Supporting Information

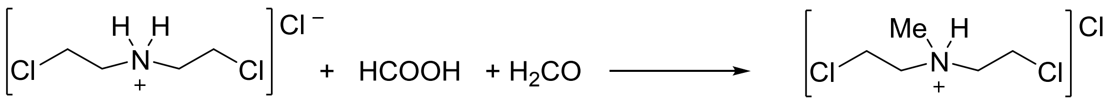
Table of Contents

1. General experimental details

Unless otherwise stated, all reactions were performed under an argon atmosphere with exclusion of moisture from reagents and glassware using standard Schlenk techniques for manipulating of air-sensitive compounds. Reaction vessels were three times flame-dried under vacuum and cooled under a stream of argon. All isolated compounds were characterized by ^{1}H NMR and ^{13}C NMR as well as mass spectrometry using EI as ionization method. NMR spectra were recorded using a Bruker AV 300 or 400. All chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. All chemical shifts are related to residual solvent peaks. ^{1}H-NMR: $CDCl_3$: 7.26, CD_2Cl_2: 5.32, C_6D_6: 7.16, MeOD: 3.31; ^{13}C-NMR: $CDCl_3$: 77.16, CD_2Cl_2: 53.84, C_6D_6: 128.06, MeOD: 49.00. Mass spectra were in general recorded on a Finnigan MAT 95-XP (Thermo Electron). All measurements were carried out at room temperature unless otherwise stated. Gas chromatography was performed on a HP 6890 with a HP5 column (Agilent).

Reagents: Unless otherwise stated, commercial reagents were used as received without further purification.

2. Synthesis of *N*-methyl bis(2-chloroethyl)amine hydrochloride



Formic acid (2.6 g, 0.06 mol) and formaldehyde (37% (aq.), 0.08 mol) were mixed in a 250 mL round-bottom flask equipped with a reflux condenser. Bis-(2-chloroethyl)amine hydrochloride (5.0 g, 0.028 mol) was dissolved and the solution was heated at 100 °C for 3 h. Afterwards the temperature was increased to 130° C for 1 h. After cooling the solution to room temperature, the solvent was evaporated to yield a white precipitate. For further purification, the solid was dissolved in 5 mL THF. After evaporation of the solvent, the product was isolated as white solid. Yield: 5.3 g (98%).

^{1}H NMR (300 MHz, MeOD) *δ* 4.03 (t, 4H), 3.68 (br.s, 4H), 3.04 (s, 3H).

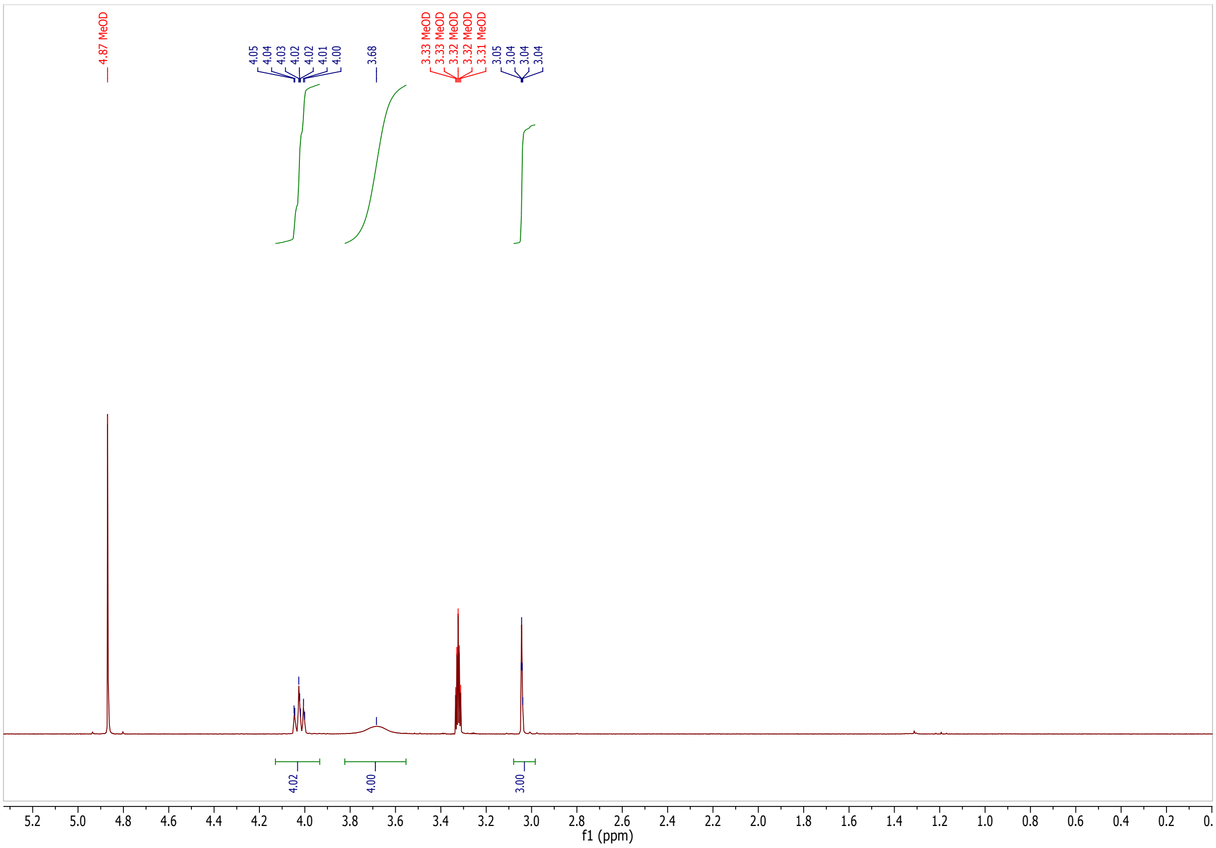
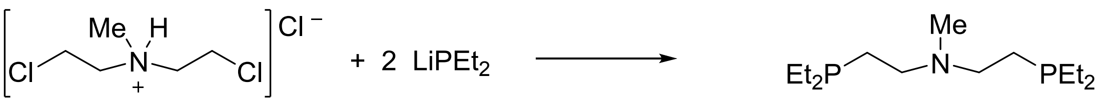


Figure SI 1. ^{1}H-NMR of *N*-methyl bis(2-chloroethyl)amine hydrochloride.

3. Synthesis of *N*-methyl bis(2-diethylphosphinoethyl)amine



Schlenk 1: To a cooled solution of heptane (25 mL, -78°C) containing Et_2PH (966 mg, 10.7 mmol) 4.4 mL (11.0 mmol) of 2.5 M BuLi in hexane was added dropwise and stirred 10 minutes at -78°C. The resulting solution was warm to room temperature and heated 4 hours under reflux.

Schlenk 2: In a separate Schlenk tube *N*-methyl bis(2-chloroethyl)amine hydrochloride (1.03 g; 5.35 mmol) are suspended in 10 mL Et_2O and cooled to -78°C followed by the dropwise addition of 2.2 mL (5.35 mmol) of 2.5 M BuLi in hexane. The reaction suspension is stirred at room temperature for 2 hours. During this time the educts is slowly dissolved and a white precipitate is formed.

The well stirred reaction mixture of Schlenk 1 (Et_2PLi solution) was again cooled to -78°C and the suspension of Schlenk 2 was added via syringe. After completion of the addition, the mixture was stirred for 15 minutes at this temperature, allowed to reach room temperature and heated to 35 °C for 13 h. The cooled solution (-78°C) was treated with water (15 mL), the phases were separated, and the aqueous layer was washed with diethyl ether (3 x 10 mL) at room temperature. The combined organic phases were dried over $MgSO_4$ and after filtration the volatiles of the liquid portion were removed in vacuo. The title compound was isolated as a yellow oil. This pincer ligand was used without further purification. Yield: 645 mg (46% with respect to silylamine).

^{1}H NMR (300 MHz, C_6D_6) δ 1.06-0.94 (m, 12H), 1.33-1.22 (m, 8H), 1.59-1.49 (m, 4H), 2.15 (s, 3H), 2.61-2.48 (m, 4H).

^{31}P NMR (122 MHz, C_6D_6) δ -25.3.

4. Synthesis of manganese complexes Mn-3c and Mn-3ck

The title compound was synthesized according to a slight modification of the reported procedure.[1]

A flame dried Schlenk flask was charged with $MnBr(CO)_5$ (970 mg, 3.5 mmol) and solved in 10 mL toluene. Ligand $[HN(CH_2CH_2P(Et)_2)_2]$ (873 mg, 3.5 mmol) dissolved in 10 mL toluene was added and the solution turned orange and a solid was formed. The suspension was heated to 120 °C for 20 h under argon flow. The reaction mixture was brought to room temperature and concentrated in vacuum and the leftover liquid was transferred to another Schlenk whereas the remaining solid was washed repeatedly with small portions of toluene until the solvent stays colorless. The pale-yellow solid was dried under vacuum, furnishing the cationic complex **Mn-3ck**. Yield: 989 mg (60%).

Afterwards the dark yellow toluene solution was evaporated and dried *in vacuo*. The remaining sticky solid was repeatedly washed with small amounts of methanol and dried under vacuum to yield the neutral complex **Mn-3c** as an orange yellow solid. Yield: 353 mg (23%).

In order to increase the share of complex **Mn-3c** the following synthesis can be conducted:

The cationic complex **Mn-3ck** was suspended in toluene and refluxed for 20 h under argon flow. The reaction mixture was cooled to room temperature and the solvent was transferred to another Schlenk flask. Then, the solid was washed several times with small amounts of toluene. The combined toluene phases were evaporated and dried under vacuum. Complex **Mn-3c** was isolated as an orange yellow solid. Yield: 367 mg (40%).

^{1}H NMR (400 MHz, C_6D_6) δ 2.68 (1H, NH), 2.53-2.19 (m, 4H), 2.21-2.05 (m, 2H), 1.89-1.58(m, 6H), 1.45-1.33 (m, 2H), 1.33-1.21 (m, 2H), 1.19-0.85 (m, 12H).

^{13}C NMR (75 MHz, C_6D_6) δ 51.33, 27.2, 19.07 (t, J_{C-P} = 16.1 Hz), 16.55 (t, J_{C-P}= 10.6 Hz), 8.28, 8.1.

^{31}P NMR (122 MHz, C_6D_6) δ 68.24.

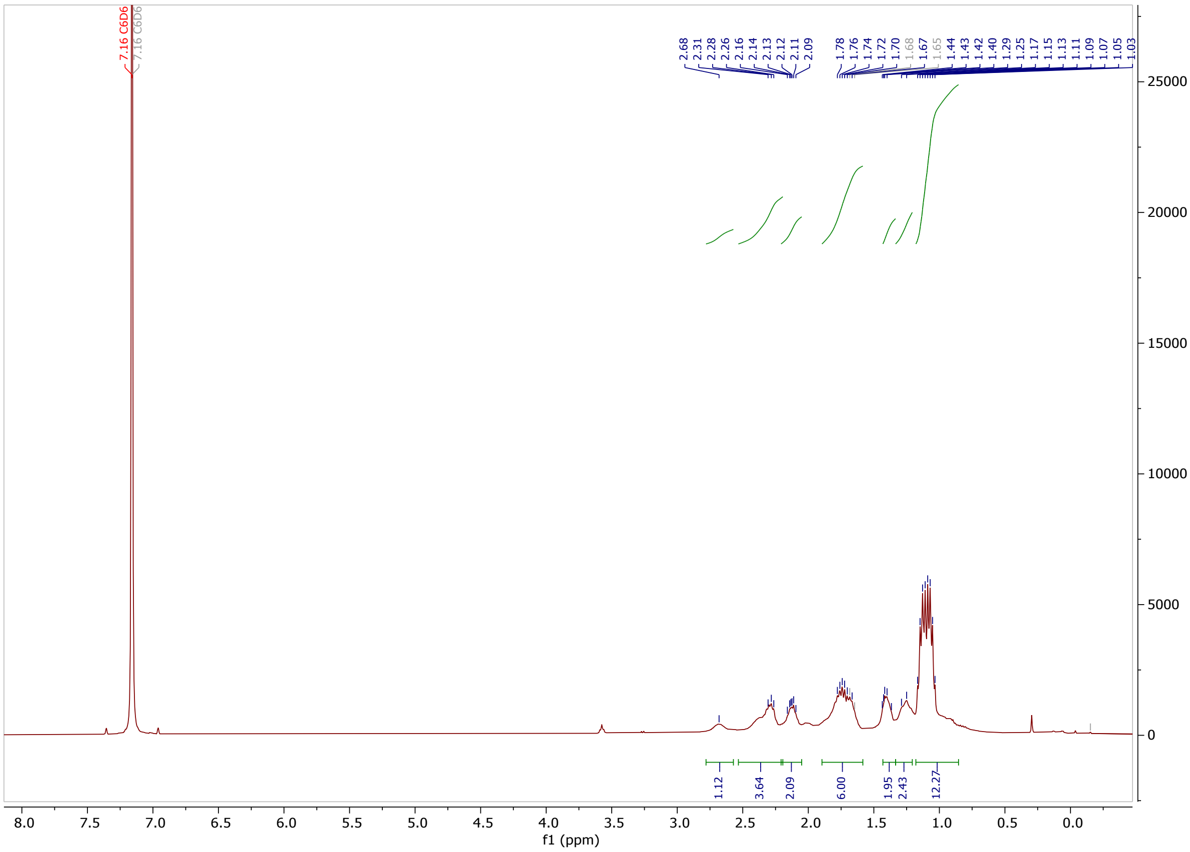


Figure SI 2. ^{1}H-NMR of manganese complex **Mn-3c**.

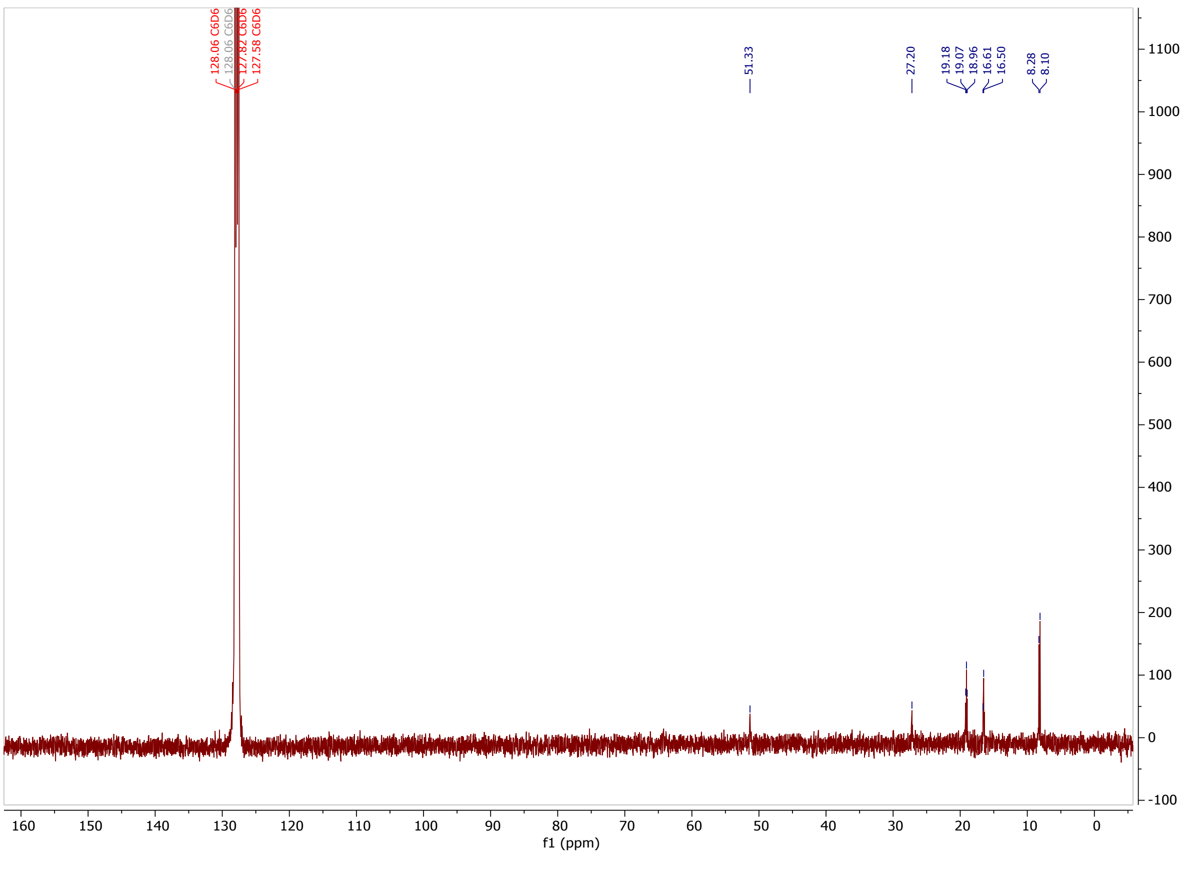


Figure SI 3. ^{13}C-NMR of manganese complex **Mn-3c**.

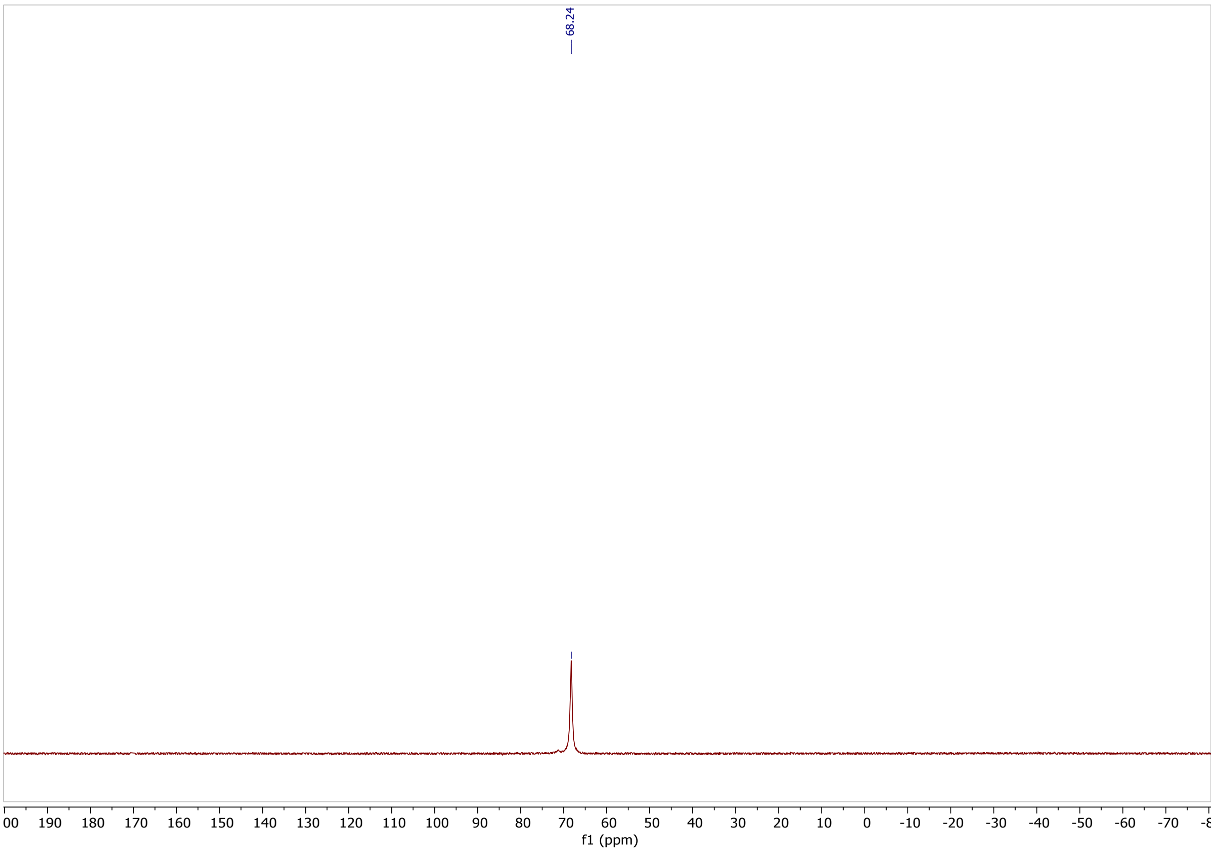


Figure SI 4. ^{31}P-NMR of manganese complex **Mn-3c**.

5. Synthesis and X-ray crystal structure analysis of manganese complex Mn-4

A flame dried Schlenk flask was charged with $MnBr(CO)_5$ (137 mg, 0.5 mmol) and solved in 15 mL toluene. Ligand $[MeN(CH_2CH_2P(Et)_2)_2]$ (132 mg, 0.5 mmol) dissolved in 2 mL toluene was added and an immediate gas evolution was observed. The solution turned orange and a solid was formed. The suspension was heated to 100 °C for 20 h under argon flow. The reaction mixture was cooled to room temperature and toluene was removed in vacuum. The residue was washed with heptane (2x 5-10 mL) and forms a pale-yellow precipitate. The pale-yellow solid was dried under vacuum, furnishing the complex **Mn-4**. Yield: 144 mg (63%). Crystals suitable for X-ray diffraction analysis were grown in methanol at 0°C.

^{1}H NMR (300 MHz, C_6D_6) δ 3.32-3.23 (m, 1H), 2.67 – 2.48 (m, 2H), 2.03 (dt, J = 13.4, 7.0 Hz, 3H), 1.91 (s, 3H), 1.75 (d, J = 8.0 Hz, 4H), 1.25-1.11 (m, J = 7.5 Hz, 6H), 1.08-0.94 (m, J = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, C_6D_6) δ 58.47, 48.56, 27.15, 27.08, 27.01, 21.76, 21.64, 21.52, 17.93, 17.82, 17.72, 8.29, 8.21.

^{31}P NMR (122 MHz, C_6D_6) δ 64.7s.

HRMS (ESI-TOF/MS) calcd. for $C_{13}H_{31}MnNP_2Br$: 397.0500, found: 397.0499 $[M]^+$-2CO; calcd. for $C_{16}H_{31}MnNP_2O_3$: 402.1165, found: 402.1161 $[M]^+$.

Selected IR frequencies (ATR, neat) 3204, 2956, 2932, 2905, 2874, 2012, 1899, 1807, 1457, 1414, 1209, 1030, 760, 750, 634 cm-1.

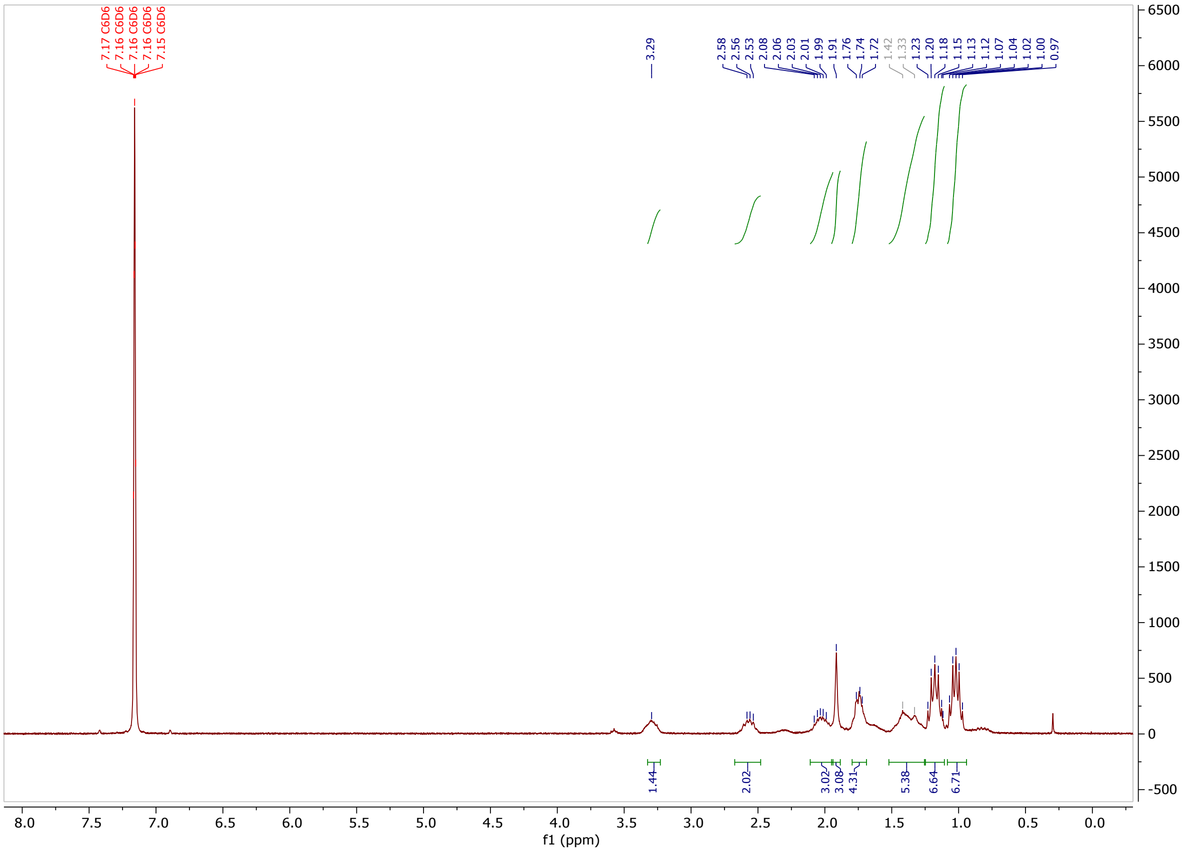


Figure SI 5. ^{1}H-NMR of manganese complex **Mn-4**.

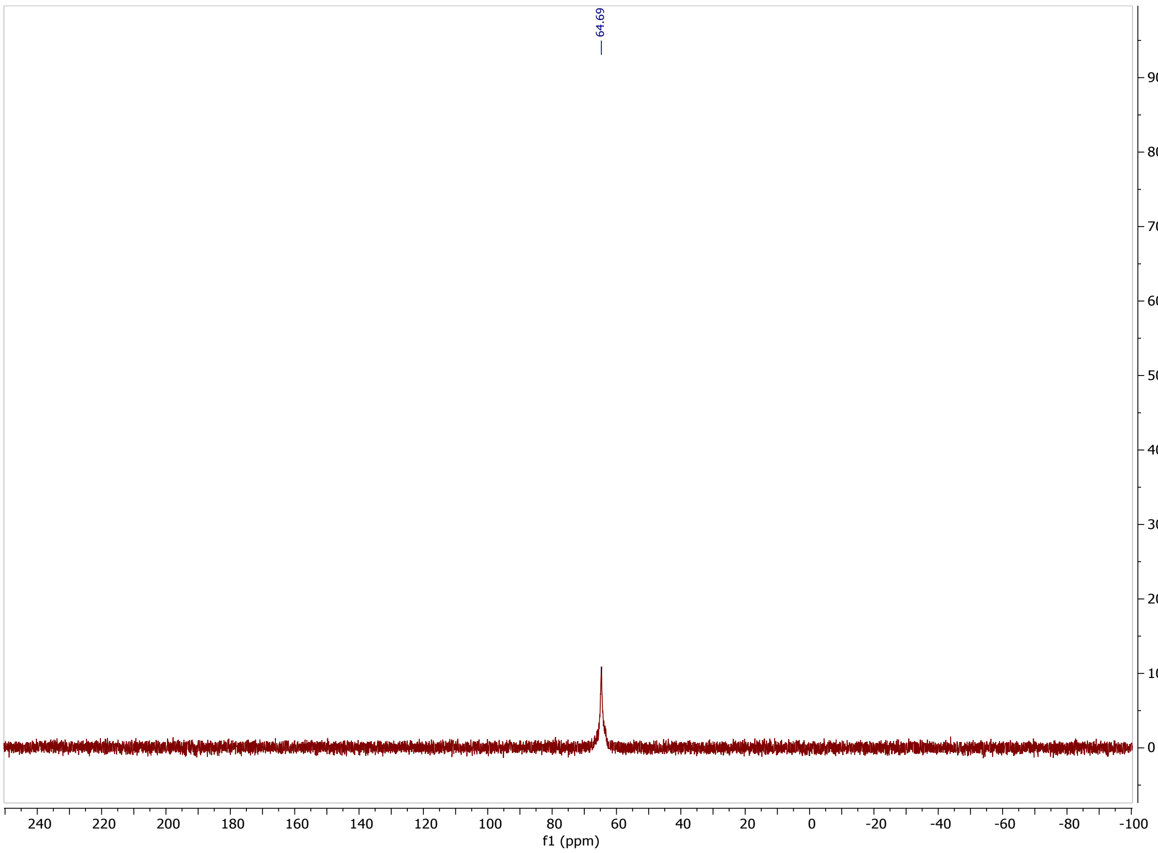


Figure SI 6. ^{31}P-NMR of manganese complex **Mn-4**.

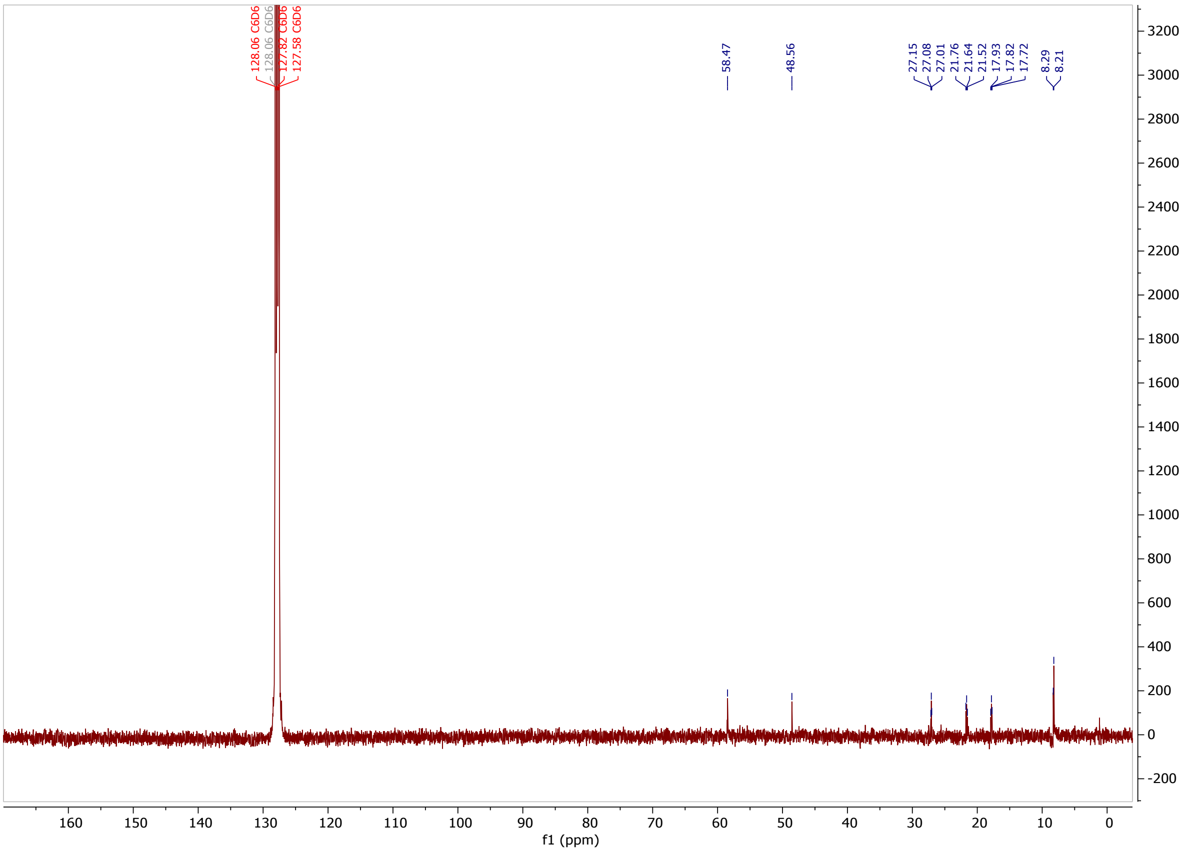


Figure SI 7. ^{13}C-NMR of manganese complex **Mn-4**.

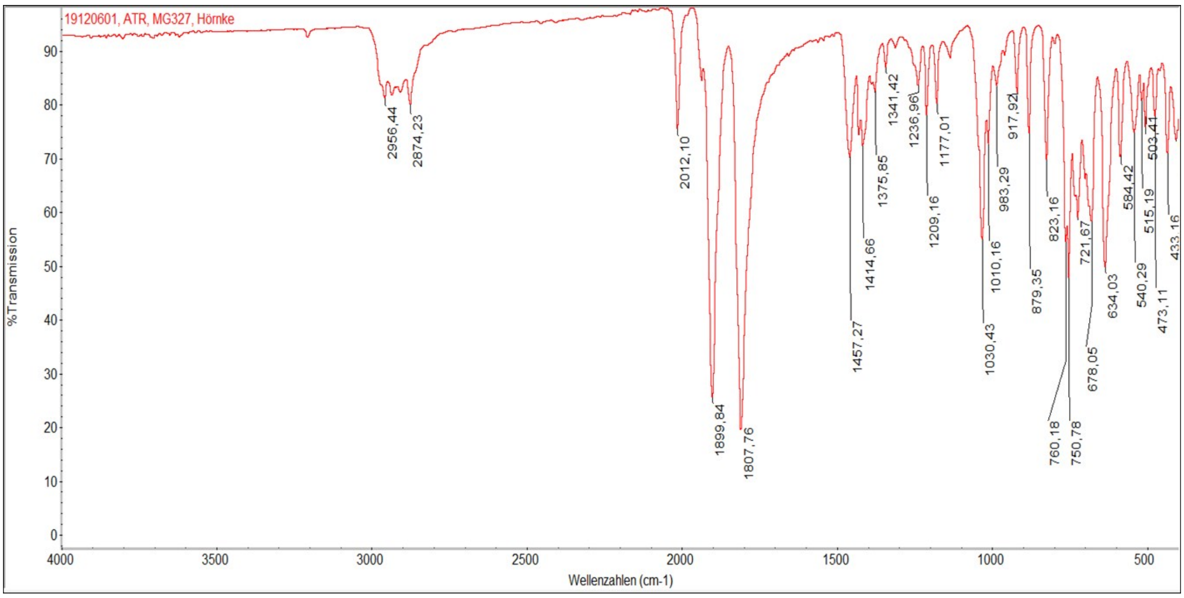


Figure SI 8. IR-ATR spectrum of manganese complex **Mn-4**.

X-ray crystal structure analysis of **Mn-4**:

Data were collected on a STOE IPDS II diffractometer. The structure was solved by direct methods (SHELXS-97: Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112.) and refined by full-matrix least-squares procedures on F^2 (SHELXL-2014: Sheldrick, G. M. *Acta Cryst.* **2015**, *C71*, 3.). XP (Bruker AXS) was used for graphical representations. CCDC 1980954 contains the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre.

Crystal data of **Mn-4**: $C_{15}H_{31}BrMnNO_2P_2$, M = 454.20, triclinic, space group $P\bar{1}$, a = 12.1238(5), b = 13.6853(6), c = 14.1422(6) Å, α = 73.803(3), β = 88.634(3), γ = 68.443(3)°, V = 2087.55(16) Å^3, T = 150(2) K, Z = 4, 36643 reflections measured, 10070 independent reflections (R_{int} = 0.0438), final R values ($I > 2\sigma(I)$): R_1 = 0.0318, wR_2 = 0.0643, final R values (all data): R_1 = 0.0601, wR_2 = 0.0688, 462 parameters.

