Supporting Information for

Mechanistic insight into catalytic redox neutral C-H bond activation involving manganese(I) carbonyls: Catalyst activation, turnover and deactivation pathways reveal an intricate network of steps

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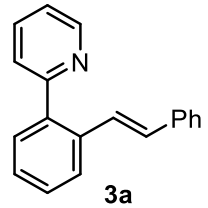
1 Characterization of Products

1.1 (*E*)-2-(2-styrylphenyl)pyridine, 3a



3a

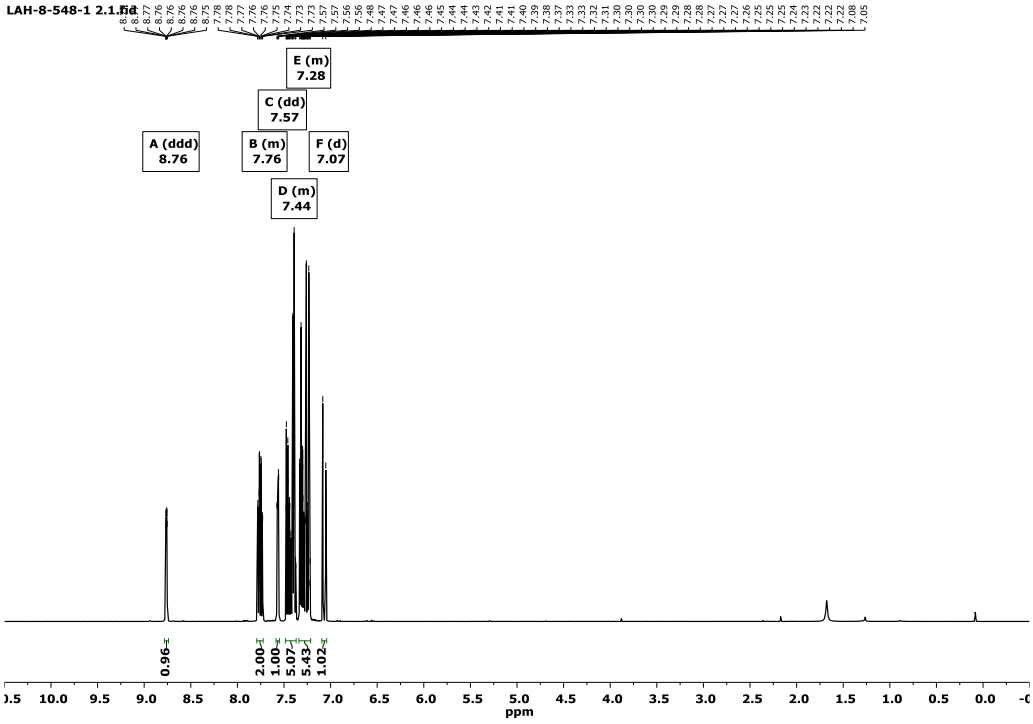


Figure S1. ^{1}H NMR spectrum of **3a** (500 MHz, $CDCl_3$).

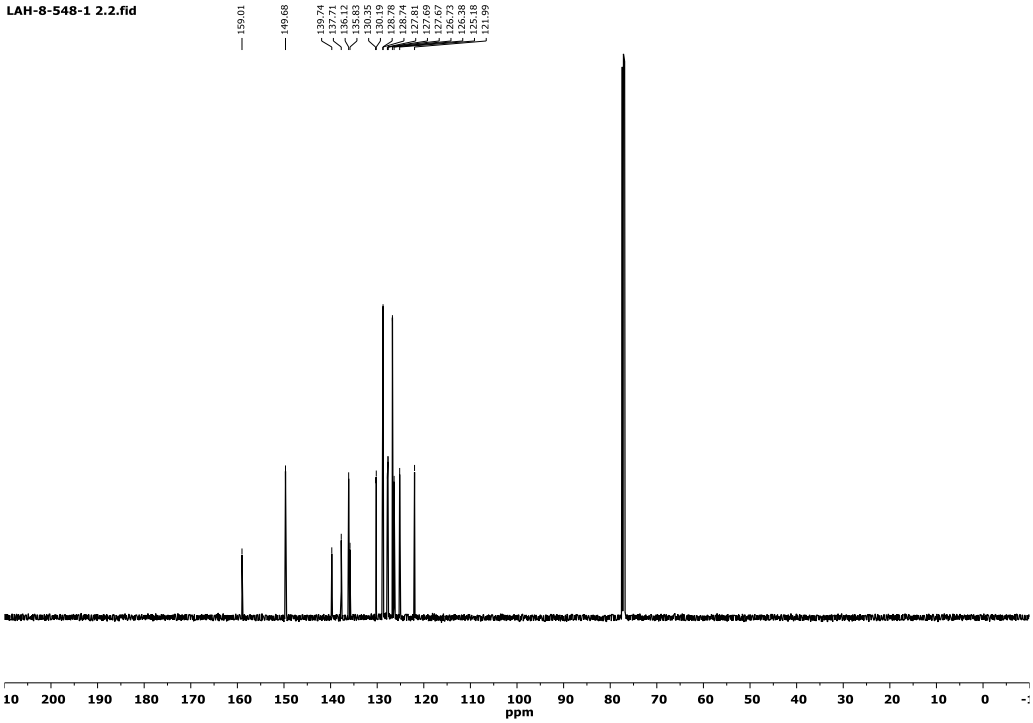
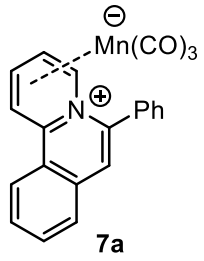


Figure S2. ^{13}C NMR spectrum of **7b** (126 MHz, CD_2Cl_2).

1.2 Reductive elimination product, 7a



7a

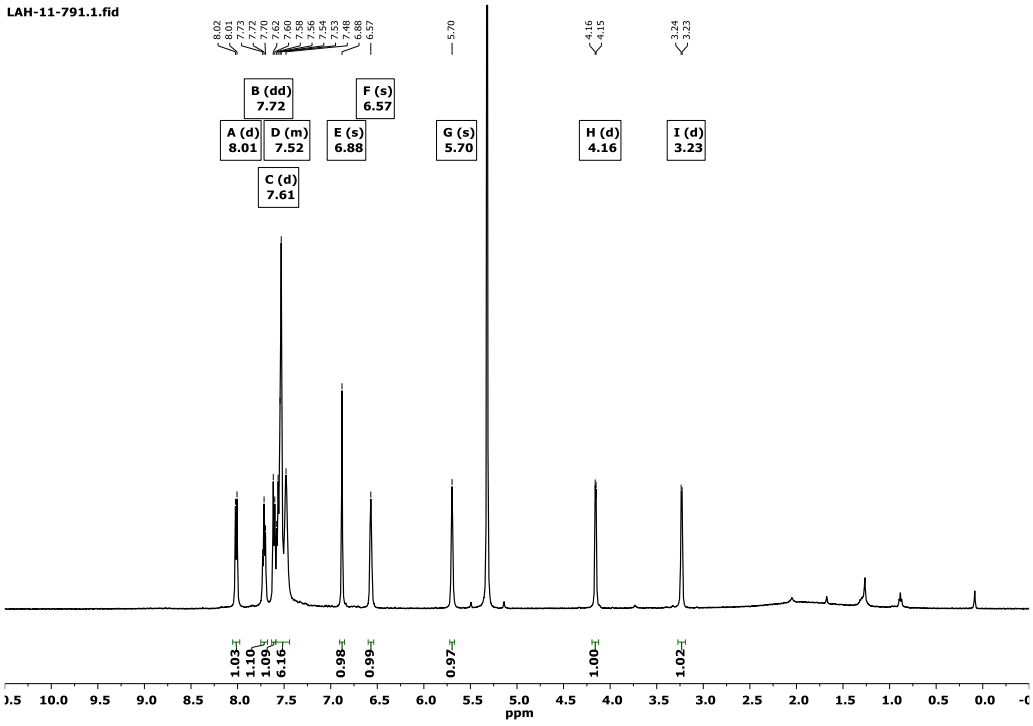


Figure S3. ^{1}H NMR spectrum of **7b** (500 MHz, CD_2Cl_2).

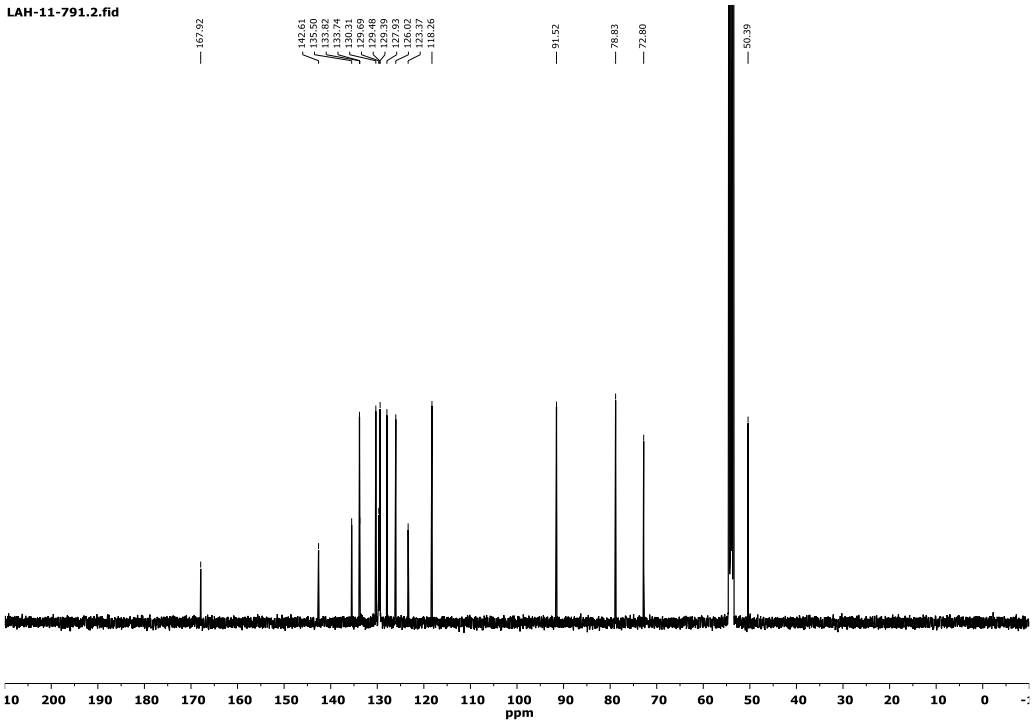
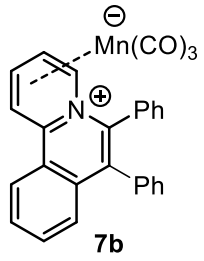


Figure S4. ^{13}C NMR spectrum of **7b** (126 MHz, CD_2Cl_2).

1.3 Reductive elimination product, 7b



7b

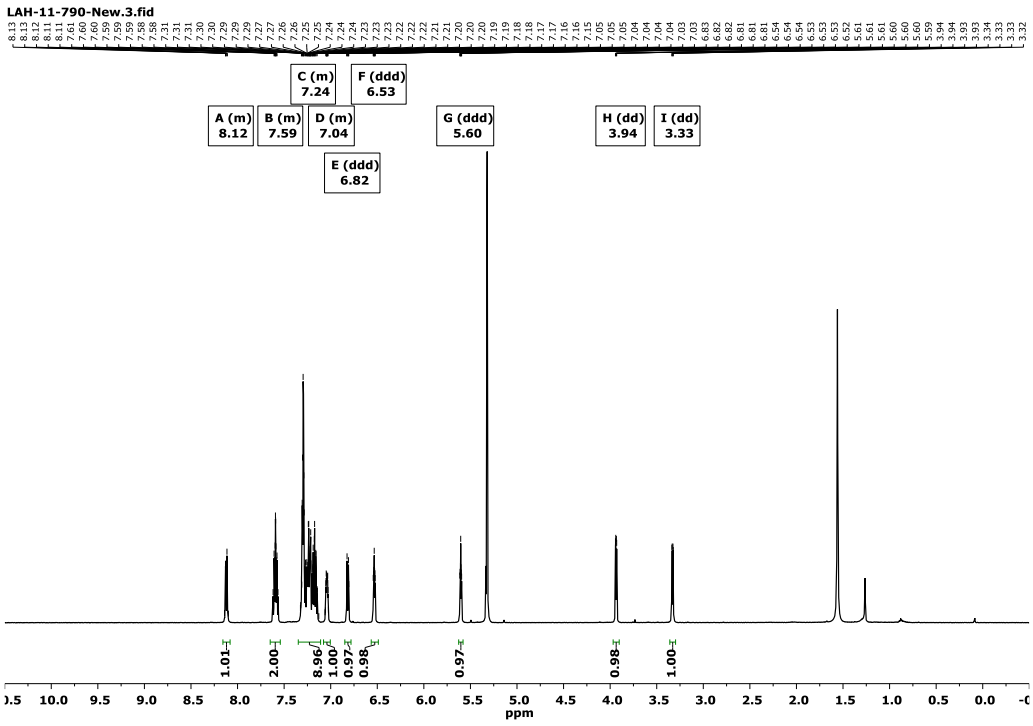


Figure S5. ^{1}H NMR spectrum of **7b** (500 MHz, CD_2Cl_2).

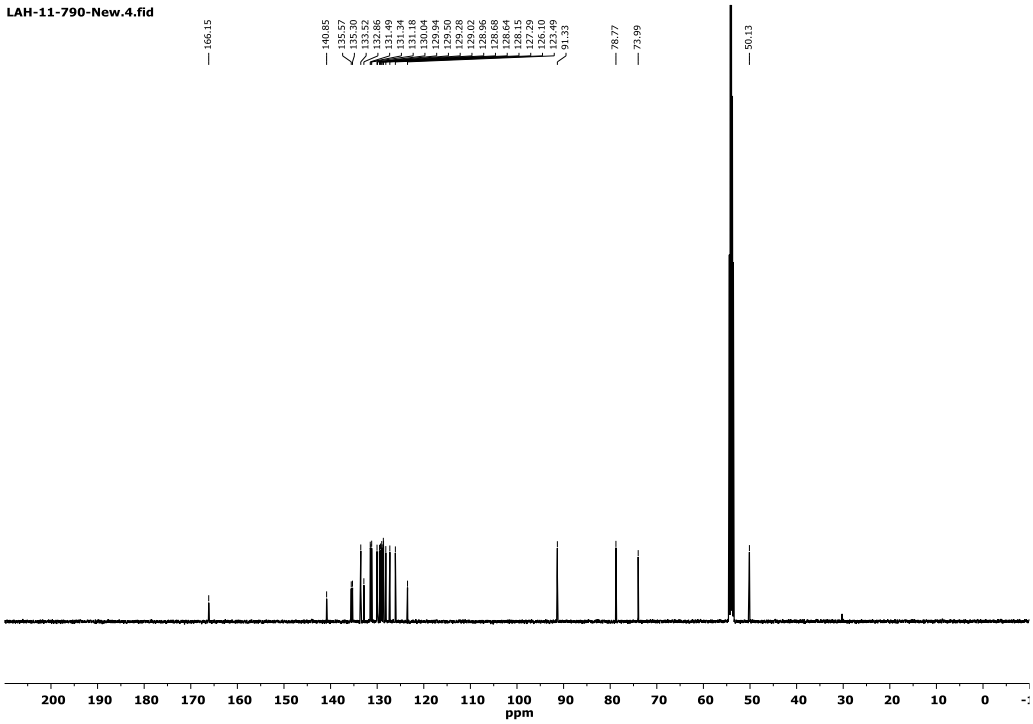
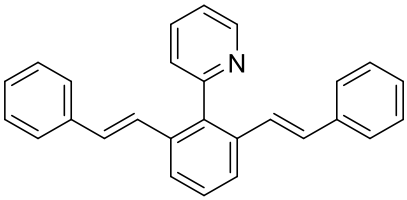


Figure S6. ^{13}C NMR spectrum of **7b** (126 MHz, CD_2Cl_2).

1.4 2-(2,6-*di*(*E*)-2-(2-styrylphenyl))pyridine, 8a



8a

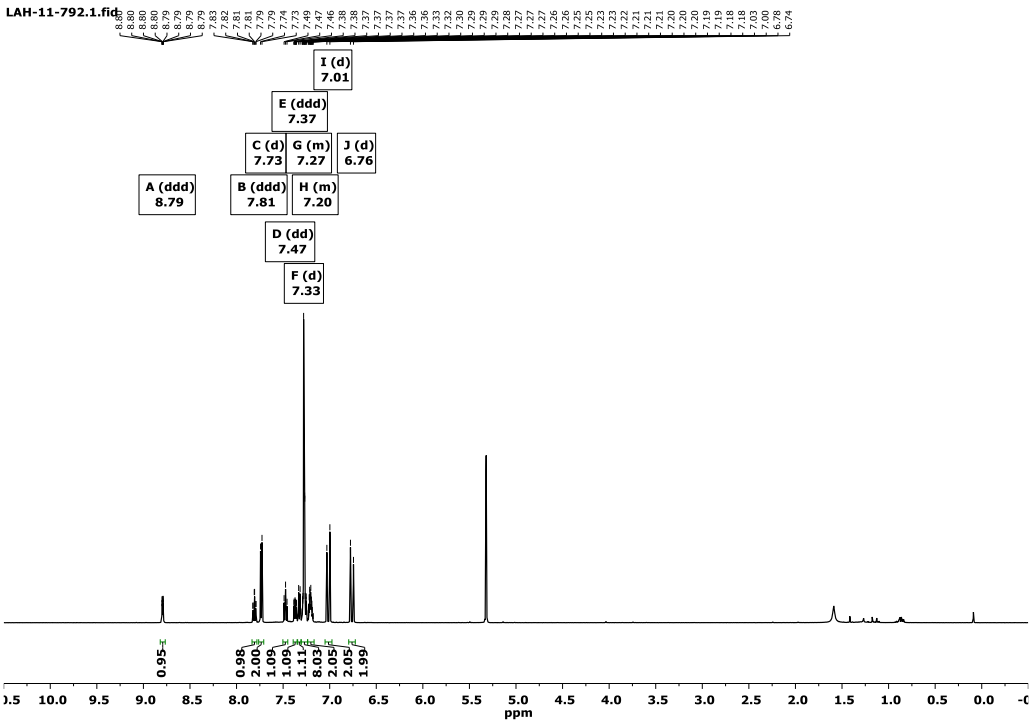


Figure S7. ^{1}H NMR spectrum of **8a** (500 MHz, CD_2Cl_2).

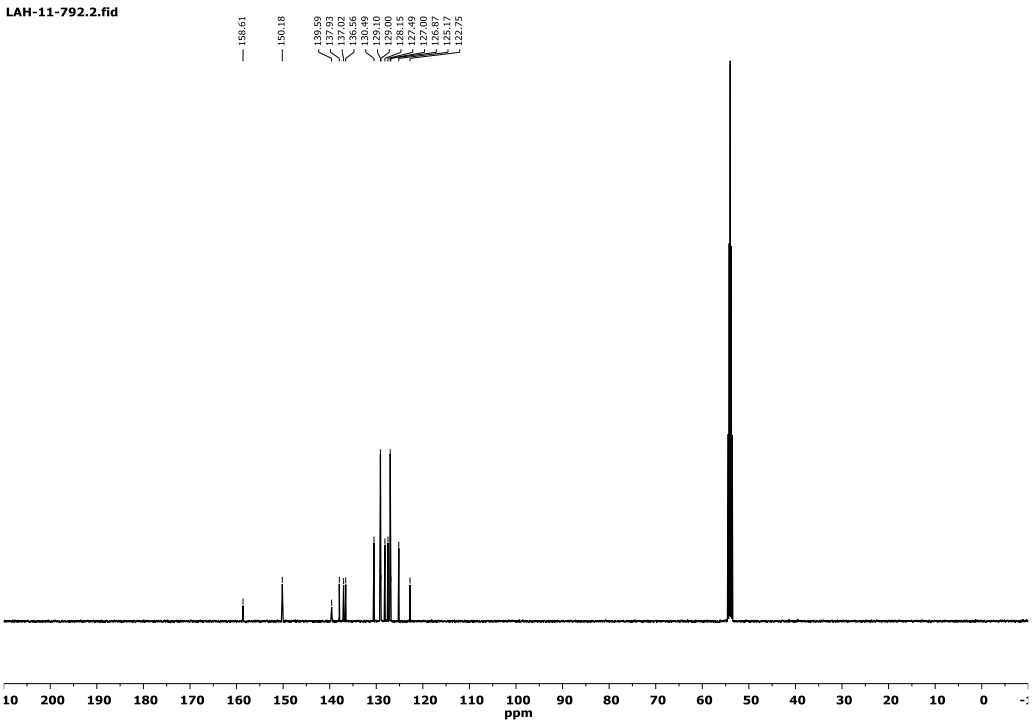
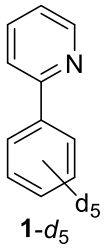


Figure S8. ^{13}C NMR spectrum of **8a** (126 MHz, CD_2Cl_2).

1.5 2-(pentadeuteriophenyl)pyridine, 1-d_5



1-d_5

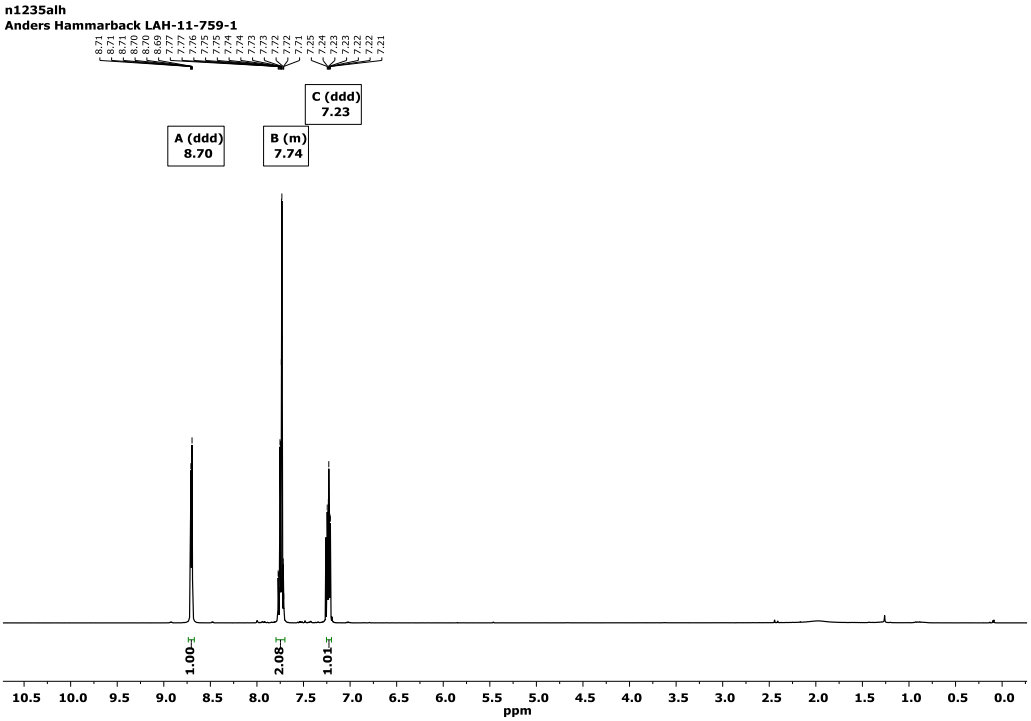


Figure S9. ^{1}H NMR spectrum of **1**-d_5 (400 MHz, $CDCl_3$).

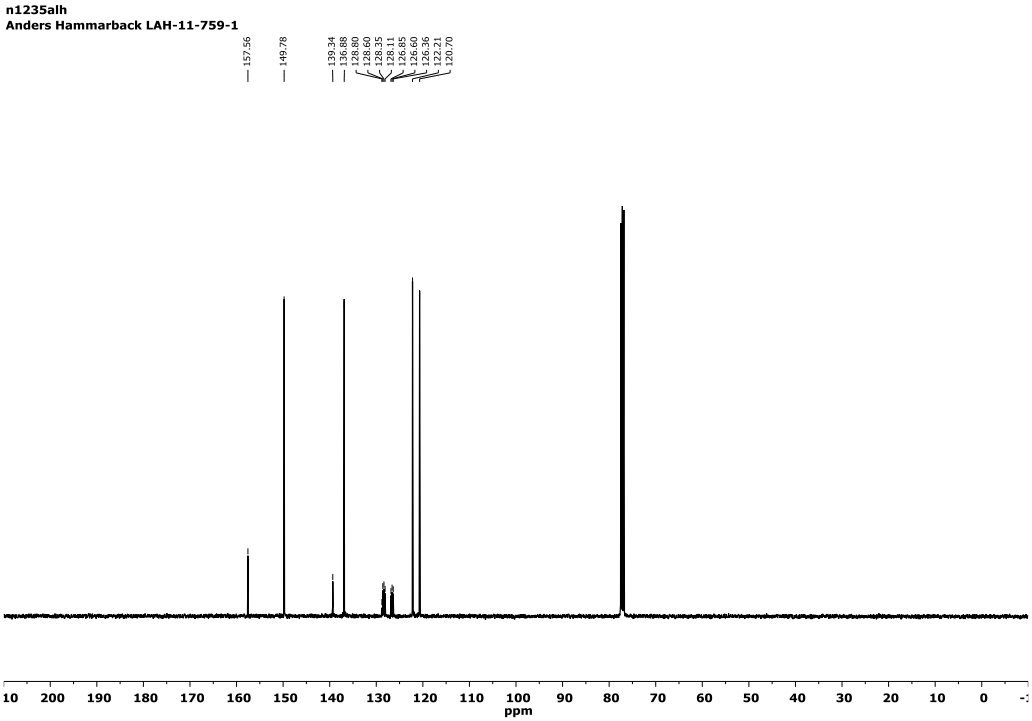
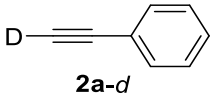


Figure S10. ^{13}C NMR spectrum of **1**-d_5 (101 MHz, $CDCl_3$).

1.6 1-(deuteriophenyl)acetylene, **2a**-*d*



2a-*d*

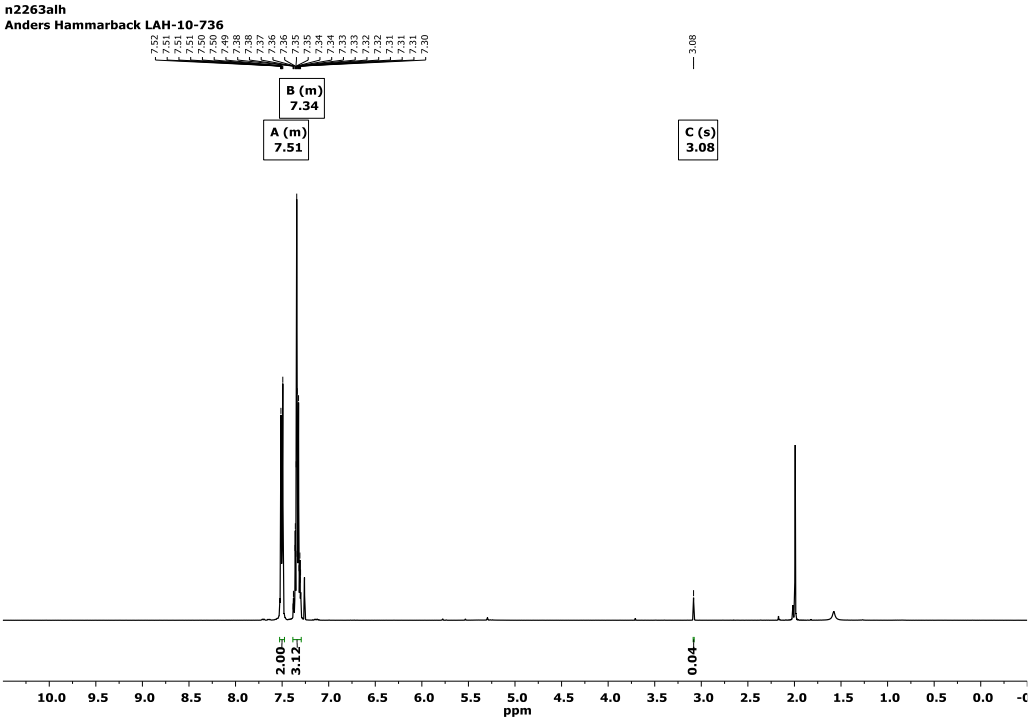


Figure S11. ^{1}H NMR spectrum of **2a**-*d* (400 MHz, $CDCl_3$).

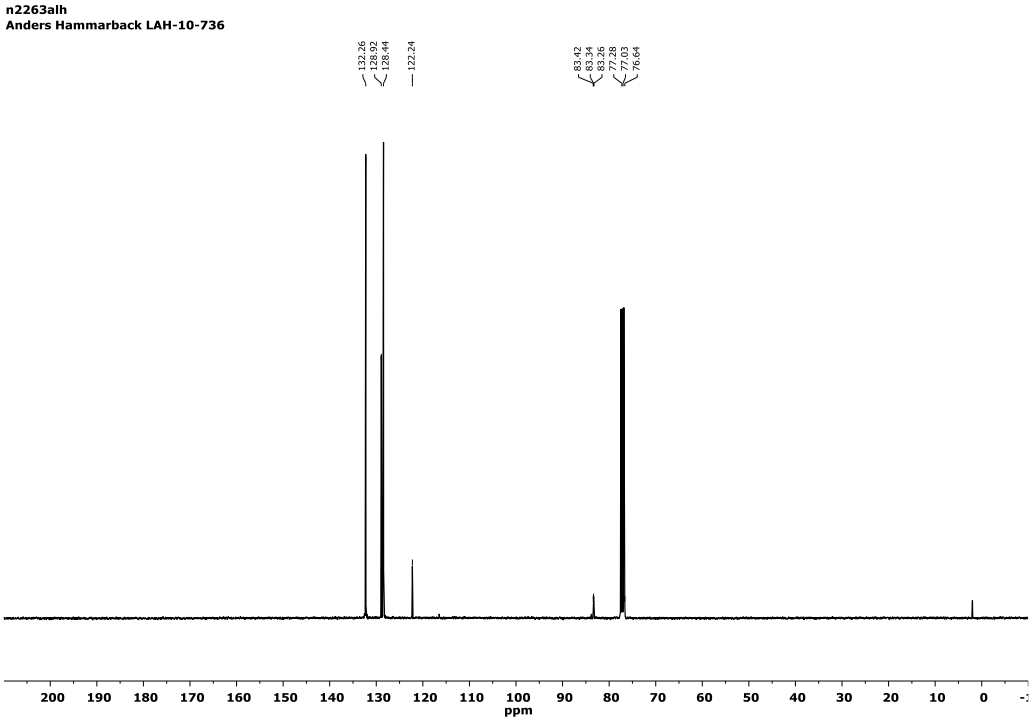
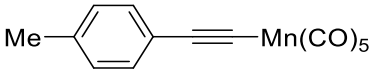


Figure S12. ^{13}C NMR spectrum of **2a**-*d* (101 MHz, $CDCl_3$).

1.7 Pentacarbonyl (2-(4'-methyl-phenyl)ethynyl-κ,C[1]) manganese(I), 14



14

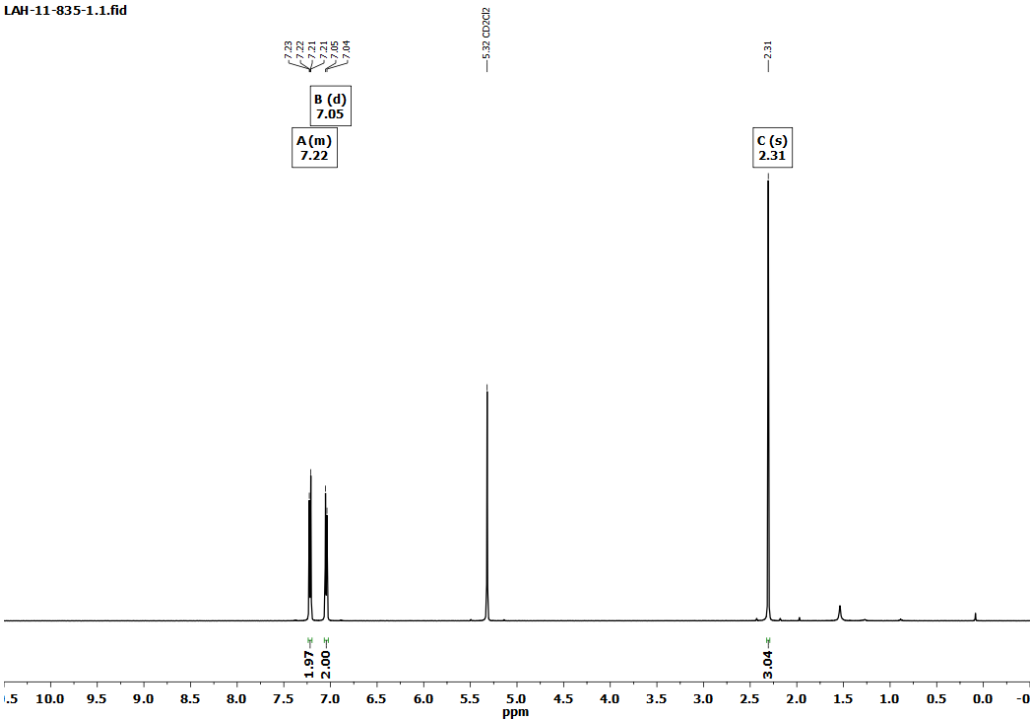


Figure S13. ^{1}H NMR spectrum of **14** (500 MHz, CD_2Cl_2).

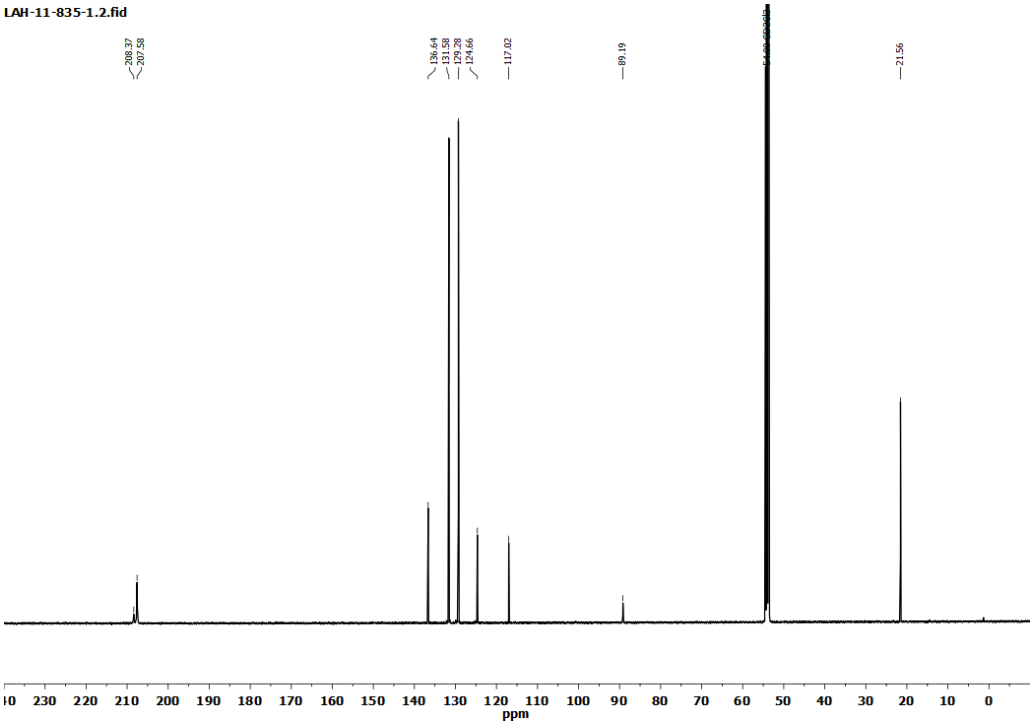
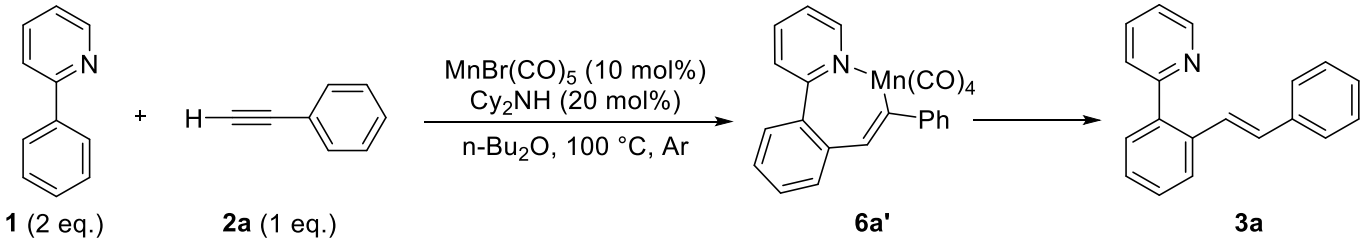


Figure S14. ^{13}C NMR spectrum of **14** (126 MHz, CD_2Cl_2).

2 Data Analysis and Individual Reaction Results

2.1 Standard reaction of 2a at 100 °C with $MnBr(CO)_5$ as precatalyst (relating to Figure 1a,b)



1 (2 eq.) **2a** (1 eq.) **6a'** **3a**

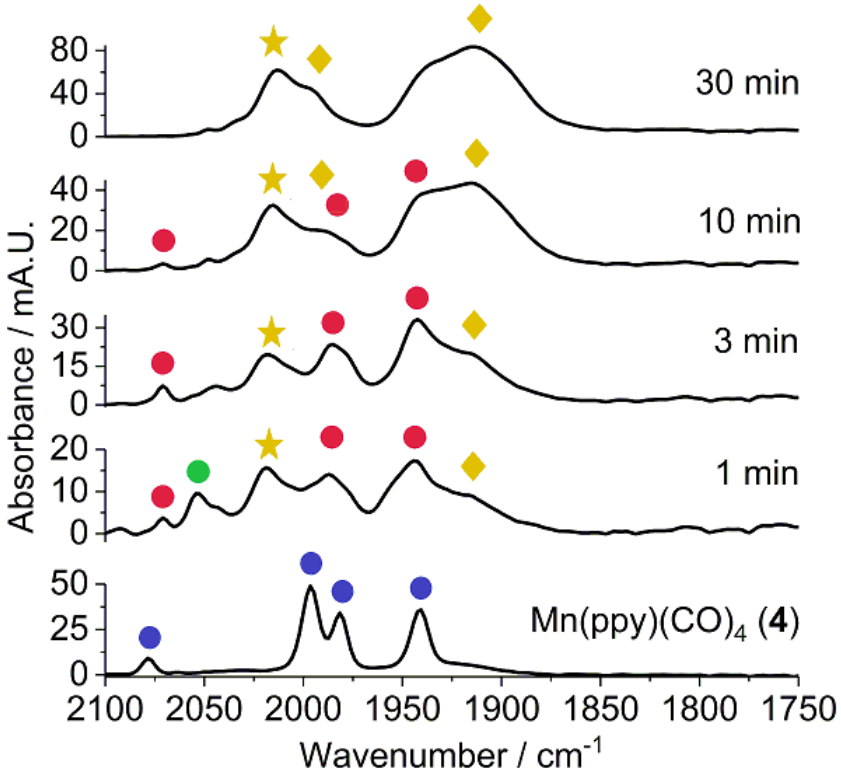


Figure S15. Reaction scheme and *in situ* IR spectra for the reaction of **2a** using $MnBr(CO)_5$ as the precatalyst, showing the formation of the alkyne insertion complex **6a'** (2071, 1986 (br), and 1943 cm^{-1}) over time from $MnBr(CO)_5$. $Mn(ppy)(CO)_4$ (**4**, 2078 cm^{-1}) cannot be observed forming during the reaction. Reaction conditions (in order of addition): n-Bu_2O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), phenylacetylene (0.45 ml, 4.16 mmol, 1 eq.), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%). Key: blue circle = **4**; red circle = **6a'**; green circle = $MnBr(CO)_5$; gold diamond / gold star = Mn carbonyl cluster species.

