887900997
Br	4.67804018499761	3.66045367903110	12.72997181668877
C	1.94445835715731	4.31653830265405	10.96146536862999
O	0.83646073707285	4.07254524331964	11.07361655003504
C	3.76362981018475	2.79056608814784	9.98426203470276
O	3.76722219008324	1.70433952922030	9.62915064078412
C	4.23821810359441	4.96310869962923	8.80408694824953
O	4.43921605989945	5.17309765788270	7.69727928950572
Se	6.99427314693733	4.76324546632893	10.43627493164542
C	6.56661831373689	6.36232350770460	11.49269985365892
H	6.42154550340298	5.97020068919094	12.49609215378401
H	7.44757061955294	6.99850614703098	11.50328267250405
C	5.35590807954933	7.14871661794331	11.02863120169922
H	5.38604992605314	8.11506123022181	11.53993619941389
H	5.39948216205873	7.34264474084429	9.95692460923935
N	4.06593511258751	6.48175495719114	11.31706618909053
H	4.04646436321843	6.29435130665406	12.31915407670161
C	2.92546121499751	7.37482717899703	11.01376705703287
H	2.01565703057942	6.80640286302807	11.18177290031822
H	2.96346854025434	7.61750023393655	9.94962031709449
C	2.84581003525866	8.65984570150091	11.82937488131402
H	1.89310583695235	9.14681380081224	11.63477205115597
H	3.63567218036853	9.37089290158687	11.59590416510268
Se	3.01321842949371	8.36447662585019	13.78235682722710
C	7.63038643894261	5.58865682608405	8.81812610432717
C	7.73117771775477	4.75223164808424	7.70562574796925
H	7.44197291266957	3.71190022357322	7.78056845353352
C	8.18981000553094	5.23980500116158	6.49208590201765
H	8.26603102422791	4.58932843369411	5.63298721048719
C	8.53887933811103	6.57987829946727	6.38398651660421
C	8.43884275979090	7.42706850474439	7.47740084217308
H	8.71581895664043	8.46711178302140	7.38180278574809
C	7.98729767453224	6.92854452490930	8.69366078081516
H	7.93098855255303	7.60217958320705	9.53563780531271

C	1.69753228627524	6.95959223571630	13.94201568055313
C	2.10293618343003	5.68944058153979	14.33839708861601
H	3.14429056946523	5.47937989093163	14.53205107816424
C	1.17613782147373	4.66073407556600	14.45220418015170
H	1.49695011804022	3.66941235149471	14.73597432757793
C	-0.15485882409176	4.91203696232409	14.15734319336126
C	-0.57537003940506	6.17698983300666	13.76145934790423
H	-1.61748174722028	6.35349505893480	13.53829221516028
C	0.35379783039278	7.20266958370163	13.66419842591244
H	0.02725429205237	8.19226012400171	13.37495258063373
Cl	9.10338425767568	7.20384976749580	4.85718129831432
Cl	-1.31812608360109	3.62230755091439	14.26688582007269

Table S 64. Coordinates of the optimized structure of compound Mn(pOCH$_3$) in S$_1$ state.

Mn	5.49132212553155	4.77437861460652	10.41846686247214
Br	5.13352766827155	2.81430654030371	11.89419169318836
C	7.24625076994213	5.29191311331384	10.88438095614873
O	8.22230779758490	5.77884665324313	11.22272428331112
C	4.96945823507061	5.78805446751017	11.84396422407277
O	4.63991229282321	6.42631747428517	12.73170147644271
C	4.55654077449902	5.98794271326099	9.39647931784595
O	4.04466837073369	6.83640631727220	8.81945103051406
Se	2.47084043363086	3.39667661537546	9.72137227110824
C	3.74310995973561	2.22542145320168	8.75858028428335
H	4.15909569415328	1.56511622280132	9.51403410842784
H	3.13650936172249	1.64138114083425	8.07163697687637
C	4.83141191002942	2.94373482279658	7.98834437787017
H	5.23394373731206	2.23594935316862	7.25864194190378
H	4.42362243388081	3.78946413632457	7.43360011478092
N	5.94487187493839	3.44271204341908	8.83390974681545
H	6.29593590969781	2.63921435282937	9.35496563279317
C	7.06261646364883	3.93134994891397	7.99325020563221
H	7.80889086786041	4.35821030858289	8.65627079078494
H	6.68170518837367	4.74118919954977	7.36741682741004
C	7.74569112040786	2.88346689522980	7.12212188895604
H	8.64060427482676	3.31716012318424	6.68179286056917
H	7.11927442802515	2.51727040683115	6.31143648910364
Se	8.26927320019480	1.25376579547580	8.12308409152411
C	1.34101960199267	3.75628638887206	8.18979171951870
C	0.37937450739472	2.82788857651255	7.80850565632453
H	0.26341907283488	1.91282374064102	8.37387657221605
C	-0.44547158709306	3.05874866057326	6.71197579053912
H	-1.18381728709374	2.31937470833626	6.44194681140143
C	-0.31360955574377	4.24360511867680	5.98790483516539
C	0.64223891712786	5.18530401727566	6.37399945063859
H	0.72595325931501	6.10266497481960	5.80759996784167
C	1.46006512306630	4.94300748086377	7.46448196528273
H	2.18731153828347	5.68593724299511	7.75507772897959
O	-1.06730932962871	4.56877502892473	4.90513729128916
C	-2.06844353256297	3.65701736317312	4.48290193377087
H	-1.63563916906145	2.69536774618480	4.19496179428588
H	-2.54221690587049	4.11253526850645	3.61776698745865
H	-2.81599776648546	3.49766246152562	5.26420597829661
C	9.16706349924490	2.12840966860901	9.58922698655661
C	8.64736677283941	2.02172514748706	10.88020830561857
H	7.73712224157176	1.46861641594372	11.06080257977203
C	9.27047178582995	2.65469829074301	11.93955911202512
H	8.85698759095943	2.59722728366384	12.93642244208789
C	10.41408863431202	3.42467439738558	11.72341520866309
C	10.94139811435301	3.53229038354625	10.43528013133293
H	11.82762943494424	4.11740454881754	10.24387332380839
C	10.32112523282478	2.87324668407326	9.37976279994133
H	10.74663900805024	2.94697978312198	8.38789008446321

O	10.93382045864528	4.03768792352637	12.81517216221955
C	12.02951555373894	4.92105330405253	12.63613092008767
H	12.91035244889387	4.39366986764146	12.26073334318354
H	12.24714637339190	5.33002751294914	13.61876768551304
H	11.77229707102911	5.73385829824350	11.95247997888117

Table S 65. Coordinates of the optimized structure of compound Mn(pCH_3) in S_1 state.

Mn	2.94903980796418	6.47944188301325	4.90364986919950
Br	4.10245214195788	5.22646297671065	3.05515386083068
C	1.31143892830378	5.52366114084143	4.74618798844167
O	0.26653331588451	5.09354190811206	4.58867618440997
C	2.31527438126118	7.60381631599979	3.62462454283167
O	1.93748303163781	8.32426380441775	2.82087144899583
C	3.03524736070692	7.97017064260495	6.00262510504391
O	2.98988473450980	8.91398071954690	6.64844665798154
Se	5.94112566910876	7.54448742507479	4.72602269796569
C	6.24247423180764	5.91701226385998	5.78075584177322
H	6.26972080160346	5.12923085546709	5.03212147462789
H	7.22923784149897	5.99099764354204	6.23018850189879
C	5.20168003007291	5.62845578765417	6.84422240639696
H	5.60873286291188	4.84428640346057	7.48833862831497
H	5.02009372144360	6.50567520925811	7.46506340017729
N	3.90125481156709	5.18379119378210	6.29525847791191
H	4.08538121954579	4.36683122836905	5.71491154339402
C	2.98100366749523	4.76042730675199	7.37516064581240
H	2.05217164583901	4.45420904618905	6.90301371775560
H	2.76026063344564	5.63729838108661	7.98783015788641
C	3.46198790980792	3.62435669107238	8.26987078508562
H	2.63931466834401	3.30371901971169	8.90502046596737
H	4.29119153492371	3.90493431851325	8.91613109447639
Se	4.12440362194866	2.04961895977903	7.26359998553916
C	6.34909791121926	8.88551700560510	6.04497213072878
C	5.98528814812392	10.19091681897500	5.71060582095674
H	5.49342516098590	10.39050260952358	4.76677222832176
C	6.24434060150729	11.23488368587366	6.58197598561795
H	5.95660852714812	12.24076446030360	6.30137100729448
C	6.85891111031881	11.01312158560024	7.81644473305399
C	7.21108530431863	9.70622659251115	8.13974265318893
H	7.69268585771579	9.50384533413518	9.08864285190203
C	6.96431104305851	8.64928858819726	7.26856058828975
H	7.26865310603555	7.65413169851161	7.55803263345565
C	7.11265305567384	12.15272558897728	8.76419383765105
H	6.17525758383574	12.55052616955510	9.16017763967086
H	7.62651686114110	12.97570768455269	8.26433809960620
H	7.72346789136602	11.83730194361248	9.60929296114960
C	2.63097673645203	1.88834976668687	6.04959497560855
C	2.81895607334040	2.14369493081570	4.69541846246124
H	3.78963927340626	2.43348796151842	4.31987840691752
C	1.74720260136923	2.05639358025040	3.81697297870337
H	1.90905136626652	2.28085710806868	2.77067773843522
C	0.47159483469187	1.72517152448659	4.26788364574056
C	0.30079471130234	1.46173562716554	5.62840980576229
H	-0.68041964738009	1.19231563979974	5.99938479343076
C	1.36711769942183	1.53318259268079	6.51415147910778
H	1.21656719818592	1.30991835675525	7.56191710306074
C	-0.69539284430079	1.69711783995232	3.32179735723869
H	-1.11844509742444	2.69862274214561	3.21038449060837
H	-1.48739568557960	1.04193337503462	3.68397587098952
H	-0.39463295579110	1.35760206388552	2.33076923832773

