SUPPORTING INFORMATION

Preparation of Organocobalt(III) Complexes via O_2 Activation

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Instrumentation

IR spectra were recorded on a PerkinElmer Spectrum 65 (FT-ATR diamond anvil) on the neat samples. All spectra have been ATR- and baseline-corrected and were normalised with regards to the most intensely absorbing band. Thermal analysis was carried out on a Perkin Elmer TGA 4000 from 30-350 °C at 5 °C/min in a nitrogen atmosphere with a purge rate of 20 mL/min. UV-vis spectra were recorded on an Agilent 8453 spectrophotometer in 1 cm quartz cuvettes, irradiation was supplied by a 365 nm LED laser, (M365FP1, 1200 mA, Thorlabs). ^{1}H NMR (400.12 MHz) and ^{13}C NMR (100.61 MHz) solution spectra were recorded on a Bruker AVANCE III 400 FT spectrophotometer at ambient temperature. Chemical shifts (δ) are denoted relative to the residual solvent peak (d_6-DMSO: δ_H = 2.50 ppm, δ_C = 39.52 ppm). ^{13}C CPMAS NMR (500 or 600 MHz) solid-state spectra were recorded on either a Varian INOVA 500 MHz NMR spectrometer (11.7 T) or a Varian INOVA 600 MHz NMR spectrometer (14.1 T) using a 3.2 mm HX MAS probe and a spinning speed of 15 kHz. Chemical shifts (δ) are corrected relative to adamantane (δ_C = 38.5 ppm). EPR spectra (X-band) were recorded on a Bruker EMX Plus CW spectrometer (Gain: 30 dB, mod. amp.: 10 G, attenuation: 10 dB) on frozen solutions at 100 K. The software packages eview and esimX were used for simulation.[1] Mass spectra are recorded with Electrospray ionisation (ESI) on a Bruker micrOTOF-Q II spectrometer (nanospray, capillary temperature = 180 °C, spray voltage = 3.7 kV).

Single crystal x-ray diffraction

The crystals used for SCXRD were taken directly from the mother liquor and mounted cryogenically using Fomblin®Y to adhere the crystal to the mounting loop. X-ray crystal diffraction data was collected at 100(2) K or 293(2) K on a Synergy, Dualflex, AtlasS2 diffractometer using CuKα radiation (λ = 1.54184 Å) and the CrysAlis PRO 1.171.40.21a suite[2] and corrected for Lorentz-polarisation effects and absorption. Using SHELXLE[3] the structure was solved by dual space methods (SHELXT[4]) and refined on F^2 using all the reflections (SHELXL-2018[5]). All the non-hydrogen atoms were refined using anisotropic atomic displacement parameters and hydrogen atoms were inserted at calculated positions using a riding model. Parameters for data collection and refinement are summarised in Table S1-S3. In Co(salen)(NO_2)(H_2O) the NO_2 group is disordered over two positions in a nitro/nitrito disorder and were refined with a final ratio of 0.37:0.63. Hydrogen atoms of the coordinate water were located from the difference maps. In [Co(salen)(NO_2)]$_2$·($CH_3CH_2NO_2$) it was not possible to model the distorted solvate molecule, therefore, a solvent mask was calculated, and

45 electrons were found in a volume of 170 Å^3 in 1 void per unit cell. This is consistent with the presence of 0.5[$C_2H_5NO_2$] per Asymmetric Unit which account for 40 electrons per unit cell. Co(salen)(CH_2COCH_3)(MeOH) is twinned in which component two (33.36 %) was rotated by 2.72° around [-1.00 -0.03 -0.01]. This phase is known (CCDC: ESACCO)[6] however has a higher R-Factor and the entry does not contain any coordinates. Co(salen)(CH_2COCH_3)(H_2O) was a weak diffractor and only room temperature data were available at meagre resolution, however, the main features of the structure are clear.

Computational details

The electronic structure calculations considered in this work are all based on (unrestricted) density functional theory (DFT) calculations performed using Jaguar[7] through the Maestro graphical interface.[8] All structures have been geometry optimised in isolation using M06-L/LACVP+* [9,10] and vibrational frequencies have also been calculated at this level of theory. Single point energies, based on the use of the M06-L/LACVP+* geometry optimized structures, have been performed using M06-L/LACV3P**. The relative energies reported are based on these single point energies but corrected for zero-point vibrational effects calculated at the M06-L/LACVP+* level. All calculations are solution phase calculations, using the Poisson-Boltzmann solvation model. The EPR *g*-tensors were calculated using the ORCA program package using the same basis set and functional as described above.[11–13]

The starting structure **V** was based on the crystal structure of [(Co(salen)DMF)$_2$$O_2$] obtained from the Cambridge Structural Database (CCDC: DOESCF10)[14] in which the DMF molecules were replaced by MeOH. Following the geometry optimization, this structure was used as basis for creating the other salen-based structures in the reaction mechanism. The crystal structure of **7** was used as the starting structure for **VIII**. Smaller molecules such as O_2, CH_2CH_2 and $EtNO_2$ etc. were created in the Jaguar program using a 2D sketcher tool.

pK_a values were calculated using the following set of formula from Smith *et al.*[15]

$$AH(DMSO) \xrightarrow{\Delta G^*_{DMSO}} A^-(DMSO) + H^+(DMSO) \quad (1)$$

$$pK_a = \frac{\Delta G^*_{DMSO}}{2.303RT} \quad (2)$$

$$\Delta G^*_{DMSO} = G^*_{DMSO}(A^-) + G^*_{DMSO}(H^+) - G^*_{DMSO}(AH) \quad (3)$$

$$G^*_{DMSO}(H^+) = G^\circ_g(H^+) + \Delta G_{DMSO,solv}(H^+) + \Delta G^{\circ\rightarrow *} \quad (4)$$

Given the deprotonation reaction shown in equation 1, the pK_a of molecule AH was calculated according to equation 2. The free energy difference was calculated directly from the Gibbs free energies of the acid and conjugated base with equation 3. The standard state free energy of the proton was calculated according to equation 4, in which the gas-phase energy of a proton ($G^\circ_g(H^+)$ = -6.29 kcal/mol) and the experimentally measured solvation free energy ($\Delta G_{DMSO,solv}(H^+)$ = -273.3) were taken from the literature.[15,16] $\Delta G^{\circ\rightarrow *}$ is used to convert from the 1 atm ideal gas standard state to the 1 M standard state. Where the superscripts ° and * the 1 atm and 1 M standard states respectively. $\Delta G^{\circ\rightarrow *} = RT\ln(24.46) = 1.89$ kcal/mol at 298 K.[15]

Synthesis

N,N'-ethylenebis(salicylideneimine)[17] and N,N'-ethylenebis(salicylideneimine)cobalt(II)[18] were prepared according to literature methods. All other chemicals were purchased from Sigma-Aldrich and were used without further purification. Reactions were carried out with the exclusion of light.

[Co(salen)(CH_2NO_2)]$_2$·(2 $MeNO_2$). Co(salen) (0.25 g) was dissolved in boiling nitromethane (25 mL) and the solution was allowed to stir for 10 minutes with continued heating. The flask was equipped with a calcium chloride drying tube and left to stand for two days during which a green crystalline solid precipitated, which was collected by filtration (0.25 g, 73.6 %). Single crystals suitable for X-ray diffraction were obtained from the crystal floating on top of the solution.

IR (ATR-FT) cm^{-1}: 1619(vs, C=C), 1594(vs, C=N), 1496(vs, ν(NO_2))

^{1}H-NMR (400.12 MHz, *d*$_6$-DMSO): δ = 8.09 (s, 2H, N=C*H*), 7.20 (dd, 2H, $^3J_{HH}$ = 7.75, $^4J_{HH}$ = 1.84, $C_{arom}H$) 7.16 (td, 2H, $^3J_{HH}$ = 7.61, $^4J_{HH}$ = 1.84, $C_{arom}H$), 6.98 (dd, 2H, $^3J_{HH}$ = 8.53, $^4J_{HH}$ = 1.14, $C_{arom}H$), 6.45 (td, 2H, $^3J_{HH}$ = 7.28, $^4J_{HH}$ = 1.19, $C_{arom}H$), 5.09 (s, 2H, CH_2), 3.77 (m, 4H, 2 × CH_2) ppm.

^{13}C NMR (101 MHz, *d*$_6$-DMSO) δ = 165.65 (2 × *C*=N), 165.14, 133.84, 133.28, 122.22, 119.16, 113.21 (6 × C_{arom}), 57.28 (2 ×*C*H_2) ppm.

[Co(salen)(NO_2)]$_2$·$CH_3CH_2NO_2$. Was prepared analogously to the compound above substituting nitromethane with nitroethane, yielding a brownish-green microcrystalline solid which was collected by filtration (0.12 g, 38.9 %).

IR (ATR-FT) cm^{-1}: 1633 (vs, C=C), 1598 (vs, C=N), 1421 (s, $\nu_a(NO_2)$), 821 (s, δ_s(ONO.

^{1}H-NMR (400.12 MHz, *d*$_6$-DMSO): δ = 8.24 (s, 2H, N=C*H*), 7.37 (dd, 2H, $^3J_{HH}$ = 7.88, $^4J_{HH}$ = 1.85, $C_{arom}H$) 7.27 (td, 2H, $^3J_{HH}$ = 7.65, $^4J_{HH}$ = 1.82, $C_{arom}H$), 7.14 (dd, 2H, $^3J_{HH}$ = 8.48, $^4J_{HH}$ = 1.09, $C_{arom}H$), 6.54 (td, 2H, $^3J_{HH}$ = 7.28, $^4J_{HH}$ = 1.22, $C_{arom}H$), 3.99 (s, 4H, 2 × CH_2) ppm.

^{13}C NMR (101 MHz, *d*$_6$-DMSO) δ = 165.92 (2 × *C*=N), 165.85, 134.24, 133.94, 122.17, 118.84, 113.47 (6 × C_{arom}), 58.02 (2 ×*C*H_2) ppm.

Co(salen)(NO_2)(H_2O). Was prepared analogously to the compound above omitting the drying tube during the crystallisation or by adding ethanol (5 mL, 96%) to the solution prior to crystallisation. After two days the compound was obtained as a brownish-green crystalline solid, which was collected by filtration (0.12 g, 40.9 %).

IR (ATR-FT) cm^{-1}: 1637 (vs, C=C), 1600 (vs, C=N), 1469 (s, ν_a(N=O)), 1432 (s, $\nu_a(NO_2)$), 1058 (m, ν_s(N–O)), 821 (vs, δ_s(ONO)).

Co(salen)(CH_2COCH_3)(MeOH). Co(salen) (0.25 g) was partially dissolved in boiling acetone/methanol (3:2 V/V, 25 mL) and the solution was allowed to stand for two days in darkness, during which the colour changed from red to green. The green solution was evaporated to dryness *in vacuo*, yielding green crystals which were collected by filtration and washed with water (0.23 g, 71.3 %). It was possible to recrystallise Co(salen)(CH_2COCH_3)(MeOH) from by slow evaporation from an aqueous ethanol solution which yielded the corresponding hydrate Co(salen)(CH_2COCH_3)(H_2O), in quantitative amount. Recrystallisation by diffusion of diethylether into a solution of Co(salen)(CH_2COCH_3)(MeOH) in benzene yielded [Co(salen)(CH_2COCH_3)]$_2$·(C_6H_6).

IR (ATR-FT) cm^{-1}: 3303 (vb, O–H), 1655 (m, ν(C=O)), 1625 (vs, C=C), 1599 (vs, C=N).

^{1}H-NMR (400.12 MHz, *d*$_6$-DMSO): δ = 8.00 (s, 2H, N=C*H*), 7.16 (dd, 2H, $^3J_{HH}$ = 7.73, $^4J_{HH}$ = 1.88, $C_{arom}H$) 7.11 (td, 2H, $^3J_{HH}$ = 7.66, $^4J_{HH}$ = 1.81, $C_{arom}H$), 6.93 (dd, 2H, $^3J_{HH}$ = 8.42, $^4J_{HH}$ = 1.08, $C_{arom}H$), 6.41 (td, 2H, $^3J_{HH}$ = 7.22, $^4J_{HH}$ = 1.13, $C_{arom}H$), 3.73 (m, 4H, 2 × CH_2), 2.88 (s, 2H, CH_2), 1.64 (s, 3H, CH_3) ppm.

^{13}C NMR (101 MHz, *d*$_6$-DMSO) δ = 217.87 (*C*=O), 165.62 (2 × *C*=N), 164.30, 133.57, 132.71, 122.43, 119.8*9, 112.85 (6 ×* C_{arom}), 57.87 (2 ×*C*H_2), 30.37 (*C*H_3) ppm.

UV-vis (DCM) λ_{max}/nm (ε/M^{-1} cm^{-1}): 250 (25550), 353 (6800), 784 (350).

[Co(salen)(CH_2COPh)]$_2$. Co(salen) (0.25 g) was dissolved in boiling acetophenone/methanol (2:3 V/V, 25 mL) and the solution was allowed to stand for two days in darkness, during which the colour changed from red to green. The solution was evaporated to almost dryness *in vacuo* and precipitated with n-hexane. The green precipitate was recrystallised from an aqueous methanol, yielding green crystals suitable for X-ray diffraction (0.18 g, 51.7 %).
IR (ATR-FT) cm^{-1}: 1681 (m, ν(C=O)), 1631 (s, C=C), 1622 (s, C=C), 1596 (s, C=N).
^{1}H-NMR (400.12 MHz, *d*$_6$-DMSO): δ = 7.90 (s, 2H, N=C*H*), 7.54 (dd, 2H, $^3J_{HH}$ = 8.13, $^4J_{HH}$ = 1.26, $C_{arom}H$) 7.11 (tt, 1H, $^3J_{HH}$ = 7.34, $^4J_{HH}$ = 1.36, $C_{arom}H$), 7.11 – 7.03 (m, 6H, $C_{arom}H$), 6.41 (dd, 2H, $^3J_{HH}$ = 8.88, $^4J_{HH}$ = 1.22, $C_{arom}H$), 6.36 (td, 2H, $^3J_{HH}$ = 7.61, $^4J_{HH}$ = 1.11**,** $C_{arom}H$), 3.77 (s, 4H, 2 × CH_2), 3.49 (s, 2H, CH_2) ppm.
^{13}C NMR (101 MHz, *d*$_6$-DMSO) δ = 211.25 (*C*=O), 165.51 (2 × *C*=N), 164.67, 139.26, 133.59, 132.66, 130.75, 127.53, 127.10, 122.50, 119.99, 112.87 (10 × C_{arom}), 57.86, (2 ×CH_2) ppm.

Co(salen)CH_2CN. Co(salen) (0.25 g) was partially dissolved in boiling acetonitrile/methanol (3:2 V/V, 25 mL) and the solution was allowed to stand for two days in darkness, during which the colour changed from red to brown. The solution was evaporated to almost dryness *in vacuo* and precipitated with n-hexane, which yielded a brown precipitate which was collected by filtration (0.16 g, 55.7 %). Single crystals suitable for X-ray diffraction were obtained by slow evaporation from a methanol/benzene solution of Co(salen)CH_2CN, yielding [Co(salen)CH_2CN]$_2$·(C_6H_6).
IR (ATR-FT) cm^{-1}: 2204 (m, ν(C≡N)) , 1627 (s, C=C), 1598 (s, C=N).
^{1}H-NMR (400.12 MHz, *d*$_6$-DMSO): δ = 8.05 (s, 2H, N=C*H*), 7.19 (dd, 2H, $^3J_{HH}$ = 7.64, $^4J_{HH}$ = 1.64, $C_{arom}H$) 7.13 (td, 2H, $^3J_{HH}$ = 7.63, $^4J_{HH}$ = 1.64, $C_{arom}H$), 6.93 (d, 2H, $^3J_{HH}$ = 8.36, $C_{arom}H$), 6.43 (t, 2H, $^3J_{HH}$ = 7.22, $C_{arom}H$), 3.80 (m, 4H, 2 × CH_2), 2.34 (s, 2H, CH_2) ppm.
^{13}C NMR (101 MHz, *d*$_6$-DMSO) δ = 165.93 (2 × *C*=N), 164.96, 134.11, 133.38 (3 × C_{arom}), 129.79 (*C*≡N), 122.45, 119.77, 113.45 (3 × C_{arom}), 57.84 (2 ×CH_2) ppm.

[Co(salen)(OCH_2CF_3)]$_2$·4 CF_3CH_2OH. Co(salen) (0.25 g) was dissolved in boiling 2,2,2-trifluoroehtanol (dry, 25 mL) and the solution was allowed to stand for one day with exposure to air, which yielded red needle crystals, suitable for X-ray diffraction, which were collected by filtration (0.33 g, 68.4 %).

^{1}H-NMR (400.12 MHz, *d*$_6$-DMSO): δ = 8.10 (s, 2H, N=C*H*), 7.32 (d, 2H, $^{3}J_{HH}$ =7.0 Hz, C$_{arom}$*H*) 7.23 (m, 4H, C$_{arom}$*H*), 6.93 (m, 2H, C$_{arom}$*H*), 3.88 (m, 4H, 2 × C*H*$_2$), 2.35 (q, 2H, $^{3}J_{HF}$ =10.7 Hz, C*H*$_2$) ppm.
^{13}C NMR (101 MHz, *d*$_6$-DMSO) δ = 166.62 (2 × *C*=N), 165.16, 134.08, 133.43 (3 × *C*$_{arom}$), 125.19 (q, $^{2}J_{CF}$ = 153.4 Hz, 1 × *C*F$_3$), 123.12 (q, $^{2}J_{CF}$ = 156.4 Hz, 1 × *C*F$_3$) 122.09, 119.20, 113.18 (3× *C*$_{arom}$), 62.32, (q, $^{3}J_{CF}$ = 29.8 Hz, *C*H$_2$), 59.19 (q, $^{3}J_{CF}$ = 33.3 Hz, *C*H$_2$), 57.96 (2 × *C*H$_2$) ppm.
^{19}F-NMR (376 MHz, *d*$_6$-DMSO) δ = -73.13 (s, C*F*$_3$), -75.22 (s, C*F*$_3$) ppm.

Photolysis of Co(salen)CH_2COCH_3

Co(salen)(CH_2COCH_3)(MeOH) (3 mg, 7.85µmol) was dissolved in 1 mL of d_6-DMSO to which was added TEMPO (10 mg, 64 µmol). The solution was then irradiated for 48 h at ambient temperature, using the fume cupboard lamp as the source of irradiation. During that time the colour of the solution changed from brown-green to red.

^{1}H-NMR (400.12 MHz, *d*$_6$-DMSO): δ = 4.40 (s, 2H, O–C*H*$_2$), 2.07 (s, 3H, CO–C*H*$_3$), 1.43 – 1.25 (bm, 6H, 3 × C*H*$_2$), 1.08 (s, 12H, 4 × C*H*$_3$) ppm.

^{13}C NMR (101 MHz, DMSO) δ = 206.01 (*C*=O), 82.62 (O–*C*H$_2$), 59.07 (2 × *C*– (CH_3)$_2$), 33.20 (2 × *C*H$_2$), 30.54 (4 × *C*H$_3$), 19.62 (CO–*C*H$_3$) ppm 16.25 (*C*H$_2$) ppm.

ESI-MS (pos. mode, MeCN): found (calcd) *m/z* = 236.153 (236.16, [TEMPO-CH_2COCH_3Na]$^+$, $C_{12}H_{23}NNaO_2$ 100%), 325.037 (325.04, [Co(salen)]$^+$, $C_{16}H_{14}CoN_2O_2$, 100%).

Figures

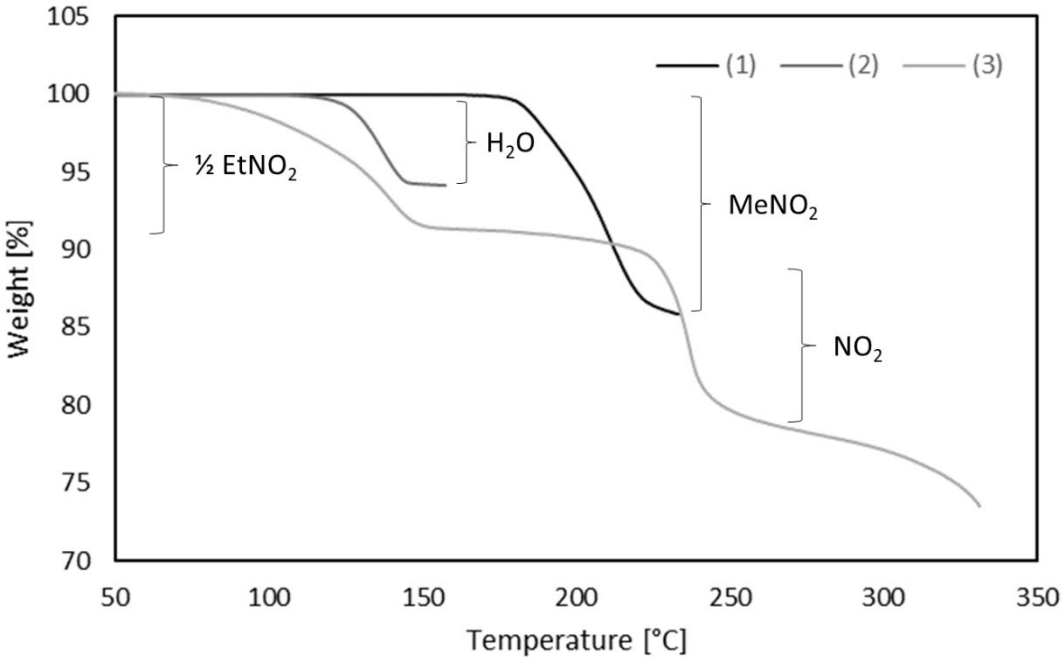

Figure S1. TGA curves of 1) $[Co(salen)(CH_2NO_2)]_2 \cdot (2\ MeNO_2)$, 2) $Co(salen)(NO_2)(H_2O)$ and 3) $[Co(salen)NO_2]_2 \cdot (EtNO_2)$.