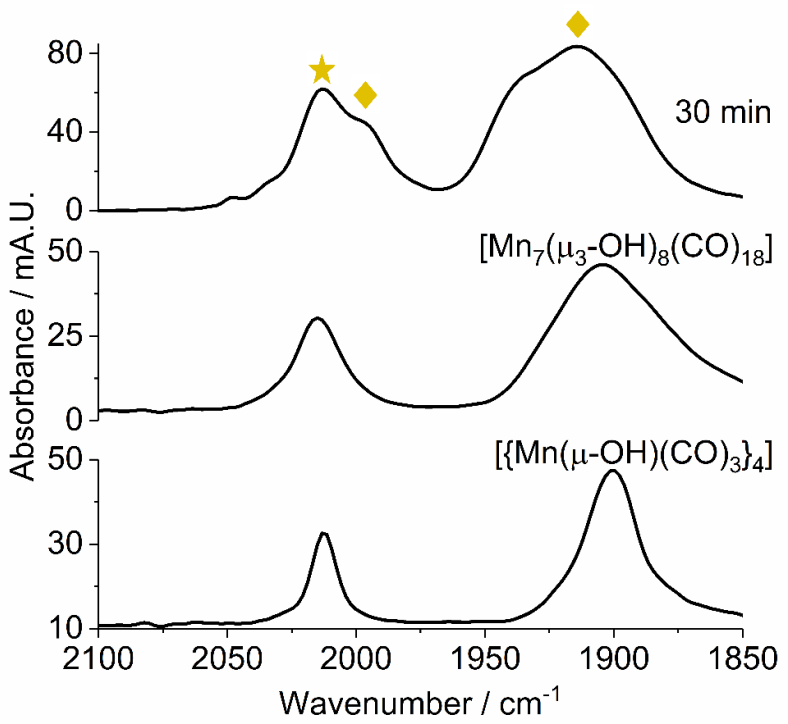


Figure S16. Comparison between the end spectrum of the reaction (30 minutes) with two Mn hydroxyl cluster compounds ([{Mn(μ_3–OH)(CO)$_3$}$_4$], and [Mn$_7$(μ_3–OH)$_8$(CO)$_{18}$]) heated at 100 °C in n-Bu$_2$O.

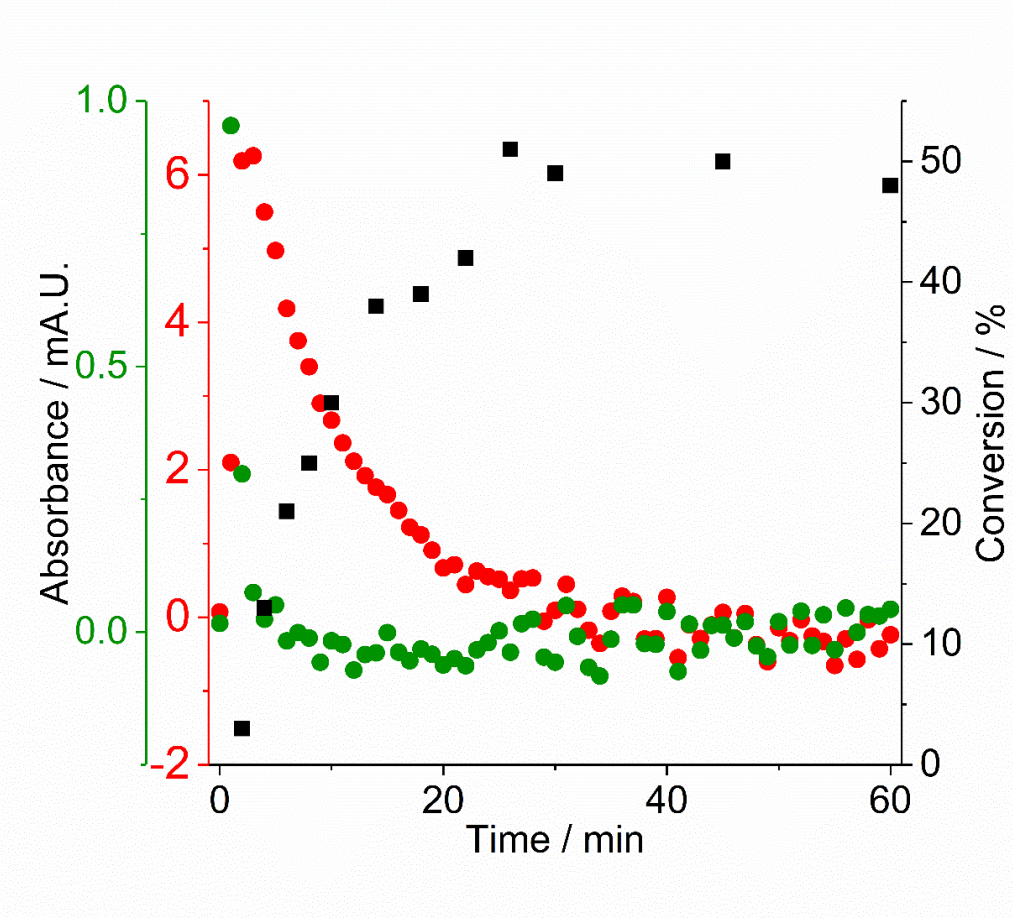
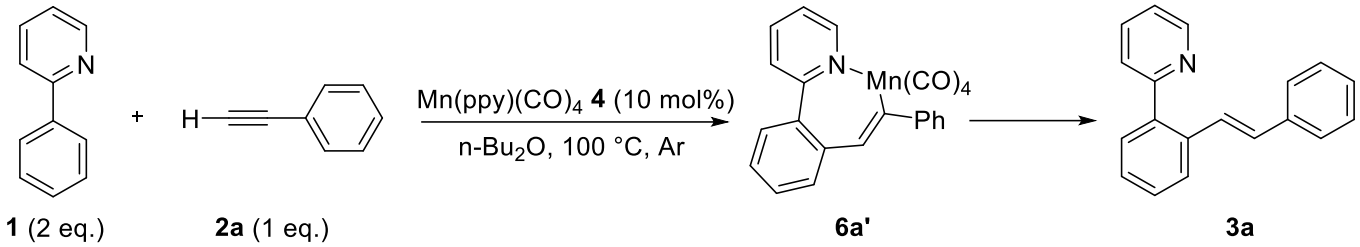


Figure S17. Kinetic plot for the formation and depletion of MnBr(CO)$_5$ (2054 cm^{-1}) and the alkyne insertion complex **6a'** (2071 cm^{-1}), compared to the conversion to alkenylated product **3a** (determined by *ex situ* ^{1}H NMR spectroscopy). Key: black square = **3a**; red circle = **6a'**; green circle = MnBr(CO)$_5$.

2.2 Reaction of 2a at 100 °C with Mn(ppy)(CO)$_4$ as precatalyst (relating to Figure 1c,d)



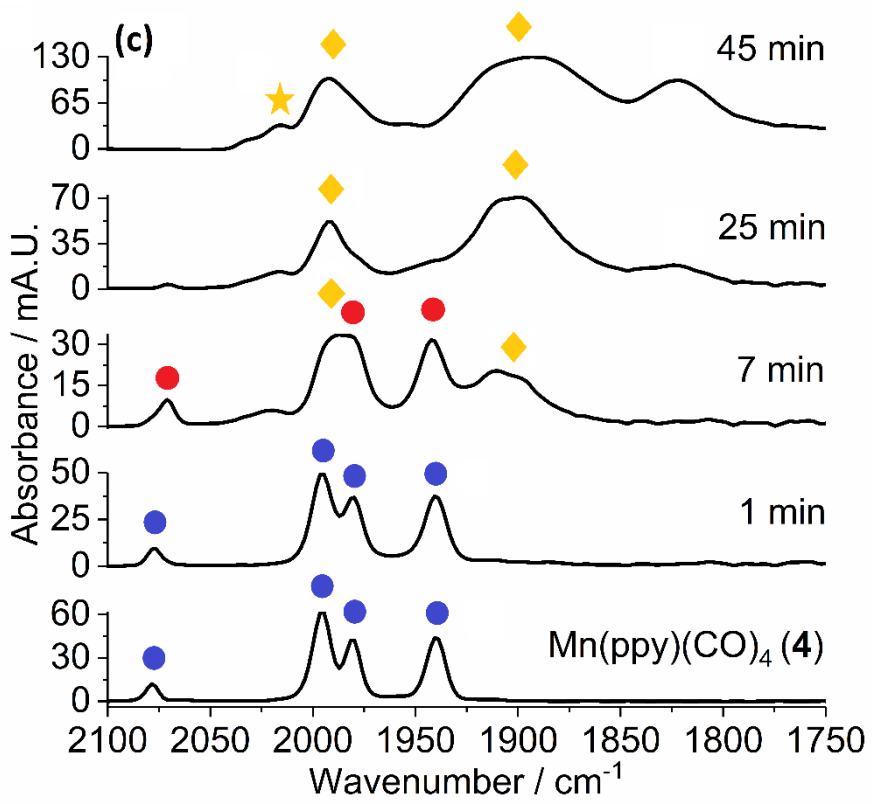


Figure S18. Reaction scheme and *in situ* IR spectra for the reaction of **2a** using Mn(ppy)(CO)$_4$ (**4**) as the precatalyst, showing the formation of alkyne insertion complex **6a'** (2071, 1989, 1982 and 1942 cm^{-1}) over time from Mn(ppy)(CO)$_4$ (2078, 1996, 1980 and 1940 cm^{-1}). Reaction conditions (in order of addition): n-Bu$_2$O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), phenylacetylene (0.45 ml, 4.16 mmol, 1 eq.) and Mn(ppy)(CO)$_4$ (0.134 g, 0.42 mmol, 10 mol%). Key: blue circle = **4**; red circle = **6a'**; gold diamond / gold star = Mn carbonyl cluster species.

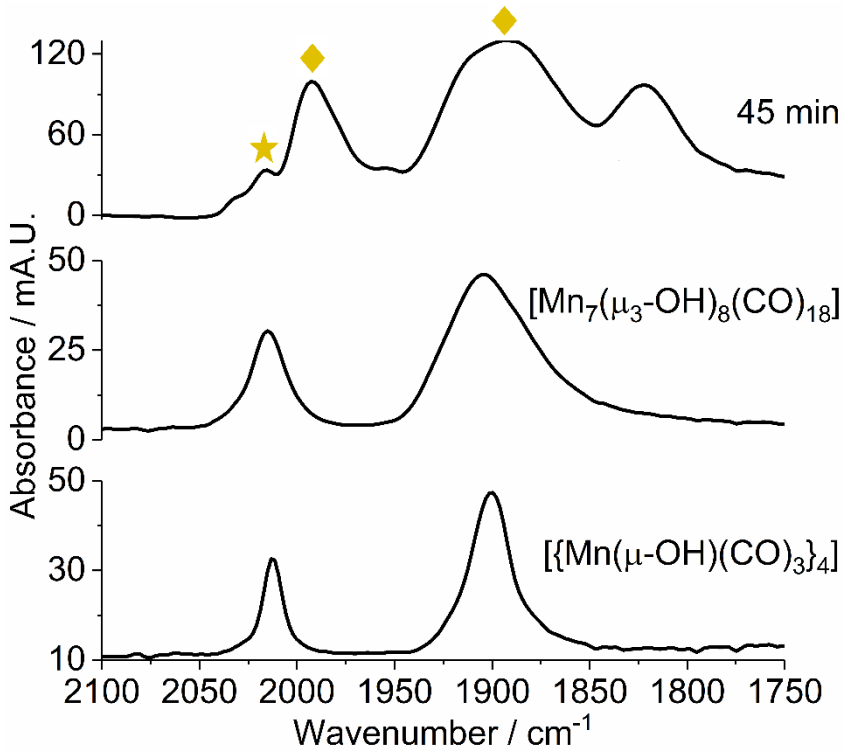


Figure S19. Comparison between the end spectrum of the reaction (45 minutes) with two Mn hydroxyl cluster compounds ([{Mn(μ_3–OH)(CO)$_3$}$_4$], and [Mn$_7$(μ_3–OH)$_8$(CO)$_{18}$]) heated at 100 °C in n-Bu$_2$O.

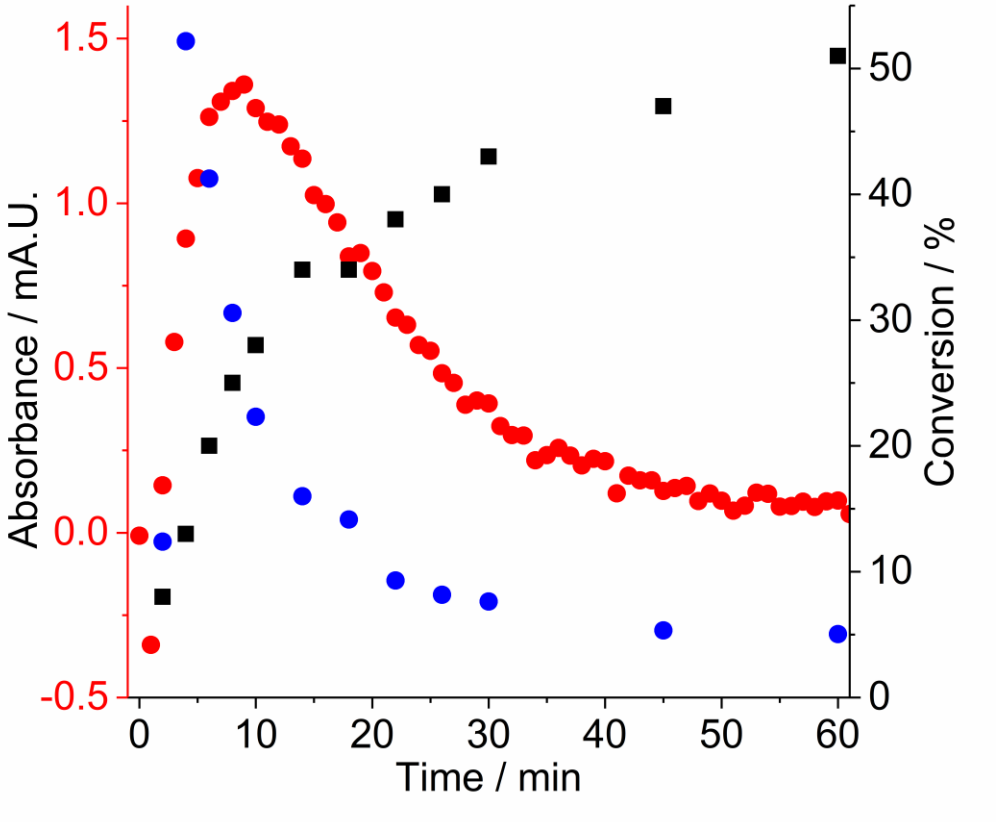


Figure S20. Kinetic plot for the formation and depletion of Mn(ppy)(CO)$_4$ (**4**, 2078 cm^{-1}) and alkyne insertion complex **6a'** (2071 cm^{-1}) compared to the conversion to alkenylated product **3a** (determined by *ex situ* ^{1}H NMR spectroscopy). Key: blue circle = **4**; red circle = **6a'**; black square = **3a**.

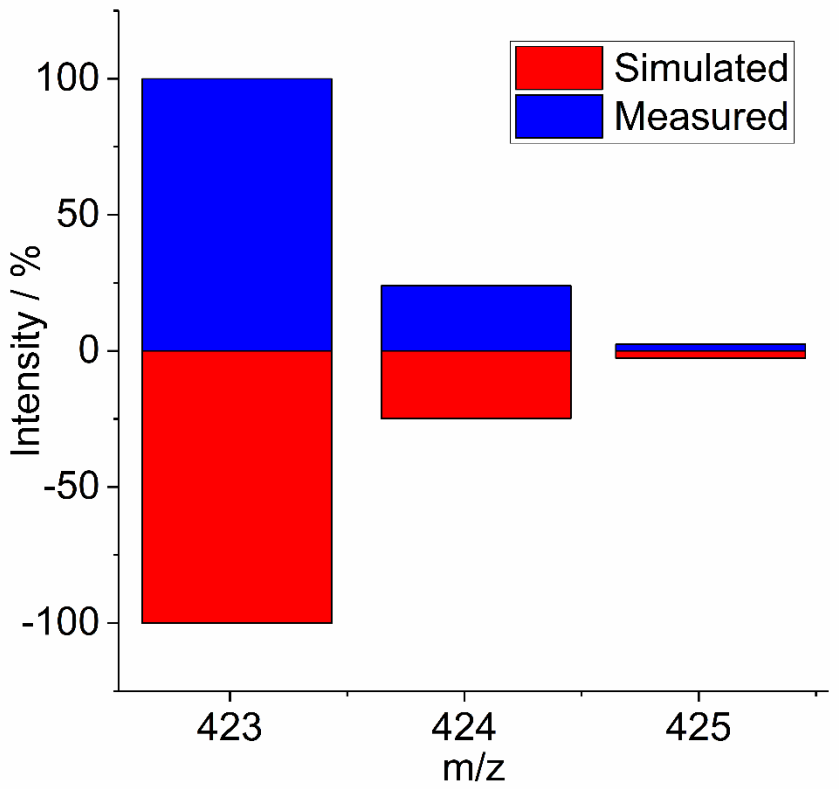


Figure S21. Expanded section of LIFDI-MS spectrum taken after 7 minutes (obtained in an independent experiment), showing the presence of the alkyne insertion complex **6a'**. Reaction conditions: n-Bu_2O (0.6 ml), 2-phenylpyridine (70 µl, 0.50 mmol, 2 eq.), phenylacetylene (27 µl, 0.25 mmol, 1 eq.) and $Mn(ppy)(CO)_4$ (8 mg, 0.025 mmol, 10 mol%). An aliquot of the reaction mixture was taken at 7 minutes and cooled immediately in ice, before a LIFDI-MS was obtained of the crude mixture.

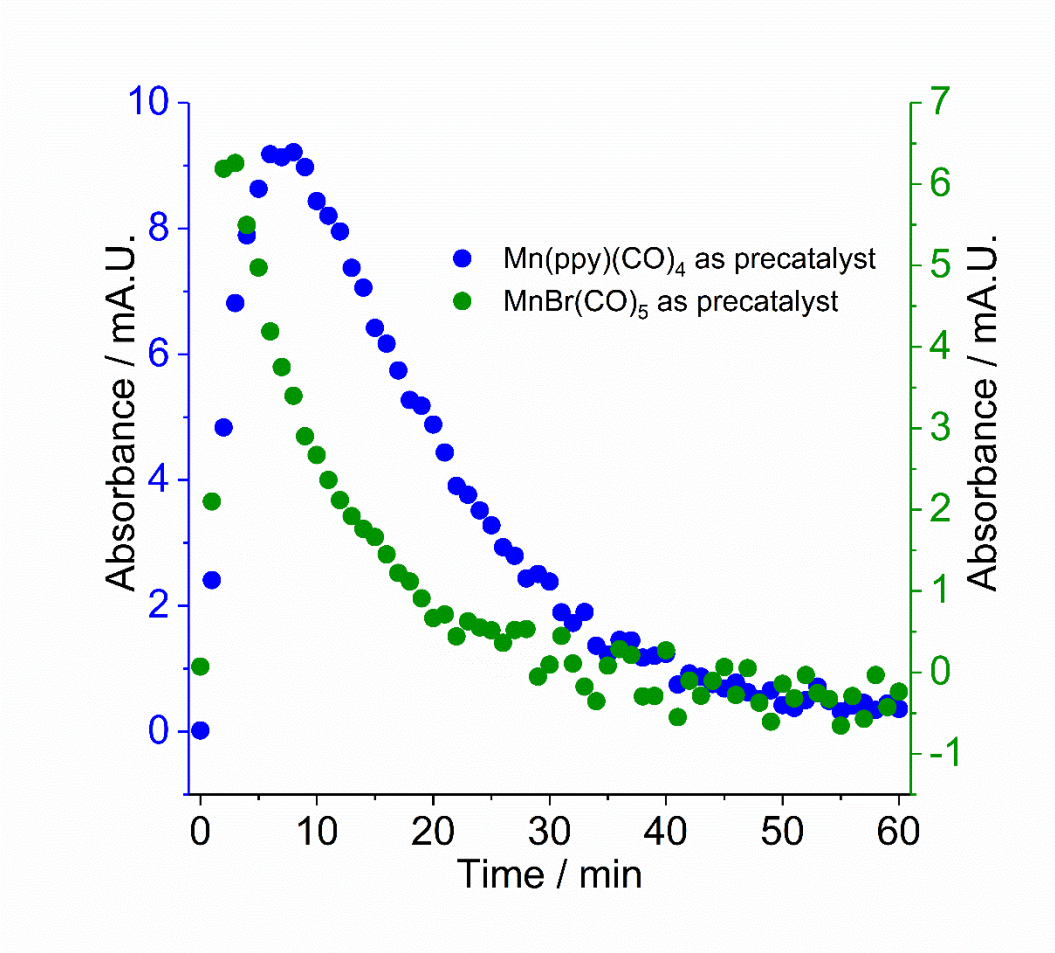
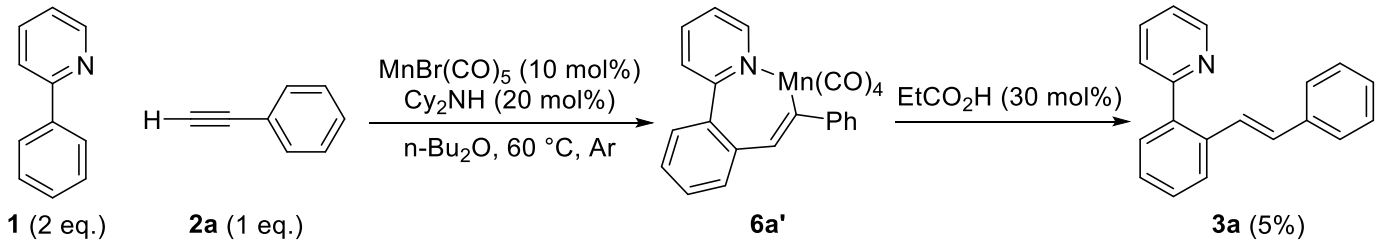


Figure S22. Comparison of the formation and depletion of the alkyne insertion complex **6a'** (2071 cm^{-1}) for the reactions employing $Mn(ppy)(CO)_4$ and $MnBr(CO)_5$ as precatalysts.

2.3 Reaction of 2a at 60 °C with $MnBr(CO)_5$ as precatalyst (relating to Figure 2a,b)



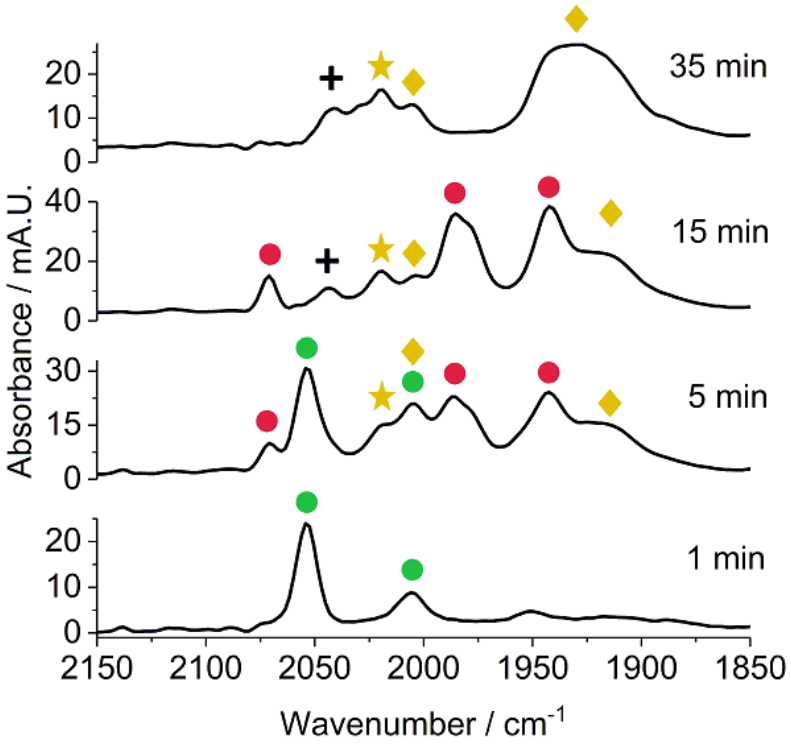


Figure S23. Reaction scheme and *in situ* IR spectra for the reaction of **2a** at 60 °C, using $MnBr(CO)_5$ as the precatalyst, showing the formation of the alkyne insertion complex **6a'** (2071, 1986, 1978, and 1942 cm^{-1}) over time from $MnBr(CO)_5$. $EtCO_2H$ (0.1 ml, 1.34 mmol, 30 mol%) was added after 30 minutes (after the formation of **6a'** had stabilized), afterwhich alkenylated product **3a** could be observed. $Mn(ppy)(CO)_4$ (**4**, 2078 cm^{-1}) cannot be observed forming during the reaction. Reaction conditions (in order of addition): n-Bu_2O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), phenylacetylene (0.45 ml, 4.16 mmol, 1 eq.), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%). Key: red circle = **6a'**; green circle = $MnBr(CO)_5$; gold diamond / gold star = Mn carbonyl cluster species; black cross = unknown Mn carbonyl species.

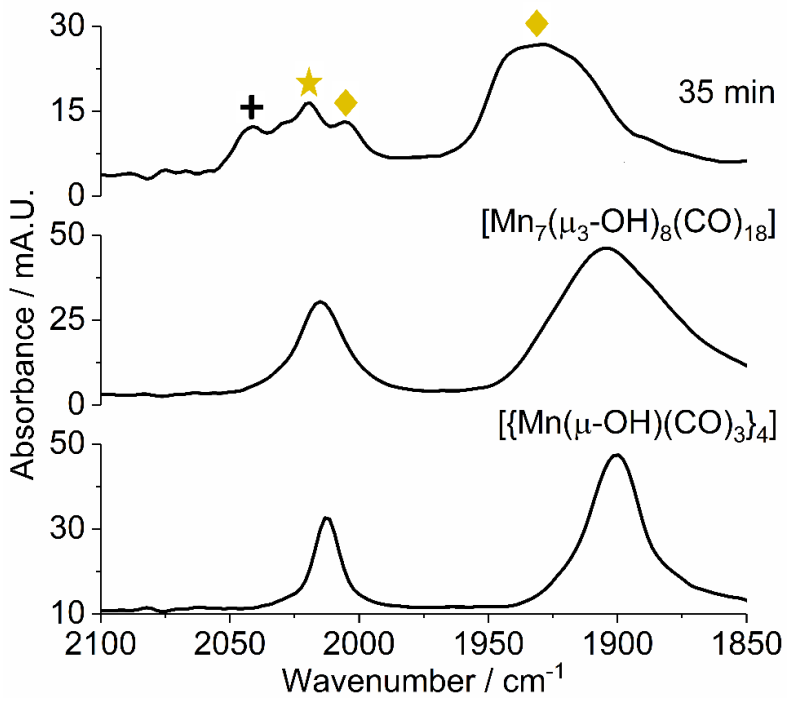


Figure S24. Comparison between the end spectrum of the reaction (35 minutes) with two Mn hydroxyl cluster compounds ([{$Mn(\mu_3$–OH)$(CO)_3\}_4$], and [$Mn_7(\mu_3$–OH$)_8(CO)_{18}$]) heated at 100 °C in n-Bu_2O.

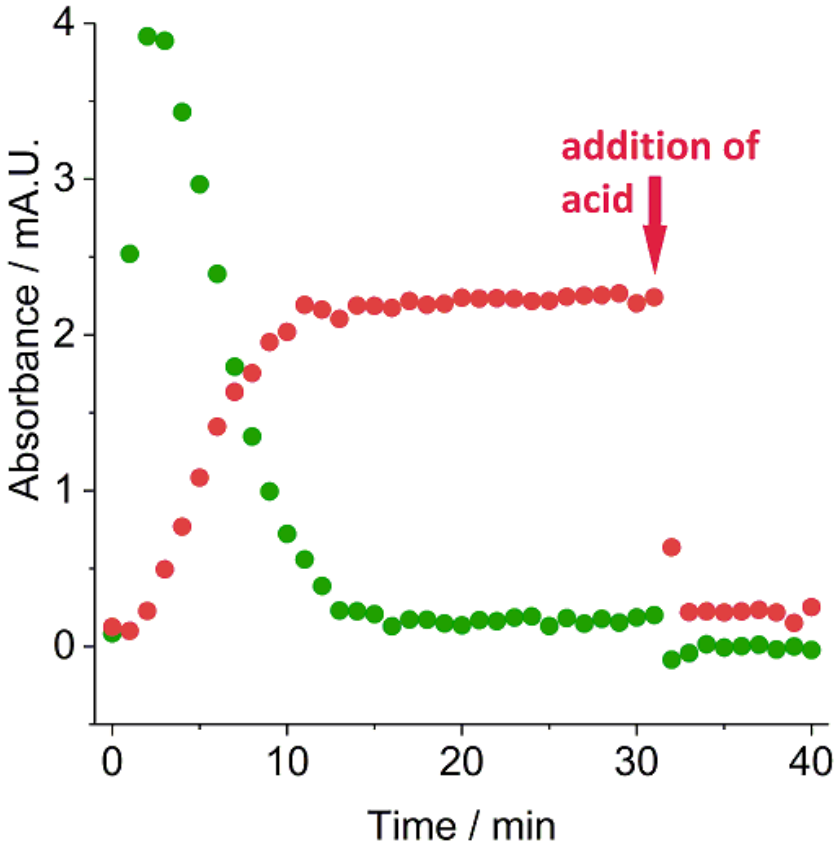
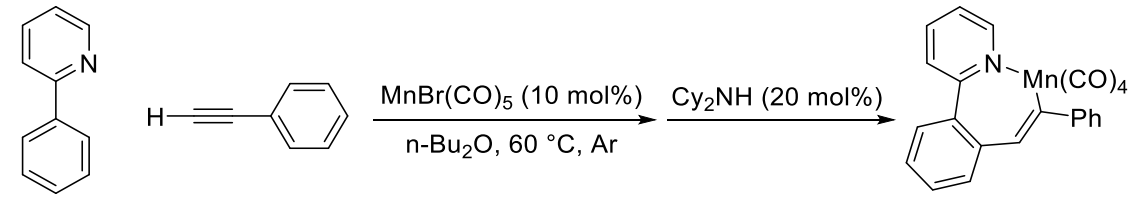


Figure S25. Kinetic plot for the formation and depletion of $MnBr(CO)_5$ (2054 cm^{-1}) the alkyne insertion complex **6a'** (2071 cm^{-1}). Key: red circle = **6a'**; green circle = $MnBr(CO)_5$.

2.4 Reaction of 2a at 60 °C with $MnBr(CO)_5$ as precatalyst, excluding Cy_2NH (relating to Figure 3a,b)



1 (2 eq.) **2a** (1 eq.) **6a'**

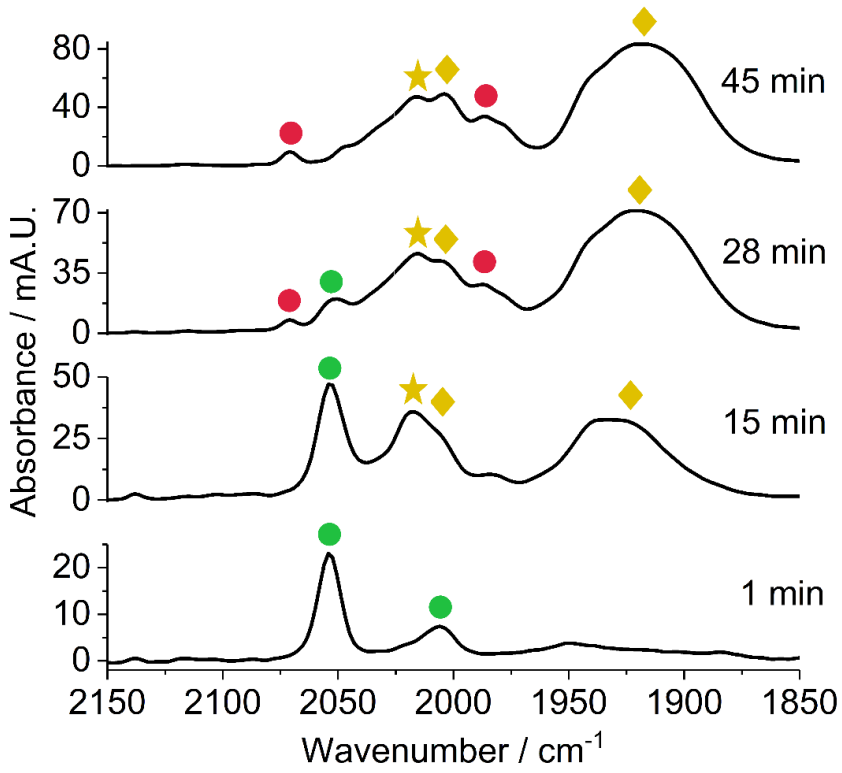


Figure S26. Reaction scheme and *in situ* IR spectra for the reaction at 60 °C without Cy_2NH, using $MnBr(CO)_5$ as the precatalyst. The reaction show no formation of alkyne insertion complex **6a'** over time from $MnBr(CO)_5$. Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) was added after 25 minutes and **6a'**,(2071, 1986, 1978, and 1942 cm^{-1}) could be observed forming. Reaction conditions (in order of addition): n-Bu_2O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), phenylacetylene (0.45 ml, 4.16 mmol, 1 eq.) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%). Key: red circle = **6a'**; green circle = $MnBr(CO)_5$; gold diamond / gold star = Mn carbonyl cluster species.

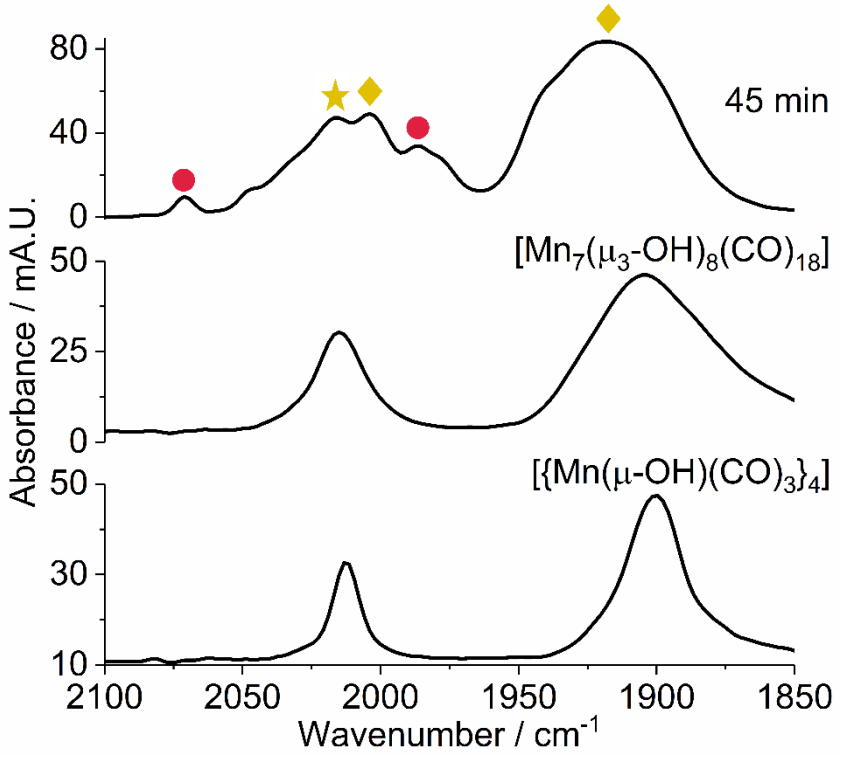


Figure S27. Comparison between the end spectrum of the reaction (45 minutes) with two Mn hydroxyl cluster compounds ([{$Mn(\mu_3–OH)(CO)_3\}_4$], and [$Mn_7(\mu_3–OH)_8(CO)_{18}$]) heated at 100 °C in n-Bu_2O.

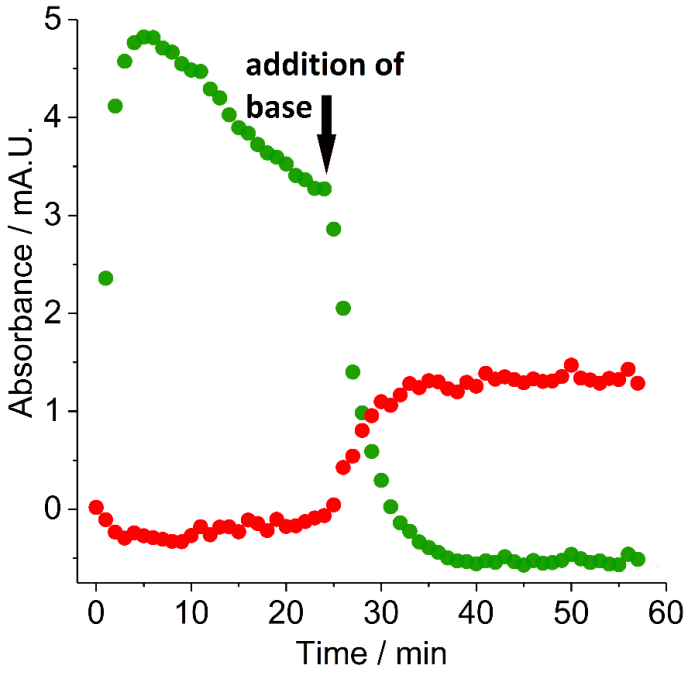


Figure S28. Kinetic plot for the formation and depletion of $MnBr(CO)_5$ (2054 cm^{-1}) the alkyne insertion complex **6a'** (2071 cm^{-1}). Key: red circle = **6a'**; green circle = $MnBr(CO)_5$.