Table S 66. Coordinates of the optimized structure of geometry b with ligand oCH_3 in S_4 state.

Mn	7.40913456535540	7.83832598702653	4.09399763309467
Br	6.52065191742975	9.86124110294627	2.98624124273554

C	8.88736513031220	7.59710576208015	3.04352340302007
O	9.68640376105639	7.32657270356140	2.25810291187567
C	6.38745758524267	6.76741643610671	3.01007309815988
O	5.94057139313758	6.11416623031528	2.17277431140750
Se	8.64361933094696	9.64692963976541	5.69405173871985
C	6.93284274876298	10.23701306439037	6.46518017069558
H	7.12589045838275	10.87159624651588	7.32646561743121
H	6.51627706410304	10.84460289470326	5.66582981269525
C	6.02046626853072	9.08016035021491	6.82331785026568
H	6.47114412656387	8.49632599265936	7.62189617062030
H	5.07638460713728	9.47962917452127	7.21557312653162
N	5.76611908958129	8.17337769695368	5.69438803747106
H	5.14896804285360	8.62619301084360	5.02860770646122
C	5.19830307851650	6.88793636757670	6.11898254216123
H	4.37525279649306	7.02770102051004	6.83259835184879
H	4.78640152793485	6.41355138139698	5.23246781983919
C	6.24689142155322	5.98951021310188	6.76046345534891
H	6.53198922822717	6.33751389911559	7.75039569205037
H	5.90474017960936	4.96527009614643	6.85114753014740
Se	7.96404017295091	6.01815618200061	5.75976631819994
C	9.45798741193749	8.81541727172013	7.24642831053773
C	10.63703830977565	8.08265238649811	7.03273455858794
C	11.22052187626773	7.44624773839488	8.12555150435855
H	12.12761407884608	6.87620887696366	7.96839350587989
C	10.67057004856250	7.52425285346589	9.39896434100438
H	11.14325192781730	7.01302333548118	10.22647098668534
C	9.52101038001362	8.27396362862848	9.59986591154436
H	9.09004490909537	8.36559983981159	10.58809559883784
C	8.92103975756865	8.92162581392583	8.52673983784217
H	8.04245172637339	9.52065505542924	8.70898951290289
C	11.26579921819903	7.97683862019348	5.67395004573059
H	10.60154101542472	7.48386880628515	4.96335672701929
H	12.19431428361666	7.41059301139061	5.71915230036199
H	11.49228823859092	8.96160329384398	5.25840240099830
C	8.19288822250888	4.30421913255115	4.87903729238953
C	7.21126349019773	3.45696685710028	4.35090691686479
C	7.65032923386365	2.31702403265097	3.67192736545848
H	6.90502147796896	1.65160545176276	3.25457732736439
C	8.99529902575067	2.02530796442759	3.50276538698165
H	9.29161632139894	1.13801214702205	2.96007572220340
C	9.95363917390653	2.88172450809271	4.02853052620383
H	11.00779230317935	2.67418398202859	3.90533297273003
C	9.54918577857530	4.01081971241111	4.72208761130984
H	10.29172723790084	4.67453129007005	5.14536863855972
C	5.73292868415793	3.68523221095302	4.48351638300957
H	5.36105378406782	3.34236824031631	5.45212056495007
H	5.19635203596417	3.13279405688243	3.71455447710154
H	5.47490555378625	4.73232442924458	4.37103873179917

Table S 67. Coordinates of the optimized structure of geometry b with ligand mCF_3 in S_4 state.

Mn	7.93773339557996	7.98155836822669	4.14754924549474
Br	6.89504208005131	9.67724501040052	2.78562971798923
C	9.53790643518041	8.14889431452599	3.28748523835564
O	10.54162956405927	8.24707700906275	2.75782620795343
C	7.27485681374913	6.75849971216788	2.96250357779582
O	6.84939473062267	6.02054303883626	2.20466338127800
Se	8.62373734330194	9.77250633967171	5.85455209295201
C	6.73064124076299	10.11747957090431	6.26017047749943
H	6.68354500779193	10.73819040138326	7.15028322700381
H	6.38420998426953	10.69556337826782	5.40940033709551
C	5.94844540533423	8.84001652709472	6.45928597329228
H	6.25511744543893	8.39481666511772	7.39979126672503
H	4.88074693581757	9.06503227460304	6.53302786792513

N	6.15663013109162	7.82229739341961	5.38782343179781
H	5.44797154318253	7.97385137557899	4.67915312903843
C	5.98832832596813	6.45449884313443	5.93278140894099
H	5.12035633054702	6.41673111287620	6.59954456853989
H	5.78936995908146	5.78242039509486	5.10096663789725
C	7.22082396538689	6.01384633695562	6.70129523076137
H	7.47392239552810	6.69209030448679	7.51404415726273
H	7.10697500907700	5.01717197660738	7.11807064085234
Se	8.84439209561892	6.03028140171793	5.59548463199196
C	9.18763433804300	8.84236020310242	7.46362813025825
C	10.34933950402008	8.12368586495094	7.34721472379804
C	10.87459573544971	7.44007404935580	8.49334303509061
C	10.16781931463656	7.54408310962896	9.71566738829333
H	10.55225398315183	7.04118875608293	10.59131264537467
C	9.01725089313919	8.28463830611930	9.80657551669186
H	8.51071935117929	8.37001077909353	10.75833861250156
C	8.47470153990670	8.95877999478537	8.66820195168084
H	7.61367101601378	9.59584675013457	8.77429726075053
C	8.53671022185903	4.45307785554829	4.50042921144599
C	7.47872257775948	3.57791219601865	4.68061121711860
C	7.34976927730319	2.47309957836968	3.84294028490028
C	8.27546445722179	2.23400120265666	2.83724244189518
H	8.16314709603034	1.37844373987683	2.18817872554051
C	9.34269928353288	3.11035670537176	2.67343056231820
H	10.07118027199769	2.93201292229350	1.89478878507260
C	9.47743990906550	4.21522326769418	3.49980612526621
H	10.31203227441157	4.89075947873081	3.36249920185889
H	6.74291437675361	3.73196546460665	5.45346920400801
H	10.89417889602824	8.09128631940328	6.41487397328481
C	6.20370358531649	1.52630189387835	4.07540030925508
F	5.07453738140828	2.18798527805039	4.41904454519627
F	5.91899289274398	0.78886517977394	2.98878632797418
F	6.46550991832204	0.66444118224069	5.08339525993253
C	12.07799774531101	6.62760322966116	8.33740906876462
F	13.17600457288959	7.33346340400850	7.90611943407500
F	12.45207679135789	5.99449526860243	9.46951383913183
F	11.94764178469819	5.63826469182042	7.37328019907364

Table S 68. Coordinates of the optimized structure of geometry b with ligand pCl in S_4 state.