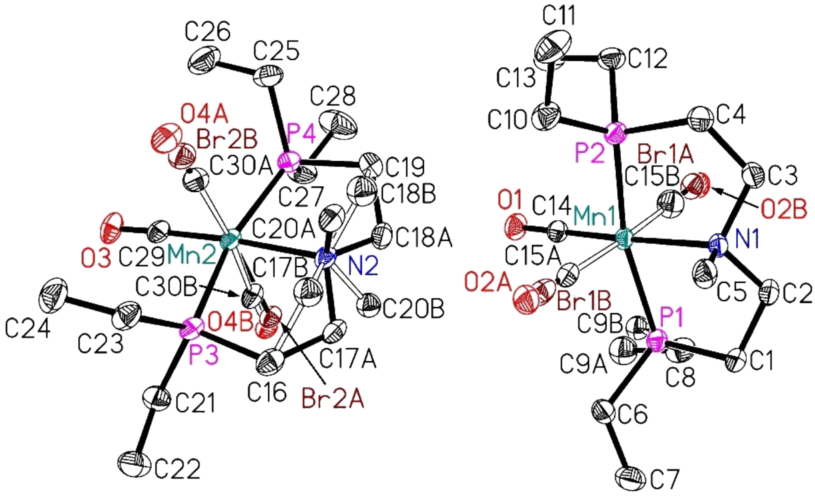
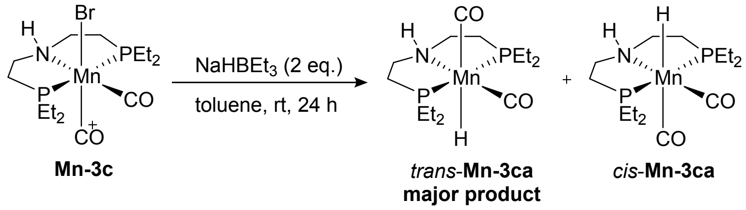


Figure SI 9. Molecular structure of **Mn-4** in the crystal.

Displacement ellipsoids correspond to 30% probability. Hydrogen atoms are omitted for clarity. Br1, C15, O2 and Br2, C30 O4 are disordered over two sites with occupancies of 0.9277(15):0.0723(15) and 0.7408(14):0.2592(14), respectively (further disorder is obtained for C9A/C9B 0.70(2):0.30(2) and C17A,C18A,C20A/C17B,C18B,C20B 0.800(4):0.200(4). Minor components of disordered parts are depicted with white coloured bonds. Following instructions were used to improve the geometry of disordered moieties: SADI, SAME, DFIX, DANG. Additionally, it was necessary to apply ISOR for C15B and EADP for Br1A, O2B and for Br2A, O4B, respectively. C9A, C9B, C17B, C18B and C20B were refined isotropically.

6. Synthesis of manganese hydride complex Mn-3ca



A flame dried Schlenk flask was charged with **Mn-3c** (50 mg, 0.114 mmol) and solved in 2 mL toluene. After heating the suspension to 60 °C a clear yellow solution was received. 2 equiv $NaBEt_3H$ (227 µl, 0.227 mmol, 1 M in THF) were added dropwise to give an orange solution. After stirring at room temperature for 24 h, the formed salt was filtered off and the resulting bright red solution was used as stock solution. In order to analyse **Mn-3ca** by NMR, the reaction was directly conducted in THF*d8*.

^{1}H NMR (300 MHz, THF-d_8) δ -5.83 (t, J = 49.82, 1H), -6.12 (t, J = 49.82, 1H).

^{31}P NMR (122 MHz, THF-d_8) δ 87.71.

ESI-HRMS (*m/z, pos*): Calculated for [$C_{14}H_{29}MnNO_2P_2$]: 360.11; found: 360.1058 [M-H]$^+$.

Calculated for [$C_{16}H_{32}MnN_2O_2P_2$]: 401.13; found: 401.1320 [M-H+ACN]$^+$.

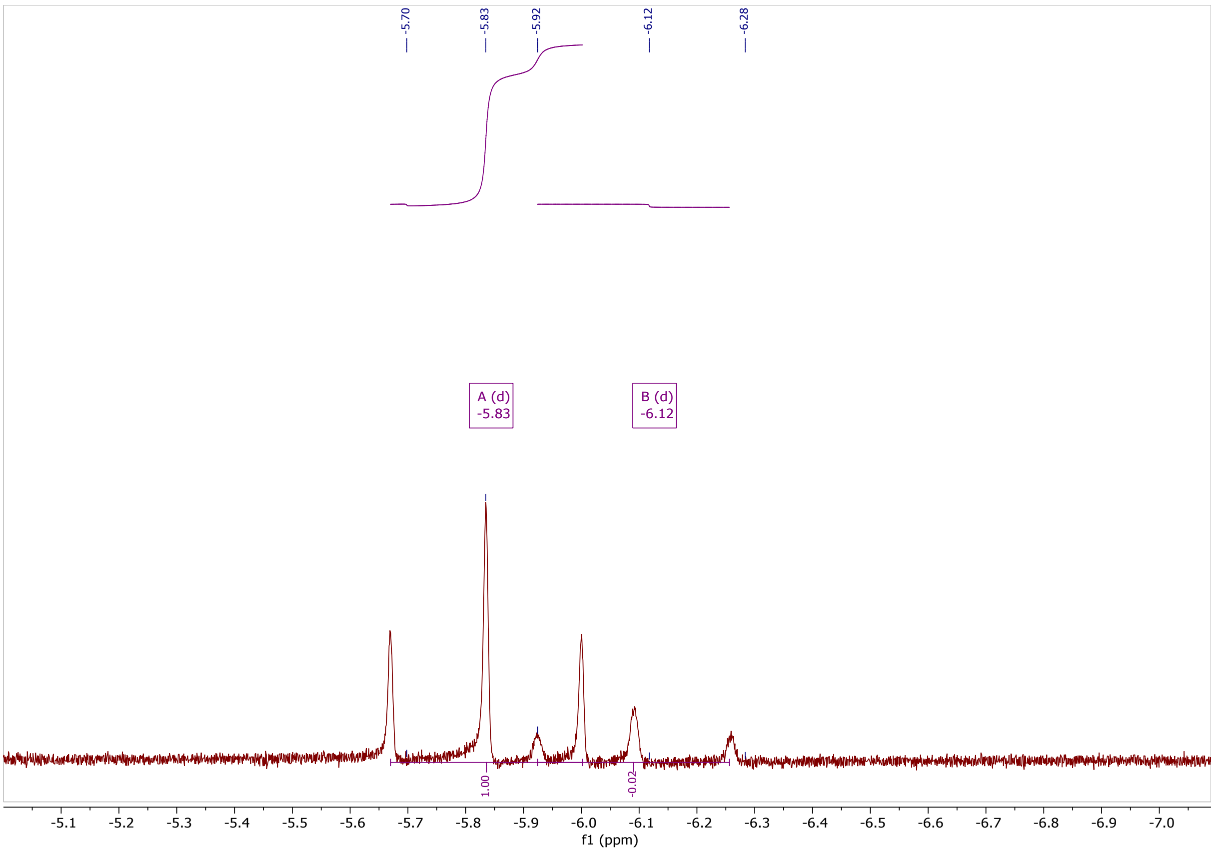


Figure SI 10. ^{1}H-NMR of manganese complex **Mn-3ca**.

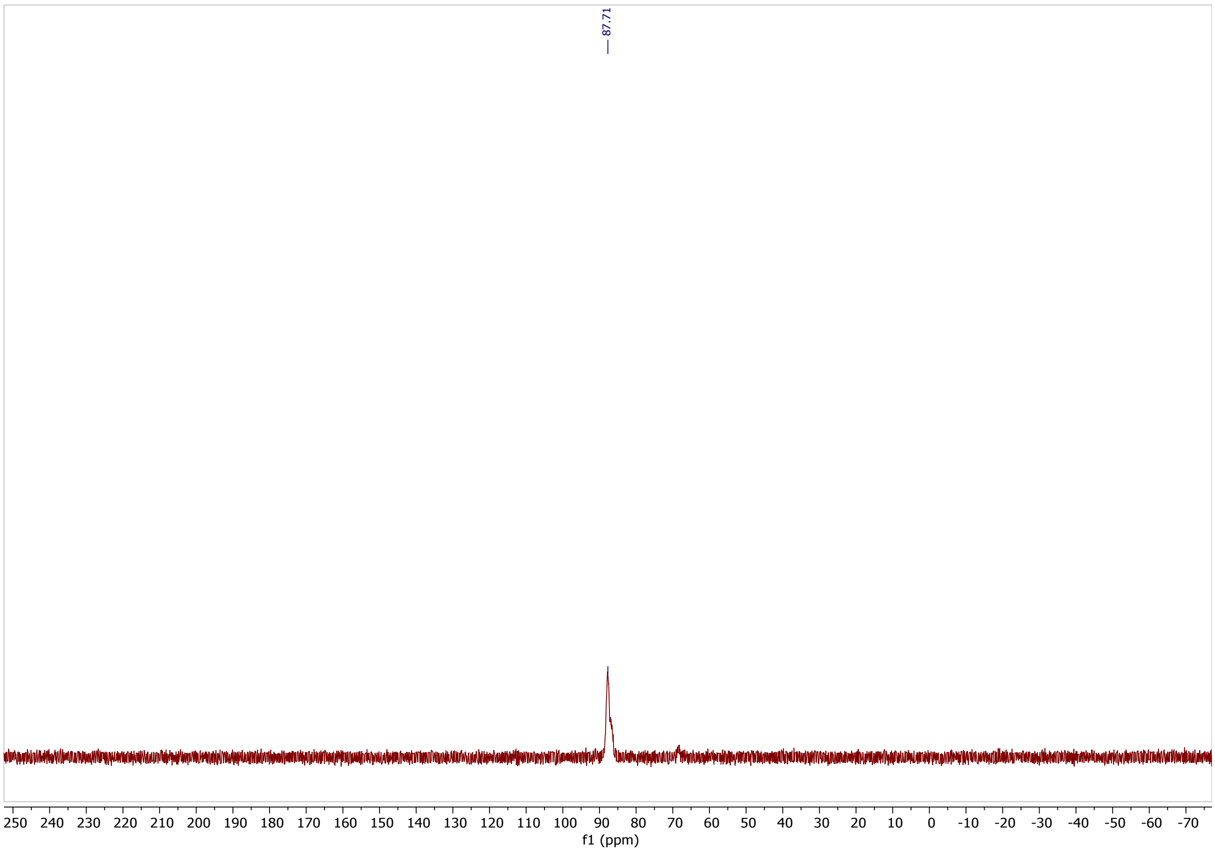


Figure SI 11. ^{31}P-NMR of manganese complex **Mn-3ca**.

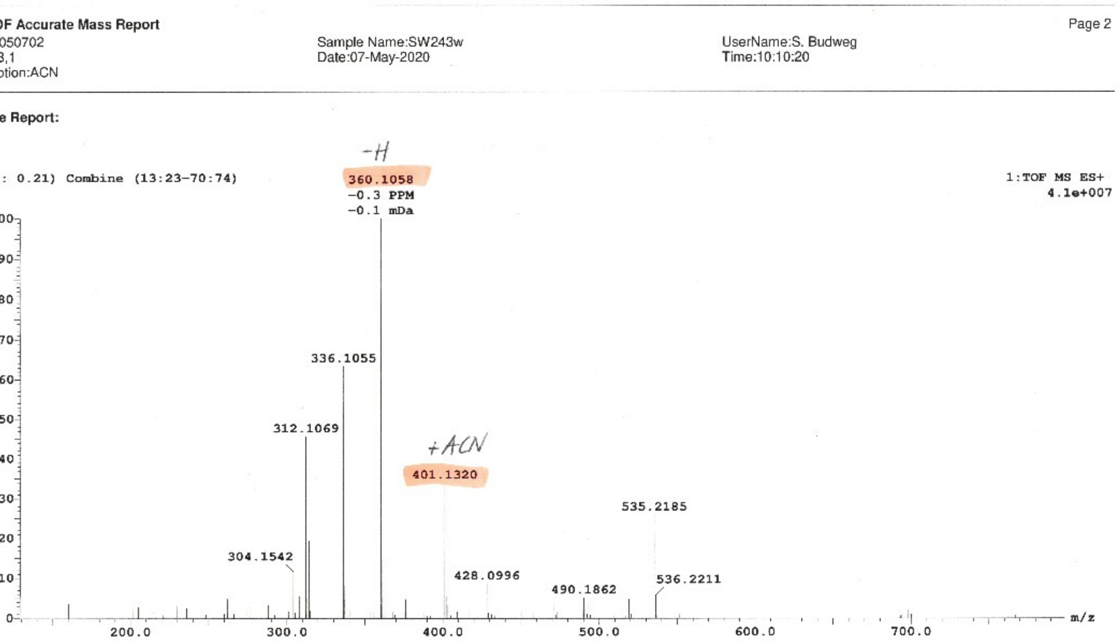


Figure SI 12. ESI-HRMS

7. General procedure for the semihydrogenation of alkynes

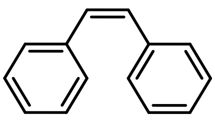
Experiments using molecular hydrogen were carried out in a Parr Instruments autoclave advanced with an internal alloy plate including up to 8 reaction vials (4 mL) equipped with a cap and needle penetrating the septum.

Representative experiment: Under an argon atmosphere, a vial was charged with complex **Mn-3c** (2 mol%, 4.4 mg) and KO*t*Bu (5 mol%, 112.2 mg), and dissolved in 1 mL of dry heptane. To the resulting orange solution, alkyne (0.5 mmol) is added and the solution is continuously stirred. The vial was put in an alloy plate, which is placed into the autoclave. Once sealed, the autoclave was purged three times with hydrogen, then pressurized to 30 bar and heated to 30 °C.

After 2 h reaction time, the autoclave was cooled to room temperature, depressurized, and the reaction mixture was analyzed by GC-FID, as well as GC-MS. Purification was accomplished by column chromatography using silica gel as stationary phase and *n*-pentane / ethylacetate mixture as eluent. Characterization of the isolated compound was done by NMR and GC-MS.

8. Analytical data of the isolated products

(*Z*)-1,2-diphenylethene[2] 2a



Chemical Formular: $C_{14}H_{12}$

Molecular Weight: 180.25 g/mol

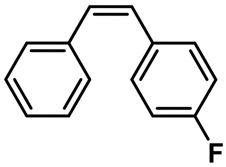
^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.30 – 7.17 (m, 10H), 6.62 (s, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) *δ* 137.38, 130.39, 129.01, 128.34, 127.22.

MS: (EI, 70eV): m/z = 181 (14), 180 ([M]$^+$, 95), 179 (100), 178 (64), 177 (10), 176 (11), 165 (50), 152 (15), 102 (10), 89 (22), 76 (18), 51 (13).

Yield: 88%.

(*Z*)-1-fluoro-4-styrylbenzene[2] 2b

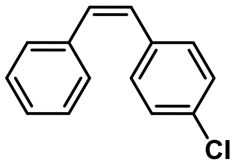


Chemical Formular: $C_{14}H_{11}F$

Molecular Weight: 198.24 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 – 7.15 (m, 7H), 7.01 – 6.87 (m, 2H), 6.63 (d, J = 12.2 Hz, 1H), 6.57 (d, J = 12.3 Hz, 1H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 161.95 (d, *J* = 246.7 Hz), 137.17, 133.31 (d, *J* = 3.6 Hz), 130.66 (d, *J* = 7.9 Hz), 130.38 (d, *J* = 1.5 Hz), 129.21, 128.94, 128.44, 127.32, 115.28 (d, *J* = 21.4 Hz).
MS: (EI, 70eV): m/z = 198 ([M]$^+$, 27), 197 (65), 183 (100), 178 (23), 121 (13), 103 (11), 90 (59), 57 (24), 39 (34).
Yield: 85%.

(*Z*)-1-chloro-4-styrylbenzene[3] 2c

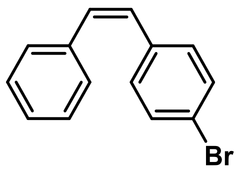


Chemical Formular: $C_{14}H_{11}Cl$

Molecular Weight: 214.69 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 – 7.10 (m, 9H), 6.65 (d, *J* = 12.2 Hz, 1H), 6.55 (d, *J* = 12.2 Hz, 1H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 137.48, 136.41, 133.12, 131.50, 130.81, 129.39, 129.32, 128.87, 128.84, 127.83.
MS: (EI, 70eV): m/z = 216 (19), 215 (13), 214 ([M]$^+$, 61), 179 (89), 178 (100), 177 (17), 176 (21), 152 (13), 89 (20), 76 (24), 51 (15).
Yield: 85%.

(*Z*)-1-bromo-4-styrylbenzene[2] 2d

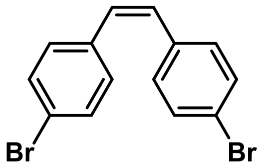


Chemical Formular: $C_{14}H_{11}Br$

Molecular Weight: 259.15 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 – 7.31 (m, 2H), 7.26 – 7.07 (m, 7H), 6.65 (d, J = 12.2 Hz, 1H), 6.51 (d, J = 12.2 Hz, 1H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 136.96, 136.24, 131.49, 131.17, 130.67, 129.07, 128.93, 128.48, 127.48, 121.07.
MS: (EI, 70eV): m/z = 260 (35), 258 (35), 180 (10), 179 (66), 178 (100), 177 (14), 176 (17), 152 (15), 89 (23), 76 (20), 51 (10).
Yield: 89%.

(*Z*)-1,2-bis(4-bromophenyl)ethene[4] 2e

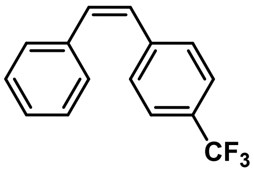


Chemical Formular: $C_{14}H_{10}Br_2$

Molecular Weight: 338.04 g/mol

^{1}H NMR (300 MHz, C_6D_6) δ 7.12 – 7.02 (m, 4H), 6.77 – 6.69 (m, 4H), 6.15 (s, 2H).
^{13}C NMR (75 MHz, C_6D_6) δ 135.89, 131.84, 130.73, 129.82, 128.38, 128.06, 127.74, 121.66
MS: (EI, 70eV): m/z = 340 (37), 339 (12), 338 ([M]$^+$, 76), 336 (38), 179 (15), 178 (100), 177 (14), 176 (23), 89 (15), 88 (14).
Yield: 81%.

(*Z*)-1-styryl-4-(trifluoromethyl)benzene[2] 2f

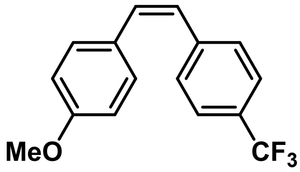


Chemical Formular: $C_{15}H_{11}F_3$

Molecular Weight: 248.08 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 – 7.44 (m, 2H), 7.34 (m, 2H), 7.26 – 7.16 (m, 5H), 6.73 (d, J = 12.3 Hz, 1H), 6.60 (d, J = 12.3 Hz, 1H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 136.68, 132.46, 129.27, 128.95, 128.88, 128.56, 127.71, 126.11, 125.36, 125.31 (q), 122.51.
MS: (EI, 70eV): m/z = 249 (16), 248 ([M]$^+$, 100), 247 (21), 233 (19), 227 (20), 207 (10), 180 (14), 179 (97), 178 (89), 177 (11), 176 (11), 152 (11), 151 (11).
Yield: 79%.

(*Z*)-1-methoxy-4-(4-trifluoromethyl)styryl)benzene[5] 2g

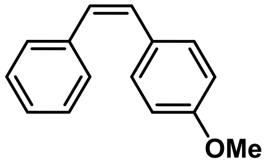


Chemical Formular: $C_{16}H_{13}F_3O$

Molecular Weight: 278.27 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 – 7.45 (m, 2H), 7.41 – 7.32 (m, 2H), 7.20 – 7.09 (m, 2H), 6.83 – 6.73 (m, 2H), 6.65 (d, J = 12.2 Hz, 1H), 6.50 (d, J = 12.2 Hz, 1H), 3.80 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 159.18, 141.47, 131.95, 130.31, 129.21, 129.04, 127.35, 125.30 (q, J = 3.9 Hz), 113.93, 55.36.
MS: (EI, 70eV): m/z = 279 (23), 278 ([M]$^+$, 100), 277 (14), 263 (14), 215 (16), 166 (32), 165 (57).
Yield: 70%.

(*Z*)-1-methoxy-4-styrylbenzene[2] 2h

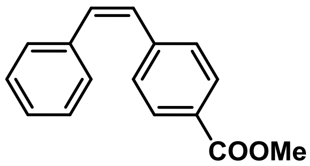


Chemical Formular: $C_{15}H_{14}O$

Molecular Weight: 210.28 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.31 – 7.13 (m, 7H), 6.76 (d, *J* = 8.6 Hz, 2H), 6.52 (d, *J* = 1.1 Hz, 2H), 3.79 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 158.78, 137.74, 130.28, 129.89, 128.94, 128.89, 128.36, 127.03, 113.71, 55.33.
MS: (EI, 70eV): m/z = 211 (23), 210 ([M]$^+$, 100), 209 (24), 195 (27), 194 (10), 179 (19), 178 (15), 167 (53), 166 (29), 165 (77), 152 (53), 139 (13), 115 (17), 89 (15), 63 (12).
Yield: 95%.

Methyl-(*Z*)-4-styrylbenzoate[6] 2i

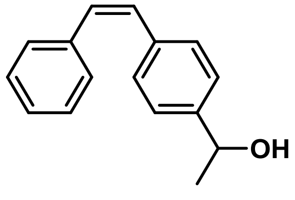


Chemical Formular: $C_{16}H_{14}O_2$

Molecular Weight: 238.29 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.92 – 7.87 (m, *J* = 7.9 Hz, 2H), 7.33 – 7.28 (m, *J* = 7.3 Hz, 2H), 7.22 (s, 5H), 6.71 (d, *J* = 12.3 Hz, 1H), 6.61 (d, *J* = 12.3 Hz, 1H), 3.90 (s, 3H). Spectra contains traces of the starting material **1i**.
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 167.05, 142.24, 136.80, 132.37, 131.88, 131.65, 129.66, 129.35, 129.00, 128.48, 127.65, 52.18.
MS: (EI, 70eV): m/z = 239 (14), 238 (75), 207 (45), 180 (12), 179 (89), 178 ([M]$^+$, 100), 177 (14), 176 (18), 152 (18), 151 (10), 103 (11), 89 (35), 76 (19), 51 (8).
Yield: 90%.

(*Z*)-1-(4-styrylphenyl)ethan-1-ol 2j[7]



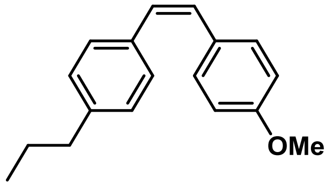
Chemical Formular: $C_{16}H_{16}O$

Molecular Weight: 224.30 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.35 – 7.13 (m, 9H), 6.59 (q, *J* = 14.4, 2.1Hz, 2H), 4.86 (q, *J* = 6.4 Hz, 1H), 1.73 (s, 2H), 1.49 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 144.71, 137.42, 136.57, 130.40, 129.99, 129.17, 128.96, 128.38, 127.25, 125.41, 70.33, 25.16.
MS: (EI, 70eV): m/z = 225 (23), 224 ([M]$^+$, 70), 209 (100), 207 (21), 206 (25), 203 (17), 202 (10), 190 (16), 189 (12), 182 (12), 181 (32), 180 (29), 179 (48), 178 (31), 177 (26), 167 (13), 166 (35), 165 (53), 153 (12), 152 (24), 150 (13), 139 (10), 127 (17), 115 (14), 104 (30), 103 (32), 102 (10), 91 (15), 89 (20), 88 (16), 77 (22), 76 (26), 64 (11), 63 (12), 45 (11), 43 (13), 39 (12).

Yield: 85%.

(*Z*)-1-methoxy-4-(4-propylstyryl)benzene 2k[8]

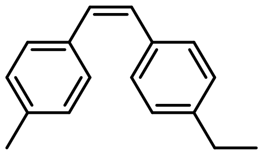


Chemical Formular: $C_{18}H_{20}O$

Molecular Weight: 252.36 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.25 – 7.16 (m, 4H), 7.05 (d, J = 8.0 Hz, 2H), 6.82 – 6.71 (m, 2H), 6.49 (s, 2H), 3.80 (s, 3H), 2.60 – 2.51 (m, 2H), 1.72 – 1.56 (m, 2H), 0.95 (t, J = 7.4 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 158.71, 141.63, 134.99, 130.23, 130.07, 129.21, 128.94, 128.81, 128.43, 113.69, 55.33, 37.94, 24.57, 14.00.
MS: (EI, 70eV): m/z = 253 (15), 252 ([M]$^+$, 76), 224 (17), 223 (100), 178 (13), 165 (22).
Yield: 85%.

(*Z*)-1-ethyl-4-(4-methylstyryl)benzene 2l[9]

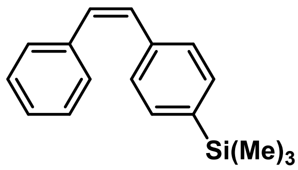


Chemical Formular: $C_{17}H_{18}$

Molecular Weight: 222.33 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.24 – 7.12 (m, 4H), 7.13 – 6.98 (m, 4H), 6.53 (s, 2H), 2.62 (q, *J* = 7.6 Hz, 2H), 2.33 (s, 3H), 1.23 (t, *J* = 7.6, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 143.23, 136.84, 134.85, 134.65, 129.66, 129.63, 129.02, 128.93, 128.87, 127.78, 28.73, 21.39, 15.56.
MS: (EI, 70eV): m/z = 223 (18), 222 ([M]$^+$, 100), 208 (13), 207 (76), 193 (28), 192 (22), 191 (24), 189 (10), 179 (13), 178 (24), 165 (11).
Yield: 74%.

(*Z*)-trimethyl(4-styrylphenyl)silane 2m[10]

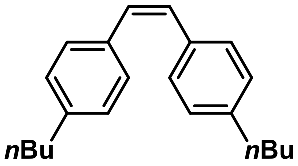


Chemical Formular: $C_{17}H_{20}Si$

Molecular Weight: 252.43 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.44 – 7.17 (m, 9H), 6.62 (d, *J* = 12.3 Hz, 1H), 6.57 (d, *J* = 12.3 Hz, 1H), 0.26 (s, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 139.51, 137.69, 137.53, 133.34, 130.53, 130.37, 128.98, 128.38, 128.27, 127.24, -0.97.
MS: (EI, 70eV): m/z = 252 ([M]$^+$, 38), 238 (24), 237 (100), 178 (14), 59 (10).
Yield: 87%.

(*Z*)-1,2-bis(4-butylphenyl)ethene 2n [11]



Chemical Formular: $C_{22}H_{28}$

Molecular Weight: 292.47 g/mol

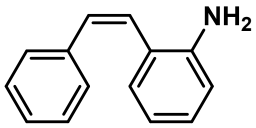
^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.25 – 7.14 (m, 4H), 7.10 – 6.99 (m, 4H), 6.52 (s, 2H), 2.58 (t, 4H), 1.64 – 1.53 (m, 4H), 1.43 – 1.26 (m, 4H), 0.93 (t, *J* = 7.3 Hz, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) *δ* 141.93, 134.86, 129.65, 128.85, 128.33, 35.55, 33.67, 22.55, 14.12.

MS: (EI, 70eV): m/z = 293 (24), 292 ([M]$^+$, 100), 250 (16), 249 (76), 207 (17), 206 (16), 191 (13).

Yield: 68%.

(*Z*)-2-styrylaniline 2o[3]



Chemical Formular: $C_{14}H_{13}N$

Molecular Weight: 195.27 g/mol

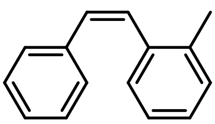
^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.28 – 7.16 (m, 5H), 7.13 – 7.05 (m, 2H), 6.76 – 6.66 (m, 2H), 6.66 (d, *J* = 12.1 Hz, 1H), 6.53 (d, *J* = 12.1 Hz, 1H), 3.65 (s, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) *δ* 143.77, 136.83, 131.81, 129.70, 128.87, 128.54, 128.33, 127.57, 126.62, 123.34, 118.56, 115.65.

MS: (EI, 70eV): m/z = 196 (16), 195 ([M]$^+$, 100), 194 (83), 193 (17), 178 (10), 167 (10), 165 (17), 152 (11), 118 (78), 117 (24), 97 (12), 91 (13), 90 (12), 89 (17), 77 (11), 63 (11), 51 (12).

Yield: 97%.

(*Z*)-1-methyl-2-styrylbenzene[3] 2p



Chemical Formular: $C_{15}H_{14}$

Molecular Weight: 194.28 g/mol

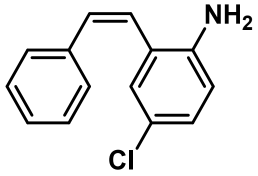
^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.25 – 7.01 (m, 9H), 6.65 (d, *J* = 2.9 Hz, 2H), 2.29 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) *δ* 137.25, 137.17, 136.23, 130.64, 130.19, 129.67, 129.04, 129.01, 128.21, 127.35, 127.16, 125.83, 20.01.

MS: (EI, 70eV): m/z = 195 (15), 194 ([M]$^+$, 81), 193 (16), 180 (18), 179 (100), 178 (79), 165 (22), 152 (16), 116 (29), 115 (46), 91 (14), 89 (16), 77 (13), 63 (12), 51 (12).

Yield: 68%.

(*Z*)-4-chloro-2-styrylaniline 2q[12]



Chemical Formular: $C_{14}H_{12}ClN$

Molecular Weight: 229.71 g/mol

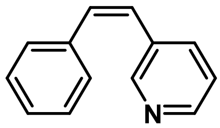
^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.21 (s, 5H), 7.07 – 7.00 (m, 2H), 6.69 (d, *J* = 12.1 Hz, 1H), 6.64 – 6.59 (m, 1H), 6.43 (d, *J* = 12.1 Hz, 1H), 3.68 (s, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) *δ* 142.36, 136.30, 132.83, 129.13, 128.82, 128.49, 128.34, 127.99, 125.25, 124.73, 123.01, 116.75, 77.58, 77.16, 76.74.

MS: (EI, 70eV): m/z = 229 ([M]$^+$, 100), 214 (10), 193 (60), 176 (10), 165 (25), 152 (63), 139 (10), 117 (33), 96 (18), 89 (15), 77 (10), 63 (11), 51 (10).

Yield: 68%.

(*Z*)-3-styrylpyridine[13] 2r



Chemical Formular: $C_{13}H_{11}N$

Molecular Weight: 181.24 g/mol

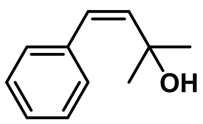
^{1}H NMR (300 MHz, $CDCl_3$) *δ* 8.48 (br.s, 2H), 7.47 (s, 1H), 7.35 – 6.95 (m, 6H), 6.77 (d, J = 12.1 Hz, 1H), 6.53 (d, J = 12.1 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) *δ* 149.81, 136.57, 132.96, 132.60, 128.78, 128.66, 128.35, 127.74, 126.61.

MS: (EI, 70eV): m/z = 181 ([M]$^+$, 43), 180 ([M]$^+$-1, 100), 152 (20), 127 (10), 116 (29), 115 (9), 102 (8), 89 (10), 76 (13), 63 (12), 51 (12).

Yield: 99%.

(*Z*)-2-methyl-4-phenylbut-3-en-2-ol 2s[14]



Chemical Formular: $C_{11}H_{14}O$

Molecular Weight: 162.23 g/mol

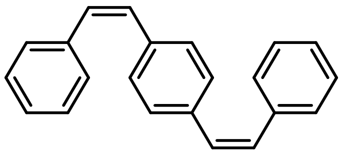
^{1}H NMR (300 MHz, $CDCl_3$) *δ* 7.38 – 7.20 (m, 6H), 6.47 (d, *J* = 12.7 Hz, 1H), 5.76 (d, *J* = 12.7 Hz, 1H), 1.36 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) *δ* 139.87, 138.08, 129.55, 128.64, 128.41, 127.53, 72.68, 31.74.

MS: (EI, 70eV): m/z = 162 ([M]$^+$, 20), 148 (11), 147 (100), 129 (67), 128 (38), 127 (13), 119 (29), 115 (12), 103 (14), 91 (68), 78 (13), 77 (25), 51 (18), 43 (50).

Yield: 43%.

1,4-di((*Z*)-styryl)benzene 2t[15]

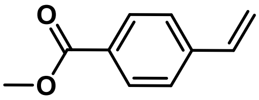


Chemical Formular: $C_{22}H_{18}$

Molecular Weight: 282.39 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) *δ* δ 7.29 – 7.14 (m, 10H), 7.10 (s, 4H), 6.61 (d, *J* = 12.4, 2H), 6.55 (d, *J* = 12.4 Hz, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 137.92, 136.70, 130.83, 130.41, 129.36, 129.24, 128.72, 127.67.
MS: (EI, 70eV): m/z = 283 (48), 282 ([M]$^+$, 100), 266 (14), 265 (27), 252 (14), 204 (12), 203 (45), 202 (45), 191 (22), 189 (17), 179 (24), 178 (60), 176 (11), 165 (17), 152 (14), 103 (11), 78 (10), 77 (15).
Yield: 90%.

Methyl-4-vinylbenzoate[16] 5c



Chemical Formular: $C_{10}H_{10}O_2$

Molecular Weight: 162.19 g/mol

^{1}H NMR (300 MHz, $CDCl_3$) *δ* 8.02 – 7.97 (m, 2H), 7.49 – 7.43 (m, 2H), 6.75 (dd, J = 17.6, 10.9 Hz, 1H), 5.87 (d, J = 16.9 Hz, 1H), 5.38 (d, J = 10.2 Hz, 1H), 3.91 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 167.02, 142.06, 136.16, 130.03, 129.41, 126.25, 116.63, 52.23.
MS: (EI, 70eV): m/z = 162 ([M]$^+$, 39), 132 (10), 131 (100), 103 (37), 102 (11), 77 (31), 51 (13).
Yield: 76%.

9. Spectra of the isolated products

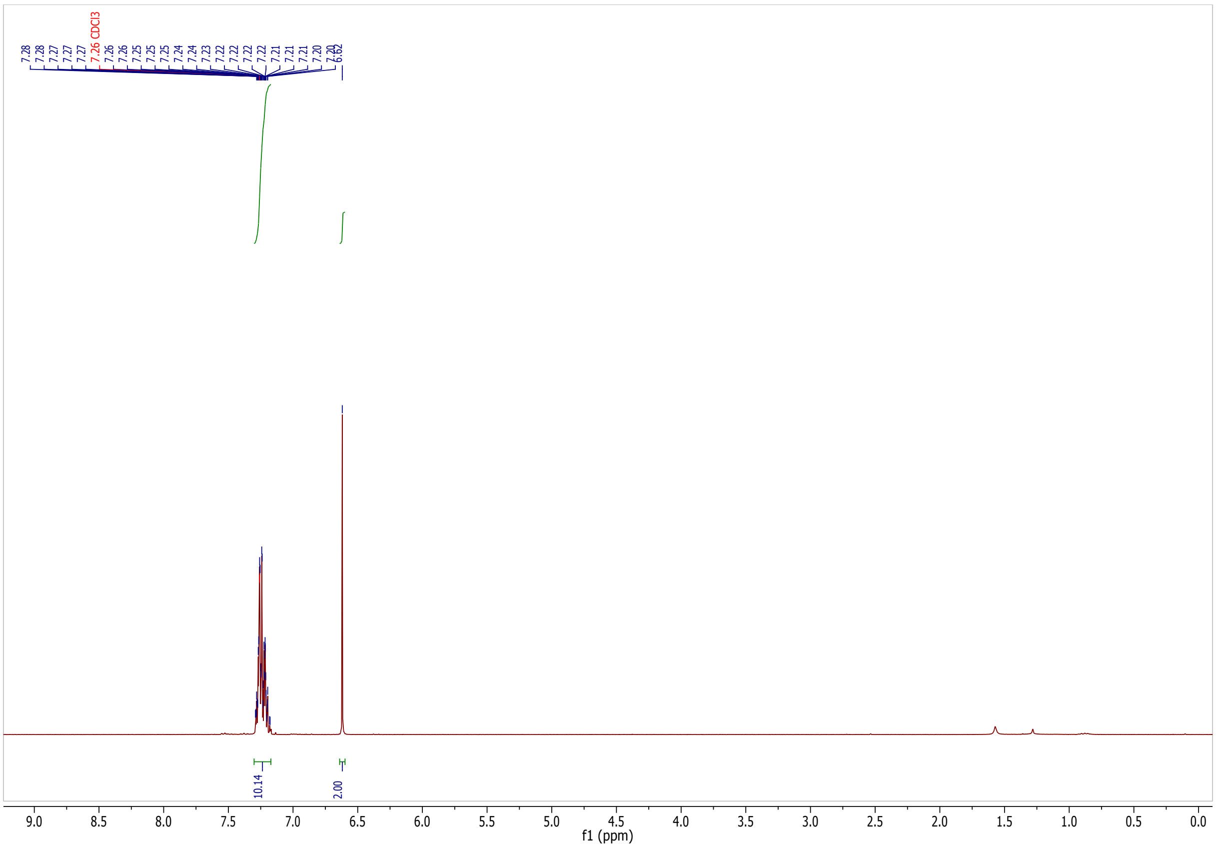


Figure SI 13.[1]H-NMR of (*Z*)-1,2-diphenylethene **2a**.

