Supporting Information:

Electronically Asynchronous Transition States for C–N Bond Formation by Electrophilic [Co^{III}(TAML)]-Nitrene Radical Complexes Involving Substrate-to-Ligand Single-Electron Transfer and a Cobalt-Centered Spin Shuttle

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General Considerations

Chemicals and solvents

All reagents were of commercial grade and used without further purification, unless noted otherwise. All reactions and measurements (except NMR studies) were performed under an inert atmosphere in a N_2-filled glovebox or by using standard Schlenk techniques (under Ar), unless noted otherwise. CH_2Cl_2 was distilled from CaH_2, toluene was distilled from sodium, THF and benzene were distilled from sodium benzophenone ketyl and CH_3CN was dried over molecular sieves prior to use. All solvents were deaerated by three freeze-pump-thaw cycles and backfilled with argon or sparged with argon prior to use. Styrene (derivatives) were filtered over basic alumina prior to use.

Li[Co^{III}(TAML^{red})] and **PPh$_4$[Co^{III}(TAML^{red})]**[1] and **[Co^{III}(TAML^{sq})]**[2] were prepared according to literature procedures.

NMR spectroscopy

^{1}H NMR spectra were recorded on a Bruker DRX 500, Bruker AMX 400, Bruker DRX 300 or Varian Mercury 300 spectrometer at r.t. and the reported ppm values are relative to $SiMe_4$ by referencing the residual solvent peak to $SiMe_4$.[3]

Mass spectrometry

ESI (electrospray ionization) mass spectra were collected on an AccuTOF LC, JMS-T100LP Mass spectrometer (JEOL, Japan) and typical measurement conditions are as follows: Positive-ion mode; Needle voltage 2500V, Orifice 1 voltage 120V, Orifice 2 voltage 9V, Ring Lens voltage 22V. Orifice 1 80 ^oC, desolvating Chamber 250 ^oC. Flow injection with a flow rate of 0.01 ml/min. All mass spectra were recorded with an average duration of 0.5 min.

FD (field desorption) Mass spectra were collected on an AccuTOF GC v 4g, JMS-T100GCV Mass spectrometer (JEOL, Japan). FD/FI probe (FD/FI) equipped with FD Emitter, Carbotec or Linden (Germany), FD 13 µm. Current rate 51.2 mA/min over 1.2 min. FI Emitter, Carbotec or Linden (Germany), FI 10 µm. Flashing current 40 mA on every spectra of 30 ms. Typical measurement conditions are: Counter electrode −10kV, Ion source 37V. LiFDi probe (FD/FI) equipped with FD Emitter, Linden CMS GmbH (Germany), FD 13 µm. Current rate 51.2 mA/min over 1.2 min. Typical measurement conditions are: Counter electrode −10kV, Ion source 37V.

EPR spectroscopy

EPR spectra were recorded on a Bruker EMX X-band spectrometer. The spectra were analyzed and simulated using the W95EPR program of Prof. F. Neese (MPI Muelheim).

EXAFS

Co K-edge XAS experiments were performed at Diamond Light Source on beamline B18 in Didcott, UK (proposal number SP22432). All measurements were done in fluorescence mode in toluene solutions. Solutions containing the complexes were kept frozen using a cryojet set to a temperature of 100K.[4] Measurements were performed with a Si(111) double monochromator in combination with a 36 element Ge detector. A typical measurement required 4 minutes. Around 25 scans were required to obtain good signal-to-noise ratio in the data. All acquired spectra were calibrated to a Co foil. EXAFS data analysis was done using the Artemis software package.[5]

UV-Vis spectroscopy

UV-Vis spectra were recorded on a Hewlett Packard 8453 or a double beam Shimadzu UV-2600 spectrometer in a 1.0 cm Teflon screw-cap quartz cuvette under Argon using the solvent as a background.

DFT calculations

DFT geometry optimizations were performed on full atomic models (no simplifications) using TURBOMOLE 7.3[6] coupled to the PQS Baker optimizer[7] via the BOpt package.[8] The calculations were performed at the BP86[9]/def2-TZVP[10] level of theory on an m4 grid, using Grimme's version 3 (disp3, "zero damping") dispersion corrections.[11] All minima (no imaginary frequencies) were characterized by numerically calculating the Hessian matrix. Transition states (saddle points) were characterized by one imaginary frequency along the reaction coordinate in the numerically calculated Hessian.

NH_3 was used as a model for the unidentified sixth axial ligand Y in **[Co^{III}(TAML^{q})(NNs)(Y)]**.

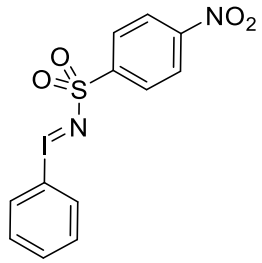
Grimme's version 3 zero-damping dispersion corrections were used to include dispersion influenced metal-ligand and ligand-substrate interactions. However, the calculated complex-substrate association/dissociation energies to/from the non-solvated **[Co^{III}(TAML^{red})]$^{-}$**, **[Co^{III}(TAML^{sq})(NNs)]$^{-}$**, **[Co^{III}(TAML^{q})(NNs)]$^{-}$**, **[Co^{III}(TAML^{sq})]**, **[Co^{III}(TAML^{sq})(NH$_3$)]**, **[Co^{III}(TAML^{q})(NNs)]** and **[Co^{III}(TAML^{q})(NNs)(NH$_3$)]** complexes are overestimated, leading to unrealistically low activation energies (< 4 kcal mol^{-1}). To compensate for this effect, we included dispersion interactions between the catalysts, nitrene intermediates and a solvent molecule (CH_2Cl_2) in solution by calculating the van der Waals adducts with CH_2Cl_2 (**A**, **[Co^{III}(TAML^{red})]$^{-}$ (CH$_2$Cl$_2$)**; **C**, **[Co^{III}(TAML^{sq})(NNs)]$^{-}$ (CH$_2$Cl$_2$)**; **D**, **[Co^{III}(TAML^{q})(NNs)]$^{-}$ (CH$_2$Cl$_2$)**; **H**, **[Co^{III}(TAML^{sq})]**; **H^{NH_3}**, **[Co^{III}(TAML^{sq})(NH$_3$)] (CH$_2$Cl$_2$)**; **J**, **[Co^{III}(TAML^{q})(NNs)] (CH$_2$Cl$_2$)**; **J^{NH_3}**, **[Co^{III}(TAML^{q})(NNs)(NH$_3$)] (CH$_2$Cl$_2$)**), and used these adducts as the energetic reference point in our calculations. However, this results in an erroneous cancelation of all translational entropy contributions to the calculated free energies because the translational entropy contributions to substrate/product association/dissociation are fully counterbalanced by the translational entropy contributions resulting from dissociation/association of the CH_2Cl_2 solvent molecule. This is not accurate for solution phase reactions, wherein the translational entropy contributions associated with substrate/product association/dissociation steps cannot be neglected. As the complexes in solution are completely surrounded by solvent molecules, these solvent association/dissociation steps lead to only small contributions to the translational entropy. These steps are of little influence on the substrate/product association/dissociation steps and therefore the latter are not cancelled by the former in solution. Therefore, we applied a +7.9 kcal mol^{-1} correction term (corresponding to the translational entropy contribution) to the calculated free energies of all substrate/product association/dissociation steps. This approach has been used previously by our group to satisfactorily describe carbene transfer reactions on cobalt-porphyrin systems.[12]