Mn	7.63779207217008	7.86193351208468	4.21203326988621
Br	6.69247182157026	9.77497667650006	2.96749479732078
C	9.26287159995488	7.71287229282021	3.39286576615393
O	10.21465870056417	7.51331033300259	2.77480797964387
C	6.80900759662336	6.69954986176987	3.04170121003786
O	6.48192605604959	6.01942188688765	2.17376526551876
Se	8.50876087739639	9.81412846889103	5.77184447734437
C	6.72929640556894	10.19319635892070	6.52686293233604
H	6.83770832029959	10.80026334578094	7.42216185407695
H	6.27184422963709	10.79662447235181	5.74628610363071
C	5.93727267469411	8.93137956354064	6.80357670671017
H	6.42908938658794	8.36456198657813	7.59091092251833
H	4.94430651458188	9.20608301363372	7.18285178481046
N	5.82122910743824	8.06214286962163	5.62445209324691
H	5.23712151007935	8.51038112028699	4.92588223148122
C	5.29673865835033	6.72931930702385	5.94545648873317
H	4.37721170029378	6.78942777134329	6.54263119828858
H	5.04884992034903	6.25045035782808	5.00066042055514
C	6.31718099582091	5.89384394246081	6.70439561056151
H	6.43825079937450	6.22226174167267	7.73331819864132
H	6.05032578428621	4.84102828252103	6.71761141789354
Se	8.13983586507800	6.04839901731337	5.92764191774576
C	9.37930020191193	8.97672755290977	7.27339813594002
C	10.57424387280015	8.31151342060009	6.98808540477894

C	11.26177778451193	7.64114657610436	7.98720777452096
C	10.75067413819252	7.62816212349668	9.27905339097973
C	9.57125075626279	8.29554022389227	9.58077981808587
H	9.19195902278449	8.29172520303660	10.59249816938888
C	8.89047075140625	8.97295210070863	8.57635409536176
H	7.98543289976783	9.50321486732552	8.83339492929294
C	8.26252076109785	4.40280150762557	4.93452626877400
C	7.16208990596655	3.74731183289370	4.39482260371527
C	7.33936973634445	2.58267754091616	3.66040358905552
C	8.62166182122332	2.09255144432970	3.45480100971912
C	9.72914040173702	2.74936539358383	3.97673204568928
H	10.72128060401675	2.35789834392049	3.80633120536060
C	9.54486808938877	3.90353125339104	4.72411916885072
H	10.40400052282817	4.40961232193013	5.14336773160174
H	6.16380670060342	4.13987681408856	4.51617109624310
H	10.96321382423588	8.30179550353251	5.97826046489604
H	6.48946964391848	2.06949343987794	3.23497327353842
H	12.18383388079252	7.12338668279196	7.76575276695808
Cl	8.84580338741889	0.63530235551561	2.52767807898191
Cl	11.60011732301763	6.76945766769187	10.53563022812861

Table S 69. Coordinates of the optimized structure of geometry b with ligand $pOCH_3$ in S_4 state.

Mn	7.76155958899058	7.68605522330955	4.24720408908270
Br	6.93081758389005	9.57135470291472	2.86708461162939
C	9.43853854793558	7.54550261024574	3.53872173988840
O	10.42508784947954	7.37191295623156	2.96850703750256
C	7.03148017229136	6.49739804823616	3.03855888072314
O	6.78475990696957	5.81225530672483	2.14613083961593
Se	8.48113609067229	9.69223458036566	5.82780911931266
C	6.64117692808529	10.05294073972255	6.42884546522658
H	6.66600691591830	10.68612716981819	7.31229307117650
H	6.23280550771996	10.62391679321627	5.59803969937555
C	5.85657410445641	8.78238993957565	6.68155645066410
H	6.30563261611495	8.24451753055635	7.51366036508949
H	4.83408498958346	9.04253433782514	6.98628251090447
N	5.83953303369576	7.88532402227336	5.51792850667232
H	5.29811719801624	8.30586689571951	4.76967599143044
C	5.31445022230757	6.55201772560101	5.83632795759918
H	4.35216533374365	6.61188965929495	6.36257102160452
H	5.14563181291005	6.04333378244643	4.88966340371064
C	6.28959602140161	5.75581278850743	6.69137301938289
H	6.33182842322280	6.11707133129571	7.71559261995937
H	6.03571853210020	4.69983580045782	6.71650200495980
Se	8.15848305892248	5.90754330342938	6.03527220253842
C	9.24132758976417	8.90183258510542	7.41781332242014
C	10.44814027381121	8.23158761120689	7.24546511117116
C	11.08007233409848	7.61007674960104	8.31565383632995
C	10.49612408695965	7.64546521321314	9.58090831225496
C	9.28812966179489	8.32266663092619	9.75848928309259
H	8.85144754998538	8.35453181522893	10.74725609185947
C	8.67087939549358	8.94944099997277	8.68864304051099
H	7.74751221519185	9.48249239479301	8.86375835996899
C	8.35079689951823	4.23392623280830	5.09982187961337
C	7.30383531067497	3.57911854495646	4.47131158364339
C	7.52738353003580	2.39279713864902	3.77898845031923
C	8.81648300137068	1.87042939374592	3.69575385687736
C	9.87311894113386	2.53848737560740	4.32098030299713
H	10.86809883023338	2.12245106076415	4.24700303447987
C	9.63973412572985	3.70576190077739	5.02273404643712
H	10.46355367125886	4.20929624879814	5.51092534712456
H	6.30406955173366	3.98667188224827	4.48762922590071
H	10.90053342748964	8.17557924178988	6.26372973591750
H	6.69561922038059	1.90503296991946	3.29503955437426

H	12.01444061137690	7.09731586033559	8.14668354124376
O	9.14252416274314	0.72936881035393	3.03513141953725
C	8.11323045685138	0.02929367815994	2.35472042076085
H	7.34094700488609	-0.31446508295208	3.04803181225726
H	7.65548255122766	0.65055979967651	1.58090743260636
H	8.59102892494308	-0.83005710369451	1.89262053017071
O	11.02205021343088	7.06061854210656	10.69056007078908
C	12.25235812996033	6.36664191172708	10.56245389394334
H	12.16601926058780	5.52923719253396	9.86496449065395
H	13.05237877979489	7.03312741413857	10.22980037280889
H	12.48735653510601	5.98778509073075	11.55326501188289

Table S 70. Coordinates of the optimized structure of geometry b with ligand pCH_3 in S_4 state.

Mn	7.93440914051154	7.79776399769838	4.19591856361590
Br	6.88518405721839	9.62872964032539	2.89862128127155
C	9.57623868409995	7.77202305084825	3.39986571276889
O	10.55058105832705	7.61272052353228	2.80252364189890
C	7.21193884748670	6.54908661258188	3.03462487972292
O	6.96678090211447	5.80745901141903	2.19021959923795
Se	8.56837317497883	9.80782961328537	5.80945436021125
C	6.70333710485382	10.12176003448374	6.35572830265018
H	6.68363360292752	10.79213176635614	7.21167917049382
H	6.29477216538520	10.63758834148345	5.49086582335999
C	5.96336115149279	8.83240030049877	6.64921437581584
H	6.36546665265179	8.38906445762737	7.55634954553323
H	4.90955021379519	9.06208206400219	6.85002104732638
N	6.07542425746321	7.83458849443099	5.57188795192569
H	5.46144478882057	8.09317641520318	4.80732955802335
C	5.76414559316941	6.47660126735722	6.03533797826791
H	4.85194126829258	6.45900588040517	6.64696310022688
H	5.58513301734990	5.86305499777779	5.15425142887422
C	6.91194601466672	5.89906065722157	6.84781942090389
H	7.12260882025025	6.48254540122898	7.74104387898464
H	6.72032427306107	4.87620589437405	7.15947887349993
Se	8.61933899880527	5.94814914078441	5.86082892585225
C	9.28911792399486	9.05078808021254	7.43294872024317
C	10.50363772063005	8.37275892902853	7.31117274141753
C	11.08706899597649	7.78093919393135	8.41874497026055
C	10.48048417486573	7.83588494843084	9.67582611041351
C	9.27508437361697	8.52475796912422	9.78478304960384
H	8.78775382069545	8.59644557147934	10.74946926718907
C	8.68402033847363	9.13391223477726	8.68200803585201
H	7.76126739848653	9.67897620785854	8.81758139253983
C	8.48736429685030	4.33720508808566	4.80271924385386
C	7.41378539974314	3.46082531789449	4.83951439993866
C	7.40977489202547	2.34019363765587	4.01458895651972
C	8.46023817068899	2.07748935002993	3.14129748792325
C	9.53016229784951	2.97567201784119	3.11788988254376
H	10.35896887069889	2.80220599074803	2.44274194638987
C	9.55071669312832	4.09273818265501	3.93585736831912
H	10.38435906939036	4.78053589463373	3.88315372147821
H	6.56939793620082	3.63080783545294	5.49039248822247
H	10.98427078259751	8.29482989314109	6.34452927265059
H	6.56400607639435	1.66487200718403	4.04996553530639
H	12.02566123719685	7.25326023561073	8.30137056740625
C	8.44577859243694	0.87592573337460	2.23748682142560
H	9.33686562590896	0.26179674568634	2.38163545466140
H	7.57289557861988	0.25120215870107	2.42297148346936
H	8.42602313107162	1.17592047222087	1.18762532544839
C	11.11791615555365	7.17579078007465	10.86704638816613
H	10.49578498108047	7.27584217194620	11.75568537468378
H	11.28078535319460	6.11101783277569	10.68821772540909
H	12.09174614790268	7.61763111751610	11.08872721919552

Table S 71. Coordinates of the optimized structure of geometry c with ligand oCH_3 in S_4 state.