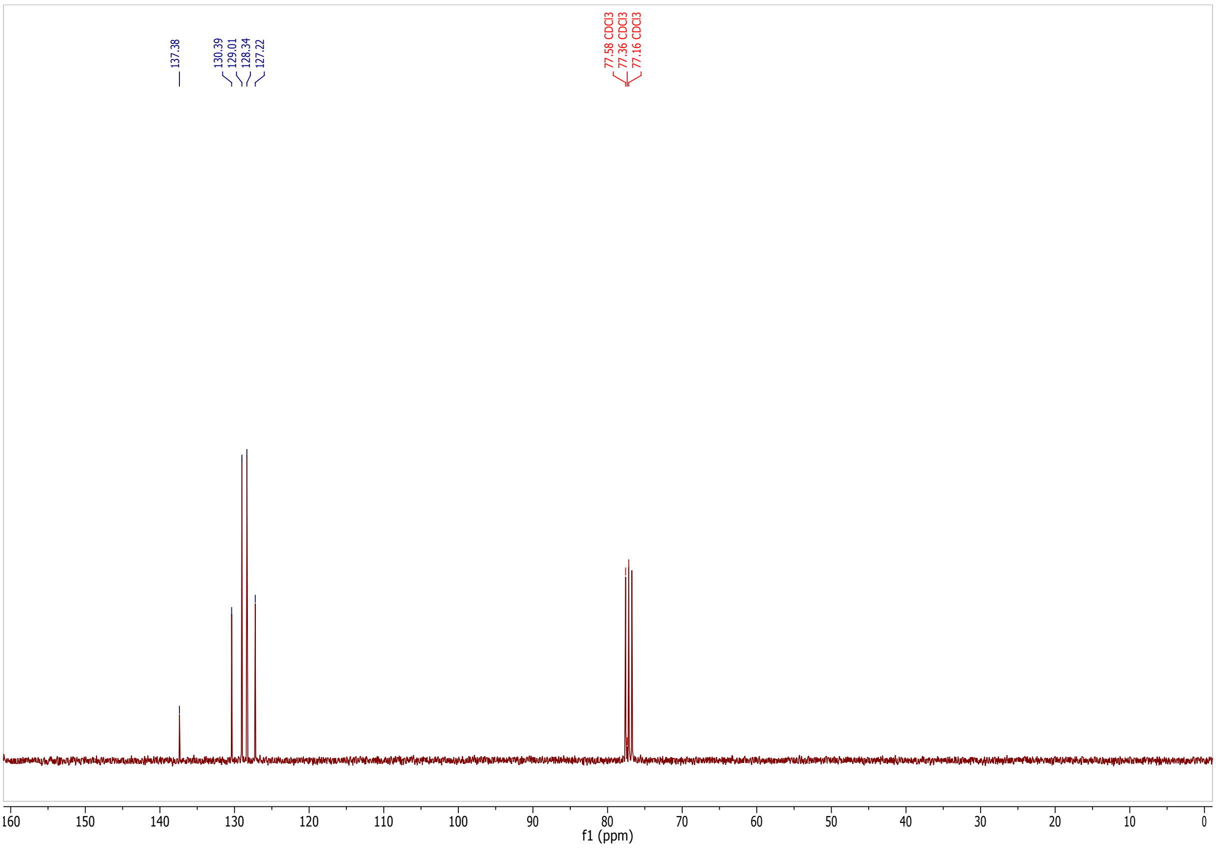


Figure SI 14. [13]C-NMR of (*Z*)-1,2-diphenylethene **2a**.

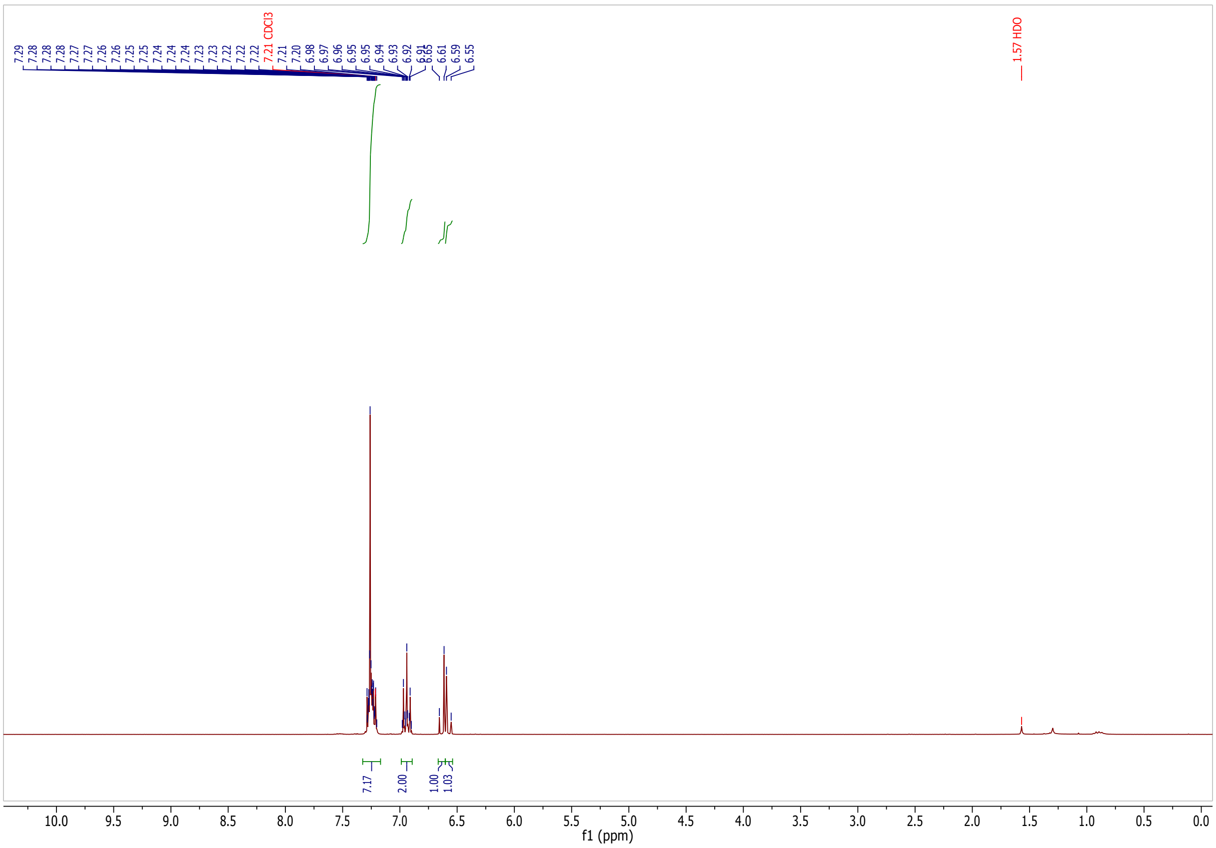


Figure SI 15.[1]H-NMR of (*Z*)-1-fluoro-4-styrylbenzene **2b**.

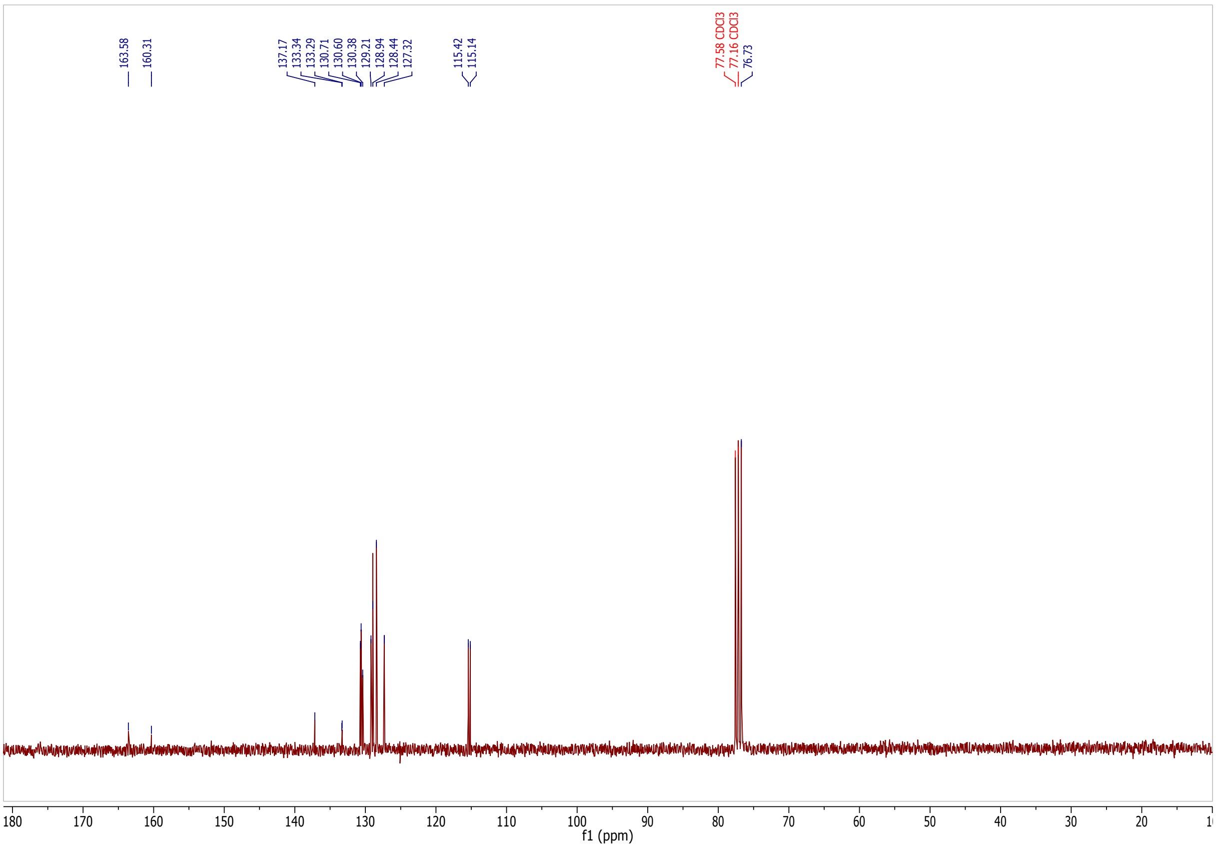


Figure SI 16. ^{13}C-NMR of (*Z*)-1-fluoro-4-styrylbenzene **2b**.

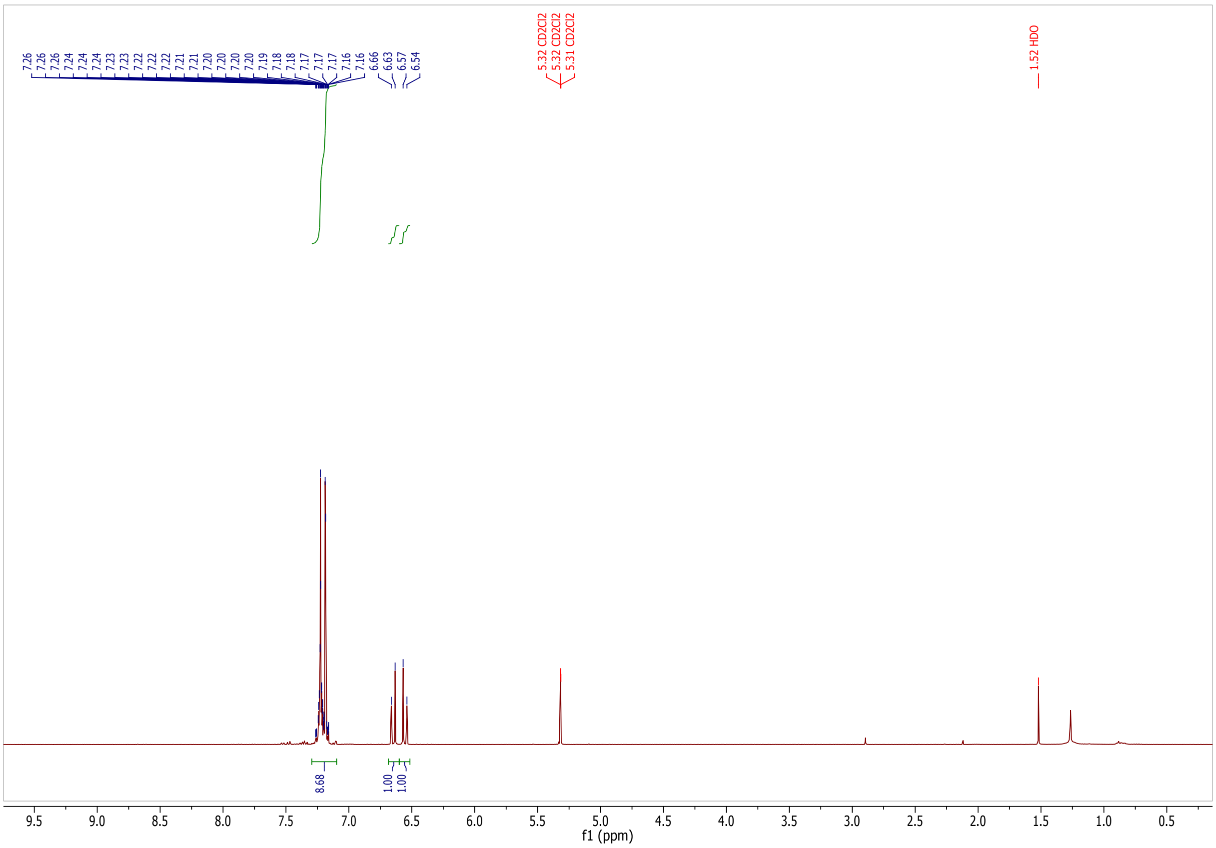


Figure SI 17. ^{1}H-NMR of (*Z*)-1-chloro-4-styrylbenzene **2c**.

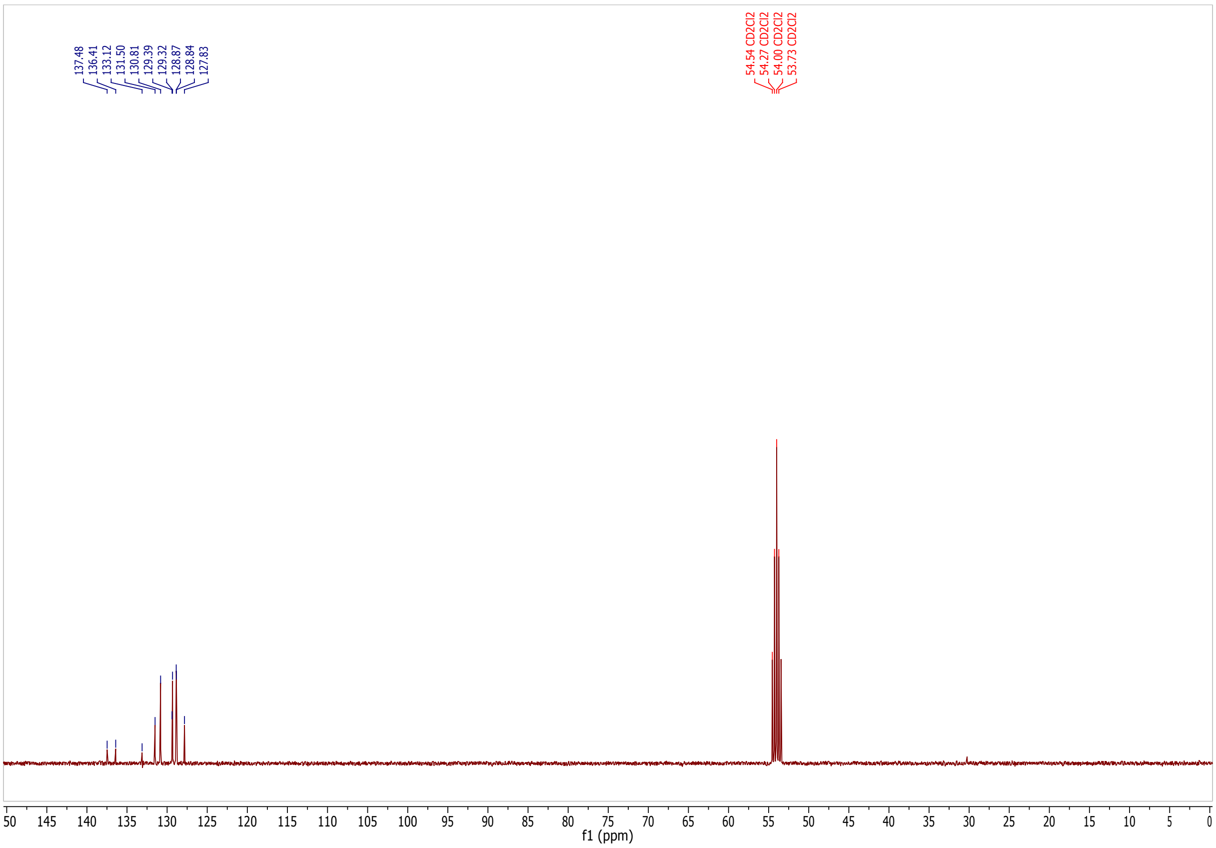


Figure SI 18. ^{13}C-NMR of (*Z*)-1-chloro-4-styrylbenzene **2c**.

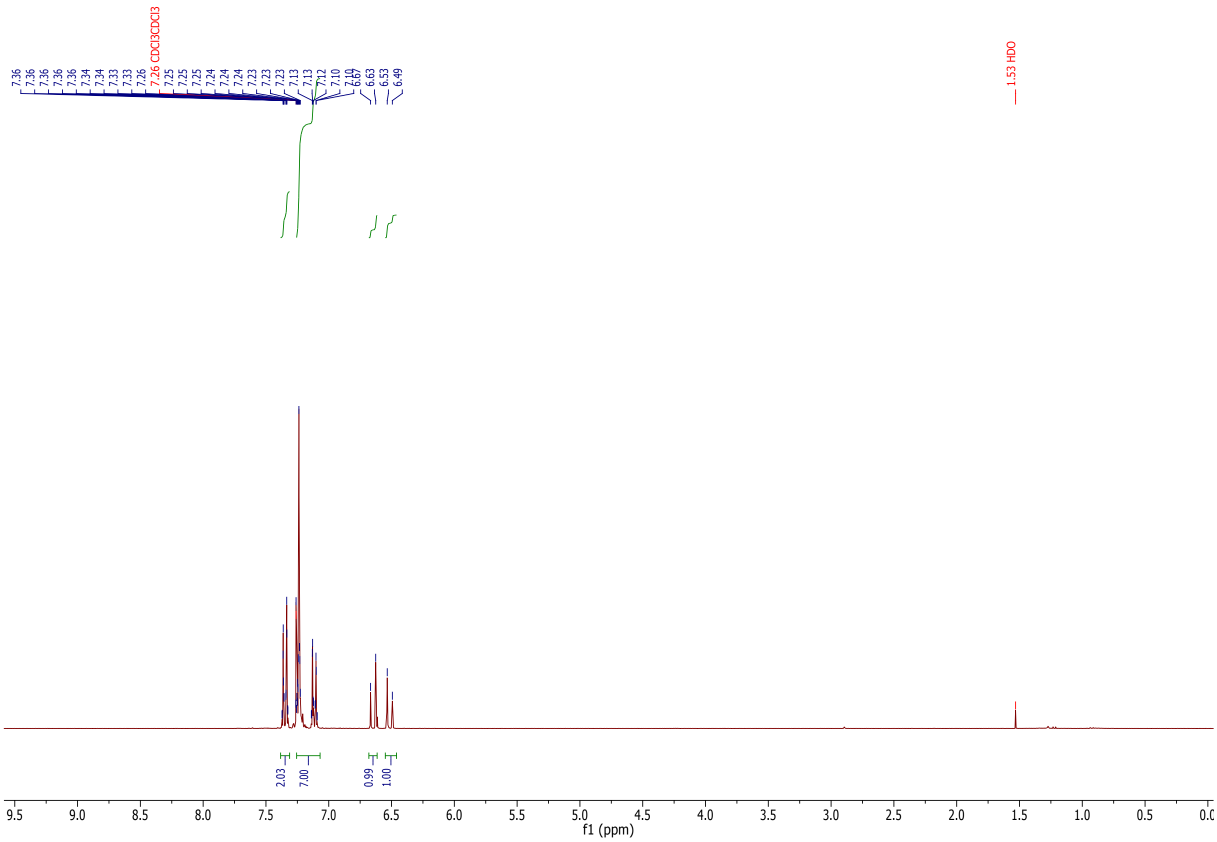


Figure SI 19. ^{1}H-NMR of (*Z*)-1-bromo-4-styrylbenzene **2d**.

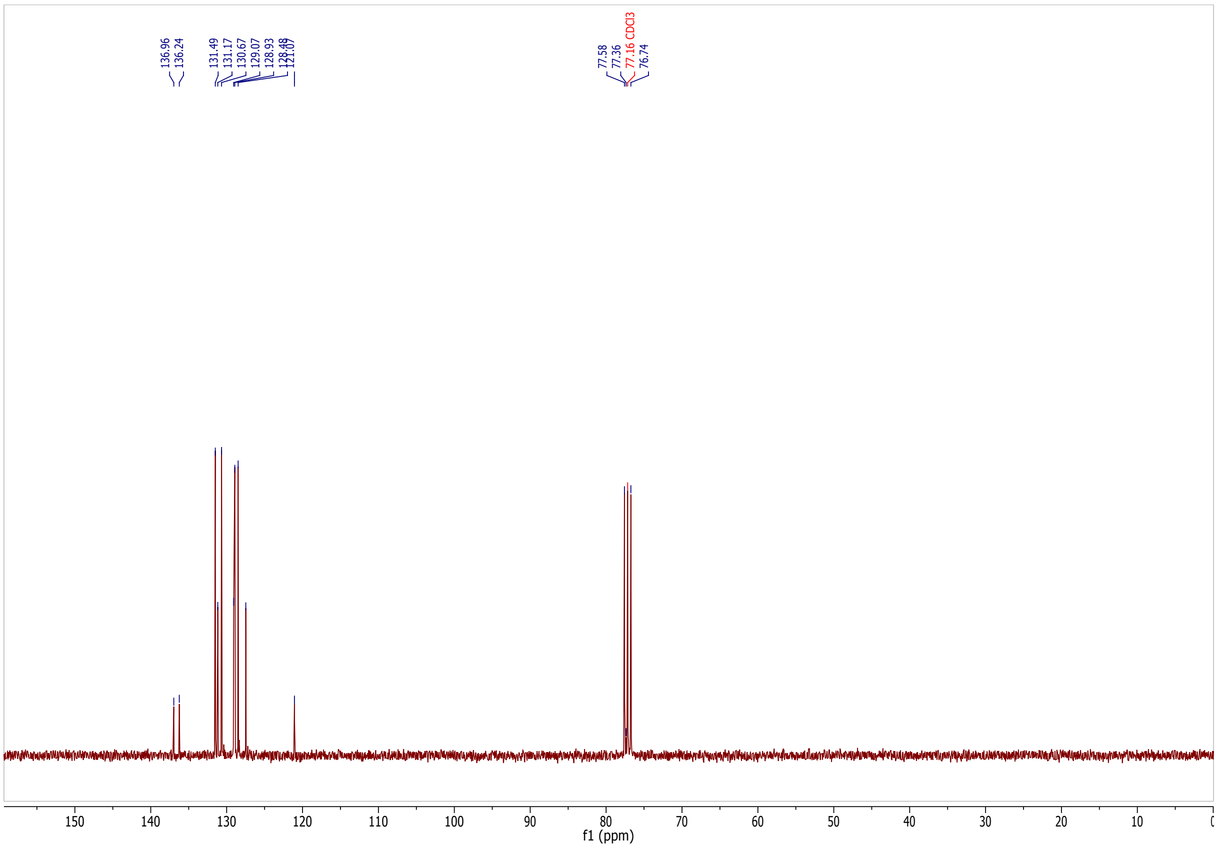


Figure SI 20.^{13}C-NMR of (*Z*)-1-bromo-4-styrylbenzene **2d**.

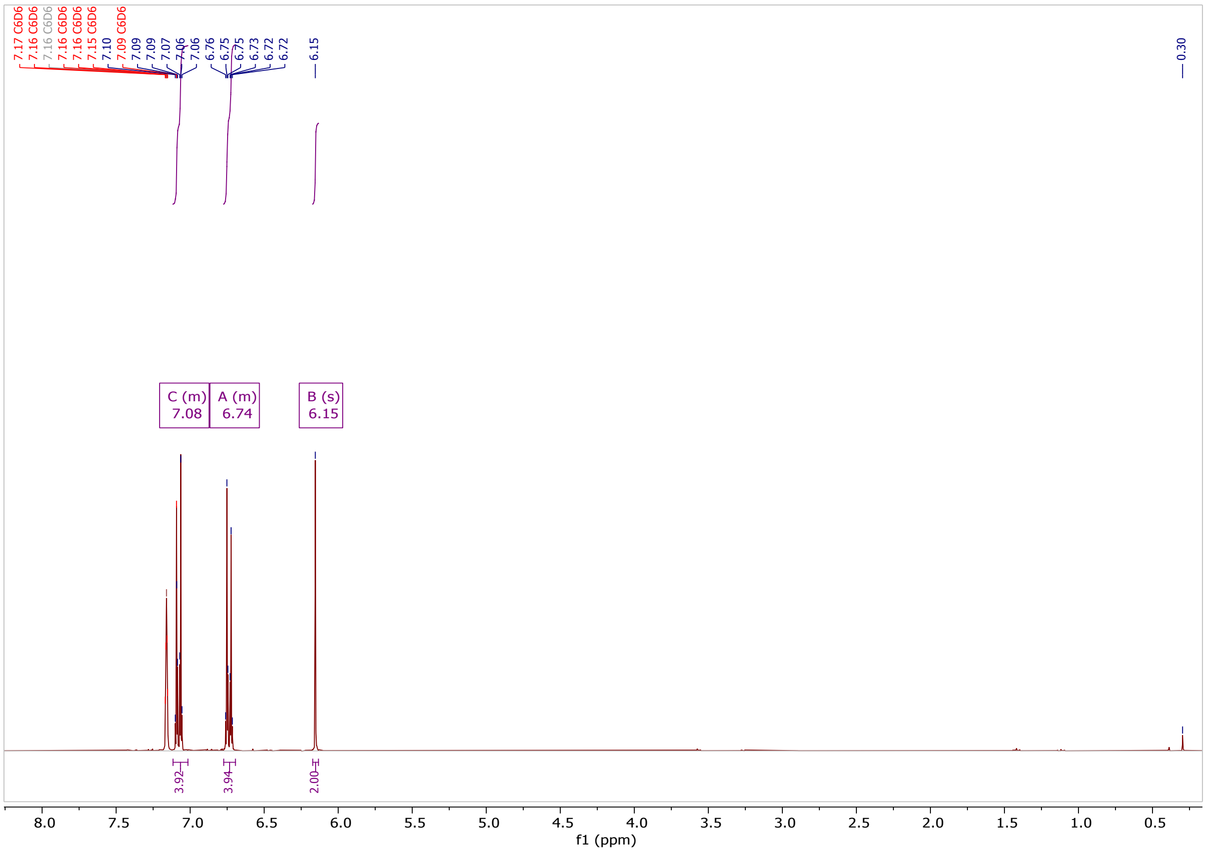


Figure SI 21. ^{1}H-NMR of (*Z*)-1,2-bis(4-bromophenyl)ethene **2e**.

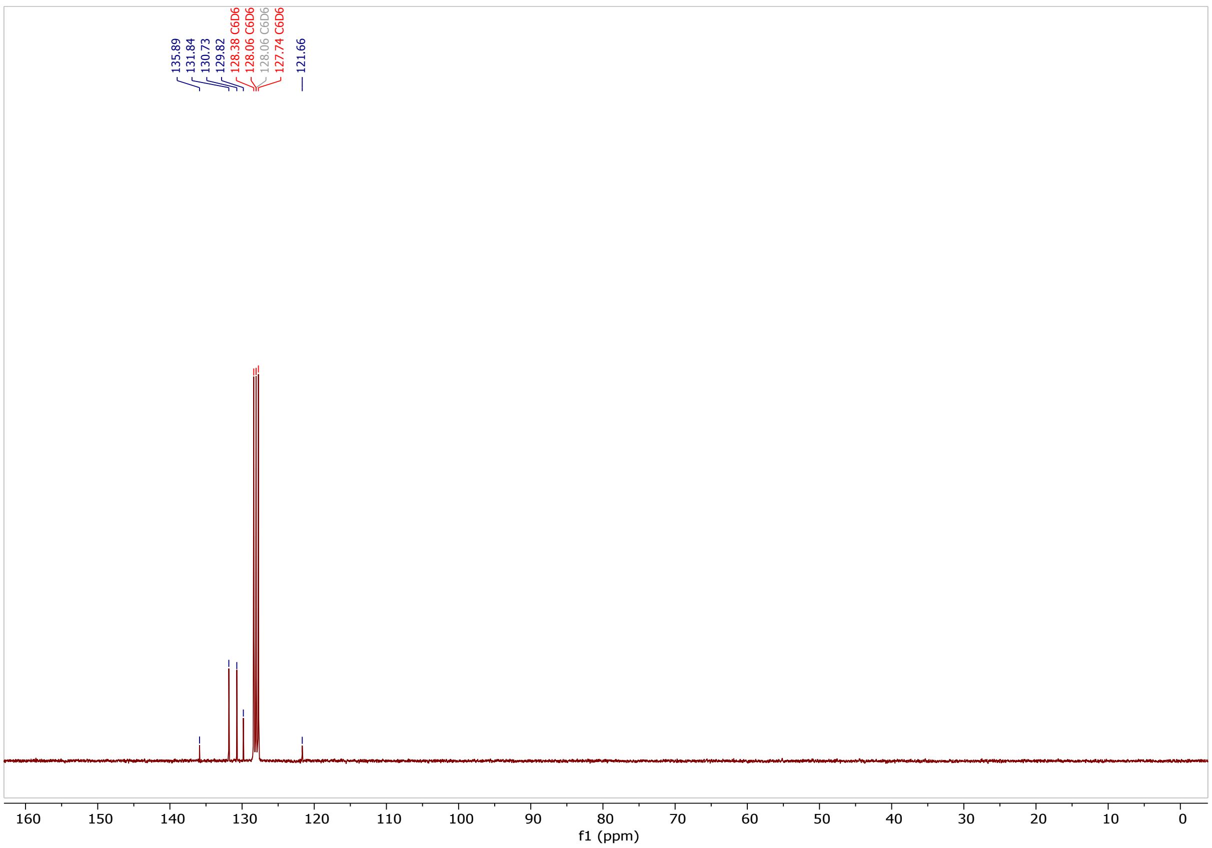


Figure SI 22. ^{13}C-NMR of (*Z*)-1,2-bis(4-bromophenyl)ethene **2e**.

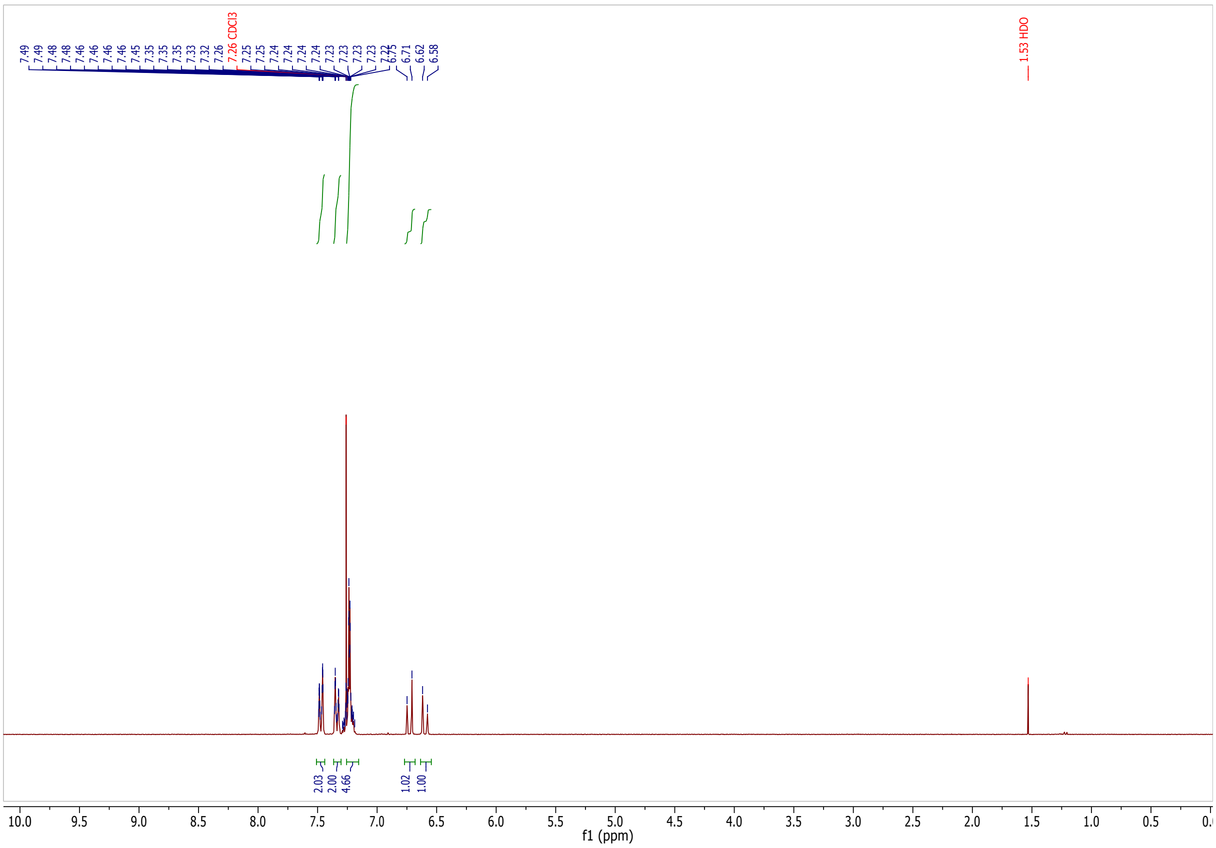


Figure SI 23. ^{1}H-NMR of (*Z*)-1-styryl-4-(trifluoromethyl)benzene **2f**.