Energy output form calculations was reported in Hartree and converted to kcal mol^{-1} by multiplication with 627.503. Graphical representations of structures is done using IboView[13] and visualization of spin densities using IQMol.[14]

NEVPT2-CASSCF calculations

NEVPT2 corrected CASSCF calculations were performed with the ORCA 4.1[15] software package on geometries optimized in TURBOMOLE at the doublet (neutral complexes) or triplet (anionic complexes) spin surface, as these were in line with experimentally found spin states. The def2-TZVP[10] basis set was used together with the RIJCOSX[16] approximation in conjunction with the def2-TZVP/C fitting basis set to reduce computational cost. In all cases, the single root spin states (doublet, quartet *or* singlet, triplet, quintet for neutral or anionic complexes, respectively) were calculated. For refined energy values, NEVPT2[17] calculations using the RI approximation were carried out on converged CASSCF wavefunctions. Energy output of the calculation was reported in Hartree and is converted to kcal mol^{-1} by multiplication with 627.503. Visualization of orbitals is done using IboView.[13]

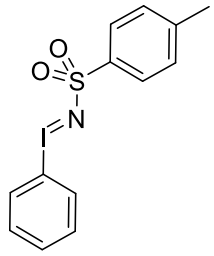
Synthesis and characterization of complexes, reagents and substrates



PhINNs

PhINNs was prepared according to a literature procedure and the spectroscopic data of the product matched those previously reported.[18] $PhI(OAc)_2$ (3.00 g; 9.3 mmol; 1.2 eq) was added portionwise to a stirred solution of KOH (1.09 g; 19.38 mmol; 2.5 eq) and $NsNH_2$ (1.57 g; 7.75 mmol; 1.0 eq) in MeOH (35 mL) at 0 °C under an N_2 atmosphere. The yellow suspension was stirred for 30 min at 0 °C and for 3 h at r.t., after which stirring was stopped and the reaction mixture was left to stand overnight in the dark. The yellow precipitate was collected by filtration, washed with ice-cold MeOH (3×5 mL) and dried *in vacuo* at 60 °C. The product was obtained as a yellow solid in 90.6% isolated yield (2.84 g; 7.03 mmol).

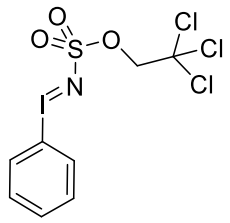
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.03 (d, ^3J = 8.8 Hz, 2H), 7.85 – 7.63 (m, 4H), 7.40 (t, ^3J = 7.4 Hz, 1H), 7.25 (t, J = 7.7 Hz, 2H).



PhINTs

PhINTs was prepared according to a literature procedure and the spectroscopic data of the product matched those previously reported.[19] $PhI(OAc)_2$ (3.22 g; 10.0 mmol; 1.0 eq) was added to a stirred solution of KOH (1.40 g; 25.0 mmol; 2.5 eq) and $TsNH_2$ (1.88 g; 11 mmol; 1.1 eq) in MeOH (40 mL) at 0 °C in absence of light. The solution was stirred for 2 h at 0-10 °C, 1 h at r.t. and poured into H_2O (230 mL). The solution was left to stand overnight, filtered and the precipitate was washed with ice-cold MeOH (12 mL), DCM (500 mL) and hexanes (200 mL). The product was obtained as a white solid 31.3% isolated yield (1.17 g; 3.13 mmol).

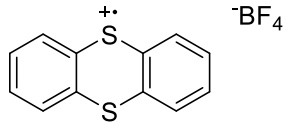
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.69 (d, J = 7.8 Hz, 2H), 7.43 (d, J = 7.6 Hz, 3H), 7.29 (t, J = 7.7 Hz, 2H), 7.06 (d, J = 7.8 Hz, 2H), 2.27 (s, 3H).



PhINTces

PhINTces was prepared according to a literature procedure and the spectroscopic data of the product matched those previously reported.[20] $TcesNH_2$ (685.4 mg; 3.0 mmol; 1.0 eq) and KOH (420.8 mg; 7.5 mmol; 2.5 eq) were dissolved in MeOH (11 mL) and cooled to -5 °C. $PhI(OAc)_2$ (966.3 mg; 3.0 mmol; 1.0 eq) was added portionwise and the yellow suspension was stirred under exclusion of light for 30 min at -5 °C and then 2.5 h at r.t., after which ice-cold H_2O (20 mL) was added. The suspension was stirred at 0 °C until a fine white solid had formed, which was collected by filtration, washed with H_2O (25 mL), ice-cold MeOH (4 mL) and EtOAc (20 mL) and then dried *in vacuo*. PhINTces was obtained as a white powder 18.9% isolated yield (244.4 mg; 0.57 mmol).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.10 (d, J = 7.8 Hz, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.52 (t, J = 7.7 Hz, 2H), 4.21 (s, 2H).



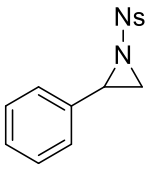
(Thi)BF_4

Thianthrenium tetrafluoroborate ((Thi)BF_4) was synthesised according to a literature procedure.[21] Under strict water-free conditions and under constant argon flow in a three necked roundbottom flask, thianthrene (510 mg, 2.36 mmol, 1.0 eq.) and (NO)BF_4 (290 mg, 2.48 mmol, 1.05 eq.) were dissolved in MeCN (40 mL) and stirred for 1 h. to afford a blue solution. The flask was closed and stirred under argon for 1h., after which Et_2O (6x20 mL portions) was added under an argon flow to yield a purple suspension, which was filtered under aerobic conditions. The purple solid was dried *in vacuo* and stored under nitrogen. Isolated yield: 77.5% (555 mg; 1.83 mmol).

X-Band EPR: g_{iso} = 2.009 (MeCN, microwave freq. 9.394585 GHz, mod. amp. 0.100 G, power 0.6325 mW).

Characterization of reaction products from catalysis reactions

Characterization of known products from the aziridination reactions was performed by ^{1}H NMR spectroscopy, and spectra are displayed in Figure S1-Figure S13. The general methods for aziridination are described on pages S14.



1

1 was prepared from styrene and PhINNs according to the general aziridination method described for **PPh$_4$[Co^{III}(TAML^{red})]** or **[Co^{III}(TAML^{sq})]** as the catalyst, and its spectral data are in accordance with literature.[22] A crude ^{1}H NMR spectrum for the formation of **1** is depicted in Figure S1. The resonance for trimethoxybenzene at δ = 6.08 and the characteristic signal for the aziridine between δ = 2.5 and 4.0 ppm were used to calculate the yield.