2.5 Reaction of Cy_2NH with $MnBr(CO)_5$ at 60 °C

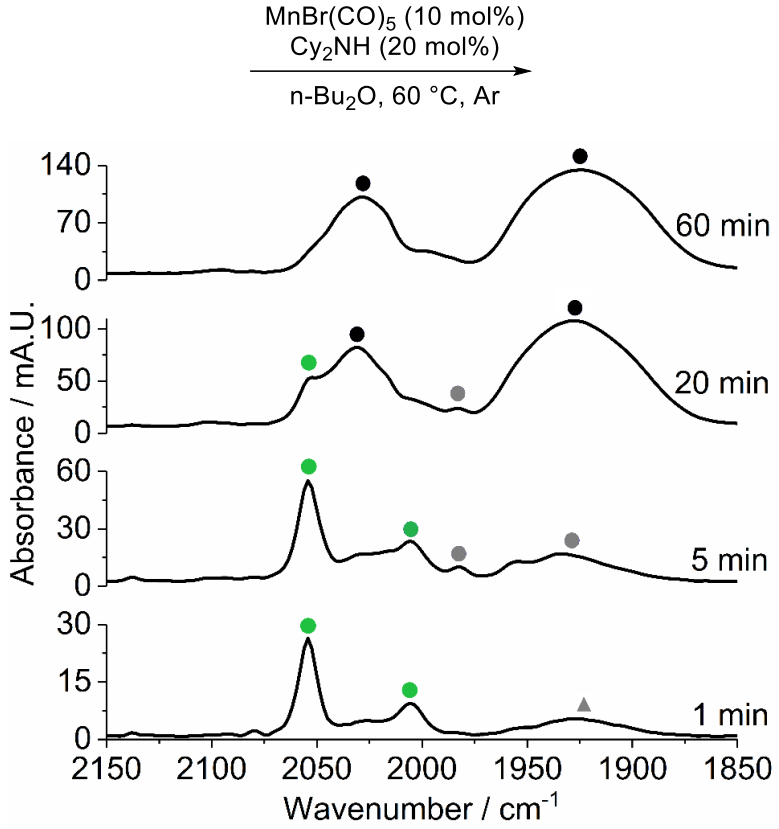
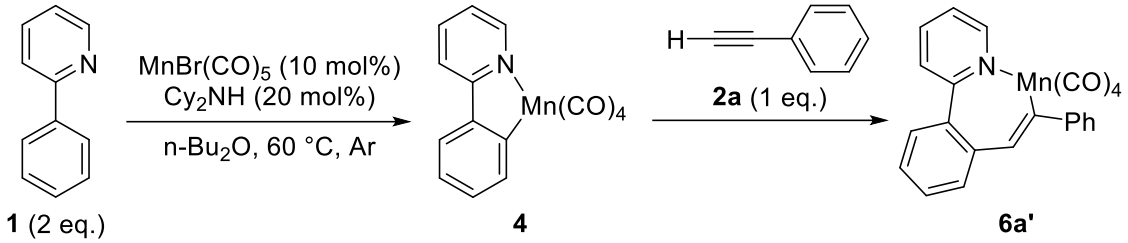


Figure S29. Reaction scheme and *in situ* IR spectra for the reaction of Cy_2NH and $MnBr(CO)_5$. Several Mn carbonyl species can be observed at early times, followed the formation of a main unknown Mn carbonyl complex (2030, 1926, br, cm^{-1}) at the end of the reaction. None of these species can be observed when **1** and **2a** are included in the reaction. Reaction conditions (in order of addition): n-Bu_2O (11.7 ml), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%). Key: green circle = $MnBr(CO)_5$; grey shapes = unknown Mn carbonyl species; black circle = unknown major Mn carbonyl species.

2.6 Reaction at 60 °C with $MnBr(CO)_5$ as precatalyst, excluding 2a (relating to Figure 3c,d)



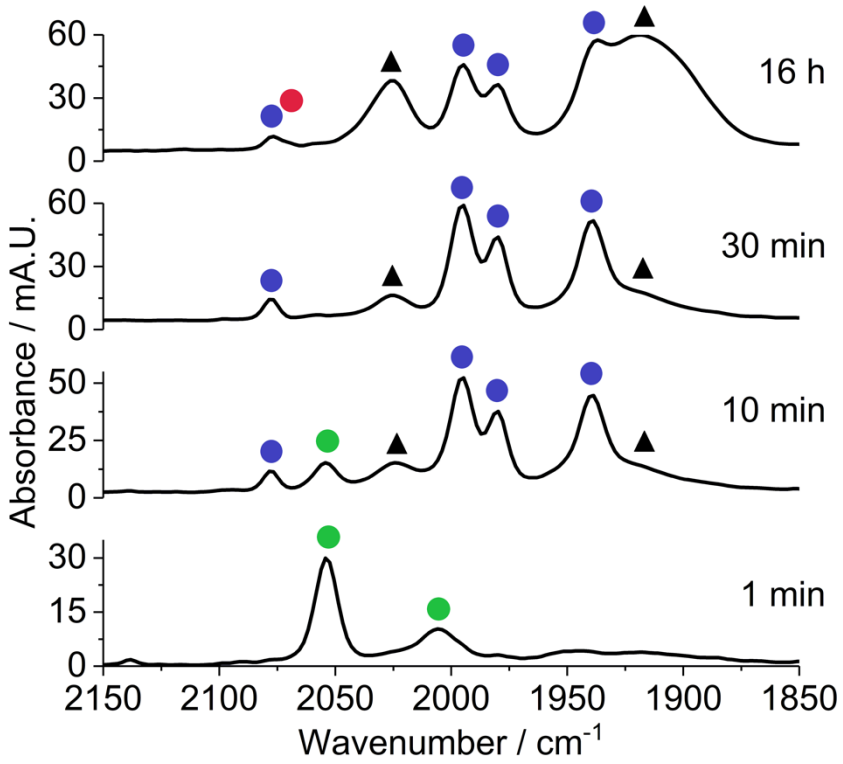


Figure S30. Reaction scheme and *in situ* IR spectra for the reaction at 60 °C without **2a**, using $MnBr(CO)_5$ as precatalyst, showing the formation of $Mn(ppy)(CO)_4$ (**4**, 2078, 1995, 1980 and 1940 cm^{-1}) over time from $MnBr(CO)_5$. Also shown is the slow formation of the alkyne insertion complex **6a'** (16 h spectrum, 2071, 1986, 1978, and 1942 cm^{-1}) following addition of **2a** (0.45 ml, 4.16 mmol, 1 eq.). Reaction conditions (in order of addition): n-Bu_2O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%). Key: blue circle = **4**; red circle = **6a'**; green circle = $MnBr(CO)_5$; black triangle = unknown Mn carbonyl species.

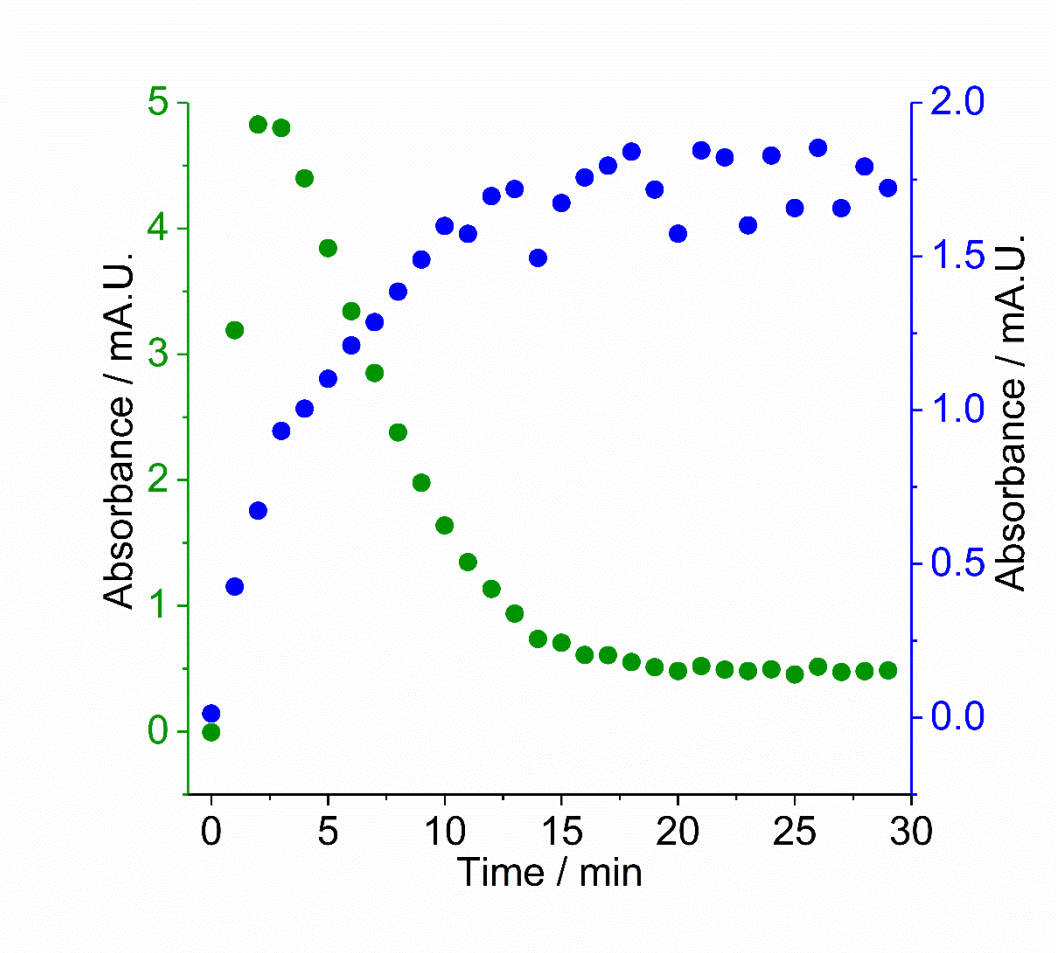


Figure S31. Kinetic plot for the formation $Mn(ppy)(CO)_4$ (**4**, 2078 cm^{-1}) over time from $MnBr(CO)_5$ (2054 cm^{-1}). Key: blue circle = **4**; green circle = $MnBr(CO)_5$.

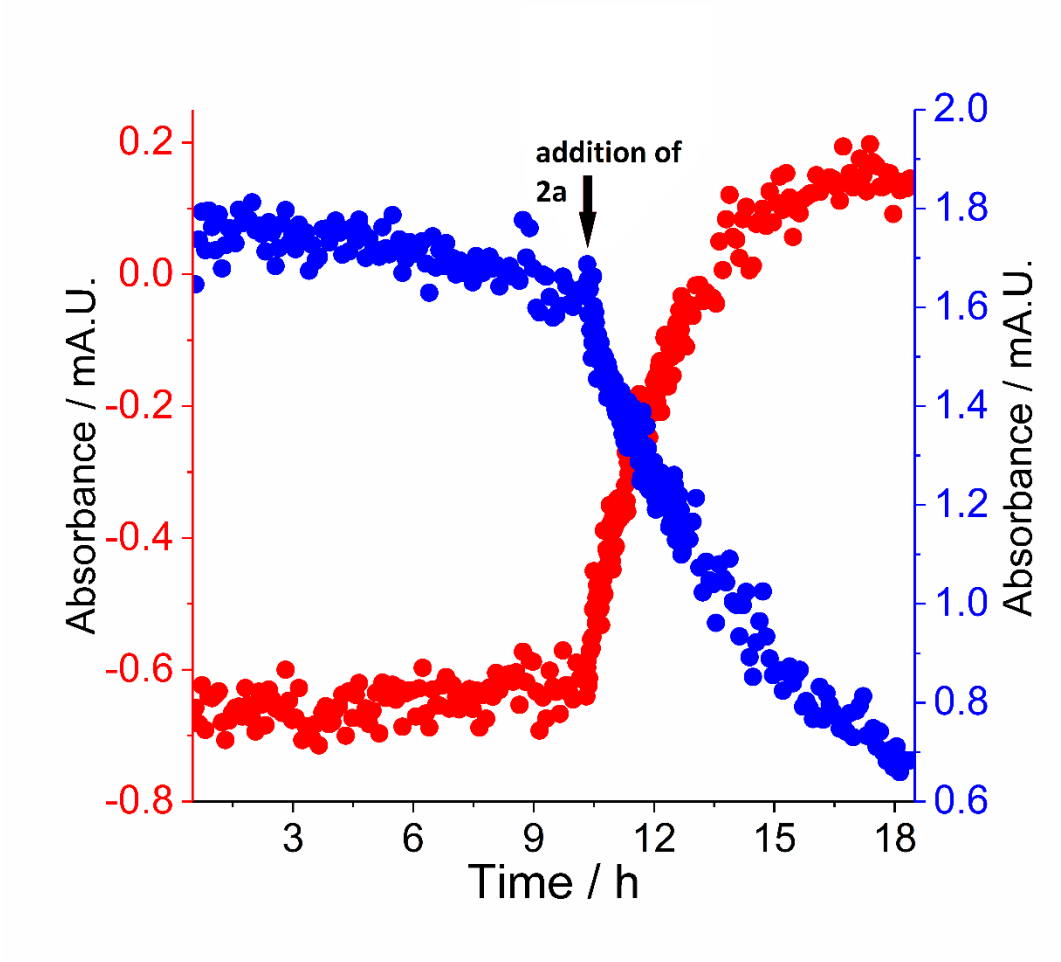
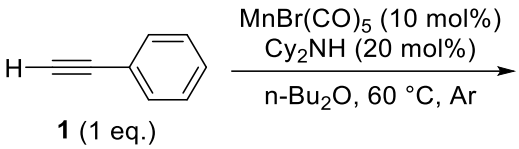


Figure S32. Kinetic plot for the slow formation of the alkyne insertion complex **6a'** (2071 cm^{-1}) from $Mn(ppy)(CO)_4$ (**4**, 2078 cm^{-1}), following the addition of PhCCH. Key: blue circle = **4**; red circle = **6a'**.

2.7 Reaction of 2a at 60 °C with $MnBr(CO)_5$ as precatalyst, excluding 1 (relating to Figure 3e)



1 (1 eq.)

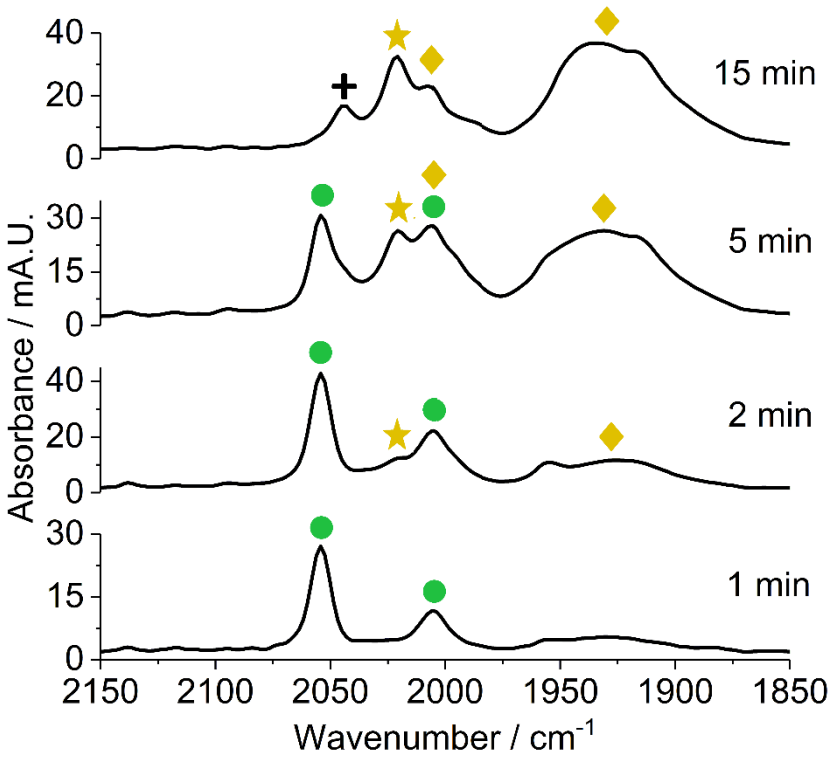


Figure S33. Reaction scheme and *in situ* IR spectra for the reaction at 60 °C without **1**, using $MnBr(CO)_5$ as the precatalyst, showing the formation of three unknown complexes (2044, 2021 and 2007 cm^{-1}) over time from $MnBr(CO)_5$. Reaction conditions (in order of addition): n-Bu_2O (11.3 ml), phenylacetylene (0.45 ml, 4.16 mmol, 1 eq.), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%). Key: green circle = $MnBr(CO)_5$; gold diamond / gold star = Mn carbonyl cluster species; black cross = unknown Mn carbonyl species.

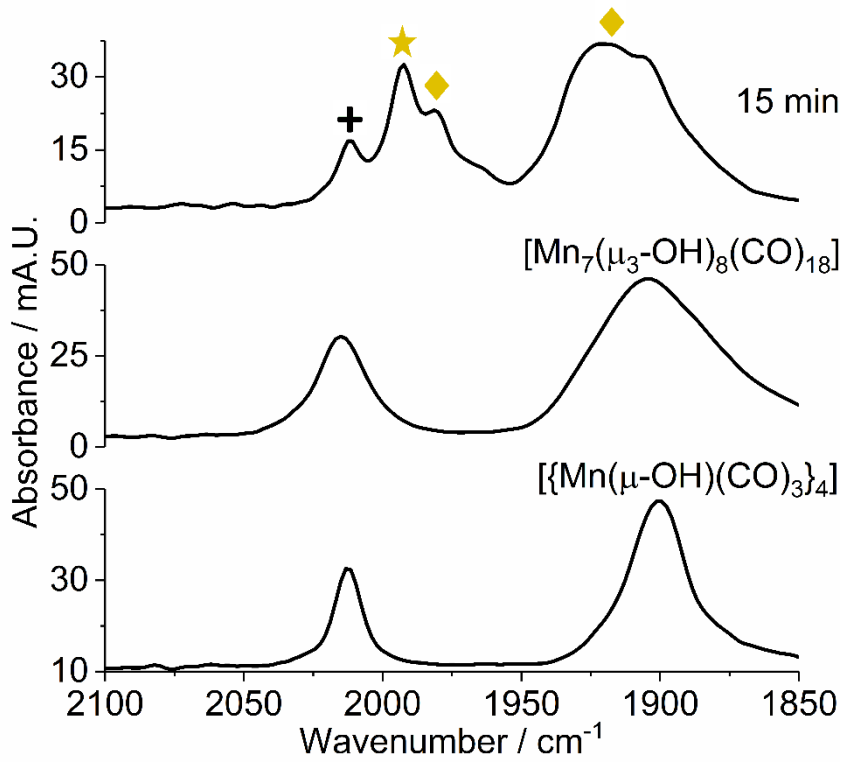
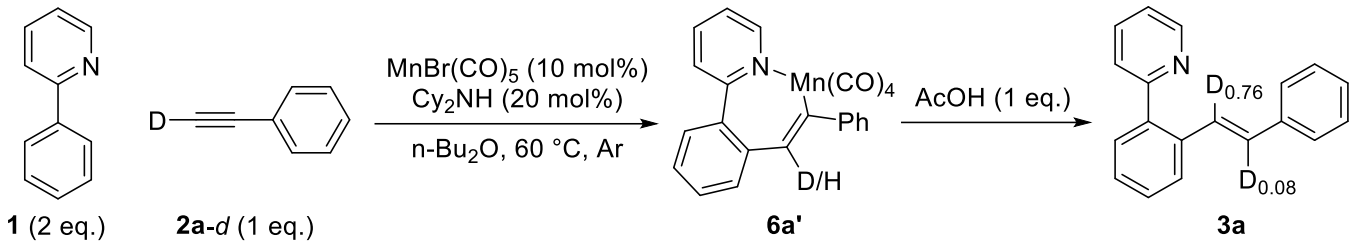


Figure S34. Comparison between the end spectrum of the reaction (15 minutes) with two Mn hydroxyl cluster compounds ([{$Mn(\mu_3–OH)(CO)_3$}$_4$], and [$Mn_7(\mu_3–OH)_8(CO)_{18}$]) heated at 100 °C in n-Bu_2O.

2.8 Reaction of 2a-*d* at 60 °C with $MnBr(CO)_5$ as precatalyst (relating to Scheme 4)



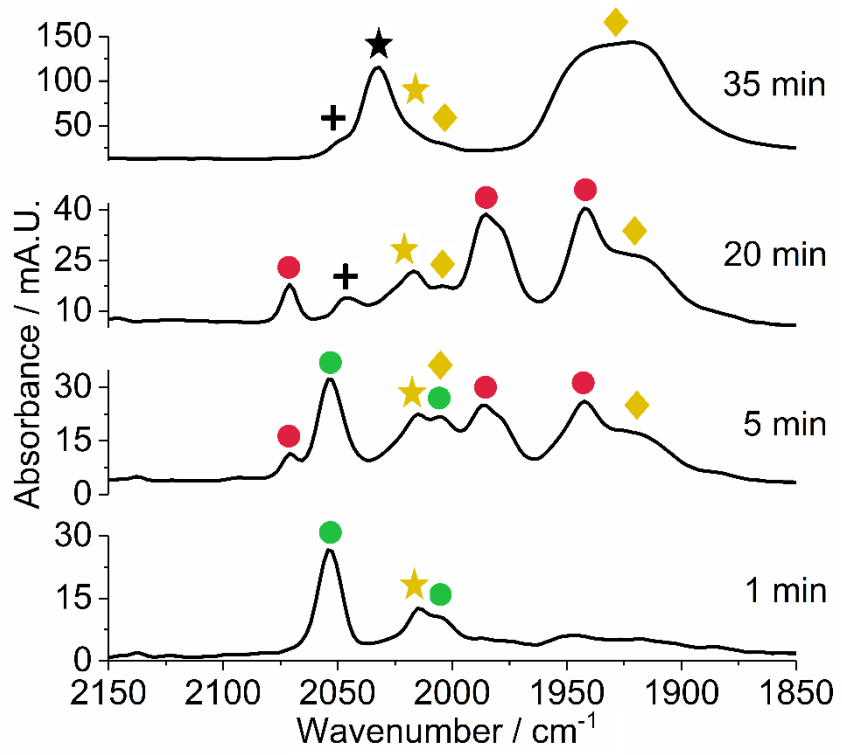


Figure S35. Reaction scheme and *in situ* IR spectra for the reaction of PhCCD using $MnBr(CO)_5$ as the precatalyst, with addition of AcOH (0.3 ml, 4.16 mmol, 1 eq.), showing the formation of the alkyne insertion complex **6a'** (2071, 1986, 1979, and 1943 cm^{-1}) over time from $MnBr(CO)_5$. Reaction conditions (in order of addition): n-Bu_2O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), phenylacetylene-D_1 (0.47 ml, 4.16 mmol, 1 eq.), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%). Deuterium incorporation was determined by ^1H NMR spectroscopy from the isolated alkenylated product (flash column chromatography, petrol/Et_2O, 8:2, *v/v*). Key: red circle = **6a'**; green circle = $MnBr(CO)_5$; gold diamond / gold star = Mn carbonyl cluster species; black cross = unknown Mn carbonyl species.

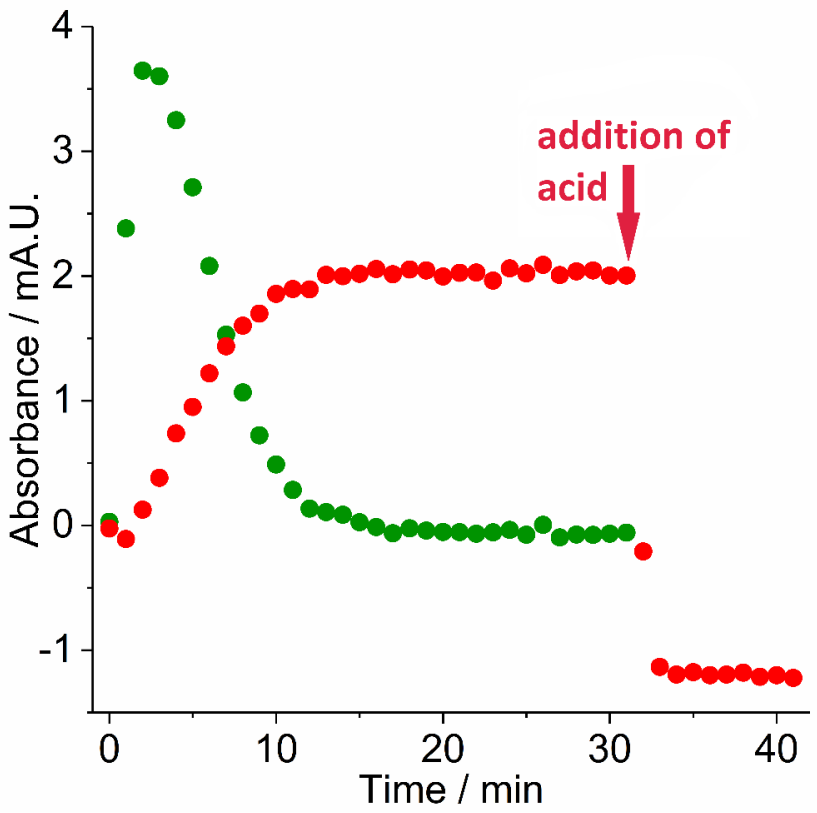


Figure S36. Kinetic plot for the formation and depletion of $MnBr(CO)_5$ (2054 cm^{-1}) the insertion complex **6a'** (2071 cm^{-1}). Key: red circle = **6a'**; green circle = $MnBr(CO)_5$.

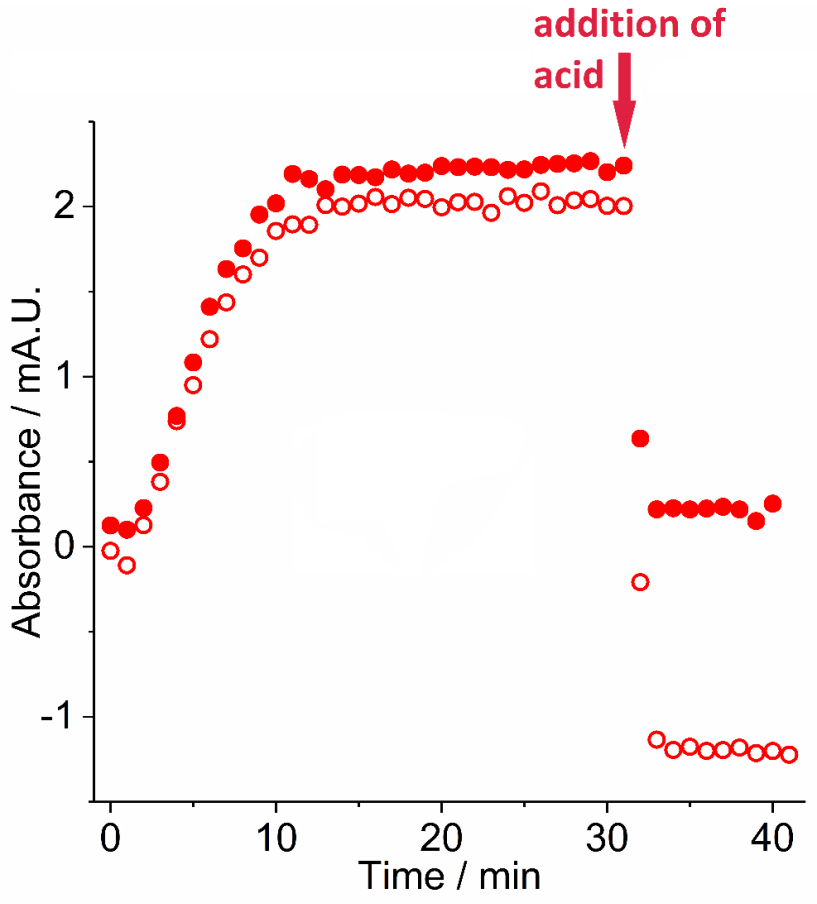


Figure S37. Comparison of the kinetic profile of the formation of the insertion complex for PhCCH and PhCCD. No KIE can be observed. Key: red circle = **6a'** from **2a**; red hollow cicle = **6a'** from **2a**-*d*.

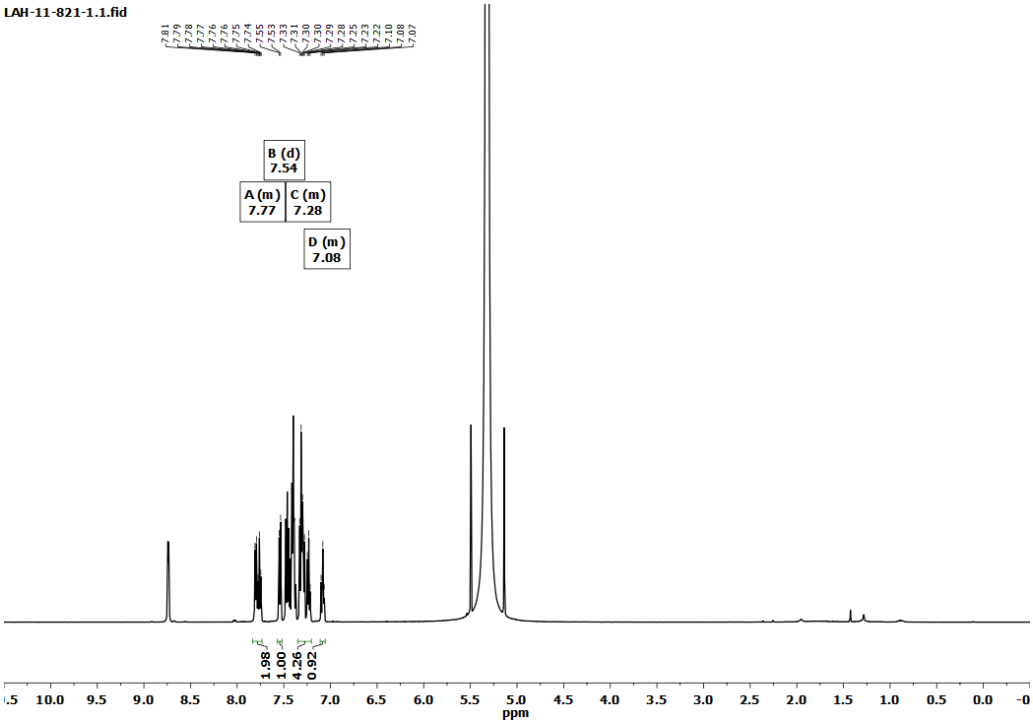


Figure S38. ^{1}H NMR spectrum of isolated **3a** from the reaction (500 MHz, CH_2Cl_2)

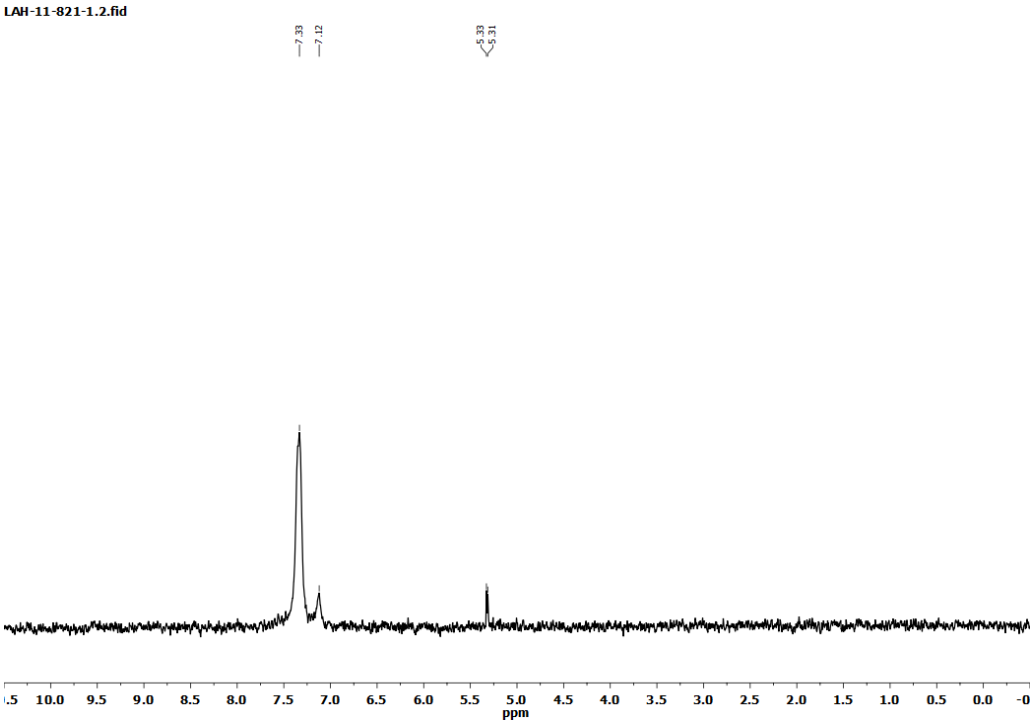
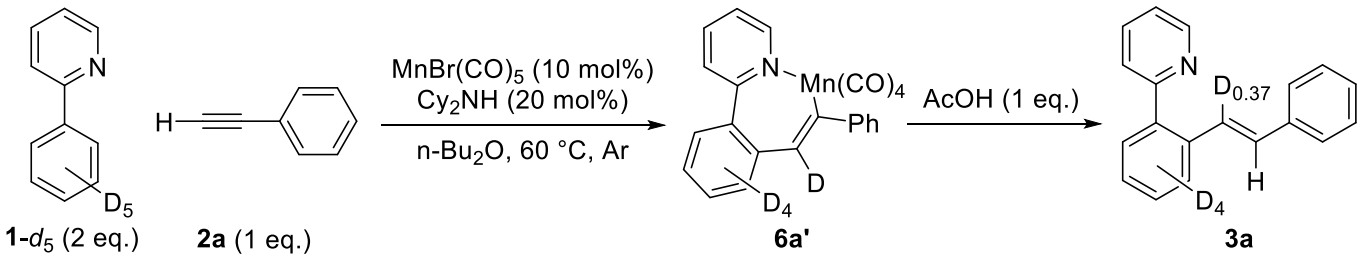


Figure S39. ^{2}H NMR spectrum of isolated **3a** from the (77 MHz, CH_2Cl_2)

2.9 Reaction of 2a and 1-d_5 at 60 °C with $MnBr(CO)_5$ as precatalyst (relating to Scheme 4)



1-d_5 (2 eq.) **2a** (1 eq.) **6a'** **3a**

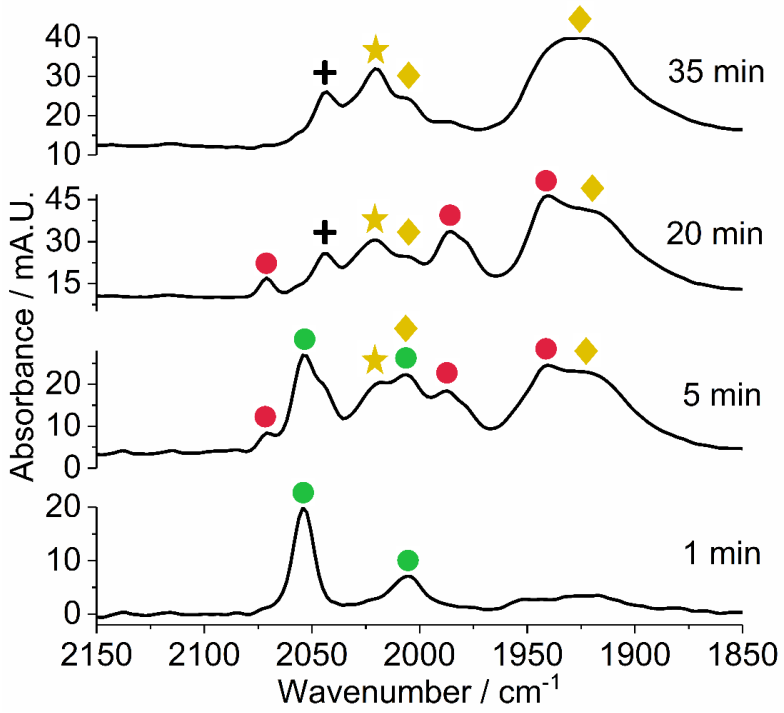


Figure S40. Reaction scheme and *in situ* IR spectra for the reaction at 60 °C with **1**-d_5, using $MnBr(CO)_5$ as the precatalyst, showing the formation of the alkyne insertion complex **6a'** (2071, 1986, 1979, and 1943 cm^{-1}) over time from $MnBr(CO)_5$. AcOH (0.3 ml, 4.16 mmol, 1 eq.) was added after the formation of **6a'** had stabilized. Reaction conditions (in order of addition): n-Bu_2O (10 ml), 2-phenylpyridine-d_5 (1.15 ml, 8.32 mmol, 2 eq.), phenylacetylene (0.45 ml, 4.16 mmol, 1 eq.), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%). Deuterium incorporation was determined by ^1H and ^2H NMR spectroscopy from the isolated alkenylated product **3a** (flash column chromatography, petrol/Et_2O, 8:2, *v/v*). Key: red circle = **6a'**; green circle = $MnBr(CO)_5$; gold diamond / gold star = Mn carbonyl cluster species; black cross = unknown Mn carbonyl species.

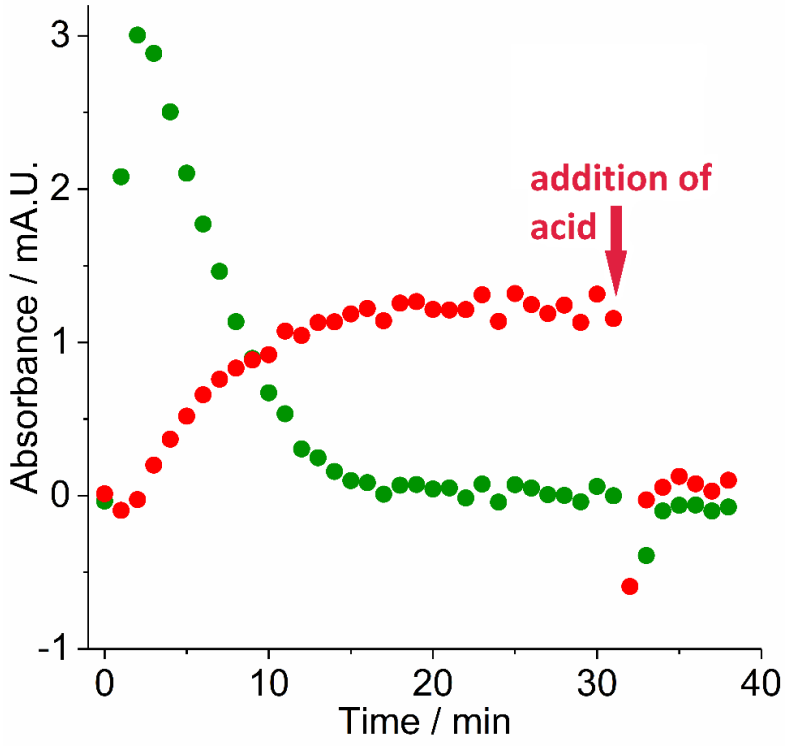


Figure S41. Kinetic plot for the formation and depletion of $MnBr(CO)_5$ (2054 cm^{-1}) the alkyne insertion complex **6a'** (2071 cm^{-1}). Key: blue circle = **4**; green circle = $MnBr(CO)_5$.