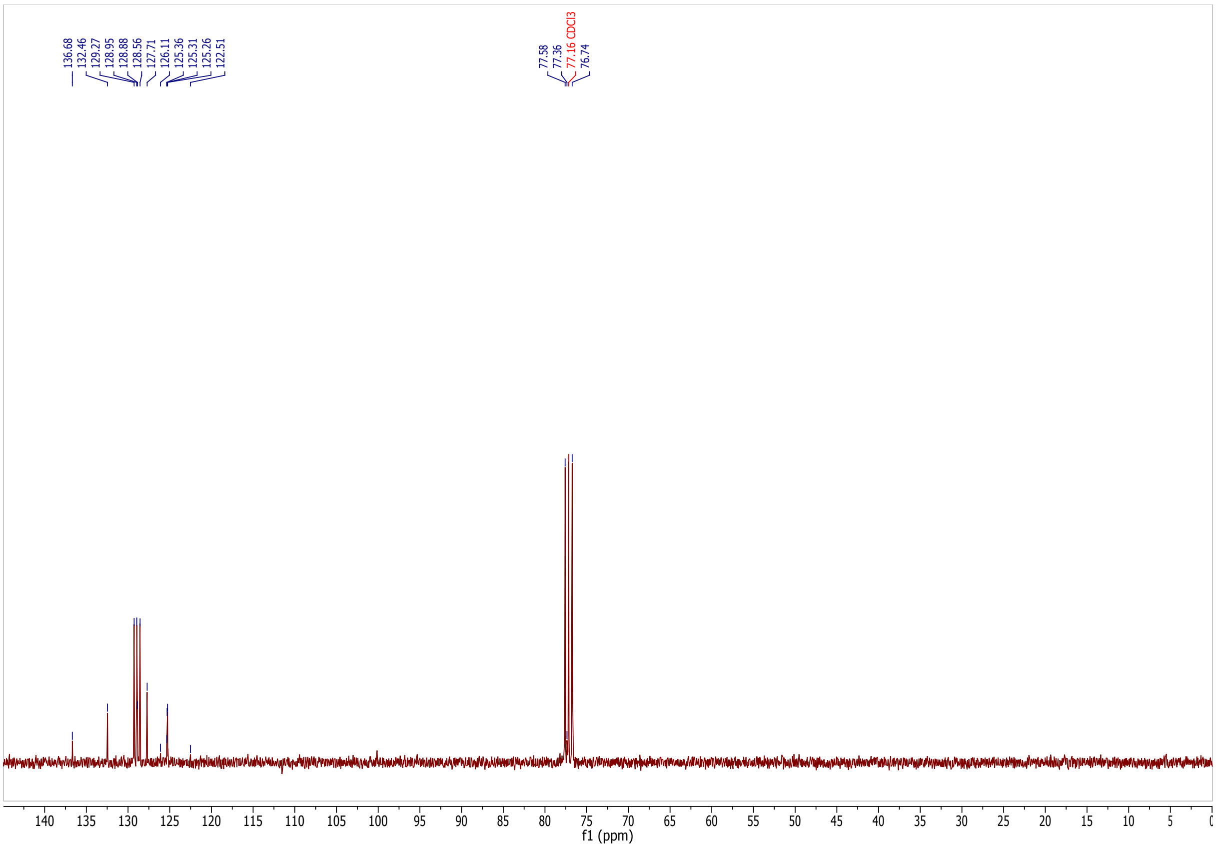


Figure SI 24. ^{13}C-NMR of (*Z*)-1-styryl-4-(trifluoromethyl)benzene **2f**.

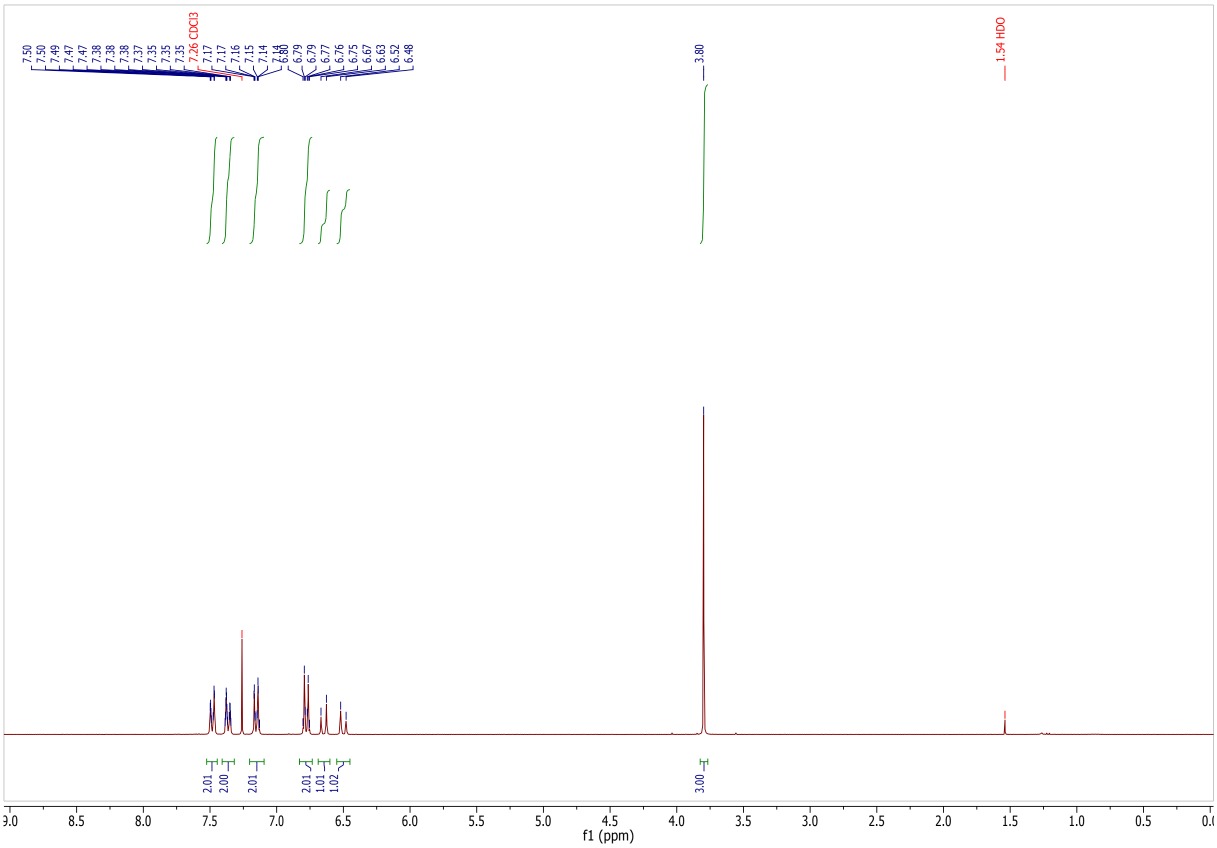


Figure SI 25. ^{1}H-NMR of (*Z*)-1-methoxy-4-(4-trifluoromethyl)styryl)benzene **2g**.

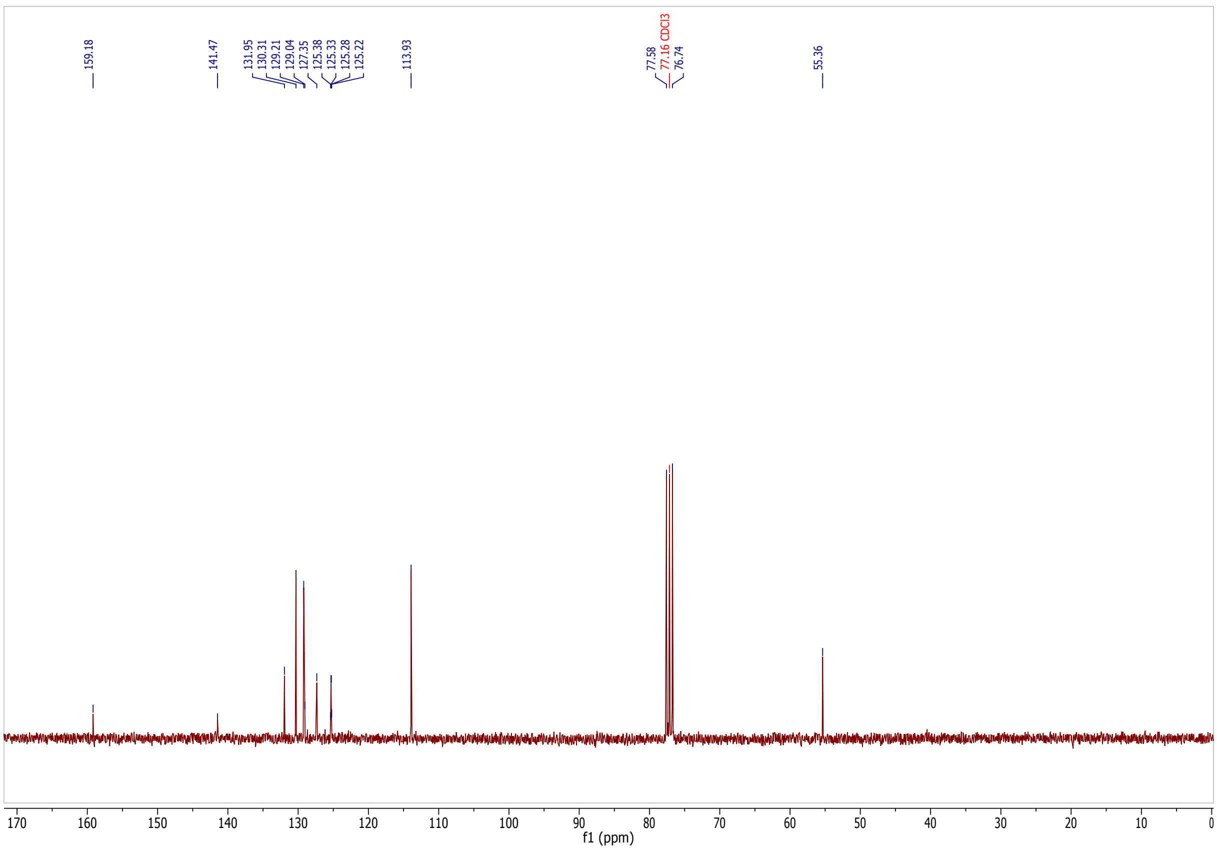


Figure SI 26. ^{13}C-NMR of (*Z*)-1-methoxy-4-(4-trifluoromethyl)styryl)benzene **2g**.

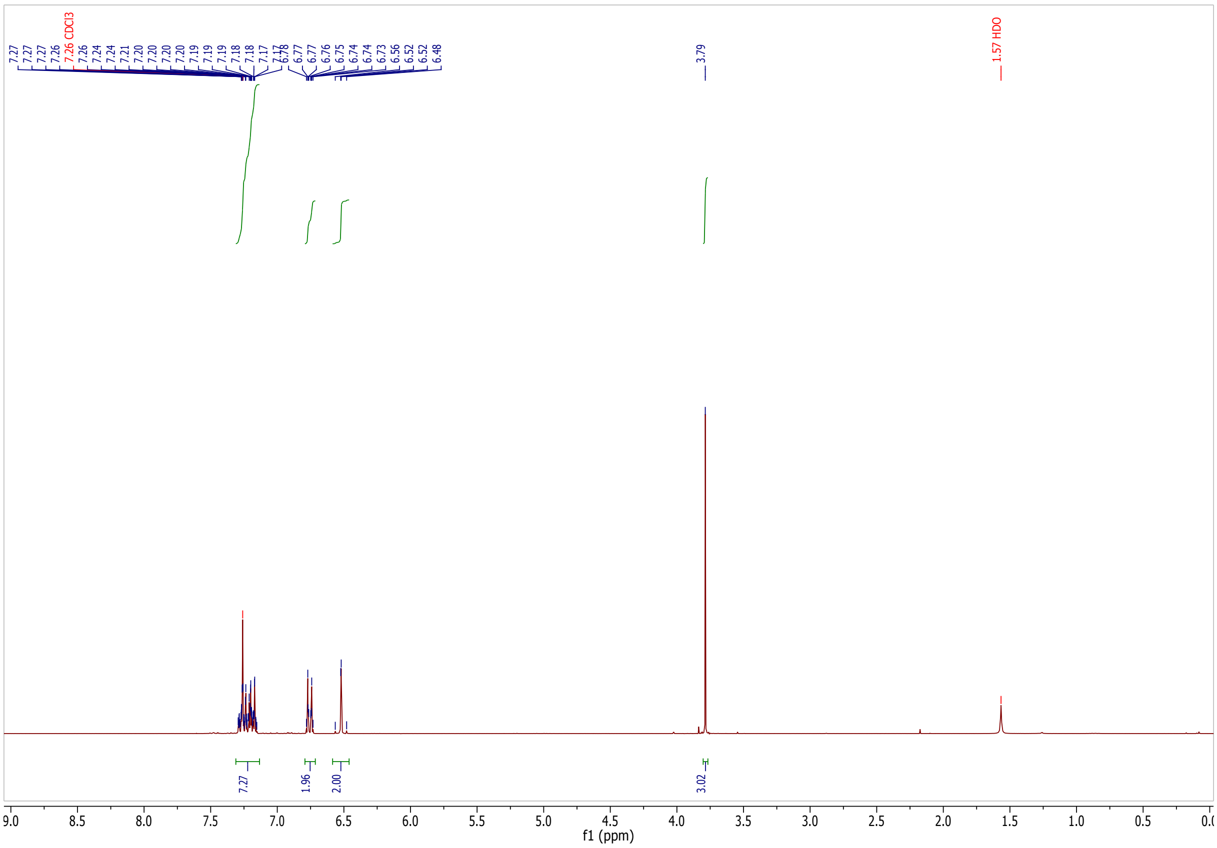


Figure SI 27. ^{1}H-NMR of (*Z*)-1-methoxy-4-styrylbenzene **2h**.

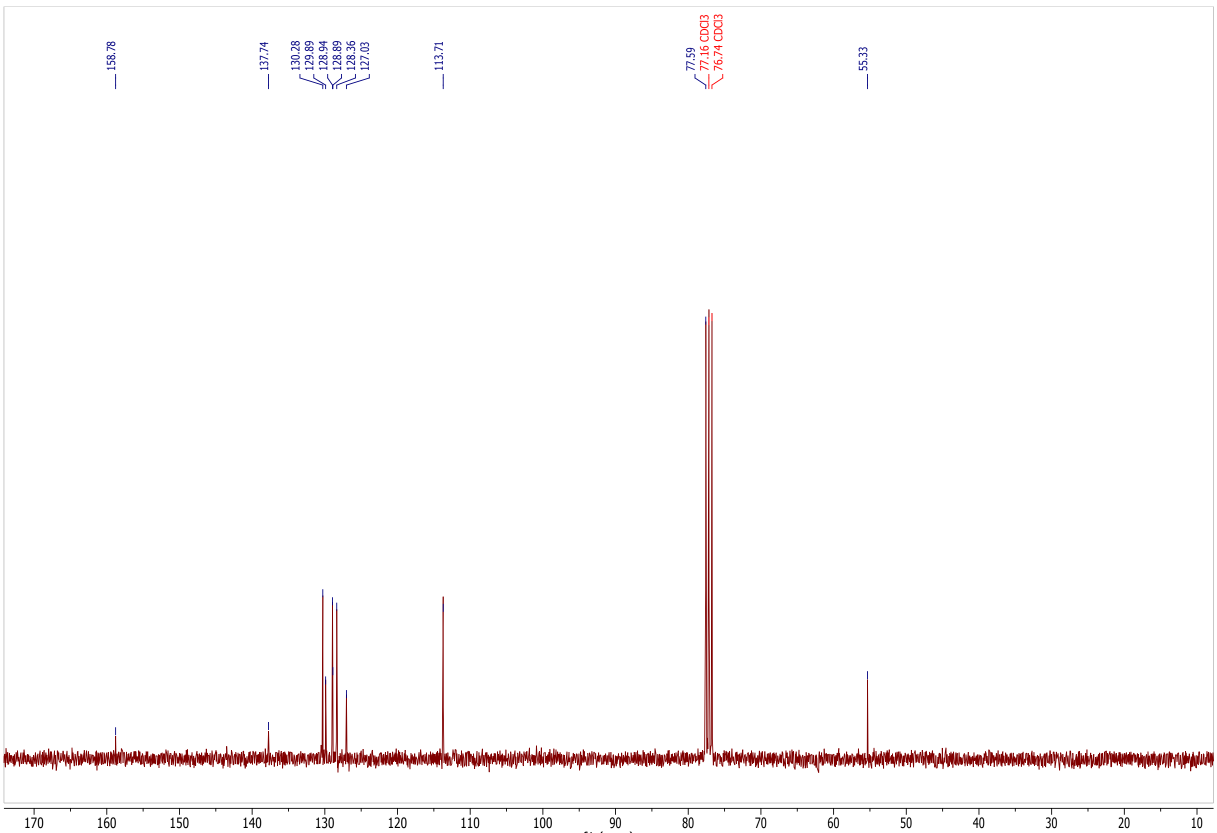


Figure SI 28. ^{13}C-NMR of (*Z*)-1-methoxy-4-styrylbenzene **2h**.

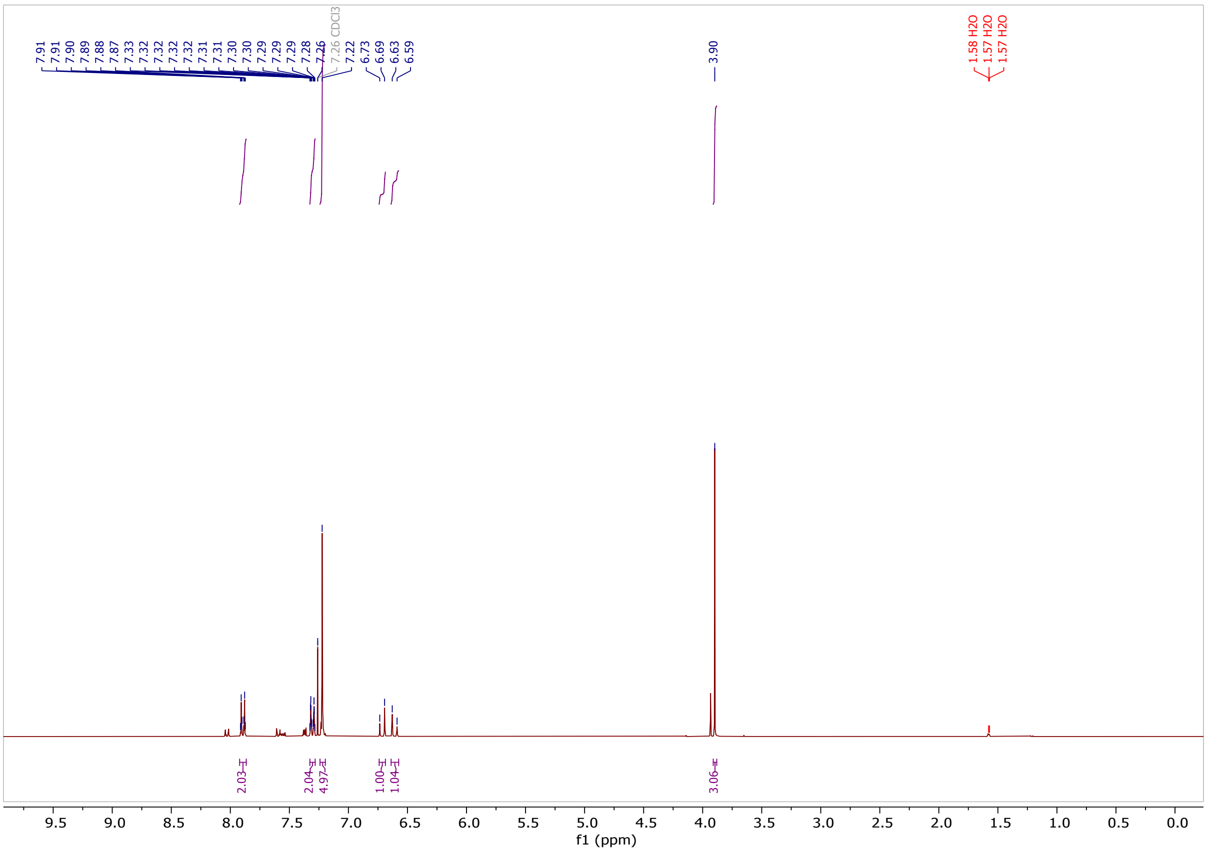


Figure SI 29. ^{1}H-NMR of Methyl-(*Z*)-4-styrylbenzoate **2i**.

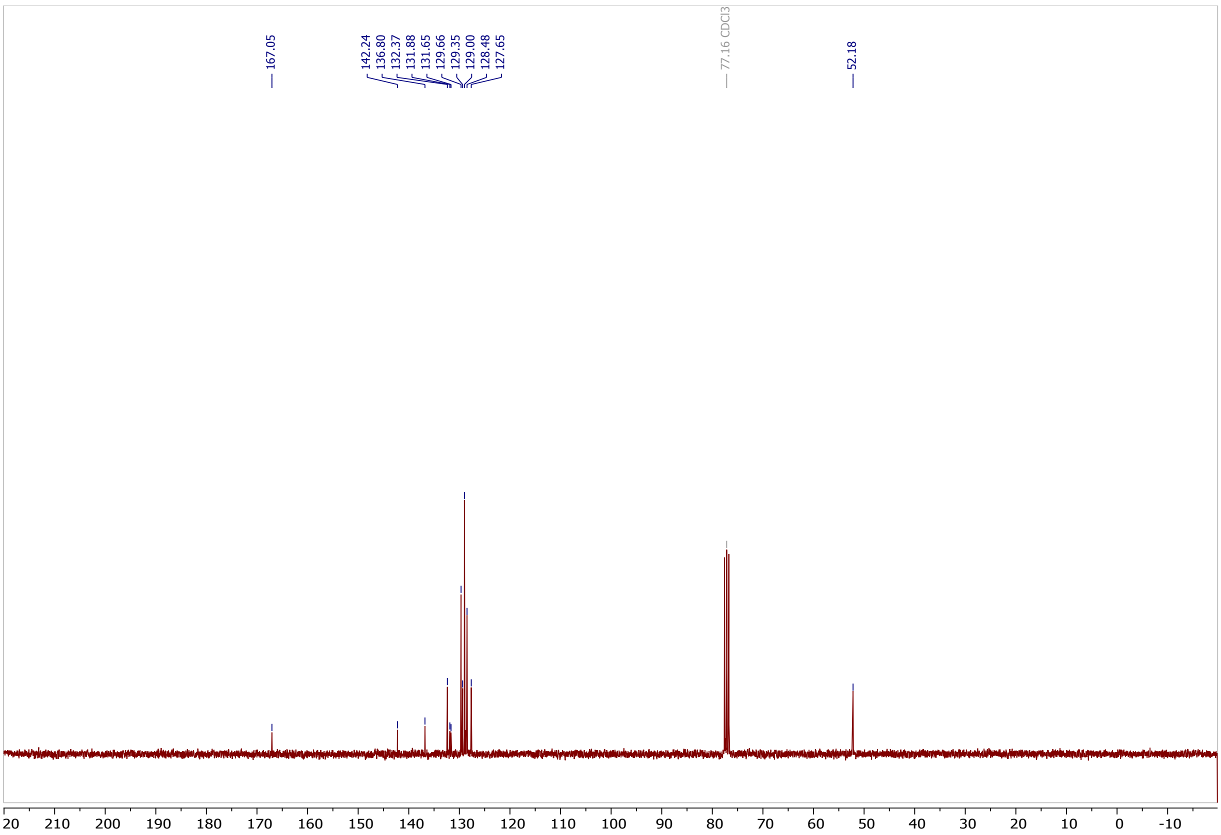


Figure SI 30. ^{13}C-NMR of Methyl-(*Z*)-4-styrylbenzoate **2i**.

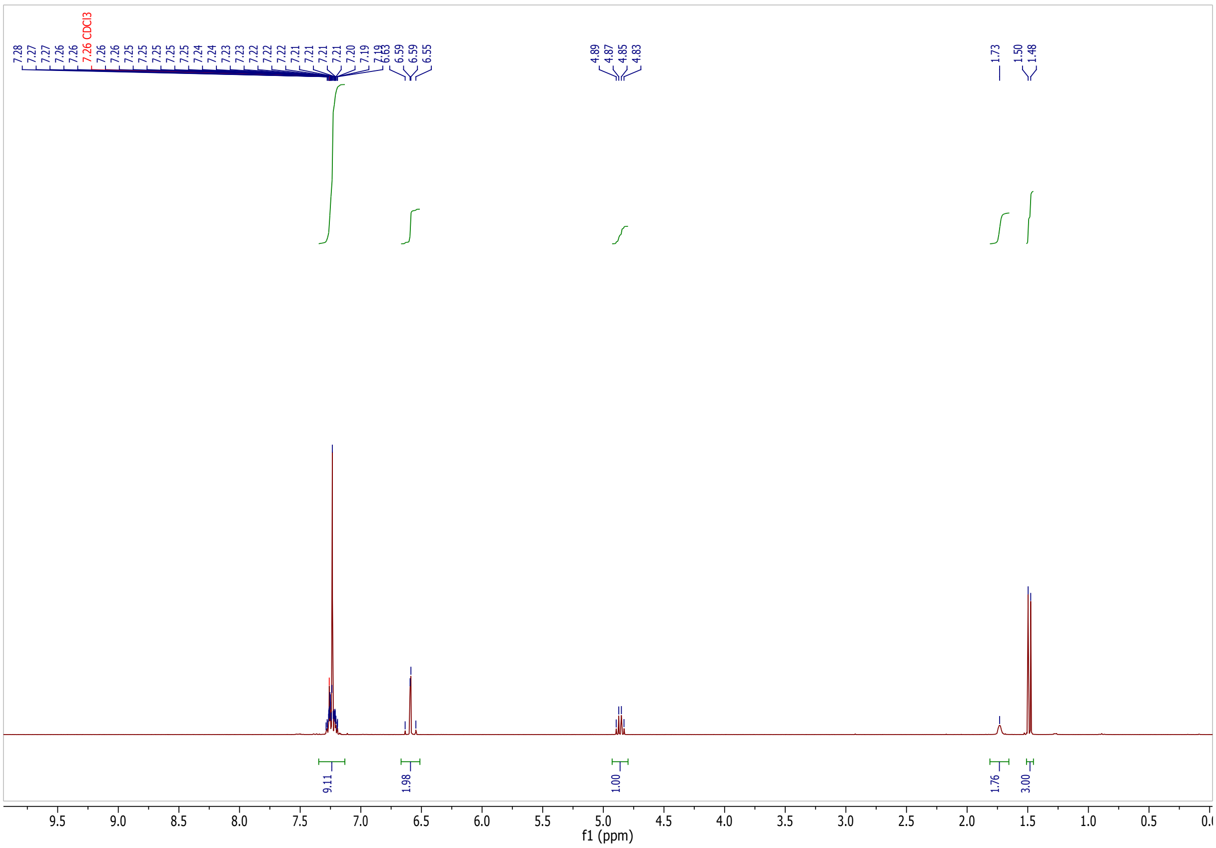


Figure SI 31. ^{1}H-NMR of (*Z*)-1-(4-styrylphenyl)ethan-1-ol **2j**.

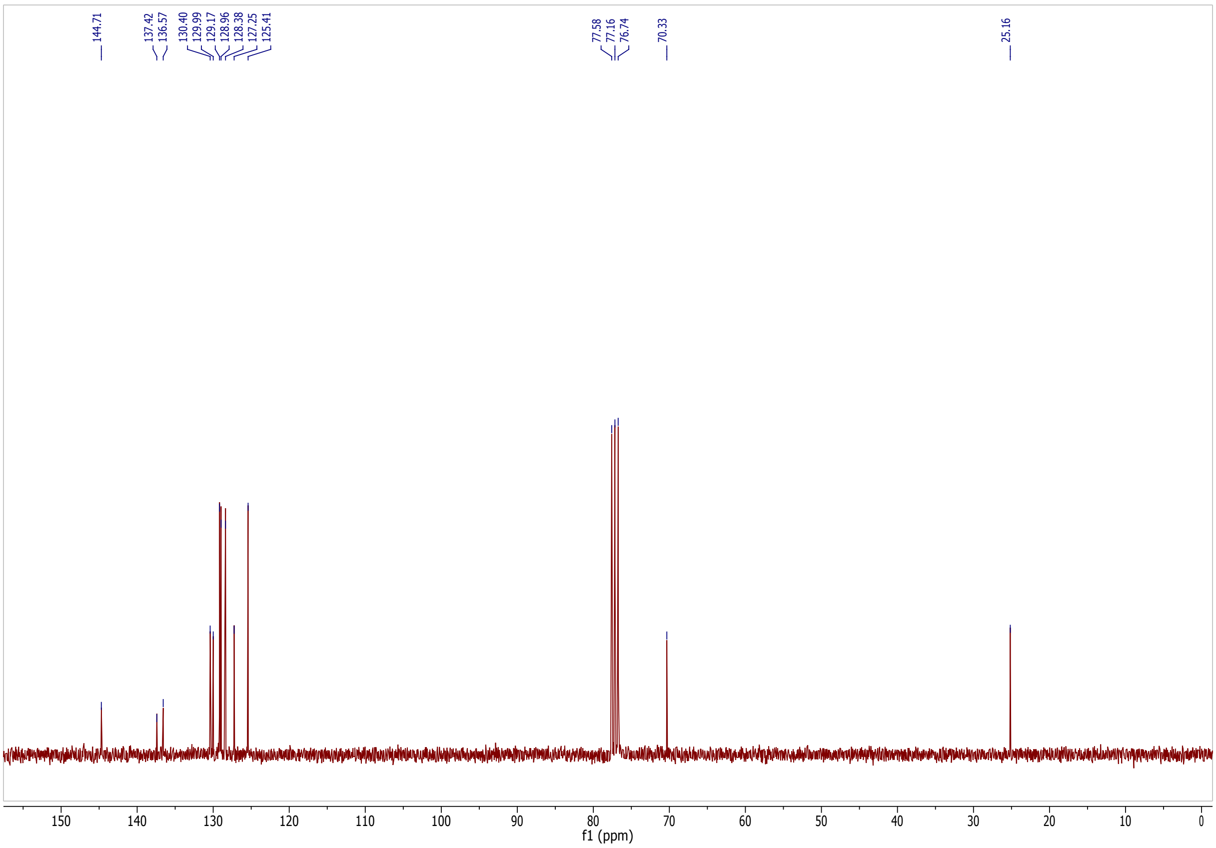


Figure SI 32.^{13}C-NMR of (*Z*)-1-(4-styrylphenyl)ethan-1-ol **2j**.

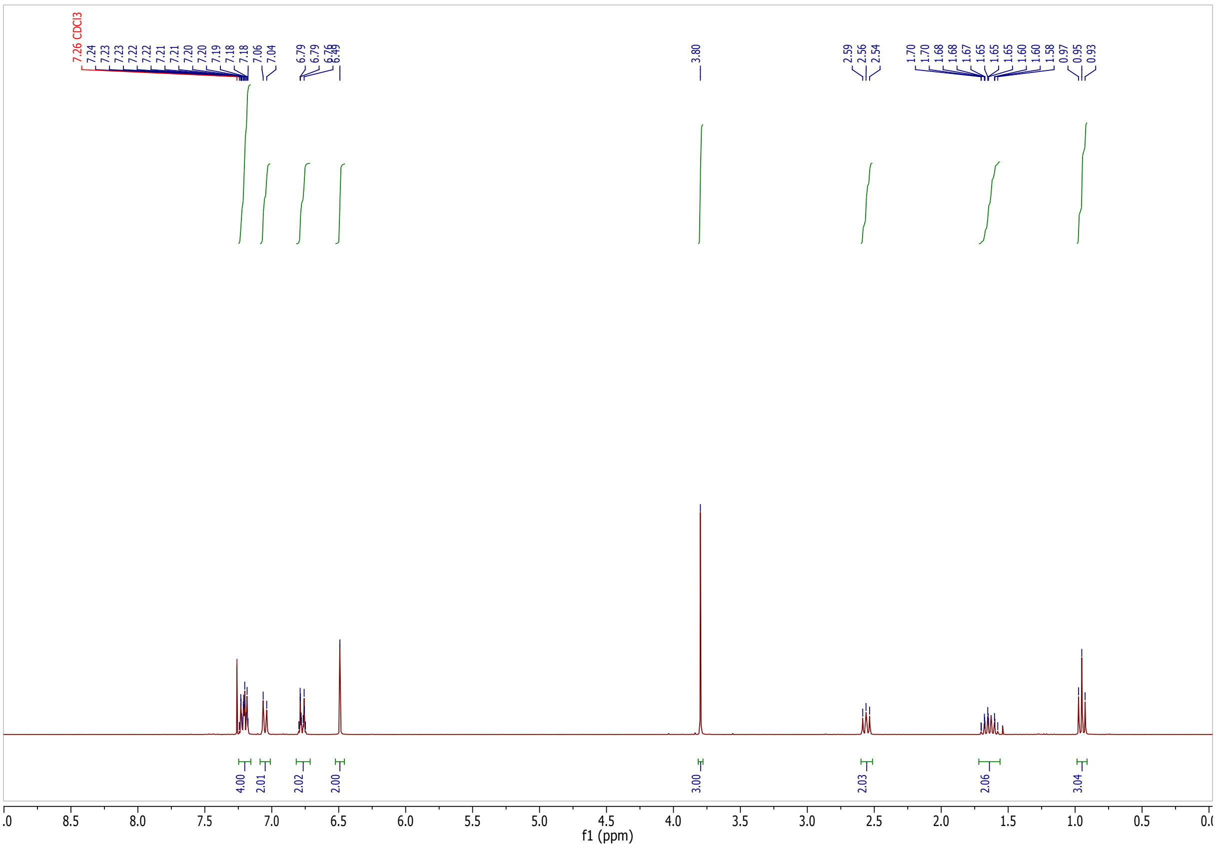


Figure SI 33. ^{1}H-NMR of (*Z*)-1-methoxy-4-(4-propylstyryl)benzene **2k**.