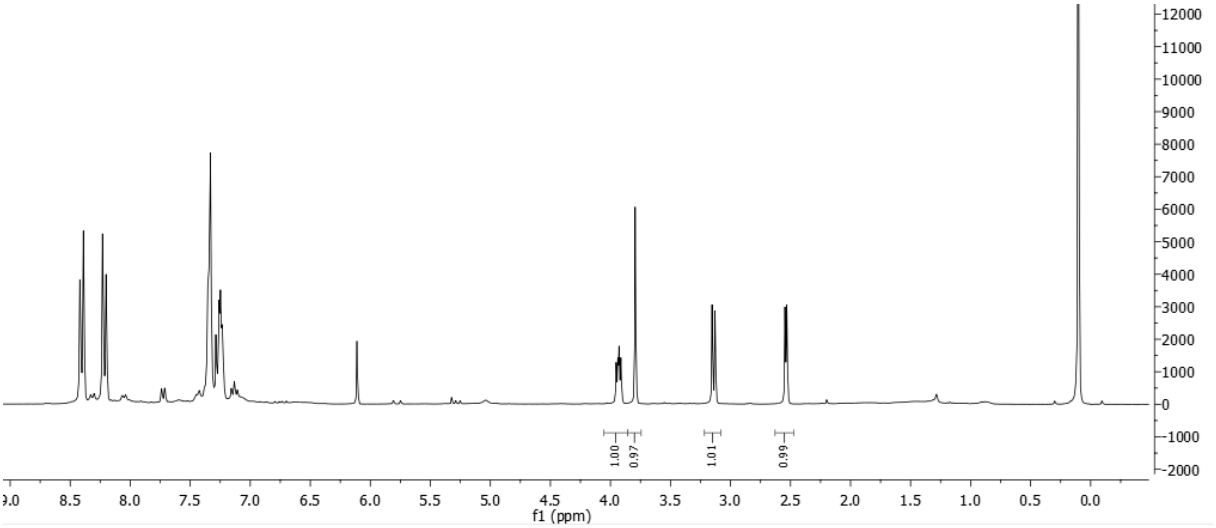
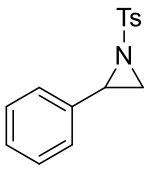


Figure S1. Crude ^{1}H NMR spectrum of **1** in $CDCl_3$ wherein **PPh$_4$[Co^{III}(TAML^{red})]** (2.5 mol%, argon) was used as the catalyst, with 6.6 µmol 1,3,5-trimethoxybenzene added as internal standard.



2

2 was prepared from styrene and PhINTs according to the general aziridination method described for **PPh$_4$[Co^{III}(TAML^{red})]** or **[Co^{III}(TAML^{sq})]** as the catalyst, and its spectral data are in accordance with literature.[23] A crude ^{1}H NMR spectrum for the formation of **2** is depicted in Figure S2. The resonance for trimethoxybenzene at δ = 6.08 and the characteristic signal for the aziridine at δ = 2.98 ppm were used to calculate the yield.

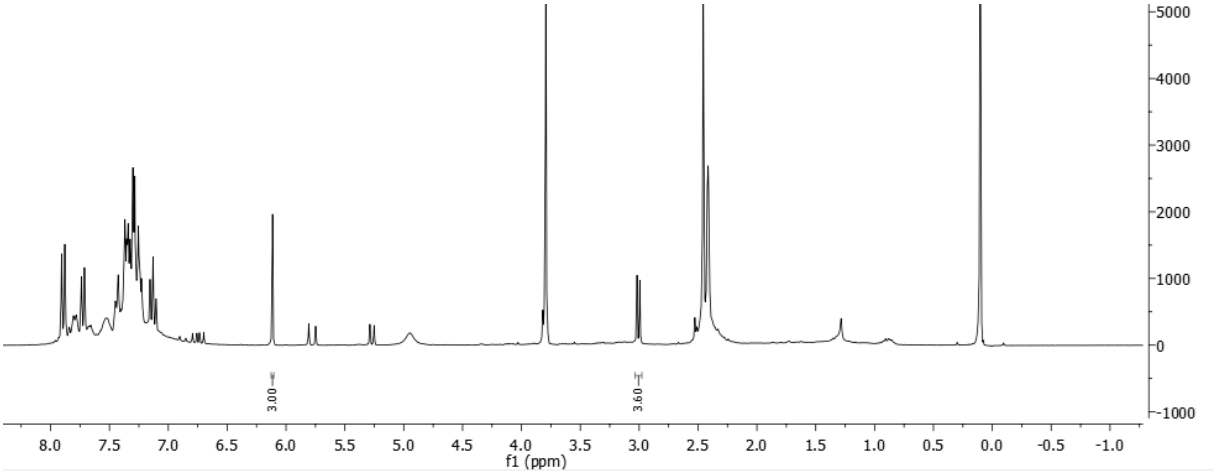
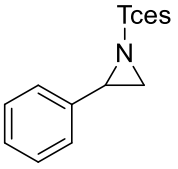


Figure S2. Crude ^{1}H NMR spectrum of **2** in $CDCl_3$ wherein **PPh$_4$[Co^{III}(TAML^{red})]** (5.0 mol%, argon) was used as the catalyst, with 8.6 µmol 1,3,5-trimethoxybenzene added as internal standard.



3

3 was prepared from styrene and PhINTces according to the general aziridination method described for **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$** as the catalyst, and its spectral data are in accordance with literature.[24] A crude ^{1}H NMR spectrum for the formation of **3** is depicted in Figure S3. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for the aziridine between δ = 2.6 and 4.0 ppm were used to calculate the yield.

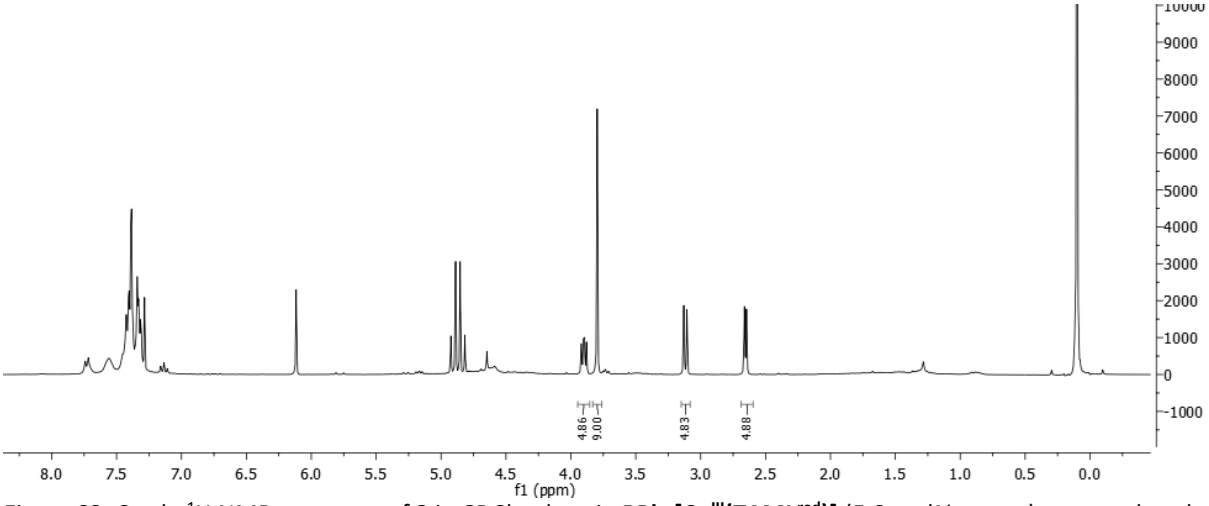
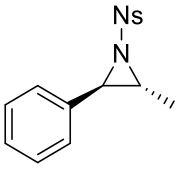


Figure S3. Crude ^{1}H NMR spectrum of **3** in $CDCl_3$ wherein **$PPh_4[Co^{III}(TAML^{red})]$** (5.0 mol%, argon) was used as the catalyst, with 8.2 µmol 1,3,5-trimethoxybenzene added as internal standard.



4

4 was prepared from *trans*-β-methylstyrene and PhINNs according to the general aziridination method described for **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$** as the catalyst, and its spectral data are in accordance with literature.[25] A crude ^{1}H NMR spectrum for the formation of **4** is depicted in Figure S4. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for the aziridine between δ = 1.5 and 4.0 ppm were used to calculate the yield and verify the selective formation of the *trans*-aziridine **4**.