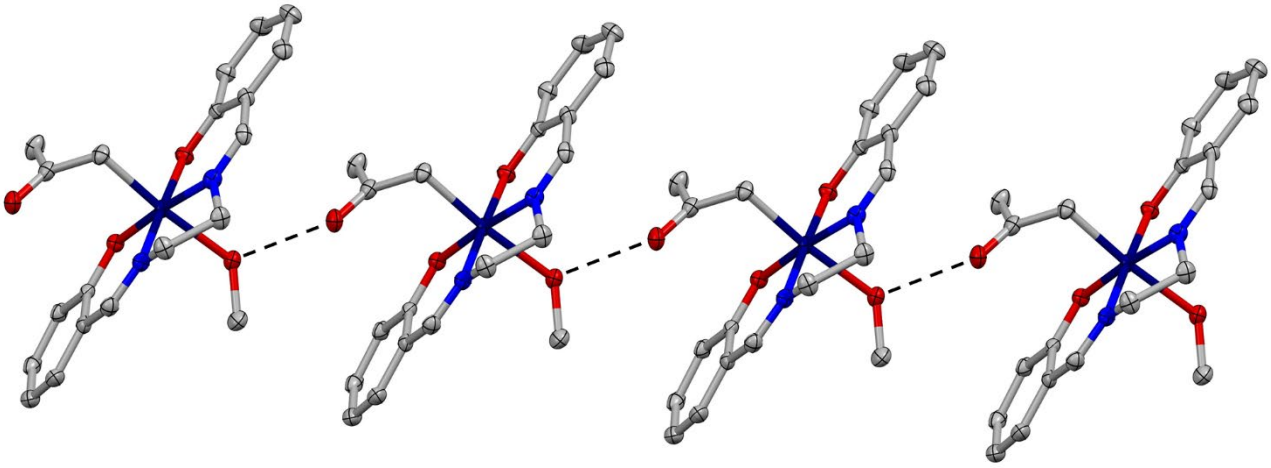

Figure S2. The hydrogen bonded 1D chain of $Co(salen)CH_2COCH_3(MeOH)$ (**3**) parallel to the a-axis. Thermal ellipsoids are drawn at 50 % probability and hydrogen atoms are omitted for clarity. The intermolecular hydrogen bond is shown with dashed lines (C=O···H-O 2.70 Å).

Figure S3. NMR tubes containing Co(salen)CH_2COCH_3 and TEMPO in d_6-DMSO under visible light irradiation at room temperature for 48 hours.

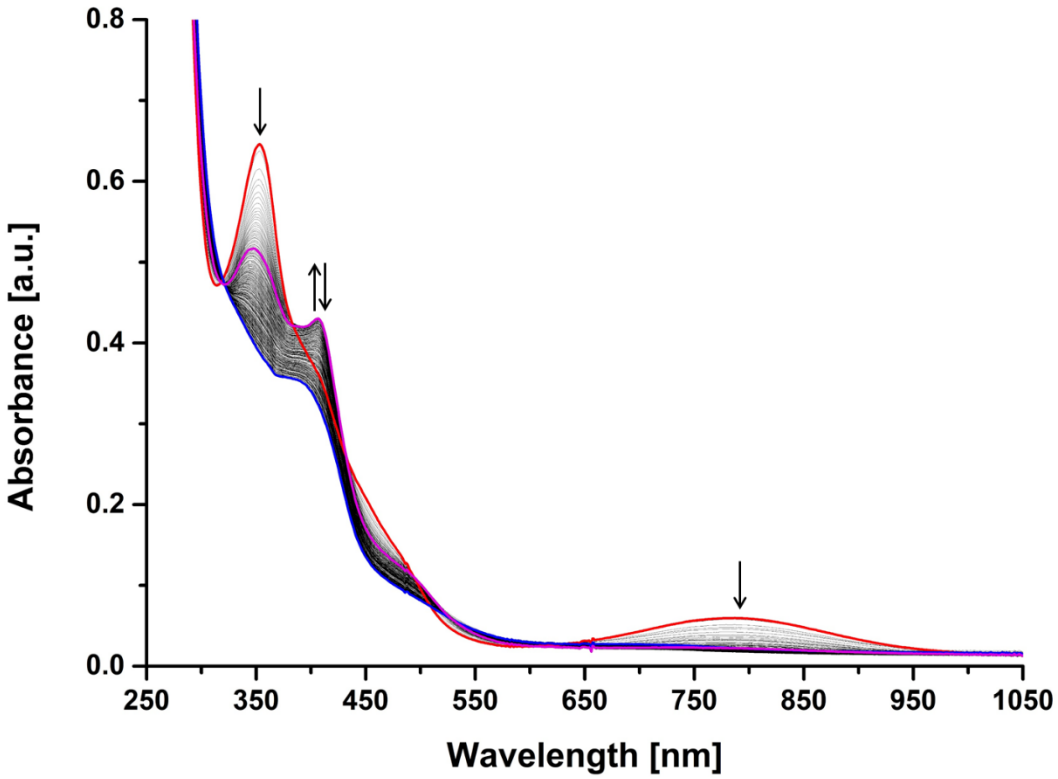

Figure S4. Time resolved UV-vis spectra of radical trapping reaction between Co(salen)CH_2COCH_3 (0.1 mM) and TEMPO (1 mM) in DCM by irradiation at 365 nm.

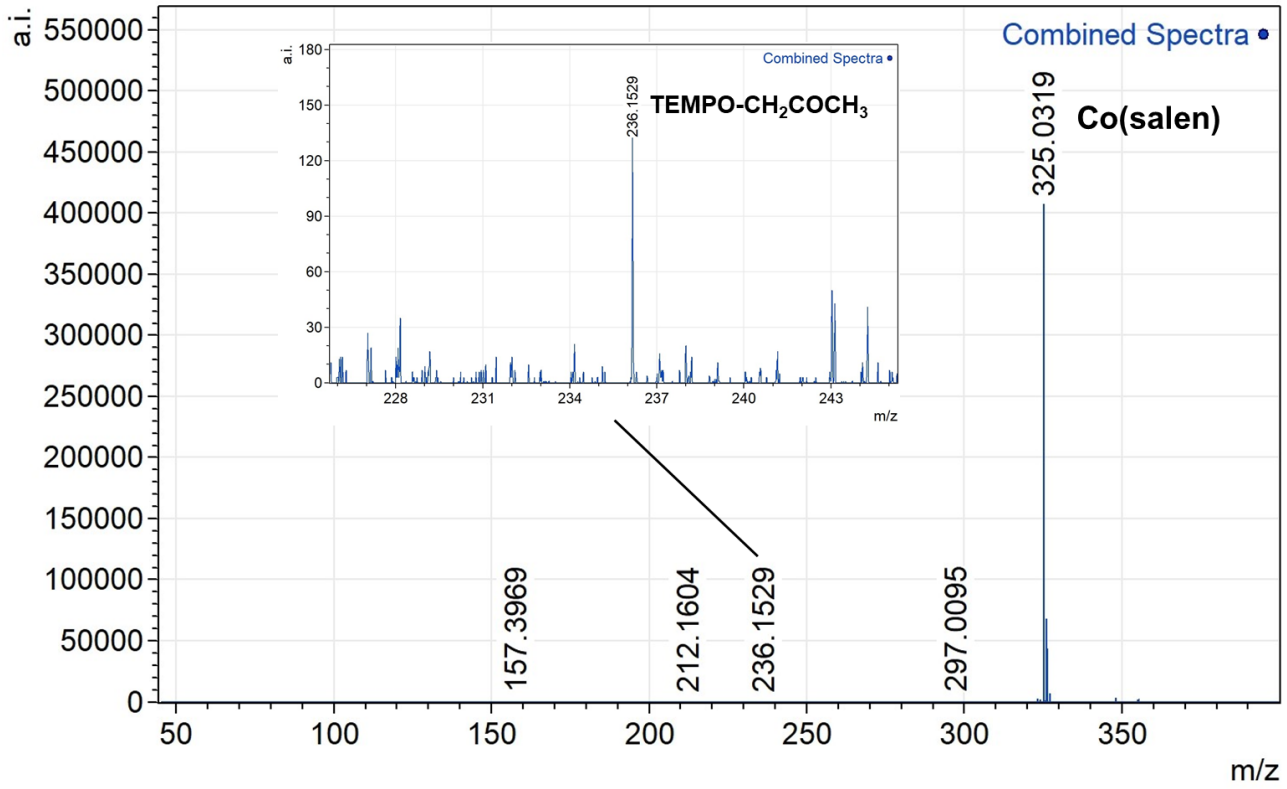

Figure S5. MS spectrum of the photoreaction between Co(salen)CH_2COCH_3 and TEMPO.

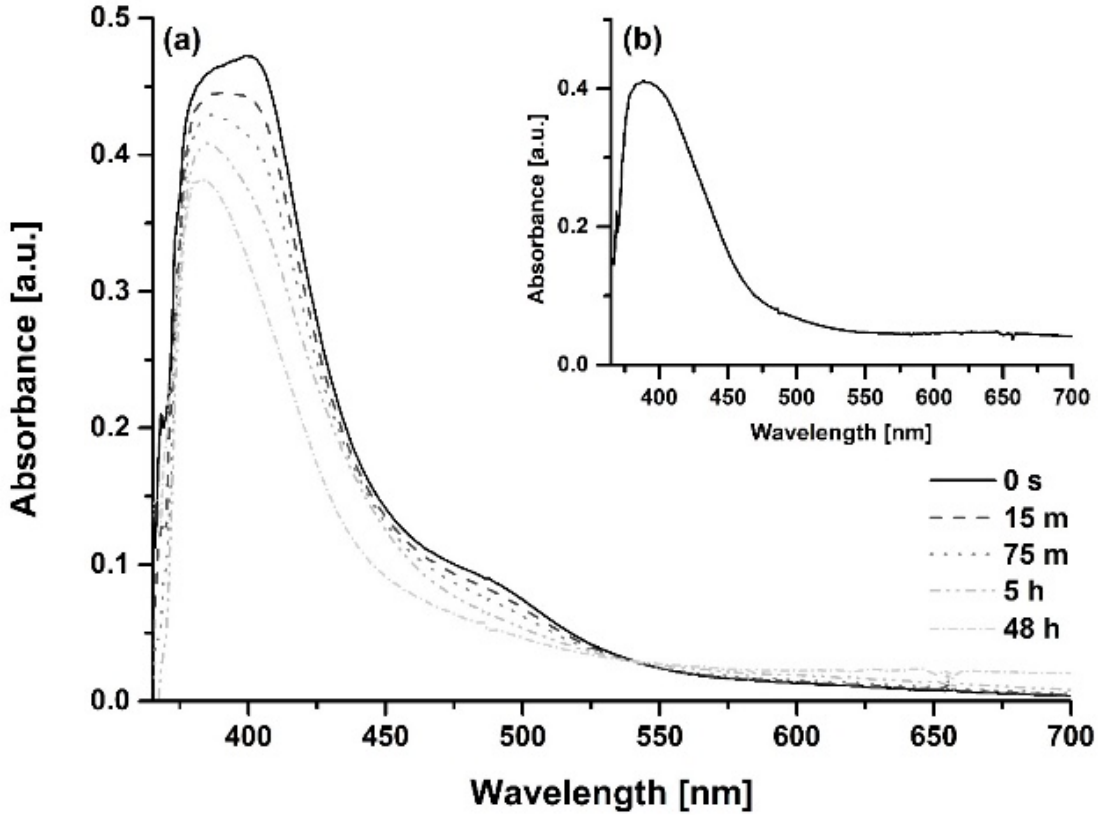

Figure S6. Time-resolved conversion of Co(salen) (0.1 mM) to Co(salen)(CH_2NO_2) upon its exposure in a degassed solution of $MeNO_2$ to air

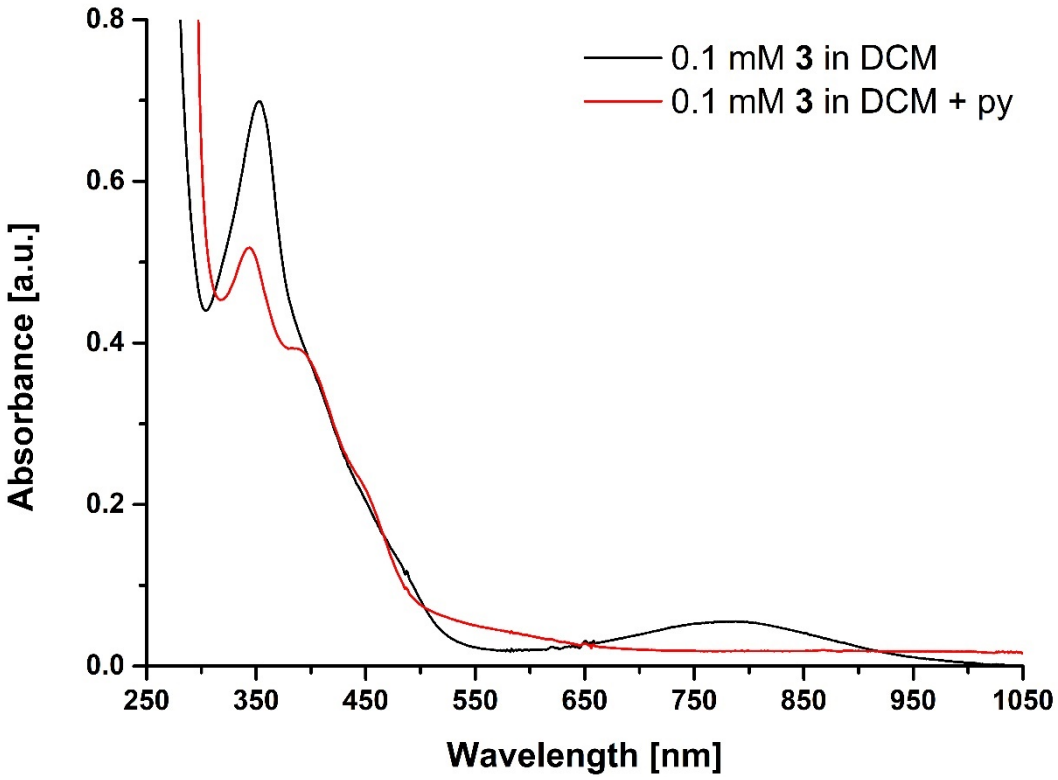

Figure S7. UV-vis spectra of Co(salen)(CH_2COCH_3) in DCM before and after the addition of pyridine (py).

Crystal data and extra images

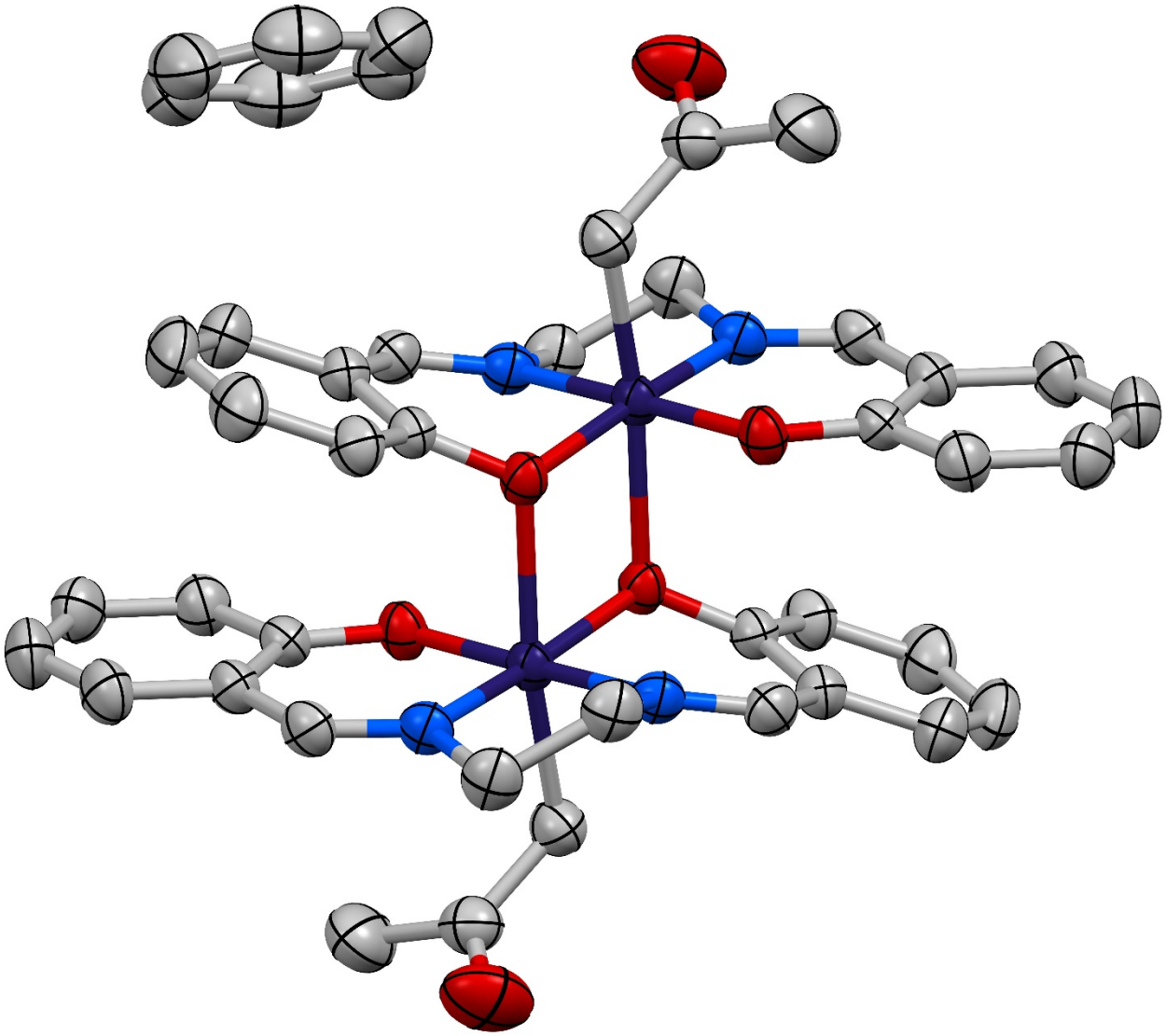

Figure S9. Crystal structure of $[Co(salen)(CH_2COCH_3)]_2 \cdot (C_6H_6)$. Thermal ellipsoids are drawn at 50 % probability and hydrogen atoms are omitted for clarity.