Mn	7.355850000	7.729093000	4.197281000
Br	7.272768000	9.448810000	2.431572000
C	7.647214000	6.483282000	5.454055000
O	7.906439000	5.679491000	6.256439000
C	8.575436000	6.894037000	3.154153000
O	9.339308000	6.329347000	2.489650000
Se	8.874701000	9.418959000	5.262895000
C	7.361638000	10.513020000	5.917290000
H	7.719741000	11.156827000	6.727403000
H	7.121832000	11.137868000	5.048046000
C	6.183872000	9.655432000	6.336297000
H	6.445455000	9.013286000	7.187434000
H	5.354808000	10.312765000	6.654224000
N	5.741875000	8.772987000	5.233176000
H	5.511015000	9.372134000	4.432060000
C	4.497155000	7.997495000	5.583540000
H	4.328295000	8.115958000	6.665235000
H	3.651155000	8.465153000	5.062337000
C	4.566223000	6.530787000	5.221305000
H	5.183170000	5.940162000	5.906939000
H	3.566299000	6.090766000	5.149570000
Se	5.399533000	6.262051000	3.341873000
C	9.530187000	8.724499000	6.960203000
C	10.602838000	7.811608000	6.882495000
C	11.095775000	7.280596000	8.080291000
H	11.925985000	6.573982000	8.032207000
C	10.555380000	7.632129000	9.318620000
H	10.958297000	7.197984000	10.233204000
C	9.503262000	8.546534000	9.375668000
H	9.077728000	8.842283000	10.334716000
C	8.991786000	9.092642000	8.197786000
H	8.182681000	9.816485000	8.266244000
C	11.205494000	7.403890000	5.567136000
H	10.527617000	6.750892000	5.000130000
H	12.141706000	6.854665000	5.720639000
H	11.424634000	8.272828000	4.928263000
C	4.026000000	7.058616000	2.297873000
C	3.099668000	6.184273000	1.645420000
C	2.028155000	6.757662000	0.967059000
H	1.324366000	6.092171000	0.462130000
C	1.827682000	8.150849000	0.909857000
H	0.978231000	8.562798000	0.367428000
C	2.752046000	8.996223000	1.547872000
H	2.635553000	10.079749000	1.494548000
C	3.833499000	8.462374000	2.232286000
H	4.579169000	9.131483000	2.654957000
C	3.267526000	4.690636000	1.669457000
H	4.239895000	4.387522000	1.249224000
H	2.474651000	4.204729000	1.087306000
H	3.236396000	4.287593000	2.694467000

Table S 72. Coordinates of the optimized structure of geometry c with ligand mCF_3 in S_4 state.

Mn	7.412131000	7.529623000	3.834227000
Br	6.832453000	9.324346000	2.323048000
C	8.116450000	6.347930000	5.026819000
O	8.571016000	5.600416000	5.762979000
C	8.847448000	7.228720000	2.753030000
O	9.736584000	7.013325000	2.074657000
Se	8.154719000	9.497496000	5.222961000
C	6.303226000	9.931676000	5.749482000
H	6.333848000	10.623879000	6.586636000

H	5.924771000	10.453117000	4.874190000
C	5.505128000	8.688244000	6.065807000
H	5.911067000	8.201785000	6.952043000
H	4.472771000	8.973455000	6.290934000
N	5.529283000	7.703859000	4.965755000
H	4.894782000	8.013975000	4.223570000
C	5.038074000	6.391361000	5.453480000
H	5.647999000	6.136857000	6.318864000
H	4.008122000	6.496339000	5.801635000
C	5.117331000	5.250782000	4.427583000
H	5.695810000	4.418747000	4.819924000
H	4.135971000	4.885276000	4.145563000
Se	6.002669000	5.714923000	2.729157000
C	8.892390000	8.855772000	6.899715000
C	10.121862000	8.212508000	6.805530000
C	10.750230000	7.757241000	7.955620000
C	10.162094000	7.943143000	9.202392000
H	10.653213000	7.578232000	10.092488000
C	8.941359000	8.595438000	9.288559000
H	8.479252000	8.747858000	10.254051000
C	8.304084000	9.057915000	8.141583000
H	7.360168000	9.573365000	8.235703000
C	4.558458000	6.694310000	1.878464000
C	3.493429000	7.163932000	2.616187000
C	2.512981000	7.992404000	1.945834000
C	2.684891000	8.248462000	0.565940000
H	1.960481000	8.868727000	0.056296000
C	3.735185000	7.719748000	-0.136497000
H	3.829404000	7.915655000	-1.194957000
C	4.729028000	6.915073000	0.520494000
H	5.599869000	6.563824000	-0.009892000
H	3.289442000	6.844316000	3.623731000
H	10.588172000	8.051430000	5.843420000
C	1.505819000	8.646935000	2.756489000
F	0.597493000	9.353310000	2.056115000
F	0.795920000	7.786413000	3.571629000
F	2.035245000	9.552738000	3.696005000
C	12.101305000	7.098705000	7.854504000
F	13.096710000	7.998997000	8.011967000
F	12.271672000	6.155632000	8.799874000
F	12.288782000	6.510677000	6.657888000

Table S 73. Coordinates of the optimized structure of geometry c with ligand pCl in S_4 state.

Mn	6.932540000	7.771080000	4.392826000
Br	6.668374000	9.428325000	2.668860000
C	7.221391000	6.513442000	5.657551000
O	7.399593000	5.665432000	6.429376000
C	8.261711000	7.001688000	3.464665000
O	9.120564000	6.497136000	2.870167000
Se	8.464475000	9.388703000	5.602942000
C	6.993524000	10.131742000	6.747350000
H	7.453773000	10.308775000	7.724103000
H	6.731702000	11.093083000	6.286076000
C	5.781756000	9.226716000	6.844714000
H	6.008534000	8.314237000	7.410202000
H	4.966906000	9.757301000	7.369545000
N	5.336664000	8.841104000	5.482765000
H	5.338072000	9.688961000	4.906661000
C	3.971828000	8.255618000	5.395030000
H	3.390983000	8.531212000	6.290695000
H	3.474366000	8.708518000	4.527557000
C	3.979570000	6.748051000	5.232344000
H	4.466974000	6.232996000	6.069020000

H	2.968851000	6.339934000	5.120840000
Se	5.072954000	6.216956000	3.663313000
C	9.579646000	8.680302000	6.982839000
C	10.960075000	8.817382000	6.751712000
C	11.873847000	8.262743000	7.673660000
C	11.370634000	7.589046000	8.797982000
C	9.999879000	7.446493000	9.034708000
H	9.649327000	6.914017000	9.915957000
C	9.082668000	7.993691000	8.107482000
H	8.016346000	7.864903000	8.275217000
C	4.020366000	6.997266000	2.238901000
C	2.660556000	7.294305000	2.358700000
C	1.966241000	7.828778000	1.272255000
C	2.640141000	8.051370000	0.069539000
C	3.996503000	7.743755000	-0.061347000
H	4.509184000	7.926643000	-1.003882000
C	4.687938000	7.221773000	1.029099000
H	5.751452000	7.005637000	0.936757000
H	2.117294000	7.103342000	3.282994000
H	11.326185000	9.362187000	5.882198000
H	0.906517000	8.063999000	1.354707000
H	12.946315000	8.365274000	7.527691000
Cl	1.775988000	8.723315000	-1.284923000
Cl	12.503137000	6.894774000	9.942467000

Table S 74. Coordinates of the optimized structure of geometry c with ligand pOCH$_3$ in S$_4$ state.