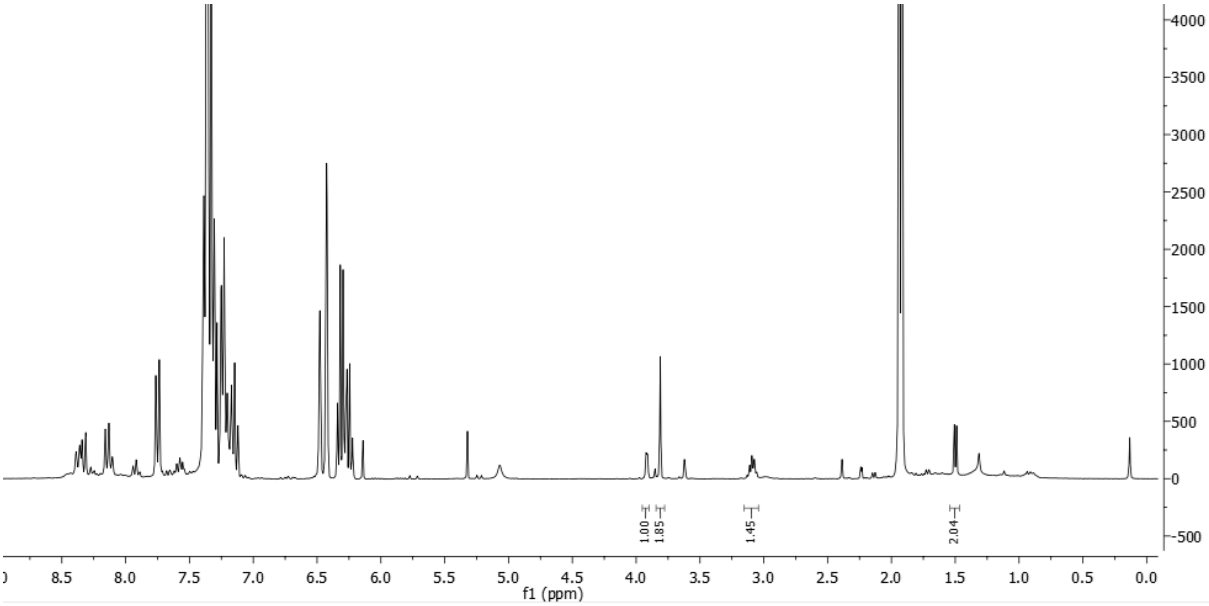
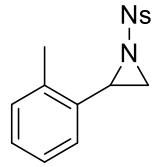


Figure S4. Crude ^{1}H NMR spectrum of **4** in $CDCl_3$ wherein **$[Co^{III}(TAML^{sq})]$** (5.0 mol%, argon) was used as the catalyst, with 8.0 µmol 1,3,5-trimethoxybenzene added as internal standard.



5

5 was prepared from 2-methylstyrene and PhINNs according to the general aziridination method described for **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$** as the catalyst, and its spectral data are in accordance with literature.[22] A crude ^1H NMR spectrum for the formation of **5** is depicted in Figure S5. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for the aziridine between δ = 1.9 and 4.2 ppm were used to calculate the yield.

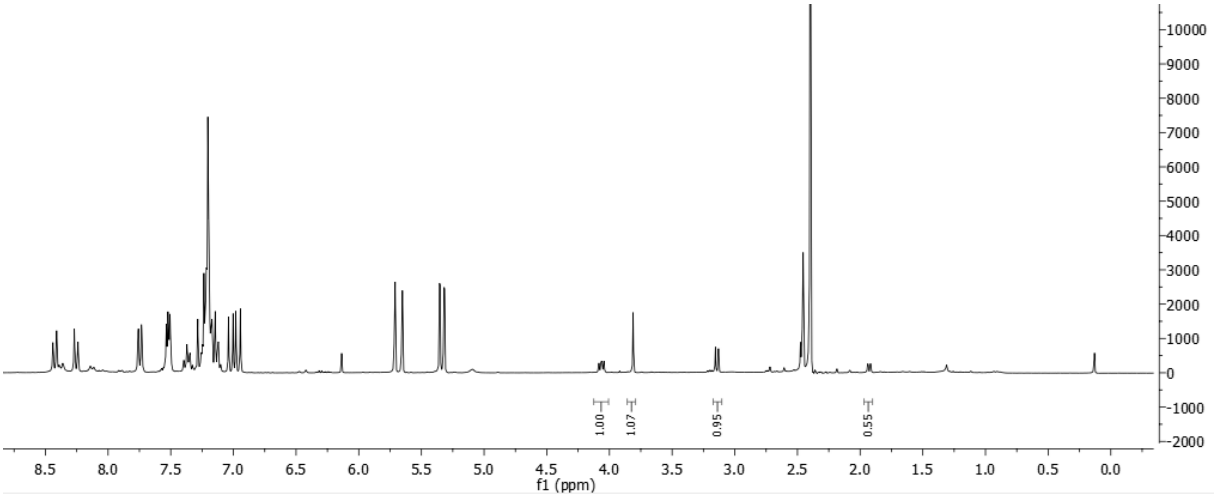
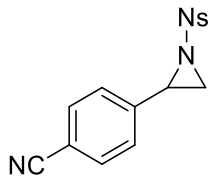


Figure S5. Crude ^1H NMR spectrum of **5** in $CDCl_3$ wherein **$[Co^{III}(TAML^{sq})]$** (5.0 mol%, argon) was used as the catalyst, with 8.0 µmol 1,3,5-trimethoxybenzene added as internal standard.



6

6 was prepared from 4-cyanostyrene and PhINNs according to the general aziridination method described for **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$** as the catalyst, and its spectral data are in accordance with literature.[22] A crude ^1H NMR spectrum for the formation of **6** is depicted in Figure S6. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for the aziridine between δ = 2.5 and 4.0 ppm were used to calculate the yield.

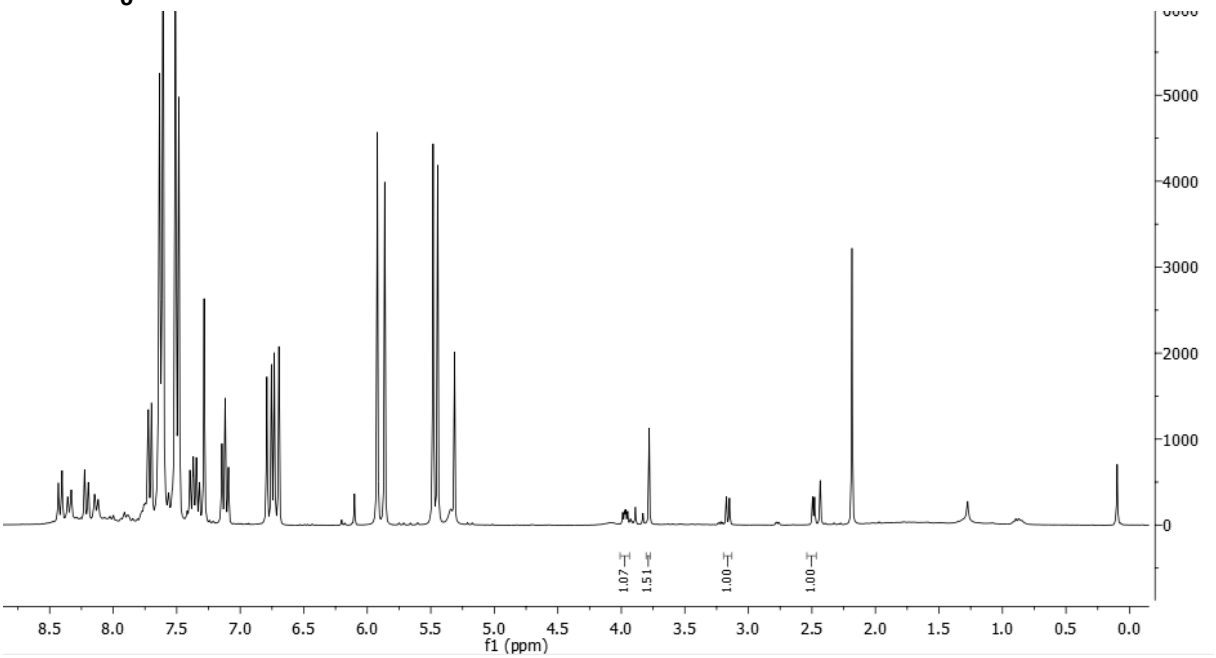
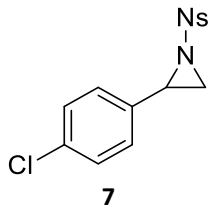