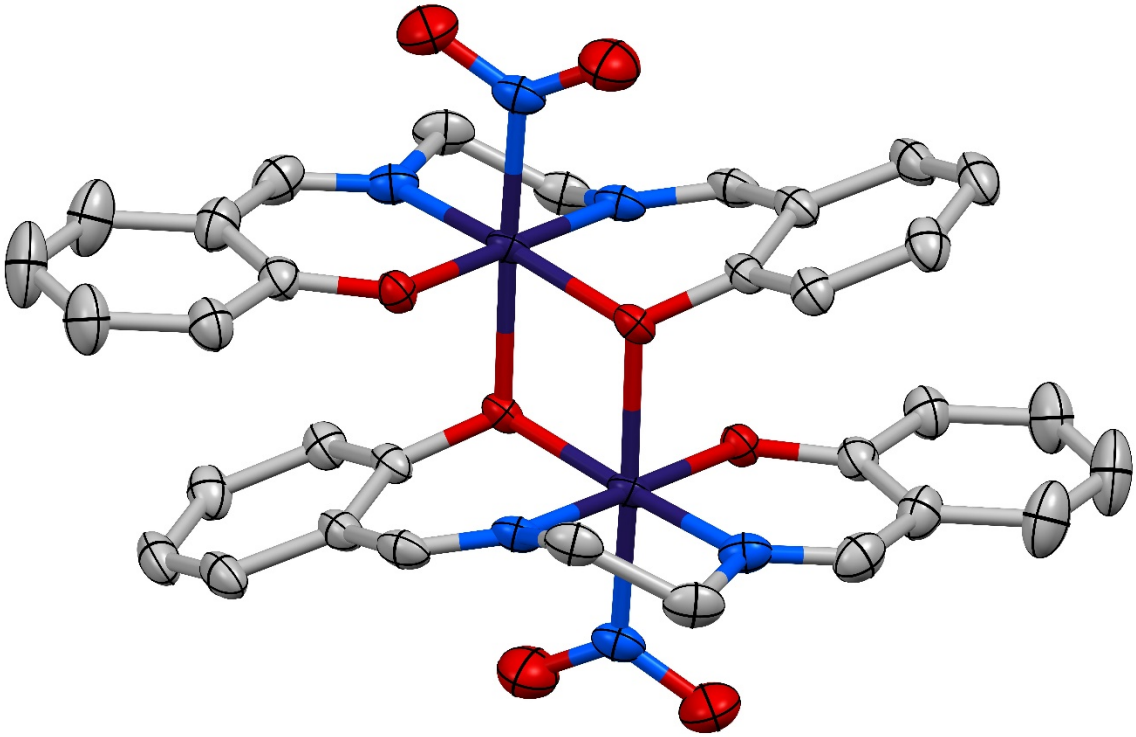

Figure S10. Crystal structure of $[Co(salen)(NO_2)]_2 \cdot (EtNO_2)$. Thermal ellipsoids are drawn at 50 % probability and protons are omitted for clarity. $EtNO_2$ removed with SQUEEZE.

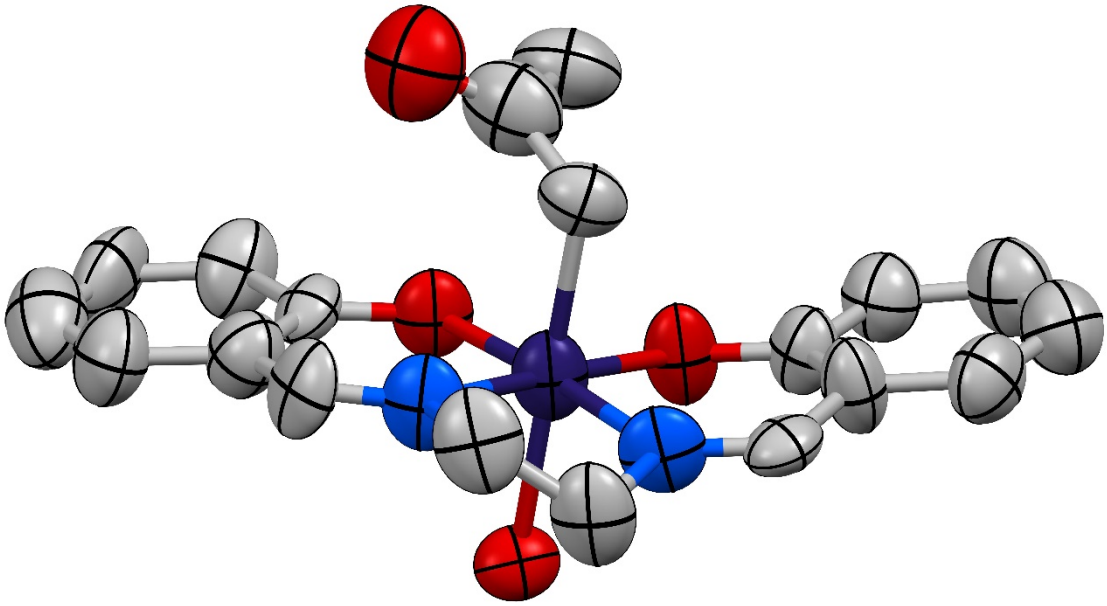

Figure S11. Crystal structure of $Co(salen)(CH_2COCH_3)(H_2O)$. Thermal ellipsoids are drawn at 50 % probability and hydrogenatoms are omitted for clarity.

Table S1. Crystallographic data for $[Co(salen)(CH_2NO_2)]_2 \cdot (2\ MeNO_2)$, $Co(salen)(CH_2COCH_3)(MeOH)$ and $[Co(salen)(CH_2COPh)]_2$.

Compound	**$[Co(salen)(CH_2NO_2)]_2 \cdot (2\ MeNO_2)$**	**$Co(salen)(CH_2COCH_3)(MeOH)$**	**$[Co(salen)(CH_2COPh)]_2$**
CCDC	2045579	2045583	2045578
Empirical formula	$C_{18}H_{19}CoN_4O_6$	$C_{20}H_{23}CoN_2O_4$	$C_{24}H_{21}CoN_2O_3$
Formula weight	446.30	414.33	444.36
Temperature [K]	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1/c$
a [Å]	10.04280(10)	7.5674(2)	10.9070(2)
b [Å]	13.78740(10)	19.9473(5)	14.9544(2)
c [Å]	13.33000(10)	12.5497(3)	13.0565(2)
α [°]	90	90	90
β [°]	97.7900(10)	99.379(3)	111.878(2)
γ [°]	90	90	90
Volume/Å^3	1828.69(3)	1869.04(8)	1976.24(6)
Z	4	4	4
ρ_{calc} [g/cm^3]	1.621	1.472	1.493
μ [mm^{-1}]	7.775	7.442	7.050
F(000)	920.0	864.0	920.0
Crystal size [mm^3]	0.091 × 0.049 × 0.042	0.082 × 0.070 × 0.018	0.065 × 0.031 × 0.022
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection [°]	9.272 to 149.594	8.404 to 149.154	8.736 to 149.252
Index ranges	$-12 \le h \le 12$ $-17 \le k \le 17$ $-16 \le l \le 16$	$-7 \le h \le 9$ $-22 \le k \le 24$ $-15 \le l \le 12$	$-13 \le h \le 13$ $-18 \le k \le 18$ $-13 \le l \le 15$
Reflections collected	40063	7723	17982
Independent reflections	3716	7723	3994
R_{int}, R_{sigma}	0.0323, 0.0134	0.0428, 0.0404	0.0231, 0.0174
Data/restraints/parameters	3716/0/263	7723/0/251	3994/0/271
Goodness-of-fit on F^2	1.051	1.048	1.045
Final R indexes [I>=2σ (I)]	$R_1 = 0.0330$, $wR_2 = 0.0934$	$R_1 = 0.0420$, $wR_2 = 0.1189$	$R_1 = 0.0277$, $wR_2 = 0.0672$
Final R indexes [all data]	$R_1 = 0.0340$, $wR_2 = 0.0943$	$R_1 = 0.0541$, $wR_2 = 0.1220$	$R_1 = 0.0316$, $wR_2 = 0.0695$
Largest diff. peak/hole [e Å^{-3}]	0.90/-0.41	0.94/-0.32	0.36/-0.34

Table S2. Crystallographic data for $[Co(salen)(CH_2CN)]_2 \cdot (C_6H_6)$, $Co(salen)(NO_2)(H_2O)$ and $[Co(salen)(OCH_2CF_3)]_2 \cdot (4\ CF_3CH_2OH)$.

Compound	**$[Co(salen)(CH_2CN)]_2 \cdot (C_6H_6)$**	**$Co(salen)(NO_2)(H_2O)$**	**$[Co(salen)(OCH_2CF_3)]_2 \cdot (4\ CF_3CH_2OH)$**
CCDC	2045576	2045584	2045581
Empirical formula	$C_{21}H_{19}CoN_3O_2$	$C_{16}H_{16}CoN_3O_5$	$C_{22}H_{22}N_2O_5F_9Co$
Formula weight	404.32	389.25	624.34
Temperature [K]	100(2)	100(2)	100(1)
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/n$	P-1
a [Å]	11.0129(2)	13.7674(9)	9.3662(2)
b [Å]	12.4615(2)	6.5594(3)	11.9220(3)
c [Å]	13.5740(3)	17.6429(10)	13.0281(2)
α [°]	90	90	105.961(2)
β [°]	104.732(2)	93.879(6)	102.9240(10)
γ [°]	90	90	109.030(2)
Volume/Å^3	1801.62(6)	1589.61(16)	1241.20(5)
Z	4	4	2
ρ_{calc} [g/cm^3]	1.491	1.626	1.671
μ [mm^{-1}]	7.644	8.779	6.404
F(000)	836.0	800.0	632.0
Crystal size [mm^3]	0.159 × 0.019 × 0.013	0.077 × 0.036 × 0.027	0.152 × 0.032 × 0.022
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection [°]	9.268 to 148.458	7.892 to 151.804	7.518 to 148.912
Index ranges	$-13 \le h \le 12$ $-15 \le k \le 14$ $-12 \le l \le 16$	$-17 \le h \le 17$ $-7 \le k \le 8$ $-21 \le l \le 22$	$-11 \le h \le 11$ $-14 \le k \le 14$ $-16 \le l \le 16$
Reflections collected	9583	33718	44153
Independent reflections	3544	3241	4979
R_{int}, R_{sigma}	0.0283, 0.0321	0.0754, 0.0242	0.0596, 0.0326
Data/restraints/parameters	3544/0/244	3241/488/259	4979/0/356
Goodness-of-fit on F^2	1.050	1.056	1.036
Final R indexes [I>=2σ (I)]	$R_1 = 0.0302$, $wR_2 = 0.0721$	$R_1 = 0.0701$, $wR_2 = 0.1842$	$R_1 = 0.0327$, $wR_2 = 0.0826$
Final R indexes [all data]	$R_1 = 0.0375$, $wR_2 = 0.0762$	$R_1 = 0.0749$, $wR_2 = 0.1923$	$R_1 = 0.0374$, $wR_2 = 0.0849$
Largest diff. peak/hole [e Å^{-3}]	0.29/-0.23	0.90/-0.26	0.29/-0.35

Table S3. Crystallographic data for $[Co(salen)(CH_2COCH_3)]_2 \cdot (C_6H_6)$, $[Co(salen)NO_2]_2 \cdot (½\ CH_3CH_2NO_2)$ and $Co(salen)(CH_2COCH_3)(H_2O)$.

Compound	**$[Co(salen)(CH_2COCH_3)]_2 \cdot (C_6H_6)$**	**$[Co(salen)NO_2]_2 \cdot (½\ CH_3CH_2NO_2)$**	**$Co(salen)(CH_2COCH_3)(H_2O)$**
CCDC	2045577	2045580	2045582
Empirical formula	$C_{22}H_{22}N_2O_3Co$	$C_{16}CoH_{14}N_3O_4$	$C_{19}H_{21}N_2O_4Co$
Formula weight	421.34	371.23	400.31
Temperature [K]	293(5)	293(2)	293(2)
Crystal system	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1
a [Å]	7.5754(2)	7.7899(2)	9.1430(8)
b [Å]	11.5841(5)	8.7278(2)	9.8383(8)
c [Å]	11.8530(4)	13.7362(3)	11.1689(7)
α [°]	110.095(3)	72.008(2)	115.062(7)
β [°]	103.433(2)	74.808(2)	100.862(7)
γ [°]	94.087(3)	79.890(2)	93.188(8)
Volume/Å^3	937.02(6)	852.63(4)	883.35(13)
Z	2	2	2
ρ_{calc} [g/cm^3]	1.493	1.446	1.505
μ [mm^{-1}]	7.396	8.112	7.853
F(000)	438.0	380.0	416.0
Crystal size [mm^3]	0.119 × 0.105 × 0.020	0.148 × 0.041 × 0.028	0.054 × 0.019 × 0.012
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection [°]	8.24 to 149.014	6.94 to 152.224	8.992 to 117.854
Index ranges	$-9 \le h \le 9$ $-13 \le k \le 14$ $-14 \le l \le 14$	$-9 \le h \le 9$ $-10 \le k \le 10$ $-17 \le l \le 17$	$-7 \le h \le 10$, $-10 \le k \le 10$, $-12 \le l \le 12$
Reflections collected	20763	30176	6165
Independent reflections	3761	3481	2522
R_{int}, R_{sigma}	0.0244, 0.0151	0.0447, 0.0229	0.1677, 0.1747
Data/restraints/parameters	3761/0/254	3481/0/217	2522/4/245
Goodness-of-fit on F^2	1.024	1.058	1.013
Final R indexes [I>=2σ (I)]	$R_1 = 0.0275$, $wR_2 = 0.0740$	$R_1 = 0.0397$, $wR_2 = 0.1056$	$R_1 = 0.0993$, $wR_2 = 0.2502$
Final R indexes [all data]	$R_1 = 0.0305$, $wR_2 = 0.0762$	$R_1 = 0.0418$, $wR_2 = 0.1073$	$R_1 = 0.1840$, $wR_2 = 0.3481$
Largest diff. peak/hole [e Å^{-3}]	0.21/-0.25	0.60/-0.45	0.53/-0.82

NMR spectra

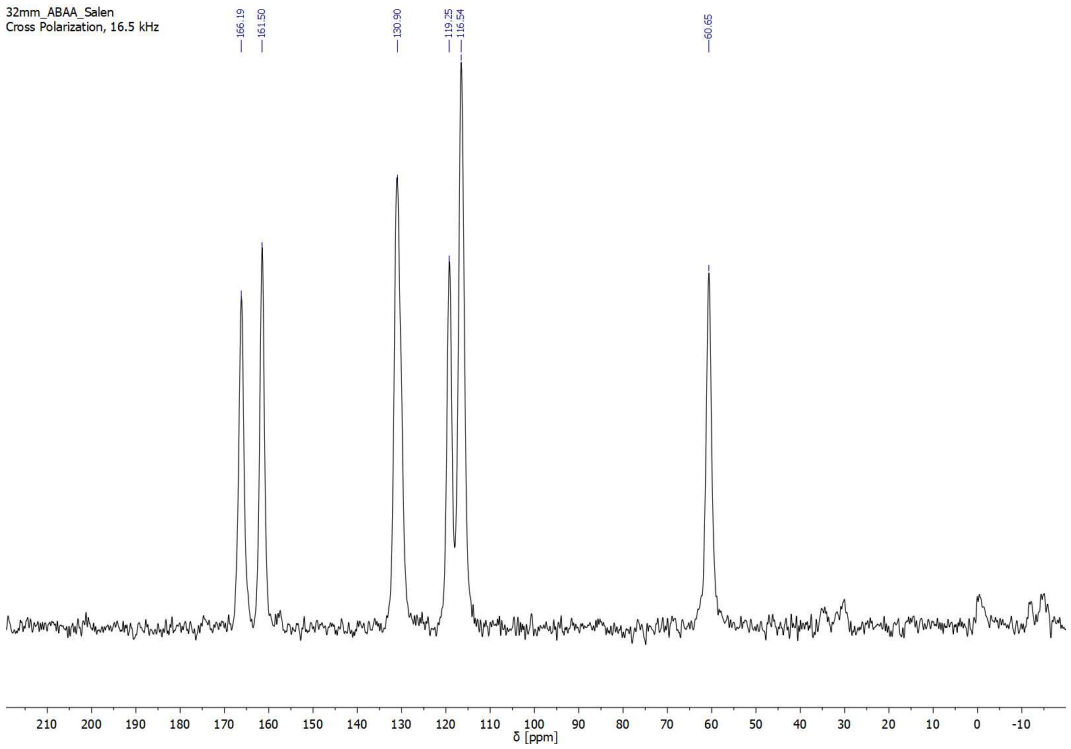

Figure S12. ^{13}C CPMAS NMR of H_2salen.

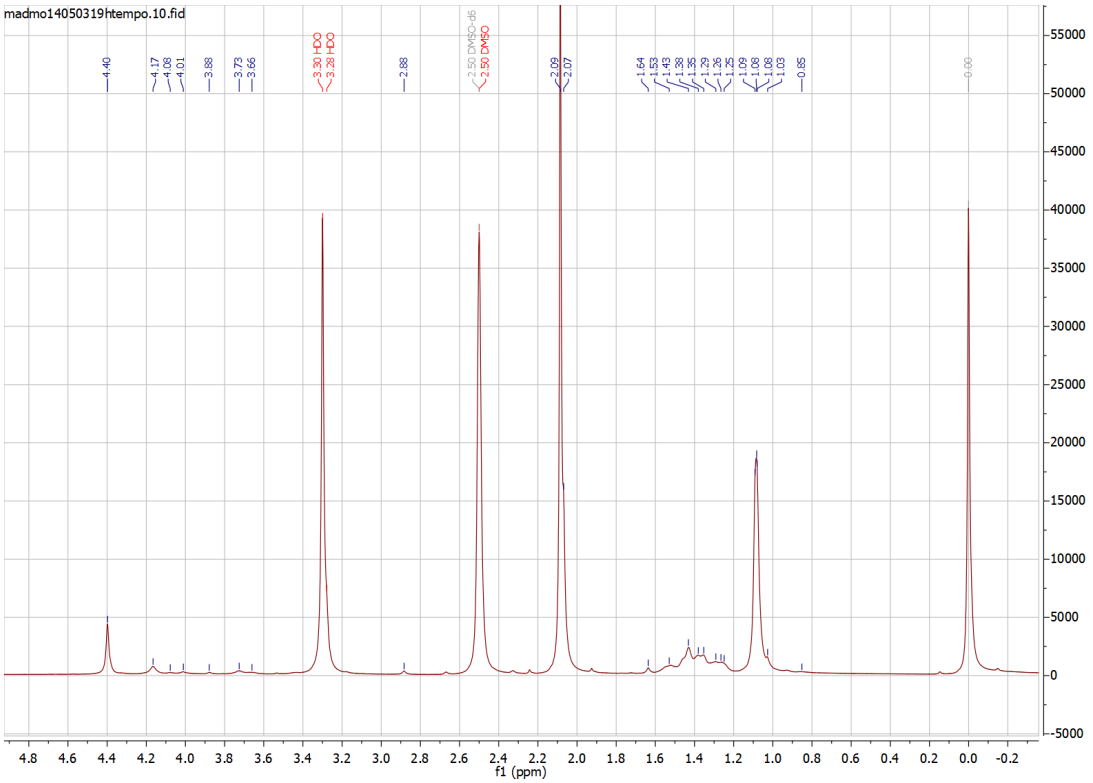

Figure S13. ^{1}H NMR spectrum of Co(salen)CH_2COCH_3 and TEMPO in d_6-DMSO under visible light irradiation at room temperature for 48 hours.

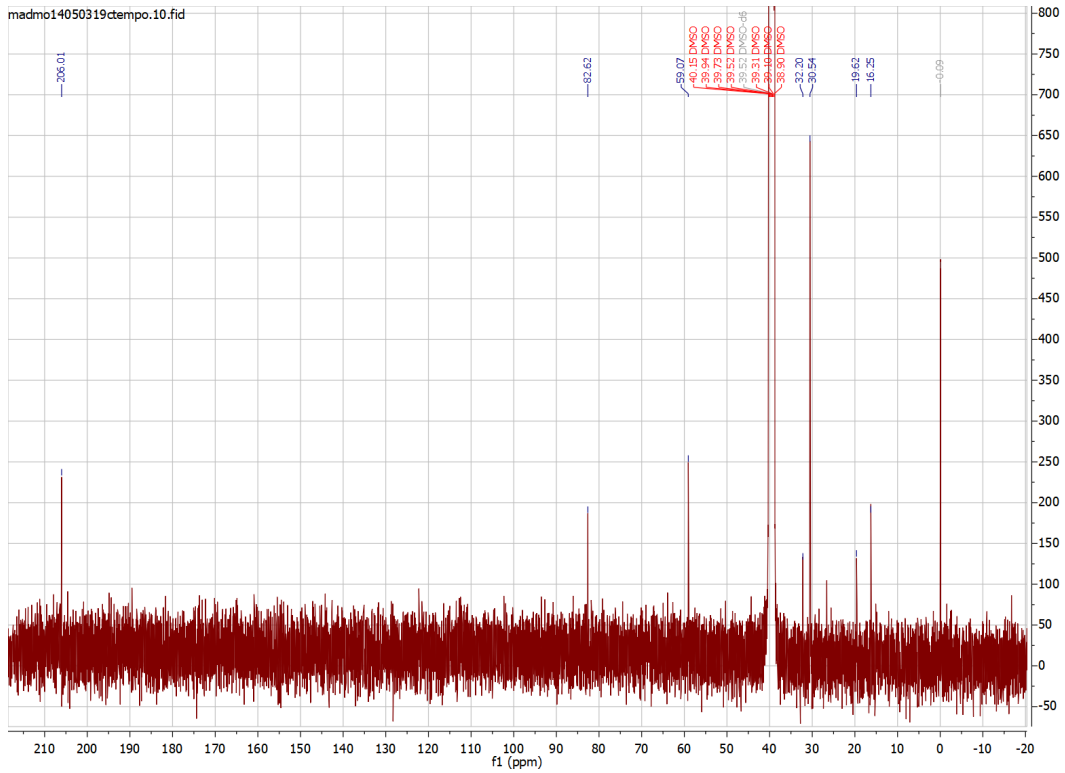

Figure S14. ^{13}C NMR spectrum of Co(salen)CH_2COCH_3 and TEMPO in d_6-DMSO under visible light irradiation at room temperature for 48 hours.