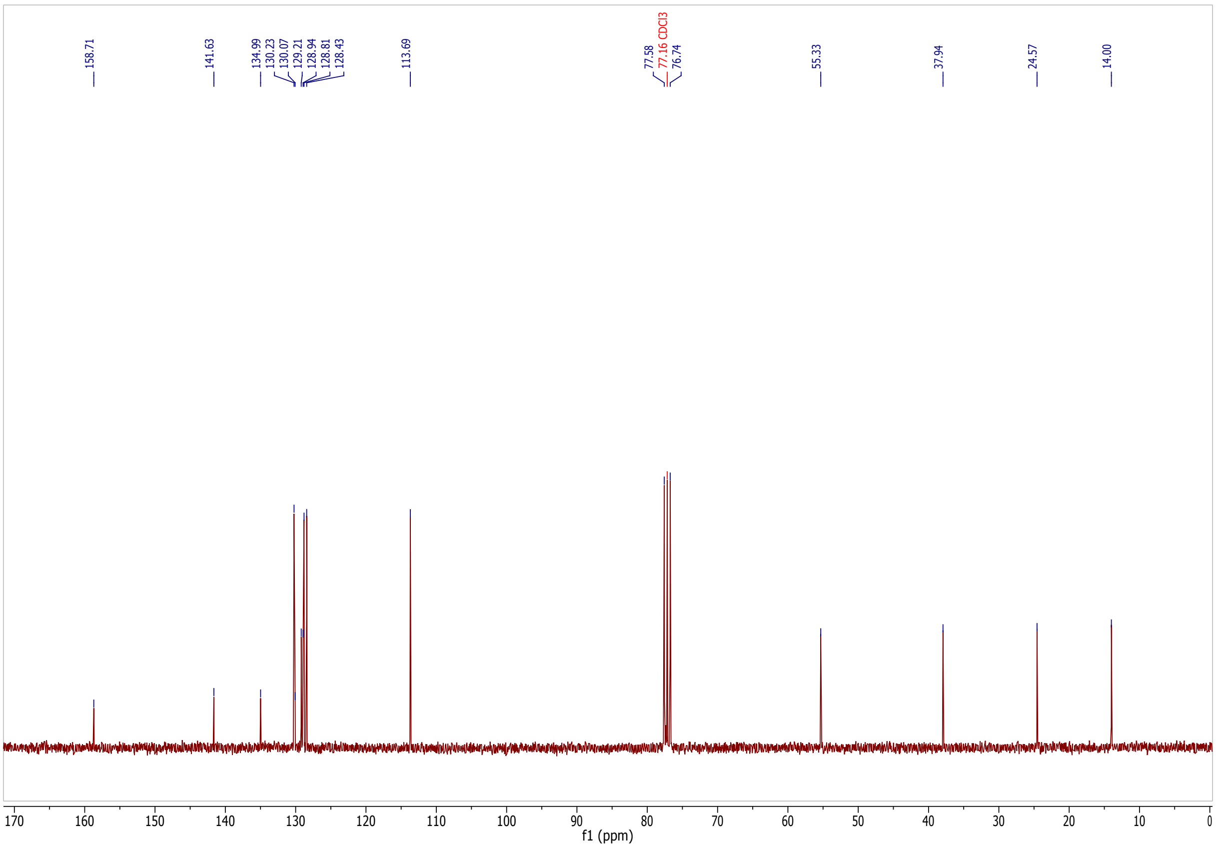


Figure SI 34.^{13}C-NMR of (*Z*)-1-methoxy-4-(4-propylstyryl)benzene **2k**.

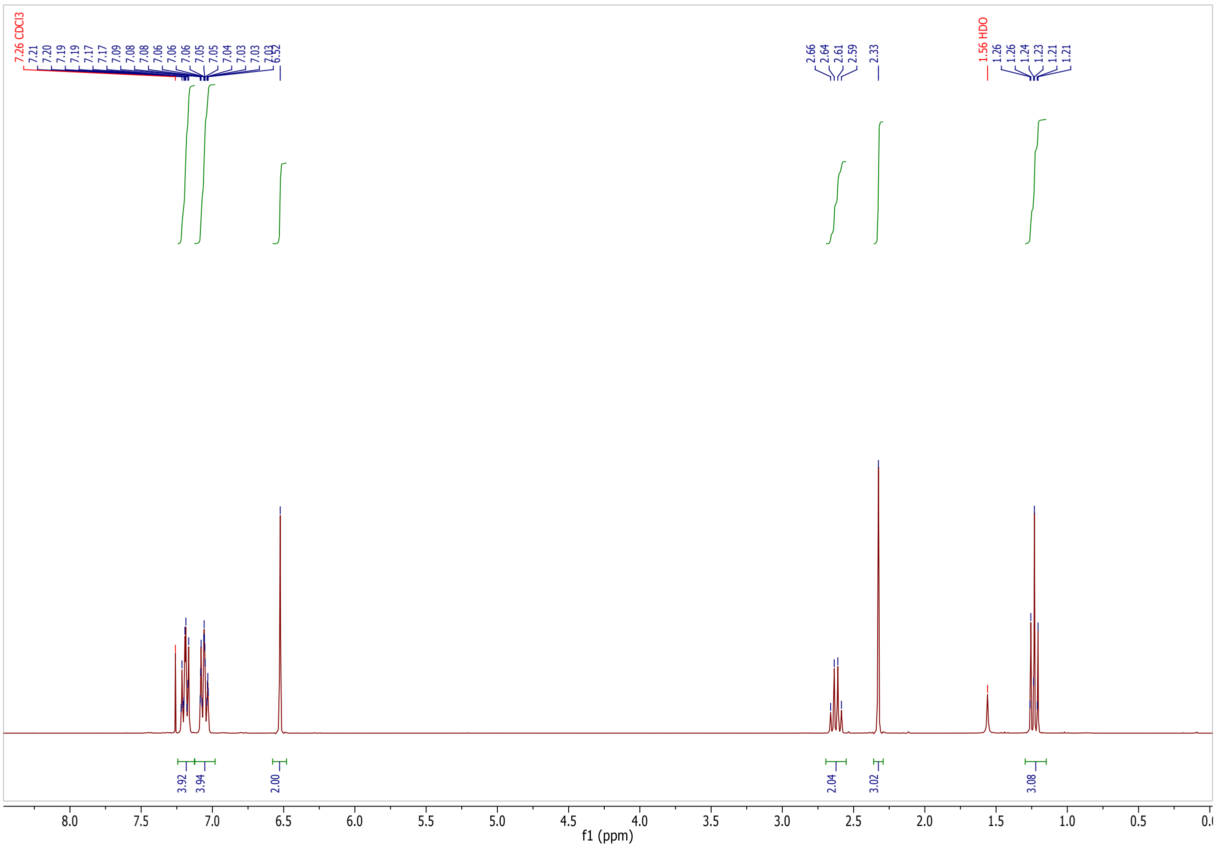


Figure SI 35.[1]H-NMR of (*Z*)-1-ethyl-4-(4-methylstyryl)benzene **2l**.

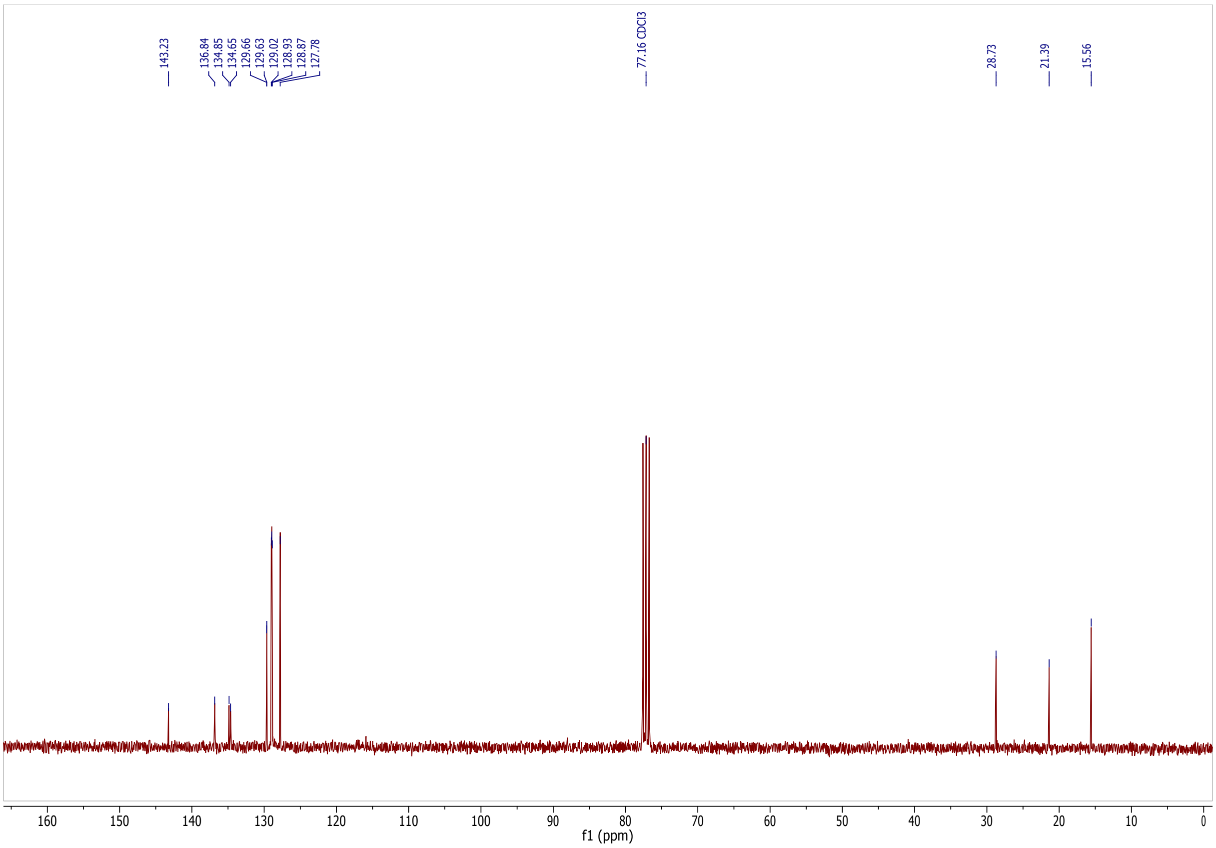


Figure SI 36. [13]C-NMR of (*Z*)-1-ethyl-4-(4-methylstyryl)benzene **2l**.

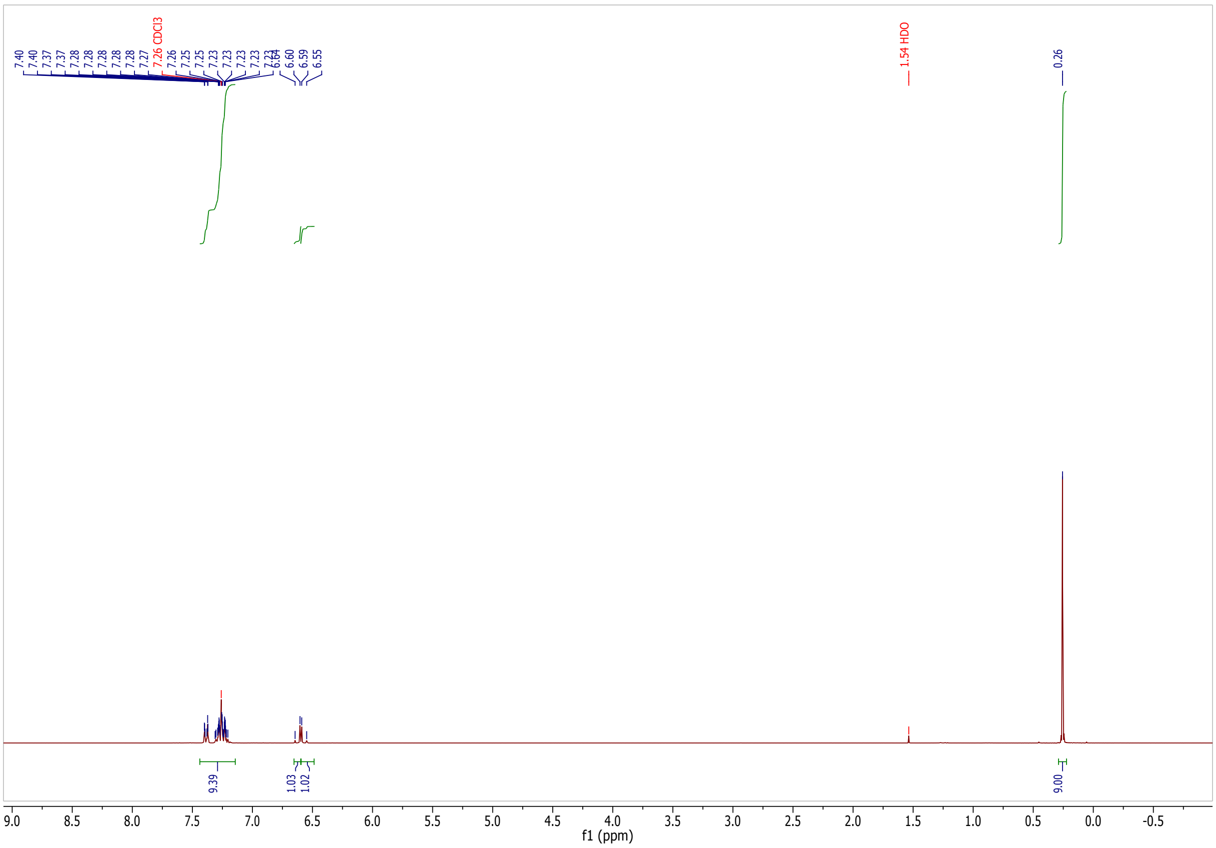


Figure SI 37.[1]H-NMR of (*Z*)-trimethyl(4-styrylphenyl)silane **2m**.

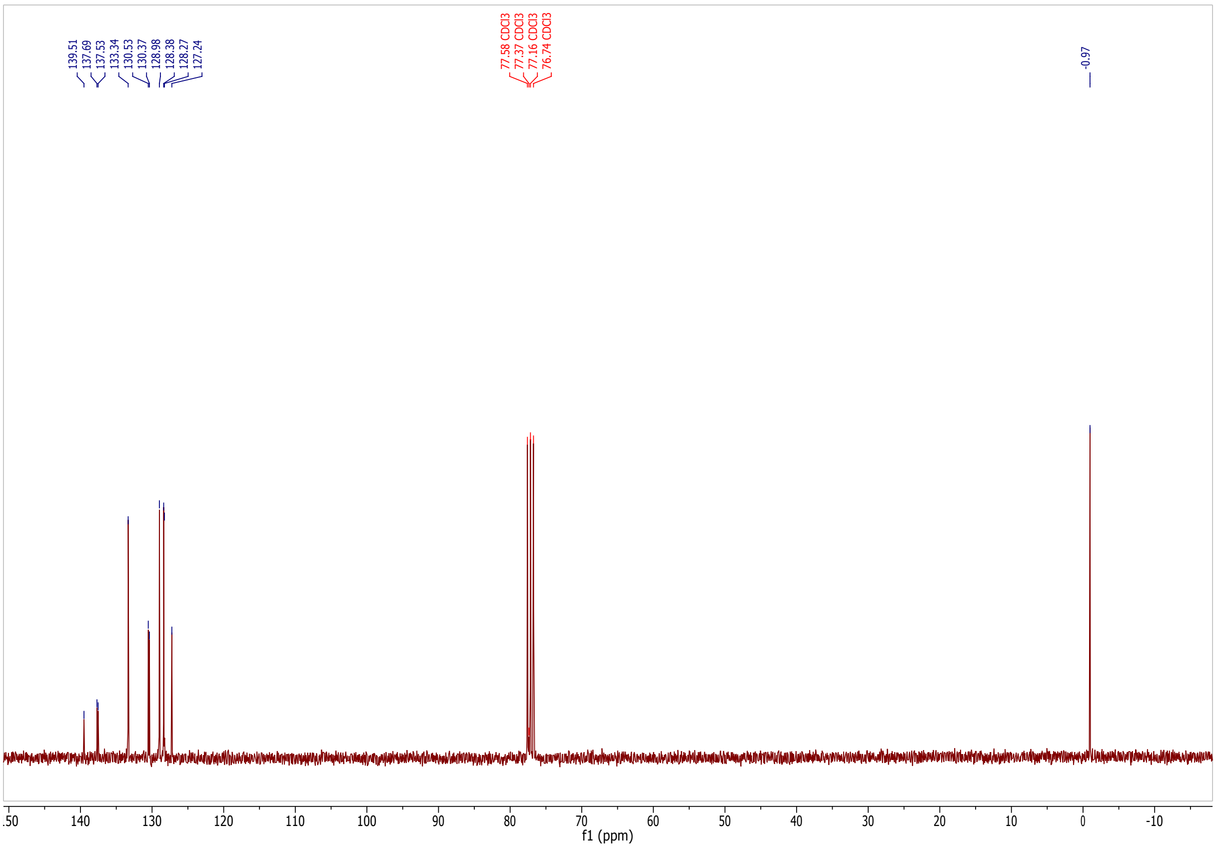


Figure SI 38. [13]C-NMR of (*Z*)-trimethyl(4-styrylphenyl)silane **2m**.

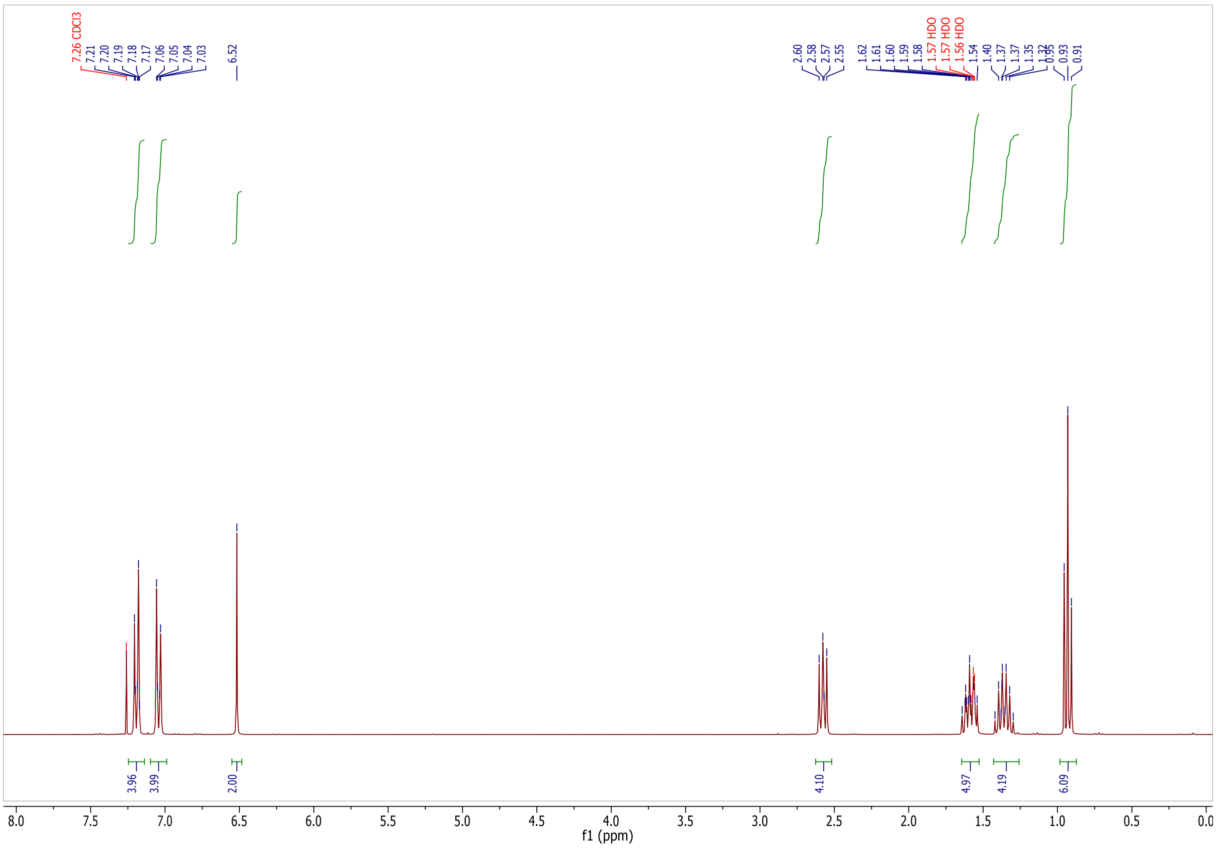


Figure SI 39. ^{1}H-NMR of (*Z*)-1,2-bis(4-butylphenyl)ethane **2n**.

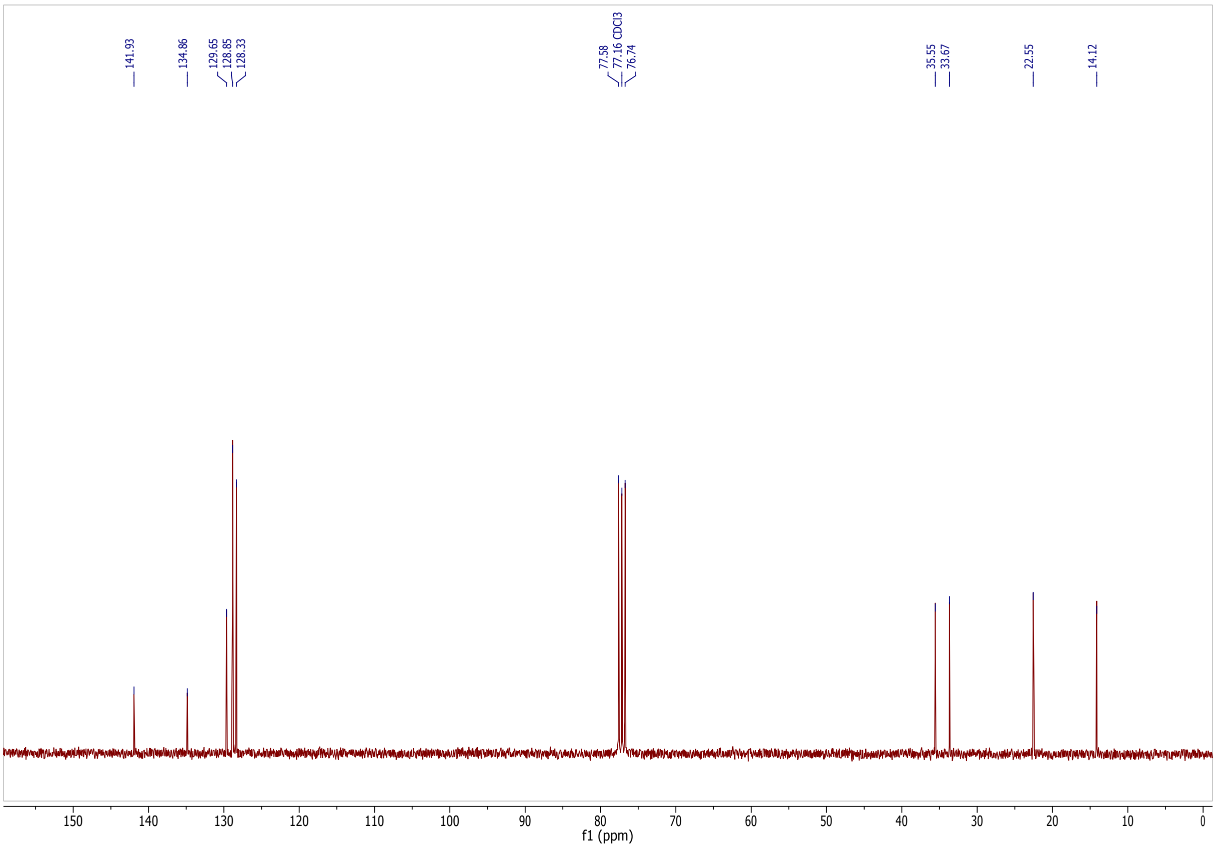


Figure SI 40.^{13}C-NMR of (*Z*)-1,2-bis(4-butylphenyl)ethane **2n.**

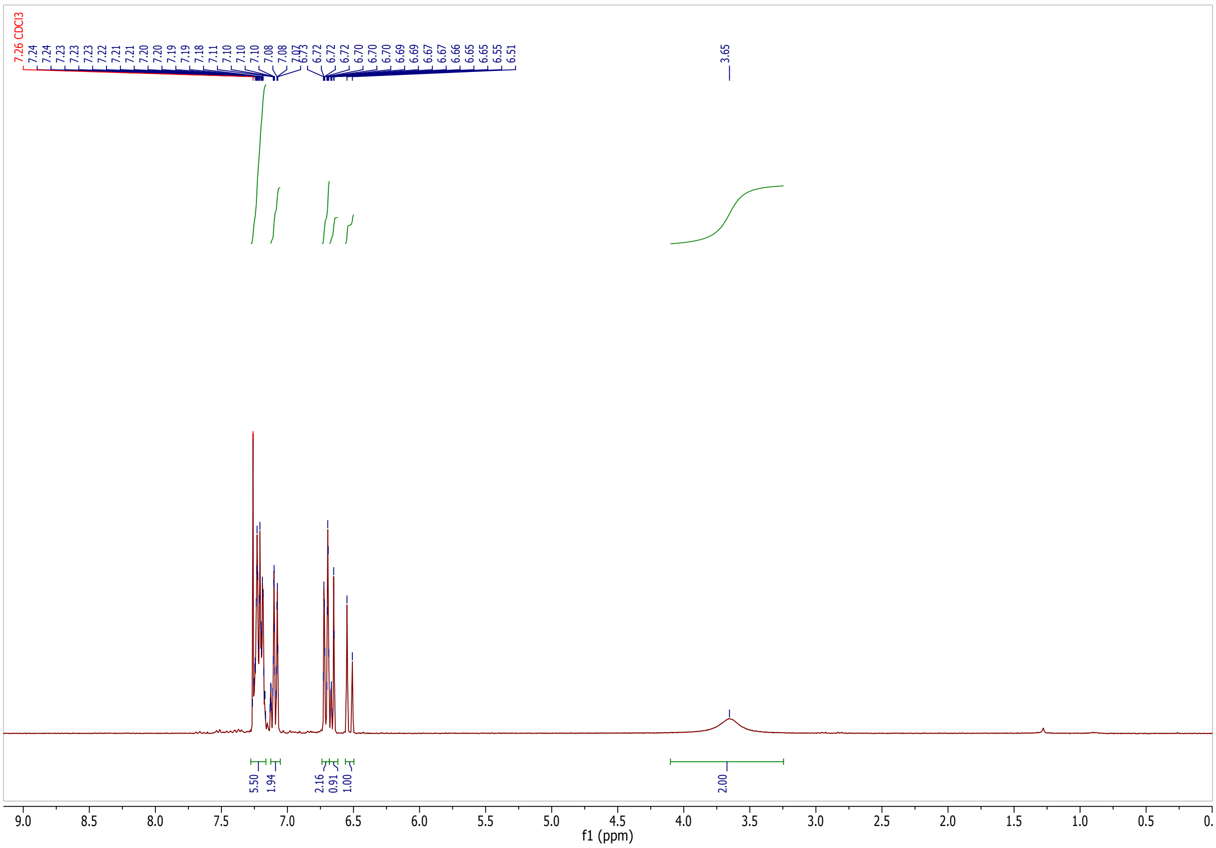


Figure SI 41. ^{1}H-NMR of (*Z*)-2-styrylaniline **2o.**

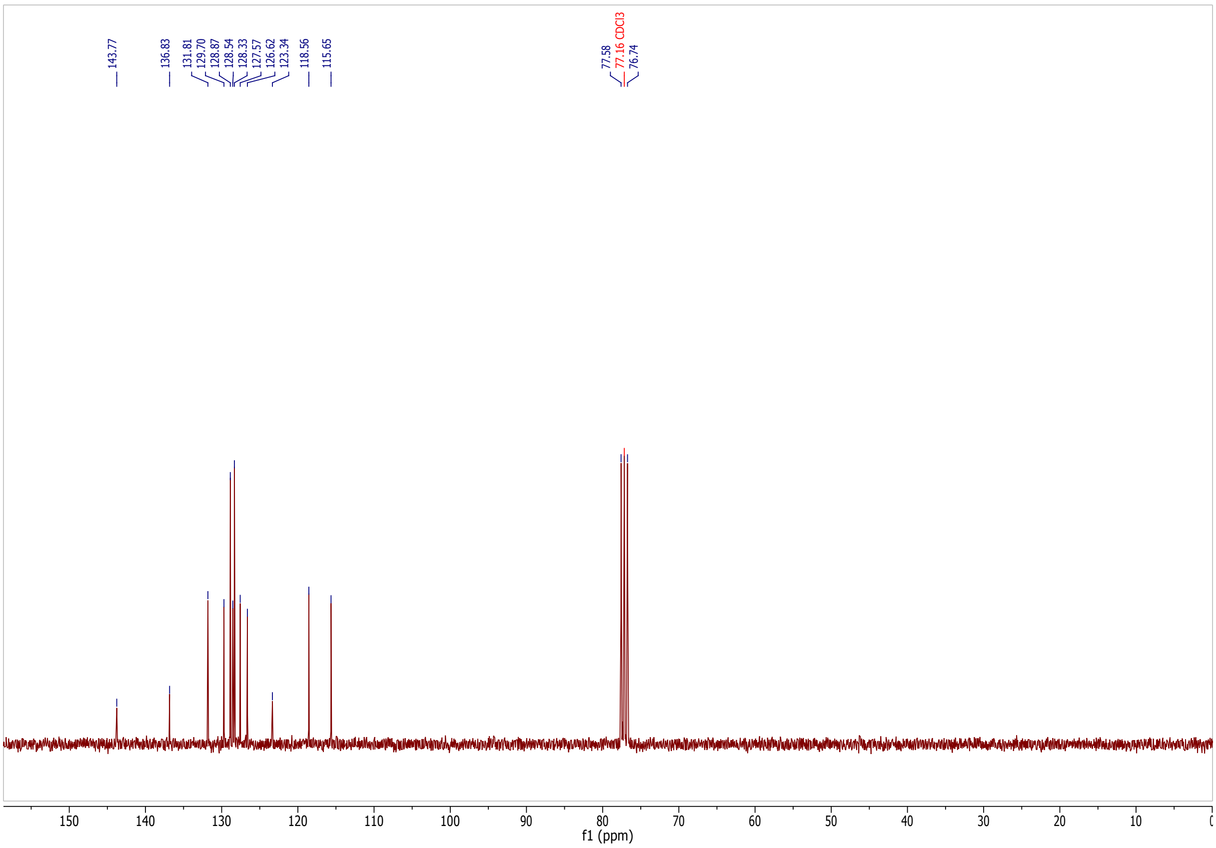


Figure SI 42.^{13}C-NMR of (*Z*)-2-styrylaniline **2o.**

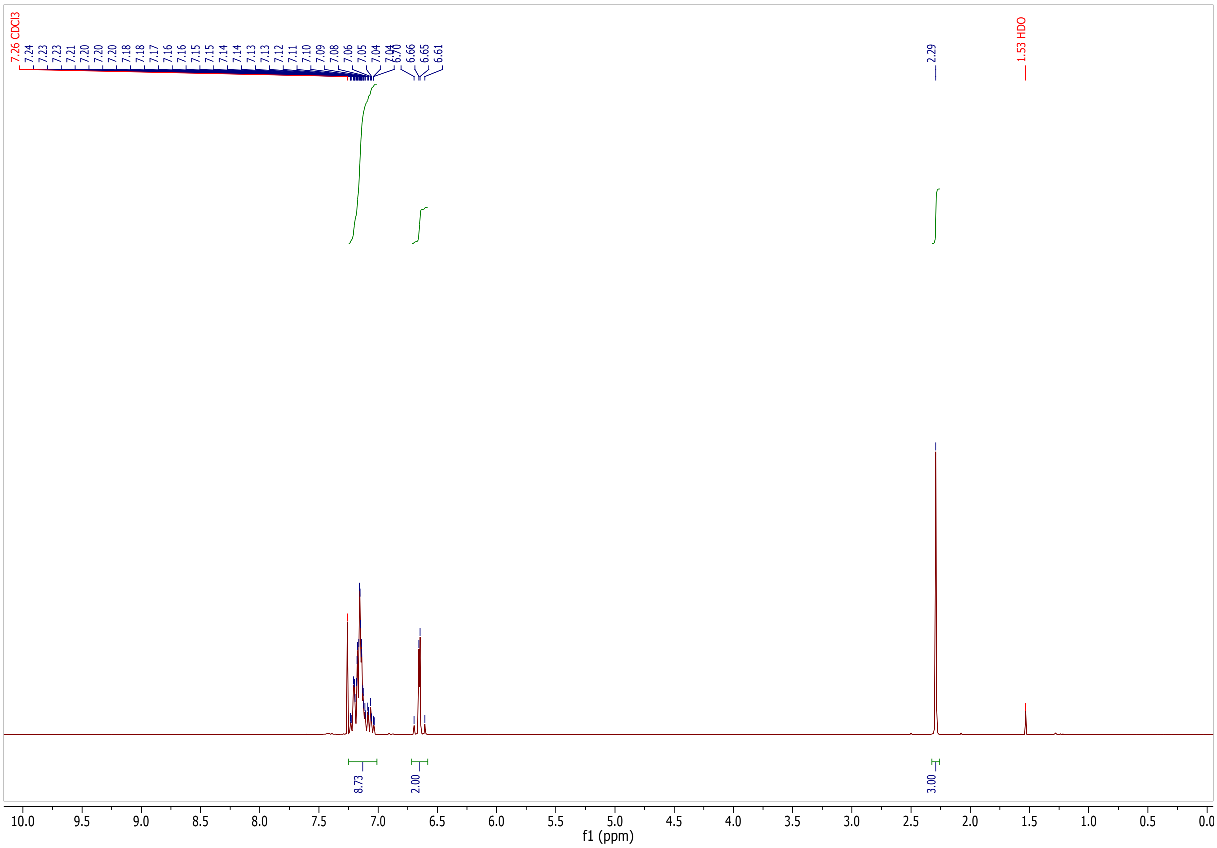


Figure SI 43.¹H-NMR of (*Z*)-1-methyl-2-styrylbenzene **2p**.

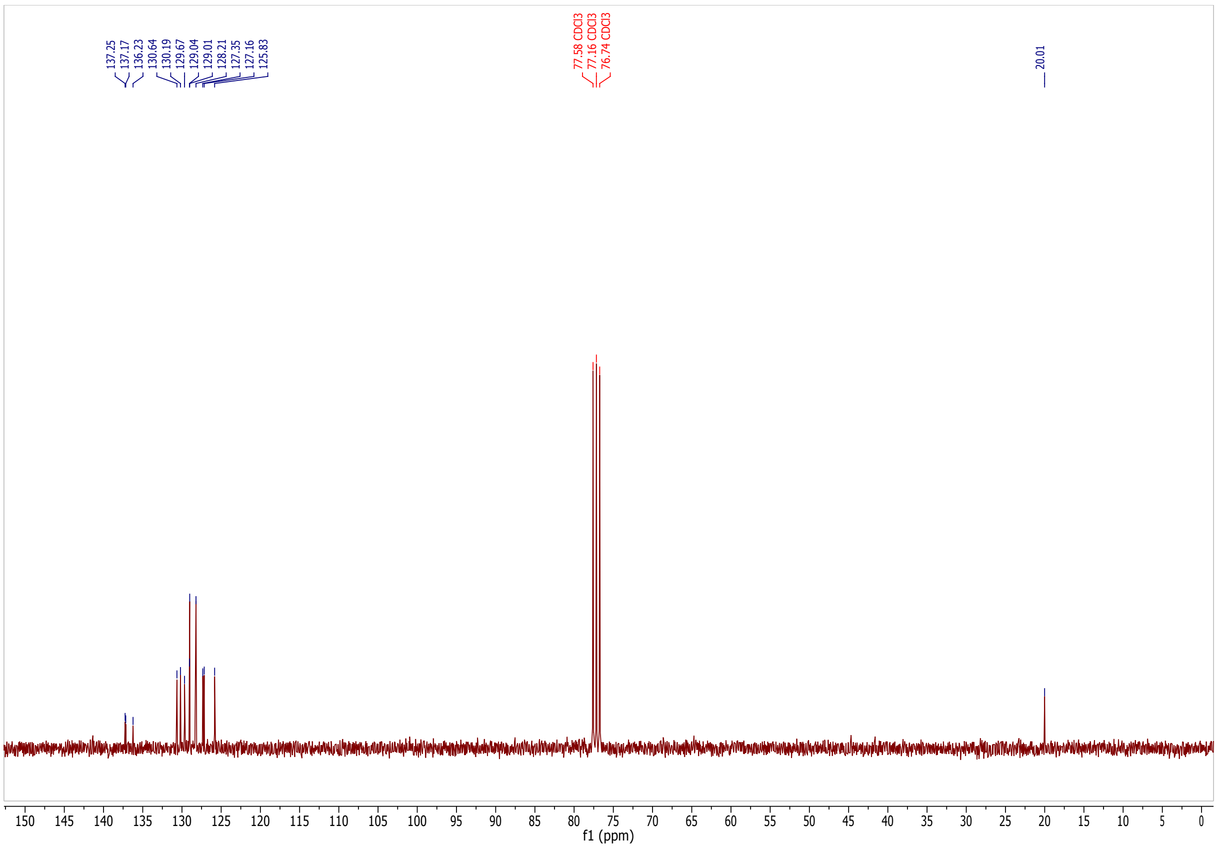


Figure SI 44. ¹³C-NMR of (*Z*)-1-methyl-2-styrylbenzene **2p**.