Mn	7.264459000	7.921581000	4.219631000
Br	7.262145000	9.848061000	2.687584000
C	7.488780000	6.650984000	5.469363000
O	7.652053000	5.801747000	6.243749000
C	8.584435000	7.158511000	3.270210000
O	9.433642000	6.658269000	2.659877000
Se	8.707873000	9.406329000	5.646333000
C	7.163296000	10.341170000	6.455674000
H	7.476324000	10.674109000	7.450275000
H	7.014294000	11.216262000	5.810761000
C	5.922266000	9.470457000	6.501905000
H	6.073878000	8.601901000	7.156212000
H	5.082516000	10.062484000	6.908582000
N	5.589654000	8.983130000	5.145174000
H	5.594910000	9.789336000	4.505259000
C	4.256209000	8.326754000	5.043656000
H	3.614152000	8.657321000	5.877064000
H	3.788199000	8.666593000	4.109048000
C	4.352037000	6.819236000	5.013862000
H	4.864407000	6.391857000	5.883031000
H	3.367072000	6.353917000	4.899904000
Se	5.431144000	6.282409000	3.405997000
C	9.380146000	8.447274000	7.181830000
C	10.607532000	7.818431000	6.967368000
C	11.172784000	7.019671000	7.991665000
C	10.489392000	6.888342000	9.208372000
C	9.262914000	7.537325000	9.421327000
H	8.762309000	7.417441000	10.380265000
C	8.692052000	8.317838000	8.392285000
H	7.735609000	8.803968000	8.567996000
C	4.186020000	6.939708000	2.091220000
C	2.968261000	6.243340000	1.961052000
C	2.033035000	6.666753000	0.998489000
C	2.323806000	7.760345000	0.179449000
C	3.553020000	8.445902000	0.313723000
H	3.761618000	9.292269000	-0.338204000
C	4.476872000	8.030880000	1.272627000

H	5.420351000	8.562527000	1.383838000
H	2.751501000	5.371187000	2.577023000
H	11.133263000	7.929129000	6.018724000
H	1.095221000	6.124325000	0.898706000
H	12.125498000	6.527090000	7.818407000
O	1.486396000	8.246795000	-0.787083000
C	0.241406000	7.578224000	-0.971250000
H	0.390772000	6.525597000	-1.261183000
H	-0.374846000	7.618825000	-0.058283000
H	-0.268694000	8.111089000	-1.780039000
O	10.945569000	6.139965000	10.262576000
C	12.183198000	5.455460000	10.090847000
H	12.130150000	4.731814000	9.261604000
H	13.009690000	6.159962000	9.903877000
H	12.363777000	4.922342000	11.030078000

Table S 75. Coordinates of the optimized structure of geometry c with ligand pCH_3 in S_4 state.

Mn	6.829798000	7.732872000	4.451504000
Br	6.551686000	9.384014000	2.719886000
C	7.128697000	6.487595000	5.725158000
O	7.314982000	5.648805000	6.506465000
C	8.141784000	6.949551000	3.518766000
O	9.000066000	6.439099000	2.925230000
Se	8.368692000	9.352179000	5.658570000
C	6.914519000	10.109770000	6.811019000
H	7.375112000	10.274219000	7.789843000
H	6.661818000	11.076758000	6.356983000
C	5.696262000	9.211598000	6.897365000
H	5.917267000	8.295410000	7.459649000
H	4.882396000	9.744151000	7.422533000
N	5.254902000	8.833998000	5.532954000
H	5.275286000	9.680265000	4.954085000
C	3.880532000	8.275582000	5.437575000
H	3.287208000	8.594411000	6.311177000
H	3.411907000	8.707929000	4.543762000
C	3.859664000	6.764126000	5.323825000
H	4.336194000	6.266403000	6.177198000
H	2.841450000	6.372865000	5.220888000
Se	4.944816000	6.171248000	3.771068000
C	9.489062000	8.615324000	7.030957000
C	10.858701000	8.657789000	6.756862000
C	11.761264000	8.056987000	7.665856000
C	11.280246000	7.434737000	8.840805000
C	9.906698000	7.420458000	9.095970000
H	9.534981000	6.939604000	10.002443000
C	8.982208000	8.002664000	8.191597000
H	7.914741000	7.935559000	8.387604000
C	3.908492000	6.927851000	2.323524000
C	2.553070000	7.247799000	2.426016000
C	1.881803000	7.762637000	1.314834000
C	2.536991000	7.957464000	0.091174000
C	3.894860000	7.611377000	0.009284000
H	4.429793000	7.750661000	-0.931547000
C	4.582624000	7.109334000	1.110352000
H	5.643339000	6.873692000	1.029694000
H	2.001653000	7.086801000	3.351685000
H	11.227919000	9.160383000	5.862638000
H	0.822067000	8.009087000	1.401971000
H	12.831628000	8.082820000	7.461064000
C	1.816966000	8.544475000	-1.093150000
H	2.145905000	8.080011000	-2.032328000
H	0.730542000	8.414849000	-1.007425000
H	2.015417000	9.624232000	-1.178349000

C	12.248331000	6.790833000	9.796984000
H	11.735174000	6.396078000	10.683627000
H	12.787570000	5.957737000	9.318476000
H	13.011564000	7.508751000	10.136767000

Table S 76. Coordinates of the optimized structure of geometry b with ligand oCH_3 in S_1 state.

Mn	6.94465359067908	9.30974450630977	4.30608870219365
Br	5.76084844322047	11.45863588212939	4.70250579764373
C	8.12976738776869	10.03556852445434	3.16723821865879
O	8.88565007541754	10.49409615754812	2.43290889109745
C	6.33380897943945	8.46364345619725	2.78317486824842
O	6.04025185715440	8.03935849272889	1.75882549274183
Se	8.46262840502695	9.80220372944577	6.30309495326419
C	6.92883374377109	9.62134210746616	7.52729574556337
H	7.27860109273381	9.58317992777153	8.55397177049353
H	6.38454565553591	10.54984015630342	7.37037474667277
C	6.10751129828540	8.40704041306049	7.16237592776612
H	6.72356582773536	7.51385725247302	7.24396053894531
H	5.27123218067392	8.30187999781503	7.86451657051324
N	5.59748720206772	8.49122431925008	5.77840252429392
H	4.98234655207381	9.30413339612539	5.72460458032467
C	4.80097416510336	7.30223350311334	5.40762172201128
H	3.93870520684981	7.20848881759509	6.07995570021324
H	4.41625336168722	7.47624108132075	4.40548759827700
C	5.57006803475417	5.99596811808685	5.46590207936508
H	5.79718122964425	5.70304153873933	6.48752234437989
H	4.97381243065701	5.20802881161291	5.01232789313119
Se	7.31518824708924	6.06470578004552	4.51856334590748
C	9.54700641018291	8.29649688102394	6.90006779899159
C	10.48657123320033	7.75172370455430	6.01423027794498
C	11.32776499971238	6.74909592829862	6.49769000857846
H	12.05172480615774	6.31335594210116	5.82125626621646
C	11.25987737176630	6.30200439949043	7.80921781461220
H	11.92523435891863	5.52063311536875	8.14941448149319
C	10.32931678744007	6.85815890462134	8.67426946305970
H	10.26496354563761	6.52803849902648	9.70240620571130
C	9.47570952797986	7.85486724494246	8.21730780869659
H	8.77217990040679	8.29145653254020	8.90969608648502
C	10.61209092935541	8.21414755866222	4.59343261472292
H	9.69629819190184	8.00906381231646	4.03733538606115
H	11.43817957569422	7.71053351462066	4.09549128911413
H	10.78832264894270	9.28964941128642	4.52802902368397
C	7.99789377471072	4.42204324137661	5.29859399506248
C	7.95478202398871	3.21574493107808	4.58567386850471
C	8.48489243182084	2.08164907263488	5.20372535177349
H	8.46109417606056	1.13881199581292	4.67175055315597
C	9.03628523970495	2.13591546418364	6.47778392590895
H	9.43956550942421	1.23771818508606	6.92659467774072
C	9.07329223292860	3.34043707530528	7.16696154637979
H	9.51177064600355	3.39833951297934	8.15439301667476
C	8.55526555230175	4.48294659955151	6.57089926487413
H	8.59954327801390	5.43027593488539	7.08690130894025
C	7.36711150462938	3.11425485537031	3.20473336027737
H	6.33659747138666	3.47046660094826	3.18265505900808
H	7.38241665987880	2.08233568738578	2.85655589925268
H	7.92072424447865	3.72533942495341	2.49099363536632

Table S 77. Coordinates of the optimized structure of geometry b with ligand mCF_3 in S_1 state.