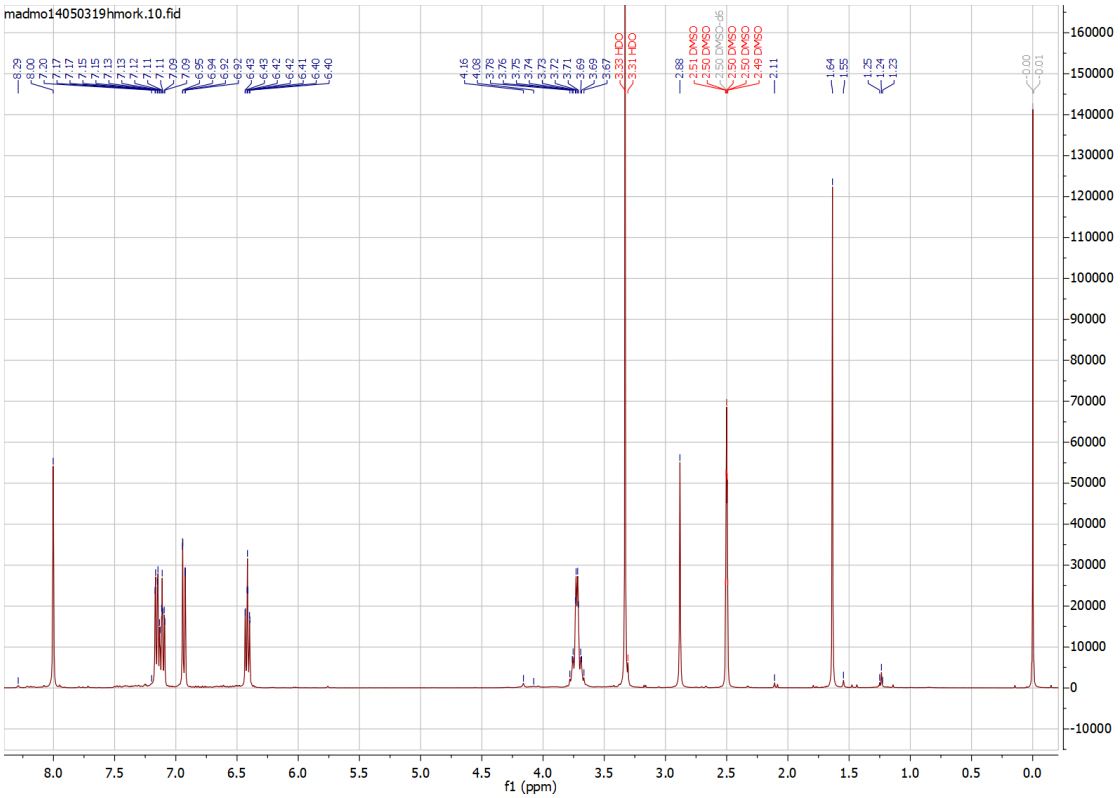

Figure S15. ^{1}H NMR spectrum of Co(salen)CH_2COCH_3 in d_6-DMSO.

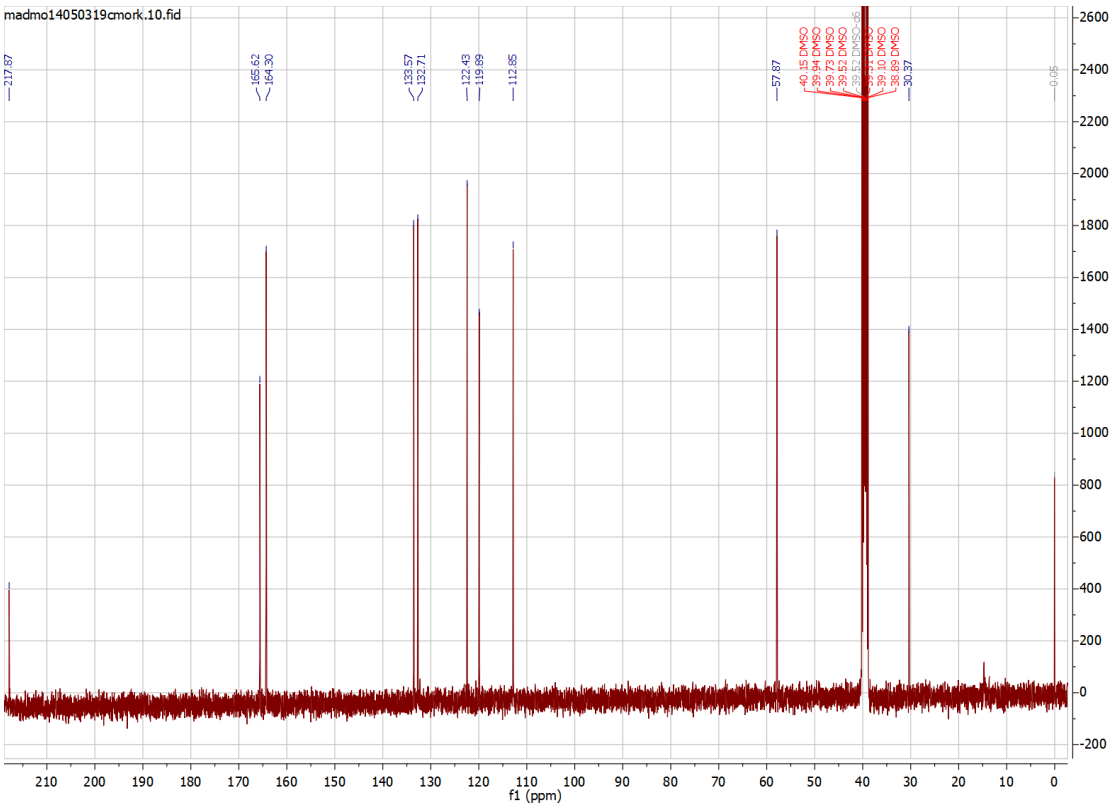

Figure S16. ^{13}C NMR spectrum of Co(salen)CH_2COCH_3 in d_6-DMSO.

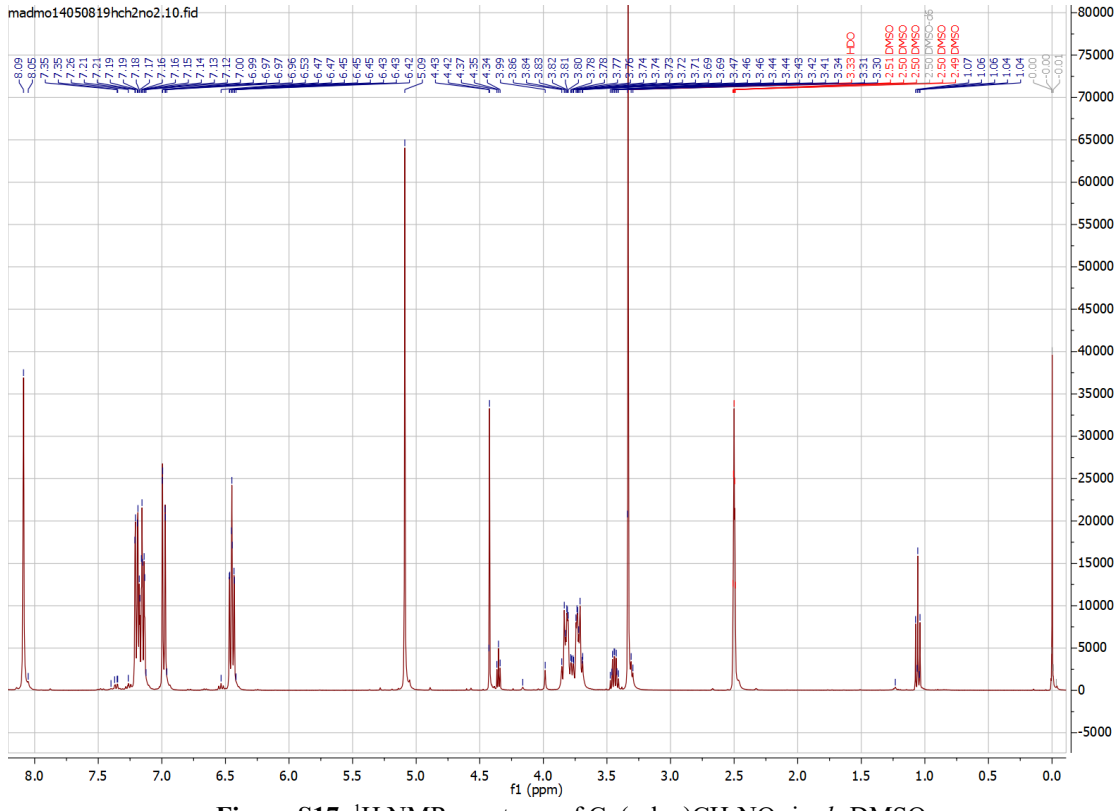

Figure S17. ^{1}H NMR spectrum of Co(salen)CH_2NO_2 in d_6-DMSO.

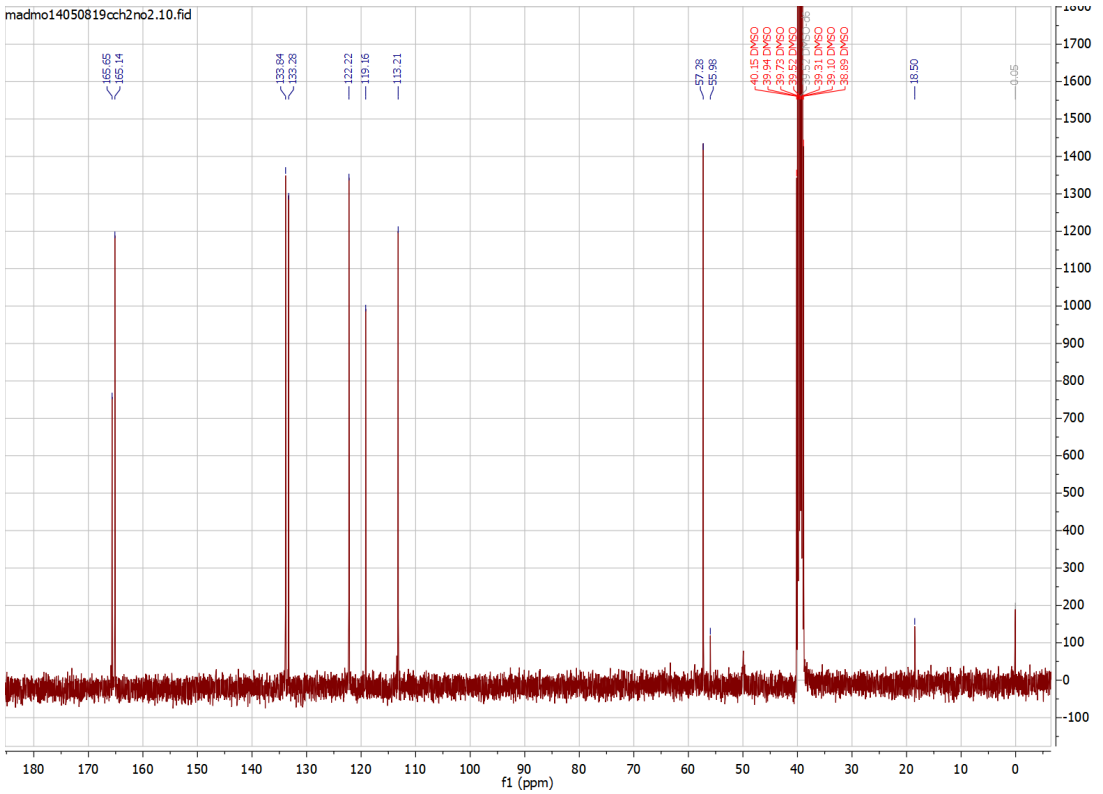

Figure S18. ^{13}C NMR spectrum of Co(salen)CH_2NO_2 in d_6-DMSO.

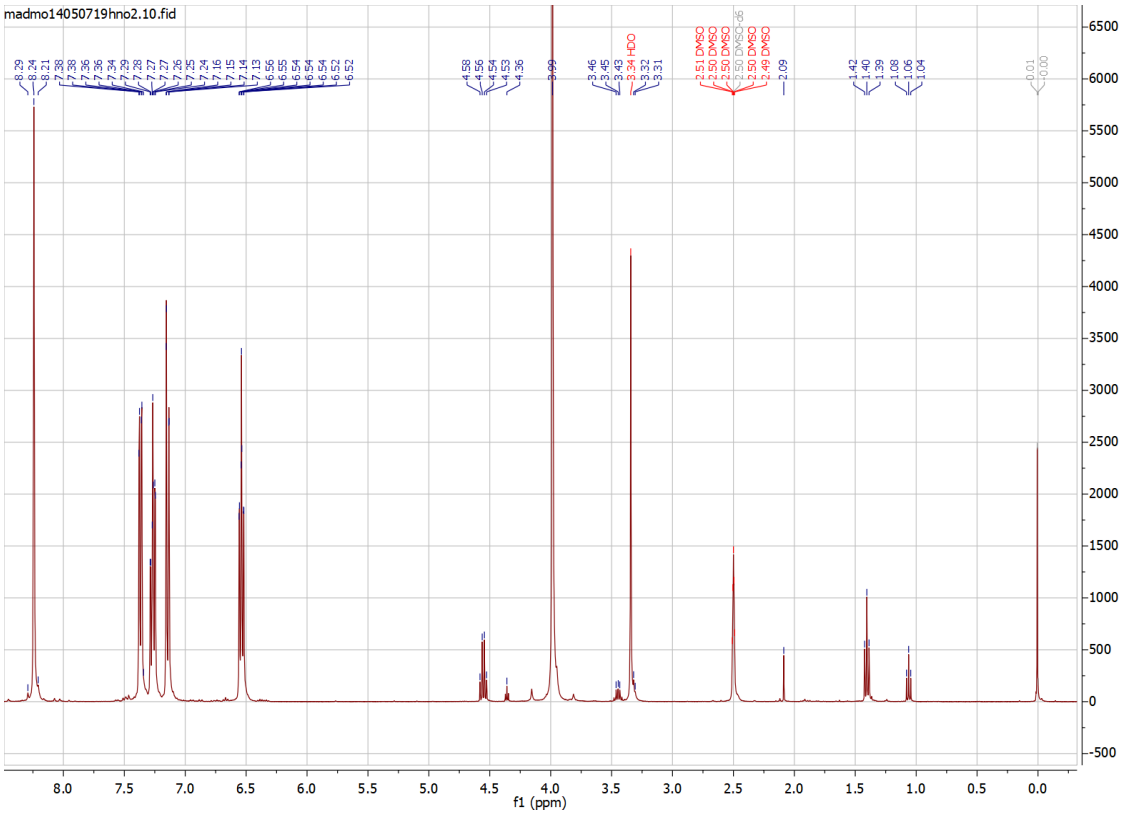

Figure S19. ^{1}H NMR spectrum of Co(salen)NO_2 in d_6-DMSO.

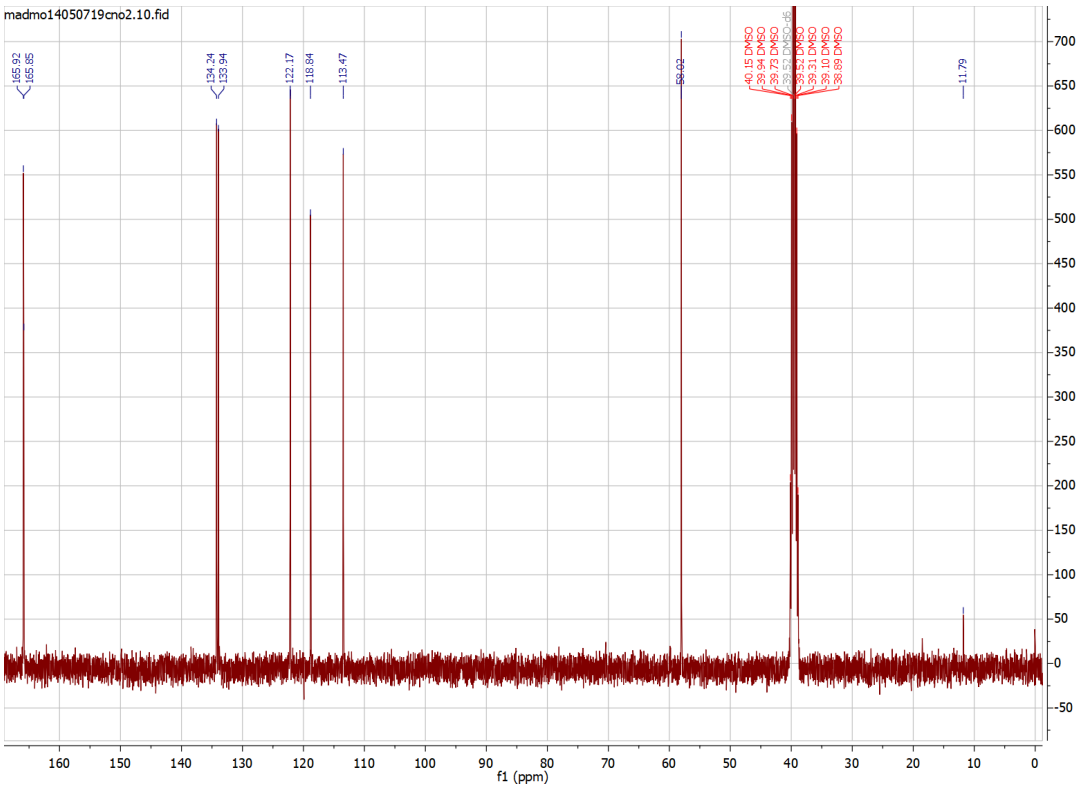

Figure S20. ^{13}C NMR spectrum of Co(salen)NO_2 in d_6-DMSO.

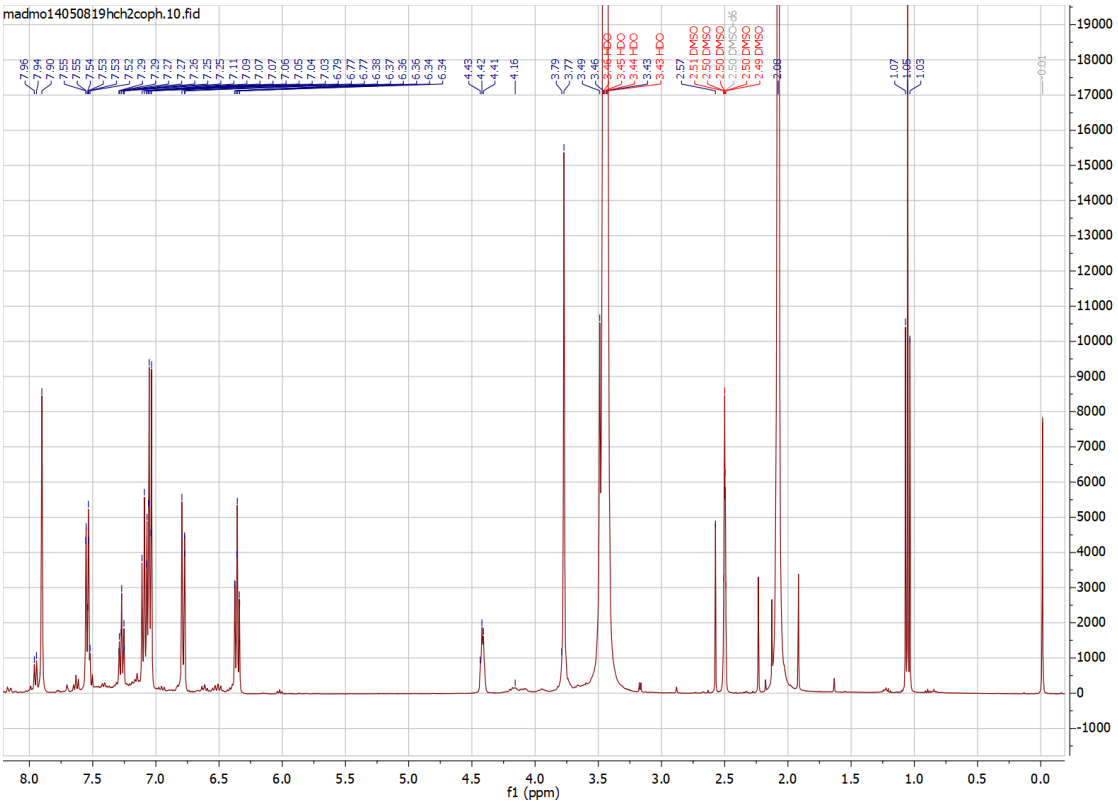

Figure S21. ^{1}H NMR spectrum of Co(salen)CH_2COPh in d_6-DMSO.