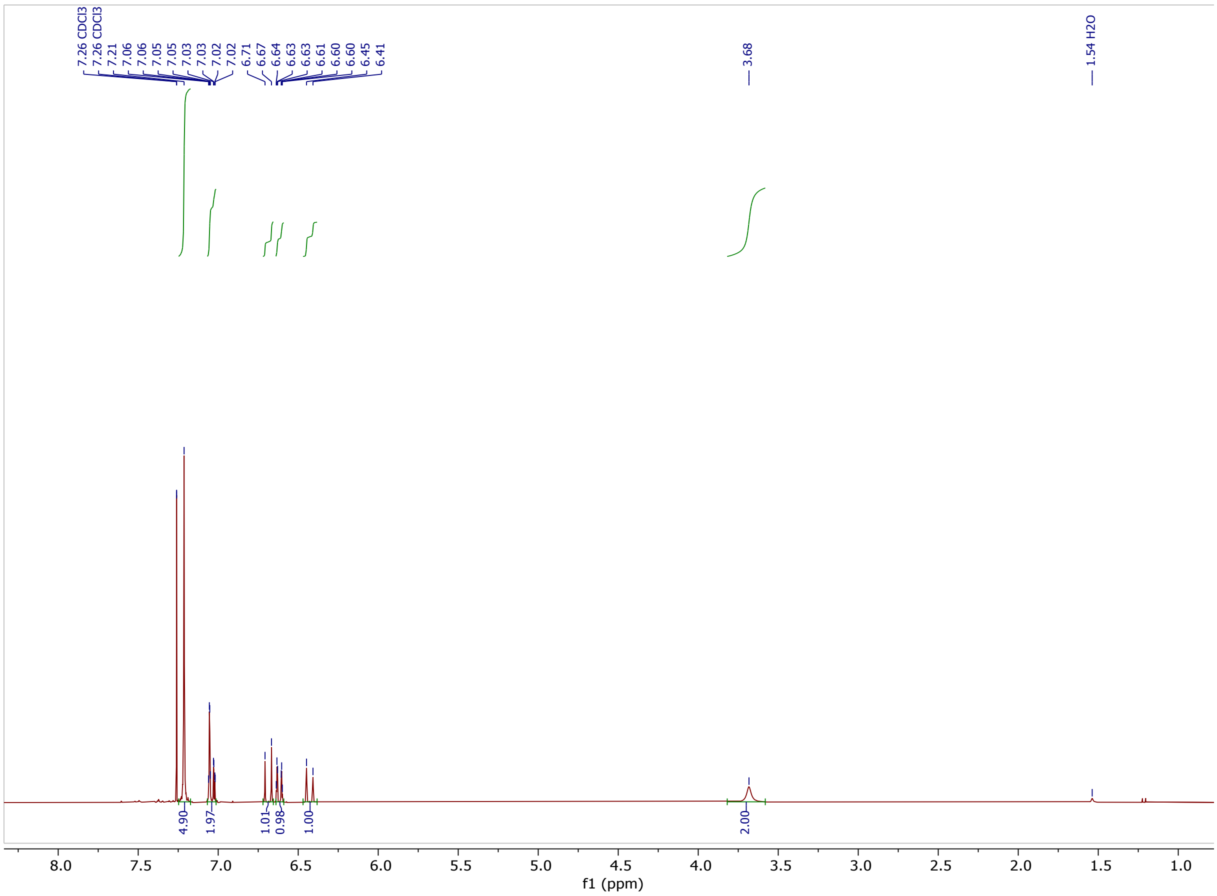


Figure SI 45.[1]H-NMR of (*Z*)-4-chloro-2-styrylaniline **2q**.

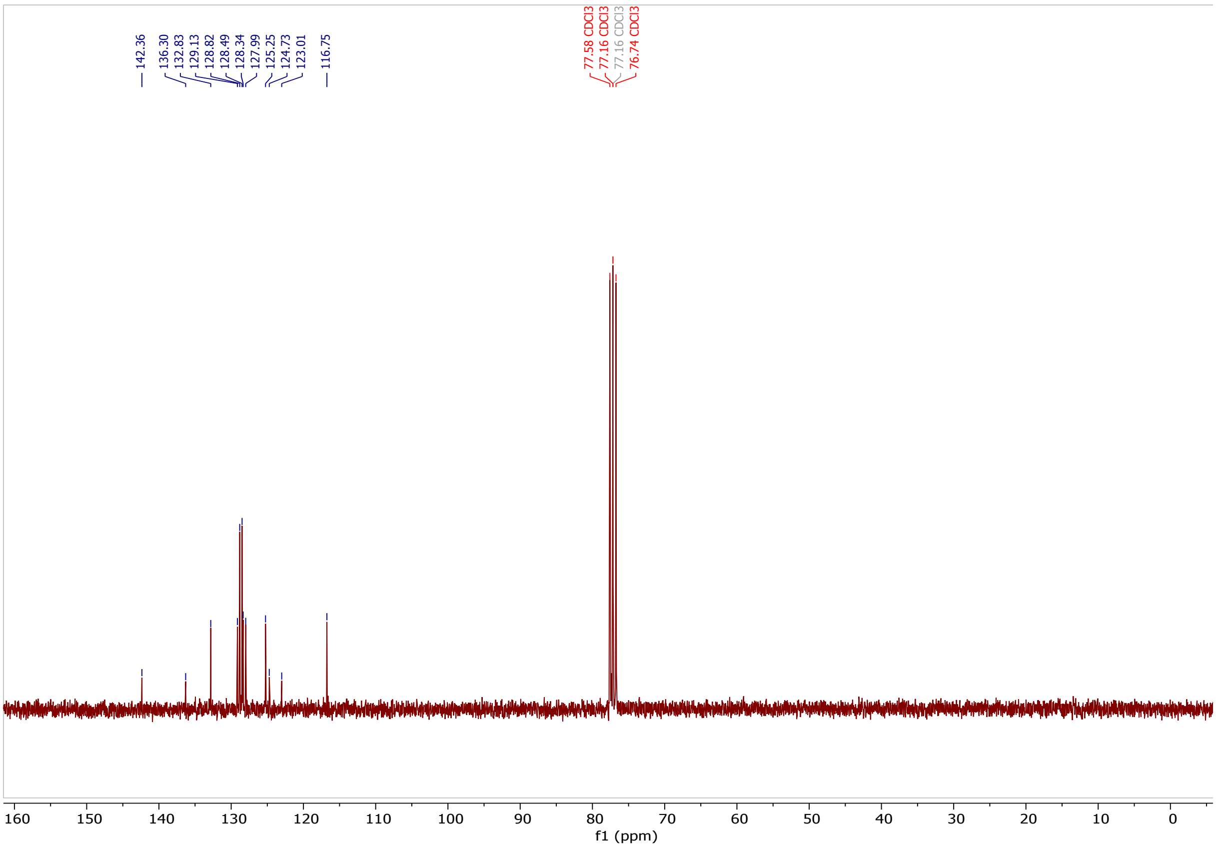


Figure SI 46. ^{13}C-NMR of (*Z*)-4-chloro-2-styrylaniline **2q**.

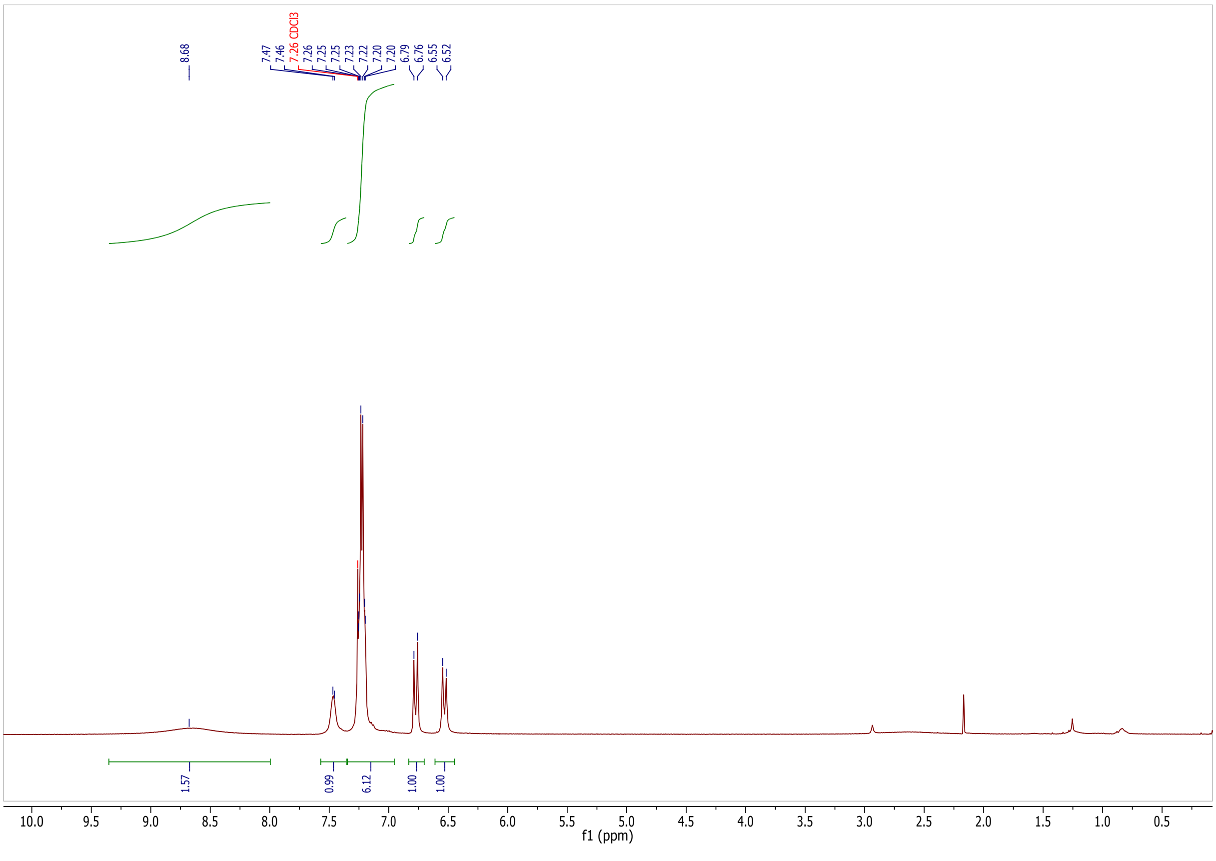


Figure SI 47. ^{1}H-NMR of (*Z*)-3-styrylpyridine **2r**.

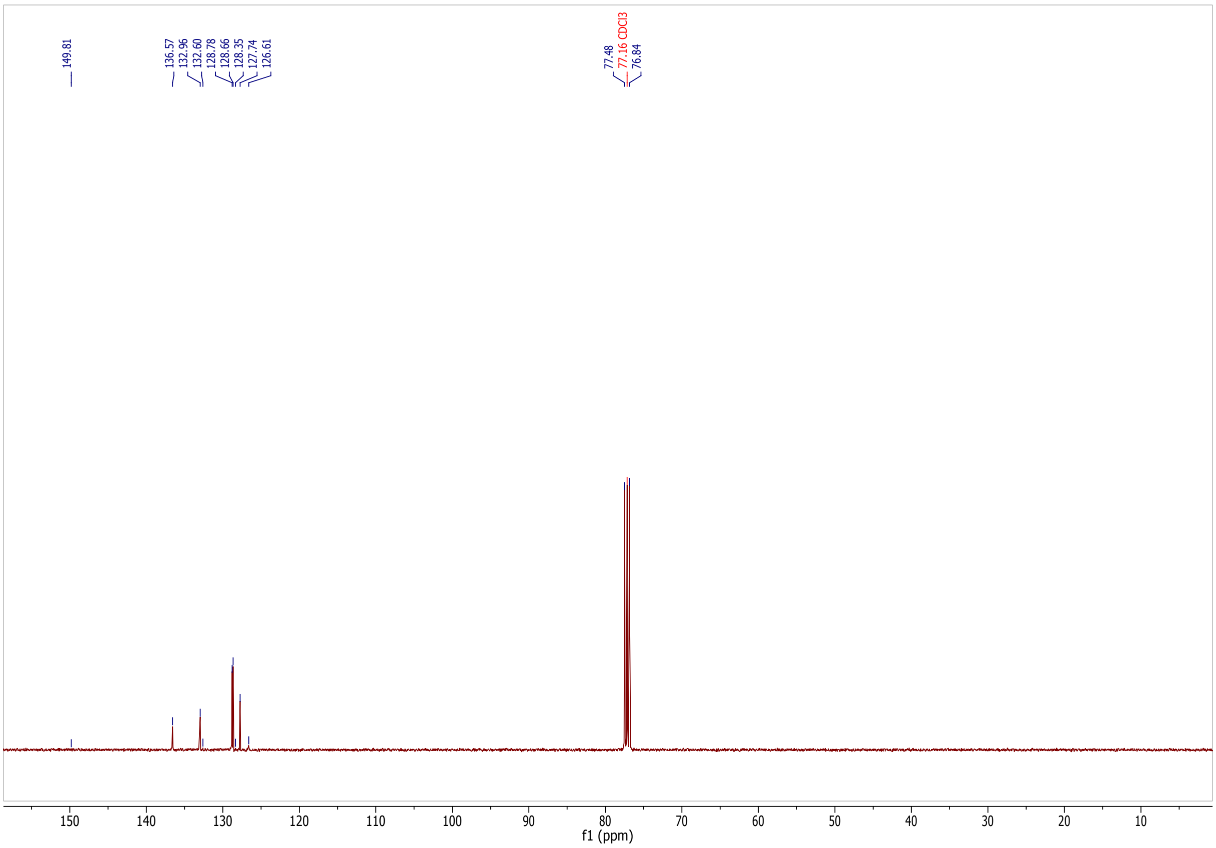


Figure SI 48. ^{13}C-NMR of (*Z*)-3-styrylpyridine **2r**.

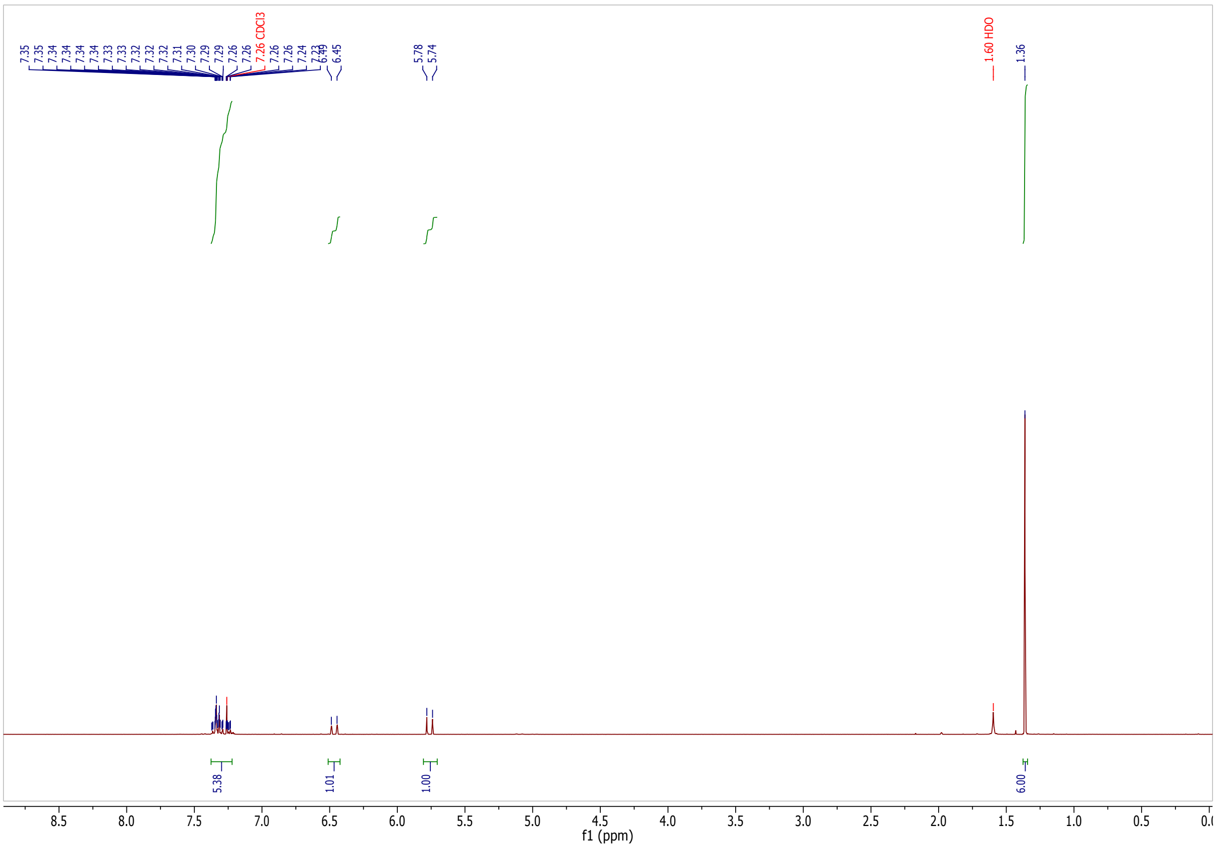


Figure SI 49.^{1}H-NMR of (*Z*)-2-methyl-4-phenylbut-3-en-2-ol **2s.**

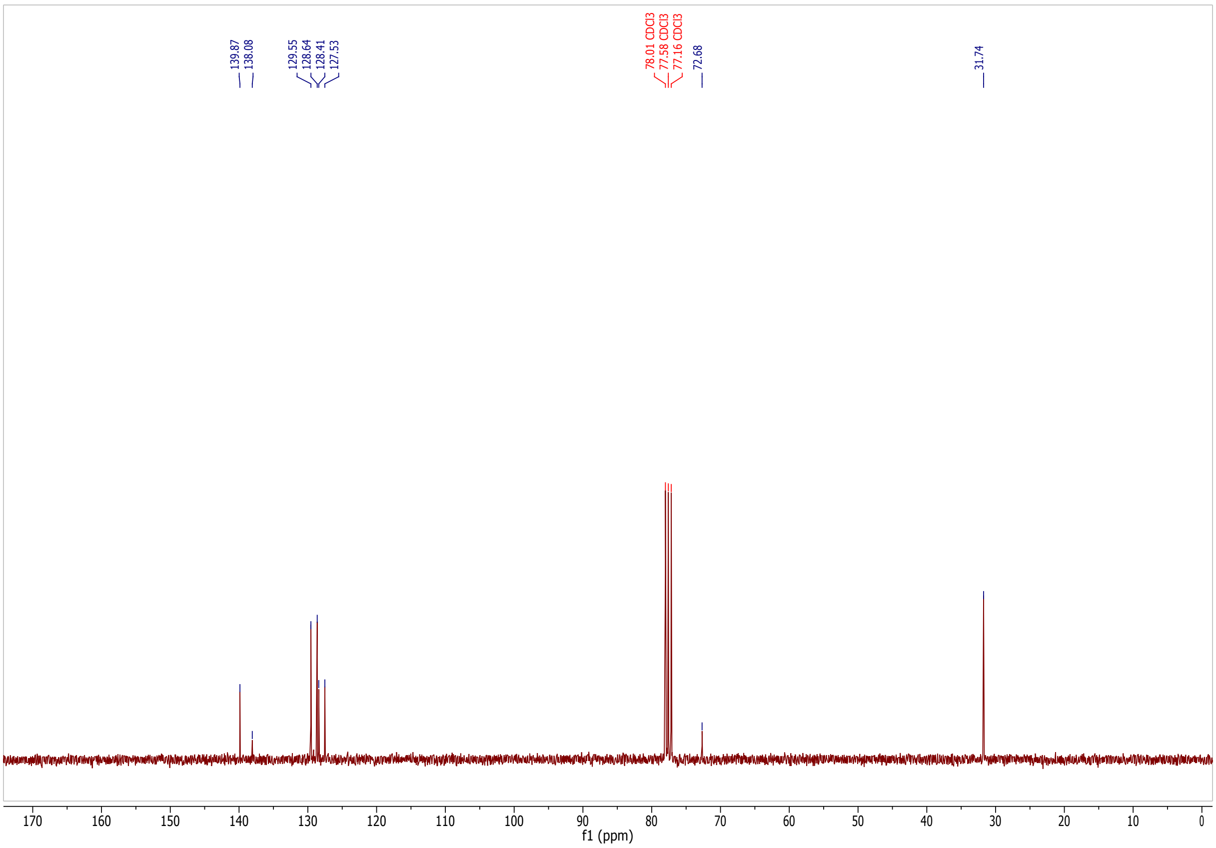


Figure SI 50. ^{13}C-NMR of (*Z*)-2-methyl-4-phenylbut-3-en-2-ol **2s.**

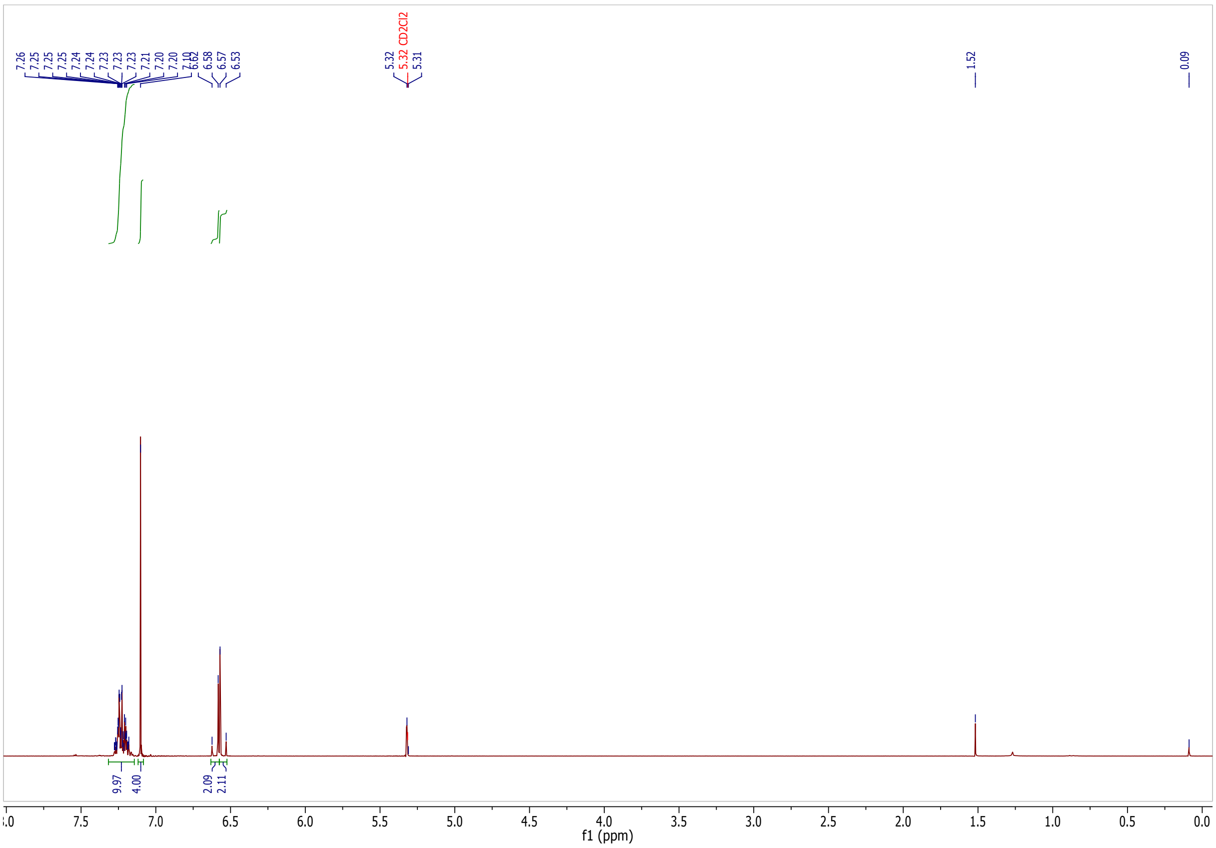


Figure SI 51. ^{1}H-NMR of 1,4-di((*Z*)-styryl)benzene **2t.**

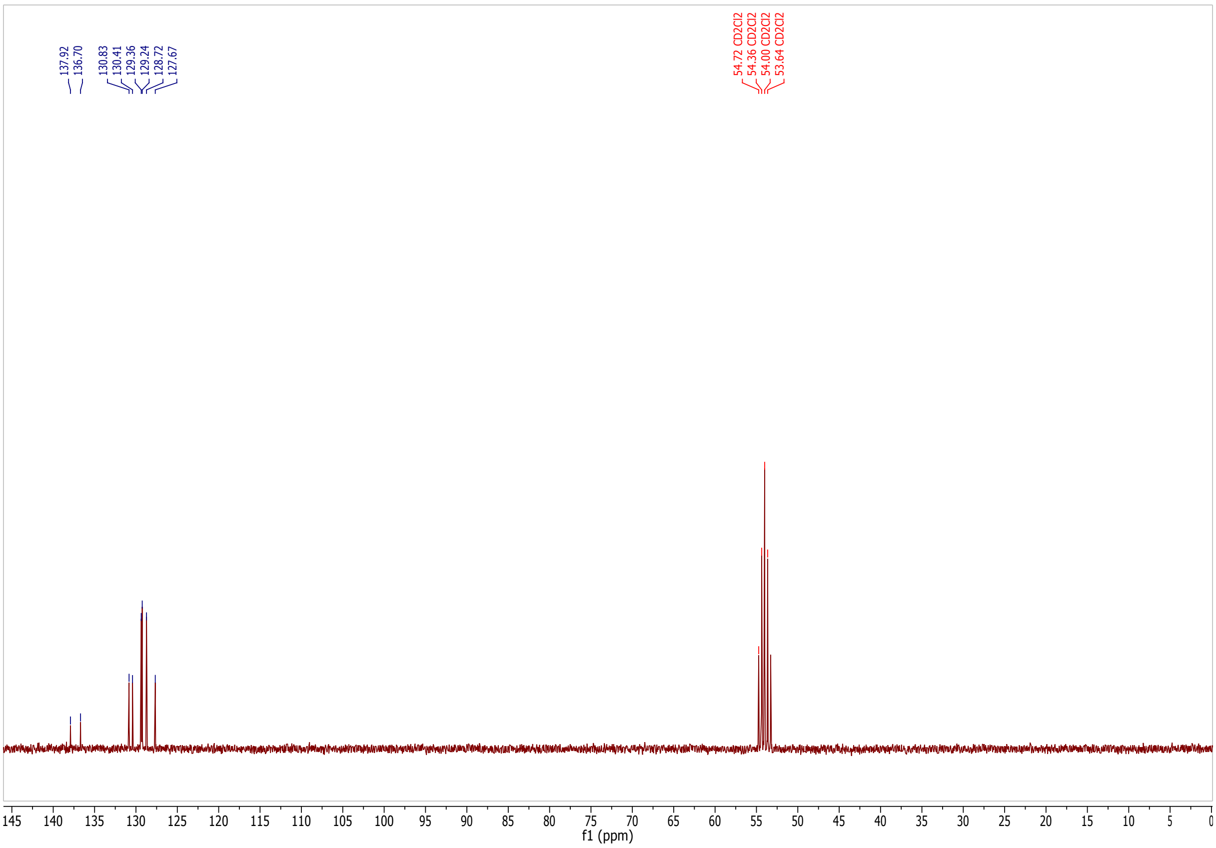


Figure SI 52. ^{13}C-NMR of 1,4-di((*Z*)-styryl)benzene **2t.**

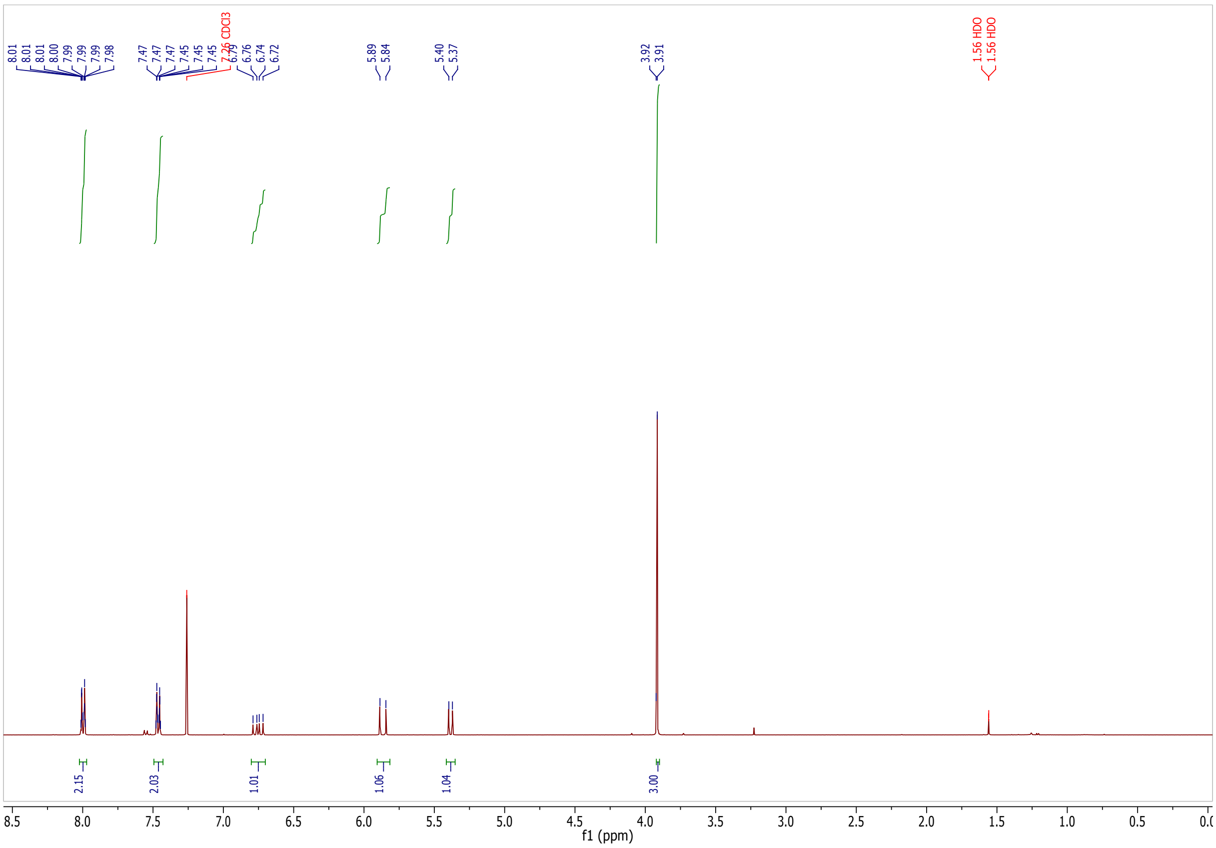


Figure SI 53.^{1}H-NMR of methyl-4-vinylbenzoate **5c**.

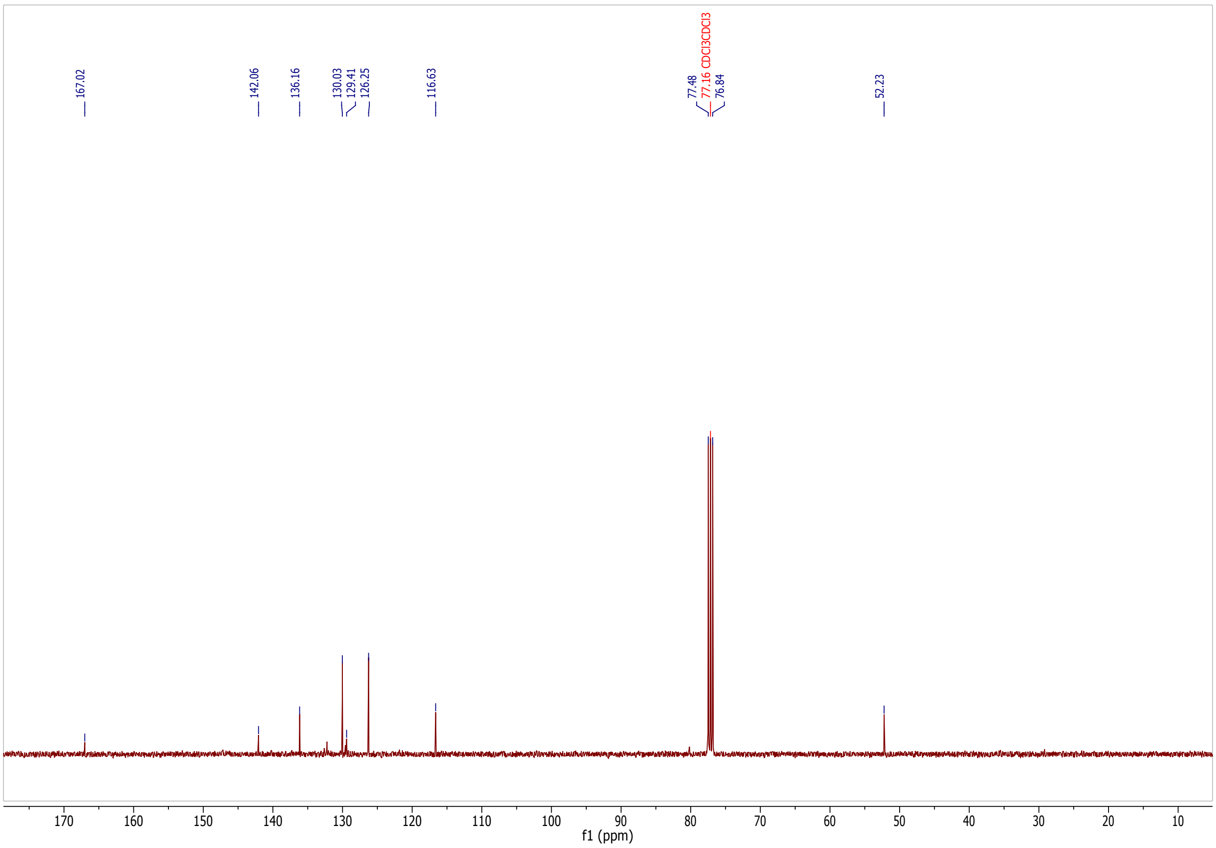


Figure SI 54. ^{13}C-NMR of methyl-4-vinylbenzoate **5c**.

11. Computational methods and models

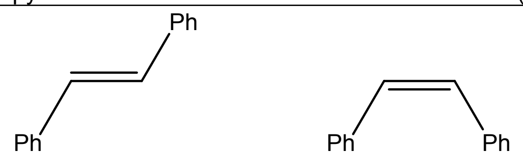
All calculations were carried out using the Gaussian 16 program.[17] Geometry optimization was carried out in gas phase at the B3PW91[18] level with the all-electron TZVP[19] (BS1) basis set (B3PW91/BS1). All optimized structures were further characterized either as energy minimums without imaginary frequencies or transition states with only one imaginary frequency by frequency calculations, which provided zero-point vibrational energies and thermodynamic corrections to enthalpy and Gibbs free energy at 298.15 K under 1 atmosphere. On the basis of the B3PW91/TZVP geometries in gas phase, single-point energies including solvation effect based on solute electron density (SMD[20]) and van der Waals dispersion (GD3BJ[21]) at different levels were computed, e.g.; B3PW91-GD3BJ/BS1//B3PW91/BS1 including dispersion correction; B3PW91-GD4BJ-SMD/BS1//B3PW91/BS1 including dispersion correction and solvation effect (THF); M062X[22]/BS1//B3PW91/BS1 and M06L/BS1//B3PW91/BS1 in gas phase as well as M062X/BS2//B3PW91/BS1 and M06L[23]/BS2//B3PW91/BS1 in gas phase with the extended basis set (BS2 = 6-311++GG(3df,3pd).[24] Finally M06L-SMD/BS2//B3PW91/BS1 including solvation effect (THF and heptane) was carried out.