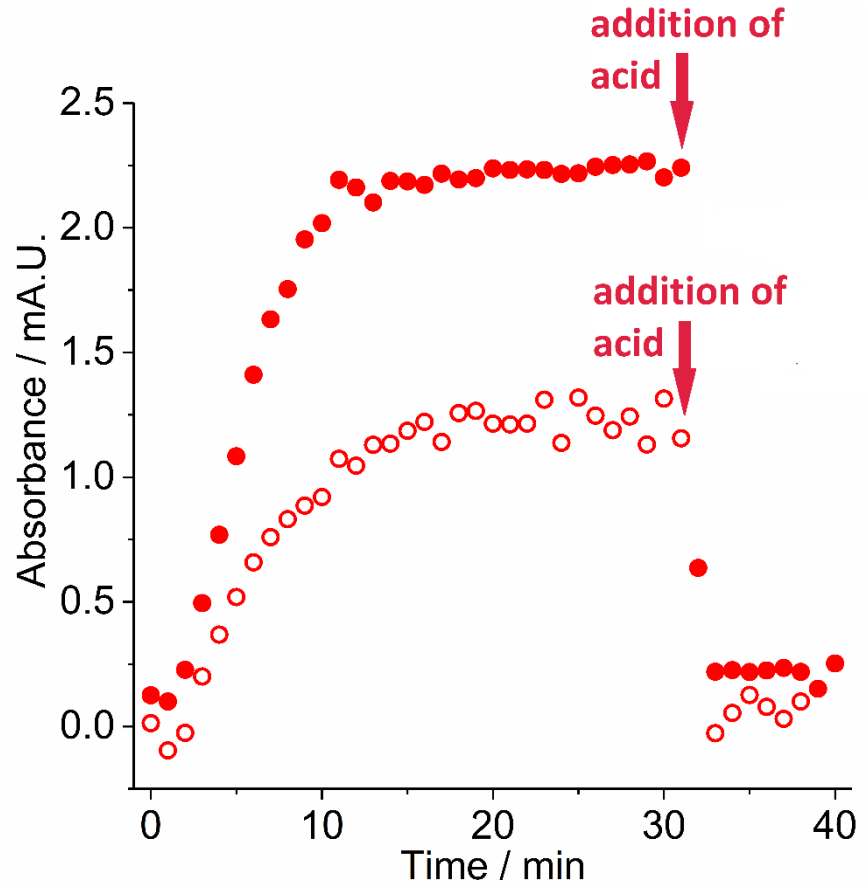


Figure S42. Comparison of the kinetic profile of the formation of the insertion complex for 2-ppy and 2-ppy-d_5. From the k_{obs} for both substrates, a kinetic isotope effect (KIE) of 1.75 ± 0.11 could be determined ((4.93 ± 0.13) × 10^{-6} s^{-1} for **1** vs (2.81 ± 0.16) × 10^{-6} s^{-1}) for **1**-d_5). Key: red circle = **6a'** from **1**; red hollow cicle = **6a'** from **1**-d_5.

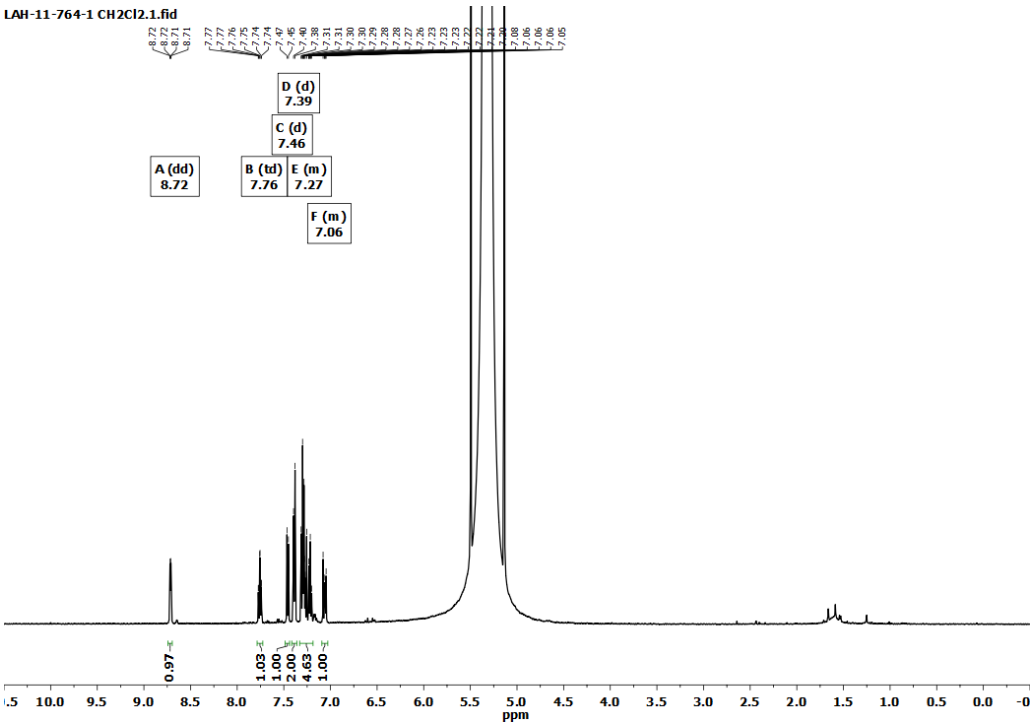


Figure S43. ^{1}H NMR spectrum of isolated **3a** from the reaction (500 MHz, CH_2Cl_2).

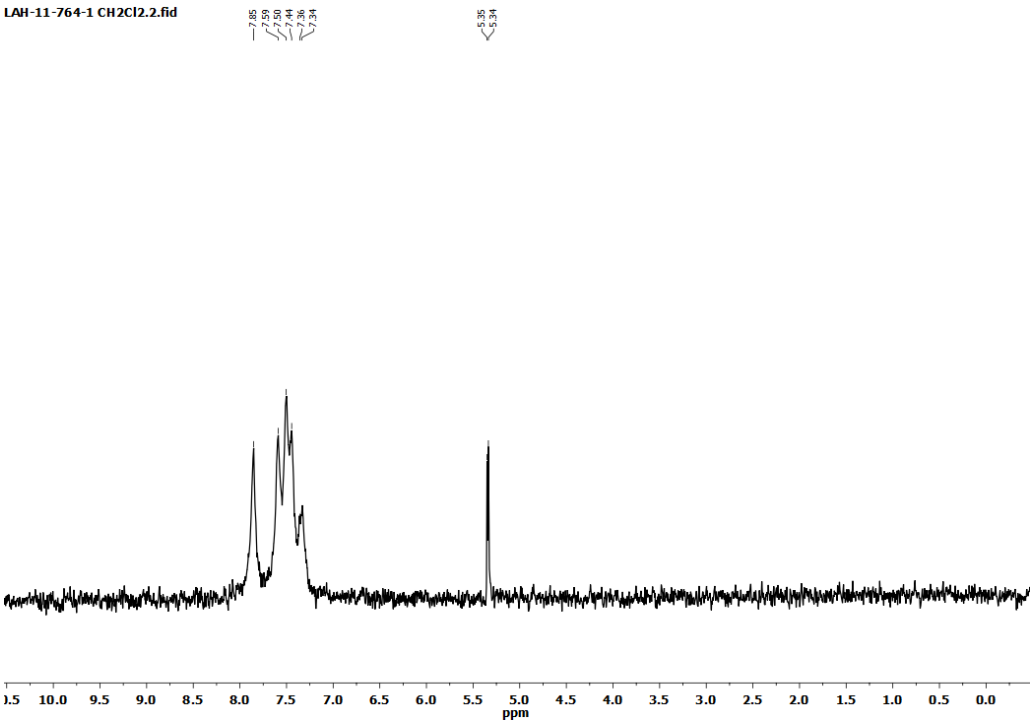
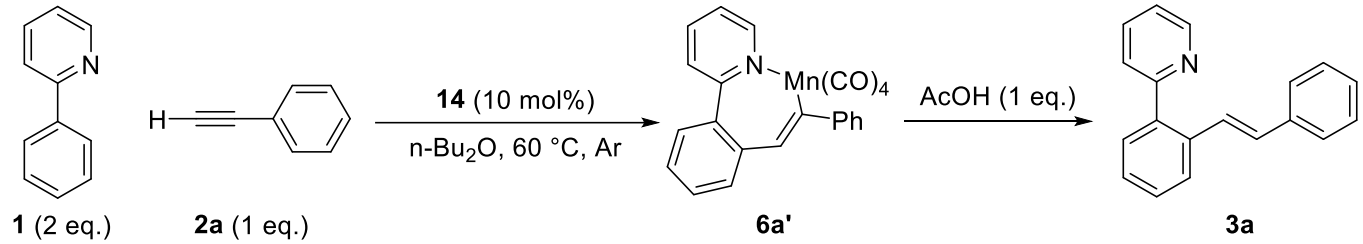


Figure S44. ^{2}H NMR spectrum of isolated **3a** from the reaction (77 MHz, CH_2Cl_2).

2.10 Reaction of 2a at 60 °C with alkynyl Mn-complex 14 as precatalyst



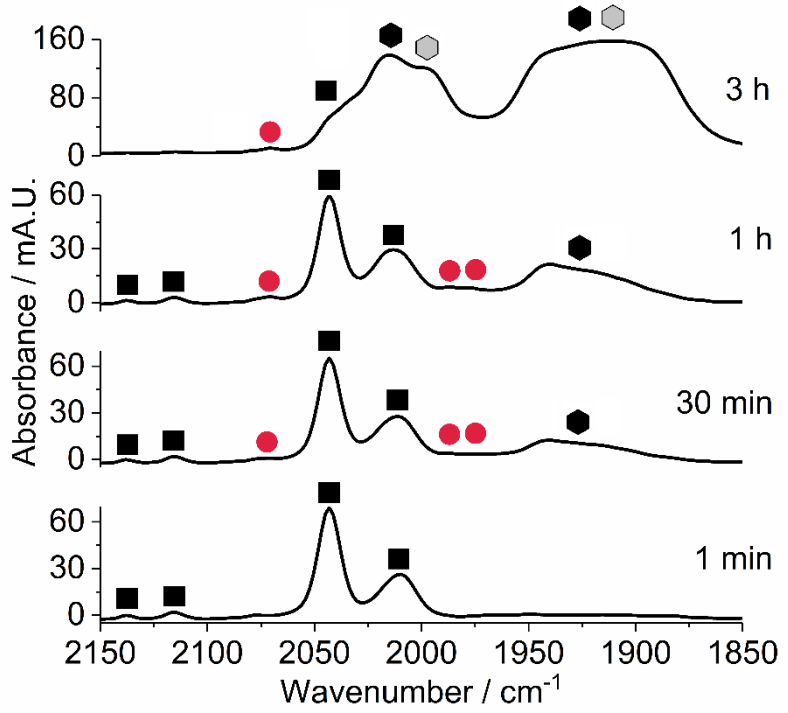


Figure S45. Reaction scheme and *in situ* IR spectra for the reaction of **2a** at 60 °C, using alkynyl Mn-complex **14** as the precatalyst, showing the formation of the alkyne insertion complex **6a'** (2071, 1986, 1978, and 1942 cm^{-1}) over time. AcOH (0.3 ml, 4.16 mmol, 1 eq.) was added after 4.5 hours (after the formation of **6a'**

had stabilized). $Mn(ppy)(CO)_4$ (**4**, 2078 cm^{-1}) cannot be observed forming during the reaction. Reaction conditions (in order of addition): n-Bu_2O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), phenylacetylene (0.45 ml, 4.16 mmol, 1 eq.), **14** (0.129 g, 0.42 mmol, 10 mol%). Key: red circle = **6a'**; black square = **14**; black and grey hexagons = unknown Mn carbonyl species.

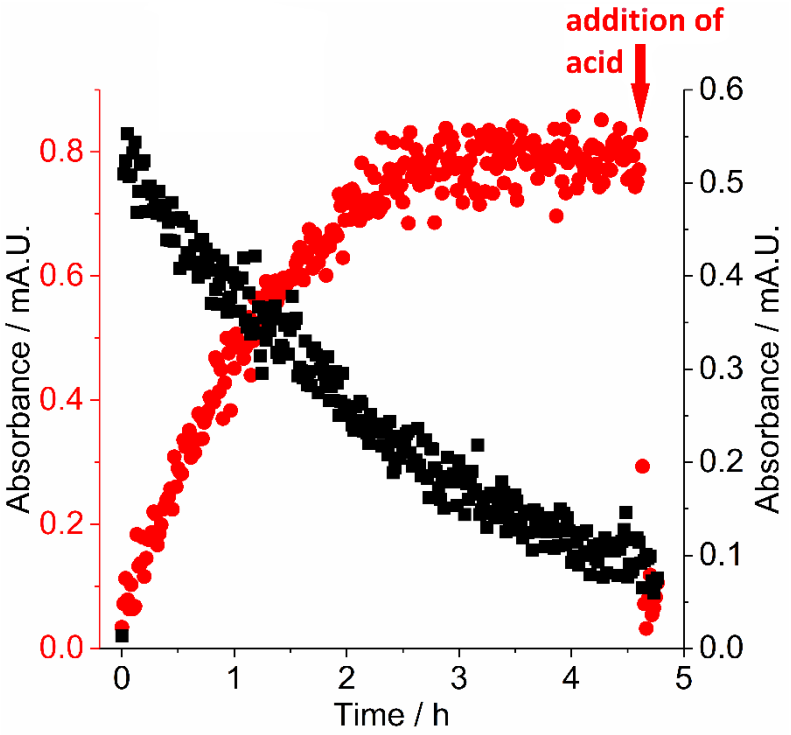
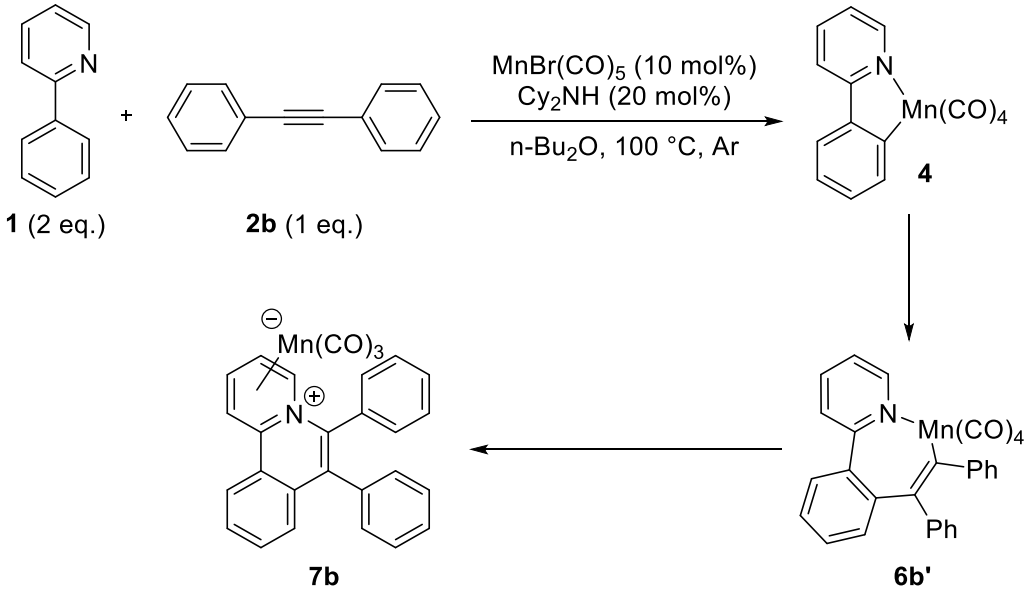


Figure S46. Kinetic plot for the depletion of **14** (2138 cm^{-1}) and formation of the alkyne insertion complex **6a'** (2071 cm^{-1}). Key: red circle = **6a'**; black squares = **14**.

2.11 Standard reaction of 2b at 100 °C with $MnBr(CO)_5$ as precatalyst (relating to Figure 4a,b)



1 (2 eq.) **2b** (1 eq.) **4** **7b** **6b'**

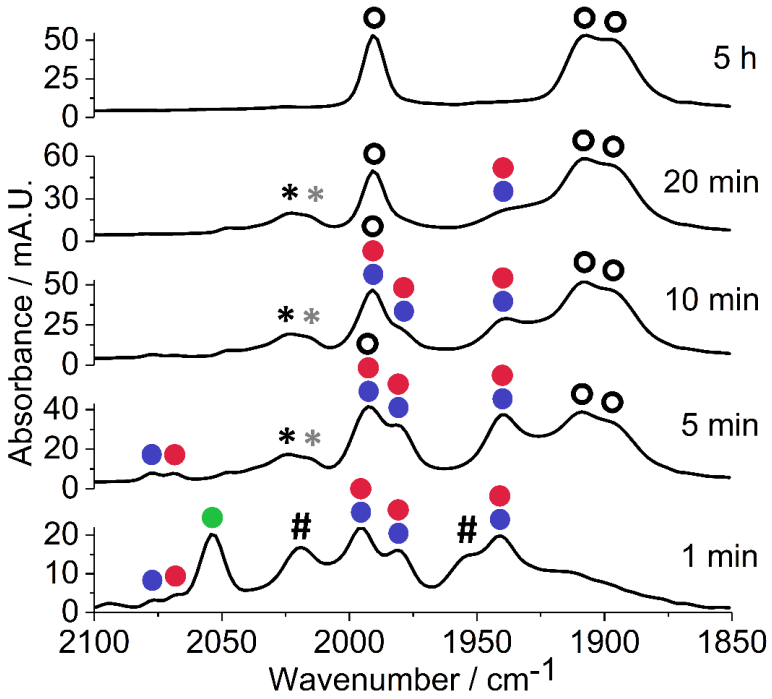


Figure S47. Reaction scheme and *in situ* IR spectra for the reaction of PhCCPh using $MnBr(CO)_5$ as the precatalyst, exhibiting formation of $Mn(ppy)(CO)_4$ (**4**, 2078 cm^{-1}), alkyne insertion complex **6b'** (2069 cm^{-1}) and the reductive elimination complex **7b** (1991, 1908 and 1897 cm^{-1}) over time from $MnBr(CO)_5$. Reaction conditions (in order of addition): n-Bu_2O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), diphenylacetylene (0.47 g, 4.16 mmol, 1 eq.), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%). Key: blue circle = **4**; red circle = **6b'**; green circle = $MnBr(CO)_5$; hollow black circle = reductive elimination product **7b**; * (both black and grey) = likely isomers of the reductive elimination product **7b**.

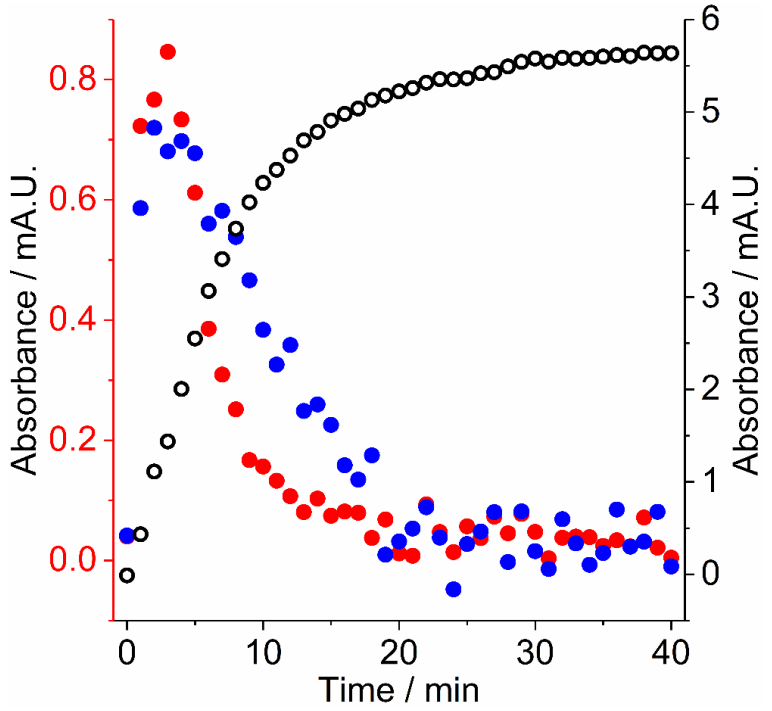
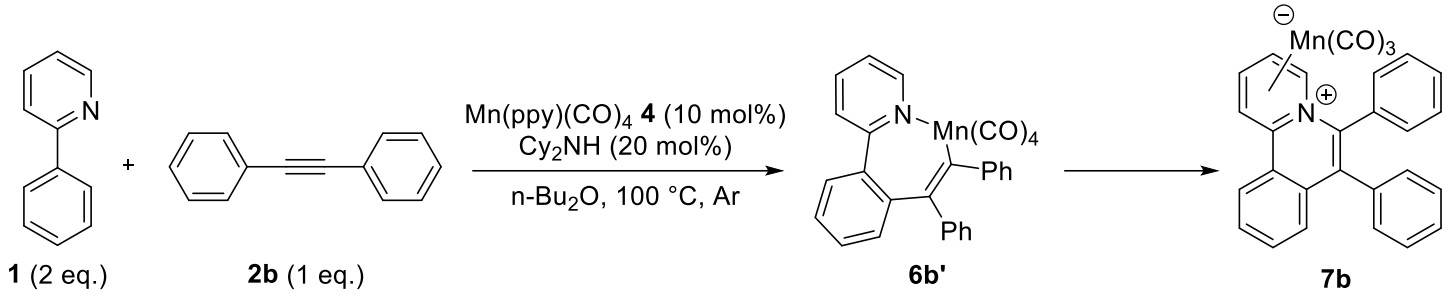


Figure S48. Kinetic plot for the formation and depletion of $Mn(ppy)(CO)_4$ (**4**, 2078 cm^{-1}), the alkyne insertion complex **6b'** (2069 cm^{-1}) and reductive elimination complex **7b** (1991 cm^{-1}). Key: blue circle = **4**; red circle = **6b'**; hollow black circle = reductive elimination product **7b**.

2.12 Reaction of 2b at 100 °C with Mn(ppy)(CO)$_4$ as precatalyst



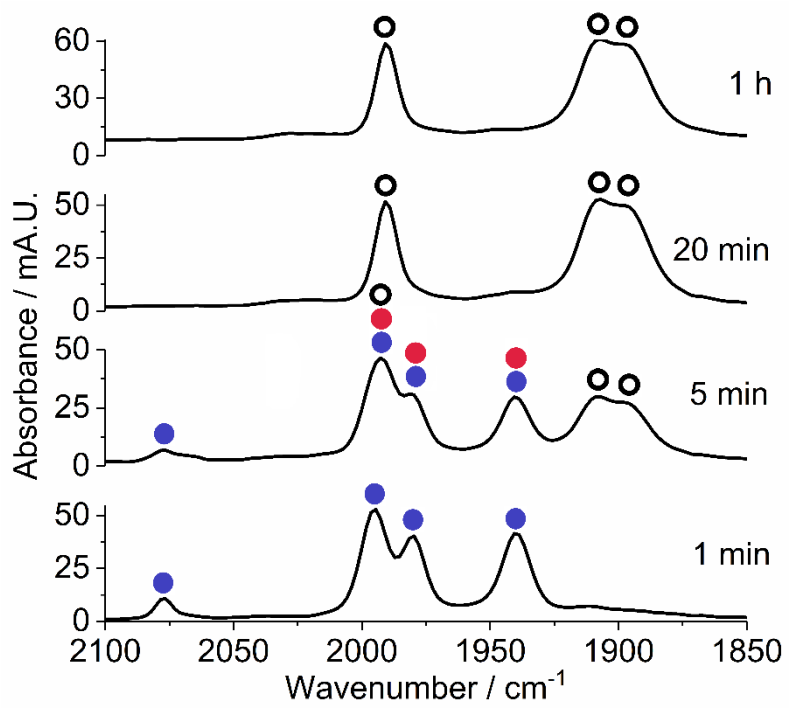


Figure S49. Reaction scheme and *in situ* IR spectra for the reaction of PhCCPh using Mn(ppy)(CO)$_4$ as the precatalyst, exhibiting formation of alkyne insertion complex **6b'** (2069 cm^{-1}) and the reductive elimination complex **7b** (1991, 1908 and 1897 cm^{-1}) over time from Mn(ppy)(CO)$_4$. Reaction conditions (in order of addition): n-Bu$_2$O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), diphenylacetylene (0.47 g, 4.16 mmol, 1 eq.) and Mn(ppy)(CO)$_4$ (0.134 g, 0.42 mmol, 10 mol%). Key: blue circle = **4**; red circle = **6b'**; green circle = MnBr(CO)$_5$; hollow black circle = reductive elimination product **7b**.

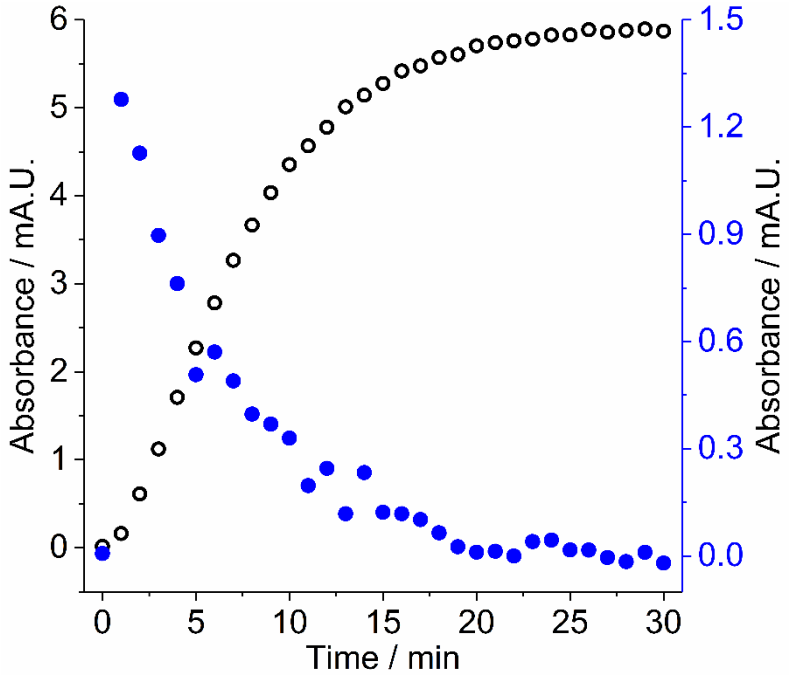


Figure S50. Kinetic plot for the depletion of $Mn(ppy)(CO)_4$ (**4**, 2078 cm^{-1}) and formation of reductive elimination complex **7b** (1991 cm^{-1}). Key: blue circle = **4**; hollow black circle = reductive elimination product **7b**.

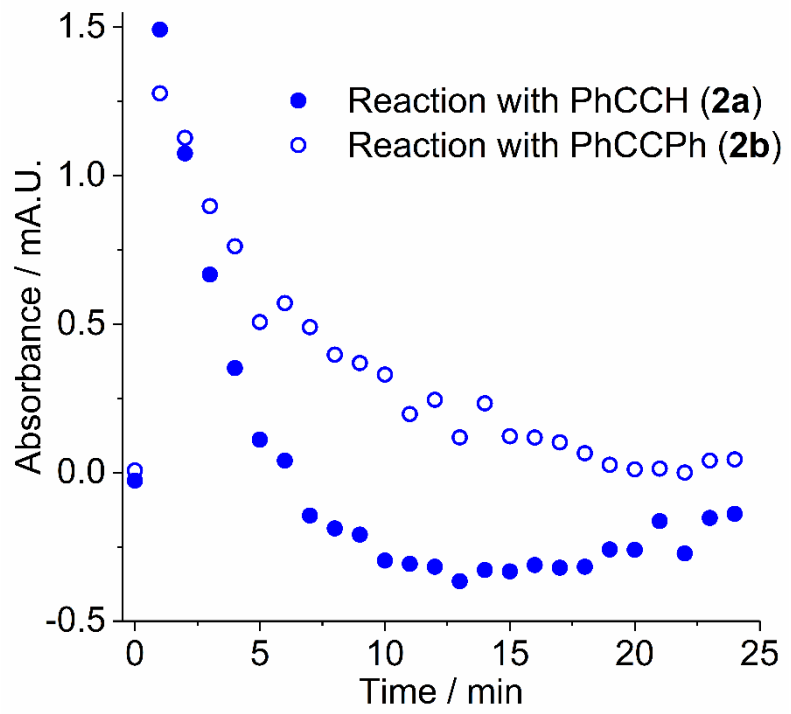


Figure S51. Comparison of the depletion of $Mn(ppy)(CO)_4$ **4** (2078 cm^{-1}) for the reactions employing $Mn(ppy)(CO)_4$ and $MnBr(CO)_5$ as precatalysts.

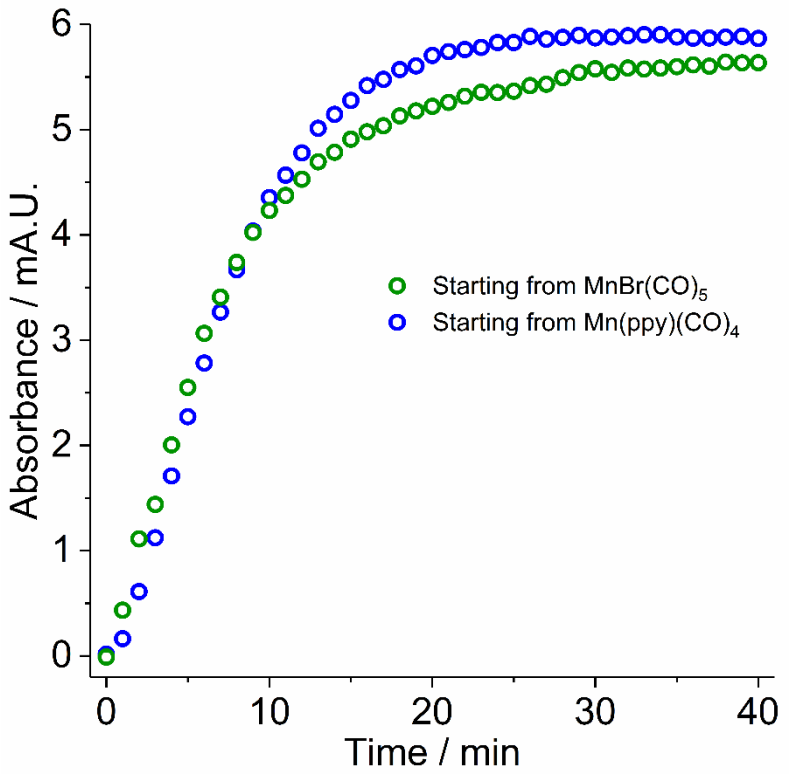
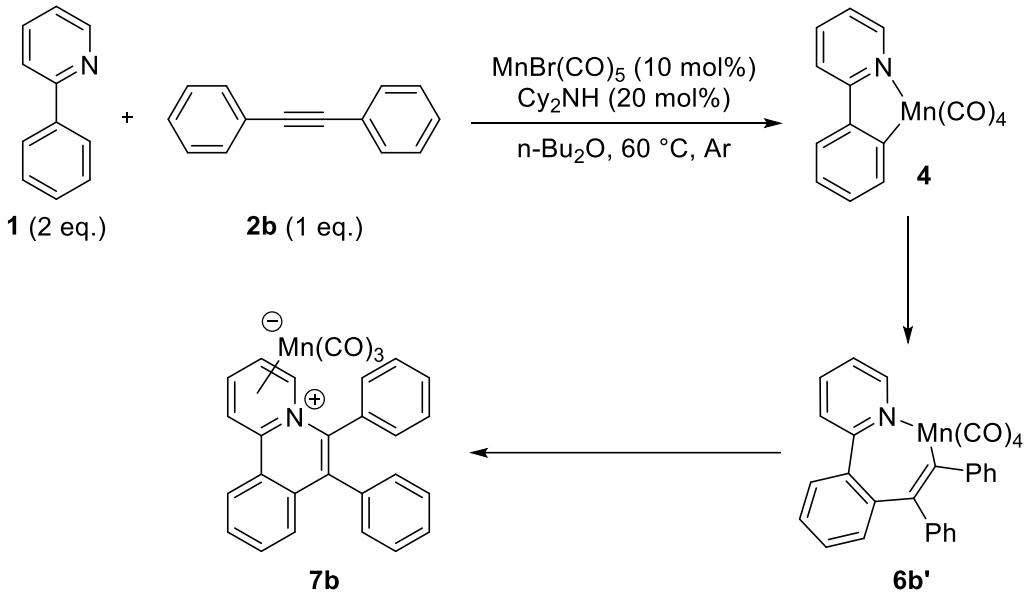


Figure S52. Comparison of the formation of reductive elimination complex **7b** (1991 cm^{-1}) for the reactions employing $Mn(ppy)(CO)_4$ and $MnBr(CO)_5$ as precatalysts.

2.13 Reaction of 2b at 60 °C with $MnBr(CO)_5$ as precatalyst



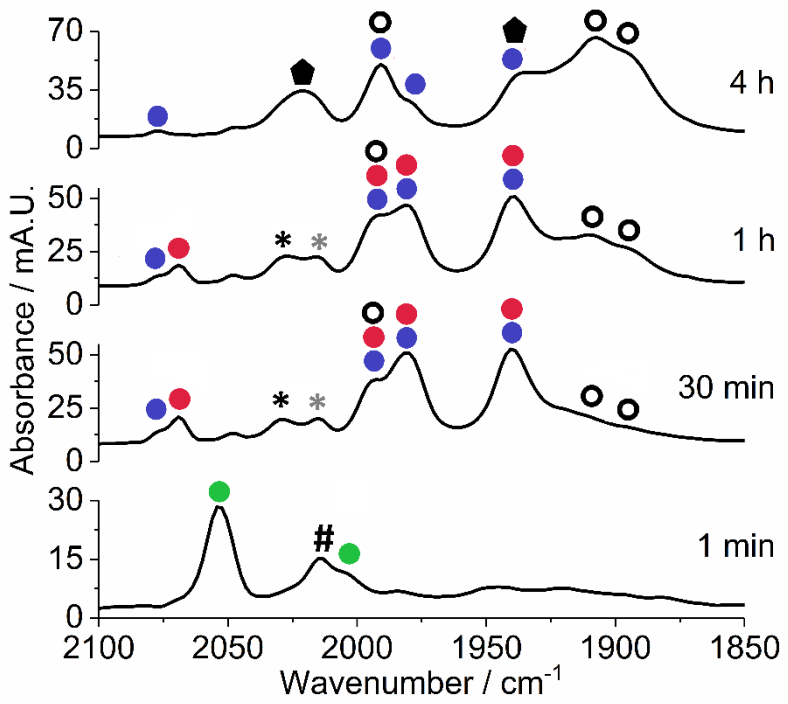


Figure S53. Reaction scheme and *in situ* IR spectra for the reaction at 60 °C of PhCCPh using $MnBr(CO)_5$ as the precatalyst, exhibiting formation of $Mn(ppy)(CO)_4$ (**4**, 2078 cm^{-1}), alkyne insertion complex **6b'** (2069 cm^{-1}) and the reductive elimination complex **7b** (1991, 1908 and 1897 cm^{-1}) over time from $MnBr(CO)_5$. Reaction conditions (in order of addition): n-Bu_2O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), diphenylacetylene (0.47 g, 4.16 mmol, 1 eq.), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%). Key: blue circle = **4**; red circle = **6b'**; green circle = $MnBr(CO)_5$; hollow black circle = reductive elimination product **7b**; * (both black and grey) = likely isomers of the reductive elimination product **7b**; black pentagon = unknown Mn carbonyl species.

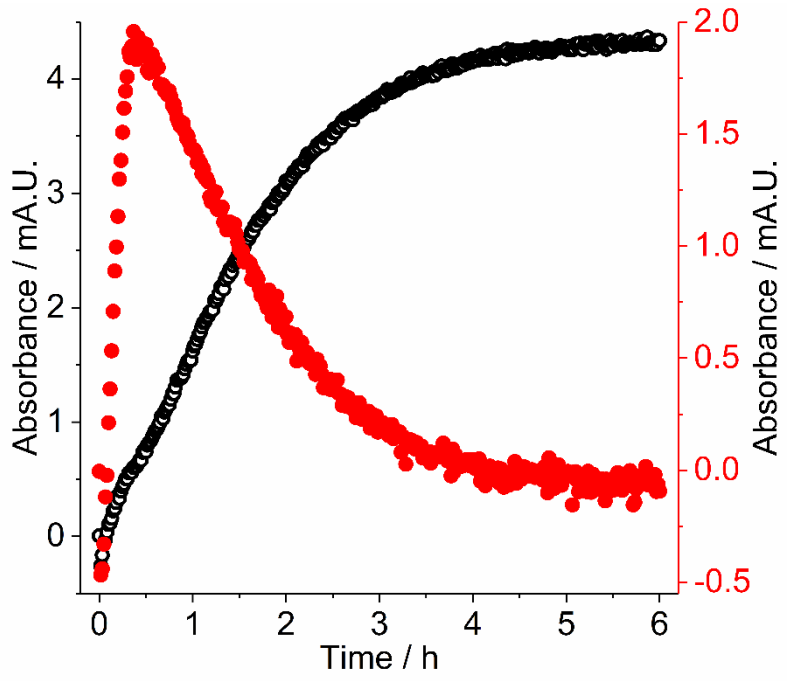
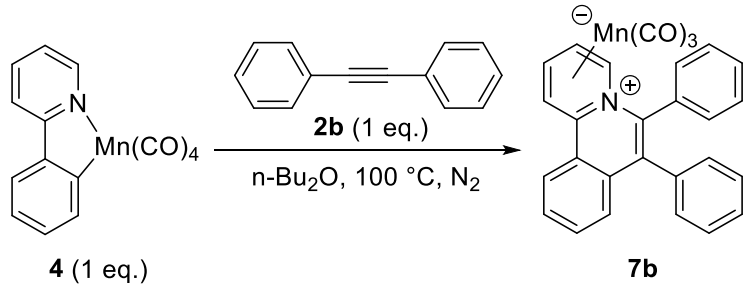


Figure S54. Kinetic plot for the formation and depletion of the alkyne insertion complex **6b'** (2069 cm^{-1}) and reductive elimination complex **7b** (1991 cm^{-1}). Key: red circle = **6b'**; hollow black circle = reductive elimination product **7b**.