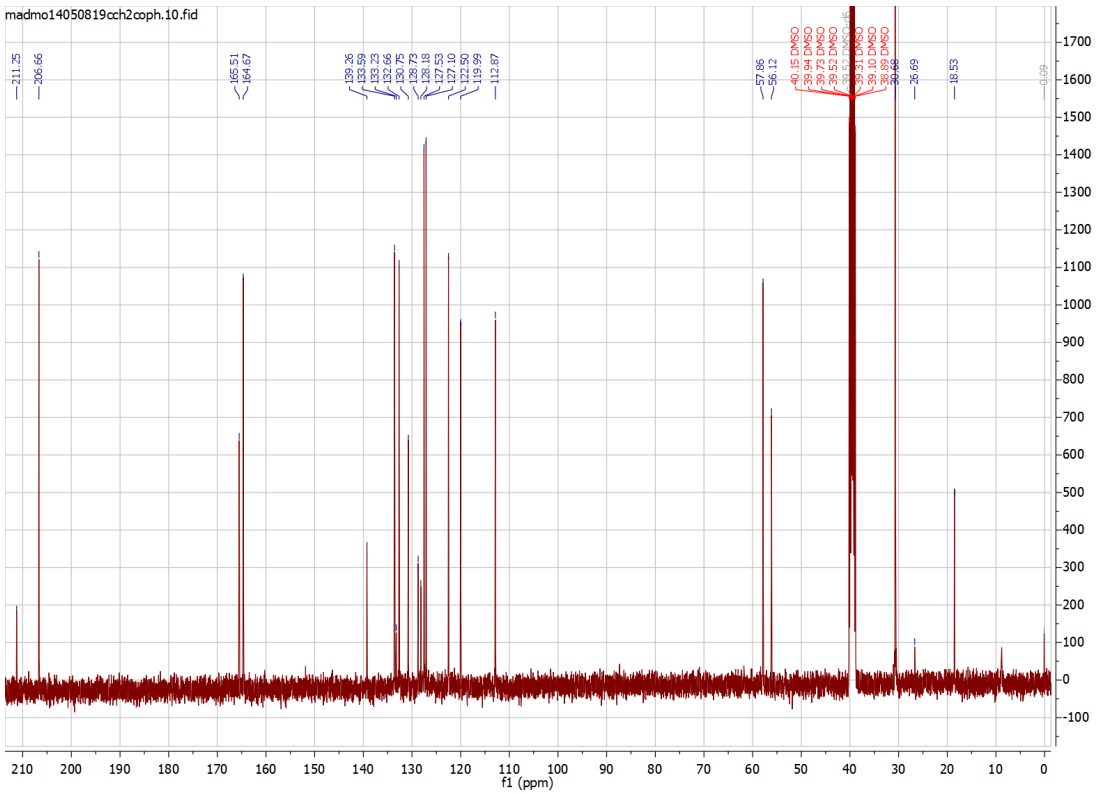

Figure S22. ^{13}C NMR spectrum of Co(salen)CH_2COPh in d_6-DMSO.

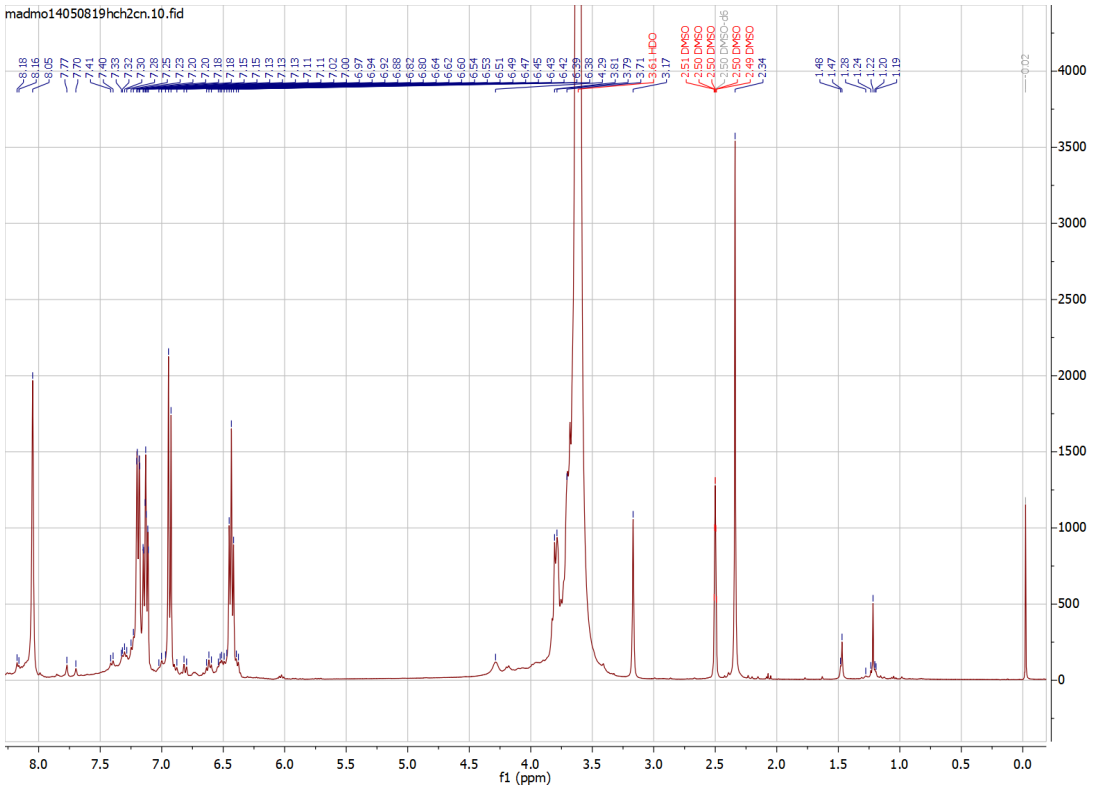

Figure S33. ^{1}H NMR spectrum of Co(salen)CH_2CN in d_6-DMSO.

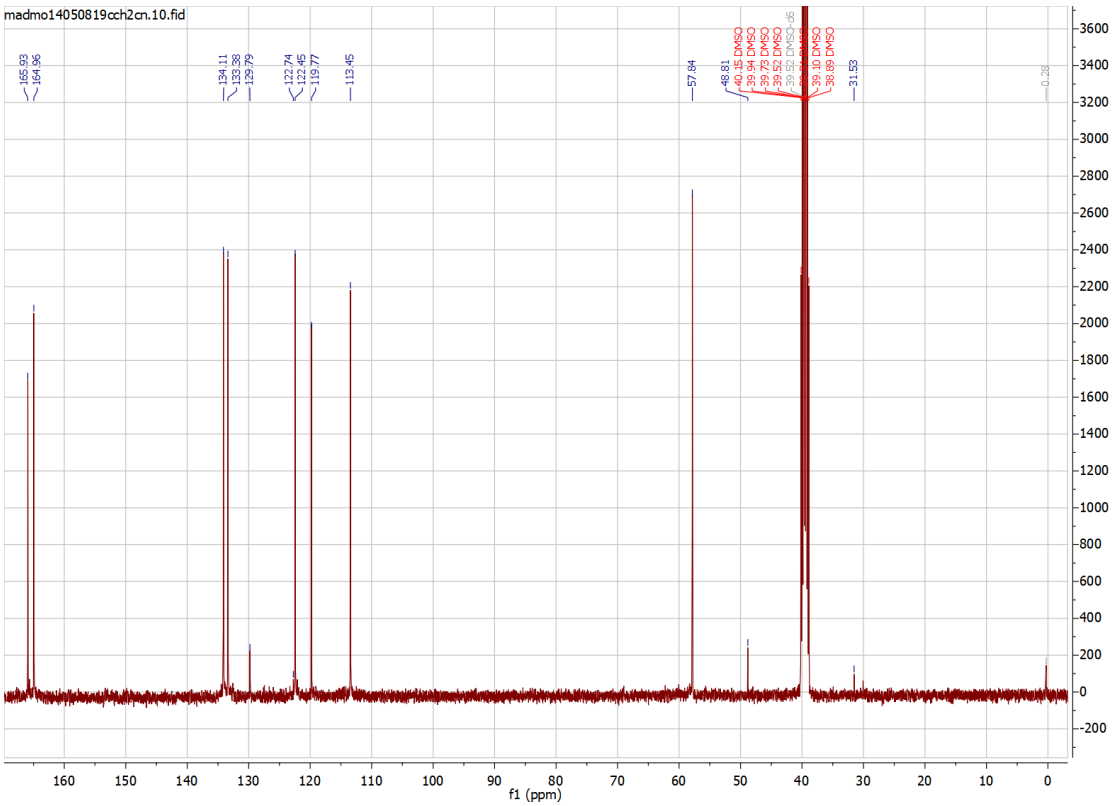

Figure S44. ^{13}C NMR spectrum of Co(salen)CH_2CN in d_6-DMSO.

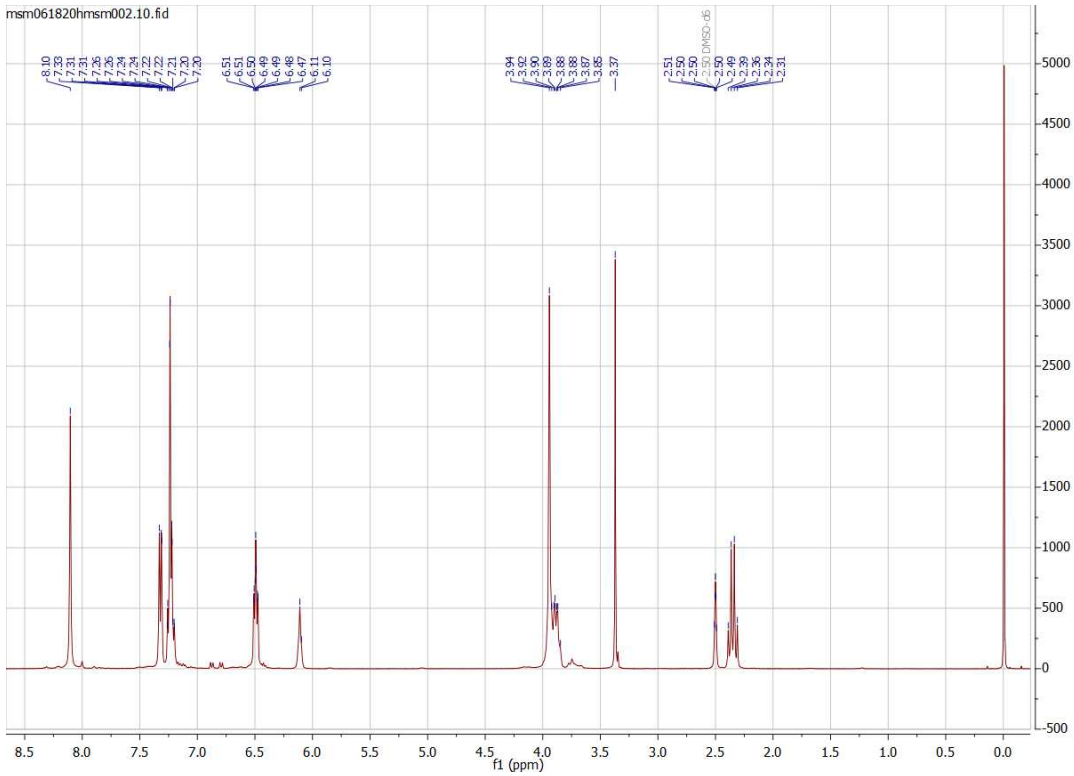

Figure S55. ^{1}H NMR spectrum of Co(salen)OCH_2CF_3 in d_6-DMSO.

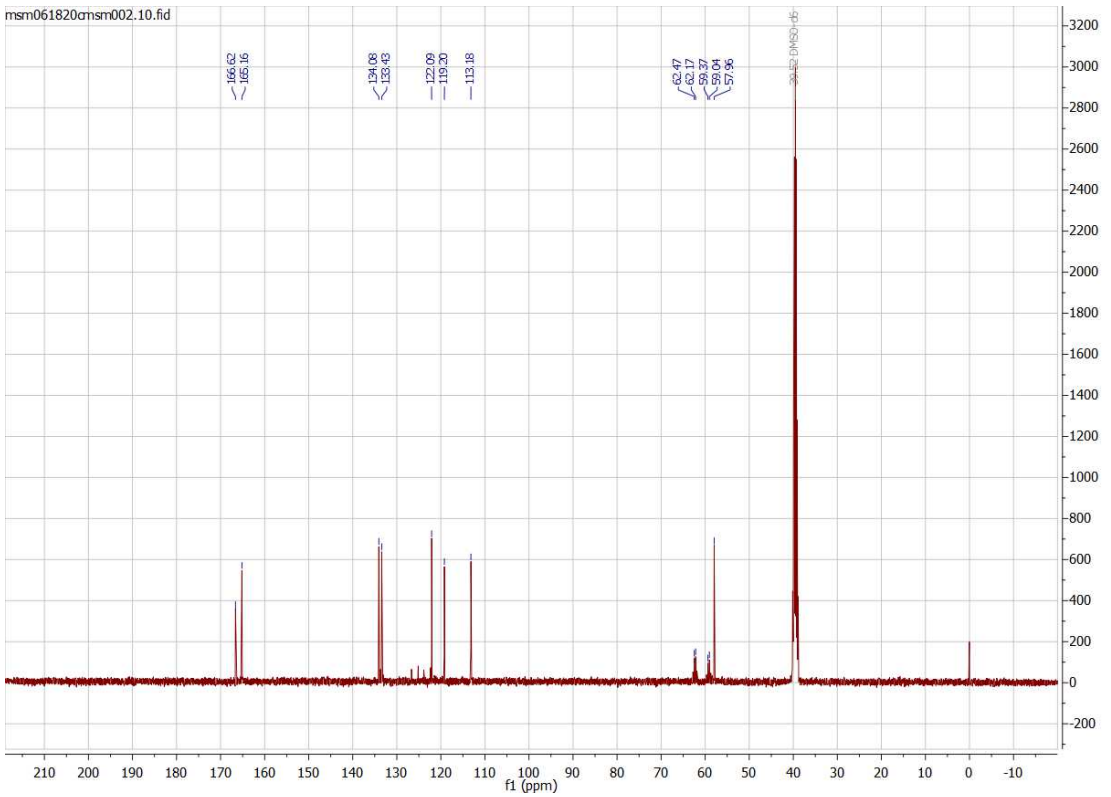

Figure S26. ^{13}C NMR spectrum of Co(salen)OCH_2CF_3 in d_6-DMSO.

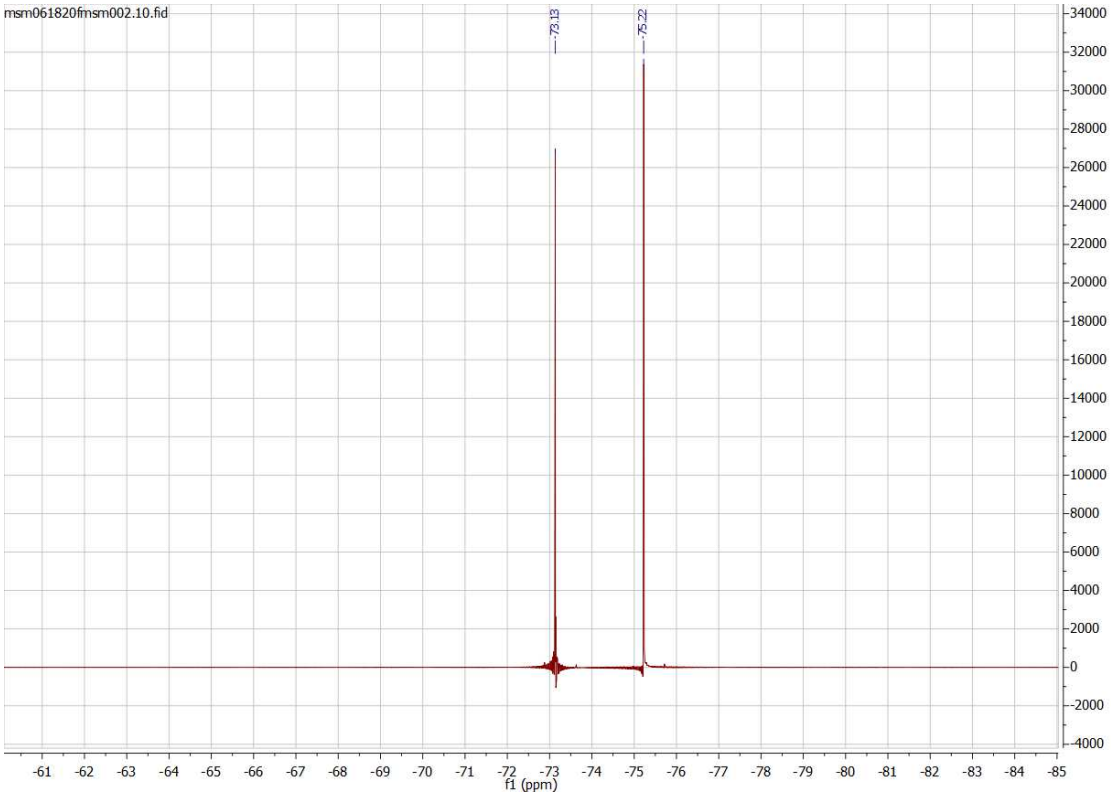

Figure S27. ^{19}F NMR spectrum of Co(salen)OCH_2CF_3 in d_6-DMSO.

DFT coordinates

Mechanism figure 8.