Figure S6. Crude ^1H NMR spectrum of **6** in $CDCl_3$ wherein **$PPh_4[Co^{III}(TAML^{red})]$** (5.0 mol%, argon) was used as the catalyst, with 8.0 µmol 1,3,5-trimethoxybenzene added as internal standard.



7

7 was prepared from 4-chlorostyrene and PhINNs according to the general aziridination method described for **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$** as the catalyst, and its spectral data are in accordance with literature.[22] A crude ^1H NMR spectrum for the formation of **7** is depicted in Figure S7. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for the aziridine between δ = 2.5 and 4.0 ppm were used to calculate the yield.

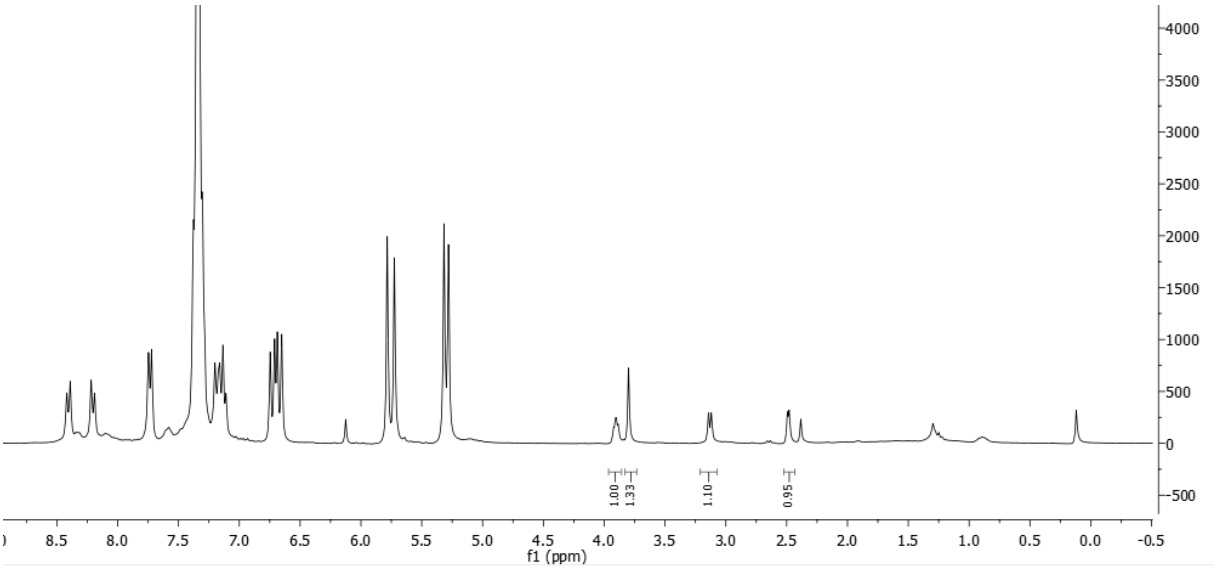
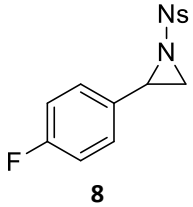


Figure S7. Crude ^1H NMR spectrum of **7** in $CDCl_3$ wherein **$PPh_4[Co^{III}(TAML^{red})]$** (5.0 mol%, argon) was used as the catalyst, with 8.0 µmol 1,3,5-trimethoxybenzene added as internal standard.



8

8 was prepared from 4-fluorostyrene and PhINNs according to the general aziridination method described for **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$** as the catalyst, and its spectral data are in accordance with literature.[22] A crude ^1H NMR spectrum for the formation of **8** is depicted in Figure S8. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for the aziridine between δ = 2.4 and 4.0 ppm were used to calculate the yield.

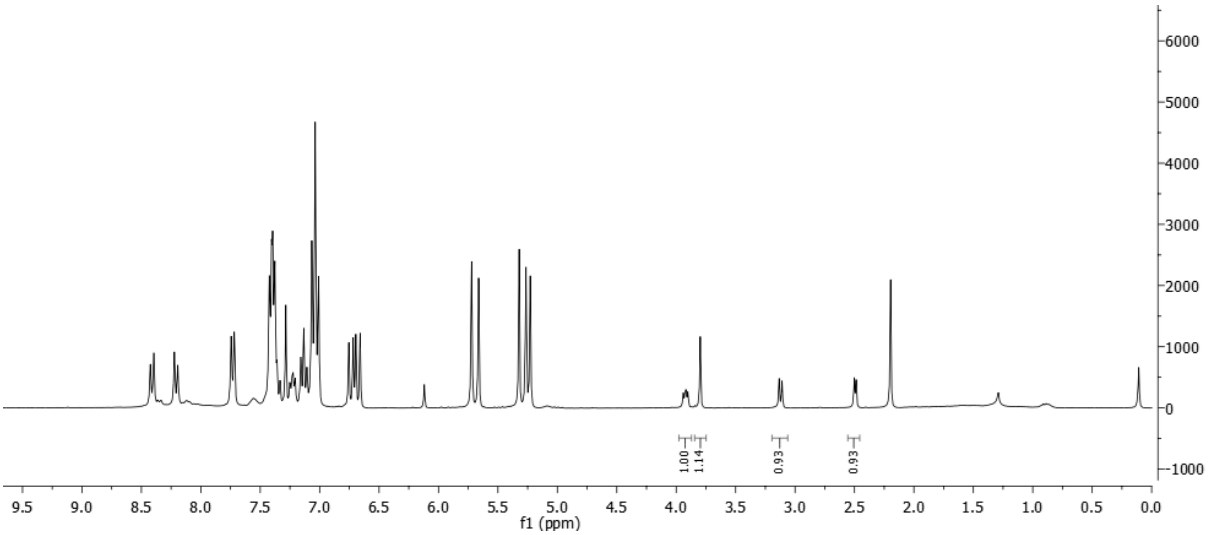
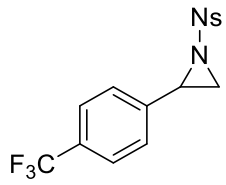


Figure S8. Crude ^1H NMR spectrum of **8** in $CDCl_3$ wherein **$PPh_4[Co^{III}(TAML^{red})]$** (5.0 mol%, argon) was used as the catalyst, with 8.0 µmol 1,3,5-trimethoxybenzene added as internal standard.