2.14 Stoichiometric reaction of 2b with Mn(ppy)(CO)$_4$



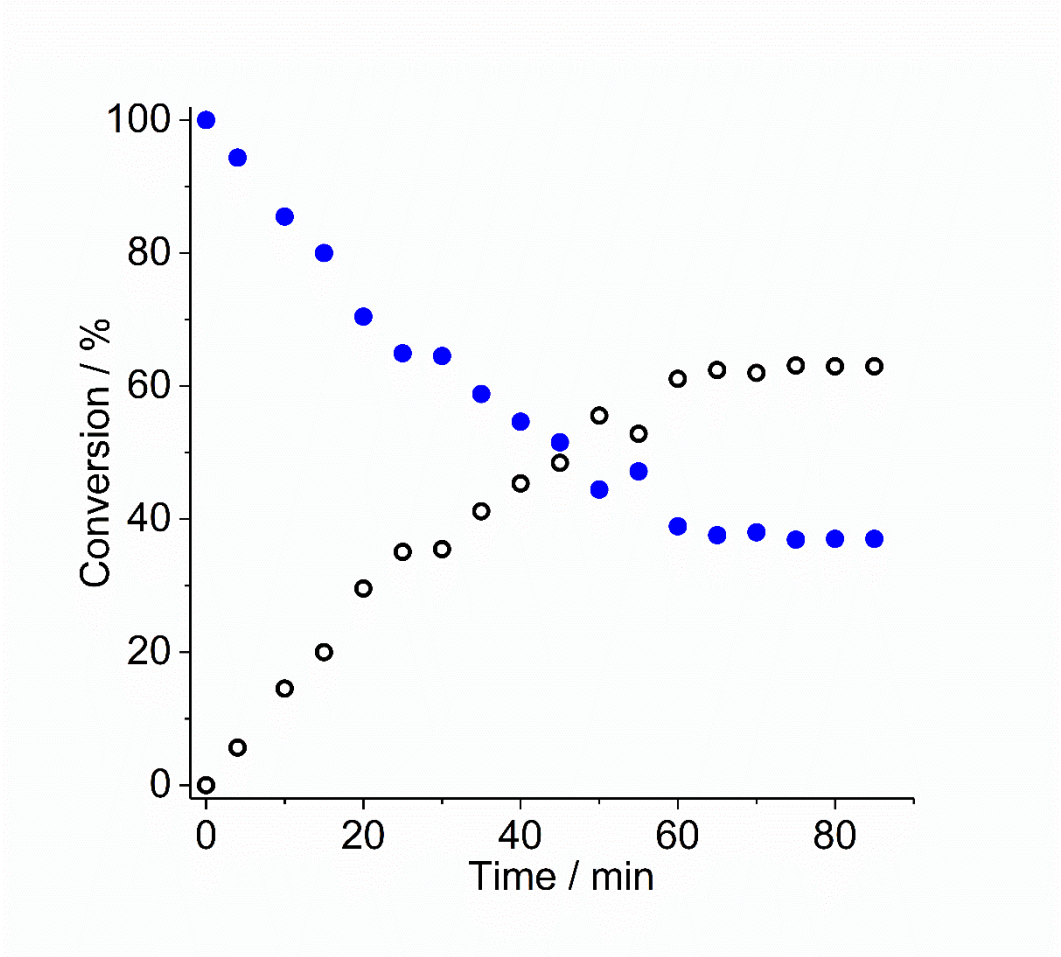
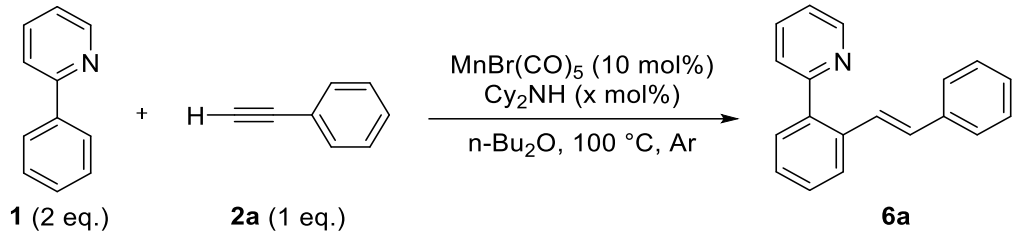


Figure S55. Reaction scheme and ^{1}H NMR kinetics for the reaction of PhCCPh and Mn(ppy)(CO)$_4$, showing the formation of the reductive elimination complex **7b** over time from Mn(ppy)(CO)$_4$. Reaction conditions: n-Bu$_2$O (0.6 ml), Mn(ppy)(CO)$_4$ (8.0 mg, 0.025 mmol, 1 eq.) and diphenylacetylene (4.5 mg, 0.025 mmol, 1 eq.). Solution was prepared in an Young's tap NMR tube, and pump thaw degassed three times using a Schlenk line vacuum, before being backfilled with N$_2$ after the final cycle. Afterwards a starting ^{1}H NMR spectrum was recorded at room temperature, followed by heating of the spectrometer to 100 °C (without the sample inside). The NMR sample was thereafter added to the spectrometer and ^{1}H NMR spectrum was recorded every 1 minutes for the length of the experiment.

2.15 Order determination w.r.t. Cy_2NH (relating to Figure 5)



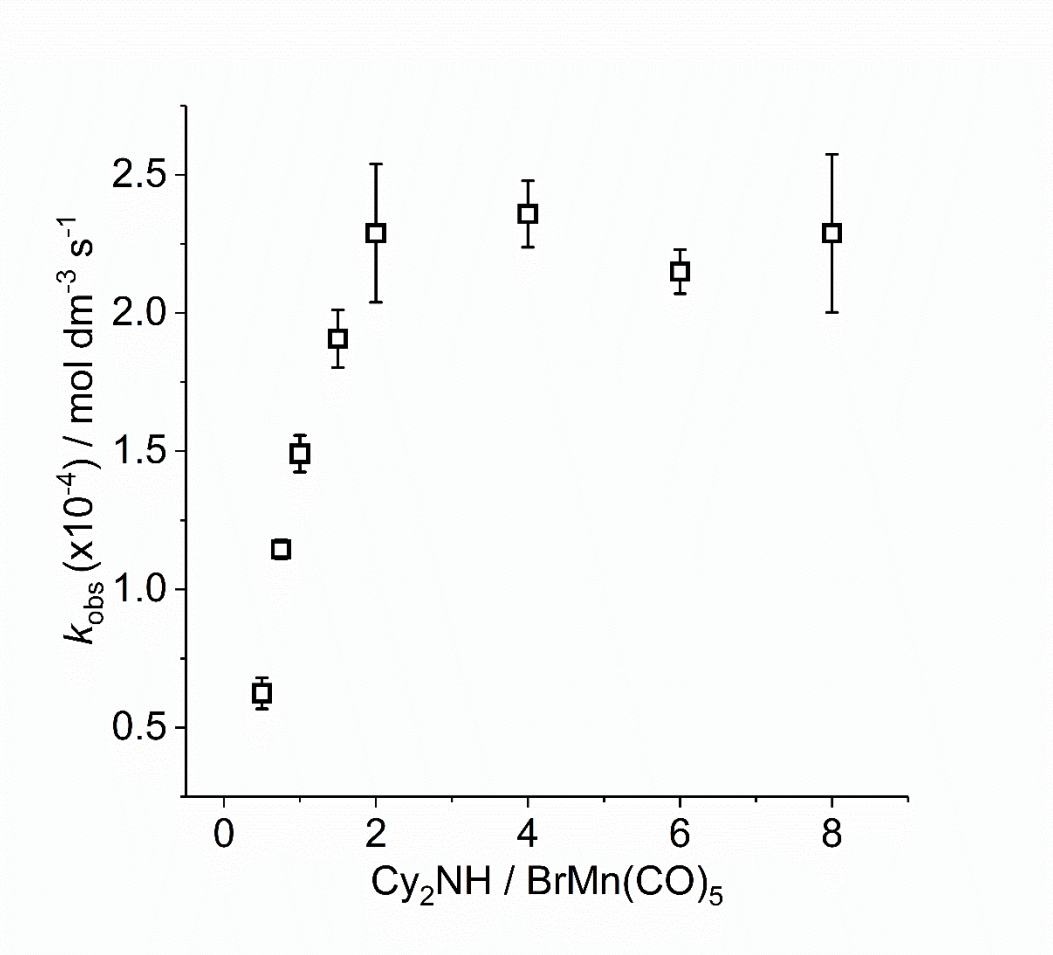


Figure S56. Plot of the dependence of the Cy_2NH/Mn ratio on the k_{obs} of the reaction. Reaction conditions (in order of addition): n-Bu_2O (10 ml), 2-phenylpyridine (1.19 ml, 8.32 mmol, 2 eq.), phenylacetylene (0.45 ml, 4.16 mmol, 1 eq.), Cy_2NH (8.3 µl/mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%).

The reactions were performed using the React-IR set up, and varied concentration of Cy_2NH (5, 7.5, 10, 15, 20, 40, 60 and 80 mol% respectively).

The reactions were in addition to *in situ* IR monitoring, also followed by *ex situ* ^1H NMR spectroscopy. The crude conversion to alkenylated product was determined from each ^1H NMR spectrum and concentration from the theoretical maximal concentration of alkenylated product obtainable. K_{obs} was determined from a linear regression of early timepoints in a graph containing [alkenylated product] vs. time in seconds.

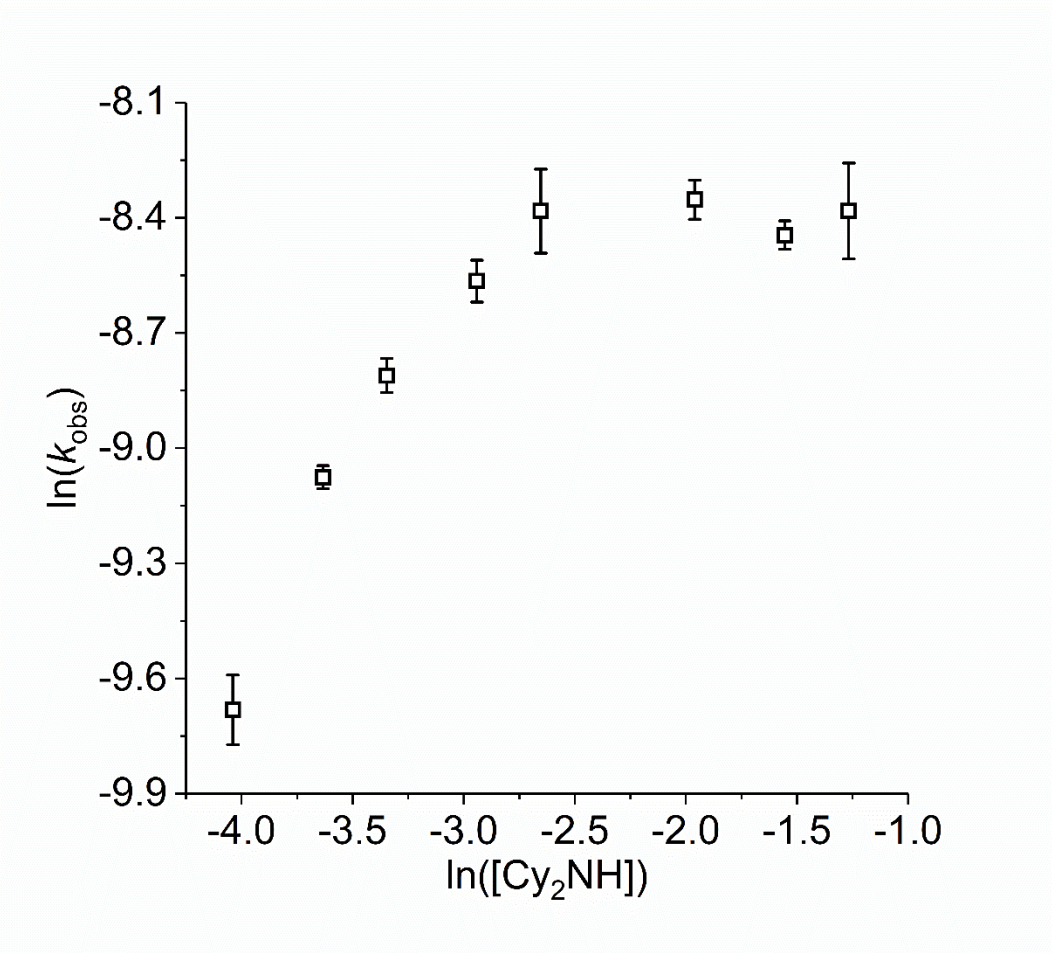
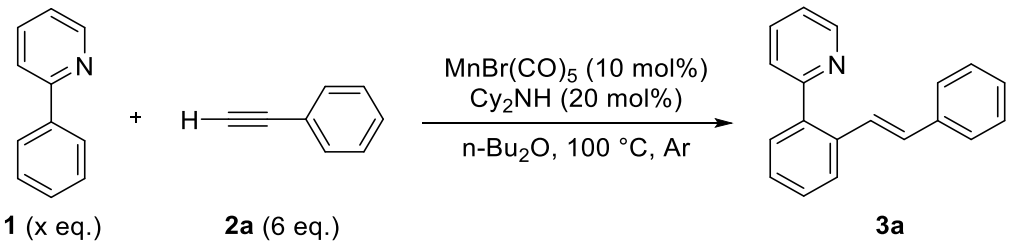


Figure S57. Plot of ln(k_{obs}) vs. ln([Cy_2H]).

2.16 Order determination w.r.t. 1



1 (x eq.) **2a** (6 eq.) **3a**

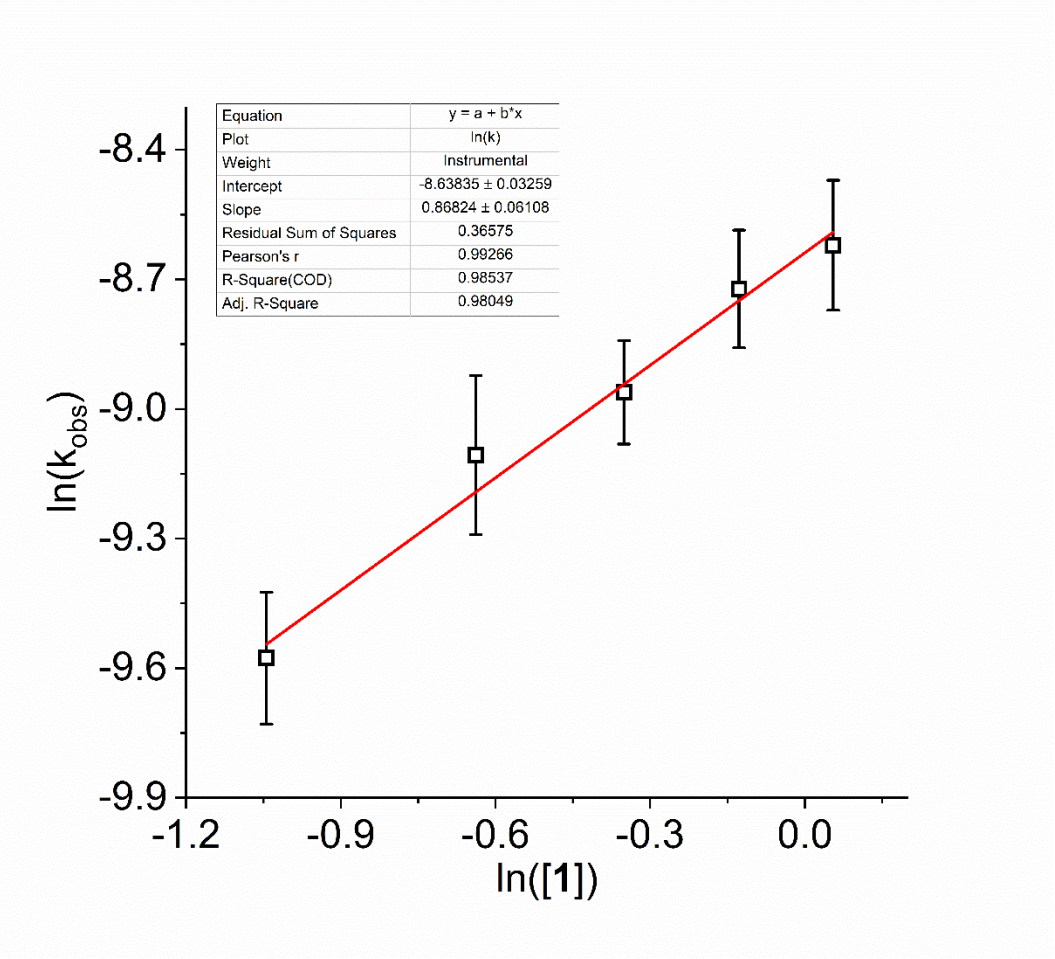
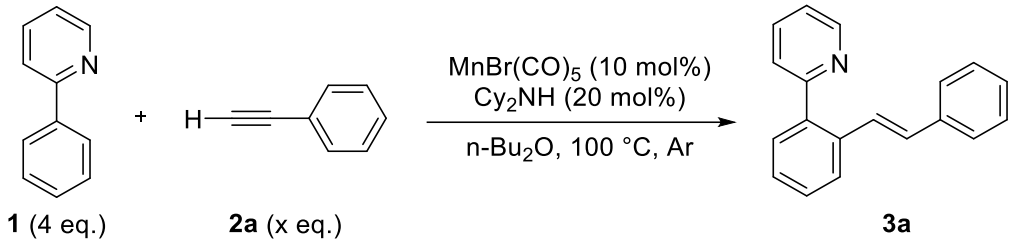


Figure S58. Plot of ln(k_{obs}) vs. ln([**1**]), giving an overall order w.r.t. **1** of 0.87±0.06. Reaction conditions (in order of addition): n-Bu_2O ((8.3−$\Delta V_{2\text{-ppy}}$) ml), 2-phenylpyridine (0.59 ml/eq.), phenylacetylene (2.74 ml, 24.96 mmol, 6 eq.), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%).

The reactions were performed using the React-IR set up, with an excess of PhCCH (6 eq.) and varied concentration of 2-ppy (1, 1.5, 2, 2.5 and 3 eq. respectively). The difference in reagent volume was adjusted in the amount of solvent added to afford the same concentration in manganese.

The reactions were in addition to *in situ* IR monitoring, also followed by *ex situ* ^{1}H NMR spectroscopy. The crude conversion to alkenylated product was determined from each ^{1}H NMR spectrum and concentration from the theoretical maximal concentration of alkenylated product obtainable. K_{obs} was determined from a linear regression of early timepoints in a graph containing [alkenylated product] vs. time in seconds.

2.17 Order determination w.r.t. 2a



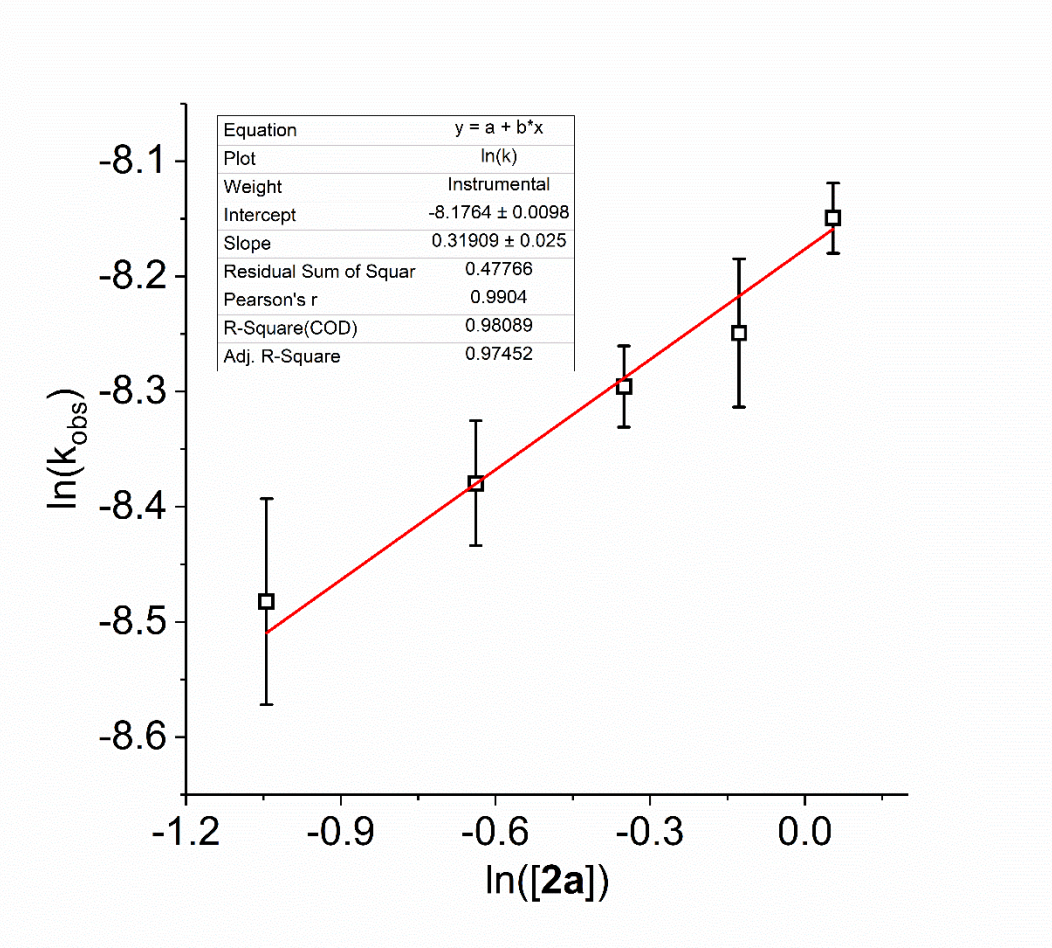


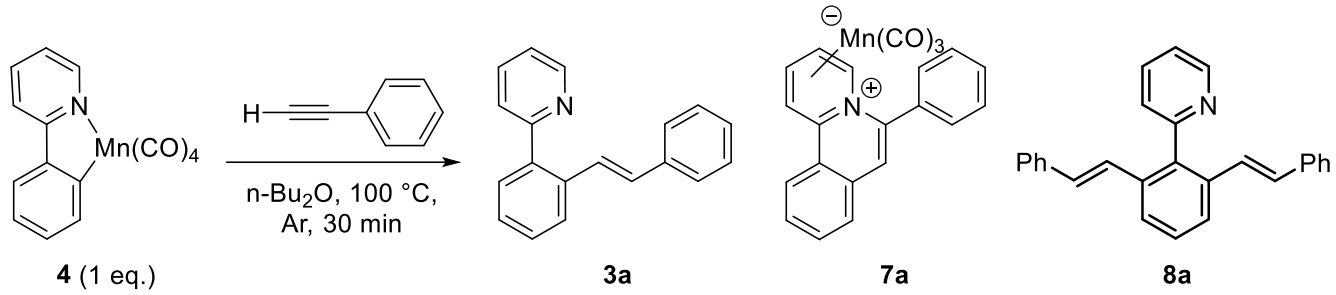
Figure S59. Plot of ln(k_{obs}) vs. ln([**2a**]), giving an overall order w.r.t. **2a** of 0.32±0.03. Reaction conditions (in order of addition): n-Bu_2O ((8.8±ΔV_{PhCCH}) ml), 2-phenylpyridine (2.58 ml, 16.64 mmol, 4 eq.), phenylacetylene (0.45 ml/eq.), Cy_2NH (0.17 ml, 0.83 mmol, 20 mol%) and $MnBr(CO)_5$ (0.114 g, 0.42 mmol, 10 mol%).

The reactions were performed using the React-IR set up, with an excess of **1** (4 eq.) and varied concentration of **2a** (0.5, 0.75, 1, 1. 5 and 2 eq. respectively). The difference in reagent volume was adjusted in the amount of solvent added to afford the same concentration in manganese.

The reactions were in addition to *in situ* IR monitoring, also followed by *ex situ* ^{1}H NMR spectroscopy. The crude conversion to alkenylated product was determined from each ^{1}H NMR spectrum and concentration from the theoretical maximal concentration of alkenylated product obtainable. K_{obs} was determined from a linear regression of early timepoints in a graph containing [alkenylated product] vs. time in seconds.

2.18 Stoichiometric reactions probing protonation pathways (relating to Figure 6)

Table S1. Summary of the stoichiometric reaction of **2a** with **4** in combination with additives.[a]



4 (1 eq.) **3a** **7a** **8a**

Entry	Eq. 2a	Additive (eq.)	3a / %[b]	7a / %[b]	8a / %[b]
1	1	-	7	76	5
2	2	-	12	64	25
3	4	-	17	32	51
4	1	H_2O (10)[c]	42	44	9
5	1	2-ppy (1.15)[d]	59	53	0
6	1	pyridine (1)[e]	22	68	0
7[f]	4 (**2a**-*d*)	-	21	50	29
8[f]	1	D_2O (10)[g]	52	40	8
9[f]	1	**1**-d_5 (1)[h]	29	60	2

[a] Standard reaction conditions: n-Bu_2O (0.6 ml), $Mn(ppy)(CO)_4$ (8 mg, 0.025 mmol, 1 eq.) and PhCCH (3 µl, 0.025 mmol, 1 eq., added as stock solution with n-Bu_2O). [b] Crude conversion determined by ^{1}H NMR spectroscopy. [c] H_2O (5 µl, 0.25 mmol, 10 eq.) added. [d] 2-phenylpyridine (4 µl, 0.029 mmol, 1.15 eq. (equivalence determined by ^{1}H NMR spectroscopy)), added as a stock solution with n-Bu_2O and PhCCH. [e] pyridine (2 µl, 0.025 mmol, 1 eq., added as a stock solution with n-Bu_2O and PhCCH. [f] Reactions performed at four times the scale of the standard reaction conditions (for every reagent and solvent). [g] D_2O (5 µl, 0.25 mmol, 10 eq.) added. [h] **1**-d_5 (4 mg, 0.025 mmol, 1 eq. (equivalence determined by ^{1}H NMR spectroscopy)), added as a stock solution with n-Bu_2O and PhCCH. Reaction time = 2 hours.

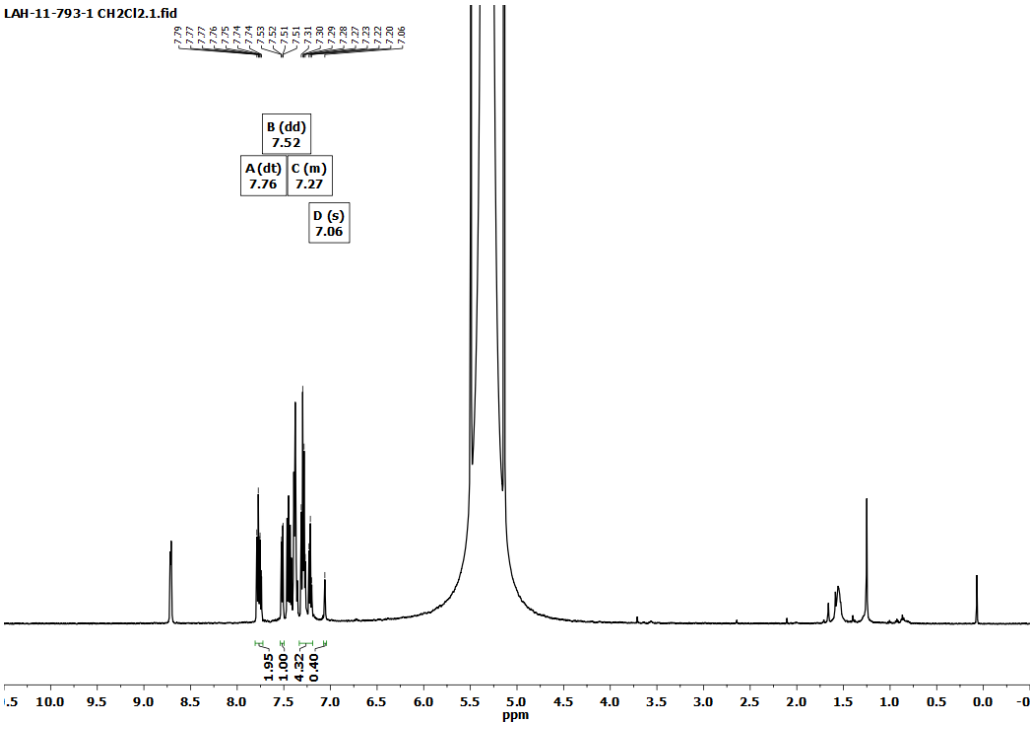


Figure S60. ^{1}H NMR spectrum of isolated **3a** from reaction with 4 eq. **2a**-*d* (500 MHz, CH_2Cl_2)

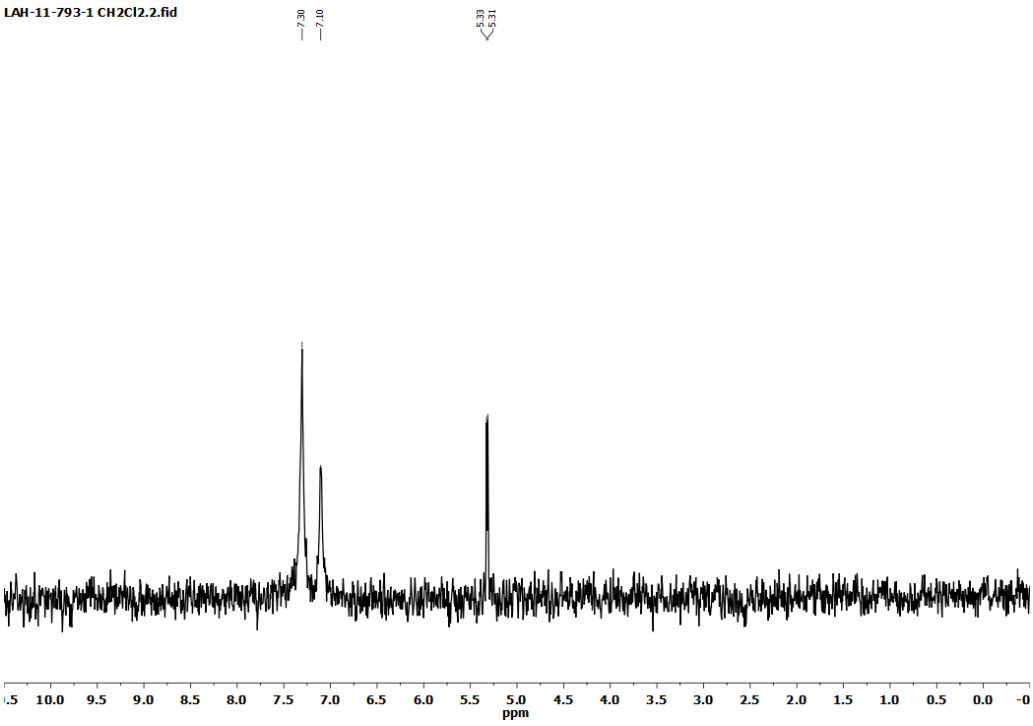


Figure S61. ^{2}H NMR spectrum of isolated **3a** from reaction with 4 eq. **2a**-*d* (77 MHz, CH_2Cl_2)

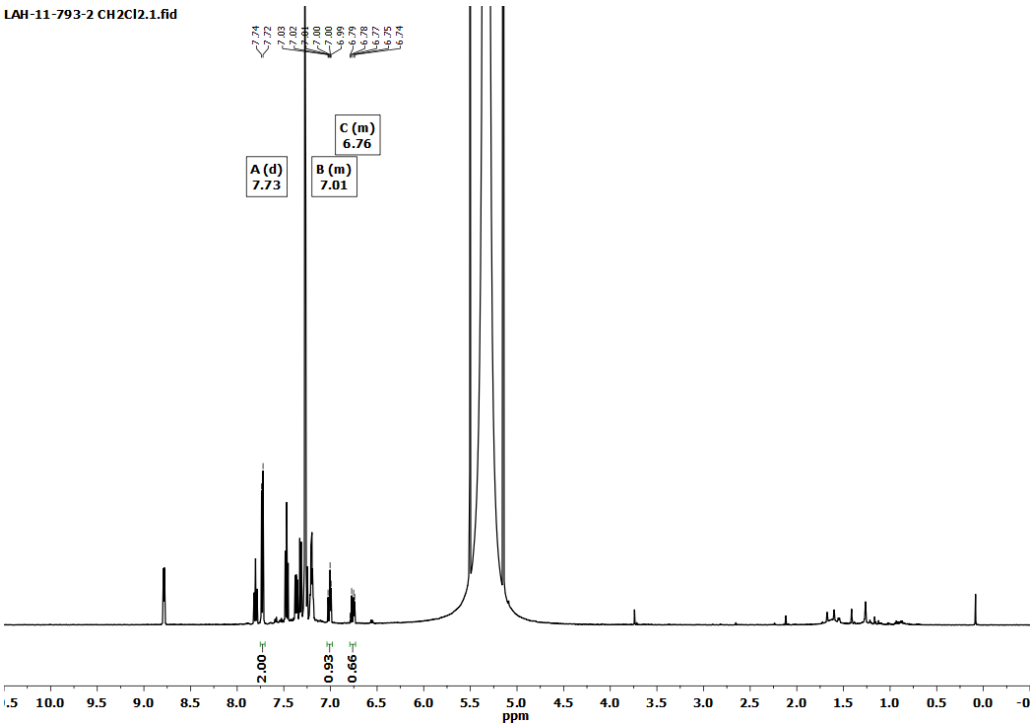


Figure S62. ^{1}H NMR spectrum of isolated **8a** from reaction with 4 eq. **2a**-*d* (500 MHz, CH_2Cl_2)

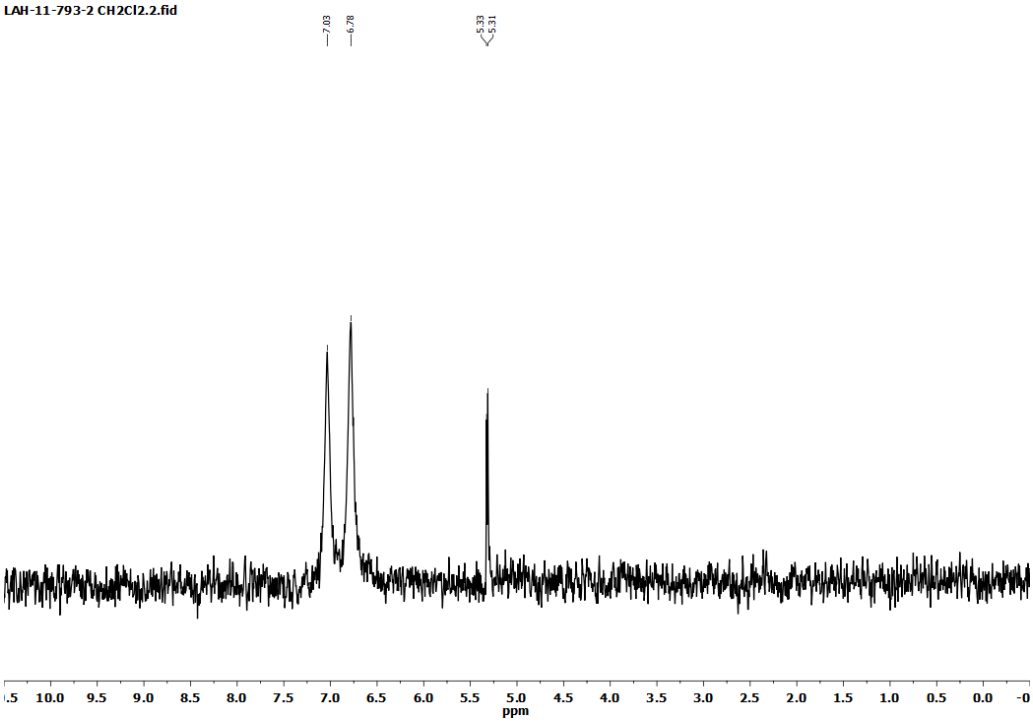


Figure S63. ^{2}H NMR spectrum of isolated **8a** from reaction with 4 eq. **2a**-*d* (77 MHz, CH_2Cl_2)

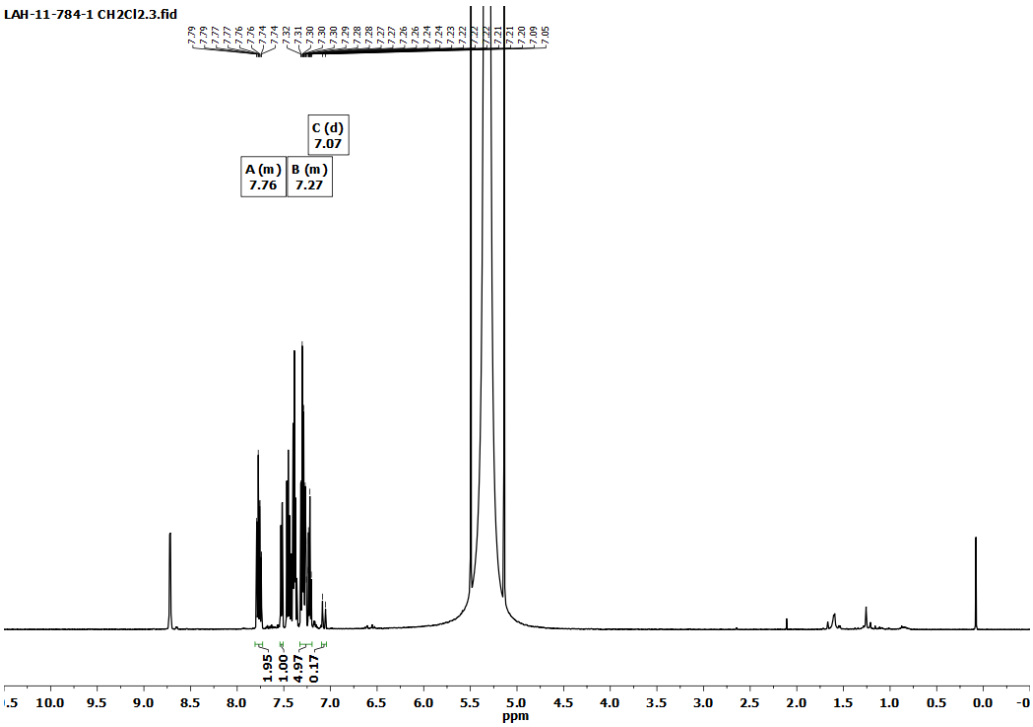


Figure S64. ^{1}H NMR spectrum of isolated **3a** from reaction with 10 eq. D_2O (500 MHz, CH_2Cl_2)