Co(salen)

atom	x	y	z
Co1	0.6958810000	2.2139670000	2.4847250000
C2	1.2590780000	-0.4508210000	3.4246920000
C3	0.0615900000	4.8475530000	1.5419520000
C4	0.3518200000	5.4502860000	2.8075120000
C5	0.2790670000	6.8599910000	2.8987160000
C6	0.5130060000	7.5264060000	4.0867350000
C7	0.8209300000	6.7736950000	5.2354660000
C8	0.8931580000	5.3931220000	5.1843360000
C9	0.6691200000	4.6791520000	3.9771270000
C13	1.5308900000	-1.3527980000	4.4877940000
C14	1.5805520000	-2.7205420000	4.2855340000
C15	1.3687230000	-3.2720630000	3.0078000000
C16	1.1118170000	-2.4196590000	1.9504700000
C17	1.0472190000	-1.0166910000	2.1215130000
C18	0.8088230000	-0.2130240000	0.9610260000
C19	0.5349980000	1.8119160000	-0.2967360000
C20	-0.2832840000	3.0557740000	-0.0157260000
H21	-0.2700200000	5.5177180000	0.7366000000
H22	0.0292810000	7.4199590000	1.9954810000
H23	0.4568200000	8.6123340000	4.1353420000
H24	1.0050850000	7.2827690000	6.1823960000
H25	1.1302730000	4.8129400000	6.0760500000
H33	1.6961840000	-0.9283600000	5.4780200000
H34	1.7876420000	-3.3775360000	5.1312020000
H35	1.4100140000	-4.3490920000	2.8557110000
H36	0.9521060000	-2.8218050000	0.9480480000
H37	0.7600810000	-0.7362720000	-0.0040860000
H38	1.5441700000	2.0918360000	-0.6323330000
H39	0.0804060000	1.1886680000	-1.0779400000
H40	-1.3498670000	2.7979610000	0.0556630000
H41	-0.1701920000	3.8095020000	-0.8060060000
N42	0.6597750000	1.0779760000	0.9672170000
N43	0.1493300000	3.5767490000	1.2852670000
O45	1.2301050000	0.8287930000	3.6882100000
O46	0.7523320000	3.3752200000	4.0021830000

Co(salen)O_2(MeOH)

atom	x	y	z
O47	-0.9620290000	1.8467220000	2.7154780000

O49	-1.9383100000	1.8158040000	1.8890690000
Co50	-3.7008690000	2.1902900000	2.5270940000
N51	-3.4961680000	1.0834460000	4.0702400000
N52	-3.0540090000	3.5862200000	3.6784000000
O53	-4.3349360000	0.7341780000	1.4291700000
O54	-3.9581150000	3.3532340000	1.0052570000
O8	-5.7844810000	2.4392300000	2.9708070000
C56	-3.3365920000	-0.1981110000	4.0480760000
C57	-3.4511860000	1.8554460000	5.3062930000
C58	-2.7188690000	4.7771090000	3.2938060000
C59	-2.6657280000	3.1189290000	5.0146150000
C60	-3.9635170000	-0.5024160000	1.6306430000
C61	-3.5015770000	4.5701330000	0.9069080000
C15	-6.2607730000	3.7813680000	3.1374810000
C63	-3.4492220000	-1.0106520000	2.8727330000
H64	-3.1083250000	-0.7086220000	4.9949610000
H65	-4.4841430000	2.1031900000	5.5914350000
H66	-3.0035910000	1.2740330000	6.1237590000
C67	-2.8911770000	5.3100440000	1.9782080000
H68	-2.2468160000	5.4393370000	4.0344060000
H69	-1.5894580000	2.8984920000	5.0001460000
H70	-2.8459440000	3.8965050000	5.7680500000
C71	-4.1050810000	-1.4298480000	0.5653530000
C72	-3.6234590000	5.2347970000	-0.3438000000
C75	-3.0986080000	-2.3746330000	2.9834170000
C76	-2.4226730000	6.6257510000	1.7476600000
C77	-3.7442990000	-2.7587910000	0.7056610000
H78	-4.5020370000	-1.0554320000	-0.3778740000
C79	-3.1533700000	6.5216760000	-0.5334860000
H80	-4.0911240000	4.6860100000	-1.1607230000
C83	-3.2289410000	-3.2481190000	1.9195090000
H84	-2.7151010000	-2.7298390000	3.9421130000
C85	-2.5391110000	7.2350460000	0.5136210000
H86	-1.9528570000	7.1554950000	2.5792440000
H87	-3.8604840000	-3.4328310000	-0.1439750000
H88	-3.2573090000	6.9852850000	-1.5153460000
H95	-2.9435490000	-4.2935370000	2.0205600000
H96	-2.1632680000	8.2439750000	0.3534400000
H40	-7.3510790000	3.7836710000	3.2402520000
H41	-5.8075220000	4.1628290000	4.0560130000
H42	-5.9620670000	4.4149490000	2.2947080000
H43	-6.2031500000	2.0556300000	2.1731990000

Co(salen)O_2(CH_3CN)

atom	x	y	z

O47	-1.0341180000	1.5775900000	2.5243470000
O49	-2.0516200000	1.6429440000	1.7496750000
Co50	-3.7111660000	2.2761300000	2.4661270000
N51	-3.5413260000	1.1636270000	4.0149100000
N52	-2.8200430000	3.5916150000	3.5549910000
O53	-4.5436570000	0.8691560000	1.4198180000
O54	-3.8258040000	3.4015730000	0.8915740000
N8	-5.5701970000	2.9761890000	3.0556220000
C56	-3.4742590000	-0.1262920000	3.9873330000
C57	-3.3334420000	1.9388140000	5.2302560000
C58	-2.4916360000	4.7822110000	3.1727570000
C59	-2.4089340000	3.0880000000	4.8678450000
C60	-4.2215740000	-0.3828100000	1.5977990000
C61	-3.3704850000	4.6185940000	0.8100950000
C15	-6.6226750000	3.4076300000	3.2937030000
C63	-3.6908720000	-0.9271690000	2.8185940000
H64	-3.2320790000	-0.6523570000	4.9223130000
H65	-4.3083560000	2.3247640000	5.5607410000
H66	-2.9191350000	1.3163870000	6.0347720000
C67	-2.7287800000	5.3404690000	1.8761650000
H68	-1.9654000000	5.4246530000	3.8941350000
H69	-1.3759330000	2.7240800000	4.7873100000
H70	-2.4351260000	3.8874310000	5.6196030000
C71	-4.4349310000	-1.2937070000	0.5293950000
C72	-3.5028300000	5.2983560000	-0.4328090000
C26	-7.9304640000	3.9421930000	3.5869350000
C75	-3.4033700000	-2.3073060000	2.9086010000
C76	-2.2634990000	6.6583220000	1.6524280000
C77	-4.1293470000	-2.6383690000	0.6473140000
H78	-4.8375820000	-0.8926350000	-0.4004190000
C79	-3.0311770000	6.5859720000	-0.6160770000
H80	-3.9831970000	4.7593960000	-1.2496880000
C83	-3.6045560000	-3.1637410000	1.8420440000
H84	-3.0060510000	-2.6889190000	3.8516170000
C85	-2.4028420000	7.2871450000	0.4304030000
H86	-1.7741300000	7.1743780000	2.4811180000
H87	-4.2952540000	-3.2968320000	-0.2063630000
H88	-3.1468760000	7.0603720000	-1.5916560000
H95	-3.3630590000	-4.2219040000	1.9248610000
H96	-2.0286740000	8.2989180000	0.2778590000
H41	-7.8343920000	4.9382920000	4.0337220000
H42	-8.5157090000	4.0198560000	2.6628170000
H43	-8.4591830000	3.2837820000	4.2878260000

Co(salen)O_2

atom	x	y	z
O47	-1.2909180000	1.9058620000	2.4603450000
O49	-2.3803320000	1.9124660000	1.8363160000
Co50	-4.1274430000	2.2658240000	2.8260970000
N51	-3.6262970000	1.0956170000	4.2403370000
N52	-3.1966600000	3.5886040000	3.8601670000
O53	-4.8614780000	0.7833930000	1.8035550000
O54	-4.5812420000	3.5008980000	1.4224910000
C56	-3.1820770000	-0.1030810000	4.0350620000
C57	-3.4524800000	1.8121010000	5.4979000000
C58	-2.5886120000	4.5896740000	3.2971170000
C59	-2.7273050000	3.1139120000	5.1740010000
C60	-4.0766060000	-0.2623070000	1.6886250000
C61	-3.6907110000	4.3801520000	1.0381590000
C63	-3.2486400000	-0.7581990000	2.7567910000
H64	-2.6895710000	-0.6349550000	4.8617970000
H65	-4.4472760000	2.0216070000	5.9131380000
H66	-2.8918690000	1.2130050000	6.2283410000
C67	-2.7188220000	4.9685320000	1.9206660000
H68	-1.8549800000	5.1522960000	3.8924320000
H69	-1.6446200000	2.9338000000	5.1098740000
H70	-2.8955710000	3.8695260000	5.9516600000
C71	-4.0165590000	-0.9578140000	0.4542350000
C72	-3.6602050000	4.7869750000	-0.3206320000
C75	-2.4180760000	-1.8785690000	2.5445210000
C76	-1.7875340000	5.9042630000	1.4144390000
C77	-3.1672710000	-2.0384270000	0.2693810000
H78	-4.6296450000	-0.5893620000	-0.3674190000
C79	-2.7173020000	5.6890830000	-0.7874520000
H80	-4.3818070000	4.3357060000	-1.0010580000
C83	-2.3543320000	-2.5105420000	1.3137250000
H84	-1.7922360000	-2.2241200000	3.3690670000
C85	-1.7675500000	6.2600720000	0.0778590000
H86	-1.0545010000	6.3274880000	2.1032110000
H87	-3.1201920000	-2.5182230000	-0.7090780000
H88	-2.7042290000	5.9473490000	-1.8473180000
H95	-1.6813850000	-3.3517810000	1.1558210000
H96	-1.0264340000	6.9627470000	-0.2989220000

Co(salen)OOH(MeOH)

atom	x	y	z
O1	-0.9185080000	2.3465780000	1.3647090000
O49	-1.6483160000	1.6082350000	2.3488340000

Co50	-3.4454480000	2.1604930000	2.5108720000
N51	-3.5109980000	1.0753830000	4.0904450000
N52	-2.9372680000	3.5567390000	3.7164720000
O53	-4.0092910000	0.7353430000	1.3302850000
O54	-3.5384170000	3.3117680000	0.9673830000
O8	-5.5583600000	2.4382490000	2.7043510000
C56	-3.5834960000	-0.2137570000	4.1117220000
C57	-3.4648450000	1.8623340000	5.3190100000
C58	-2.7865080000	4.8063600000	3.4181290000
C59	-2.5735600000	3.0546900000	5.0398170000
C60	-3.9269230000	-0.5307350000	1.6332710000
C61	-3.3586000000	4.6013340000	0.9739730000
C15	-6.1304220000	3.7456570000	2.8344090000
C63	-3.7167120000	-1.0504720000	2.9570960000
H64	-3.5549880000	-0.7147480000	5.0904990000
H65	-4.4861300000	2.2007590000	5.5516560000
H66	-3.1053310000	1.2620720000	6.1655990000
C67	-3.0049830000	5.3825810000	2.1280170000
H68	-2.4648520000	5.4885400000	4.2186540000
H69	-1.5215960000	2.7380990000	5.0046990000
H70	-2.6775740000	3.8377790000	5.8026640000
C71	-4.0918680000	-1.4827000000	0.5922080000
C72	-3.5367770000	5.3102820000	-0.2457060000
C75	-3.6878260000	-2.4476860000	3.1691010000
C76	-2.8553610000	6.7842840000	2.0135020000
C77	-4.0524090000	-2.8442600000	0.8338450000
H78	-4.2540980000	-1.1004710000	-0.4153130000
C79	-3.3861940000	6.6832260000	-0.3210970000
H80	-3.8023310000	4.7301920000	-1.1287300000
C83	-3.8466180000	-3.3467340000	2.1317760000
H84	-3.5360790000	-2.8065780000	4.1894500000
C85	-3.0420040000	7.4418640000	0.8131230000
H86	-2.5849530000	7.3450180000	2.9106750000
H87	-4.1834040000	-3.5353290000	0.0005610000
H88	-3.5364280000	7.1822160000	-1.2794020000
H95	-3.8166250000	-4.4189720000	2.3161520000
H96	-2.9230110000	8.5217210000	0.7451900000
H48	-1.2167120000	1.9543560000	0.5184490000
H41	-7.2208190000	3.6740190000	2.9006790000
H42	-5.7386470000	4.1688430000	3.7608400000
H43	-5.8544400000	4.3898610000	1.9933320000
H44	-5.8690230000	2.0398940000	1.8675380000

Co(salen)CH$_2$CN(MeOH)

atom	x	y	z

Co50	-3.4851320000	2.5509860000	2.6066440000
N51	-3.3845870000	1.4073150000	4.1267390000
N52	-3.1506860000	3.9566760000	3.8561720000
O53	-3.8817560000	1.1026240000	1.3965550000
O54	-3.7005660000	3.7334430000	1.1030970000
O6	-5.6536930000	2.5805180000	2.8414900000
C56	-3.2151450000	0.1251950000	4.0993590000
C57	-3.5425640000	2.1369550000	5.3818760000
C58	-2.9624970000	5.2057040000	3.5605770000
C59	-2.8561220000	3.4768570000	5.2102210000
C60	-3.5189640000	-0.1324510000	1.6131940000
C61	-3.3948330000	5.0005060000	1.0877720000
C13	-6.2999130000	3.8558970000	2.9026800000
C63	-3.1654360000	-0.6635860000	2.9021450000
H64	-3.1102220000	-0.4047650000	5.0571200000
H65	-4.6187960000	2.2814340000	5.5565560000
H66	-3.1330700000	1.5695790000	6.2283860000
C67	-3.0419420000	5.7711870000	2.2492380000
H68	-2.6952350000	5.8905580000	4.3782390000
H69	-1.7654630000	3.3580800000	5.3023240000
H70	-3.1787100000	4.2048590000	5.9657010000
C71	-3.4924750000	-1.0314620000	0.5140140000
C72	-3.4291150000	5.6871490000	-0.1566480000
C75	-2.8114710000	-2.0265700000	3.0258020000
C76	-2.7343790000	7.1458000000	2.1125380000
C77	-3.1332880000	-2.3587770000	0.6701920000
H78	-3.7616660000	-0.6352210000	-0.4649340000
C79	-3.1207250000	7.0324500000	-0.2533360000
H80	-3.6991740000	5.1098860000	-1.0406990000
C83	-2.7828540000	-2.8725430000	1.9326260000
H84	-2.5558380000	-2.4028840000	4.0183390000
C85	-2.7640380000	7.7802810000	0.8853430000
H86	-2.4598580000	7.7023950000	3.0110550000
H87	-3.1199870000	-3.0130550000	-0.2024550000
H88	-3.1500690000	7.5166460000	-1.2305280000
H95	-2.4985380000	-3.9170910000	2.0463610000
H96	-2.5147530000	8.8367050000	0.7994050000
C46	-1.5627330000	2.2800480000	2.1479840000
H47	-1.3364450000	1.2334960000	2.3890180000
C49	-0.6159300000	3.1404890000	2.7721020000
N41	0.1543530000	3.8507270000	3.3028360000
H42	-1.5679570000	2.4263150000	1.0620640000
H43	-6.0093910000	4.4885640000	2.0552860000
H44	-5.9370450000	2.1253530000	2.0248230000
H45	-5.9744900000	4.3280670000	3.8335860000

H46	-7.3884730000	3.7314370000	2.9199370000

(MeOH)Co(salen)O$_2$Co(salen)(MeOH)

atom	x	y	z
Co1	0.7961170000	2.1905690000	2.3984170000
C2	1.2388150000	-0.5001970000	3.1905270000
C3	0.1267900000	4.8685150000	1.6356050000
C4	0.4248480000	5.3919250000	2.9367500000
C5	0.3033190000	6.7875970000	3.1209970000
C6	0.5078600000	7.3853420000	4.3509680000
C7	0.8477390000	6.5699770000	5.4469250000
C8	0.9832420000	5.2010570000	5.3016960000
C9	0.7868580000	4.5548030000	4.0488140000
C10	3.6674620000	3.4350690000	2.6438910000
C13	1.4143080000	-1.4537200000	4.2264530000
C14	1.1015810000	-2.7911670000	4.0473060000
C15	0.6010650000	-3.2590020000	2.8209650000
C16	0.4264320000	-2.3555020000	1.7871920000
C17	0.7256200000	-0.9858910000	1.9375870000
C18	0.5711540000	-0.1406970000	0.7890820000
C19	0.5635870000	1.9631960000	-0.3942230000
C20	-0.2759250000	3.1715730000	-0.0136650000
H21	-0.1851150000	5.5958780000	0.8714220000
H22	0.0311380000	7.3947720000	2.2548200000
H23	0.4079100000	8.4631270000	4.4701990000
H24	1.0115090000	7.0216680000	6.4267790000
H25	1.2516270000	4.5724570000	6.1511450000
H33	1.8046300000	-1.0932640000	5.1781810000
H34	1.2474600000	-3.4873440000	4.8747140000
H35	0.3505740000	-4.3104460000	2.6874780000
H36	0.0428260000	-2.6946050000	0.8223990000
H37	0.3460000000	-0.6314040000	-0.1693850000
H38	1.5692150000	2.2875220000	-0.6978890000
H39	0.1157690000	1.3975180000	-1.2229120000
H40	-1.3295560000	2.8758830000	0.0847780000
H41	-0.1955450000	3.9782480000	-0.7551690000
N42	0.6952320000	1.1443700000	0.8022370000
N43	0.1702840000	3.6191270000	1.3035600000
O45	1.5988290000	0.7349810000	3.4087100000
O46	0.9536260000	3.2664030000	3.9878180000
O47	-0.8788310000	1.4951620000	2.9340060000
O38	2.8985600000	2.5685730000	1.8038250000
O49	-1.8501120000	1.4944070000	2.0091900000
Co50	-3.5264510000	2.1881240000	2.5447760000
N51	-3.4162440000	1.1494890000	4.1465670000

N52	-2.8975840000	3.6206990000	3.6339190000
O53	-4.3250890000	0.7224190000	1.5419950000
O54	-3.6906710000	3.2597490000	0.9526500000
O48	-5.6283460000	2.5530240000	3.1170810000
C56	-3.2864430000	-0.1346700000	4.1656310000
C57	-3.2869050000	1.9727410000	5.3399670000
C58	-2.8460850000	4.8682330000	3.2959560000
C59	-2.4500460000	3.1804380000	4.9535820000
C60	-3.9581410000	-0.5104740000	1.7676020000
C61	-3.5090010000	4.5463680000	0.8844790000
C52	-6.3616360000	3.5372440000	2.3809660000
C63	-3.4376800000	-0.9858580000	3.0206720000
H64	-3.0575880000	-0.6202540000	5.1257390000
H65	-4.2928690000	2.2959420000	5.6430530000
H66	-2.8375030000	1.4113700000	6.1705750000
C67	-3.1390260000	5.3862860000	1.9919260000
H68	-2.5307310000	5.5976150000	4.0567960000
H69	-1.3958210000	2.8865330000	4.8567530000
H70	-2.5315750000	3.9911470000	5.6903780000
C71	-4.1291790000	-1.4702290000	0.7374830000
C72	-3.6959170000	5.1874910000	-0.3721740000
C75	-3.1254180000	-2.3519130000	3.1758860000
C76	-3.0032590000	6.7796490000	1.8005820000
C77	-3.8036220000	-2.8042330000	0.9208830000
H78	-4.5262100000	-1.1182260000	-0.2145430000
C79	-3.5449520000	6.5541250000	-0.5250230000
H80	-3.9678560000	4.5570120000	-1.2192040000
C83	-3.2943680000	-3.2618320000	2.1467900000
H84	-2.7355340000	-2.6825740000	4.1406510000
C85	-3.1990810000	7.3724830000	0.5669780000
H86	-2.7258580000	7.3883430000	2.6641220000
H87	-3.9463780000	-3.5047280000	0.0966430000
H88	-3.7012980000	7.0010160000	-1.5082980000
H95	-3.0328000000	-4.3100160000	2.2840780000
H96	-3.0867510000	8.4484150000	0.4420400000
H77	-7.4103530000	3.5499290000	2.7025500000
H79	-5.9028670000	4.5042940000	2.6058640000
H81	4.7191750000	3.4298920000	2.3344260000
H82	3.2586920000	4.4402740000	2.5164190000
H83	3.5825810000	3.1448390000	3.6968420000
H85	-6.3012870000	3.3551210000	1.3012660000
H89	3.2423730000	1.6626830000	1.9207410000
H90	-5.9883790000	1.6750140000	2.8824150000

Co(salen)O(MeOH)

atom	x	y	z
O49	-1.8857320000	1.8728080000	2.0876250000
Co50	-3.5590470000	2.2073580000	2.4650240000
N51	-3.4978270000	1.0985490000	4.0278450000
N52	-3.0092700000	3.6100720000	3.6552010000
O53	-4.2055520000	0.7757250000	1.3350390000
O54	-3.8366780000	3.3766340000	0.9627490000
O7	-5.6700720000	2.4387730000	2.8594010000
C56	-3.4402540000	-0.1917210000	4.0162800000
C57	-3.4397980000	1.8789720000	5.2582740000
C58	-2.7470790000	4.8286650000	3.3090300000
C59	-2.5931520000	3.0990060000	4.9616560000
C60	-3.9322350000	-0.4787710000	1.5664550000
C61	-3.4819460000	4.6315920000	0.9092250000
C14	-6.2267160000	3.7530020000	2.9722150000
C63	-3.5476060000	-1.0087550000	2.8460100000
H64	-3.3104960000	-0.7061270000	4.9794240000
H65	-4.4635330000	2.1812540000	5.5230690000
H66	-3.0317810000	1.2832960000	6.0853870000
C67	-2.9529220000	5.3881900000	2.0092160000
H68	-2.3244310000	5.4971050000	4.0733310000
H69	-1.5341570000	2.8132390000	4.8902050000
H70	-2.6926720000	3.8693300000	5.7368940000
C71	-4.0693800000	-1.4056250000	0.4992620000
C72	-3.6500480000	5.3157920000	-0.3246440000
C75	-3.3266740000	-2.3972900000	2.9953960000
C76	-2.6068040000	6.7481390000	1.8242890000
C77	-3.8388360000	-2.7582350000	0.6786980000
H78	-4.3636490000	-1.0127700000	-0.4736010000
C79	-3.3028560000	6.6471570000	-0.4687260000
H80	-4.0559510000	4.7500870000	-1.1625720000
C83	-3.4592080000	-3.2715060000	1.9329970000
H84	-3.0444090000	-2.7704900000	3.9820810000
C85	-2.7703010000	7.3814550000	0.6076130000
H86	-2.1968930000	7.2937450000	2.6766500000
H87	-3.9528330000	-3.4336210000	-0.1702000000
H88	-3.4408710000	7.1300050000	-1.4369760000
H95	-3.2778220000	-4.3368690000	2.0644220000
H96	-2.4921270000	8.4265880000	0.4828720000
H39	-7.3121940000	3.6910710000	3.1092570000
H40	-5.7764770000	4.2113320000	3.8573480000
H41	-5.9962990000	4.3607330000	2.0885510000
H42	-6.0663130000	1.9917240000	2.0838070000