9

9 was prepared from 4-trifluoromethylstyrene and PhINNs according to the general aziridination method described for **PPh$_4$[Co^{III}(TAML^{red})]** or **[Co^{III}(TAML^{sq})]** as the catalyst, and its spectral data are in accordance with literature.[22] A crude ^{1}H NMR spectrum for the formation of **9** is depicted in Figure S9. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for the aziridine between δ = 2.5 and 4.0 ppm were used to calculate the yield.

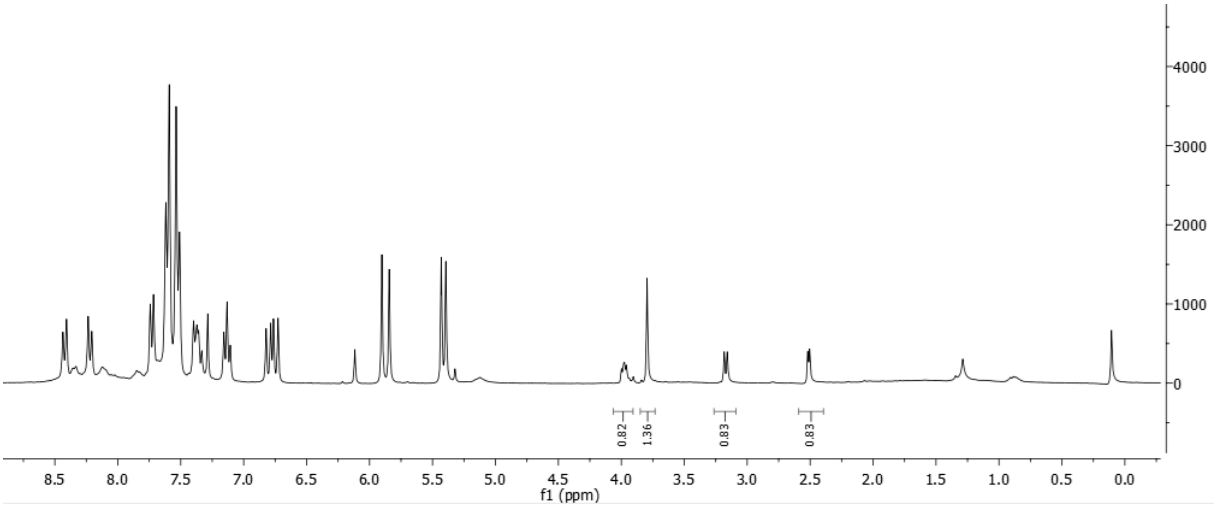
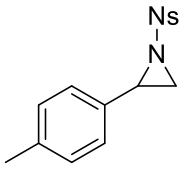


Figure S9. Crude ^{1}H NMR spectrum of **9** in $CDCl_3$ wherein **PPh$_4$[Co^{III}(TAML^{red})]** (5.0 mol%, argon) was used as the catalyst, with 8.0 µmol 1,3,5-trimethoxybenzene added as internal standard.



10

10 was prepared from 4-methylstyrene and PhINNs according to the general aziridination method described for **PPh$_4$[Co^{III}(TAML^{red})]** or **[Co^{III}(TAML^{sq})]** as the catalyst, and its spectral data are in accordance with literature.[22] A crude ^{1}H NMR spectrum for the formation of **10** is depicted in Figure S10. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for the aziridine between δ = 2.5 and 4.0 ppm were used to calculate the yield.

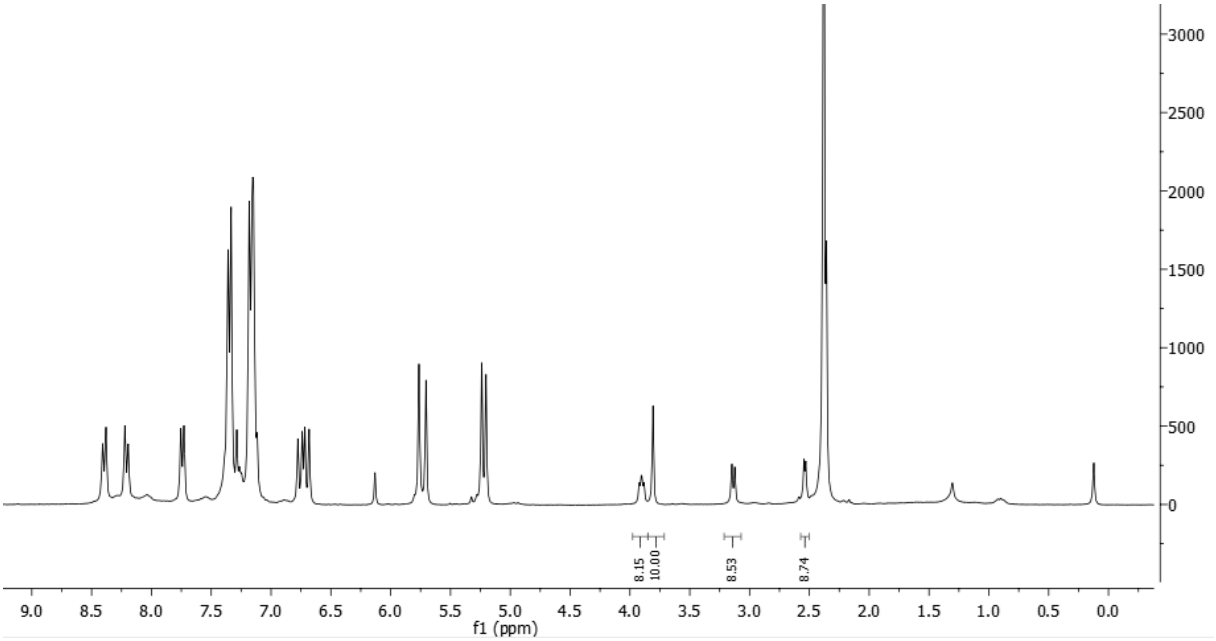
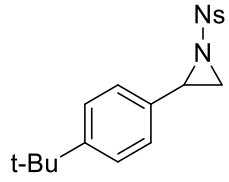


Figure S10. Crude ^{1}H NMR spectrum of **10** in $CDCl_3$ wherein **PPh$_4$[Co^{III}(TAML^{red})]** (5.0 mol%, argon) was used as the catalyst, with 8.0 µmol 1,3,5-trimethoxybenzene added as internal standard.



11

11 was prepared from 4-*tert*-butylstyrene and PhINNs according to the general aziridination method described for **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$** as the catalyst, and its spectral data are in accordance with literature.[22] A crude ^1H NMR spectrum for the formation of **11** is depicted in Figure S11. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for the aziridine between δ = 2.5 and 4.0 ppm were used to calculate the yield.