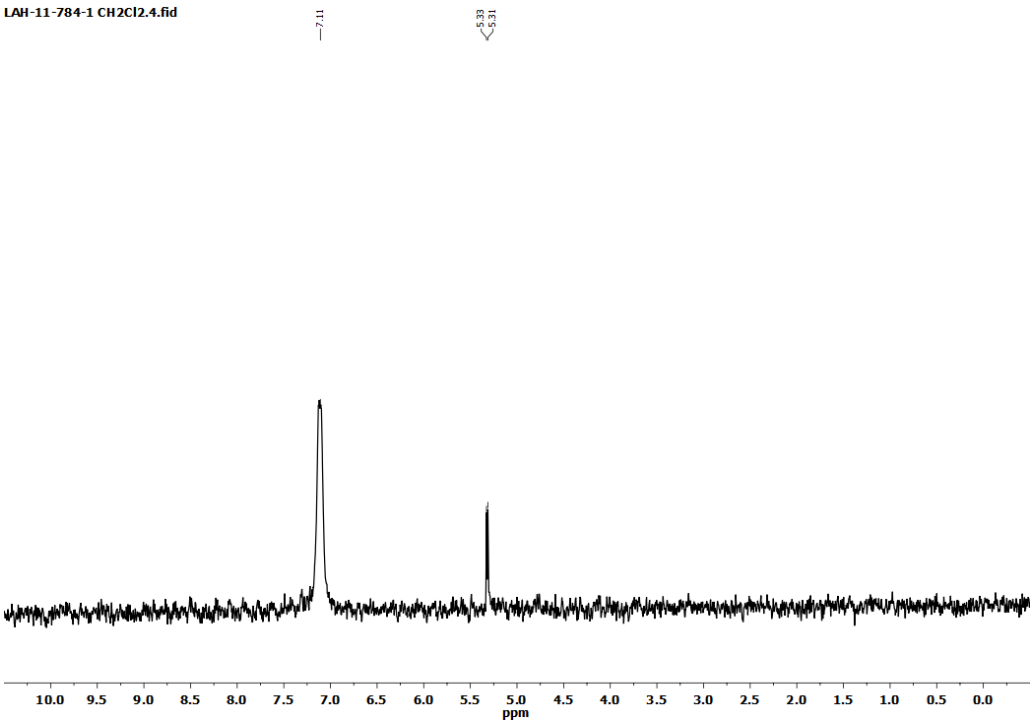


Figure S65. ^{2}H NMR spectrum of isolated **3a** from reaction with 10 eq. D_2O (77 MHz, CH_2Cl_2)

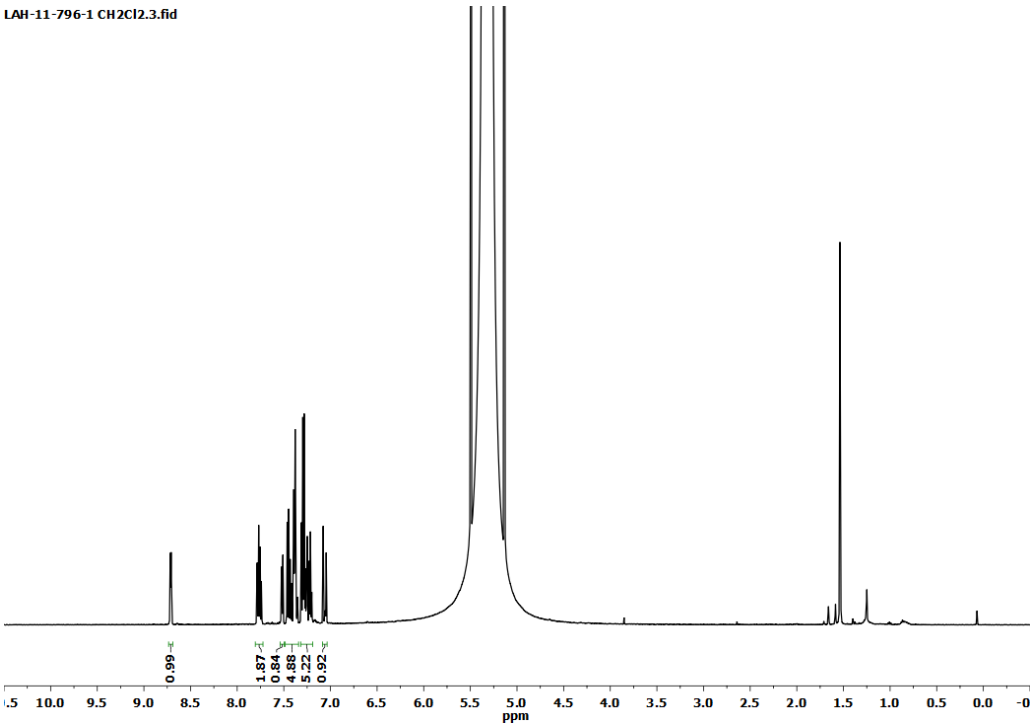


Figure S66. ^{1}H NMR spectrum of isolated **3a** from reaction with 1 eq. **1**-d_5 (500 MHz, CH_2Cl_2)

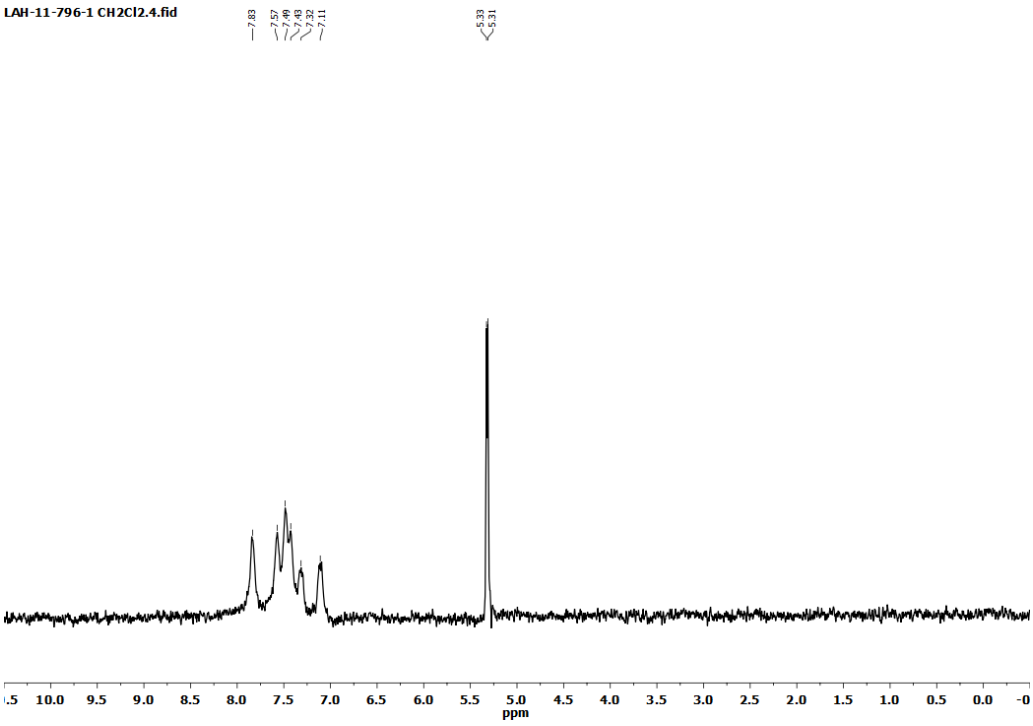


Figure S67. ^{2}H NMR spectrum of isolated **3a** from reaction with 1 eq. **1**-d_5 (77 MHz, CH_2Cl_2)

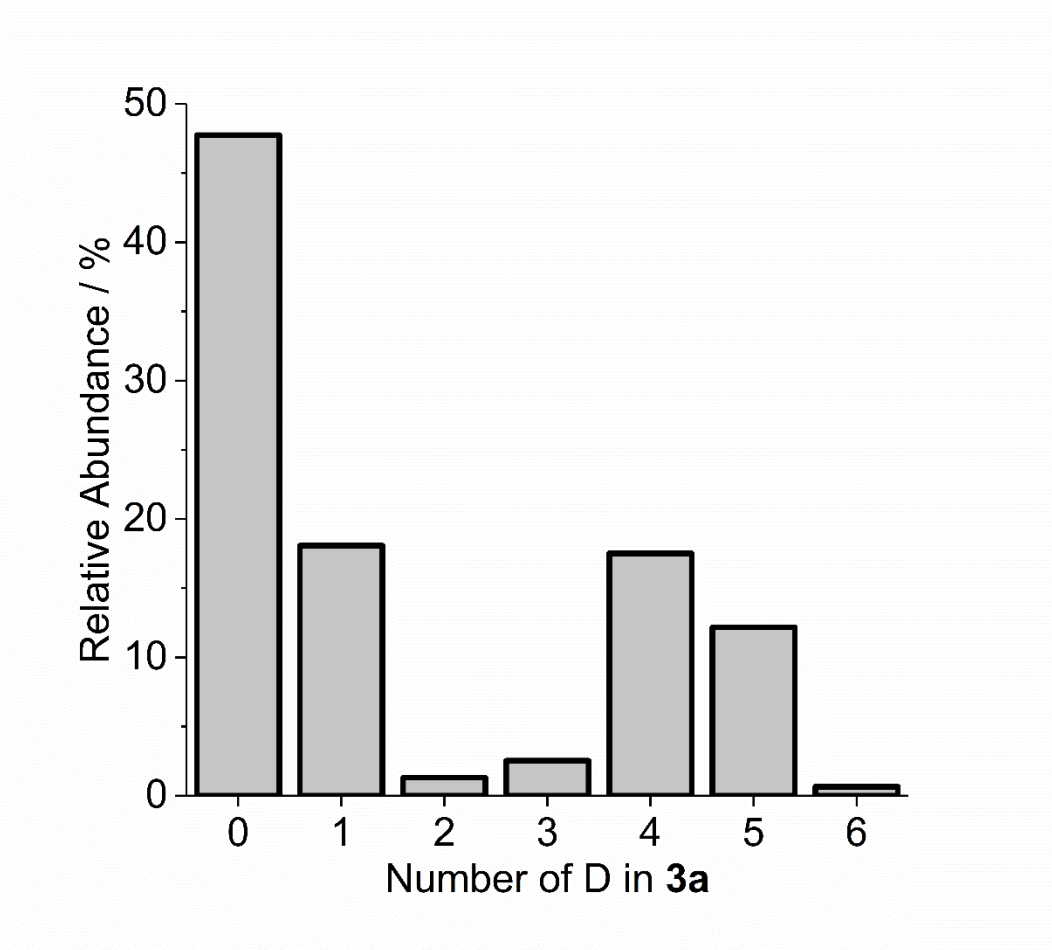


Figure S68. Combinded ESI-MS data, showing the amount of deutuerium incorporation into the isolated product **3a** from reaction with 1 eq. **1**-d_5.

3 X-ray crystallography

3.1 General details

Diffraction data for complex **7b** were collected at 110 K on a Bruker Smart Apex diffractometer with Mo-K_α radiation (λ = 0.71073 Å) using a SMART CCD camera. Diffractometer control, data collection and initial unit cell determination was performed using "SMART".[1] Frame integration and unit-cell refinement was carried out with "SAINT+".[2] Absorption corrections were applied by SADABS.[3] Structures were solved by "direct methods" using SHELXS-97 (Sheldrick, 1997)[4] and refined by full-matrix least squares using SHELXL-97 (Sheldrick, 1997).[5] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using a "riding model" and included in the refinement at calculated positions.

3.2 X-ray data for complex 7b

Table S2. X-ray data for complex **7b**.[a]

Identification code	ijsf1809
Empirical formula	$C_{28}H_{18}MnNO_3$
Formula weight	471.37
Temperature/K	109.95(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	19.1024(2)
b/Å	7.84458(12)
c/Å	32.2257(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4829.03(12)
Z	8
ρ_{calc}g/cm^3	1.297
μ/mm^{-1}	4.674
F(000)	1936.0
Crystal size/mm^3	0.275 × 0.226 × 0.02
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.178 to 134.13
Index ranges	-22 ≤ h ≤ 22, -6 ≤ k ≤ 9, -38 ≤ l ≤ 28
Reflections collected	9268
Independent reflections	4294 [R_{int} = 0.0312, R_{sigma} = 0.0438]
Data/restraints/parameters	4294/0/298
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0457, wR_2 = 0.1022
Final R indexes [all data]	R_1 = 0.0637, wR_2 = 0.1095
Largest diff. peak/hole / e Å^{-3}	0.50/-0.38

[a] Refinement Special Details: The crystal contained disordered solvent for which a suitable discrete atom model could not be obtained therefore a solvent mask was used. There were 4 solvent voids per unit cell each with a volume of Ca 200 A^3 containing an estimated 51 electrons. This is consistent with there being approximately one DCM or pentane per void.

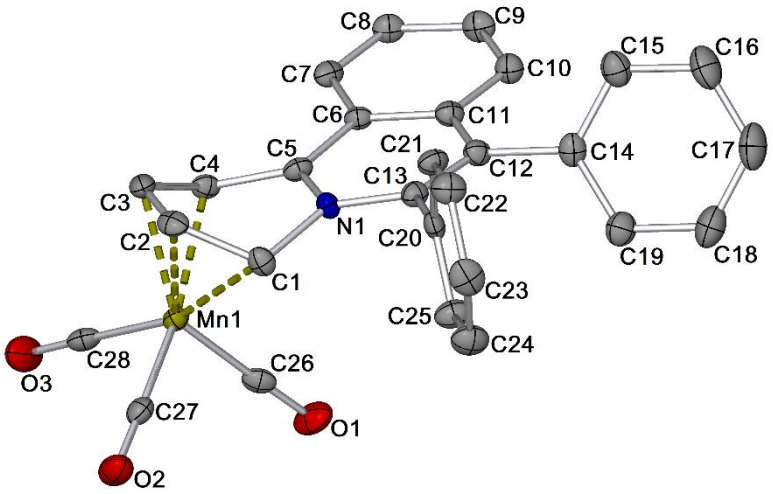


Figure S69. X-ray structure of **7b**. Selected bond lengths and angles: C1-C2: 1.446(4) Å; C1-Mn1: 2.091(3) Å; C1-N1: 1.476(3) Å; C2-C3: 1.382(4) Å; C2-Mn1: 2.095(3) Å; C3-C4: 1.445(4) Å; C3-Mn1: 2.083(3) Å; C4-C5: 1.442(4) Å; C4-Mn1: 2.162(3) Å; C5-N1: 1.342(3) Å; C12-C13: 1.372(4) Å; C13-N1: 1.387(4) Å; C26-Mn1: 1.804(3) Å; C27-Mn1: 1.161(3) Å; C28-Mn1: 1.798(3) Å; C2-C1-N1: 115.7(2) °; C3-C2-C1: 113.1(3) °; N1-C5-C4: 155.5(2) °; C12-C13-N1: 119.7(2) °; O1-C26-Mn1: 178.5(3) °; C1-Mn1-C2: 40.41(11) °; C1-Mn1-C4: 74.07(11) °; C3-Mn1-C2: 38.63(11) °; C26-Mn1-C1: 97.38(13) °; C27-Mn1-C1: 96.86(12) °; C28-Mn1-C1: 163.33(13) °.

4 Computational Chemistry

4.1 Collated xyz coordinates, energies and vibrational frequencies (first 50 lines)

1

SCF Energy (au) BP86/SV(P) -479.0045858023
SCF Energy (au) PBE0/def2-TZVPP -478.9367212604
SCF Energy (au) PBE0/def2-TZVPP -478.9452850324 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.1651040
Chemical potential (kJ mol^{-1}) 340.38
Dispersion correction (au) PBE0/def2-TZVPP -0.02166655

xyz coordinates
21

N	1.87154	-0.26360	-0.08786
C	1.69751	1.81974	-1.95475
C	0.54837	1.33529	-1.31584
C	2.96287	0.20417	-0.70452
C	0.66657	0.28622	-0.37084
C	2.94206	1.24911	-1.64560
H	1.61811	2.63507	-2.69314
H	-0.43360	1.76534	-1.56336
C	-0.51068	-0.27951	0.35365
H	3.91943	-0.28295	-0.43353
H	3.87230	1.59763	-2.12257
C	-2.70130	-1.42192	1.75177
C	-1.42931	-2.01856	1.81661
C	-0.34724	-1.45260	1.12869
C	-1.79450	0.31301	0.30181
C	-2.87729	-0.25150	0.99347
H	-3.55341	-1.86557	2.29324
H	-1.27954	-2.93564	2.41066
H	0.65597	-1.90292	1.17244
H	-1.96030	1.23822	-0.27244
H	-3.86756	0.23096	0.94210

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	25.69	0.64130	YES	YES
8	a	91.43	1.74849	YES	YES
9	a	163.47	1.69537	YES	YES
10	a	220.13	0.20869	YES	YES
11	a	324.70	0.00134	YES	YES
12	a	395.22	2.89099	YES	YES
13	a	403.62	1.04727	YES	YES
14	a	412.14	0.46624	YES	YES
15	a	442.90	2.01388	YES	YES
16	a	553.66	0.13999	YES	YES
17	a	600.64	4.38401	YES	YES
18	a	615.67	4.22415	YES	YES
19	a	630.97	4.02773	YES	YES
20	a	691.38	25.05439	YES	YES

21	a	733.57	30.53182	YES	YES
22	a	742.93	48.60575	YES	YES
23	a	750.61	0.54612	YES	YES
24	a	814.69	1.23608	YES	YES
25	a	832.52	0.40531	YES	YES
26	a	876.33	0.49994	YES	YES
27	a	920.02	0.71077	YES	YES
28	a	945.09	0.08071	YES	YES
29	a	962.98	0.24601	YES	YES
30	a	977.79	0.02968	YES	YES
31	a	978.33	3.07719	YES	YES
32	a	985.43	1.13949	YES	YES
33	a	990.50	0.30905	YES	YES
34	a	1015.85	5.33587	YES	YES
35	a	1034.61	2.86208	YES	YES
36	a	1054.04	1.26209	YES	YES
37	a	1074.43	9.98607	YES	YES
38	a	1086.86	3.32494	YES	YES
39	a	1136.79	1.78749	YES	YES
40	a	1139.94	0.72265	YES	YES
41	a	1163.07	6.67363	YES	YES
42	a	1261.40	3.80308	YES	YES
43	a	1275.60	13.03919	YES	YES
44	a	1301.44	0.78901	YES	YES
45	a	1335.12	0.67112	YES	YES
46	a	1369.72	1.00346	YES	YES
47	a	1419.34	22.87245	YES	YES
48	a	1446.66	33.13184	YES	YES
49	a	1462.37	38.24392	YES	YES
50	a	1491.24	1.76897	YES	YES

2a

SCF Energy (au) BP86/SV(P) -308.1698939972
SCF Energy (au) PBE0/def2-TZVPP -308.1232351678
SCF Energy (au) PBE0/def2-TZVPP -308.1303056182 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.1064946
Chemical potential (kJ mol^{-1}) 199.25
Dispersion correction (au) PBE0/def2-TZVPP -0.01224568

xyz coordinates
14

C	0.06253	-0.51956	0.51746
C	1.20573	0.18505	0.05791
C	1.08074	1.17386	-0.92774
C	-0.17983	1.47832	-1.47222
C	-1.31941	0.78636	-1.02417
C	-1.20440	-0.20407	-0.03883
H	2.19157	-0.05609	0.48600
H	1.97749	1.71311	-1.27539
H	-0.27456	2.25635	-2.24760
H	-2.31009	1.02126	-1.44742
H	-2.09512	-0.74750	0.31411
C	0.18593	-1.53070	1.52457
C	0.29314	-2.39627	2.38625
H	0.38630	-3.16013	3.14705

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	137.62	1.54239	YES	YES
8	a	152.55	1.03541	YES	YES
9	a	359.94	2.76692	YES	YES
10	a	399.86	0.00003	YES	YES
11	a	458.49	0.36532	YES	YES
12	a	517.31	2.56247	YES	YES
13	a	545.24	5.37218	YES	YES
14	a	599.90	35.42594	YES	YES
15	a	614.16	0.52393	YES	YES
16	a	644.63	35.19285	YES	YES
17	a	692.49	31.23483	YES	YES
18	a	758.17	2.37031	YES	YES
19	a	760.72	32.28818	YES	YES
20	a	831.08	0.00007	YES	YES
21	a	909.88	3.38795	YES	YES
22	a	957.19	0.00017	YES	YES
23	a	982.21	0.08346	YES	YES
24	a	983.86	0.16195	YES	YES
25	a	1025.10	3.71162	YES	YES
26	a	1071.38	5.62927	YES	YES
27	a	1142.08	0.00035	YES	YES
28	a	1158.70	0.00087	YES	YES
29	a	1204.65	0.89088	YES	YES
30	a	1290.24	0.08234	YES	YES

31	a	1356.94	0.05075	YES	YES
32	a	1438.07	4.75311	YES	YES
33	a	1482.44	13.36586	YES	YES
34	a	1581.64	1.09448	YES	YES
35	a	1614.48	1.64749	YES	YES
36	a	2144.36	3.12605	YES	YES
37	a	3091.78	0.38767	YES	YES
38	a	3100.56	5.07513	YES	YES
39	a	3110.97	15.11875	YES	YES
40	a	3118.68	16.60336	YES	YES
41	a	3122.26	3.97788	YES	YES
42	a	3386.07	81.84204	YES	YES

$end

H_2O

SCF Energy (au) BP86/SV(P) -76.3451982082
SCF Energy (au) PBE0/def2-TZVPP -76.379976764
SCF Energy (au) PBE0/def2-TZVPP -76.3899545235 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.0199812
Chemical potential (kJ mol^{-1}) 5.89
Dispersion correction (au) PBE0/def2-TZVPP -0.00027693

xyz coordinates
3

O	0.00000	0.00000	-0.40473
H	-0.77070	0.00000	0.20252
H	0.77070	0.00000	0.20252

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a1	1604.23	61.98164	YES	YES
8	a1	3526.13	0.10543	YES	YES
9	b1	3640.35	16.43822	YES	YES

$end

CO

SCF Energy (au) BP86/SV(P) -113.2300640696
SCF Energy (au) PBE0/def2-TZVPP -113.2302273127
SCF Energy (au) PBE0/def2-TZVPP -113.2310218702 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.0049005
Chemical potential (kJ mol^{-1}) -37.48
Dispersion correction (au) PBE0/def2-TZVPP -0.00033780

xyz coordinates
2

C	0.00000	0.00000	0.57100
O	0.00000	0.00000	-0.57100

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6	a1	2151.08	60.66925	YES	YES

$end

4

SCF Energy (au) BP86/SV(P) -2082.6115690800
SCF Energy (au) PBE0/def2-TZVPP -2082.210872156
SCF Energy (au) PBE0/def2-TZVPP -2082.2211822344 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.1903172
Chemical potential (kJ mol^{-1}) 374.35
Dispersion correction (au) PBE0/def2-TZVPP -0.04156702

xyz coordinates
29

Mn	0.05709	-1.83673	0.00000
C	1.39028	-3.08100	0.00000
O	2.22362	-3.89701	0.00000
N	1.35181	-0.19364	0.00000
C	2.93541	2.12139	0.00000
C	3.53263	0.84888	0.00000
C	2.70110	-0.27530	0.00000
C	0.74982	1.03954	0.00000
C	1.54177	2.21179	0.00000
H	3.55260	3.03453	0.00000
H	4.62570	0.71936	0.00000
H	3.12942	-1.28921	0.00000
H	1.05067	3.19566	0.00000
C	-0.06024	-1.70106	-1.83368
C	-0.06024	-1.70106	1.83368
O	-0.16495	-1.60118	-2.98357
O	-0.16495	-1.60118	2.98357
C	-1.22732	-3.09417	0.00000
O	-2.07196	-3.89682	0.00000
C	-1.31074	-0.28499	0.00000
C	-2.90927	2.08078	0.00000
C	-3.51042	0.80796	0.00000
C	-2.71880	-0.35473	0.00000
C	-0.71565	1.01075	0.00000
C	-1.51391	2.18080	0.00000
H	-3.52927	2.99194	0.00000
H	-4.61029	0.71866	0.00000
H	-3.22683	-1.33364	0.00000
H	-1.04708	3.17969	0.00000

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a"	42.18	0.06728	YES	YES
8	a"	57.40	0.13603	YES	YES
9	a'	61.06	0.06177	YES	YES
10	a'	77.36	0.22319	YES	YES
11	a"	80.59	1.08367	YES	YES
12	a"	90.24	0.00173	YES	YES
13	a'	102.66	0.52273	YES	YES
14	a'	105.29	0.00805	YES	YES
15	a"	105.40	0.04324	YES	YES
16	a"	109.78	0.11409	YES	YES

17	a"	183.47	1.05450	YES	YES
18	a'	195.37	0.26564	YES	YES
19	a'	234.49	0.20849	YES	YES
20	a"	252.32	0.49250	YES	YES
21	a'	284.87	0.26555	YES	YES
22	a'	360.74	1.94986	YES	YES
23	a"	401.30	0.02468	YES	YES
24	a"	409.07	4.16118	YES	YES
25	a"	431.47	0.77571	YES	YES
26	a'	433.07	0.47282	YES	YES
27	a'	456.14	0.95061	YES	YES
28	a"	460.64	0.01647	YES	YES
29	a"	468.92	10.55912	YES	YES
30	a'	487.14	0.92925	YES	YES
31	a'	491.94	0.53093	YES	YES
32	a"	502.93	10.05195	YES	YES
33	a'	504.21	0.13227	YES	YES
34	a'	552.00	18.18756	YES	YES
35	a"	556.90	1.51145	YES	YES
36	a"	567.86	2.43793	YES	YES
37	a'	620.93	1.53210	YES	YES
38	a'	626.28	2.10180	YES	YES
39	a'	647.40	0.16550	YES	YES
40	a'	656.73	89.12384	YES	YES
41	a"	657.99	70.50823	YES	YES
42	a'	688.29	113.45156	YES	YES
43	a"	721.10	14.33326	YES	YES
44	a"	734.19	13.59702	YES	YES
45	a"	746.02	86.99424	YES	YES
46	a'	756.91	1.53917	YES	YES
47	a"	803.95	0.27180	YES	YES
48	a"	861.00	0.56600	YES	YES
49	a"	871.33	0.70478	YES	YES
50	a"	931.17	0.30242	YES	YES

6a

SCF Energy (au) BP86/SV(P) -2277.5454614300
SCF Energy (au) PBE0/def2-TZVPP -2277.104426951
SCF Energy (au) PBE0/def2-TZVPP -2277.1196227593 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.2916092
Chemical potential (kJ mol^{-1}) 622.45
Dispersion correction (au) PBE0/def2-TZVPP -0.06485843

xyz coordinates
41

Mn	1.2036008	0.6106628	0.8522765
C	1.6744594	0.8952513	2.5996280
C	2.8473914	0.0459172	0.3776595
C	1.5911029	2.2600181	0.4058252
O	1.8151640	3.3749548	0.1224248
O	3.9082732	-0.3104898	0.0510345
O	2.0053518	1.0917446	3.7007502
C	-1.3227856	-0.2379977	1.6400043
C	-1.5435172	2.0145716	1.0272904
C	-2.9079081	2.0118246	1.3452868
C	-3.4880860	0.8331982	1.8413069
C	-2.6826598	-0.3075575	1.9890141
C	-0.3858537	-1.3933135	1.7625586
C	0.2684015	-1.9505773	0.6109429
C	1.0046730	-3.1537928	0.7947670
C	1.1266907	-3.7632905	2.0454927
C	0.5022348	-3.1927154	3.1746089
C	-0.2553715	-2.0286898	3.0253299
H	-1.0385621	2.9154598	0.6440124
H	-3.5010334	2.9288071	1.2049194
H	-4.5580140	0.7990083	2.1030172
H	-3.0974468	-1.2587283	2.3570313
H	1.4894566	-3.6036832	-0.0875235
H	1.7149517	-4.6900600	2.1489986
H	0.6023407	-3.6634756	4.1659099
H	-0.7646556	-1.5866450	3.8977602
N	-0.7721961	0.9179128	1.1840420
C	0.4618969	0.5684594	-2.2842737
C	1.4956238	1.4053105	-2.7767161
C	1.4172409	1.9808854	-4.0534696
C	0.2931146	1.7554251	-4.8682955
C	-0.7507065	0.9415658	-4.3932670
C	-0.6663964	0.3544298	-3.1217575
H	2.3830739	1.5885554	-2.1508602
H	2.2421910	2.6177027	-4.4145169
H	0.2279000	2.2188777	-5.8668102
H	-1.6422056	0.7651665	-5.0188331
H	-1.4944769	-0.2707101	-2.7486092
C	0.5386977	-0.0685731	-0.9603080
C	0.1585599	-1.3605615	-0.7492654
H	-0.1005158	-2.0548483	-1.5773864

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	30.30	0.17649	YES	YES
8	a	36.56	0.28182	YES	YES
9	a	45.26	0.15260	YES	YES
10	a	53.87	0.01646	YES	YES
11	a	59.64	0.18618	YES	YES
12	a	71.73	0.36926	YES	YES
13	a	75.92	0.28896	YES	YES
14	a	85.62	0.08104	YES	YES
15	a	95.10	1.35102	YES	YES
16	a	100.25	0.88608	YES	YES
17	a	106.07	0.11247	YES	YES
18	a	109.83	0.57407	YES	YES
19	a	145.93	0.39566	YES	YES
20	a	164.65	1.78214	YES	YES
21	a	176.36	0.65196	YES	YES
22	a	201.48	0.39951	YES	YES
23	a	225.56	0.91647	YES	YES
24	a	241.41	1.04958	YES	YES
25	a	290.50	0.85078	YES	YES
26	a	305.47	0.62366	YES	YES
27	a	340.84	2.00198	YES	YES
28	a	359.20	1.66114	YES	YES
29	a	407.29	0.27575	YES	YES
30	a	411.66	2.09249	YES	YES
31	a	430.33	2.45302	YES	YES
32	a	448.21	0.79307	YES	YES
33	a	458.90	0.39480	YES	YES
34	a	476.58	0.31871	YES	YES
35	a	479.07	5.09467	YES	YES
36	a	491.65	1.11579	YES	YES
37	a	505.52	8.07195	YES	YES
38	a	505.80	6.51906	YES	YES
39	a	535.03	0.56159	YES	YES
40	a	540.90	5.74542	YES	YES
41	a	548.35	4.66086	YES	YES
42	a	555.33	0.93242	YES	YES
43	a	564.16	0.93933	YES	YES
44	a	613.21	0.87378	YES	YES
45	a	621.74	35.33440	YES	YES
46	a	622.91	1.39939	YES	YES
47	a	630.52	26.30650	YES	YES
48	a	633.59	22.26462	YES	YES
49	a	644.97	6.16755	YES	YES
50	a	696.00	24.05472	YES	YES

6a'

SCF Energy (au) BP86/SV(P) -2390.8151653250
SCF Energy (au) PBE0/def2-TZVPP -2390.369700332
SCF Energy (au) PBE0/def2-TZVPP -2390.3837338351 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.3008799
Chemical potential (kJ mol^{-1}) 641.09
Dispersion correction (au) PBE0/def2-TZVPP -0.06673312

xyz coordinates
43

Mn	0.34634	1.72585	0.59734
C	0.01135	2.87140	1.98187
C	1.03425	3.00182	-0.45947
C	-1.26908	2.21113	-0.19516
O	-2.17189	2.73211	-0.70403
O	1.45669	3.85606	-1.13096
O	-0.18658	3.60587	2.86364
C	-1.55670	-0.60866	1.42640
C	0.17338	-0.17176	2.93109
C	-0.23392	-1.17699	3.80973
C	-1.36286	-1.93833	3.47608
C	-2.01894	-1.64290	2.27944
H	1.04881	0.44317	3.18329
H	0.33450	-1.34871	4.73680
H	-1.72000	-2.75105	4.12940
H	-2.89502	-2.22834	1.96257
N	-0.45091	0.12200	1.75957
C	2.07592	-0.13438	-1.28280
C	2.57770	-1.44045	-1.04605
C	3.86506	-1.81655	-1.46335
C	4.68561	-0.89927	-2.14075
C	4.20313	0.39769	-2.39127
C	2.92233	0.77760	-1.96102
H	1.93941	-2.16380	-0.51194
H	4.22842	-2.83750	-1.25642
H	5.69634	-1.19178	-2.47053
H	4.83187	1.12586	-2.93103
H	2.56310	1.79450	-2.18042
C	0.69587	0.21157	-0.83550
C	-0.30311	-0.55652	-1.36576
H	-0.02599	-1.27631	-2.16573
C	2.05557	1.40362	1.19921
O	3.14645	1.28474	1.57664
C	-2.33287	-0.37634	0.17836
C	-4.00815	-0.36081	-2.10084
C	-2.62362	-0.50030	-2.23872
C	-1.74924	-0.46885	-1.12206
C	-3.73895	-0.24919	0.30408
C	-4.57211	-0.21304	-0.81919
H	-4.65294	-0.35771	-2.99517
H	-2.17966	-0.60832	-3.24254
H	-4.17990	-0.16332	1.31137
H	-5.65968	-0.08380	-0.69613

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
#					
1		0.00	0.00000	-	-

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.07	0.28937	YES	YES
8	a	30.27	0.06649	YES	YES
9	a	46.14	0.03769	YES	YES
10	a	55.36	0.10874	YES	YES
11	a	60.28	0.20908	YES	YES
12	a	65.11	0.30858	YES	YES
13	a	81.26	0.56985	YES	YES
14	a	90.05	0.09006	YES	YES
15	a	97.90	0.57055	YES	YES
16	a	100.74	0.33146	YES	YES
17	a	112.48	0.25482	YES	YES
18	a	116.40	0.25885	YES	YES
19	a	123.87	0.38054	YES	YES
20	a	135.16	0.07832	YES	YES
21	a	155.67	0.21153	YES	YES
22	a	175.89	1.18274	YES	YES
23	a	184.62	0.32611	YES	YES
24	a	198.18	0.09214	YES	YES
25	a	228.76	1.12219	YES	YES
26	a	245.44	0.34560	YES	YES
27	a	288.62	0.66357	YES	YES
28	a	301.36	0.26318	YES	YES
29	a	351.11	1.13105	YES	YES
30	a	367.59	2.23127	YES	YES
31	a	402.86	0.45234	YES	YES
32	a	409.54	0.20205	YES	YES
33	a	418.17	0.43104	YES	YES
34	a	426.87	1.76791	YES	YES
35	a	433.72	2.72331	YES	YES
36	a	448.18	1.00728	YES	YES
37	a	468.55	2.22660	YES	YES
38	a	480.09	4.17398	YES	YES
39	a	485.15	22.03254	YES	YES
40	a	494.10	14.76074	YES	YES
41	a	505.06	1.74967	YES	YES
42	a	523.53	6.79554	YES	YES
43	a	541.40	3.46013	YES	YES
44	a	544.48	3.81708	YES	YES
45	a	549.19	8.48106	YES	YES
46	a	557.34	0.88342	YES	YES
47	a	564.20	6.73318	YES	YES
48	a	575.27	4.00036	YES	YES
49	a	613.79	2.66719	YES	YES
50	a	623.17	1.81939	YES	YES

7a'

SCF Energy (au) BP86/SV(P) -2277.5279704610
SCF Energy (au) PBE0/def2-TZVPP -2277.079674398
SCF Energy (au) PBE0/def2-TZVPP -2277.0925557051 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.2917488
Chemical potential (kJ mol^{-1}) 627.54
Dispersion correction (au) PBE0/def2-TZVPP -0.06221297

xyz coordinates
41

C	0.11506	-1.04987	3.18138
C	-1.68297	0.45180	2.43257
C	0.31260	0.57413	0.27310
C	-1.76216	-2.15299	1.64126
C	0.94879	-1.80162	0.31960
C	1.76034	-2.86925	0.88414
C	1.38624	-4.23726	-1.10464
C	0.60048	-3.26183	-1.68617
H	0.14836	-3.44426	-2.67454
C	0.30797	-2.04059	-0.99567
C	-0.57325	-1.05158	-1.44162
C	-1.26645	-0.97664	-2.68050
H	-0.99258	-1.70203	-3.46262
C	-2.28428	-0.06818	-2.89947
H	-2.81642	-0.03737	-3.86213
C	-2.65410	0.82982	-1.83348
H	-3.51039	1.51282	-1.94626
C	-1.94850	0.86450	-0.66902
H	-2.16299	1.56174	0.15142
Mn	-0.62872	-0.72563	1.59418
N	-0.83937	-0.01135	-0.42963
O	0.63751	-1.28326	4.20177
O	-2.37178	1.20690	3.00169
C	1.22756	-0.42029	0.67577
O	-2.49985	-3.05191	1.67499
C	1.95914	-4.04590	0.20352
H	2.14796	-0.13225	1.20634
C	0.56900	2.03534	0.29445
C	1.16792	4.79965	0.31461
C	1.26649	4.04592	1.49866
C	0.96133	2.67743	1.49129
C	0.47767	2.79885	-0.89348
C	0.77121	4.17235	-0.87830
H	1.39778	5.87775	0.32383
H	1.56998	4.53125	2.44082
H	1.00509	2.09287	2.42499
H	0.19284	2.30994	-1.83878
H	0.69645	4.75463	-1.81160
H	1.56699	-5.18307	-1.64113
H	2.57072	-4.84681	0.64980
H	2.22836	-2.70377	1.86882

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	42.29	0.06425	YES	YES
8	a	43.48	0.33674	YES	YES
9	a	46.29	0.13526	YES	YES
10	a	60.05	0.09926	YES	YES
11	a	62.05	0.07407	YES	YES
12	a	78.97	0.03583	YES	YES
13	a	85.71	0.13077	YES	YES
14	a	91.86	0.32603	YES	YES
15	a	103.36	0.53113	YES	YES
16	a	110.74	0.83272	YES	YES
17	a	126.78	1.10937	YES	YES
18	a	137.77	0.93380	YES	YES
19	a	156.55	1.89229	YES	YES
20	a	180.23	0.61820	YES	YES
21	a	217.19	0.67051	YES	YES
22	a	233.50	0.58195	YES	YES
23	a	248.73	0.13804	YES	YES
24	a	275.88	0.68066	YES	YES
25	a	286.15	2.56865	YES	YES
26	a	381.92	0.29874	YES	YES
27	a	398.21	1.38131	YES	YES
28	a	403.64	4.93022	YES	YES
29	a	407.23	1.25098	YES	YES
30	a	417.28	6.92016	YES	YES
31	a	428.34	4.42897	YES	YES
32	a	457.59	3.33767	YES	YES
33	a	458.71	5.10217	YES	YES
34	a	471.10	2.94826	YES	YES
35	a	479.48	3.18296	YES	YES
36	a	487.64	7.41628	YES	YES
37	a	491.33	3.65691	YES	YES
38	a	507.64	5.88200	YES	YES
39	a	522.66	25.16936	YES	YES
40	a	539.35	8.21135	YES	YES
41	a	555.45	3.25448	YES	YES
42	a	560.12	8.86594	YES	YES
43	a	586.56	25.68173	YES	YES
44	a	599.04	8.41344	YES	YES
45	a	603.64	7.86430	YES	YES
46	a	620.56	13.89848	YES	YES
47	a	637.99	50.84300	YES	YES
48	a	648.56	25.86957	YES	YES
49	a	667.20	21.13953	YES	YES
50	a	674.67	28.95069	YES	YES