Co(salen)OH(MeOH)

atom	x	y	z
O49	-1.4960270000	1.8329700000	2.2378010000
Co50	-3.3417760000	2.1860970000	2.4489150000
N51	-3.3944810000	1.1165880000	4.0323210000
N52	-2.9219890000	3.6187730000	3.6413090000
O53	-3.8312340000	0.7511780000	1.2600080000
O54	-3.4161240000	3.3123620000	0.8874130000
O7	-5.4270610000	2.3924760000	2.5843990000
C56	-3.5540070000	-0.1603780000	4.0731630000
C57	-3.3213300000	1.9067820000	5.2600280000
C58	-2.8530840000	4.8710910000	3.3372700000
C59	-2.4972190000	3.1377260000	4.9529710000
C60	-3.9169310000	-0.5032810000	1.6031690000
C61	-3.3823430000	4.6134610000	0.8925450000
C14	-6.0807250000	3.6493330000	2.7978220000
C63	-3.7738210000	-1.0062830000	2.9396670000
H64	-3.5503880000	-0.6455280000	5.0587880000
H65	-4.3431610000	2.1976420000	5.5422060000
H66	-2.9027960000	1.3224740000	6.0871210000
C67	-3.1228840000	5.4265310000	2.0469360000
H68	-2.5687050000	5.5747960000	4.1313230000
H69	-1.4332960000	2.8764870000	4.8881620000
H70	-2.6095800000	3.9142600000	5.7179760000
C71	-4.2031910000	-1.4525720000	0.5884530000
C72	-3.6381270000	5.2944800000	-0.3263840000
C75	-3.9186960000	-2.3890430000	3.1872330000
C76	-3.1251700000	6.8345680000	1.9292310000
C77	-4.3425700000	-2.7976880000	0.8682060000
H78	-4.3204230000	-1.0805030000	-0.4280480000
C79	-3.6431500000	6.6732560000	-0.4017520000
H80	-3.8419470000	4.6881970000	-1.2071530000
C83	-4.1977970000	-3.2858730000	2.1777530000
H84	-3.8119950000	-2.7376690000	4.2153380000
C85	-3.3840030000	7.4648760000	0.7305660000
H86	-2.9199210000	7.4241620000	2.8240380000
H87	-4.5712790000	-3.4875490000	0.0563500000
H88	-3.8523520000	7.1514640000	-1.3585510000
H95	-4.3106700000	-4.3460230000	2.3921050000
H96	-3.3871220000	8.5506260000	0.6622850000
H39	-1.4085640000	1.8454840000	1.2734060000
H40	-7.1621420000	3.5010570000	2.8538100000
H41	-5.7262080000	4.0390590000	3.7515660000
H42	-5.8498280000	4.3639300000	2.0029790000
H43	-5.7215690000	2.0206310000	1.7357730000

CH_3CN

atom	x	y	z
C1	0.0104990000	1.2859810000	0.0000000000
C2	0.0030330000	-0.1580540000	0.0000000000
N3	-0.0140990000	-1.3250710000	0.0000000000
H4	1.0421930000	1.6574510000	0.0000000000
H5	-0.5037090000	1.6617640000	-0.8926880000
H6	-0.5037090000	1.6617640000	0.8926880000

CH_2CN

atom	x	y	z
C1	0.0948210000	0.1120550000	0.1966230000
C2	1.4580690000	-0.0040810000	0.0110870000
N3	2.6224190000	-0.1099200000	-0.1528390000
H4	-0.4375180000	0.9734470000	-0.2050030000
H5	-0.4444800000	-0.6592640000	0.7454150000

O_2

atom	x	y	z
O47	0.0000000000	0.0000000000	0.6086740000
O49	0.0000000000	0.0000000000	-0.6086740000

H_2O_2

atom	x	y	z
O1	-0.7328820000	-0.0613730000	0.0000000000
O2	0.7328820000	0.0613730000	0.0000000000
H3	-0.9867770000	0.8855320000	0.0000000000
H4	0.9867770000	-0.8855320000	0.0000000000

MeOH

atom	x	y	z
O1	0.0477050000	-0.6918060000	0.0000000000
C2	0.0049620000	0.7283310000	0.0000000000
H3	-0.8654980000	-1.0297510000	0.0000000000
H4	1.0389870000	1.0849240000	0.0000000000
H5	-0.4948410000	1.1260850000	-0.8933970000
H6	-0.4948410000	1.1260850000	0.8933970000

H_2O

atom	x	y	z
O1	0.0000000000	0.0000000000	-0.0673550000
H2	0.0000000000	0.7637350000	0.5344900000
H3	0.0000000000	-0.7637350000	0.5344900000

Mechanism figure 9b.

Co(salen)

atom	x	y	z
Co1	0.7057600000	2.2154160000	2.4824200000
C2	1.2577420000	-0.4470210000	3.4220290000
C3	0.0629390000	4.8478650000	1.5433890000
C4	0.3508570000	5.4501510000	2.8073780000
C5	0.2654860000	6.8590280000	2.9047320000
C6	0.4943930000	7.5216610000	4.0947240000
C7	0.8114420000	6.7664410000	5.2401690000
C8	0.8974160000	5.3878530000	5.1836250000
C9	0.6783490000	4.6766250000	3.9731180000
C13	1.5294370000	-1.3463710000	4.4879560000
C14	1.5729970000	-2.7136520000	4.2897770000
C15	1.3555470000	-3.2702100000	3.0147010000
C16	1.0988090000	-2.4218640000	1.9553470000
C17	1.0397600000	-1.0177310000	2.1215160000
C18	0.8016770000	-0.2153700000	0.9626430000
C19	0.5333280000	1.8093610000	-0.2963870000
C20	-0.2805140000	3.0564890000	-0.0148480000
H21	-0.2744460000	5.5163460000	0.7388920000
H22	0.0092470000	7.4208100000	2.0044860000
H23	0.4274130000	8.6066760000	4.1482360000
H24	0.9918130000	7.2733460000	6.1888670000
H25	1.1405080000	4.8052370000	6.0716640000
H33	1.6992230000	-0.9176310000	5.4751010000
H34	1.7799400000	-3.3683370000	5.1372100000
H35	1.3927720000	-4.3479490000	2.8675160000
H36	0.9348310000	-2.8274000000	0.9551290000
H37	0.7497130000	-0.7381620000	-0.0026560000
H38	1.5425560000	2.0860040000	-0.6349390000
H39	0.0751390000	1.1869680000	-1.0765880000
H40	-1.3479200000	2.8012330000	0.0573650000
H41	-0.1669720000	3.8092120000	-0.8063580000
N42	0.6570240000	1.0770660000	0.9673660000
N43	0.1559310000	3.5769600000	1.2842550000
O45	1.2347340000	0.8311220000	3.6804020000
O46	0.7731470000	3.3758480000	3.9923530000

Co(salen)O_2(CF_3CH_2OH)

atom	x	y	z
O47	-0.6766400000	1.7438130000	2.5444340000
O49	-1.6995990000	1.7530650000	1.7900860000
Co50	-3.4045990000	2.2032740000	2.5459340000

N51	-3.1647210000	1.0844830000	4.0747010000
N52	-2.6478170000	3.5715600000	3.6493580000
O53	-4.2007950000	0.7836550000	1.5040240000
O54	-3.7514030000	3.3824660000	1.0655630000
O8	-5.5455350000	2.4155120000	3.0986420000
C56	-3.1103170000	-0.2064210000	4.0559040000
C57	-2.9917950000	1.8528900000	5.3011640000
C58	-2.3751600000	4.7818570000	3.2768820000
C59	-2.1760500000	3.0815230000	4.9476070000
C60	-3.9170880000	-0.4794740000	1.6914320000
C61	-3.3255630000	4.6099320000	0.9542790000
C15	-6.2487420000	3.6376380000	2.9435700000
C63	-3.3665650000	-1.0176140000	2.9034070000
H64	-2.8641540000	-0.7266200000	4.9927820000
H65	-3.9887520000	2.1478350000	5.6579630000
H66	-2.5118240000	1.2519610000	6.0853850000
C67	-2.6597580000	5.3443460000	1.9942950000
H68	-1.8733330000	5.4387940000	4.0017070000
H69	-1.1160790000	2.8097940000	4.8453840000
H70	-2.2573610000	3.8626000000	5.7149280000
C71	-4.2045460000	-1.3957370000	0.6483650000
C72	-3.5508600000	5.2931750000	-0.2713410000
C75	-3.1311070000	-2.4059280000	3.0110470000
C76	-2.2520250000	6.6796310000	1.7636630000
C77	-3.9536500000	-2.7495970000	0.7843200000
H78	-4.6254380000	-0.9925640000	-0.2719410000
C79	-3.1354500000	6.5983230000	-0.4627920000
H80	-4.0553800000	4.7440890000	-1.0651850000
C83	-3.4080720000	-3.2718960000	1.9703150000
H84	-2.7193650000	-2.7862790000	3.9478550000
C85	-2.4757550000	7.3106240000	0.5562840000
H86	-1.7418390000	7.2062840000	2.5725610000
H87	-4.1815370000	-3.4185600000	-0.0460780000
H88	-3.3191000000	7.0790100000	-1.4244140000
H95	-3.2125250000	-4.3378220000	2.0679370000
H96	-2.1474150000	8.3358500000	0.3945490000
H40	-7.2456410000	3.4757500000	2.5189260000
C41	-6.4106460000	4.2576840000	4.3104020000
H42	-5.6974680000	4.3348070000	2.3000910000
H43	-5.8391910000	1.7867490000	2.4075550000
F44	-7.0545410000	5.4406420000	4.2080490000
F45	-7.1234860000	3.4793980000	5.1504470000
F46	-5.2257470000	4.4959220000	4.9139180000

Co(salen)OOH(CF_3CH_2OH)

atom	x	y	z
O1	-0.9385870000	2.3340440000	1.4133570000
O49	-1.6885610000	1.5305770000	2.3180550000
Co50	-3.4512500000	2.1307260000	2.5247220000
N51	-3.5304080000	1.0273310000	4.0891860000
N52	-2.9050550000	3.5056920000	3.7274960000
O53	-4.1330300000	0.7261390000	1.3725910000
O54	-3.5387110000	3.2890840000	0.9924890000
O8	-5.5892000000	2.4459320000	2.7109970000
C56	-3.5775000000	-0.2638750000	4.0949400000
C57	-3.4506060000	1.8052040000	5.3204750000
C58	-2.7549150000	4.7593410000	3.4414340000
C59	-2.5286070000	2.9753890000	5.0351260000
C60	-3.9817470000	-0.5474960000	1.6281970000
C61	-3.3669430000	4.5795370000	1.0069940000
C15	-6.1719800000	3.6801480000	2.3280080000
C63	-3.7097970000	-1.0874220000	2.9298850000
H64	-3.5214380000	-0.7772490000	5.0657520000
H65	-4.4596520000	2.1712950000	5.5616030000
H66	-3.0981400000	1.1918290000	6.1604740000
C67	-2.9964680000	5.3510220000	2.1624750000
H68	-2.4190990000	5.4308730000	4.2447080000
H69	-1.4885340000	2.6253600000	4.9707740000
H70	-2.5893580000	3.7495270000	5.8114880000
C71	-4.1413070000	-1.4713730000	0.5649580000
C72	-3.5824510000	5.2981360000	-0.2007770000
C75	-3.6201690000	-2.4865360000	3.1044020000
C76	-2.8620790000	6.7553620000	2.0591700000
C77	-4.0403540000	-2.8366500000	0.7689640000
H78	-4.3461760000	-1.0657130000	-0.4250840000
C79	-3.4490740000	6.6727210000	-0.2629790000
H80	-3.8648960000	4.7221970000	-1.0812800000
C83	-3.7758160000	-3.3622250000	2.0460400000
H84	-3.4216470000	-2.8679520000	4.1078590000
C85	-3.0848520000	7.4223300000	0.8714230000
H86	-2.5755050000	7.3094610000	2.9551770000
H87	-4.1671350000	-3.5120380000	-0.0778080000
H88	-3.6299990000	7.1819690000	-1.2105140000
H95	-3.6972320000	-4.4369020000	2.1984910000
H96	-2.9801580000	8.5041180000	0.8126610000
H48	-1.2565170000	2.0362040000	0.5361860000
C41	-7.5803480000	3.7648860000	2.8685190000
H42	-5.5830270000	4.4854110000	2.7771850000
H43	-6.1913050000	3.8116970000	1.2405910000

H44	-5.7532950000	1.7792530000	2.0097160000
F45	-8.1511540000	4.9386780000	2.5208730000
F46	-8.3621110000	2.7718840000	2.3909240000
F47	-7.6159660000	3.6818080000	4.2156410000

Co(salen)(CF_3CHOH)(CF_3CH_2OH)

atom	x	y	z
Co1	2.0680620000	5.7332810000	1.6751610000
F2	-0.6379190000	7.4437560000	1.2994630000
F3	-0.9465730000	6.3444870000	3.1681460000
F4	-0.6711220000	8.4955570000	3.1872850000
F5	2.9011850000	4.3437100000	-3.2352230000
F6	4.4730190000	3.4242700000	-2.0389950000
F7	4.0277120000	5.5341740000	-1.7997140000
O11	1.8462840000	6.7952620000	0.1053480000
O12	0.4322990000	4.9123270000	1.1633750000
O13	1.5317730000	7.1475600000	4.1341560000
O14	3.0315950000	4.0600620000	0.3312340000
H15	3.2362080000	3.1620620000	0.6466170000
N18	3.7978320000	6.4314360000	2.0335710000
N19	2.4053890000	4.5536570000	3.1289110000
C20	2.4687630000	7.9105240000	-0.1353720000
C21	1.9560540000	8.7680220000	-1.1462510000
H22	1.0475800000	8.4510050000	-1.6575620000
C23	2.5794710000	9.9595640000	-1.4668230000
H24	2.1516430000	10.5945090000	-2.2439850000
C25	3.7539930000	10.3666760000	-0.8048460000
H26	4.2370620000	11.3067040000	-1.0663470000
C27	4.2828930000	9.5503910000	0.1768980000
H28	5.1992480000	9.8396680000	0.6957750000
C29	3.6664010000	8.3303050000	0.5391910000
C30	4.3058090000	7.5105520000	1.5245550000
H31	5.3075530000	7.8179000000	1.8563940000
C32	4.5733320000	5.5766230000	2.9283620000
H33	5.3447480000	6.1503770000	3.4589610000
H34	5.0795510000	4.8203540000	2.3117730000
C35	3.6054710000	4.9049080000	3.8885360000
H36	4.0502770000	4.0178140000	4.3579030000
H37	3.3205520000	5.6091220000	4.6801070000
C38	1.6950890000	3.5100230000	3.4353240000
H39	2.0380840000	2.8819680000	4.2701680000
C40	0.5005140000	3.0950320000	2.7658940000
C41	-0.1378790000	1.9150340000	3.2190420000
H42	0.3075350000	1.3808550000	4.0608750000
C43	-1.2905170000	1.4362210000	2.6276760000

H44	-1.7658780000	0.5266970000	2.9914700000
C45	-1.8432680000	2.1477830000	1.5436030000
H46	-2.7546890000	1.7838640000	1.0671180000
C47	-1.2505250000	3.3039670000	1.0751000000
H48	-1.6773880000	3.8610760000	0.2415360000
C49	-0.0627450000	3.8237540000	1.6614770000
C50	1.2506460000	7.1722990000	2.7584510000
H52	1.7406360000	8.0701430000	2.3618760000
C53	-0.2424410000	7.3444250000	2.5710890000
C54	2.4327370000	3.9899580000	-0.9508010000
H55	1.6283170000	4.7327930000	-0.9903900000
H56	2.0188740000	2.9971550000	-1.1651060000
C57	3.4611730000	4.3293820000	-2.0025190000
H53	1.0056970000	6.4485890000	4.5640730000

Co(salen)(CF_3CH_2O)(CF_3CH_2OH)

atom	x	y	z
Co1	1.9829610000	5.8288770000	1.5063490000
F2	-2.1839950000	7.9255830000	2.8604940000
F3	-1.0884350000	6.1609350000	3.5181880000
F4	-0.6411550000	8.0948560000	4.3877880000
F5	2.8306930000	3.9868080000	-3.1890670000
F6	4.3185760000	3.1865210000	-1.8101100000
F7	3.9708020000	5.3259820000	-1.9048070000
O11	1.8215810000	6.8251940000	-0.1128060000
O12	0.2820240000	5.0832620000	1.0437920000
O13	1.3194900000	7.2789340000	2.5077140000
O14	2.8432910000	4.2218630000	0.3795120000
H15	2.9976250000	3.3741800000	0.8337670000
N18	3.7294150000	6.4970170000	1.9083630000
N19	2.1907100000	4.7763310000	3.0815860000
C20	2.4625840000	7.9334650000	-0.3459760000
C21	1.9844360000	8.7788930000	-1.3822840000
H22	1.0855350000	8.4631640000	-1.9112660000
C23	2.6273160000	9.9593640000	-1.7070710000
H24	2.2242490000	10.5842770000	-2.5050790000
C25	3.7865420000	10.3666560000	-1.0208350000
H26	4.2844520000	11.2989410000	-1.2811600000
C27	4.2790270000	9.5608560000	-0.0109020000
H28	5.1792480000	9.8543030000	0.5329020000
C29	3.6443270000	8.3517280000	0.3535590000
C30	4.2343910000	7.5740070000	1.4021850000
H31	5.1955780000	7.9288540000	1.8019900000
C32	4.3729800000	5.7556200000	2.9844070000
H33	5.1212680000	6.3695550000	3.5033610000

H34	4.8860790000	4.8837980000	2.5504970000
C35	3.2647900000	5.2916320000	3.9201160000
H36	3.6151130000	4.5369160000	4.6368910000
H37	2.8695780000	6.1522490000	4.4780560000
C38	1.4603570000	3.7606940000	3.4129320000
H39	1.7120480000	3.2248070000	4.3396230000
C40	0.3424140000	3.2730690000	2.6608900000
C41	-0.2786740000	2.0802450000	3.0993660000
H42	0.1374510000	1.5772420000	3.9745750000
C43	-1.3793020000	1.5511360000	2.4537980000
H44	-1.8398950000	0.6294570000	2.8044810000
C45	-1.8997860000	2.2305600000	1.3353340000
H46	-2.7709460000	1.8289960000	0.8160390000
C47	-1.3266270000	3.4039530000	0.8838770000
H48	-1.7313250000	3.9360330000	0.0231930000
C49	-0.1895940000	3.9707990000	1.5219900000
C50	0.0733440000	7.7379960000	2.1375220000
H51	-0.3031620000	7.2888560000	1.2060160000
H52	0.0862510000	8.8340140000	1.9848120000
C53	-0.9516300000	7.4693850000	3.2192380000
C54	2.2720500000	3.9950880000	-0.9051850000
H55	1.5094260000	4.7622090000	-1.0735180000
H56	1.8184800000	3.0010130000	-0.9801290000
C57	3.3545540000	4.1307230000	-1.9507570000

CF_3CHOH

atom	x	y	z
F5	-1.1731250000	-0.8368260000	5.0779750000
F6	-0.1033610000	-2.5978930000	4.3868760000
F7	0.7197890000	-0.5902140000	4.0479210000
O14	1.3719340000	-0.3718330000	6.7557340000
C54	0.8332850000	-1.4844070000	6.2084780000
H55	0.5802950000	-2.2678650000	6.9179030000
C57	0.0795860000	-1.3849090000	4.9484320000
H8	1.5996840000	0.2997670000	6.0810950000

CF_3CH_2O

atom	x	y	z
F5	-1.0989830000	-0.8385230000	5.1895320000
F6	-0.1128290000	-2.5911980000	4.3501110000
F7	0.6941520000	-0.5987910000	3.9937670000
O14	1.2077920000	-0.3445540000	6.7831190000
C54	0.9591120000	-1.5204340000	6.1726840000
H55	0.4762790000	-2.2179700000	6.8885070000
H56	1.9173550000	-2.0244460000	5.9283380000

C57	0.1047640000	-1.3840950000	4.9188530000

O_2

atom	x	y	z
O47	0.0000000000	0.0000000000	0.6086740000
O49	0.0000000000	0.0000000000	-0.6086740000

CF_3CH_2OH

atom	x	y	z
F5	-1.1230510000	-0.9195770000	5.2029360000
F6	-0.0565350000	-2.6171150000	4.3575360000
F7	0.6471490000	-0.5865010000	3.9923350000
O14	1.1935200000	-0.2389990000	6.7506070000
C54	0.9840870000	-1.5002060000	6.1626590000
C57	0.1089440000	-1.4021030000	4.9303380000
H7	1.8825830000	0.2392130000	6.2546610000
H8	0.4648500000	-2.1306640000	6.8926840000
H9	1.9194440000	-2.0001410000	5.8778640000

Mechanism figure 10.