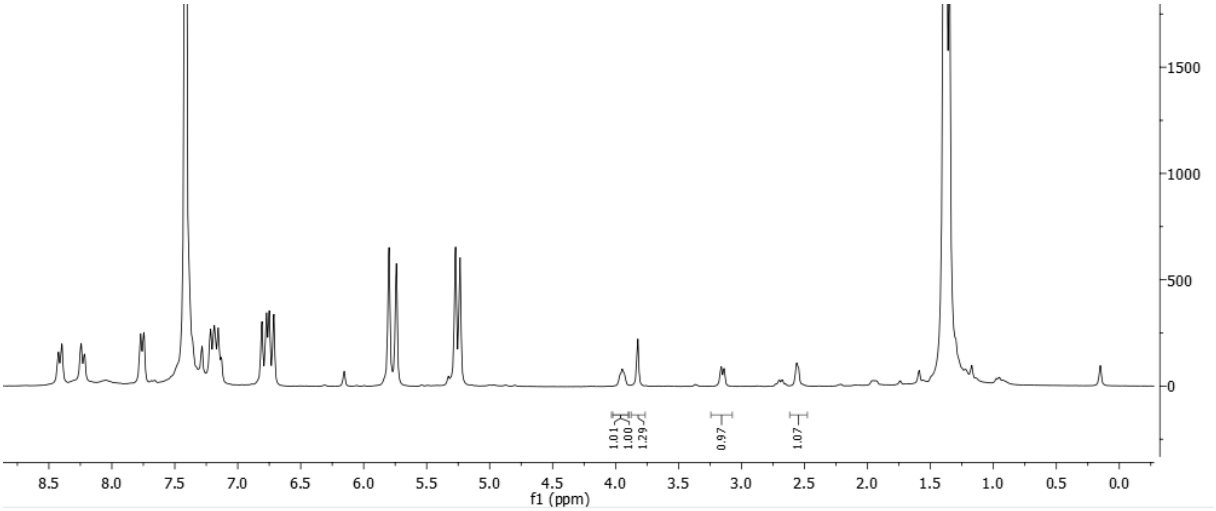
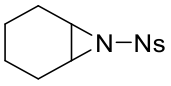
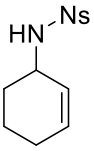


Figure S11. Crude ^1H NMR spectrum of **11** in $CDCl_3$ wherein **$PPh_4[Co^{III}(TAML^{red})]$** (5.0 mol%, argon) was used as the catalyst, with 8.0 µmol 1,3,5-trimethoxybenzene added as internal standard.



12a

12a was prepared from cyclohexene and PhINNs according to the general aziridination method described for **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$** as the catalyst, and its spectral data are in accordance with literature. **12a** was obtained as a mixture with **12b**.[26] A crude ^1H NMR spectrum for the formation of **12a** and **12b** is depicted in Figure S12. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signal for the aziridine at δ = 3.13 ppm were used to calculate the yield.



12b

12b was prepared from cyclohexene and PhINNs according to the general aziridination method described for **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$** as the catalyst, and its spectral data are in accordance with literature. **12b** was obtained as a mixture with **12a**.[26] A crude ^1H NMR spectrum for the formation of **12a** and **12b** is depicted in Figure S12. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for **12b** at δ = 4.69, 5.36 and 5.84 ppm were used to calculate the yield.

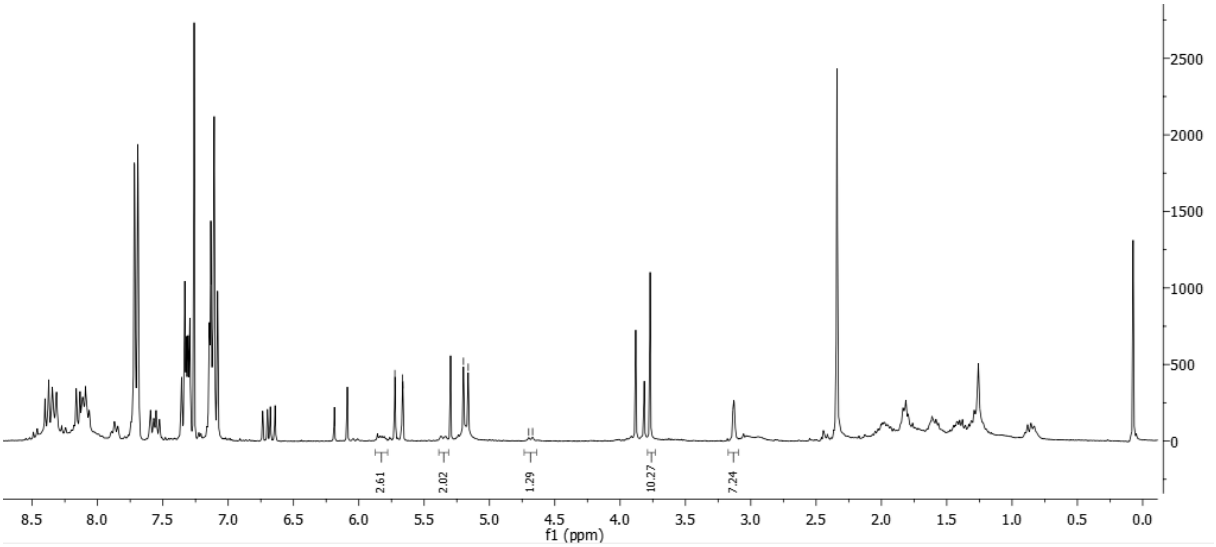
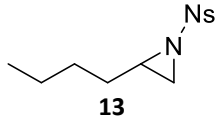


Figure S12. Crude ^{1}H NMR spectrum of **12a** and **12b** in $CDCl_3$ wherein **PPh_4[Co^{III}($TAML^{red}$)]** (5.0 mol%, argon) was used as the catalyst, with 8.0 µmol 1,3,5-trimethoxybenzene added as internal standard.



13

13 was prepared from 1-hexene and PhINNs according to the general aziridination method described for **PPh_4[Co^{III}($TAML^{red}$)]** or **[Co^{III}($TAML^{sq}$)]** as the catalyst, and its spectral data are in accordance with literature.[26] A crude ^{1}H NMR spectrum for the formation of **13** is depicted in Figure S13. The resonance for trimethoxybenzene at δ = 3.80 and the characteristic signals for the aziridine between δ = 2.0 and 34.0 ppm were used to calculate the yield.

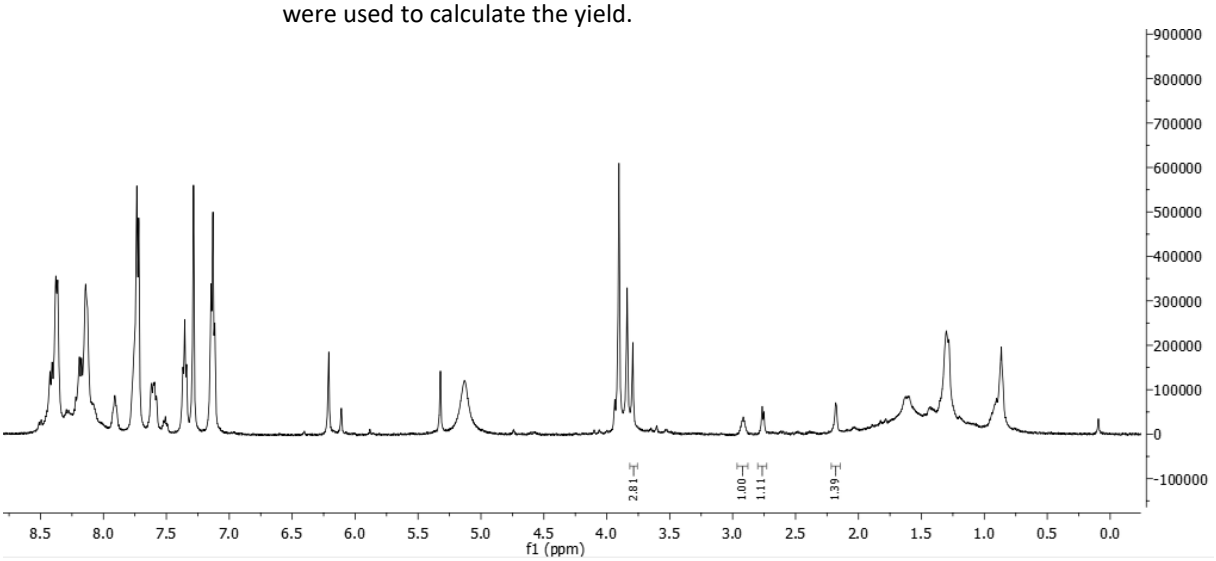


Figure S13. Crude ^{1}H NMR spectrum of **13** in $CDCl_3$ wherein **PPh_4[Co^{III}($TAML^{red}$)]** (2.5 mol%, aerobic) was used as the catalyst, with 8.0 µmol 1,3,5-trimethoxybenzene added as internal standard.