8a

SCF Energy (au) BP86/SV(P) -2277.5161934120
SCF Energy (au) PBE0/def2-TZVPP -2277.070662383
SCF Energy (au) PBE0/def2-TZVPP -2277.0842359540 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.2897634
Chemical potential (kJ mol^{-1}) 615.48
Dispersion correction (au) PBE0/def2-TZVPP -0.06121589

xyz coordinates
41

Mn	1.30245	-0.02169	0.74661
C	1.62450	0.20050	2.50505
C	2.95518	-0.65910	0.47892
C	1.80850	1.68376	0.37645
O	2.16975	2.77915	0.19703
O	4.02418	-1.09454	0.30725
O	1.83742	0.33700	3.64134
C	-1.50058	-0.52608	1.56873
C	-1.27856	1.65238	0.71772
C	-2.63581	1.93251	0.90926
C	-3.45321	0.92907	1.45802
C	-2.88049	-0.30226	1.78637
C	-0.79093	-1.77234	1.87664
C	0.60334	-1.78573	1.57636
C	1.32783	-2.95859	1.87556
C	0.69738	-4.08534	2.43189
C	-0.68244	-4.06455	2.71326
C	-1.42254	-2.90964	2.43720
H	-0.60440	2.41196	0.29343
H	-3.03434	2.92083	0.63358
H	-4.52759	1.10675	1.62928
H	-3.49983	-1.10273	2.21649
H	2.41075	-3.00739	1.67158
H	1.29065	-4.98956	2.65166
H	-1.17666	-4.94690	3.15149
H	-2.50135	-2.89703	2.66437
N	-0.71744	0.46477	1.03412
C	0.73330	1.04190	-2.46476
C	1.87490	1.75765	-2.90758
C	1.75933	2.72560	-3.91464
C	0.50805	3.00721	-4.49220
C	-0.63158	2.30703	-4.05887
C	-0.52486	1.33316	-3.05520
H	2.85681	1.54056	-2.45926
H	2.65784	3.26873	-4.25112
H	0.42142	3.77294	-5.28063
H	-1.61579	2.51924	-4.50883
H	-1.41520	0.77891	-2.71836
C	0.82108	0.00599	-1.46154
C	0.69860	-1.14191	-0.94251
H	0.51034	-2.21220	-1.03415

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.92	0.18196	YES	YES
8	a	29.12	0.18730	YES	YES
9	a	39.44	0.04922	YES	YES
10	a	57.29	0.28357	YES	YES
11	a	69.45	0.06837	YES	YES
12	a	74.51	0.10817	YES	YES
13	a	85.75	1.34343	YES	YES
14	a	90.69	0.27811	YES	YES
15	a	99.33	0.44510	YES	YES
16	a	109.87	0.12107	YES	YES
17	a	113.33	0.10699	YES	YES
18	a	118.28	0.53725	YES	YES
19	a	129.86	0.33981	YES	YES
20	a	162.72	1.55487	YES	YES
21	a	164.97	5.40992	YES	YES
22	a	189.65	1.22846	YES	YES
23	a	222.86	0.69322	YES	YES
24	a	242.13	2.15168	YES	YES
25	a	262.03	0.56601	YES	YES
26	a	283.38	1.93927	YES	YES
27	a	320.56	23.66758	YES	YES
28	a	358.49	1.90009	YES	YES
29	a	401.23	0.01985	YES	YES
30	a	410.51	1.59782	YES	YES
31	a	420.06	11.11831	YES	YES
32	a	437.09	2.13531	YES	YES
33	a	454.94	15.46878	YES	YES
34	a	456.15	2.06895	YES	YES
35	a	471.44	3.94462	YES	YES
36	a	480.07	5.73117	YES	YES
37	a	486.53	2.17161	YES	YES
38	a	492.67	5.76252	YES	YES
39	a	501.93	9.24113	YES	YES
40	a	508.11	12.94047	YES	YES
41	a	524.80	34.54409	YES	YES
42	a	539.50	10.09634	YES	YES
43	a	550.69	5.86095	YES	YES
44	a	556.63	1.71211	YES	YES
45	a	609.36	20.54643	YES	YES
46	a	614.44	8.33273	YES	YES
47	a	623.38	6.75777	YES	YES
48	a	625.77	13.21340	YES	YES
49	a	643.19	9.46298	YES	YES
50	a	654.08	72.32014	YES	YES

9aa

SCF Energy (au) BP86/SV(P) -2585.7120861790
SCF Energy (au) PBE0/def2-TZVPP -2585.222285558
SCF Energy (au) PBE0/def2-TZVPP -2585.2395859905 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.4004348
Chemical potential (kJ mol^{-1}) 882.18
Dispersion correction (au) PBE0/def2-TZVPP -0.08677851
xyz coordinates
55

Mn	0.47599	1.17442	-0.62969
C	1.31857	2.43262	0.37135
C	-0.59765	2.46948	-1.28481
O	-1.23951	3.35150	-1.69136
O	1.83716	3.31149	0.93752
C	-1.38400	-0.39149	1.50387
C	-1.50879	1.93498	1.52669
C	-2.43384	1.95709	2.57210
C	-2.85712	0.73386	3.11131
C	-2.32460	-0.43568	2.56769
C	-0.90505	-1.71097	1.00664
C	-1.02091	-2.11982	-0.35406
C	-0.81530	-3.49461	-0.64744
C	-0.41746	-4.41738	0.32595
C	-0.23297	-3.98950	1.65335
C	-0.50288	-2.65595	1.98307
H	-1.16393	2.88629	1.09812
H	-2.80964	2.92278	2.94429
H	-3.59579	0.69078	3.92836
H	-2.65168	-1.42021	2.93345
H	-0.95104	-3.82630	-1.69098
H	-0.24341	-5.47041	0.04901
H	0.10250	-4.69446	2.43133
H	-0.38699	-2.32429	3.02810
N	-0.97846	0.80485	0.98649
C	-1.33083	0.48812	-3.15884
C	-0.47478	0.70276	-4.26652
C	-0.98134	1.13426	-5.50270
C	-2.35628	1.38007	-5.66380
C	-3.22095	1.17841	-4.57501
C	-2.71524	0.73351	-3.34260
H	0.60338	0.50647	-4.16634
H	-0.29104	1.27882	-6.35090
H	-2.75071	1.72868	-6.63277
H	-4.30218	1.36938	-4.68363
H	-3.39891	0.58099	-2.49084
C	-0.83300	-0.01931	-1.84314
C	-1.33993	-1.24055	-1.49092
H	-1.97822	-1.74383	-2.24954
C	2.80441	0.15007	1.72207
C	2.31373	0.72454	2.92147
C	3.14648	0.85405	4.04166
C	4.48380	0.42256	3.98758
C	4.98481	-0.14382	2.80155
C	4.15783	-0.27961	1.67821
H	1.26840	1.06661	2.96809
H	2.74777	1.30149	4.96712
H	5.13737	0.53211	4.86857
H	6.03344	-0.48058	2.74873

H	4.54887	-0.71921	0.74707
C	1.97402	-0.05769	0.55995
C	1.51200	-0.66021	-0.45103
H	1.42922	-1.53501	-1.09392
C	1.65177	1.43071	-1.94377
O	2.46291	1.59715	-2.76615

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.82	0.03519	YES	YES
8	a	23.00	0.22563	YES	YES
9	a	27.88	0.41776	YES	YES
10	a	33.18	0.28278	YES	YES
11	a	36.95	0.00657	YES	YES
12	a	51.08	0.11682	YES	YES
13	a	61.76	0.23887	YES	YES
14	a	68.22	0.20227	YES	YES
15	a	79.15	0.03369	YES	YES
16	a	88.73	0.35772	YES	YES
17	a	97.17	0.18178	YES	YES
18	a	101.80	0.34931	YES	YES
19	a	109.97	0.68153	YES	YES
20	a	113.52	0.48190	YES	YES
21	a	121.90	0.52662	YES	YES
22	a	129.47	0.35119	YES	YES
23	a	137.53	0.12192	YES	YES
24	a	146.80	2.99958	YES	YES
25	a	156.96	0.73343	YES	YES
26	a	172.92	0.25159	YES	YES
27	a	196.27	3.02614	YES	YES
28	a	198.58	2.21502	YES	YES
29	a	220.79	0.52067	YES	YES
30	a	235.83	1.14163	YES	YES
31	a	245.22	0.31159	YES	YES
32	a	284.88	0.40943	YES	YES
33	a	301.62	0.84880	YES	YES
34	a	320.28	22.97572	YES	YES
35	a	350.52	1.02195	YES	YES
36	a	372.12	1.28637	YES	YES
37	a	399.00	1.27625	YES	YES
38	a	402.75	0.45898	YES	YES
39	a	404.75	3.50659	YES	YES
40	a	432.33	0.96303	YES	YES
41	a	440.62	2.09758	YES	YES
42	a	462.99	3.80011	YES	YES
43	a	469.93	0.57574	YES	YES
44	a	472.91	4.84551	YES	YES
45	a	486.06	3.28811	YES	YES
46	a	492.19	27.96598	YES	YES
47	a	495.50	22.18241	YES	YES
48	a	512.97	4.46311	YES	YES
49	a	515.69	9.32231	YES	YES
50	a	527.11	6.29771	YES	YES

10aa

SCF Energy (au) BP86/SV(P) -2585.7050644730
SCF Energy (au) PBE0/def2-TZVPP -2585.213754528
SCF Energy (au) PBE0/def2-TZVPP -2585.2318519835 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.3989997
Chemical potential (kJ mol^{-1}) 871.08
Dispersion correction (au) PBE0/def2-TZVPP -0.08167977
xyz coordinates
55

Mn	-0.86075	1.13851	-0.46339
C	-0.10093	2.77846	-0.20155
C	-2.46776	1.88489	-0.65290
O	-3.49450	2.41869	-0.80131
O	0.37363	3.83150	-0.05244
C	-0.51295	-0.10744	2.42223
C	-1.80465	1.83210	2.29195
C	-2.05870	1.84626	3.66445
C	-1.51242	0.82625	4.45636
C	-0.73741	-0.14659	3.82219
C	0.33760	-1.19309	1.85836
C	-0.10161	-2.06740	0.81651
C	0.69197	-3.21288	0.53841
C	1.90227	-3.45720	1.19291
C	2.35604	-2.56010	2.17871
C	1.56566	-1.45630	2.51543
H	-2.22129	2.62718	1.65816
H	-2.67838	2.64975	4.09178
H	-1.69383	0.78335	5.54268
H	-0.30907	-0.98194	4.39558
H	0.33818	-3.91095	-0.23902
H	2.50193	-4.34441	0.92987
H	3.31761	-2.72754	2.69060
H	1.90724	-0.76340	3.30245
N	-1.05707	0.88849	1.65841
C	-3.11037	-0.90142	-1.26836
C	-3.27874	-0.67816	-2.65708
C	-4.52348	-0.86676	-3.27717
C	-5.64347	-1.26458	-2.52574
C	-5.49944	-1.48452	-1.14592
C	-4.24971	-1.31154	-0.52910
H	-2.41525	-0.37474	-3.26831
H	-4.61897	-0.69887	-4.36335
H	-6.62316	-1.39956	-3.01383
H	-6.36836	-1.79435	-0.54062
H	-4.14378	-1.48225	0.55539
C	-1.80332	-0.73934	-0.56629
C	-1.33465	-1.87634	0.03887
H	-1.87401	-2.82607	-0.16800
C	3.78210	1.18391	-1.19172
C	4.67526	1.72676	-0.22487
C	5.98834	2.05823	-0.58005
C	6.44037	1.85742	-1.89799
C	5.56802	1.32139	-2.86397
C	4.25275	0.98589	-2.52103
H	4.31654	1.88435	0.80430
H	6.66882	2.47997	0.17813
H	7.47488	2.12078	-2.17344
H	5.91817	1.16499	-3.89759

H	3.56522	0.56919	-3.27362
C	2.44841	0.84738	-0.84198
C	1.25386	0.63198	-0.56262
H	0.57605	-0.18825	-0.21105
C	-0.64697	1.20610	-2.23849
O	-0.47589	1.27219	-3.39091

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.40	0.22149	YES	YES
8	a	19.89	0.24179	YES	YES
9	a	20.05	0.06659	YES	YES
10	a	27.26	0.49056	YES	YES
11	a	36.22	0.13026	YES	YES
12	a	53.20	0.27819	YES	YES
13	a	55.61	0.06434	YES	YES
14	a	62.71	0.25604	YES	YES
15	a	66.14	0.62558	YES	YES
16	a	82.56	0.29297	YES	YES
17	a	88.12	0.12419	YES	YES
18	a	92.91	0.32222	YES	YES
19	a	97.29	0.11725	YES	YES
20	a	106.15	0.82195	YES	YES
21	a	108.67	0.42865	YES	YES
22	a	114.11	0.58421	YES	YES
23	a	121.17	0.49938	YES	YES
24	a	141.00	0.46852	YES	YES
25	a	163.96	0.38394	YES	YES
26	a	179.27	0.46066	YES	YES
27	a	192.70	5.15066	YES	YES
28	a	199.22	0.42403	YES	YES
29	a	215.89	20.18297	YES	YES
30	a	232.79	10.76479	YES	YES
31	a	244.79	1.68296	YES	YES
32	a	265.57	6.59472	YES	YES
33	a	288.62	0.99226	YES	YES
34	a	298.08	1.98236	YES	YES
35	a	346.95	1.02710	YES	YES
36	a	368.14	1.51827	YES	YES
37	a	392.51	7.33798	YES	YES
38	a	396.15	47.65546	YES	YES
39	a	402.92	0.94968	YES	YES
40	a	427.23	4.20308	YES	YES
41	a	434.70	10.69372	YES	YES
42	a	443.24	2.76032	YES	YES
43	a	465.39	3.79834	YES	YES
44	a	473.43	5.86640	YES	YES
45	a	482.87	30.20988	YES	YES
46	a	489.00	11.74662	YES	YES
47	a	492.41	1.68076	YES	YES
48	a	499.86	4.29008	YES	YES
49	a	512.37	1.88990	YES	YES
50	a	513.96	8.09141	YES	YES

12aa

SCF Energy (au) BP86/SV(P) -2585.7461640620
SCF Energy (au) PBE0/def2-TZVPP -2585.259938642
SCF Energy (au) PBE0/def2-TZVPP -2585.2803286597 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.4022033
Chemical potential (kJ mol^{-1}) 882.64
Dispersion correction (au) PBE0/def2-TZVPP -0.08241356
xyz coordinates
55

Mn	0.01290	1.68683	-0.18082
C	1.07773	2.74322	0.79788
C	-1.09994	3.03775	-0.68500
O	-1.74213	3.96679	-0.98646
O	1.79267	3.41150	1.42705
C	-1.59111	0.22040	2.19103
C	-1.50397	2.55010	2.32144
C	-2.23146	2.58549	3.51418
C	-2.67742	1.37252	4.05833
C	-2.35916	0.19301	3.38246
C	-1.26410	-1.05728	1.51843
C	-1.20652	-1.14239	0.10001
C	-0.91513	-2.39012	-0.49185
C	-0.64950	-3.52508	0.28832
C	-0.68644	-3.43345	1.68847
C	-1.00154	-2.20819	2.29265
H	-1.16130	3.49053	1.86669
H	-2.44609	3.55431	3.99084
H	-3.27457	1.34614	4.98445
H	-2.72690	-0.77506	3.75298
H	-0.91346	-2.47140	-1.59043
H	-0.41325	-4.48411	-0.20099
H	-0.46110	-4.31260	2.31324
H	-0.99016	-2.13271	3.39171
N	-1.17676	1.41198	1.66039
C	-1.38825	0.96046	-3.14558
C	-0.60847	0.99124	-4.32835
C	-1.08390	1.61089	-5.49340
C	-2.35296	2.21395	-5.50239
C	-3.14285	2.18750	-4.33784
C	-2.66843	1.56709	-3.17483
H	0.38918	0.52262	-4.32711
H	-0.45789	1.62311	-6.40068
H	-2.73005	2.70154	-6.41653
H	-4.14227	2.65288	-4.33802
H	-3.30830	1.54777	-2.27866
C	-0.85671	0.24759	-1.96547
C	-1.49886	0.03593	-0.74879
H	-2.45972	0.54556	-0.55319
C	3.27170	-1.37026	1.07850
C	3.60639	-1.57904	2.44576
C	4.62996	-2.46435	2.81037
C	5.34928	-3.16782	1.82684
C	5.03336	-2.97228	0.46974
C	4.01186	-2.08785	0.09764
H	3.04707	-1.02648	3.21777
H	4.87229	-2.60647	3.87739
H	6.15502	-3.86291	2.11619
H	5.59351	-3.51556	-0.31031

H	3.76935	-1.93376	-0.96612
C	2.23249	-0.46586	0.70116
C	1.30062	0.29302	0.37774
H	0.02981	-0.37955	-2.16589
C	1.12535	1.95316	-1.55592
O	1.89013	2.13967	-2.41503

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.01	0.00385	YES	YES
8	a	15.57	0.01558	YES	YES
9	a	20.84	0.13766	YES	YES
10	a	28.82	0.57255	YES	YES
11	a	42.77	0.09474	YES	YES
12	a	48.98	0.12729	YES	YES
13	a	51.53	0.52488	YES	YES
14	a	62.95	1.22310	YES	YES
15	a	74.97	0.67223	YES	YES
16	a	83.63	0.42445	YES	YES
17	a	90.59	1.05657	YES	YES
18	a	94.05	0.73019	YES	YES
19	a	101.70	1.50337	YES	YES
20	a	107.04	1.31684	YES	YES
21	a	107.72	0.45034	YES	YES
22	a	121.72	0.83483	YES	YES
23	a	128.27	0.13181	YES	YES
24	a	152.60	4.62867	YES	YES
25	a	162.22	0.63572	YES	YES
26	a	174.48	0.17281	YES	YES
27	a	176.69	1.87810	YES	YES
28	a	190.58	3.13033	YES	YES
29	a	217.64	0.43701	YES	YES
30	a	252.20	0.67843	YES	YES
31	a	275.65	0.17920	YES	YES
32	a	283.28	2.77329	YES	YES
33	a	298.55	0.51402	YES	YES
34	a	315.04	1.85625	YES	YES
35	a	346.58	4.69166	YES	YES
36	a	384.33	1.57518	YES	YES
37	a	391.92	6.79024	YES	YES
38	a	401.50	0.53221	YES	YES
39	a	402.85	0.00541	YES	YES
40	a	406.54	4.42489	YES	YES
41	a	444.40	2.34286	YES	YES
42	a	459.54	2.48149	YES	YES
43	a	466.74	1.77026	YES	YES
44	a	479.50	0.98956	YES	YES
45	a	486.58	3.63794	YES	YES
46	a	493.67	5.36757	YES	YES
47	a	505.44	16.01629	YES	YES
48	a	508.92	2.29273	YES	YES
49	a	510.87	0.67256	YES	YES
50	a	519.02	14.69989	YES	YES

9ab

SCF Energy (au) BP86/SV(P) -2756.5483165690
SCF Energy (au) PBE0/def2-TZVPP -2756.041057054
SCF Energy (au) PBE0/def2-TZVPP -2756.0620348227 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.4596312
Chemical potential (kJ mol^{-1}) 1030.81
Dispersion correction (au) PBE0/def2-TZVPP -0.10222235

xyz coordinates
62

Mn	0.59254	-0.86562	-0.10740
C	0.93827	-1.89298	-1.56840
C	-0.30670	-2.17854	0.69152
O	-0.76601	-3.09982	1.25103
O	1.26353	-2.57362	-2.46245
C	-2.21209	-0.49016	-1.62750
C	-1.16844	1.46191	-0.91633
C	-2.16694	2.27693	-1.45870
C	-3.24238	1.67159	-2.11933
C	-3.25607	0.27385	-2.19452
C	-2.33662	-1.97862	-1.75379
C	-3.05903	-2.70808	-0.78546
C	-3.29285	-4.08145	-0.95823
C	-2.82154	-4.73964	-2.10632
C	-2.11963	-4.01629	-3.08536
C	-1.88634	-2.64235	-2.91518
N	-1.15717	0.10479	-0.99247
C	1.99211	-1.63640	0.70015
O	2.82610	-2.27444	1.21148
C	0.30243	0.43093	1.53895
H	-0.31896	1.91074	-0.38480
H	-2.09302	3.36938	-1.34451
H	-4.05727	2.26961	-2.55936
H	-4.08081	-0.25884	-2.69241
H	-1.34286	-2.07966	-3.69095
H	-3.43367	-2.19308	0.11353
H	-1.74841	-4.52338	-3.99105
H	-3.00392	-5.81878	-2.24017
H	-3.84519	-4.64092	-0.18558
C	1.32562	1.01130	2.24373
C	-1.05461	0.80324	2.04854
C	2.77675	0.83669	2.08969
H	1.06161	1.58783	3.15727
C	5.59216	0.36960	2.03032
C	4.91030	0.41324	3.25987
C	3.53356	0.65475	3.27739
C	3.48472	0.85590	0.85078
C	4.88270	0.61295	0.84943
H	6.67285	0.15695	1.99184
H	5.45289	0.24685	4.20532
H	2.99517	0.67742	4.24000
C	2.89923	1.26592	-0.45656
H	5.41854	0.59902	-0.11422
C	2.11733	2.00120	-3.03012
C	3.20270	2.67056	-2.44707
C	3.58756	2.28955	-1.15959
N	1.79964	0.66797	-1.01003
C	1.45741	1.02848	-2.27602

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H          1.77380        2.22263       -4.05260
H          3.74323        3.46649       -2.98506
H          4.43208        2.78576       -0.65975
H          0.60569        0.48801       -2.71036
C         -3.59671        1.60865        3.09568
C         -2.63701        2.57121        2.74148
C         -1.39003        2.17303        2.23272
C         -2.04273       -0.14714        2.41202
C         -3.28518        0.24703        2.93412
H         -4.57668        1.91557        3.49769
H         -2.85820        3.64554        2.86397
H         -0.64485        2.94107        1.96373
H         -1.82087       -1.21971        2.32300
H         -4.01774       -0.52459        3.22643

$vibrational spectrum (first 50 lines)
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              11.71         0.08347      YES     YES
     8        a              21.14         0.38916      YES     YES
     9        a              23.67         0.25976      YES     YES
    10        a              40.29         0.28157      YES     YES
    11        a              42.45         0.33243      YES     YES
    12        a              54.13         0.03060      YES     YES
    13        a              56.26         0.18021      YES     YES
    14        a              66.39         0.32488      YES     YES
    15        a              74.21         0.18959      YES     YES
    16        a              80.09         0.36183      YES     YES
    17        a              89.47         0.52874      YES     YES
    18        a              99.61         0.21931      YES     YES
    19        a             107.60         1.16067      YES     YES
    20        a             113.85         0.33784      YES     YES
    21        a             118.20         0.74920      YES     YES
    22        a             128.46         0.44705      YES     YES
    23        a             130.72         1.38669      YES     YES
    24        a             135.70         0.49475      YES     YES
    25        a             140.34         0.28170      YES     YES
    26        a             160.02         0.41843      YES     YES
    27        a             173.00         0.31882      YES     YES
    28        a             184.19         0.77344      YES     YES
    29        a             185.92         0.29087      YES     YES
    30        a             199.80         1.00472      YES     YES
    31        a             205.24         0.05404      YES     YES
    32        a             234.77         0.51979      YES     YES
    33        a             246.91         0.61783      YES     YES
    34        a             284.70         0.69318      YES     YES
    35        a             303.51         0.31171      YES     YES
    36        a             307.30         0.78876      YES     YES
    37        a             309.74         0.09480      YES     YES
    38        a             334.20         0.71365      YES     YES
    39        a             354.59         0.67598      YES     YES
    40        a             370.23         1.52010      YES     YES
    41        a             400.96         0.02300      YES     YES
    42        a             406.40         0.66074      YES     YES
```

43	a	430.83	1.25681	YES	YES
44	a	440.34	0.36065	YES	YES
45	a	448.34	1.82836	YES	YES
46	a	464.10	0.12076	YES	YES
47	a	473.72	3.66405	YES	YES
48	a	484.51	0.87570	YES	YES
49	a	496.52	2.95187	YES	YES
50	a	505.35	2.87312	YES	YES

10ab

SCF Energy (au) BP86/SV(P) -2756.5345191470
SCF Energy (au) PBE0/def2-TZVPP -2756.026803533
SCF Energy (au) PBE0/def2-TZVPP -2756.0475772785 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.4576515
Chemical potential (kJ mol^{-1}) 1017.89
Dispersion correction (au) PBE0/def2-TZVPP -0.09903071

xyz coordinates
62

Mn	-0.29760	0.32681	1.78382
C	-0.89022	-0.28520	3.38949
C	0.25709	1.87117	2.42418
O	0.60843	2.91229	2.83034
O	-1.23771	-0.62603	4.44965
C	-3.15540	-0.14857	1.05670
C	-2.72731	2.11799	1.46598
C	-4.06997	2.46176	1.27934
C	-4.98833	1.44981	0.95931
C	-4.52066	0.13669	0.84529
C	-2.59935	-1.51247	0.97215
C	-1.19902	-1.66186	0.79494
C	-0.60842	-2.93759	0.75056
C	-1.40461	-4.08222	0.90699
C	-2.79282	-3.94685	1.09791
C	-3.38522	-2.67543	1.13049
N	-2.26709	0.84911	1.36647
C	1.26674	-0.49038	2.13391
O	2.18933	-1.13259	2.44758
C	0.36525	1.18952	-0.06291
H	-1.98143	2.88739	1.71027
H	-4.37778	3.51397	1.37510
H	-6.05240	1.68156	0.79108
H	-5.20847	-0.67697	0.57108
H	-4.46723	-2.59090	1.31976
H	-0.58457	-0.80362	0.36306
H	-3.42070	-4.84248	1.23381
H	-0.94416	-5.08339	0.88116
H	0.47760	-3.02765	0.58983
C	1.63219	1.24892	-0.56611
C	-0.67960	1.80751	-0.93556
C	2.93308	0.89283	0.06324
H	1.74271	1.62767	-1.60234
C	5.44525	0.38075	1.29971
C	4.64817	1.44644	1.74320
C	3.41263	1.69270	1.12621
C	3.75398	-0.18407	-0.39428
C	4.99366	-0.42095	0.24224
H	6.42290	0.17757	1.76732
H	4.98810	2.09420	2.56854
H	2.79459	2.53793	1.46673
C	3.33432	-1.09148	-1.50229
H	5.63414	-1.24186	-0.12128
C	2.58293	-2.72079	-3.62050
C	3.22363	-3.30270	-2.51474
C	3.60136	-2.48349	-1.44185
N	2.70590	-0.54277	-2.56664
C	2.34615	-1.33529	-3.58536

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H          2.26670       -3.32407       -4.48711
H          3.42119       -4.38761       -2.48320
H          4.08329       -2.91640       -0.55103
H          1.83648       -0.83478       -4.43110
C         -2.60774        3.04362       -2.63464
C         -2.47697        1.64329       -2.60496
C         -1.52954        1.03539       -1.76511
C         -0.82203        3.21674       -0.98409
C         -1.77208        3.82747       -1.82111
H         -3.35007        3.52055       -3.29617
H         -3.11344        1.01623       -3.25252
H         -1.42572       -0.06283       -1.76979
H         -0.15862        3.83747       -0.35814
H         -1.85150        4.92794       -1.84462

$vibrational spectrum (first 50 lines)
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a               9.23         0.49381      YES     YES
     8        a              15.79         0.03672      YES     YES
     9        a              25.49         0.24814      YES     YES
    10        a              30.45         0.23980      YES     YES
    11        a              38.84         0.83831      YES     YES
    12        a              41.77         0.43886      YES     YES
    13        a              48.19         0.33606      YES     YES
    14        a              55.13         0.96917      YES     YES
    15        a              58.92         0.01939      YES     YES
    16        a              67.16         0.23668      YES     YES
    17        a              76.36         0.15814      YES     YES
    18        a              80.66         0.32235      YES     YES
    19        a              88.73         1.86777      YES     YES
    20        a              96.92         1.01991      YES     YES
    21        a             103.12         0.61236      YES     YES
    22        a             110.74         1.44338      YES     YES
    23        a             113.75         0.80794      YES     YES
    24        a             120.24         0.73285      YES     YES
    25        a             123.33         0.84594      YES     YES
    26        a             141.49         0.26701      YES     YES
    27        a             164.28         0.34712      YES     YES
    28        a             172.87         1.05727      YES     YES
    29        a             176.86         0.57617      YES     YES
    30        a             195.31         1.70267      YES     YES
    31        a             218.48         0.76357      YES     YES
    32        a             224.95         0.29082      YES     YES
    33        a             225.74         0.43223      YES     YES
    34        a             271.90         0.59569      YES     YES
    35        a             272.68         0.10316      YES     YES
    36        a             305.23         0.11604      YES     YES
    37        a             338.34         1.56522      YES     YES
    38        a             342.11         1.58051      YES     YES
    39        a             369.13         1.56656      YES     YES
    40        a             399.12         0.62362      YES     YES
    41        a             401.80         0.85414      YES     YES
    42        a             405.39         5.97737      YES     YES
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43	a	417.36	4.72451	YES	YES
44	a	430.71	0.79450	YES	YES
45	a	436.91	9.36921	YES	YES
46	a	449.04	3.45482	YES	YES
47	a	468.56	2.87312	YES	YES
48	a	471.87	2.03653	YES	YES
49	a	478.97	5.45966	YES	YES
50	a	482.97	2.69789	YES	YES

11ab

SCF Energy (au) BP86/SV(P) -2756.5637604820
SCF Energy (au) PBE0/def2-TZVPP -2756.054270722
SCF Energy (au) PBE0/def2-TZVPP -2756.0741859173 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.4592741
Chemical potential (kJ mol^{-1}) 1030.75
Dispersion correction (au) PBE0/def2-TZVPP -0.10388960

xyz coordinates
62

Mn	-0.06071	-0.09079	1.92092
C	-0.77729	-0.90543	3.34687
C	0.72200	1.11916	3.02328
O	1.17662	1.83670	3.82671
O	-1.22582	-1.44202	4.27814
C	-2.87864	0.38755	1.19158
C	-1.89437	2.36157	1.99922
C	-3.08283	3.08503	1.86187
C	-4.21773	2.41660	1.37066
C	-4.10952	1.06542	1.03631
C	-2.65164	-1.02508	0.87400
C	-1.32555	-1.50188	1.09496
C	-1.06559	-2.85912	0.80480
C	-2.06554	-3.70505	0.29305
C	-3.37004	-3.21817	0.07875
C	-3.66107	-1.88149	0.37239
N	-1.77955	1.05344	1.67720
C	1.31419	-1.23571	1.99404
O	2.18069	-2.01653	2.06776
C	0.35086	0.27980	-0.36078
H	-0.99004	2.84564	2.39945
H	-3.11152	4.14841	2.14494
H	-5.17717	2.94591	1.25063
H	-4.98238	0.52107	0.64782
H	-4.68406	-1.50633	0.20548
H	0.77833	-0.69495	-0.63312
H	-4.15749	-3.88331	-0.31184
H	-1.82706	-4.75863	0.06645
H	-0.06002	-3.27953	0.97593
C	1.16612	1.18591	0.33959
C	-0.78636	0.67695	-1.22260
C	2.64599	1.14780	0.50461
H	0.76263	2.20680	0.46768
C	5.44689	1.22802	1.05604
C	4.58987	2.17982	1.63014
C	3.21930	2.13046	1.35203
C	3.53729	0.23659	-0.14379
C	4.91418	0.27952	0.17211
H	6.52812	1.23997	1.27012
H	4.98535	2.95910	2.30216
H	2.55501	2.87102	1.82509
C	3.15084	-0.70574	-1.24518
H	5.58853	-0.43091	-0.33469
C	2.59659	-2.33871	-3.40565
C	3.13947	-2.91564	-2.24711
C	3.42396	-2.08976	-1.14867
N	2.62469	-0.15125	-2.36062
C	2.35757	-0.95176	-3.40261

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H          2.35951       -2.94687       -4.29386
H          3.33723       -3.99958       -2.19541
H          3.83389       -2.50629       -0.21530
H          1.92603       -0.45800       -4.29408
C         -2.88520        1.34536       -3.02859
C         -2.46989        0.01037       -2.88626
C         -1.43751       -0.31676       -1.99488
C         -1.20930        2.01920       -1.39193
C         -2.24606        2.34792       -2.27657
H         -3.69395        1.60650       -3.73138
H         -2.95353       -0.78673       -3.47508
H         -1.12117       -1.36715       -1.88868
H         -0.70489        2.82924       -0.84276
H         -2.54825        3.40233       -2.39135

$vibrational spectrum (first 50 lines)
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              16.60         0.15339       YES     YES
     8        a              19.49         0.48021       YES     YES
     9        a              36.93         0.28771       YES     YES
    10        a              40.30         0.08635       YES     YES
    11        a              51.24         1.83370       YES     YES
    12        a              58.36         0.34018       YES     YES
    13        a              62.69         0.20910       YES     YES
    14        a              67.40         0.57340       YES     YES
    15        a              73.02         0.53680       YES     YES
    16        a              75.41         0.70260       YES     YES
    17        a              81.09         0.56041       YES     YES
    18        a              90.30         0.73744       YES     YES
    19        a              91.36         0.01049       YES     YES
    20        a              99.79         0.28472       YES     YES
    21        a             107.85         0.27191       YES     YES
    22        a             111.06         0.18373       YES     YES
    23        a             117.76         0.40036       YES     YES
    24        a             125.44         0.63618       YES     YES
    25        a             132.64         0.97723       YES     YES
    26        a             149.38         7.89428       YES     YES
    27        a             168.70         2.03588       YES     YES
    28        a             183.86         1.74960       YES     YES
    29        a             200.26         1.93949       YES     YES
    30        a             212.37         0.04339       YES     YES
    31        a             227.79         0.13559       YES     YES
    32        a             236.79         0.93852       YES     YES
    33        a             262.84         9.79322       YES     YES
    34        a             266.98         1.24644       YES     YES
    35        a             289.90         0.55201       YES     YES
    36        a             326.41        12.44131       YES     YES
    37        a             336.14         0.14601       YES     YES
    38        a             340.43         2.56365       YES     YES
    39        a             359.88         2.29554       YES     YES
    40        a             403.30         7.92755       YES     YES
    41        a             404.80         0.40726       YES     YES
    42        a             410.23         3.11681       YES     YES
```

43	a	420.04	2.54304	YES	YES
44	a	431.73	0.45480	YES	YES
45	a	452.58	7.29790	YES	YES
46	a	457.60	1.45102	YES	YES
47	a	469.03	1.40250	YES	YES
48	a	473.24	2.20641	YES	YES
49	a	490.10	4.17173	YES	YES
50	a	493.56	0.56611	YES	YES

12ab

SCF Energy (au) BP86/SV(P) -2756.5667234480
SCF Energy (au) PBE0/def2-TZVPP -2756.056934554
SCF Energy (au) PBE0/def2-TZVPP -2756.0752461204 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.4595577
Chemical potential (kJ mol^{-1}) 1031.38
Dispersion correction (au) PBE0/def2-TZVPP -0.10222821

xyz coordinates
62

Mn	-0.30337	-0.21690	1.52379
C	-0.70425	-0.60884	3.21313
C	0.32204	1.42952	1.98555
O	0.74871	2.45041	2.36981
O	-0.96268	-0.87460	4.31865
C	-3.18103	-0.66336	1.00973
C	-2.78858	1.57262	1.62068
C	-4.15088	1.88793	1.57801
C	-5.05990	0.87554	1.22823
C	-4.56879	-0.40111	0.94024
C	-2.55133	-1.96839	0.77903
C	-1.13876	-2.01998	1.00355
C	-0.52664	-3.28747	0.86598
C	-1.25370	-4.43120	0.48745
C	-2.63635	-4.34737	0.23806
C	-3.28410	-3.11576	0.39009
N	-2.30820	0.33942	1.34706
C	1.27612	-1.01261	1.82386
O	2.24908	-1.59056	2.10682
C	-0.40679	0.27546	-0.90881
H	-2.04297	2.33697	1.88412
H	-4.48205	2.90999	1.81592
H	-6.14251	1.07886	1.18319
H	-5.26110	-1.21294	0.67308
H	-4.37028	-3.05549	0.20745
H	-0.92528	-0.62626	-1.27401
H	-3.20776	-5.24133	-0.06145
H	-0.73492	-5.40086	0.38990
H	0.55310	-3.40148	1.05845
C	0.95729	0.20090	-0.64020
C	-1.14244	1.52939	-1.16569
C	1.86910	-0.89717	-1.02212
H	1.47701	1.13571	-0.38954
C	3.58933	-2.99510	-1.89556
C	2.19595	-3.13323	-2.00938
C	1.36059	-2.09676	-1.58076
C	3.29445	-0.74866	-0.92627
C	4.11839	-1.81132	-1.36777
H	4.26344	-3.80740	-2.21306
H	1.75569	-4.05216	-2.42994
H	0.27321	-2.22089	-1.68338
C	3.97973	0.47792	-0.41098
H	5.21052	-1.71579	-1.25942
C	5.28429	2.69832	0.63623
C	5.84195	2.04655	-0.47524
C	5.18426	0.93059	-1.00984
N	3.43935	1.13188	0.64283
C	4.07133	2.20310	1.14447

```
H          5.76688        3.57820        1.09139
H          6.77819        2.40993       -0.93119
H          5.58751        0.42609       -1.90151
H          3.57301        2.69531        2.00008
C         -2.61907        3.86912       -1.83925
C         -3.15051        2.59594       -2.10506
C         -2.42210        1.44465       -1.77015
C         -0.62126        2.82342       -0.90710
C         -1.35095        3.97377       -1.23715
H         -3.18656        4.77699       -2.10275
H         -4.14055        2.49681       -2.58050
H         -2.84494        0.44959       -1.98866
H          0.37055        2.93708       -0.44338
H         -0.92043        4.96698       -1.02671
```

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.20	0.39963	YES	YES
8	a	24.89	0.70672	YES	YES
9	a	36.43	0.07796	YES	YES
10	a	46.23	0.63503	YES	YES
11	a	48.87	0.05705	YES	YES
12	a	53.72	0.25864	YES	YES
13	a	56.39	0.54247	YES	YES
14	a	66.84	0.11787	YES	YES
15	a	69.14	0.46647	YES	YES
16	a	74.25	0.12704	YES	YES
17	a	80.09	0.56925	YES	YES
18	a	88.65	1.58347	YES	YES
19	a	100.29	0.25180	YES	YES
20	a	101.89	1.07502	YES	YES
21	a	107.32	0.34081	YES	YES
22	a	114.53	1.13117	YES	YES
23	a	115.48	5.82360	YES	YES
24	a	117.77	0.60404	YES	YES
25	a	130.76	0.02074	YES	YES
26	a	136.57	0.14504	YES	YES
27	a	171.21	2.12258	YES	YES
28	a	196.06	0.99612	YES	YES
29	a	201.21	0.12590	YES	YES
30	a	203.87	0.22027	YES	YES
31	a	219.60	0.71007	YES	YES
32	a	237.47	0.44406	YES	YES
33	a	262.78	1.50084	YES	YES
34	a	276.63	7.46040	YES	YES
35	a	287.39	0.27596	YES	YES
36	a	295.60	1.21941	YES	YES
37	a	313.16	0.32519	YES	YES
38	a	350.97	5.25921	YES	YES
39	a	361.39	4.09952	YES	YES
40	a	379.49	0.43029	YES	YES
41	a	403.51	0.37007	YES	YES
42	a	411.04	2.00234	YES	YES