(a) Benchmark calculation

On the basis of the experimentally observed kinetic and thermodynamic parameters for various PNP pincer-type complexes, especially PNP manganese complexes, it is found that solvation and dispersion can affect the kinetic and thermodynamic parameters of the reaction; i.e.; barriers (kinetics) can be either underestimated or overestimated; and the same is found for reaction energies (thermodynamics). No general trends can be seen; and it depends on catalysts and substrates. Therefore, it is necessary to have benchmark calculations on the basis of available experimental results.

The first example is the difference in standard enthalpy of formation of *cis*- and *trans*-stilbene. The standard enthalpy of formation of *cis*- and *trans*-stilbene is 60.30 and 56.43 kcal/mol,[25] respectively, and their difference is 3.87 kcal/mol. Taking this difference we evaluated the computed results at different levels of theory (Table S1); and the difference in gas phase at B3PW91, M062X, M06L, M062X/BS2, M06L/BS2 as well as B3PW91-GD3BJ is 4.88, 2.90, 2.97, 4.80, 4.61 and 2.97 kcal/mol, respectively. The deviation is within ±1 kcal/mol. In THF solution with dispersion (B3PW91-GD3BJ-SMD), the difference is 4.01 kcal/mol. At M06L/BS2 including solvation in THF and heptane, the difference is 5.44 and 5.08 kcal/mol, respectively.

Table S1. Difference of enthalpy of formation between *cis*- and *trans*-stilbene (kcal/mol)



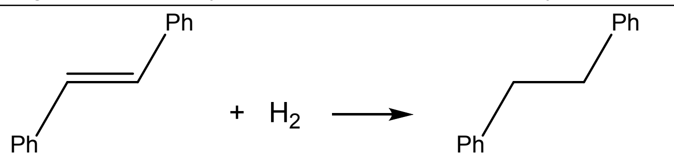
ΔH_f° = 56.43 kcal/mol ΔH_f° = 60.30 kcal/mol

	$\Delta\Delta H_f^\circ$ (*trans* – *cis*)	Deviation
Standard/gas phase	–3.87	0.00
B3PW91/BS1	–4.88	–1.01
B3PW91-GD3BJ/BS1//B3PW91/BS1	–2.97	+0.90
B3PW91-GD3BJ-SMD-THF/BS1//B3PW91/BS1	–4.01	–0.14
M062X/BSI//B3PW91/BS1//B3PW91/BS1	–2.90	+0.97
M062X/BS2//B3PW91/BS1	–2.97	+0.90
M06L/BS1//B3PW91/BS1	–4.80	–0.93

M06L/BS2//B3PW91/BS1	–4.61	–0.74
M06L-SMD-THF//BS2//B3PW91/BS1	–5.44	–1.57
M06L-SMD-Heptane//BS2//B3PW91/BS1	–5.08	–1.21

The second example is the enthalpy of hydrogenation (–22.28 kcal/mol) of *trans*-stilbene to 1,2-diphenylethane on the basis of their standard enthalpies of formation (Table S2). The computed enthalpy of hydrogenation at B3PW91, M062X, M06L, M062XL/BS2, M06L/BS2 and B3PW91-GD3BJ is –22.78, –25.37, –25.04, –23.00, –22.90, –24.48 kcal/mol, respectively. In THF solution with dispersion (B3PW91-GD3BJ-SMD), the difference is –24.34 kcal/mol. At M06L/BS2 including THF and heptane solution, the difference is –23.05 and –23.10 kcal/mol, respectively. Among these values, the best agreement is found at B3PW91, M06L and M06L/BS2 in gas phase with the smallest deviation (–0.50, –0.72 and –0.62 kcal/mol, respectively). The largest deviation is –3.09 kcal/mol at M062X.

Table S2. Table S2. Hydrogenation enthalpy of trans-stilbene to 1,2-diphenylethane (kcal/mol)

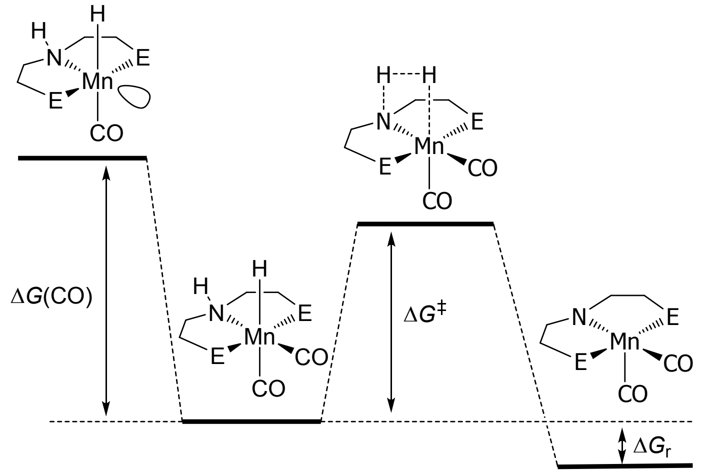


ΔH_f° = 56.43 kcal/mol ΔH_f° = 34.15 kcal/mol

	ΔH_r	Deviation
Standard/gas phase	–22.28	0.00
B3PW91/BS1	–22.78	–0.50
B3PW91-GD3BJ/BS1//B3PW91/BS1	–24.48	–2.22
B3PW91-GD3BJ-SMD-THF/BS1// B3PW91/BS1	–24.34	–2.06
M062X/BSI//B3PW91/BS1	–25.37	–3.09
M062X/BS2//B3PW91/BS1	–25.04	–2.76
M06L/BS1//B3PW91/BS1	–23.00	–0.72
M06L/BS2//B3PW91/BS1	–22.90	–0.62
M06L-SMD-THF/BS2//B3PW91/BS1	–23.05	–0.77
M06L-SMD-Heptane/BS2//B3PW91/BS1	–23.10	–0.82

Next, we tested the stability of the amine active catalyst either towards H_2 elimination to form the amido active catalyst or toward the equatorial CO dissociation (Table S3). For H_2 elimination in gas phase, the computed barriers are very close in the range of 18-19.5 kcal/mol and the reaction is slightly exergonic; and the same trend is found including dispersion correction (19.46, –2.02 kcal/mol). All these reveal the possibility of reversibility and equilibrium. Including dispersion corrections, the barrier becomes higher by about 5 kcal/mol and the reaction changes from exergonic to endergonic (24.58, 2.41 as well as 23.55, 4.00 kcal/mol) and such changes have been found in other PNP pincer catalysts.[26] As expected from the previous and current experimental work, CO dissociation needs much higher energy than H_2 elimination by over 22 kcal/mol. At M062X, however, CO dissociation free energies are much smaller (26.7 kcal/mol), but they are still higher than the free energy barriers of H_2 elimination by about 8 kcal/mol. Nevertheless, all these results show that under certain conditions CO coordination is stable for the hydrogenations. At M06L/BS2 including THF and heptane solution, the barrier is 23.55 and 20.60 kcal/mol, respectively, and the reaction is endergonic by 4.00 and 1.55 kcal/mol, respectively.

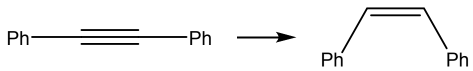
Table S3. Catalyst stability towards either H_2 elimination or CO dissociation (kcal/mol)



	$\Delta G^{\ddagger}$ ($\Delta H^{\ddagger}$)	ΔG_r (ΔH_r)	ΔG_{CO} (ΔH_{CO})
B3PW91/BS1	19.53 (19.61)	–1.99 (7.55)	42.47 (54.14)
B3PW91-GD3BJ/BS1//B3PW91/SB1	19.46 (19.54)	–2.02 (7.73)	45.61 (57.29)
B3PW91-GD3BJ-SMD-THF/BS1//B3PW91/SB1	24.58 (24.66)	2.41 (12.16)	47.49 (59.17)
M062X/BSI//B3PW91/SB1	18.88 (18.96)	–1.69 (8.06)	26.74 (38.42)
M062X/BS2//B3PW91/SB1	17.99 (18.07)	–3.20 (6.54)	26.74 (38.42)
M06L/BS1//B3PW91/SB1	18.44 (18.52)	0.01 (9.76)	46.70 (58.38)
M06L/BS2//B3PW91/SB1	18.49 (18.41)	–0.61 (9.14)	48.22 (59.90)
M06L-SMD-THF/BS2//B3PW91/SB1	23.55 (23.63)	4.00 (13.73)	49.62 (61.30)
M06L-SMD-Heptane/BS2//B3PW91/SB1	20.60 (20.68)	1.55 (11.30)	50.19 (61.87)

Having these results in hand we computed the hydrogenation 1,2-diphenylacetylene as well as *cis*- and *trans*-stilbenes (Table S4). In agreement with the previous results, the hydrogenation of *cis*-and *trans*-stilbenes follows a stepwise outer-sphere bifunctional mechanism; and the Mn-H transfer has the highest barrier and that of N-H transfer is lower; and one intermediate connects the transitions states of Mn-H and N-H transfers. For the hydrogenation 1,2-diphenylacetylene, only the first Mn-H transfer transition state has been located; and that of the N-H transfer as well as the corresponding intermediate were not able be located and optimized; and all attempts led to the direct formation of *cis*-stilbene. However, this does not affect the comparison of the catalytic activity, since only the first step is needed for the discussion and comparison.

Table S4a. Related free energies (kcal/mol) of the catalyzed hydrogenation of 1,2-diphenylacetylene

			
	$\Delta G^{\ddagger}$ ($\Delta H^{\ddagger}$)	ΔG_r (ΔH_r)	$\Delta G^{\ddagger}$ ($\Delta H^{\ddagger}$)
	TS1(Mn-H)	Int	TS2(N-H)
B3PW91/BS1	27.64 [15.38]	#	#
B3PW91-GD3BJ/BS1//B3PW91/BS1	6.41 [–6.01]		
B3PW91-GD3BJ-SMD-THF/BS1//B3PW91/BS1	12.05 [–0.37]		
M062X/BSI//B3PW91/BS1	16.81 [4.55]		
M062X/BS2//B3PW91/BS1	15.91 [3.50]		
M06L/BS1//B3PW91/BS1	14.35 [1.94]		
M06L/BS2//B3PW91/BS1	13.65 [1.24]		
M06L-SMD-THF/BS2//B3PW91/BS1	19.12 [6.72]		
M06L-SMD-Heptane/BS2//B3PW91/BS1	17.28 [4.86]		

Not located

Table S4b. Related free energies (kcal/mol) of the catalyzed hydrogenation of cis-stilbene

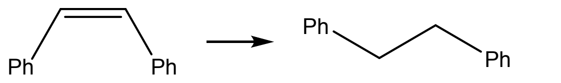
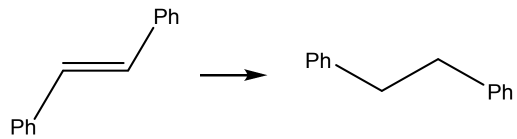
			
	$\Delta G^{\ddagger}$ ($\Delta H^{\ddagger}$)	ΔG_r (ΔH_r)	$\Delta G^{\ddagger}$ ($\Delta H^{\ddagger}$)
	TS1(Mn-H)	Int	TS2(N-H)
B3PW91/BS1	33.18 [19.28]	31.55 [18.41]	30.59 [16.78]
B3PW91-GD3BJ/BS1//B3PW91/BS1	5.29 [-8.60]	4.95 [-8.46]	4.56 [-9.24]
B3PW91-GD3BJ-SMD-THF/BS1//B3PW91/BS1	10.11 [-3.78]	8.34 [-5.06]	9.03 [-4.78]
M062X/BSI//B3PW91/BS1	20.81 [6.91]	16.09 [2.68]	14.74 [0.93]
M062X/BS2//B3PW91/BS1	19.74 [5.84]	14.92 [1.52]	14.02 [0.21
M06L/BS1//B3PW91/BS1	18.10 [4.20]	15.07 [1.66]	16.01 [2.21]
M06L/BS2//B3PW91/BS1	18.06 [4.16]	15.36 [1.95]	16.42 [2.62]
M06L-SMD-THF/BS2//B3PW91/BS1	22.76 [8.87]	18.87 [5.47]	20.90 [7.09]
M06L-SMD-Heptane/BS2//B3PW91/BS1	22.27 [7.38]	18.05 [4.64]	19.58 [5.77]

Table S4b. Related free energies (kcal/mol) of the catalyzed hydrogenation of trans-stilbene

			
	TS1(Mn-H)	Int	TS2(N-H)
B3PW91/BS1	35.29 [20.53]	34.13 [20.26]	32.87 [18.81]
B3PW91-GD3BJ/BS1//B3PW91/BS1	5.73 [–9.03]	6.32 [–7.55]	5.90 [–8.16]
B3PW91-GD3BJ-SMD-THF/BS1//B3PW91/BS1	11.67 [–3.09]	11.11 [–2.75]	11.48 [–2.58]
M062X/BSI//B3PW91/BS1	20.79 [6.02]	18.15 [4.28]	16.88 [2.18]
M062X/BS2//B3PW91/BS1	19.67 [4.90]	17.12 [3.25]	16.31 [2.24]
M06L/BS1//B3PW91/BS1	19.62 [4.86]	18.39 [4.51]	19.04 [4.97]
M06L/BS2//B3PW91/BS1	19.36 [4.59]	18.51 [4.64]	19.29 [5.23]
M06L-SMD/BS2//B3PW91/BS1	25.00 [10.24]	23.11 [9.24]	24.55 [10.49]
M06L-SMD-THF/BS2//B3PW91/BS1	23.20 [8.43]	21.72 [7.85]	22.74 [8.70]

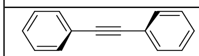
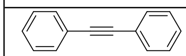
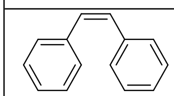
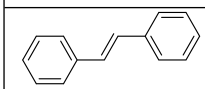
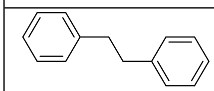
As shown in Table S4, some trends can be seen. At B3PW91 in gas phase, the highest barrier (27.64 kcal/mol) of 1,2-diphenylacetylene hemi-hydrogenation to *cis*-stilbene is much lower than that of *cis*- and *trans*-stilbenes to 1,2-diphenylethane (33.18 and 35.29 kcal/mol, respectively). AT M062X and M06L, all barriers become lower, but the highest barrier (16.81, 14.34 and 15.91 kcal/mol) of 1,2-diphenylacetylene hemi-hydrogenation to *cis*-stilbene is lower than that of *cis*- and *trans*-stilbenes to 1,2-diphenylethane (20.81, 18.10 and 19.74 as well as 20.97, 19.62 and 19.67 kcal/mol, respectively). All these indicate that 1,2-diphenylacetylene should be easily hydrogenated than the hydrogenation of cis- and trans-stilbene; and this agrees with our experiment.

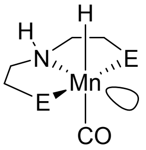
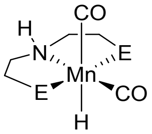
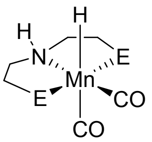
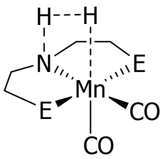
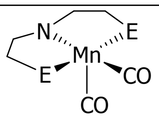
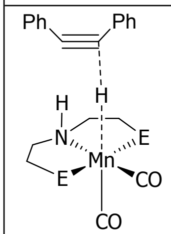
In gas phase including dispersion correction, however, all barriers become extreme low (6.41, 5.29 and 5.73 kcal/mol, respectively); and they are too low to be true; and especially all three barriers are close, and this disagrees with the experiment. Taking correction of solvation and dispersion into account, the barriers (12.05, 10.11 and 11.67 kcal/mol, respectively) are also lower than those in gas phase; and they are also close. This trend does also not agree with the experiment.

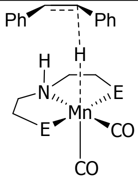
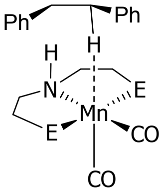
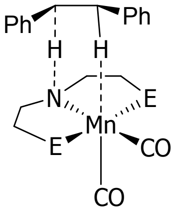
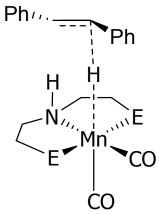
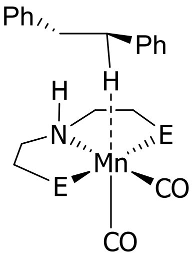
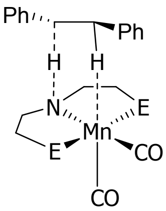
Under the consideration of all these benchmark results, it seems that the M06L gas phase results are reasonable, e.g.; the agreement between the difference of the enthalpy of formation of *cis*- and *trans*-stilbene (–3.87 vs. –4.80

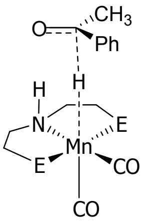
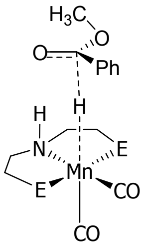
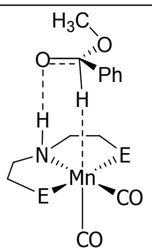
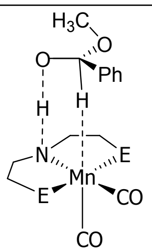
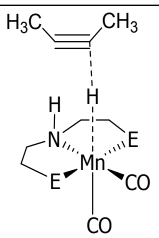
kcal/ml) and the reasonable agreement in the hydrogenation enthalpy of trans-stilbene (–22.28 vs. –23.00 kcal/mol). Finally, it is noted that the M06L gas phase catalytic activity agrees qualitatively and quantitatively. For example, 1,2-diphenylacetylene can be hydrogenated at mild condition (nearly ambient condition); and *trans*-stilbene can be hydrogenated at relatively higher temperature and higher H_2 pressure.

Table S5a. Total electronic energy (HF, au), Sum of electronic and thermal Enthalpies (Htot, au), Sum of electronic and thermal Free Energies (Gtot, au) as well as Zero-point vibrational energy (ZPE, au), and the number of imaginary frequencies (NImag) as well as the thermal correction to enthalpy (H, au) and thermal correction to Gibbs free energy (G, au)

	B3PW91	M06L-BS2-SMD-Heptane	M06L-BS2-SMD-THF
H2	HF=-1.178636 ZPE=0.010064 NImag=0 H=0.013368 G=-0.001430 Htot=-1.165268 Gtot =-1.180066	HF=-1.1718555 Htot= 1.1584875 Gtot= 1.1732855	HF=-1,1718296 Htot=1,1584616 Gtot= 1,1732596
	HF=-539.4137308 ZPE= NImag=0 H=0.203049 G= 0.152780 Htot=-539.210681 Gtot= -539.260951	HF=-539.5714373 Htot= 539.3683883 Gtot= 539.4186573	HF=-539,570527 Htot=539,367478 Gtot= 539,417747
	HF=-539.4137299 ZPE=0.190934 NImag=0 H=0.203066 G=0.152553 Htot=-539.210663 Gtot= -539.261177	HF=-539.5714383 Htot= 539.3683723 Gtot= 539.4188853	HF=-539,5705272 Htot=539,3674612 Gtot= 539,4179742
	HF=-540.6571549 ZPE=0.214627 NImag=0 H=0.226724 G=0.176517 Htot=-540.430431 Gtot= -540.480638	HF=-540.8099911 Htot= 540.5832671 Gtot= 540.6334741	HF=-540,8092019 Htot=540,5824779 Gtot= 540,6326849
	HF=-540.664665 ZPE=0.214087 NImag=0 H=0.226461 G=0.175046 Htot=-540.438204 Gtot= -540.489619	HF=-540.8178306 Htot= 540.5913696 Gtot= 540.6427846	HF=-540,8174566 Htot=540,5909956 Gtot= 540,6424106
	HF=-541.8903136 ZPE=0.237794 NImag=0 H=0.250532 G=0.197925 Htot=-541.639782	HF =-542.0372036 Htot=541.7866716 Gtot= 541.8392786	HF=-542,0367159 Htot=541,7861839 Gtot= 541,8387909

	Gtot= -541.692388		
	HF=-2477.0611803 ZPE=0.416307 NImag=0 H=0.441974 G= 0.362699 Htot=-2476.619206 Gtot= -2476.698481	HF=-2477.2757156 Htot= 2476.8337416 Gtot= 2476.9130166	HF=-2477,2842448 Htot=2476,8422708 Gtot= 2476,9215458
CO	HF=-113.3043308 ZPE=0.005076 NImag=0 H=0.008381 G=-0.014043 Htot=-113.295950 Gtot= -113.318374	HF=-113.3338691 Htot= 113.3254881 Gtot= 113.3479121	HF=-113,333762 Htot=113,325381 Gtot= 113,347805
	HF=- 2590.4565993 ZPE= 0.426491 NImag=0 H=0.454111 G=0.370486 Htot=-2590.002489 Gtot= -2590.086113	HF=-2590.7138433 Htot= 2590.2597323 Gtot= 2590.3433573	
	HF=-2590.4556062 ZPE=0.426644 NImag=0 H=0.454157 G=0.371066 Htot=-2590.001449 Gtot= -2590.084540	HF=-2590.7119849 Htot= 2590.2578279 Gtot= 2590.3409189	HF=-2590,7194923 Htot=2590,2653353 Gtot= 2590,3484263
	HF=-2590.4182153 ZPE=0.420566 NImag=1 (-761 i) H=0.448021 G=0.364800 Htot=-2589.970194 Gtot= -2590.053416	HF =-2590.6728858 Htot= 2590.2248648 Gtot= 2590.3080858	HF=-2590,6756942 Htot=2590,2276732 Gtot= 2590,3108942
	HF=-2589.2566624 ZPE=0.405468 NImag=0 H=0.432839 G=0.349017 Htot=-2588.823824 Gtot= -2588.907646	HF=-2589.5141791 Htot= 2589.0813401 Gtot= 2589.1651621	HF=-2589,5178262 Htot=2589,0849872 Gtot= 2589,1688092
	HF=-3129.8441486 ZPE=0.616552 NImag=1 (-495 i) H=0.656526 G=0.542711 Htot=-3129.187623 Gtot= -3129.301438	HF=-3130.2749794 Htot= 3129.6184534 Gtot= 3129.7322684	HF=-3130,2786328 Htot=3129,6221068 Gtot= 3129,7359218

	HF=-3131.0814271 ZPE=0.640477 NImag=1 (-748 i) H=0.680278 G=0.569126 Htot=-3130.401149 Gtot= -3130.512301	HF=-3131.5096201 Htot= 3130.8293421 Gtot= 3130.9404941	HF =-3131,5139606 Htot=3130,8336826 Gtot= 3130,9448346
	HF=-3131.0857257 ZPE=0.642587 NImag=0 H=0.682766 G=0.570829 Htot=-3130.402959 Gtot= -3130.514896	HF=-3131.5164645 Htot= 3130.8336985 Gtot= 3130.9456355	HF=-3131,5218699 Htot=3130,8391039 Gtot= 3130,9510409
	HF=-3131.0846096 ZPE=0.639647 NImag=1 (-673 i) H=0.679471 G=0.568174 Htot=-3130.405139 Gtot= -3130.516435	HF=-3131.5113654 Htot= 3130.8318944 Gtot= -3130.9431914	HF=-3131,5159816 Htot=3130,8365106 Gtot= 3130,9478076
	HF=-3131.086867 ZPE=0.640119 NImag=1 (-677 i) H=0.679928 G=0.568949 Htot=-3130.406939 Gtot= -3130.517918	HF=-3131.5156866 Htot= 3130.8357586 Gtot= 3130.9467376	HF=-3131,5199429 Htot=3130,8400149 Gtot= 3130,9509939
	HF=-3131.0896449 ZPE=0.642081 NImag=0 H=0.682273 G=0.569869 Htot=-3130.407371 Gtot= -3130.519776	HF=-3131.5189555 Htot= 3130.8366825 Gtot= 3130.9490865	HF=-3131,523876 Htot=3130,841603 Gtot=3130,954007
	HF=-3131.0889791 ZPE=0.639465 NImag=1 (-478 i) H=0.679302 G=0.567207 Htot=-3130.409677 Gtot= -3130.521772	HF=-3131.5146684 Htot=3130.8353664 Gtot= 3130.9474614	HF=-3131,5189193 Htot=3130,8396173 Gtot= 3130,9517123
Ph-CHOH-CH3	HF=-386.0771798 ZPE=0.161141 NImag=0 H=0.170465 G=0.127807 Htot=-385.906715 Gtot=-385.949373	HF=-386.177749 Htot= 386.007284 Gtot= 386.049942	HF=-386,1788132 Htot=386,0083482 Gtot= 386,0510062
Ph-CO-CH3	HF=-384.8714153 ZPE=0.137520	HF=-384.9813811	HF=-384,9831106

	NImag=0 H=0.146394 G=0.104515 Htot=-384.725022 Gtot=-384.766900	Htot= 384.8349871 Gtot= 384.8768661	Htot=384,8367166 Gtot= 384,8785956
	HF=-2975.3126691 ZPE = 0.564872 NImag=1 (-389 i) H= 0.600788 G= 0.499692 Htot= -2974.711881 Gtot= -2974.812977	HF=-2975.6928157 Htot=2975.0920277 Gtto= 2975.1931237	HF=-2975,6876646 Htot=2975,0868766 Gtot= 2975,1879726
	HF=-3050.5306486 ZPE=0.569749 NImag= 1 (-431 i) H=0.607054 G=0.502167 Htot=-3049.923595 Gtot= -3050.028482	HF=-3050.9317867 Htot=3050.3247327 Gtot= 3050.4296197	
	HF=-3050.5408367 ZPE=0.571994 NImag=0 H=0.609441 G=0.504357 Htot=-3049.931396 Gtot=-3050.036480	HF=-3050.9373549 Htot=3050.3279139 Gtot= 3050.4329979	
	HF=-3050.5390866 ZPE=0.568832 NImag= 1 (-777 i) H=0.606057 G=0.501075 Htot=-3049.933030 Gtot= -3050.038011	HF=-3050.9301841 Htot=3050.3241271 Gtot= 3050.4291091	
Ph-COOCH3	HF=-460.1021776 ZPE=0.143276 NImag=0 H=0.153071 G=0.108767 Htot=-459.949107 Gtot= -459.993411	HF=-460.232335 Htot= 460.079264 Gtot= 460.123568	
	HF=-2746.3950967 ZPE=0.510030 NImag=1 (-494.7382) H=0.543820 G=0.446922 Htot= -2745.851276 Gtot= -2745.948175	HF=-2746.7016069 Htot= 2746.1577869 Gtot= 2746.2546849	
2-Butyne	HF=-155.9718872 ZPE=0.084057 NImag=0	HF=-156.0154203 Htot= 155.9246793	

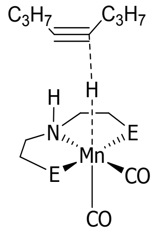
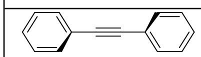
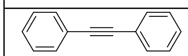
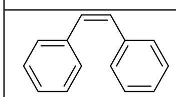
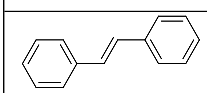
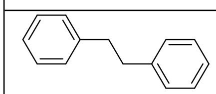
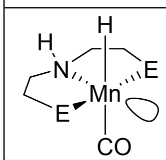
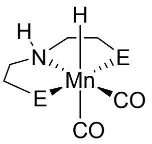
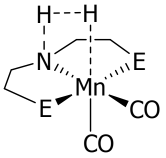
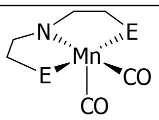
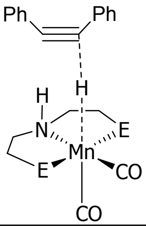
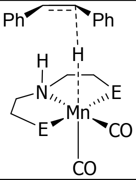
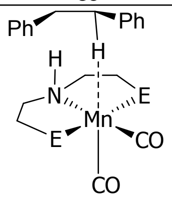
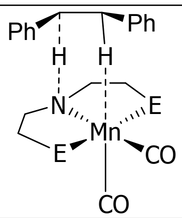
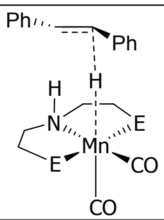
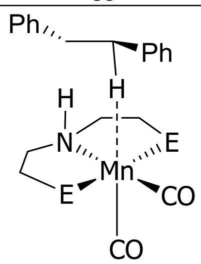
	H=0.090741 G=0.055294 Htot=-155.881146 Gtot= -155.916593	Gtot= 155.9601263	
	HF=-2903.6442215 ZPE=0.623952 NImag=1 (-459.6154) H=0.663159 G=0.551871 Htot=-2902.981062 Gtot= -2903.092350	HF=-2903.989399 Htot=2903.32624 Gtot= 2903.437528	
4-Octyne	HF=-313.2212269 ZPE=0.198700 NImag=0 H=0.210300 G=0.160401 Htot=-313.010927 Gtot= -313.060826	HF=-313.2995044 Htot=313.0892044 Gtot= 313.1391034	

Table S5b. Total electronic energy (HF, au), Sum of electronic and thermal Enthalpies (Htot, au), Sum of electronic and thermal Free Energies (Gtot, au)

	M062X	B3PW91-GD3BJ	B3PW91-SMD-THF-GD3BJ
H2	HF=-1,1684428 Htot= 1,1550748 Gtot= 1,1698728	HF=-1,178773 Htot=1,165405 Gtot= 1,180203	HF=-1,178293 Htot=-1,164925 Gtot= -1,179723
	HF= -539,3992043 Htot=-539,1961553 Gtot= -539,2464243	HF=-539,4617937 Htot=-539,2587447 Gtot= -539,3090137	HF=-539,478114 Htot=-539,275065 Gtot= -539,325334
	HF=-539,3992196 Htot=-539,1961536 Gtot=- 539,2466666	HF=-539,4617921 Htot= 539,2587261 Gtot= 539,3092391	HF=-539,4781145 Htot= -539,2750485 Gtot=- 539,3255615
	HF=-540,6354423 Htot=-540,4087183 Gtot= -540,4589253	HF=-540,7130182 Htot=540,4862942 Gtot= 540,5365012	HF=-540,7285282 Htot=-540,5018042 Gtot= -540,5520112
	HF=-540,6397929 Htot=540,4133319 Gtot= 540,4647469	HF=-540,7174939 Htot=-540,4910329 Gtot= -540,5424479	HF=-540,7346597 Htot= -540,5081987 Gtot= -540,5596137
	HF=-541,8593753 Htot=541,6088433 Gtot= 541,6614503	HF=-541,9459793 Htot=541,6954473 Gtot=541,7480543	HF =-541,9624444 Htot=541,7119124 Gtot= 541,7645194
	HF=-2476,915995 Htot=2476,474021 Gtot= 2476,553296	HF=-2477,1847817 Htot=2476,7428077 Gtot= 2476,8220827	HF=-2477,2102642 Htot=2476,7682902 Gtot= 2476,8475652
CO	HF=-113,3157285	HF=-113,3050411	HF=-113,300808

	Htot=113,3073475 Gtot= 113,3297715	Htot=113,2966601 Gtot= 113,3190841	Htot=113,292427 Gtot= 113,314851
	HF=-2590,2967498 Htot=2589,8425928 Gtot= 2589,9256838	HF=-2590,5849214 Htot= 2590,1307644 Gtot= 2590,2138554	HF=-2590,6091651 Htot= -2590,1550081 Gtot= -2590,2380991
	HF=-2590,2603976 Htot=2589,8123766 Gtot= -2589,8955976	HF=-2590,5476403 Htot= 2590,0996193 Gtot= 2590,1828403	HF =-2590,5637305 Htot= -2590,1157095 Gtot= -2590,1989305
	HF=-2589,1075177 Htot=2588,6746787 Gtot= 2588,7585007	HF=-2589,3858876 Htot=2588,9530486 Gtot= 2589,0368706	HF=-2589,4035503 Htot= -2588,9707113 Gtot= -2589,0545333
	HF=-3129,6880309 Htot=3129,0315049 Gtot= 3129,1453199	HF=-3130,0555917 Htot=3129,3990657 Gtot= -3129,5128807	HF=-3130,0871678 Htot=-3129,4306418 Gtot= -3129,5444568
	HF=-3130,920577 Htot=3130,240299 Gtot= 3130,351451	HF=-3131,311049 Htot=3130,630771 Gtot= 3130,741923	HF=-3131,3431175 Htot=3130,6628395 Gtto= 3130,7739915
	HF=-3130,9297987 Htot=3130,2470327 Gtot= 3130,3589697	HF=-3131,3133037 Htot=3130,6305377 Gtot= 3130,7424747	HF=-3131,3476433 Htot=-3130,6648773 Gtot= -3130,7768143
	HF=-3130,9293005 Htot=3130,2498295 Gtot= 3130,3611265	HF=-3131,3112607 Htot=3130,6317897 Gtot= 3130,7430867	HF=-3131,3438995 Htot=-3130,6644285 Gtot= -3130,7757255
	HF=-3130,9262545 Htot=3130,2463265 Gtot= 3130,3573055	HF=-3131,3161214 Htot= 3130,6361934 Gtot= 3130,7471724	HF=-3131,3480568 Htot=-3130,6681288 Gtot= -3130,7791078
	HF=-3130,9313717 Htot=3130,2490987 Gtot= 3130,3615027	HF=-3131,3160982 Htot=3130,6338252 Gtot= 3130,7462292	HF=-3131,3498691 Htot= -3130,6675961 Gtot= -3130,7800001

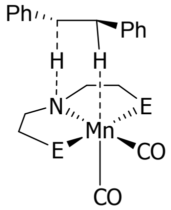
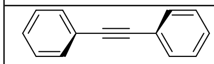
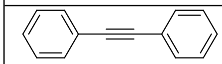
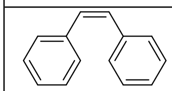
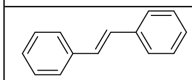
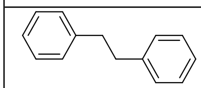
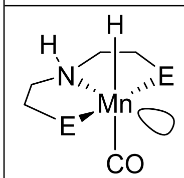
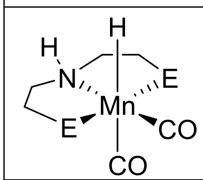
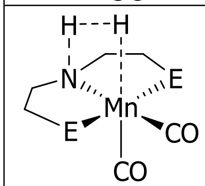
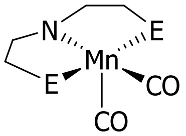
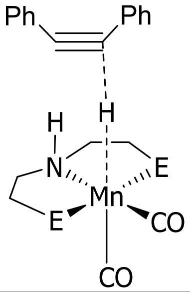
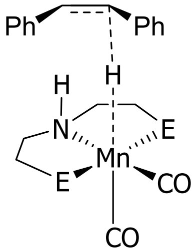
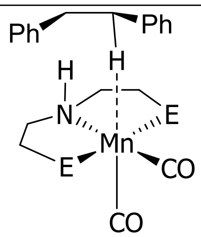
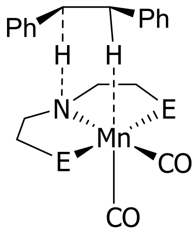
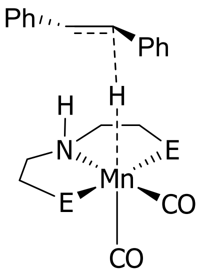
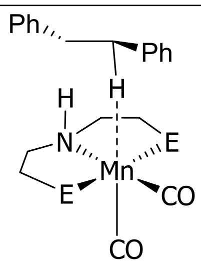
	HF=-3130,9307441 Htot=3130,2514421 Gtot= 3130,3635371	HF=-3131,3141061 Htot=3130,6348041 Gtot= 3130,7468991	HF=-3131,3466268 Htot= -3130,6673248 Gtot= -3130,7794198