Mn	7.87664223164844	7.98627994453684	4.22533227433662
Br	6.73578832099263	9.83862840959240	2.95177299115706
C	9.58929894514494	7.47167652886070	3.75088913152663
O	10.62183848421402	7.09023263425139	3.43000356664984
C	7.29351492449700	6.74254386683377	3.07830268832887

O	6.92632828514014	5.95690111076608	2.32266332488662
Se	8.51411516116572	9.87879263701407	5.74412693628515
C	6.67596766239510	10.07152119602655	6.43297895869976
H	6.68396250336183	10.68378537507912	7.33023579677835
H	6.18283740420522	10.61456873927455	5.63071692058269
C	6.05379083294678	8.71802465695452	6.68411862485119
H	6.59774529997686	8.21674983611890	7.48135747164133
H	5.02030192868062	8.84960246452730	7.02798562298355
N	6.08574149818167	7.85286769509958	5.48755432659689
H	5.50855772805035	8.29042966928983	4.77119440708369
C	5.54133656323930	6.50885215418999	5.75819211510651
H	4.51571295125899	6.58656519097709	6.14172979035787
H	5.49635246644727	5.97899414291171	4.81027986468619
C	6.35041995298060	5.71307896508343	6.77123028824959
H	6.30283908882378	6.15205951952339	7.76512087808835
H	5.95352524585524	4.70518934642964	6.85951126596445
Se	8.28121515183244	5.59264273535168	6.42513681903510
C	9.34668538255518	9.07184615791471	7.30550248251955
C	10.42596993060995	8.22692490753267	7.08160227620859
C	11.05790660900886	7.60962551225140	8.15383011290748
C	10.62420390504356	7.83109768448984	9.45508623482488
H	11.11026761164016	7.33561480183277	10.28184465528998
C	9.55584869030474	8.69043074121006	9.67475292610096
H	9.21396758855004	8.87671046069608	10.68368829330334
C	8.92118930542667	9.31513333845501	8.60765018010990
H	8.09880869294063	9.98766367093399	8.80389952560569
C	8.33687734002882	4.24105164323779	5.06100826128817
C	7.23944005576072	3.48398699559243	4.67746717406123
C	7.37639156363462	2.53433232874507	3.67090204272795
C	8.59852574323020	2.33278210627904	3.04376836893284
H	8.69103048678823	1.60071373789157	2.25530197290213
C	9.69340025309319	3.09233920514364	3.43697368066545
H	10.64981533925637	2.95076918597645	2.95296903393583
C	9.56944606844599	4.04165001674003	4.43990567150275
H	10.42805341343153	4.63175953136926	4.72881779076755
H	6.27269504592457	3.62003931157378	5.13451566457547
H	10.76098914904492	8.02172992126289	6.07582025808576
C	6.19379488348948	1.68086542813681	3.30581651993528
F	5.02161663143115	2.32321921217269	3.49869052791516
F	6.22509071843624	1.28201035182228	2.02141433926148
F	6.14386051342700	0.55679847697228	4.06178970858066
C	12.21848214508992	6.69502548047146	7.87055877383019
F	13.32604842174050	7.38692283788432	7.52765519734016
F	12.54036369475978	5.93102954051921	8.92936160525804
F	11.95188331286106	5.85877901619479	6.84010308668258

Table S 78. Coordinates of the optimized structure of geometry b with ligand pCl in S_1 state.

Mn	7.81999432358896	8.00433829856659	4.23453722123286
Br	6.67717716706850	9.85621190227931	2.95400065339547
C	9.52305933015998	7.44894403545009	3.77691607550004
O	10.55411337727262	7.03997225373782	3.48298023787329
C	7.20544864013715	6.76309466694235	3.10048437742355
O	6.81580991913348	5.98146860035862	2.35164034306147
Se	8.51391095567245	9.89186008296629	5.72888665050289
C	6.69135934955897	10.13709876616365	6.43675627496258
H	6.72709325452206	10.75374339380950	7.33087278534941
H	6.20627499268916	10.69071308910249	5.63677209219249
C	6.02760184338494	8.80567309010669	6.70131285796842
H	6.55052712175047	8.29927542740074	7.50817203801842
H	4.99640203446384	8.97287349451806	7.03650957946092
N	6.03978029216807	7.91891292651485	5.52008596535197
H	5.46070320131248	8.34858492815080	4.80067213572679
C	5.48607152510838	6.58705101305525	5.82577153511585

H	4.46893573701116	6.68305852925840	6.22827060025695
H	5.41822011031058	6.04060096585063	4.88858823878133
C	6.30795733810379	5.80133143398786	6.83673087276608
H	6.29579317737409	6.26415700509099	7.82063902742562
H	5.89725574653627	4.80265381780390	6.95950500636634
Se	8.22315123213580	5.63422429322556	6.43482878479743
C	9.36550383339917	9.06623600622093	7.26604502986871
C	10.52926070845671	8.33983941128055	7.02576134497763
C	11.20069293788638	7.72077285877817	8.06854687154503
C	10.69827055338530	7.82280577408098	9.35969995606040
C	9.54806145197367	8.55352851693067	9.61602528059980
H	9.17347941666880	8.63611243728313	10.62597560121557
C	8.88798110721150	9.18218019385398	8.56566060175692
H	8.00411797812362	9.76283911193999	8.78510267755496
C	8.19934974524515	4.25039965844091	5.10020546654173
C	7.07431628640134	3.51074882443892	4.75574377744325
C	7.15292087369303	2.53035131333548	3.77477224513191
C	8.36207901186026	2.29011699241036	3.14106877409885
C	9.49408409812979	3.02120248852930	3.47628029517565
H	10.43042628779344	2.83181902119593	2.97221497084172
C	9.40874037865097	4.00042498621852	4.45343499739672
H	10.29090940373691	4.57550222953125	4.69922223616036
H	6.12096221762200	3.68246635244894	5.23172936871164
H	10.91290573474268	8.23828950515968	6.02044633877821
H	6.27676369521237	1.96083985828865	3.50142711401468
H	12.09991294556609	7.15242508146264	7.88092115931935
Cl	8.46153319103469	1.06249632437360	1.90829357337904
Cl	11.52112410074134	7.02436139245574	10.67004286289648

Table S 79. Coordinates of the optimized structure of geometry b with ligand pOCH₃ in S_1 state.

Mn	7.69790929049043	7.89356412614225	4.22507369852284
Br	6.62534999706425	9.79976097802325	2.92881337139248
C	9.36887894410187	7.16648346345009	3.89235784088020
O	10.36129113677039	6.62815662675188	3.69117126250436
C	7.04966888089509	6.71307397120762	3.05700413442830
O	6.63263678143686	5.97248140136198	2.27773914696124
Se	8.43948319231211	9.76944566814976	5.72104141932825
C	6.62459198478372	10.05240381081599	6.43606305581804
H	6.68255769106826	10.64727149418622	7.34358027199529
H	6.15407426749994	10.63961799447670	5.65136087518948
C	5.91456825046122	8.73865953068772	6.67149021769156
H	6.42743046712657	8.18644905413499	7.45560937449328
H	4.89417641826742	8.93340124513784	7.02563815179352
N	5.88207145389602	7.89610586804996	5.46070157484849
H	5.34169411092525	8.38539365631494	4.74911582401805
C	5.25602261748502	6.58544760694270	5.70702008461094
H	4.23245204065602	6.71663032788206	6.08198721387129
H	5.18931578214042	6.07904985984808	4.74823619274642
C	6.01201328517458	5.72783464637178	6.71491021040859
H	5.84108468376353	6.06792620302618	7.73336929771721
H	5.68341885492681	4.69347701414971	6.65523811216315
Se	7.97690828022287	5.72533912325113	6.53268039456366
C	9.28585409082616	8.93527463116002	7.25581671695989
C	10.44988034806975	8.21741681725841	7.01706834850619
C	11.11544626603841	7.57152377609110	8.05140879372493
C	10.60836749146805	7.63656578626719	9.34889081704919
C	9.44844823579096	8.37186925026264	9.59372545496288
H	9.07033361730765	8.42528039641247	10.60521962328929
C	8.79824437716957	9.02069494951448	8.55694483738569
H	7.90909664877271	9.59160400366836	8.78166637853293
C	8.24552959304634	4.14415557100246	5.47587182170659
C	7.33214261264177	3.67207486412397	4.54605229314256
C	7.61669883879225	2.54558826188978	3.77908668603127

C	8.83854669650103	1.89433619709688	3.92784849167707
C	9.76499409054139	2.37672100810007	4.85589735727205
H	10.70978239556068	1.86214981748162	4.96308901309787
C	9.46791211253374	3.48563644909815	5.62494765157867
H	10.18924578651789	3.83984680561170	6.34952506647844
H	6.39403459914056	4.17858658456672	4.38186633607466
H	10.84490164348072	8.13505202807176	6.01409469278940
H	6.88745876350881	2.20771083729250	3.05925701007301
H	12.01376480052965	7.01640322456786	7.82978334374470
O	9.21760425232116	0.79515458778643	3.22281733332500
C	8.32268658551173	0.28178980016995	2.24963332736512
H	7.38128431122200	-0.03854083019325	2.70414186209180
H	8.11542155765819	1.02048824606926	1.47125412309977
H	8.82052472722514	-0.57756465226934	1.80890036056346
O	11.16762227529861	7.02635321025050	10.42553908764619
C	12.33840562383720	6.25067920517258	10.22392255471743
H	12.15191479576225	5.42375815830753	9.53387937981763
H	13.16023377346677	6.86233773058827	9.84307506571892
H	12.60588136398813	5.85398696521550	11.19921842562911

Table S 80. Coordinates of the optimized structure of geometry b with ligand pCH_3 in S_1 state.