43	a	418.14	5.08471	YES	YES
44	a	429.85	0.60281	YES	YES
45	a	450.87	1.61605	YES	YES
46	a	457.07	0.97428	YES	YES
47	a	470.61	7.53521	YES	YES
48	a	480.78	1.47564	YES	YES
49	a	485.01	0.96138	YES	YES
50	a	490.86	1.82252	YES	YES

13ab SCF Energy (au) BP86/SV(P) -2756.5794388400
SCF Energy (au) PBE0/def2-TZVPP -2756.070609560
SCF Energy (au) PBE0/def2-TZVPP -2756.0909349003 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.4594418
Chemical potential (kJ mol^{-1}) 1025.29
Dispersion correction (au) PBE0/def2-TZVPP -0.09864428

xyz coordinates
62

Mn	1.78256	-2.27044	1.42220
C	3.02410	-3.52670	0.97608
O	3.80638	-4.36868	0.74670
N	3.09990	-0.64173	1.44938
C	4.70776	1.65978	1.51364
C	5.29014	0.38806	1.36710
C	4.44510	-0.72620	1.33846
C	2.52016	0.58658	1.64504
C	3.32104	1.75378	1.65591
H	5.33213	2.56814	1.52919
H	6.37903	0.25365	1.27670
H	4.85875	-1.74148	1.22526
H	2.84540	2.73591	1.79300
N	1.48206	-1.76961	-0.73342
C	2.08455	-2.44151	3.16700
O	2.27201	-2.54240	4.31512
C	0.51984	-3.51743	1.61493
O	-0.26446	-4.34701	1.87403
C	0.48764	-0.75769	1.89826
C	-1.03718	1.59481	2.52073
C	-1.62934	0.31772	2.56788
C	-0.87702	-0.82981	2.26150
C	1.07517	0.54665	1.89010
C	0.31641	1.70722	2.18407
H	-1.62741	2.49521	2.75609
H	-2.69201	0.21661	2.84794
H	-1.38098	-1.80951	2.30956
H	0.78493	2.70598	2.17136
C	1.57752	-0.50376	-3.27545
C	0.36244	-0.84456	-2.67568
C	0.33046	-1.50210	-1.42176
C	2.65247	-1.48464	-1.36024
C	2.75679	-0.86369	-2.60802
H	1.60164	0.00006	-4.25558
H	-0.59289	-0.64165	-3.18266
C	-0.99415	-2.02686	-0.97602
H	3.56614	-1.77243	-0.82409
H	3.75258	-0.66938	-3.03589
C	-3.53050	-3.18436	-0.53026
C	-2.40219	-4.00930	-0.67574
C	-1.14689	-3.42656	-0.89852
C	-2.13978	-1.17992	-0.85128
C	-3.39535	-1.79288	-0.61464
H	-4.52158	-3.62782	-0.33835
H	-2.49504	-5.10504	-0.60878
H	-0.26226	-4.06709	-1.03916
C	-2.01119	0.28174	-0.94324
H	-4.27907	-1.15323	-0.45934
C	-2.99612	1.13628	-1.34383

H	-1.02274	0.69146	-0.67082
C	-2.91952	2.59882	-1.43475
H	-3.96051	0.70542	-1.67184
C	-2.86363	5.43308	-1.68574
C	-3.96950	4.70405	-2.15526
C	-3.99559	3.30739	-2.02908
C	-1.81564	3.35403	-0.95798
C	-1.78951	4.74868	-1.08502
H	-2.83945	6.53122	-1.78113
H	-4.81990	5.22764	-2.62318
H	-4.86764	2.74186	-2.40048
H	-0.97430	2.84025	-0.46543
H	-0.92177	5.31340	-0.70458

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.20	0.38896	YES	YES
8	a	17.37	0.28400	YES	YES
9	a	26.63	0.13389	YES	YES
10	a	28.99	0.13648	YES	YES
11	a	43.34	0.18544	YES	YES
12	a	49.15	0.27759	YES	YES
13	a	53.30	0.10833	YES	YES
14	a	57.92	0.51089	YES	YES
15	a	68.54	0.26487	YES	YES
16	a	74.81	0.17847	YES	YES
17	a	83.98	0.79056	YES	YES
18	a	88.17	0.09100	YES	YES
19	a	93.28	0.14313	YES	YES
20	a	95.95	1.04244	YES	YES
21	a	102.61	0.03664	YES	YES
22	a	107.89	0.33318	YES	YES
23	a	121.05	0.47973	YES	YES
24	a	125.73	0.90682	YES	YES
25	a	131.24	0.26652	YES	YES
26	a	151.19	0.92143	YES	YES
27	a	165.82	0.06516	YES	YES
28	a	186.90	0.15496	YES	YES
29	a	195.91	0.75625	YES	YES
30	a	209.77	0.49721	YES	YES
31	a	224.43	2.24810	YES	YES
32	a	235.22	0.28708	YES	YES
33	a	248.64	0.75774	YES	YES
34	a	259.02	0.18242	YES	YES
35	a	264.87	0.03646	YES	YES
36	a	285.08	0.09297	YES	YES
37	a	311.41	0.29328	YES	YES
38	a	343.14	0.23724	YES	YES
39	a	359.75	2.13139	YES	YES
40	a	369.58	0.15044	YES	YES
41	a	402.26	0.24490	YES	YES
42	a	414.19	5.87883	YES	YES
43	a	430.19	0.79806	YES	YES

44	a	433.95	0.77502	YES	YES
45	a	450.70	0.20418	YES	YES
46	a	455.64	1.61610	YES	YES
47	a	456.99	1.89089	YES	YES
48	a	481.56	0.82749	YES	YES
49	a	486.46	1.65996	YES	YES
50	a	493.29	0.96071	YES	YES

9ac SCF Energy (au) BP86/SV(P) -2353.9080695410
SCF Energy (au) PBE0/def2-TZVPP -2353.491408085
SCF Energy (au) PBE0/def2-TZVPP -2353.5093718975 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.3164094
Chemical potential (kJ mol^{-1}) 680.05
Dispersion correction (au) PBE0/def2-TZVPP -0.06898599

xyz coordinates
44

Mn	1.21529	-0.06531	1.43360
C	1.29900	-0.28786	3.24924
C	2.94387	-0.48575	1.28371
C	1.66861	1.64237	1.53791
O	1.99150	2.76413	1.61870
O	4.07355	-0.78280	1.23193
O	1.37634	-0.39068	4.40889
C	-1.92846	-0.32165	1.02378
C	-1.19826	1.47360	2.31701
C	-2.49413	1.95441	2.51533
C	-3.56307	1.26299	1.92824
C	-3.26667	0.11845	1.18480
C	-1.73838	-1.56758	0.22479
C	-0.91324	-1.62775	-0.94688
C	-1.04579	-2.77444	-1.77746
C	-1.86726	-3.85656	-1.44082
C	-2.61328	-3.82402	-0.24819
C	-2.55968	-2.67683	0.55602
H	-0.35030	2.00220	2.77337
H	-2.64724	2.86076	3.12124
H	-4.60317	1.61005	2.04004
H	-4.06766	-0.44745	0.68604
H	-3.17243	-2.62820	1.47190
N	-0.89149	0.36910	1.58413
C	1.67915	1.17572	-1.40353
C	3.09325	1.21701	-1.48310
C	3.75003	2.18793	-2.25449
C	3.01590	3.16564	-2.94920
C	1.61323	3.15087	-2.87430
C	0.95620	2.16481	-2.12059
H	3.69071	0.46222	-0.95030
H	4.85179	2.18232	-2.30906
H	3.53569	3.93687	-3.54171
H	1.02173	3.91385	-3.40852
H	-0.14528	2.16153	-2.06322
C	0.93326	0.15060	-0.61654
C	0.03528	-0.58206	-1.36018
H	0.07918	-0.46620	-2.46520
O	0.87664	-2.18476	1.22554
H	-0.45249	-2.80782	-2.70682
H	-1.91787	-4.73537	-2.10470
H	-3.24592	-4.67689	0.04564
H	1.06898	-2.33970	0.26936
H	-0.08711	-2.39775	1.29360

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.60	3.39747	YES	YES
8	a	29.01	4.05320	YES	YES
9	a	43.97	12.93097	YES	YES
10	a	53.83	0.04405	YES	YES
11	a	55.31	1.69774	YES	YES
12	a	68.83	0.42125	YES	YES
13	a	71.69	3.16007	YES	YES
14	a	84.28	2.42924	YES	YES
15	a	98.56	0.22422	YES	YES
16	a	102.00	0.34825	YES	YES
17	a	104.71	0.60598	YES	YES
18	a	119.09	1.26170	YES	YES
19	a	124.82	1.26975	YES	YES
20	a	140.24	3.18645	YES	YES
21	a	154.46	1.23581	YES	YES
22	a	178.38	1.53876	YES	YES
23	a	181.91	0.60159	YES	YES
24	a	196.52	0.71421	YES	YES
25	a	219.73	1.91893	YES	YES
26	a	232.37	2.19541	YES	YES
27	a	252.75	2.34834	YES	YES
28	a	288.92	1.17415	YES	YES
29	a	299.73	1.45735	YES	YES
30	a	330.78	7.49843	YES	YES
31	a	346.37	3.24849	YES	YES
32	a	368.69	3.25924	YES	YES
33	a	402.16	0.99844	YES	YES
34	a	426.50	1.74948	YES	YES
35	a	441.97	3.83338	YES	YES
36	a	460.90	3.94412	YES	YES
37	a	469.00	0.98072	YES	YES
38	a	489.47	8.47252	YES	YES
39	a	494.89	4.97530	YES	YES
40	a	497.33	7.33793	YES	YES
41	a	507.94	9.43828	YES	YES
42	a	530.95	10.39302	YES	YES
43	a	538.45	3.59239	YES	YES
44	a	549.87	4.10504	YES	YES
45	a	557.20	0.09607	YES	YES
46	a	559.15	3.83434	YES	YES
47	a	575.22	3.35883	YES	YES
48	a	604.79	28.64783	YES	YES
49	a	615.18	12.55702	YES	YES
50	a	622.97	0.97583	YES	YES

12ac

SCF Energy (au) BP86/SV(P) -2353.9227332610
SCF Energy (au) PBE0/def2-TZVPP -2353.501508738
SCF Energy (au) PBE0/def2-TZVPP -2353.5239608610 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.3164092
Chemical potential (kJ mol^{-1}) 672.27
Dispersion correction (au) PBE0/def2-TZVPP -0.06423512

xyz coordinates
44

Mn	-0.09666	-1.49987	1.87240
C	-0.08087	-1.72862	3.61343
C	1.08424	-2.83594	1.66631
C	1.24364	-0.29927	1.99314
O	2.09126	0.50560	2.05543
O	1.86426	-3.68631	1.51853
O	-0.14332	-1.94536	4.76455
C	-2.21701	0.57647	0.73539
C	-1.50620	0.93988	2.93006
C	-2.27961	2.09658	3.06194
C	-3.05116	2.51667	1.96875
C	-3.01237	1.74470	0.80330
C	-2.28726	-0.23080	-0.52411
C	-1.16740	-0.44085	-1.38670
C	-1.37917	-1.20828	-2.55917
C	-2.62956	-1.75051	-2.87743
C	-3.73156	-1.51439	-2.03847
C	-3.55513	-0.74663	-0.87868
H	-0.89225	0.59060	3.77274
H	-2.26624	2.65160	4.01267
H	-3.66879	3.42810	2.02108
H	-3.59037	2.03547	-0.08722
H	-4.41221	-0.56380	-0.20859
N	-1.45831	0.17952	1.80468
C	2.64471	0.38229	-1.48618
C	3.78920	-0.31798	-1.94832
C	5.07172	0.24034	-1.85453
C	5.24222	1.52041	-1.30028
C	4.11776	2.23417	-0.84334
C	2.83769	1.67550	-0.93503
H	3.66161	-1.32440	-2.38249
H	5.94452	-0.32758	-2.21707
H	6.24867	1.96444	-1.22580
H	4.24281	3.24050	-0.41046
H	1.97129	2.25508	-0.57926
C	1.33043	-0.25110	-1.62170
C	0.13775	0.17220	-1.10680
H	0.12513	1.06403	-0.45495
O	-1.35283	-2.51826	0.99931
H	-0.54161	-1.35110	-3.26007
H	-2.74946	-2.34262	-3.79958
H	-4.72502	-1.92195	-2.28569
H	1.33666	-1.18970	-2.20596
H	-2.19122	-2.01882	0.88419

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.46	0.36002	YES	YES
8	a	23.72	0.16481	YES	YES
9	a	34.86	0.15531	YES	YES
10	a	39.81	0.22353	YES	YES
11	a	44.37	0.14638	YES	YES
12	a	49.86	0.32824	YES	YES
13	a	69.40	0.50383	YES	YES
14	a	73.71	0.36313	YES	YES
15	a	83.22	0.58282	YES	YES
16	a	89.28	0.26094	YES	YES
17	a	94.23	0.18275	YES	YES
18	a	99.56	1.08011	YES	YES
19	a	116.72	0.18958	YES	YES
20	a	123.52	0.27379	YES	YES
21	a	143.66	1.21305	YES	YES
22	a	155.96	0.89083	YES	YES
23	a	172.33	1.16968	YES	YES
24	a	183.89	0.33394	YES	YES
25	a	220.48	1.17237	YES	YES
26	a	243.89	0.17746	YES	YES
27	a	249.26	2.05215	YES	YES
28	a	271.38	0.37234	YES	YES
29	a	308.26	1.43123	YES	YES
30	a	342.12	0.32987	YES	YES
31	a	358.44	0.29734	YES	YES
32	a	402.27	0.04352	YES	YES
33	a	410.40	12.05107	YES	YES
34	a	429.32	0.18855	YES	YES
35	a	448.11	0.13352	YES	YES
36	a	459.46	1.64603	YES	YES
37	a	477.11	15.12820	YES	YES
38	a	482.73	3.46338	YES	YES
39	a	487.72	0.45018	YES	YES
40	a	505.74	51.02190	YES	YES
41	a	517.06	44.01398	YES	YES
42	a	528.05	12.40923	YES	YES
43	a	530.01	10.45242	YES	YES
44	a	544.00	28.86367	YES	YES
45	a	547.11	9.42416	YES	YES
46	a	557.49	2.24012	YES	YES
47	a	597.46	43.88134	YES	YES
48	a	612.02	0.09426	YES	YES
49	a	620.14	1.10454	YES	YES
50	a	624.83	0.65600	YES	YES

TS_{8a-6a}

SCF Energy (au) BP86/SV(P) -2277.5084109160
SCF Energy (au) PBE0/def2-TZVPP -2277.059171549
SCF Energy (au) PBE0/def2-TZVPP -2277.0724955365 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.2894069
Chemical potential (kJ mol^{-1}) 617.36
Dispersion correction (au) PBE0/def2-TZVPP -0.06065131

xyz coordinates
41

Mn	1.54771	0.37033	0.77601
C	1.90922	0.62895	2.52872
C	3.24140	-0.11505	0.46337
C	1.95376	2.07699	0.34740
O	2.25077	3.17945	0.09864
O	4.34482	-0.44157	0.26518
O	2.13108	0.78743	3.66028
C	-1.25257	-0.25182	1.59649
C	-1.09401	1.97436	0.86730
C	-2.45843	2.20000	1.06765
C	-3.25128	1.13811	1.54032
C	-2.64471	-0.09211	1.79905
C	-0.50252	-1.47892	1.85703
C	0.85104	-1.50084	1.39103
C	1.63475	-2.64377	1.70773
C	1.10095	-3.71846	2.42376
C	-0.24841	-3.70067	2.84500
C	-1.04014	-2.58582	2.56068
H	-0.44310	2.77510	0.48495
H	-2.88633	3.19025	0.84886
H	-4.33388	1.27053	1.70011
H	-3.24405	-0.94267	2.15554
H	2.68380	-2.69141	1.36963
H	1.74052	-4.58496	2.66285
H	-0.66924	-4.55134	3.40486
H	-2.08268	-2.56067	2.91786
N	-0.49743	0.78851	1.12252
C	0.34801	0.66034	-2.37847
C	0.95629	1.84675	-2.86602
C	0.54552	2.41442	-4.08065
C	-0.49223	1.83066	-4.82884
C	-1.11497	0.66209	-4.35225
C	-0.70219	0.08143	-3.14640
H	1.76593	2.31854	-2.29063
H	1.04080	3.32980	-4.44524
H	-0.81766	2.28588	-5.77877
H	-1.93161	0.19565	-4.92854
H	-1.19149	-0.83284	-2.77347
C	0.75854	0.00615	-1.15816
C	0.94124	-1.13956	-0.58432
H	1.15278	-2.17924	-0.85105

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-229.92	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	17.41	0.06220	YES	YES
9	a	25.16	0.19062	YES	YES
10	a	45.64	0.05440	YES	YES
11	a	58.62	0.10755	YES	YES
12	a	71.56	0.08061	YES	YES
13	a	82.91	0.01235	YES	YES
14	a	89.59	0.27702	YES	YES
15	a	92.91	1.10365	YES	YES
16	a	100.44	0.45908	YES	YES
17	a	110.09	0.06448	YES	YES
18	a	116.49	0.03755	YES	YES
19	a	132.59	0.36059	YES	YES
20	a	162.30	1.18698	YES	YES
21	a	181.99	0.55163	YES	YES
22	a	187.34	0.53494	YES	YES
23	a	217.21	0.99851	YES	YES
24	a	233.62	0.81122	YES	YES
25	a	259.66	0.64011	YES	YES
26	a	278.88	0.12099	YES	YES
27	a	343.64	8.47045	YES	YES
28	a	359.48	1.38284	YES	YES
29	a	385.75	2.26724	YES	YES
30	a	402.48	0.07176	YES	YES
31	a	415.90	3.19141	YES	YES
32	a	430.60	1.17126	YES	YES
33	a	447.49	0.40574	YES	YES
34	a	453.68	8.55989	YES	YES
35	a	463.23	5.74678	YES	YES
36	a	474.04	0.97570	YES	YES
37	a	488.66	0.39341	YES	YES
38	a	496.54	7.45279	YES	YES
39	a	503.72	5.28052	YES	YES
40	a	523.08	0.38776	YES	YES
41	a	544.07	14.03546	YES	YES
42	a	546.45	13.87922	YES	YES
43	a	553.17	0.60215	YES	YES
44	a	583.23	24.53609	YES	YES
45	a	610.37	10.84840	YES	YES
46	a	614.29	13.13794	YES	YES
47	a	620.34	1.05032	YES	YES
48	a	625.79	33.77338	YES	YES
49	a	639.14	0.32541	YES	YES
50	a	656.22	9.58836	YES	YES

$TS_{8a-7a'}$

SCF Energy (au) BP86/SV(P) -2277.5152698420
SCF Energy (au) PBE0/def2-TZVPP -2277.063594120
SCF Energy (au) PBE0/def2-TZVPP -2277.0766276445 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.2901506
Chemical potential (kJ mol^{-1}) 622.05
Dispersion correction (au) PBE0/def2-TZVPP -0.06117935

xyz coordinates
41

C	2.13062	-0.13639	2.64741
C	-0.01201	1.08548	2.88500
C	0.55785	0.73144	0.05408
C	-0.06920	-1.57224	2.91070
C	1.17578	-1.70836	0.11918
C	2.28150	-2.63539	0.26517
C	0.90983	-4.47087	-0.57712
C	-0.17989	-3.62644	-0.72307
H	-1.14108	-4.03308	-1.07719
C	-0.10668	-2.25495	-0.33982
C	-1.20261	-1.35462	-0.36593
C	-2.40481	-1.51193	-1.11198
H	-2.49419	-2.37574	-1.78917
C	-3.44192	-0.60392	-0.98755
H	-4.37160	-0.72501	-1.56518
C	-3.27636	0.50507	-0.09916
H	-4.08999	1.22910	0.06327
C	-2.08589	0.68241	0.56272
H	-1.90627	1.54603	1.21910
Mn	0.54097	-0.23865	1.83350
N	-1.00989	-0.19505	0.42834
O	3.18378	-0.08842	3.15322
O	-0.35081	1.94662	3.60353
C	1.47758	-0.29365	-0.11618
O	-0.50274	-2.40464	3.59996
C	2.14755	-3.96836	-0.05890
H	2.51725	-0.03088	-0.37784
C	0.50683	2.05634	-0.54851
C	0.36846	4.60026	-1.79227
C	0.35517	4.49677	-0.38863
C	0.41156	3.23909	0.22815
C	0.51880	2.17685	-1.96587
C	0.44619	3.43510	-2.57804
H	0.31543	5.59038	-2.27458
H	0.30329	5.40566	0.23168
H	0.40172	3.16320	1.32618
H	0.57822	1.26347	-2.57953
H	0.45213	3.50999	-3.67791
H	0.81846	-5.53758	-0.83767
H	3.00135	-4.65341	0.07150
H	3.24563	-2.24366	0.62945

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-375.68	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	24.73	0.07562	YES	YES
9	a	39.04	0.01211	YES	YES
10	a	49.50	0.08305	YES	YES
11	a	56.39	0.42235	YES	YES
12	a	64.74	0.04942	YES	YES
13	a	78.81	0.26565	YES	YES
14	a	87.66	0.01769	YES	YES
15	a	94.35	0.64672	YES	YES
16	a	100.92	1.80641	YES	YES
17	a	108.27	0.03835	YES	YES
18	a	123.20	1.45140	YES	YES
19	a	138.31	1.93404	YES	YES
20	a	152.49	1.42015	YES	YES
21	a	189.87	1.47018	YES	YES
22	a	212.44	2.83311	YES	YES
23	a	228.73	0.09515	YES	YES
24	a	254.23	0.39767	YES	YES
25	a	267.59	1.01387	YES	YES
26	a	292.14	2.24154	YES	YES
27	a	364.19	6.19346	YES	YES
28	a	374.72	0.17344	YES	YES
29	a	402.92	0.33476	YES	YES
30	a	413.71	5.16361	YES	YES
31	a	418.27	2.47638	YES	YES
32	a	436.42	2.34749	YES	YES
33	a	459.64	1.11727	YES	YES
34	a	467.63	3.99259	YES	YES
35	a	479.17	3.23969	YES	YES
36	a	485.07	1.46773	YES	YES
37	a	488.11	3.60391	YES	YES
38	a	517.21	6.91137	YES	YES
39	a	526.75	1.86171	YES	YES
40	a	537.20	20.33485	YES	YES
41	a	545.51	2.46971	YES	YES
42	a	548.80	10.02944	YES	YES
43	a	569.56	3.71402	YES	YES
44	a	601.09	18.49537	YES	YES
45	a	605.97	7.56066	YES	YES
46	a	617.33	17.18411	YES	YES
47	a	627.79	3.96100	YES	YES
48	a	632.90	11.10528	YES	YES
49	a	648.27	21.55982	YES	YES
50	a	677.61	8.97962	YES	YES

$TS_{10aa-12aa}$

SCF Energy (au) BP86/SV(P) -2585.6969763850
SCF Energy (au) PBE0/def2-TZVPP -2585.208683995
SCF Energy (au) PBE0/def2-TZVPP -2585.226247436 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.3967098
Chemical potential (kJ mol^{-1}) 871.84
Dispersion correction (au) PBE0/def2-TZVPP -0.08313758
xyz coordinates
55

Mn	0.16710	1.92451	-0.18383
C	1.19924	2.88928	0.94856
C	-0.86580	3.30158	-0.74661
O	-1.48952	4.20367	-1.14190
O	1.88844	3.47104	1.68370
C	-1.64071	0.45829	2.07144
C	-1.65156	2.78578	2.04951
C	-2.53345	2.87482	3.12716
C	-3.00933	1.68679	3.69785
C	-2.55371	0.48305	3.16015
C	-1.22362	-0.90306	1.62627
C	-1.41377	-1.40056	0.30574
C	-1.28765	-2.79843	0.09329
C	-0.90426	-3.67517	1.11268
C	-0.65000	-3.16937	2.40063
C	-0.83121	-1.80386	2.64812
H	-1.27237	3.71018	1.59385
H	-2.83768	3.86612	3.49717
H	-3.72372	1.69625	4.53721
H	-2.91665	-0.47619	3.55753
H	-1.47420	-3.18953	-0.92100
H	-0.79674	-4.75205	0.90250
H	-0.33124	-3.83998	3.21538
H	-0.65878	-1.41134	3.66358
N	-1.20456	1.62078	1.50478
C	-1.40067	1.00756	-2.69710
C	-0.45921	0.92041	-3.75020
C	-0.79978	1.31271	-5.05401
C	-2.08497	1.80891	-5.33539
C	-3.02952	1.90133	-4.29960
C	-2.69258	1.50240	-2.99565
H	0.54834	0.52241	-3.54748
H	-0.05099	1.22704	-5.85923
H	-2.34819	2.12353	-6.35884
H	-4.04125	2.28967	-4.50582
H	-3.43633	1.58270	-2.18542
C	-1.07881	0.54467	-1.31773
C	-1.71400	-0.58701	-0.88549
H	-2.40244	-1.07948	-1.60409
C	3.28887	-1.44826	0.63280
C	3.09019	-2.61625	1.41833
C	4.14238	-3.51524	1.63729
C	5.41309	-3.27279	1.08439
C	5.62489	-2.12064	0.30527
C	4.57823	-1.21745	0.07800
H	2.09282	-2.80316	1.84623
H	3.97040	-4.41770	2.24773
H	6.23857	-3.98249	1.26030
H	6.61842	-1.92456	-0.13136

H	4.74175	-0.31521	-0.53251
C	2.22826	-0.52204	0.40131
C	1.31559	0.30239	0.21237
H	0.26400	0.28858	-0.64737
C	1.31042	2.31808	-1.50290
O	2.08825	2.61727	-2.31760

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-818.71	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	18.30	0.19721	YES	YES
9	a	21.28	0.01915	YES	YES
10	a	26.40	0.75626	YES	YES
11	a	33.40	0.19587	YES	YES
12	a	42.15	0.09230	YES	YES
13	a	50.64	0.08912	YES	YES
14	a	57.19	0.13653	YES	YES
15	a	67.34	0.68076	YES	YES
16	a	75.41	0.20046	YES	YES
17	a	84.28	0.13377	YES	YES
18	a	91.22	0.17735	YES	YES
19	a	97.03	0.68962	YES	YES
20	a	101.39	0.27732	YES	YES
21	a	106.48	0.31659	YES	YES
22	a	115.84	1.61207	YES	YES
23	a	117.76	0.45182	YES	YES
24	a	126.50	0.19292	YES	YES
25	a	144.88	0.28042	YES	YES
26	a	168.61	0.87078	YES	YES
27	a	187.86	7.01953	YES	YES
28	a	190.45	4.95554	YES	YES
29	a	216.18	1.64198	YES	YES
30	a	218.75	0.32496	YES	YES
31	a	244.43	0.22518	YES	YES
32	a	266.79	8.56109	YES	YES
33	a	282.94	0.69383	YES	YES
34	a	302.88	10.82200	YES	YES
35	a	321.54	0.78416	YES	YES
36	a	359.86	12.20792	YES	YES
37	a	371.06	8.14164	YES	YES
38	a	400.89	0.86041	YES	YES
39	a	402.33	0.27258	YES	YES
40	a	404.56	5.61992	YES	YES
41	a	437.79	5.59958	YES	YES
42	a	446.77	1.14749	YES	YES
43	a	470.12	3.85869	YES	YES
44	a	476.75	6.23337	YES	YES
45	a	480.72	2.71564	YES	YES
46	a	489.31	4.01073	YES	YES
47	a	493.95	3.24537	YES	YES
48	a	508.99	0.94088	YES	YES
49	a	516.54	7.40170	YES	YES
50	a	520.12	4.68768	YES	YES

$TS_{10ab-11ab}$

SCF Energy (au) BP86/SV(P) -2756.5226020510
SCF Energy (au) PBE0/def2-TZVPP -2756.011798844
SCF Energy (au) PBE0/def2-TZVPP -2756.0305548883 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.4538519
Chemical potential (kJ mol^{-1}) 1009.71
Dispersion correction (au) PBE0/def2-TZVPP -0.10059645

xyz coordinates
62

Mn	-0.29543	0.00814	1.94767
C	-0.93746	-0.84032	3.40235
C	0.41233	1.37468	2.87560
O	0.85337	2.26415	3.49457
O	-1.35984	-1.40260	4.33202
C	-3.10572	0.18049	1.06343
C	-2.48565	2.10293	2.25764
C	-3.76583	2.65334	2.15347
C	-4.75268	1.93024	1.46335
C	-4.41474	0.69020	0.91533
C	-2.65293	-1.11942	0.54684
C	-1.25974	-1.41033	0.67707
C	-0.78825	-2.65215	0.19827
C	-1.66437	-3.59406	-0.36606
C	-3.03797	-3.30469	-0.47303
C	-3.52816	-2.07294	-0.01951
N	-2.15169	0.90187	1.73335
C	1.19764	-0.97795	2.11799
O	2.10053	-1.69594	2.30003
C	0.28033	0.93258	-0.02715
H	-1.68658	2.64396	2.78611
H	-3.97434	3.63614	2.60376
H	-5.77267	2.33190	1.34957
H	-5.16506	0.10880	0.36053
H	-4.60747	-1.86481	-0.09744
H	-0.35871	-0.38765	0.33111
H	-3.73045	-4.04267	-0.91048
H	-1.27501	-4.56149	-0.72455
H	0.28734	-2.88563	0.26352
C	1.56383	1.09103	-0.45692
C	-0.77626	1.56682	-0.87875
C	2.85718	0.76405	0.20774
H	1.69418	1.63672	-1.41392
C	5.36863	0.41967	1.49593
C	4.50594	1.44723	1.90560
C	3.27066	1.61069	1.26127
C	3.74065	-0.27385	-0.21422
C	4.98116	-0.42613	0.44818
H	6.34842	0.28238	1.98227
H	4.79166	2.12993	2.72289
H	2.60304	2.42928	1.56945
C	3.39286	-1.20506	-1.32453
H	5.67690	-1.21134	0.11064
C	2.77768	-2.85025	-3.47236
C	3.52153	-3.38041	-2.40559
C	3.82919	-2.55435	-1.31653
N	2.65794	-0.71016	-2.34583
C	2.36414	-1.50970	-3.38012

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H          2.51464       -3.46153       -4.35091
H          3.85352       -4.43222       -2.41587
H          4.38442       -2.95417       -0.45404
H          1.76229       -1.05363       -4.18919
C         -2.69971        2.81647       -2.56227
C         -2.41014        1.44939       -2.70968
C         -1.46245        0.83151       -1.87597
C         -1.07856        2.94321       -0.74619
C         -2.02629        3.56188       -1.57809
H         -3.44094        3.30279       -3.21831
H         -2.91935        0.85676       -3.48860
H         -1.22679       -0.23587       -2.01740
H         -0.54517        3.53326        0.01762
H         -2.23560        4.63883       -1.46164

$vibrational spectrum (first 50 lines)
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1        a             -949.44         0.00000       YES     YES
     2                         0.00         0.00000         -       -
     3                         0.00         0.00000         -       -
     4                         0.00         0.00000         -       -
     5                         0.00         0.00000         -       -
     6                         0.00         0.00000         -       -
     7                         0.00         0.00000         -       -
     8        a                7.64         0.65295       YES     YES
     9        a               13.15         0.10592       YES     YES
    10        a               26.93         0.23165       YES     YES
    11        a               31.53         1.20591       YES     YES
    12        a               37.72         0.69751       YES     YES
    13        a               44.40         0.20482       YES     YES
    14        a               53.61         0.58940       YES     YES
    15        a               59.64         0.17213       YES     YES
    16        a               62.79         0.09790       YES     YES
    17        a               69.15         0.30552       YES     YES
    18        a               73.52         0.38082       YES     YES
    19        a               82.85         0.08291       YES     YES
    20        a               90.89         2.09571       YES     YES
    21        a               95.08         0.46816       YES     YES
    22        a              105.19         0.03953       YES     YES
    23        a              116.34         0.35562       YES     YES
    24        a              118.28         0.86927       YES     YES
    25        a              121.67         0.64390       YES     YES
    26        a              129.83         0.35348       YES     YES
    27        a              163.95         1.32535       YES     YES
    28        a              179.59         0.12722       YES     YES
    29        a              188.67         1.96370       YES     YES
    30        a              194.65         0.46353       YES     YES
    31        a              210.89         0.32865       YES     YES
    32        a              225.40         0.51077       YES     YES
    33        a              233.07         1.26121       YES     YES
    34        a              265.09         1.29702       YES     YES
    35        a              270.25         0.63942       YES     YES
    36        a              279.33         0.33896       YES     YES
    37        a              307.89         0.26142       YES     YES
    38        a              355.27         1.30954       YES     YES
    39        a              360.09         1.09378       YES     YES
    40        a              368.14         0.38854       YES     YES
    41        a              404.22         0.13154       YES     YES
    42        a              404.71         7.46588       YES     YES
```

43	a	416.02	2.68073	YES	YES
44	a	429.44	0.75542	YES	YES
45	a	434.06	5.30971	YES	YES
46	a	454.14	1.65645	YES	YES
47	a	457.95	1.47259	YES	YES
48	a	471.27	1.85618	YES	YES
49	a	480.42	0.90037	YES	YES
50	a	489.36	2.18628	YES	YES

$TS_{9ac\text{-}12ac}$

SCF Energy (au) BP86/SV(P) -2353.8814385400
SCF Energy (au) PBE0/def2-TZVPP -2353.459711057
SCF Energy (au) PBE0/def2-TZVPP -2353.4788473423 (CH_2Cl_2 Correction)
Zero Point Energy (au) 0.3122974
Chemical potential (kJ mol^{-1}) 674.38
Dispersion correction (au) PBE0/def2-TZVPP -0.06460211

xyz coordinates
44

Mn	1.11232	-0.12097	1.49861
C	1.09574	-0.47172	3.25802
C	2.86619	-0.48373	1.50690
C	1.49056	1.61941	1.69441
O	1.76567	2.74885	1.81981
O	4.00144	-0.73285	1.57999
O	1.07516	-0.73146	4.39509
C	-2.08265	-0.30356	1.01857
C	-1.32502	1.28107	2.54516
C	-2.61525	1.70646	2.86458
C	-3.69945	1.09381	2.22173
C	-3.41880	0.08642	1.29752
C	-1.94183	-1.38959	0.00123
C	-1.25158	-1.22035	-1.23526
C	-1.48715	-2.16311	-2.26715
C	-2.28609	-3.29529	-2.06969
C	-2.89709	-3.50458	-0.82114
C	-2.74529	-2.54329	0.18634
H	-0.46735	1.74965	3.04535
H	-2.75190	2.50832	3.60650
H	-4.73849	1.39907	2.42665
H	-4.23232	-0.40654	0.74492
H	-3.26224	-2.68168	1.15059
N	-1.03168	0.30271	1.64376
C	1.91512	0.95431	-1.32893
C	3.24506	0.50368	-1.51585
C	4.20835	1.33182	-2.11170
C	3.87269	2.63497	-2.52097
C	2.55931	3.09927	-2.33577
C	1.59141	2.26683	-1.75104
H	3.52095	-0.51731	-1.20708
H	5.23440	0.95416	-2.25601
H	4.63466	3.28797	-2.97782
H	2.28476	4.12194	-2.64466
H	0.56542	2.64122	-1.59573
C	0.87227	0.06506	-0.75246
C	-0.24761	-0.17352	-1.50957
H	-0.29889	0.26598	-2.52756
O	0.86923	-2.05719	0.85960
H	-0.98540	-2.01096	-3.23754
H	-2.42067	-4.02367	-2.88617
H	-3.50800	-4.40331	-0.63798
H	0.99394	-1.07789	-0.08255
H	-0.07990	-2.31041	0.90730

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-895.81	0.00000	YES	YES

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	24.26	0.60203	YES	YES
9	a	43.38	0.12015	YES	YES
10	a	49.58	0.12610	YES	YES
11	a	53.32	0.15978	YES	YES
12	a	66.01	0.62205	YES	YES
13	a	71.93	0.34420	YES	YES
14	a	81.19	0.06548	YES	YES
15	a	94.60	0.42666	YES	YES
16	a	100.07	0.26267	YES	YES
17	a	105.48	0.10661	YES	YES
18	a	114.10	0.90737	YES	YES
19	a	114.80	0.21290	YES	YES
20	a	137.82	0.02505	YES	YES
21	a	150.37	1.22588	YES	YES
22	a	169.27	0.28205	YES	YES
23	a	187.93	0.04500	YES	YES
24	a	195.72	4.70464	YES	YES
25	a	205.29	1.10379	YES	YES
26	a	243.66	0.46406	YES	YES
27	a	276.72	0.42970	YES	YES
28	a	293.38	0.41756	YES	YES
29	a	321.11	3.33132	YES	YES
30	a	359.46	1.71273	YES	YES
31	a	378.60	17.56262	YES	YES
32	a	403.82	0.82106	YES	YES
33	a	423.48	11.60077	YES	YES
34	a	431.65	12.95518	YES	YES
35	a	441.96	17.65693	YES	YES
36	a	460.86	4.53111	YES	YES
37	a	469.58	1.73096	YES	YES
38	a	485.23	3.93093	YES	YES
39	a	489.28	2.10087	YES	YES
40	a	496.85	10.50382	YES	YES
41	a	501.93	23.75879	YES	YES
42	a	514.05	19.93158	YES	YES
43	a	522.05	15.07431	YES	YES
44	a	537.86	2.17505	YES	YES
45	a	544.56	8.19397	YES	YES
46	a	549.69	4.30984	YES	YES
47	a	564.88	8.04376	YES	YES
48	a	580.29	0.47970	YES	YES
49	a	613.16	0.24279	YES	YES
50	a	622.27	2.64742	YES	YES

5 References

(1) "SMART" - control software Bruker SMART Apex X-ray Diffractometer. v5.625, Bruker-AXS GMBH, Karlsruhe, Germany.

(2) "SAINT+" - integration software for Bruker SMART detectors. v6.45, Bruker-AXS GMBH, Karlsruhe, Germany.

(3) "SADABS" - program for absorption correction. v2.10. Sheldrick, G. M. Bruker AXS Inc., Madison, Wisconsin, USA, **2007**.

(4) "SHELXS-97" - program for structure solution. Sheldrick, G. M. University of Göttingen, Göttingen, Germany, 1997.

(5) "SHELXL-97" - program for the Refinement of Crystal Structures. Sheldrick, G. M. University of Göttingen, Göttingen, Germany, 1997.