Table S5c. Total electronic energy (HF, au), Sum of electronic and thermal Enthalpies (Htot, au), Sum of electronic and thermal Free Energies (Gtot, au)

	M062X-BS2	M06L	M06L-BS2
H2	HF=-1,1689148 Htot=1,1555468 Gtot= 1,1703448	HF=-1,171711 Htot=1,158343 Gtot= 1,173141	HF=-1,1722883 Htot=1,1589203 Gtot= 1,1737183
	HF=-539,3997529 Htot=539,1967039 Gtot= 539,2469729	HF=-539,5497289 Htot=539,3466799 Gtot= 539,3969489	HF=-539,5564197 Htot=539,3533707 Gtot= 539,4036397
	HF=-539,3997709 Htot=539,1967049 Gtot= 539,2472179	HF=-539,5497257 Htot=539,3466597 Gtot= 539,3971727	HF=-539,5564173 Htot=539,3533513 Gtot= 539,4038643
	HF=-540,6364418 Htot=540,4097178 Gtot= 540,4599248	HF=-540,7884697 Htot=540,5617457 Gtot=540,6119527	HF=-540,7960666 Htot=540,5693426 Gtot= 540,6195496
	HF=-540,6409112 Htot=540,4144502 Gtot= 540,4658652	HF=-540,795843 Htot=540,569382 Gtot= 540,620797	HF=-540,8031534 Htot=540,5766924 Gtot= 540,6281074
	HF=-541,8604277 Htot=541,6098957 Gtot= 541,6625027	HF=-542,0149138 Htot=541,7643818 Gtot= 541,8169888	HF=-542,022642 Htot=541,77211 Gtot= 541,824717
	HF=-2476,9195598 Htot=2476,4775858 Gtot= 2476,5568608	HF=-2477,2585919 Htot=2476,8166179 Gtot= 2476,8958929	HF=-2477,2592666 Htot=2476,8172926 Gtot= 2476,8965676
CO	HF=-113,3173601 Htot=113,3089791 Gtot= 113,3314031	HF=-113,3383124 Htot=113,3299314 Gtot= 113,3523554	HF=-113,3379484 Htot=113,3295674 Gtot= 113,3519914
	HF=-2590,3019426 Htot=2589,8477856 Gtot= 2589,9308766	HF=-2590,6937415 Htot=2590,2395845 Gtot= 2590,3226755	HF=-2590,6964729 Htot=2590,2423159 Gtot= 2590,3254069
	HF=-2590,2670102 Htot=2589,8189892 Gtot= 2589,9022102	HF=-2590,6580841 Htot=2590,2100631 Gtot= 2590,2932841	HF=-2590,6608709 Htot= 2590,2128499 Gtot= 2590,2960709

	HF=-2589,1146531 Htot=2588,6818141 Gtot= 2588,7656361	HF=-2589,4985276 Htot=2589,0656886 Gtot= 2589,1495106	HF=-2589,5016734 Htot=2589,0688344 Gtot= 2589,1526564
	HF=-3129,6954446 Htot=3129,0389186 Gtot= 3129,1527336	HF=-3130,2396778 Htot=3129,5831518 Gtot= 3129,6969668	HF=-3130,2502358 Htot=3129,5937098 Gtot= 3129,7075248
	HF=-3130,9284651 Htot=3130,2481871 Gtot= 3130,3593391	HF=-3131,4749113 Htot=3130,7946333 Gtot= 3130,9057853	HF=-3131,4853057 Htot=3130,8050277 Gtot= 3130,9161797
	HF=-3130,9378521 Htot=3130,2550861 Gtot= 3130,3670231	HF=-3131,481449 Htot=3130,798683 Gtot= 3130,91062	HF=-3131,4913141 Htot=3130,8085481 Gtot= 3130,9204851
	HF=-3130,9366382 Htot=3130,2571672 Gtot= 3130,3684642	HF=-3131,4772855 Htot=3130,7978145 Gtot= 3130,9091115	HF=-3131,4869611 Htot=3130,8074901 Gtot= 3130,9187871
	HF=-3130,9343464 Htot=3130,2544184 Gtot= 3130,3653974	HF=-3131,4811568 Htot=3130,8012288 Gtot= 3130,9122078	HF=-3131,4916152 Htot=3130,8116872 Gtot= 3130,9226662
	HF=-3130,9393228 Htot=3130,2570498 Gtot= 3130,3694538	HF=-3131,4840395 Htot=3130,8017665 Gtot=3130,9141705	HF=-3131,4938808 Htot=3130,8116078 Gtot= 3130,9240118

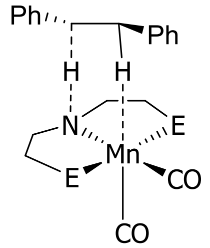
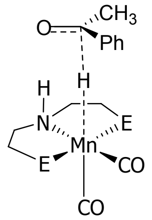
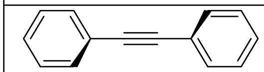
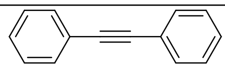
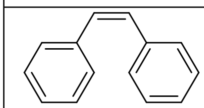
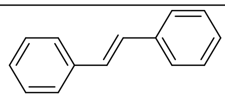
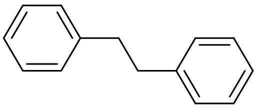
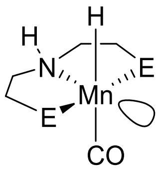
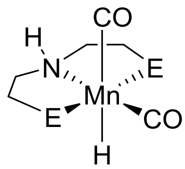
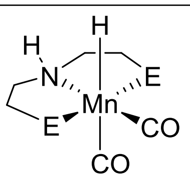
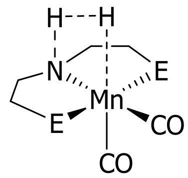
	HF=-3130,9379623 Htot=3130,2586603 Gtot= 3130,3707553	HF=-3131,4803451 Htot=3130,8010431 Gtot= 3130,9131381	HF=-3131,4899814 Htot=3130,8106794 Gtot= 3130,9227744
Ph-CHOH-CH3			HF=-386,1685729 Htot=385,9981079 Gtot= 386,0407659
Ph-CO-CH3			HF=-384,9712345 Htot=384,8248405 Gtot= 384,8667195
			HF=-3132,9457594 Htot=3132,2263274 Gtot= 3132,3374604

Table S6. B3PW91 computed Cartesian Coordinates in gas phase

H2 H,0,0.,0.,0.372594 H,0,0.,0.,-0.372594	CO C,0,0.,0.,0.5632035413 O,0,0.,0.,-0.5632035413
 C,0,-0.0000000147,-0.0000000028,0.9711045251 C,0,-0.0000000098,-0.0000000039,3.7687018837 C,0,-0.808070984,-0.8971583271,1.6850537215 C,0,0.808070957,0.8971583209,1.6850537194 C,0,0.8047752869,0.8934962789,3.0705757324 C,0,-0.804775309,-0.8934962862,3.0705757345 H,0,-1.434473984,-1.5926220122,1.1393365605 H,0,1.4344739552,1.5926220065,1.1393365568 H,0,1.4343946973,1.592513803,3.6097446804 H,0,-1.4343947175,-1.5925138107,3.6097446841 H,0,-0.0000000079,-0.0000000044,4.8528199451 C,0,-0.0000000172,-0.0000000022,-0.4482273353 C,0,-0.0000000193,-0.0000000017,-1.6584400617 C,0,-0.0000000218,-0.0000000011,-3.077771922 C,0,-0.0000000268,0.0000000001,-5.8753692807 C,0,0.8077596069,0.89743865,-3.7917211184 C,0,-0.8077596531,-0.8974386516,-3.7917211164 C,0,-0.8044622383,-0.8937781804,-5.1772431294 C,0,0.8044621872,0.89377818,-5.1772431315 H,0,1.4339229229,1.5931181434,-3.2460039574 H,0,-1.4339229672,-1.5931181454,-3.2460039537 H,0,-1.4338236486,-1.5930280041,-5.7164120774 H,0,1.4338235957,1.5930280042,-5.7164120811 H,0,-0.0000000287,0.0000000006,-6.9594873421	 C,0,0.0000000022,0.,1.0478996089 C,0,-0.0000000022,0.,2.2582823911 C,0,0.0000000074,0.,-0.3718771393 C,0,0.0000000176,0.,-3.1690267956 C,0,0.00000001,1.2073626561,-1.0854452417 C,0,0.00000001,-1.2073626561,-1.0854452417 C,0,0.0000000151,-1.2023513457,-2.4710014767 C,0,0.0000000151,1.2023513457,-2.4710014767 H,0,0.000000008,2.1434263884,-0.5402960155 H,0,0.000000008,-2.1434263884,-0.5402960155 H,0,0.0000000171,-2.143065353,-3.0100283773 H,0,0.0000000171,2.143065353,-3.0100283773 H,0,0.0000000216,0.,-4.2531284707 C,0,-0.0000000074,0.,3.6780591393 C,0,-0.0000000176,0.,6.4752087956 C,0,-0.00000001,-1.2073626561,4.3916272417 C,0,-0.00000001,1.2073626561,4.3916272417 C,0,-0.0000000151,1.2023513457,5.7771834767 C,0,-0.0000000151,-1.2023513457,5.7771834767 H,0,-0.000000008,-2.1434263884,3.8464780155 H,0,-0.000000008,2.1434263884,3.8464780155 H,0,-0.0000000171,2.143065353,6.3162103773 H,0,-0.0000000171,-2.143065353,6.3162103773 H,0,-0.0000000216,0.,7.5593104707
 C,0,0.0356515133,-0.3558197874,1.0932705591 H,0,0.0093860476,0.6221954727,1.5695006963 C,0,0.1043141288,-0.3515634233,-0.2467611025 H,0,0.2035184424,0.6265678827,-0.7130405462 C,0,0.0459498625,-1.4643638857,-1.204592578 C,0,-0.0756235535,-3.5020244871,-3.1309458471 C,0,0.7886520757,-1.3834020899,-2.3881396036 C,0,-0.782963267,-2.5770226005,-1.0206705212 C,0,-0.8410308836,-3.5833756282,-1.9724806127 C,0,0.7385484833,-2.3953896196,-3.3363029351 H,0,1.4193353391,-0.5166843224,-2.5589955215 H,0,-1.3933641502,-2.6437285972,-0.1284257099 H,0,-1.4947082844,-4.4340831567,-1.8133302214 H,0,1.3309722073,-2.315709878,-4.2412110283 H,0,-0.1233828063,-4.2907030219,-3.873481873 C,0,0.0106222443,-1.4795500965,2.039725059 C,0,-0.0206132697,-3.5400713583,3.9452313466 C,0,0.7544453151,-2.6489212033,1.8441945779 C,0,-0.7244369364,-1.3555334437,3.2243147864 C,0,-0.7501928865,-2.3780225755,4.1621289683 C,0,0.7370494871,-3.6664218878,2.7857095576	 C,0,0.119053952,-0.2592852645,1.0936105544 H,0,0.1402146174,0.6955998553,1.6129685228 C,0,0.0875567797,-0.2638461359,-0.2475517306 H,0,0.0301791161,-1.2177016284,-0.7660626448 C,0,0.1012198762,0.8992034872,-1.130402161 C,0,0.0954189712,3.0648419754,-2.9246174307 C,0,-0.0847531015,0.703728865,-2.5051548008 C,0,0.2943949242,2.2125113097,-0.6784827807 C,0,0.2888292451,3.2778820792,-1.5626861566 C,0,-0.0899692719,1.7705671066,-3.3918250257 H,0,-0.2312688446,-0.3050032167,-2.8782905253 H,0,0.4597596392,2.4038396655,0.3754293927 H,0,0.441725423,4.2845672104,-1.189143585 H,0,-0.2384842546,1.5898506243,-4.4507490234 H,0,0.0938692843,3.9017589655,-3.6137090605 C,0,0.1078808298,-1.422405676,1.9764027486 C,0,0.0629404145,-3.5866016193,3.7718047715 C,0,0.2048503177,-2.7439621317,1.51769738 C,0,-0.0022701166,-1.2185124303,3.3580812243 C,0,-0.0266299091,-2.2845098453,4.2454431808 C,0,0.1801100536,-3.8084713216,2.4026095605

H,0,1.3585217877,-2.7518295407,0.951086958 H,0,-1.2888904836,-0.4460368143,3.4042061034 H,0,-1.3353807784,-2.2636445721,5.068024211 H,0,1.3256211488,-4.5617848224,2.617677106 H,0,-0.0319996588,-4.3376194737,4.6796984193	H,0,0.3096717329,-2.9429717152,0.4574660116 H,0,-0.0736812112,-0.2035848209,3.7363138877 H,0,-0.115015644,-2.0970584193,5.3099078842 H,0,0.2579815368,-4.8217170374,2.023669725 H,0,0.0460629835,-4.4229947377,4.4613273804
 H,0,-0.3120253029,-0.2581653222,0.249850372 C,0,-0.0436446308,-0.0727524731,1.2940503876 H,0,-0.3529478898,-0.9582837649,1.8570118494 C,0,1.4872863674,0.073101933,1.3965696546 H,0,1.7965896264,0.9586332248,0.8336081928 H,0,1.7556670394,0.258514782,2.4407696701 C,0,2.221060142,-1.1387606901,0.8873367847 C,0,3.5229282931,-3.4290282038,-0.0772101724 C,0,2.5822659211,-1.245292741,-0.4559586919 C,0,2.5263924196,-2.201196846,1.7383732381 C,0,3.1709777935,-3.3362771592,1.2636452617 C,0,3.2269936491,-2.3779376086,-0.9362773714 H,0,2.3615560013,-0.4255623281,-1.1332029987 H,0,2.2616745418,-2.1343705214,2.7894628428 H,0,3.4033484532,-4.1486166203,1.9437992234 H,0,3.5033463025,-2.4378171889,-1.9834376181 H,0,4.0289303511,-4.3128432374,-0.4493372425 C,0,-0.7774184055,1.13911015,1.8032832574 C,0,-2.0792865566,3.4293776637,2.7678302145 C,0,-1.1386241846,1.2456422009,3.146578734 C,0,-1.0827506831,2.2015463059,0.952246804 C,0,-1.7273360569,3.3366266191,1.4269747804 C,0,-1.7833519125,2.3782870684,3.6268974136 H,0,-0.9179142648,0.425911788,3.8238230408 H,0,-0.8180328053,2.1347199812,-0.0988428007 H,0,-1.9597067167,4.1489660802,0.7468208187 H,0,-2.059704566,2.4381666487,4.6740576602 H,0,-2.5852886146,4.3131926973,3.1399572846	
 C,0,0.4833127417,1.8478306493,0. O,0,0.8093771694,2.9738525999,0. Mn,0,-0.0348588293,0.1521533482,0. P,0,0.0928050492,-0.0809790083,2.2247817926 P,0,0.0928050492,-0.0809790083,-2.2247817926 C,0,1.806377247,-0.8099581621,2.4397457284 C,0,1.806377247,-0.8099581621,-2.4397457284 H,0,1.7015630337,-1.8982090594,2.496598843 H,0,1.7015630337,-1.8982090594,-2.496598843 H,0,2.2877617666,-0.4825456841,3.3637355801 H,0,2.2877617666,-0.4825456841,-3.3637355801 C,0,2.6419170467,-0.4263312751,1.2284194344 C,0,2.6419170467,-0.4263312751,-1.2284194344 H,0,3.5965165711,-0.9722086063,1.2229017975 H,0,3.5965165711,-0.9722086063,-1.2229017975 H,0,2.8683299673,0.6429536916,1.2402719121	 C,0,-2.4048266722,0.0295035899,0. O,0,-3.5662111755,0.1153522714,0. Mn,0,-0.6197159489,-0.0493183392,0. P,0,-0.38832085,-0.2721254493,2.2060518986 P,0,-0.38832085,-0.2721254493,-2.2060518986 C,0,-0.3896035499,-2.120668252,2.4626914064 C,0,-0.3896035499,-2.120668252,-2.4626914064 H,0,-1.4298813397,-2.4320565668,2.6020588658 H,0,-1.4298813397,-2.4320565668,-2.6020588658 H,0,0.1640800659,-2.4331352574,3.3514687334 H,0,0.1640800659,-2.4331352574,-3.3514687334 C,0,0.1944809343,-2.7535633572,1.2137221315 C,0,0.1944809343,-2.7535633572,-1.2137221315 H,0,0.1154238712,-3.8492147531,1.2507382834 H,0,0.1154238712,-3.8492147531,-1.2507382834 H,0,1.2538801644,-2.4995031346,1.1295256778

H,0,2.8683299673,0.6429536916,-1.2402719121 N,0,1.8769551978,-0.6931198561,0. C,0,-0.96251185,-1.2937875078,-3.1604675476 C,0,-0.96251185,-1.2937875078,3.1604675476 H,0,-0.8221353634,-2.2448275416,-2.6402069565 H,0,-0.8221353634,-2.2448275416,2.6402069565 C,0,0.109839273,1.4096413412,-3.349031163 C,0,0.109839273,1.4096413412,3.349031163 H,0,0.8816724175,2.065818332,-2.9362360955 H,0,0.8816724175,2.065818332,2.9362360955 C,0,0.3183880814,1.1943726102,4.8422098247 C,0,0.3183880814,1.1943726102,-4.8422098247 H,0,1.2437992015,0.652998717,5.0558211397 H,0,1.2437992015,0.652998717,-5.0558211397 H,0,-0.5027581151,0.6327025554,5.2926052851 H,0,-0.5027581151,0.6327025554,-5.2926052851 H,0,0.3793917626,2.1538900938,5.363499761 H,0,0.3793917626,2.1538900938,-5.363499761 H,0,-0.8339240338,1.9320025442,3.1656536062 H,0,-0.8339240338,1.9320025442,-3.1656536062 C,0,-2.437813359,-0.9128834375,-3.1445147796 C,0,-2.437813359,-0.9128834375,3.1445147796 H,0,-2.6224555155,0.0321439434,-3.6621134426 H,0,-2.6224555155,0.0321439434,3.6621134426 H,0,-2.7947868834,-0.8094989345,-2.1168395615 H,0,-2.7947868834,-0.8094989345,2.1168395615 H,0,-3.0456069801,-1.6780757924,-3.6343213121 H,0,-3.0456069801,-1.6780757924,3.6343213121 H,0,-0.5966694952,-1.415548627,-4.1845245182 H,0,-0.5966694952,-1.415548627,4.1845245182 H,0,-0.6641822011,-1.3763060742,0. H,0,1.6098079028,-1.6753774354,0.	H,0,1.2538801644,-2.4995031346,-1.1295256778 N,0,-0.4590239044,-2.2246726191,0. C,0,-1.6924721319,0.2787637104,-3.4108266233 C,0,-1.6924721319,0.2787637104,3.4108266233 H,0,-2.6228161975,-0.1803859412,-3.0646767113 H,0,-2.6228161975,-0.1803859412,3.0646767113 C,0,1.195313795,0.3028090947,-2.9942992826 C,0,1.195313795,0.3028090947,2.9942992826 H,0,1.9851104808,-0.1883894758,-2.4196052879 H,0,1.9851104808,-0.1883894758,2.4196052879 C,0,-0.3778714375,1.6998223051,0. O,0,-0.163824891,2.8412593301,0. C,0,1.3778496123,0.0842029166,4.4901533947 C,0,1.3778496123,0.0842029166,-4.4901533947 H,0,1.2833923622,-0.9688638102,4.7682330373 H,0,1.2833923622,-0.9688638102,-4.7682330373 H,0,0.6502059348,0.6474428889,5.0780474894 H,0,0.6502059348,0.6474428889,-5.0780474894 H,0,2.3722166281,0.4124335593,4.8051952862 H,0,2.3722166281,0.4124335593,-4.8051952862 H,0,1.2777747999,1.3638969959,2.7420016652 H,0,1.2777747999,1.3638969959,-2.7420016652 C,0,-1.8563467285,1.7930327824,-3.476888526 C,0,-1.8563467285,1.7930327824,3.476888526 H,0,-0.9509240033,2.2861504726,-3.838897395 H,0,-0.9509240033,2.2861504726,3.838897395 H,0,-2.088023484,2.2070189538,-2.494167009 H,0,-2.088023484,2.2070189538,2.494167009 H,0,-2.6702199195,2.0627341371,-4.1545902223 H,0,-2.6702199195,2.0627341371,4.1545902223 H,0,-1.4767646299,-0.134988109,-4.4008520736 H,0,-1.4767646299,-0.134988109,4.4008520736 H,0,0.9840104141,-0.1412098416,0. H,0,-1.4238897547,-2.545436749,0.
 C,0,0.5749688322,1.9010360149,0. O,0,0.9507269364,3.0032451475,0. Mn,0,-0.0597953469,0.2312045964,0. P,0,0.0980838034,-0.0677033358,2.2089103535 P,0,0.0980838034,-0.0677033358,-2.2089103535 C,0,1.8059388092,-0.8037414713,2.4399637734 C,0,1.8059388092,-0.8037414713,-2.4399637734 H,0,1.6936963666,-1.890569412,2.5092592663 H,0,1.6936963666,-1.890569412,-2.5092592663 H,0,2.2843083356,-0.4706300513,3.3632952854 H,0,2.2843083356,-0.4706300513,-3.3632952854 C,0,2.6493107648,-0.4401021015,1.2290165284 C,0,2.6493107648,-0.4401021015,-1.2290165284 H,0,3.5971707618,-0.9971394516,1.2304516643 H,0,3.5971707618,-0.9971394516,-1.2304516643 H,0,2.8916558799,0.6257115995,1.2359819377 H,0,2.8916558799,0.6257115995,-1.2359819377 N,0,1.8855189386,-0.7056136086,0. C,0,-0.9580941941,-1.3006433426,-3.1123642822 C,0,-0.9580941941,-1.3006433426,3.1123642822 H,0,-0.8505127035,-2.2298659939,-2.5466187825 H,0,-0.8505127035,-2.2298659939,2.5466187825	 C,0,0.4389860325,-1.6056801762,0. O,0,0.8440039006,-2.690148857,0. Mn,0,-0.1682139383,0.0691956383,0. P,0,0.0519470595,0.2696455056,-2.2529065093 P,0,0.0519470595,0.2696455056,2.2529065093 C,0,1.6389186928,1.2181910816,-2.429635408 C,0,1.6389186928,1.2181910816,2.429635408 H,0,1.376767606,2.2801045392,-2.4537541575 H,0,1.376767606,2.2801045392,2.4537541575 H,0,2.1664253253,0.9816651715,-3.3563193665 H,0,2.1664253253,0.9816651715,3.3563193665 C,0,2.4829188727,0.9223931974,-1.1979586111 C,0,2.4829188727,0.9223931974,1.1979586111 H,0,3.3496714367,1.6046882086,-1.184929766 H,0,3.3496714367,1.6046882086,1.184929766 H,0,2.9029717352,-0.0998768145,-1.2837151413 H,0,2.9029717352,-0.0998768145,1.2837151413 N,0,1.6974347941,1.0802258913,0. C,0,-1.1392196958,1.2877959061,3.2509173153 C,0,-1.1392196958,1.2877959061,-3.2509173153 H,0,-1.2203680436,2.2405521997,2.7199016187 H,0,-1.2203680436,2.2405521997,-2.7199016187

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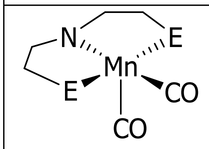

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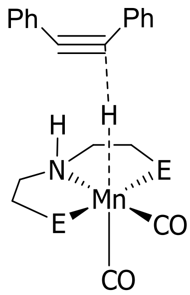

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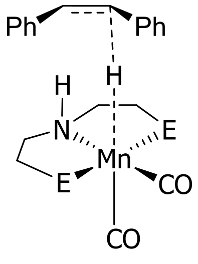
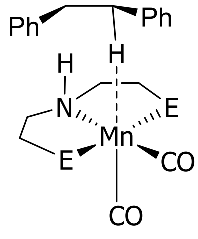
 N,0,0.5920692803,0.6489791466,-1.7472365632	 N,0,0.07224252,-0.8509456468,-1.6497800339 Mn,0,1.3323155241,-0.9127557716,0.0089634999

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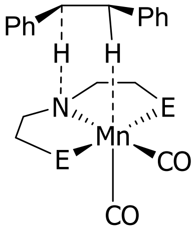
<td>

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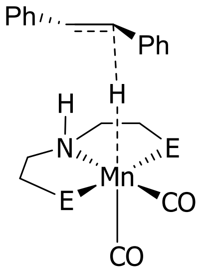
<td>

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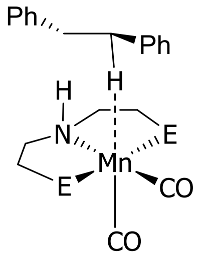

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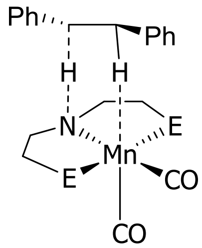

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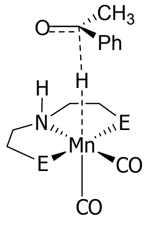
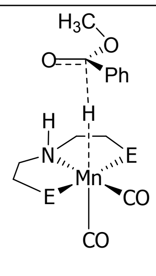
 O,0,-1.8925716659,2.668084776,0.9638595901 P,0,1.4344621908,1.4242235054,-0.0613679668 P,0,-2.4987959623,-0.8279497076,-0.06445118 C,0,1.6417159452,1.4180494715,-1.9073311498 C,0,-2.5981607848,-1.0200986399,-1.9123021494 H,0,2.1826276006,0.5059348,-2.1725307431 H,0,-2.0947458942,-1.9513510715,-2.1843655595 H,0,2.2142055231,2.2732626657,-2.2729625981 H,0,-3.6255139532,-1.0750376247,-2.2790647359 C,0,0.2517101003,1.3792785296,-2.5193669872 C,0,-1.8556556369,0.15586392,-2.5264053316 H,0,0.3167520589,1.2370183819,-3.6065087985 H,0,-1.7600740151,0.0211715399,-3.612186539 H,0,-0.2803516337,2.319423463,-2.3431405913 H,0,-2.4028940247,1.088994849,-2.3599932334 N,0,-0.5249159749,0.2856294358,-1.9080389683 C,0,-2.9837099478,-2.495823182,0.5952637607	 N,0,-0.4466571612,0.3878798593,2.1245836815 P,0,-2.4583987083,-0.6033304828,0.2232743032 P,0,1.5387171499,1.4993403956,0.2988330339 C,0,-0.299035881,0.226074146,-1.7516042014 H,0,0.2799984728,-1.0980874599,0.1895338063 C,0,0.9919653507,-2.2972303367,1.0262513184 O,0,1.2971565671,-1.8383621537,2.1358996614 O,0,-0.05511864,-3.2283693929,0.9365028564 C,0,2.0404969426,-2.622312594,-0.0108934331 C,0,-2.5523082292,-0.8850545534,2.0609498813 C,0,1.708666574,1.5458580776,2.1528756272 H,0,-2.0872576654,-1.8528155008,2.2573365845 H,0,2.2745931304,0.6574671329,2.4445752489 H,0,-3.5787628233,-0.9296224376,2.4316235678 H,0,2.251862141,2.4261919482,2.5030549193 C,0,-1.7713601692,0.222177662,2.7498373975 C,0,0.3145529863,1.4836375581,2.7529663523

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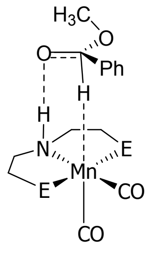
<td>

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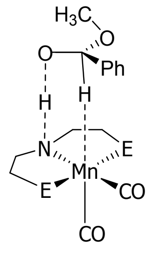
<td>

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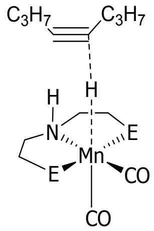
H,0,5.7826995625,-2.7955038072,-0.7509188763	H,0,5.8771457835,-2.7759914669,-0.4294662573
H,0,1.5752465357,-2.4133275025,-1.4907488882	H,0,1.7176288381,-2.5571935636,-1.4503731695
H,0,3.8500900601,-2.9641260903,-2.2925664905	H,0,4.0524239313,-3.078741204,-2.0790942942
C,0,0.2332781312,-3.8156957501,1.6640429904	C,0,0.222731078,-3.8419874324,1.6295437069
H,0,-0.5292194906,-4.5766206376,1.4884149271	H,0,-0.5226103947,-4.617354493,1.4470650913
H,0,1.2193873641,-4.2559144745,1.4720528489	H,0,1.2206939246,-4.2677209076,1.4723285632
H,0,0.1891408107,-3.487287713,2.7066311303	H,0,0.1430772741,-3.4949301433,2.6638412163
C,0,-1.6777435913,2.0704729349,-0.8362324533	C,0,-1.7507844961,2.1550336798,-0.8920136048
O,0,-2.3158899019,2.9838950395,-1.1594264559	O,0,-2.3833513158,3.0731113192,-1.2128833902

Mn,0,-0.7171695109,0.6853021706,-0.3493125452	Mn,0,-0.8047876453,0.7734730211,-0.3836489615
s	2-Butyne C,0,-0.0010851761,0.0032361433,1.0713597464 C,0,0.0011049258,-0.0032740009,2.2748181089 C,0,-0.0037369807,0.0111079193,-0.3815784196 H,0,0.9798790101,0.2796880865,-0.7765372349 H,0,-0.7273632878,0.7324882686,-0.7709498896 H,0,-0.2659052019,-0.9724163372,-0.7810489631 C,0,0.003743306,-0.0111087031,3.7277641592 H,0,0.9889512356,0.2526411623,4.1220140838 H,0,-0.2575299135,-0.9987579975,4.1175219452 H,0,-0.7180591665,0.7063954586,4.1275464627
 C,0,-1.7748829847,0.0399935794,-1.8578647285 O,0,-2.8888481464,0.1012573298,-2.1837823792 P,0,0.2186948263,2.1710434052,-1.1297490538 P,0,-0.0268448349,-2.2982322732,-1.1247071673 C,0,1.8420948445,2.2906543458,-0.2216466265 C,0,1.5640743933,-2.5926355464,-0.1992800919 H,0,1.607014605,2.3672806902,0.8434432295 H,0,1.3103162652,-2.6306719243,0.8637756448 H,0,2.420698751,3.1738822035,-0.5002755182 H,0,2.0413253029,-3.5386519021,-0.4636260655 C,0,2.6206105472,1.0140649948,-0.4828295693 C,0,2.4845715747,-1.414881255,-0.4643941733 H,0,3.4888895297,0.9497722103,0.1881331539 H,0,3.3485651785,-1.4413581524,0.2147540596 H,0,2.9984156445,0.9909381047,-1.5088161098 H,0,2.8717718207,-1.4453847671,-1.4867644459 N,0,1.7397867564,-0.1533834316,-0.2975540883 C,0,-1.2371988933,-3.2615849834,-0.0956519519 C,0,-0.8710633394,3.2549102263,-0.0857451694 H,0,-1.2610041873,-2.7508882231,0.870339782 H,0,-0.9375519165,2.7471354437,0.8798437774 C,0,0.1294259984,-3.333268404,-2.6646191968 C,0,0.4661410176,3.186673807,-2.6706032503 H,0,0.9743455674,-2.9099306088,-3.2146365355 H,0,1.252041732,2.6753181231,-3.2331638729 C,0,0.5638044934,-0.0904080446,-2.9909869755 O,0,0.9687413368,-0.1119855976,-4.082160758 C,0,0.7929315551,4.6654825096,-2.508457778 C,0,0.2906909518,-4.8390913905,-2.501767984 H,0,-0.4437858343,3.0545659187,-3.2632132731 H,0,-0.7519905894,-3.1017053726,-3.2696111984 C,0,-2.637021715,-3.3491356967,-0.6919543504 C,0,-2.2611081429,3.4904804882,-0.6646699982 H,0,-2.6397636955,-3.8802901419,-1.6468171095 H,0,-2.2198922215,4.0215475732,-1.6187073578 H,0,-3.0618396316,-2.3596325263,-0.8667011576 H,0,-2.7894104624,2.5513551078,-0.8352618367 H,0,-3.3077571421,-3.8884731823,-0.01804411 H,0,-2.8632739314,4.0954349616,0.0182493063 H,0,-0.8283332315,-4.2612575102,0.0822224189 H,0,-0.3573920338,4.2056557319,0.088503295 H,0,-0.621585956,-0.0179349341,0.2741124874	4-Octyne C,0,-0.0425403451,0.0468184529,1.0709619704 C,0,-0.0426487229,0.0379907338,2.2758374185 C,0,-0.0187513591,0.0683991773,-0.3850372367 C,0,1.3704090214,0.3505661355,-0.9726926254 H,0,-0.7255977627,0.8247804792,-0.7469112937 H,0,-0.3847453961,-0.892526384,-0.766260177 C,0,-0.05359438,0.0036230825,3.7317437217 H,0,0.9084165957,0.3712042535,4.1086781492 C,0,-0.3252936113,-1.3909943477,4.3113511424 H,0,-0.8104903453,0.704419629,4.1041553159 C,0,1.36343533,0.367354828,-2.4951713378 H,0,1.7285664163,1.3096086229,-0.58739262 H,0,2.0688499017,-0.4080782948,-0.6077824239 H,0,2.360602195,0.5695667918,-2.8928269376 H,0,1.033508011,-0.5928594391,-2.9021902887 H,0,0.6907002782,1.138517056,-2.8814954417 C,0,-0.3309849656,-1.3950831836,5.8339227805 H,0,-1.28552815,-1.7506616323,3.930452197 H,0,0.433754034,-2.0833704215,3.9358747976 H,0,-0.525894478,-2.3959838373,6.2258020008 H,0,0.6307201131,-1.0638294664,6.2363181572 H,0,-1.1022542803,-0.7285934357,6.2307163311

H,0,1.3968956598,-0.1314358568,0.6961272587 C,0,-0.6492619968,-0.0523224103,1.8171210365 C,0,0.4450174454,-0.1311891036,2.4029004937 C,0,1.3080064295,-0.2406953216,3.5908107818 C,0,-2.1293152747,0.0329241304,1.9254677377 Mn,0,-0.0838799369,-0.0532132901,-1.3406018747 H,0,0.4258536242,-5.3144148569,-3.4771274217 H,0,1.162049505,-5.0968857792,-1.8944933771 H,0,-0.5841242089,-5.2973815598,-2.0362142919 H,0,0.9640561309,5.1259931014,-3.4852789817 H,0,-0.0195088854,5.2150535949,-2.0288738899 H,0,1.6964383165,4.8251478112,-1.9145805792 H,0,-2.4777894269,0.9379845724,1.4159144837 H,0,-2.581887771,-0.7945750511,1.3678965882 C,0,-2.619594643,0.0239011129,3.3731556486 H,0,1.6920770647,-1.2669359252,3.6562828462 C,0,2.5003219317,0.7215048734,3.6206157613 H,0,0.7169867902,-0.0867849057,4.5062544459 C,0,3.3398512688,0.5753025517,4.8830441141 H,0,3.1231307407,0.5472060959,2.7370481735 H,0,2.1300884627,1.7484708964,3.5389548078 C,0,-4.1379853311,0.1086655974,3.4730676034 H,0,-2.2635912024,-0.8862410011,3.8659587125 H,0,-2.1633385181,0.8612269021,3.9104515548 H,0,4.1827836614,1.2704443344,4.8844945522 H,0,2.7456219653,0.7744895256,5.7793712461 H,0,3.7446709237,-0.4368757531,4.9750743671 H,0,-4.4681632609,0.1007646338,4.5147726838 H,0,-4.5161619406,1.0257252543,3.012455872 H,0,-4.6172557259,-0.7341999601,2.9670715739	

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