Mn	7.77724092087194	8.00483913612181	4.24043169210418
Br	6.62205958071414	9.86600971972091	2.96683577187926
C	9.48336454851428	7.44274978139811	3.79625417378785
O	10.51363331254091	7.02534899031366	3.51265169788580
C	7.16980633554160	6.76855482530707	3.10071812195371
O	6.78365839248598	5.98886434143440	2.34686104287389
Se	8.46324652632233	9.88714432740992	5.74452270705971
C	6.64354313975439	10.11428713699941	6.46573742513119
H	6.68496288528534	10.71187513930252	7.37265417328102
H	6.15250919617895	10.68397892271742	5.68079062373928
C	5.97936357573408	8.77848520262532	6.70829753817643
H	6.50554888334439	8.25670887883609	7.50297173375213
H	4.94957982506592	8.94008929506407	7.05148525102035
N	5.98611342439665	7.91395604768017	5.51152852019031
H	5.41110579015732	8.35858869834132	4.79804025324504
C	5.43195188124650	6.57708909110760	5.79209404856922
H	4.41064850623758	6.66438828212669	6.18637784279024
H	5.37511871023763	6.04547831095423	4.84593500121195
C	6.24923210618462	5.77995723082431	6.79925494054926
H	6.17716430528856	6.19812272952578	7.80037403355511
H	5.88298886768396	4.75835359995679	6.85906722860544
Se	8.18474917691992	5.71511678443528	6.46451932423795
C	9.33676039298633	9.05023907948210	7.26243269639773
C	10.53153864799456	8.38211609259742	7.00361466510059
C	11.20908506320176	7.74549461139563	8.02981991413732
C	10.71500423551564	7.74753698214482	9.33630564734550
C	9.53073248700049	8.43506248120972	9.58155922999581
H	9.13106441418654	8.46769754742205	10.58758674415688
C	8.84697840422545	9.08878293686953	8.55985484278868
H	7.93980157364267	9.62521296724891	8.79759170358427
C	8.29817619704676	4.27887266189692	5.19018976728642
C	7.21396895503689	3.55486779959112	4.71508459382492
C	7.41193800780259	2.53501570855607	3.79018687829666
C	8.68103522265994	2.21636159290376	3.31839679845324
C	9.75940646486767	2.96182943590415	3.79991734421019
H	10.75928625713287	2.74735089982401	3.44299640679191
C	9.57709957468710	3.97912372870793	4.72180496840235
H	10.43153021212457	4.54571655191563	5.06826279123201
H	6.20745424659202	3.77369210807974	5.03806745038307
H	10.92797348149275	8.34296792962919	5.99835757865101
H	6.55336477119882	1.98602624401004	3.42394277395545
H	12.13406444731573	7.22680034714765	7.80960186814023

C	8.89374563374598	1.10537644332163	2.32744779389800
H	9.41280256463443	0.26119347339283	2.78796394504951
H	7.94605750645550	0.73812720362386	1.93516892020884
H	9.50161620036550	1.43826136616145	1.48467311890781
C	11.43618122030728	7.01317758058705	10.43197987641178
H	11.04668980005958	7.28172367706103	11.41318357120444
H	11.32511024500805	5.93261681295932	10.31402206386382
H	12.50481370500331	7.23202242515174	10.41856127272061

Table S 81. Coordinates of the optimized structure of geometry c with ligand oCH_3 in S_1 state.

Mn	7.36135457372065	8.10490845616761	4.08272105567791
Br	7.03018493716572	10.15018890907935	2.68094801456155
C	7.87227427048040	6.72159624280855	5.20772199190599
O	8.29094281506137	5.86268940709205	5.84374418979422
C	8.62943799210972	7.49814000230855	2.96008248578869
O	9.43573649907077	7.09108226855288	2.24865351929667
Se	8.87606605706928	9.76000884579709	5.73212497087076
C	7.21911731728616	10.40738135068120	6.56610264100673
H	7.44751802075984	10.78236541954731	7.55950505729274
H	6.94348206142160	11.25551867103278	5.94058027137467
C	6.10367228096073	9.37998964699981	6.59563546919607
H	6.39532318942613	8.49744406393577	7.16426861021523
H	5.23858560181015	9.82868897905041	7.09979557245508
N	5.73269334805620	8.96761307382281	5.23003163054087
H	5.66535674860334	9.80975157712962	4.65997830134399
C	4.41941439005986	8.28607387485105	5.15434137246203
H	3.81515549611306	8.55034038603922	6.02884044543603
H	3.89778445607789	8.66931690455038	4.27762454121035
C	4.51706309046300	6.78052943081627	5.04648663362621
H	5.13678903124147	6.34524299612565	5.82781269969399
H	3.53138481771936	6.32467735352020	5.08967914163423
Se	5.37326851985438	6.24406002582160	3.34296646090149
C	9.60041189980835	8.69059928443484	7.17082673246776
C	10.77014716096619	7.97038492710906	6.88249134660219
C	11.31476160204670	7.17853204900001	7.89060724806552
H	12.21667084163077	6.61840310593622	7.67818294213771
C	10.72983420199444	7.08941492644481	9.14722695464258
H	11.17404802386585	6.46303530850082	9.90875492593318
C	9.57379272773282	7.80748197729248	9.41511460473066
H	9.10567101005092	7.75199090499785	10.38895844395077
C	9.01008539838978	8.60561196610014	8.42723237120944
H	8.11343452263216	9.15977398726473	8.65831693620266
C	11.42322268669176	8.03800918135068	5.53170100244480
H	10.76107388651937	7.66695258397073	4.74779289678899
H	12.33237905172413	7.44022902231312	5.51080908097596
H	11.68916632981099	9.06430582832855	5.26632819087378
C	3.97386121785907	6.85441602677371	2.14443780121218
C	2.79814101729600	6.11003153332286	1.96273156085379
C	1.86095890791188	6.60168844754820	1.05339680058466
H	0.94623560808659	6.04395218568936	0.89544193093526
C	2.07996519261246	7.77498995764191	0.34173909055927
H	1.33433141699338	8.12377749681312	-0.36056958235841
C	3.25512944271157	8.48875819848386	0.52657397511131
H	3.44151332651492	9.40049251356545	-0.02463349453423
C	4.20379345121668	8.02634459429911	1.43070935269525
H	5.11825858124435	8.58094712272822	1.58734716249073
C	2.52298532190809	4.82602547282916	2.69533030793918
H	3.38360605979997	4.15827496719598	2.66593338411365
H	1.66793159504723	4.31232858327095	2.25874774230718
H	2.29597500240218	5.00304296106361	3.74908421477839

Table S 82. Coordinates of the optimized structure of geometry c with ligand mCF_3 in S_1 state.

Mn	7.27366129597156	8.01109729276261	4.30119869399912

Br	6.59901608317340	9.73907738559041	2.64442152690249
C	7.81292649319222	6.70483052280247	5.50037776031269
O	8.19854653157941	5.86253661516098	6.17831458035104
C	8.72229252296483	7.55714054795923	3.33122346065221
O	9.65612462656659	7.26332343843708	2.72991321073700
Se	8.46419558966061	9.98402976596311	5.82889594514836
C	6.75522219496201	10.33586625985188	6.74080117461632
H	6.95673607617861	10.68180983807164	7.75044853362577
H	6.34694288004622	11.17513692249302	6.17820869299004
C	5.79202697990831	9.16324531865863	6.72697036055555
H	6.18951495817181	8.32106885835879	7.29300750194377
H	4.86332766303334	9.48247353136599	7.21562562655586
N	5.51902768512431	8.73208283140224	5.34451916317609
H	5.41306106354537	9.56495652827392	4.76634505590165
C	4.27042033619891	7.95484694253872	5.18223029322158
H	3.57768257466157	8.18826647863598	5.99770108408337
H	3.80118034128130	8.28897719619350	4.25798297278239
C	4.47476919654474	6.45567151197912	5.11718070088247
H	5.05492092957059	6.07482742595064	5.95572218175261
H	3.52134360073297	5.93375467648622	5.10406198840733
Se	5.51816651489094	5.92190327997976	3.52794785503404
C	9.36701403089585	8.90606836359802	7.14475425228332
C	10.50298938284320	8.23569747482908	6.69497358852908
C	11.19745929436369	7.40218925268467	7.55871958424000
C	10.77160950128468	7.22547028737834	8.87209669572094
H	11.31013288111036	6.56268098229204	9.53318036114783
C	9.64148287410730	7.89715954714331	9.31209669415409
H	9.29868645066822	7.76475898275657	10.32930071762051
C	8.93792941258318	8.73701347606919	8.45577832195643
H	8.06080572679742	9.24680470440115	8.82533422812073
C	4.35014996121797	6.57944038173986	2.14367326819355
C	2.96710659925117	6.50482098665105	2.24596138321129
C	2.17650937417592	6.99525827356238	1.21289702376587
C	2.75893223701384	7.52931473730078	0.06787433512361
H	2.13674598201015	7.91049330401542	-0.72862854398279
C	4.14215967352411	7.58288661947560	-0.03114026822356
H	4.60465003825847	8.01296424810716	-0.90854253536864
C	4.94116636715704	7.12279456309304	1.00683076807928
H	6.01486230759239	7.21843206577665	0.94569968714503
H	2.49466652149162	6.07416297937653	3.11571533728763
H	10.83024386530575	8.33715812389290	5.66962156268827
C	0.68109553437505	6.89452615002486	1.31815500670558
F	0.05637470356343	7.89513318893315	0.66727280742817
F	0.21472849583297	5.73771944145997	0.79370383948148
F	0.25943982201176	6.93099185824546	2.60219544494050
C	12.44207126775663	6.70291208370066	7.08137541820399
F	13.55428140912902	7.40698097568767	7.39765393899015
F	12.58238171240453	5.48567565484737	7.64465699661457
F	12.45380943531424	6.53246012404063	5.74716672231098

Table S 83. Coordinates of the optimized structure of geometry c with ligand pCl in S_1 state.