$Co(salen)(CH_3CHNO_2)(CH_3CH_2NO_2)$

atom	x	y	z
Co50	-3.0576240000	2.5291560000	2.6878530000
N51	-3.2720860000	1.3580430000	4.1775080000
N52	-2.7748200000	3.8791990000	3.9912550000
O53	-3.5698630000	1.2032820000	1.4220110000
O54	-3.1309950000	3.7318770000	1.2170110000
O55	-5.4157940000	3.0140740000	2.9944460000
C56	-3.5373650000	0.0879960000	4.1294290000
C57	-3.2739210000	2.0583500000	5.4666050000
C58	-2.8577570000	5.1580590000	3.7912280000
C59	-2.4620640000	3.3299580000	5.3078320000
C60	-3.6857810000	-0.0766920000	1.6331210000
C61	-3.1879940000	5.0280090000	1.3008610000
N62	-6.2255120000	2.5107970000	2.1997540000
C63	-3.6926490000	-0.6810820000	2.9349030000
H64	-3.6629840000	-0.4453630000	5.0824470000
H65	-4.3154320000	2.3125440000	5.7105520000
H66	-2.8830140000	1.4168820000	6.2671830000
C67	-3.0798510000	5.7784840000	2.5218390000
H68	-2.7405610000	5.8228140000	4.6583100000
H69	-1.3842000000	3.1068390000	5.3424410000
H70	-2.6772750000	4.0540030000	6.1042980000

C71	-3.8271380000	-0.9320180000	0.5092980000
C72	-3.3790930000	5.7630690000	0.0990290000
O73	-7.0863970000	1.7069080000	2.5394010000
C74	-6.1301010000	2.9355930000	0.7640490000
C75	-3.8524330000	-2.0791350000	3.0538010000
C76	-3.1717450000	7.1897680000	2.4843880000
C77	-3.9752890000	-2.2980110000	0.6622380000
H78	-3.8064070000	-0.4714390000	-0.4780520000
C79	-3.4722960000	7.1417760000	0.1021720000
H80	-3.4533710000	5.1950180000	-0.8280500000
H81	-6.4413350000	3.9887120000	0.7842380000
C82	-6.9609720000	2.0855240000	-0.1540290000
C83	-3.9903720000	-2.8875590000	1.9408690000
H84	-3.8569150000	-2.5165780000	4.0542190000
C85	-3.3694590000	7.8741840000	1.3010440000
H86	-3.0820070000	7.7358540000	3.4257050000
H87	-4.0771000000	-2.9266230000	-0.2234260000
H88	-3.6260040000	7.6679520000	-0.8408810000
H92	-6.6503660000	1.0359290000	-0.1111140000
H93	-8.0273690000	2.1426360000	0.0828160000
H94	-6.8175580000	2.4387430000	-1.1810740000
H95	-4.1061280000	-3.9645640000	2.0496810000
H96	-3.4415530000	8.9603030000	1.2932520000
H91	-5.0538490000	2.9095490000	0.5516350000
C46	-1.0818270000	2.2439090000	2.5379930000
H47	-0.7950220000	1.9613930000	3.5542140000
N48	-0.8352840000	1.0317890000	1.7288340000
C49	-0.3427780000	3.4282350000	1.9882860000
H50	0.7415640000	3.2409950000	1.9986030000
H51	-0.6434040000	3.6522490000	0.9627920000
H52	-0.5371900000	4.3088430000	2.6089940000
O56	-0.6092730000	1.1444820000	0.5195890000
O57	-0.8584630000	-0.0627460000	2.3120090000

Co(salen)(CH$_3$CHNO$_2$)

atom	x	y	z
Co50	-3.5911610000	2.4887630000	2.6617300000
N51	-3.4404130000	1.1910000000	4.0341610000
N52	-3.1737230000	3.7470930000	4.0313570000
O53	-4.1839410000	1.1899190000	1.4011340000
O54	-3.9835860000	3.8368240000	1.3725580000
C56	-3.2846430000	-0.0859150000	3.8610580000
C57	-3.5840910000	1.7705920000	5.3706980000
C58	-2.8457140000	4.9865380000	3.8217590000
C59	-2.9654010000	3.1575710000	5.3621460000

C60	-3.7372420000	-0.0411950000	1.4022540000
C61	-3.4056220000	5.0120450000	1.3703250000
C63	-3.2776100000	-0.7224310000	2.5785320000
H64	-3.1492940000	-0.7206010000	4.7482230000
H65	-4.6597180000	1.8351010000	5.5877710000
H66	-3.1256720000	1.1251010000	6.1319620000
C67	-2.8452010000	5.6284550000	2.5409750000
H68	-2.5015140000	5.5845760000	4.6769990000
H69	-1.8849810000	3.0985080000	5.5422150000
H70	-3.4038120000	3.7933290000	6.1416710000
C71	-3.7048540000	-0.7568250000	0.1788620000
C72	-3.3171510000	5.7278020000	0.1494970000
C75	-2.8173230000	-2.0533140000	2.4844690000
C76	-2.2425180000	6.9039880000	2.4387200000
C77	-3.2234470000	-2.0532260000	0.1155430000
H78	-4.0416600000	-0.2397220000	-0.7192850000
C79	-2.7021290000	6.9662210000	0.0816120000
H80	-3.7276850000	5.2577450000	-0.7433390000
C83	-2.7722160000	-2.7156400000	1.2715120000
H84	-2.4714960000	-2.5487520000	3.3937540000
C85	-2.1569630000	7.5682600000	1.2296580000
H86	-1.8190160000	7.3495480000	3.3408700000
H87	-3.1860600000	-2.5625130000	-0.8484110000
H88	-2.6301810000	7.4747230000	-0.8808060000
H95	-2.3902640000	-3.7330660000	1.2099700000
H96	-1.6685820000	8.5380260000	1.1643700000
C46	-1.6833820000	2.5223200000	1.9931620000
H47	-1.4363600000	3.5723960000	2.1678980000
N48	-0.7974220000	1.7683180000	2.9024150000
C49	-1.5147780000	2.0962930000	0.5647490000
H50	-0.4976820000	2.3449020000	0.2240110000
H51	-1.6589850000	1.0221350000	0.4238740000
H52	-2.2334080000	2.6322710000	-0.0615920000
O56	-0.5182910000	0.5959400000	2.6304430000
O57	-0.3807000000	2.3384640000	3.9227840000

Co(salen)NO_2

atom	x	y	z
Co50	-3.5455740000	2.3247240000	2.6745820000
N51	-3.4491760000	1.1190000000	4.1505070000
N52	-3.0139480000	3.6513230000	3.9428310000
O53	-4.0748990000	0.9647070000	1.4425970000
O54	-3.7793920000	3.5583160000	1.2497720000
C56	-3.3253000000	-0.1669580000	4.0518480000
C57	-3.3893820000	1.8004180000	5.4446200000

C58	-2.7724810000	4.8986250000	3.6746000000
C59	-2.6218410000	3.0924660000	5.2423900000
C60	-3.7216770000	-0.2883060000	1.5776010000
C61	-3.3563420000	4.7931160000	1.2344660000
C63	-3.3305540000	-0.8932660000	2.8179440000
H64	-3.1595250000	-0.7418370000	4.9737770000
H65	-4.4175960000	2.0092380000	5.7705880000
H66	-2.9143070000	1.1610690000	6.2000720000
C67	-2.8680180000	5.5012450000	2.3832370000
H68	-2.4012170000	5.5333650000	4.4911910000
H69	-1.5439620000	2.8879090000	5.2091930000
H70	-2.8110290000	3.8098760000	6.0506380000
C71	-3.6777330000	-1.1009490000	0.4144110000
C72	-3.3277220000	5.4742980000	-0.0117380000
C75	-2.9095580000	-2.2439090000	2.8386150000
C76	-2.3848510000	6.8242930000	2.2391300000
C77	-3.2456460000	-2.4146950000	0.4674540000
H78	-3.9460920000	-0.6392850000	-0.5350200000
C79	-2.8401260000	6.7642910000	-0.1173110000
H80	-3.6614640000	4.9280420000	-0.8930870000
C83	-2.8594970000	-3.0041020000	1.6856150000
H84	-2.5935530000	-2.6726250000	3.7916210000
C85	-2.3723700000	7.4607660000	1.0138410000
H86	-1.9928600000	7.3283340000	3.1243840000
H87	-3.1894300000	-2.9946700000	-0.4548220000
H88	-2.8063110000	7.2417030000	-1.0973740000
H95	-2.5039950000	-4.0327080000	1.7137410000
H96	-1.9735820000	8.4689920000	0.9163320000
N48	-1.7221530000	2.0341070000	2.1866950000
O56	-1.4552660000	1.9749170000	0.9943790000
O57	-0.8850870000	1.9141760000	3.0837310000

$Co(salen)NO_2(CH_3CH_2NO_2)$

atom	x	y	z
Co50	-3.2747550000	2.3314170000	2.5890190000
N51	-3.4018570000	1.1531310000	4.0944000000
N52	-2.8232810000	3.6672590000	3.8892660000
O53	-3.8885770000	0.9859540000	1.3775300000
O54	-3.2249670000	3.5250270000	1.1078060000
O55	-5.3647090000	2.8758720000	2.9951000000
C56	-3.3841380000	-0.1397340000	4.0340100000
C57	-3.4472970000	1.8729080000	5.3639440000
C58	-2.7214500000	4.9372890000	3.6577510000
C59	-2.5822210000	3.1132230000	5.2224130000
C60	-3.6741710000	-0.2898020000	1.5481750000

C61	-3.1180730000	4.8194410000	1.1766290000
N62	-6.3585310000	2.7824600000	2.2471300000
C63	-3.4077040000	-0.8999250000	2.8200160000
H64	-3.3536220000	-0.6995790000	4.9794850000
H65	-4.4909070000	2.1617170000	5.5501280000
H66	-3.1147220000	1.2331840000	6.1917470000
C67	-2.8830640000	5.5639140000	2.3814810000
H68	-2.4941650000	5.5957140000	4.5082810000
H69	-1.5214800000	2.8448950000	5.2966270000
H70	-2.8092020000	3.8551330000	5.9985810000
C71	-3.7309550000	-1.1415000000	0.4144750000
C72	-3.2430370000	5.5557080000	-0.0327100000
O73	-7.4687700000	2.5194550000	2.6827690000
C74	-6.1867060000	3.0533750000	0.7803830000
C75	-3.2117790000	-2.2976240000	2.9001670000
C76	-2.7785230000	6.9734660000	2.3213260000
C77	-3.5240460000	-2.5048550000	0.5276280000
H78	-3.9282420000	-0.6809520000	-0.5527480000
C79	-3.1432640000	6.9339720000	-0.0511950000
H80	-3.4149700000	4.9897540000	-0.9479040000
H81	-6.0595330000	4.1434930000	0.7405480000
C82	-7.3508730000	2.5665150000	-0.0354110000
C83	-3.2578170000	-3.0998600000	1.7752220000
H84	-3.0151220000	-2.7370000000	3.8800820000
C85	-2.9078370000	7.6621350000	1.1308200000
H86	-2.5891880000	7.5143640000	3.2503960000
H87	-3.5619230000	-3.1250250000	-0.3690020000
H88	-3.2459950000	7.4613410000	-1.0003780000
H92	-7.4910120000	1.4857250000	0.0740200000
H93	-8.2838720000	3.0688690000	0.2340270000
H94	-7.1411360000	2.7746650000	-1.0902290000
H95	-3.0916800000	-4.1729580000	1.8513780000
H96	-2.8259900000	8.7470610000	1.1049920000
H91	-5.2254410000	2.6002220000	0.5203880000
N48	-1.4549620000	1.8588060000	2.2807540000
O56	-1.1109580000	1.6397930000	1.1251240000
O57	-0.6856680000	1.7916860000	3.2452350000

Co(salen)NO$_2$(H$_2$O)

atom	x	y	z
Co50	-3.5973690000	2.3632910000	2.7183810000
N51	-3.3712250000	1.1496030000	4.1810670000
N52	-2.9605570000	3.6892860000	3.9635710000
O53	-4.2183120000	0.9454720000	1.5631280000
O54	-3.9168990000	3.6461930000	1.3206210000

O55	-5.6620970000	2.6262140000	3.1440520000
C56	-3.1050770000	-0.1094950000	4.0607750000
C57	-3.3739020000	1.8386510000	5.4652180000
C58	-2.5368460000	4.8665590000	3.6268740000
C59	-2.6152000000	3.1411230000	5.2826370000
C60	-3.6971800000	-0.2539180000	1.6273520000
C61	-3.3065700000	4.7968760000	1.2324700000
C63	-3.1239530000	-0.8211230000	2.8158900000
H64	-2.8426100000	-0.6735520000	4.9676000000
H65	-4.4179950000	2.0388550000	5.7416530000
H66	-2.9237770000	1.2141080000	6.2487080000
C67	-2.6231840000	5.4405790000	2.3195950000
H68	-2.0390690000	5.4711030000	4.3989580000
H69	-1.5334900000	2.9515700000	5.2997720000
H70	-2.8505270000	3.8606540000	6.0771520000
C71	-3.7226990000	-1.0676780000	0.4676710000
C72	-3.3280910000	5.4780320000	-0.0123950000
C75	-2.6040130000	-2.1345640000	2.7889490000
C76	-1.9935750000	6.6903550000	2.1124360000
C77	-3.1950270000	-2.3478180000	0.4719470000
H78	-4.1572830000	-0.6431620000	-0.4369000000
C79	-2.6965860000	6.6973240000	-0.1810080000
H80	-3.8450870000	4.9957930000	-0.8411440000
C83	-2.6220820000	-2.8952860000	1.6343220000
H84	-2.1734690000	-2.5399080000	3.7069600000
C85	-2.0147370000	7.3182560000	0.8821560000
H86	-1.4721040000	7.1493550000	2.9547120000
H87	-3.2191220000	-2.9355070000	-0.4464210000
H88	-2.7215320000	7.1777320000	-1.1598160000
H95	-2.2017490000	-3.8995570000	1.6244770000
H96	-1.5112730000	8.2719940000	0.7362070000
N48	-1.7783820000	2.0920100000	2.1340150000
O56	-1.5792100000	2.0090140000	0.9244050000
O57	-0.8691950000	2.0138340000	2.9697450000
H40	-5.9336560000	3.3632200000	2.5619950000
H41	-6.0665960000	1.8460430000	2.7144480000

$CH_3CH_2NO_2$

atom	x	y	z
O55	-5.4322300000	3.1203400000	2.9991700000
N62	-6.3599910000	2.7849930000	2.2624010000
O73	-7.4027270000	2.2737150000	2.6598430000
C74	-6.1773010000	3.0290290000	0.7849770000
H81	-5.9686300000	4.1021900000	0.7176520000
C82	-7.3581550000	2.5914620000	-0.0336030000

H92	-7.5474830000	1.5188550000	0.0716810000
H93	-8.2665510000	3.1330740000	0.2471950000
H94	-7.1486950000	2.7993590000	-1.0883010000
H91	-5.2511640000	2.4973360000	0.5414070000

C_2H_4

atom	x	y	z
C1	0.0000000000	0.0000000000	0.6670630000
C2	0.0000000000	0.0000000000	-0.6670630000
H3	0.0000000000	0.9253030000	1.2449140000
H4	0.0000000000	-0.9253030000	1.2449140000
H5	0.0000000000	-0.9253030000	-1.2449140000
H6	0.0000000000	0.9253030000	-1.2449140000

H_2O

atom	x	y	z
O55	-0.0668750000	-0.0080230000	0.0000000000
H40	0.6216640000	-0.6947500000	0.0000000000
H41	0.4396910000	0.8220820000	0.0000000000

pK_a calculations

Co(salen)OH

atom	x	y	z
O49	-1.4960270000	1.8329700000	2.2378010000
Co50	-3.3417760000	2.1860970000	2.4489150000
N51	-3.3944810000	1.1165880000	4.0323210000
N52	-2.9219890000	3.6187730000	3.6413090000
O53	-3.8312340000	0.7511780000	1.2600080000
O54	-3.4161240000	3.3123620000	0.8874130000
O7	-5.4270610000	2.3924760000	2.5843990000
C56	-3.5540070000	-0.1603780000	4.0731630000
C57	-3.3213300000	1.9067820000	5.2600280000
C58	-2.8530840000	4.8710910000	3.3372700000
C59	-2.4972190000	3.1377260000	4.9529710000
C60	-3.9169310000	-0.5032810000	1.6031690000
C61	-3.3823430000	4.6134610000	0.8925450000
C14	-6.0807250000	3.6493330000	2.7978220000
C63	-3.7738210000	-1.0062830000	2.9396670000
H64	-3.5503880000	-0.6455280000	5.0587880000
H65	-4.3431610000	2.1976420000	5.5422060000
H66	-2.9027960000	1.3224740000	6.0871210000
C67	-3.1228840000	5.4265310000	2.0469360000
H68	-2.5687050000	5.5747960000	4.1313230000
H69	-1.4332960000	2.8764870000	4.8881620000

H70	-2.6095800000	3.9142600000	5.7179760000
C71	-4.2031910000	-1.4525720000	0.5884530000
C72	-3.6381270000	5.2944800000	-0.3263840000
C75	-3.9186960000	-2.3890430000	3.1872330000
C76	-3.1251700000	6.8345680000	1.9292310000
C77	-4.3425700000	-2.7976880000	0.8682060000
H78	-4.3204230000	-1.0805030000	-0.4280480000
C79	-3.6431500000	6.6732560000	-0.4017520000
H80	-3.8419470000	4.6881970000	-1.2071530000
C83	-4.1977970000	-3.2858730000	2.1777530000
H84	-3.8119950000	-2.7376690000	4.2153380000
C85	-3.3840030000	7.4648760000	0.7305660000
H86	-2.9199210000	7.4241620000	2.8240380000
H87	-4.5712790000	-3.4875490000	0.0563500000
H88	-3.8523520000	7.1514640000	-1.3585510000
H95	-4.3106700000	-4.3460230000	2.3921050000
H96	-3.3871220000	8.5506260000	0.6622850000
H39	-1.4085640000	1.8454840000	1.2734060000
H40	-7.1621420000	3.5010570000	2.8538100000
H41	-5.7262080000	4.0390590000	3.7515660000
H42	-5.8498280000	4.3639300000	2.0029790000
H43	-5.7215690000	2.0206310000	1.7357730000

Co(salen)OH_2^+

atom	x	y	z
O49	-1.4960270000	1.8329700000	2.2378010000
Co50	-3.3417760000	2.1860970000	2.4489150000
N51	-3.3944810000	1.1165880000	4.0323210000
N52	-2.9219890000	3.6187730000	3.6413090000
O53	-3.8312340000	0.7511780000	1.2600080000
O54	-3.4161240000	3.3123620000	0.8874130000
O7	-5.4270610000	2.3924760000	2.5843990000
C56	-3.5540070000	-0.1603780000	4.0731630000
C57	-3.3213300000	1.9067820000	5.2600280000
C58	-2.8530840000	4.8710910000	3.3372700000
C59	-2.4972190000	3.1377260000	4.9529710000
C60	-3.9169310000	-0.5032810000	1.6031690000
C61	-3.3823430000	4.6134610000	0.8925450000
C14	-6.0807250000	3.6493330000	2.7978220000
C63	-3.7738210000	-1.0062830000	2.9396670000
H64	-3.5503880000	-0.6455280000	5.0587880000
H65	-4.3431610000	2.1976420000	5.5422060000
H66	-2.9027960000	1.3224740000	6.0871210000
C67	-3.1228840000	5.4265310000	2.0469360000
H68	-2.5687050000	5.5747960000	4.1313230000

H69	-1.4332960000	2.8764870000	4.8881620000
H70	-2.6095800000	3.9142600000	5.7179760000
C71	-4.2031910000	-1.4525720000	0.5884530000
C72	-3.6381270000	5.2944800000	-0.3263840000
C75	-3.9186960000	-2.3890430000	3.1872330000
C76	-3.1251700000	6.8345680000	1.9292310000
C77	-4.3425700000	-2.7976880000	0.8682060000
H78	-4.3204230000	-1.0805030000	-0.4280480000
C79	-3.6431500000	6.6732560000	-0.4017520000
H80	-3.8419470000	4.6881970000	-1.2071530000
C83	-4.1977970000	-3.2858730000	2.1777530000
H84	-3.8119950000	-2.7376690000	4.2153380000
C85	-3.3840030000	7.4648760000	0.7305660000
H86	-2.9199210000	7.4241620000	2.8240380000
H87	-4.5712790000	-3.4875490000	0.0563500000
H88	-3.8523520000	7.1514640000	-1.3585510000
H95	-4.3106700000	-4.3460230000	2.3921050000
H96	-3.3871220000	8.5506260000	0.6622850000
H39	-1.4085640000	1.8454840000	1.2734060000
H40	-7.1621420000	3.5010570000	2.8538100000
H41	-5.7262080000	4.0390590000	3.7515660000
H42	-5.8498280000	4.3639300000	2.0029790000
H43	-5.7215690000	2.0206310000	1.7357730000
H44	-1.1940973670	0.8471161904	2.621116487

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