Mn	7.42288912473619	8.07552801844595	4.24056643704312
Br	7.18790740703947	9.93392136832597	2.58078780564748
C	7.73113070550265	6.72697789266086	5.46047749231643
O	8.01385982322961	5.86277105783535	6.16222003136918
C	8.79971722718746	7.34340176458632	3.32765491512145
O	9.68574894693916	6.85979313515755	2.78047496226248
Se	8.84582079512098	9.85045906604990	5.74709517995251
C	7.18849981170899	10.52039798010476	6.56749211167572
H	7.41182330660697	10.88602397745106	7.56584600888446
H	6.93387796173587	11.37826379340683	5.94602071954154
C	6.05822697461808	9.51023492541110	6.57815618863479
H	6.31034685700125	8.64473936318818	7.19071521428231

H	5.17863563167958	9.98812465203502	7.02663300650027
N	5.74494263903283	9.05106406240632	5.21203030098470
H	5.73571735309821	9.86445013972385	4.59828980971108
C	4.41415228020407	8.40641112911449	5.10014429460448
H	3.77997842137476	8.72340862342935	5.93465124089115
H	3.94498108895839	8.77269577610396	4.18773250176481
C	4.46336538382642	6.89486934322511	5.05313889723244
H	5.02233735792196	6.46632643229489	5.88203916734806
H	3.45976969580996	6.47601689516140	5.05498906026801
Se	5.37088558168030	6.25863419207348	3.41041802697379
C	9.54777699894017	8.75388985156925	7.16522443009058
C	10.64614964497637	7.96521390426458	6.82511768465512
C	11.22084843163986	7.12084279330713	7.76114242045526
C	10.68824720102445	7.06004500226726	9.04288085368753
C	9.59394380812601	7.83624577593223	9.39275026172599
H	9.18820516170166	7.77863105757584	10.39240158469494
C	9.02453274011633	8.68520342209156	8.45051593350560
H	8.17501123326299	9.28396741657078	8.74325188030564
C	4.00731900205646	6.87426099801871	2.17980700751701
C	2.82858619501166	6.14499933293462	2.04002779922123
C	1.83828533599731	6.57916654208821	1.16957142200926
C	2.04486350492494	7.74007558235210	0.43382079013444
C	3.22128186641305	8.46587527466042	0.55351319062710
H	3.36686141749854	9.36424558470097	-0.02872126279743
C	4.20667476893519	8.03008387458449	1.43264536490654
H	5.12071436532551	8.59811915377137	1.54057823976733
H	2.68169767200992	5.23428125691640	2.60477066365645
H	11.04963710469457	7.99518542441103	5.82123445617527
H	0.91981908299642	6.02185996243964	1.05537539385966
H	12.06899035143637	6.50647089263854	7.49667105241809
Cl	0.80322337535578	8.28868432698674	-0.66002448925832
Cl	11.39806136254272	5.99014498172587	10.22118794963208

Table S 84. Coordinates of the optimized structure of geometry c with ligand $pOCH_3$ in S_1 state.

Mn	7.41772145390475	8.03616307808272	4.28812489769556
Br	7.28099801081975	9.86900779763507	2.59163636187143
C	7.62576068116873	6.67501072236603	5.52011812063495
O	7.84300488744942	5.79498163663110	6.22553284158211
C	8.80753433990778	7.26716165760995	3.43785367237674
O	9.70440036252552	6.76144065546293	2.92674981301965
Se	8.82503987631990	9.76823057812417	5.84574802055064
C	7.15966297867204	10.47625378712375	6.61736982234101
H	7.35694822534034	10.81605685309468	7.63015077969860
H	6.95418619969657	11.35331109927778	6.00433516647753
C	5.99860491494120	9.50264391714534	6.56639498581586
H	6.19792169253007	8.62329141032625	7.17865268797874
H	5.11411601566989	10.00207483587916	6.98111123577589
N	5.73577072952165	9.07185858579045	5.18106968926035
H	5.79365275833501	9.89038450426470	4.57681098600897
C	4.38824380643568	8.48791863009173	4.98640993647451
H	3.70773021235281	8.86763778971851	5.75657632285809
H	4.01302389011766	8.84123970326377	4.02656485334769
C	4.36644693940842	6.97518998303050	4.99420467357274
H	4.85744031028923	6.55328036840275	5.86880999940116
H	3.34499777464880	6.60424735188489	4.95321126605933
Se	5.32567351068519	6.23266661533406	3.42643351892245
C	9.44786932853235	8.63671590438396	7.27700177951932
C	10.51724471898740	7.80584034533435	6.96653870200933
C	11.04224036699168	6.93666832566160	7.91416914513796
C	10.48538097498154	6.88583806314070	9.19124518124090
C	9.40867567836696	7.71685456422424	9.50197971273386
H	8.98384831526894	7.66712826086851	10.49502954523217
C	8.89544831894532	8.58594030465275	8.55370320051942

H	8.06310471701566	9.21705458003114	8.82862656255248
C	4.06059190218731	6.82540575936682	2.09074060716052
C	2.91735192211834	6.07480153244059	1.84586627978787
C	1.99370039524690	6.48062413268211	0.88797100909046
C	2.22514123614230	7.64830296856201	0.15956356932820
C	3.38105532894373	8.39530120750512	0.39753330384738
H	3.54918717371897	9.29358750377567	-0.18042767853401
C	4.29357069816429	7.98764109930794	1.35462365902259
H	5.18625258901944	8.57211660569122	1.53144042690939
H	2.74070097562143	5.16198595653834	2.39898339481121
H	10.94444334869104	7.81689281038638	5.97193825615212
H	1.11342960270906	5.88061585305858	0.71552196462419
H	11.87000167191663	6.30147227031042	7.63970951198477
O	1.39012921562962	8.13093617084177	-0.79667978950599
C	0.21440071283988	7.39783437462587	-1.09942913214691
H	0.45372256760991	6.39416417660634	-1.46006923796052
H	-0.44335575788505	7.32257132564739	-0.22950572115680
H	-0.28993599370180	7.95289794959167	-1.88556984370975
O	10.91514838972459	6.06553528259205	10.18677300635880
C	12.00212386820818	5.19592343373353	9.91331603577207
H	11.76140473314353	4.50114823527524	9.10463719348296
H	12.90369145593675	5.75650141829940	9.65241651652563
H	12.17691897418417	4.63788802432335	10.82894018748595

Table S 85. Coordinates of the optimized structure of geometry c with ligand pCH_3 in S_1 state.

Mn	7.45167741978598	8.10199590816027	4.25871691299463
Br	7.23479228838103	9.91975804906065	2.55377938886713
C	7.72751603112424	6.76127331091250	5.49840630718253
O	7.98920600397221	5.89928796678497	6.21092642502163
C	8.82689371314584	7.34387245190970	3.37234465399486
O	9.71265866430146	6.84251873879721	2.83904480177295
Se	8.87018579424704	9.87813737919973	5.74437337683309
C	7.21944875739188	10.56588927976180	6.56393117725974
H	7.44513710270475	10.92085930651270	7.56553359395743
H	6.97577378426521	11.43069542488393	5.94765381952451
C	6.07755291473622	9.56852900009435	6.56447204224907
H	6.31533630406702	8.70187315057929	7.18094232932708
H	5.19759513231823	10.05578030932855	7.00253424197521
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C	1.02005499368758	8.13118374535065	-0.60613767488067
H	1.44093998026166	8.75747773637596	-1.39200255689758
H	0.51753272084493	7.28503378153843	-1.07572820981155
H	0.25508784765987	8.71855776852281	-0.09146370073414
C	11.36185936881678	6.17091025388840	10.09165313267065
H	10.78821895903899	6.15171739387733	11.01750149789765
H	11.42657305873179	5.14896342998279	9.71359463314912
H	12.37785352252318	6.49072136684292	10.33411129231104