EXAFS Studies

All sample preparations were performed in a glovebox containing an Ar atmosphere with less than 1 ppm of O_2 and H_2O. The analyte solutions were filtered prior to use over a syringe filter (PTFE 0.45 μm) and transferred to a Kapton® tube. The solutions were taken out of the glovebox, rapidly frozen into liquid nitrogen and transferred to the beamline for measurement.

Co K-edge EXAFS measurements of **$PPh_4[Co^{III}(TAML^q)(NNs)_2]$** were hampered by the low solubility of the complex in toluene. The analysis of the XANES region is discussed in our previous publication on these complexes.[2]

$PPh_4[Co^{III}(TAML^{red})]$ (33.5 mg; 0.040 mmol) was dissolved in toluene (4.0 mL) in an argon filled glovebox. The experimental Co K-edge EXAFS data and our fitting model is shown in Table S1 and Figure S14. A fit was obtained by including a Co–N shell containing 4 atoms at a distance of 1.79(1) Å and a Co–C shell containing 8 atoms at a distance of 2.73(2) Å. A multiple scattering shell (arising from scattering within the ligand framework) was included to further improve the quality of the fit. The coordination numbers and bond distances are in close agreement with the crystal structure and are in agreement with a square-planar geometry of the complex.

Table S1. Fitting parameters for the experimental Co K-edge EXAFS spectrum of **$PPh_4[Co^{III}(TAML^{red})]$** and the Co–N bond lengths as derived from a single crystal XRD measurement.[2] The experimental and simulated spectrum is shown in Figure S4. CN = coordination number, DW = Debye Waller factor, R = distance, Abs-Sc = Absorber Scatterer, MS = multiple scattering path.

Abs-Sc	**CN**	**R(Å)**	**DW ($Å^{-2}$)**	**Co–N from XRD (Å)**
CoN	4	1.79(1)	0.0006(8)	1.8244(15)
CoC	8	2.73(2)	0.001(1)	1.8273(15)
CoNC (MS)	12	2.95(2)	0.001(1)	1.8337(15)
				1.8267(15)

E_0=-4(2) eV, Amp=0.95, R factor = 0.008, 2.7<k<12; 1.11<R<3.0; k^1, k^2, k^3 weighted fit.

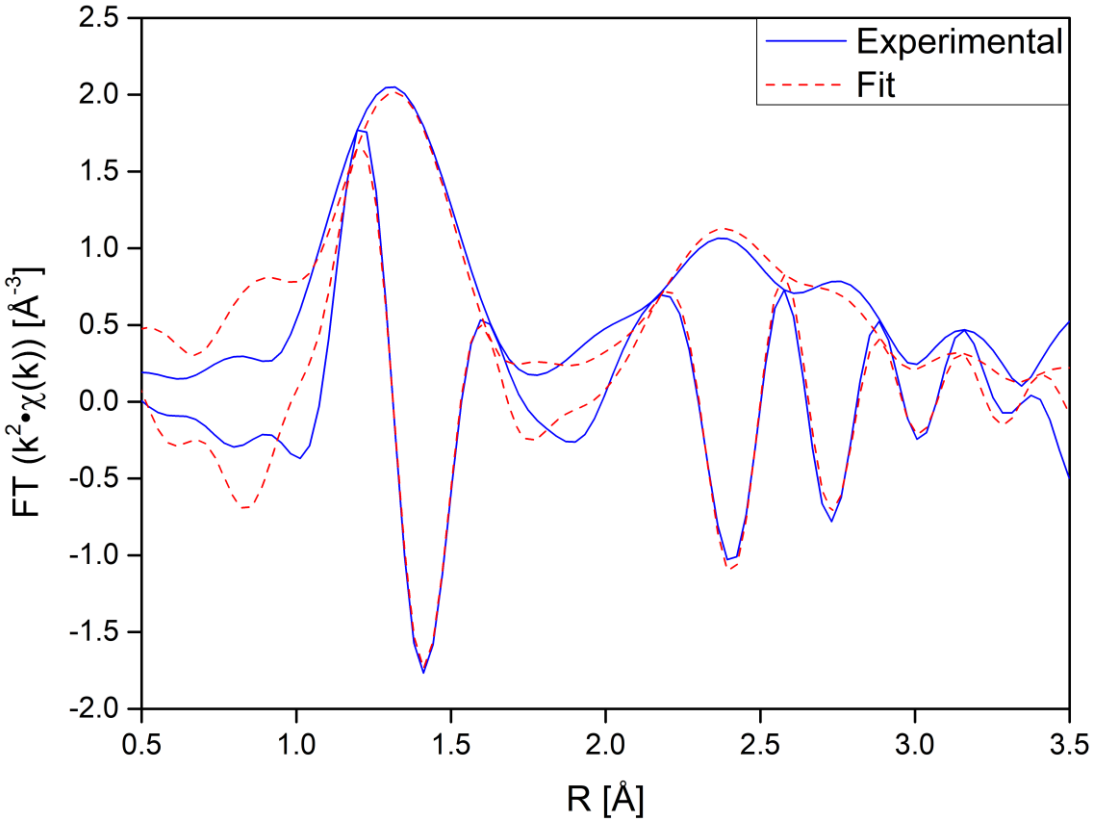


Figure S14. Experimental (solid blue) and fitted (dashed red) Co K-edge EXAFS spectrum of **PPh_4[Co^{III}($TAML^{red}$)]**.

[Co^{III}($TAML^{sq}$)] was prepared according to our previously reported method via oxidation of **Li[Co^{III}($TAML^{red}$)]** with (Thi)BF_4 in MeCN in an argon filled glovebox,[2] to afford a 10 mM concentration in toluene (4.0 mL). The experimental Co K-edge EXAFS data and our fitting model is shown in Table S2 and Figure S15. A fit was obtained by including a Co–N shell containing 4 atoms at a distance of 1.80(2) Å and a Co–C shell containing 8 atoms at a distance of 2.81(4) Å. A multiple scattering shell (arising from scattering within the ligand framework) was included to further improve the quality of the fit. The coordination numbers and bond distances are in close agreement with the DFT calculated structure[2] and are in agreement with a square-planar geometry of the complex.

Table S2. Fitting parameters for the experimental Co K-edge EXAFS spectrum of **[Co^{III}($TAML^{sq}$)]** and the DFT calculated Co–N bond lengths. The experimental and simulated spectrum is shown in Figure S15. CN = coordination number, DW = Debye Waller factor, R = distance, Abs-Sc = Absorber Scatterer, MS = multiple scattering path.

Abs-Sc	**CN**	**R(Å)**	**DW ($Å^{-2}$)**	**Co–N from DFT (Å)**
CoN	4	1.80(2)	0.002(2)	1.832
CoC	8	2.81(4)	0.003(3)	1.832
CoNC (MS)	12	2.97(5)	0.003(8)	1.819
				1.817
E_0=-1(2) eV, Amp=0.95, R factor = 0.05, 2.7<k<10.9; 1.15<R<3.15; k^1, k^2 weighted fit.				

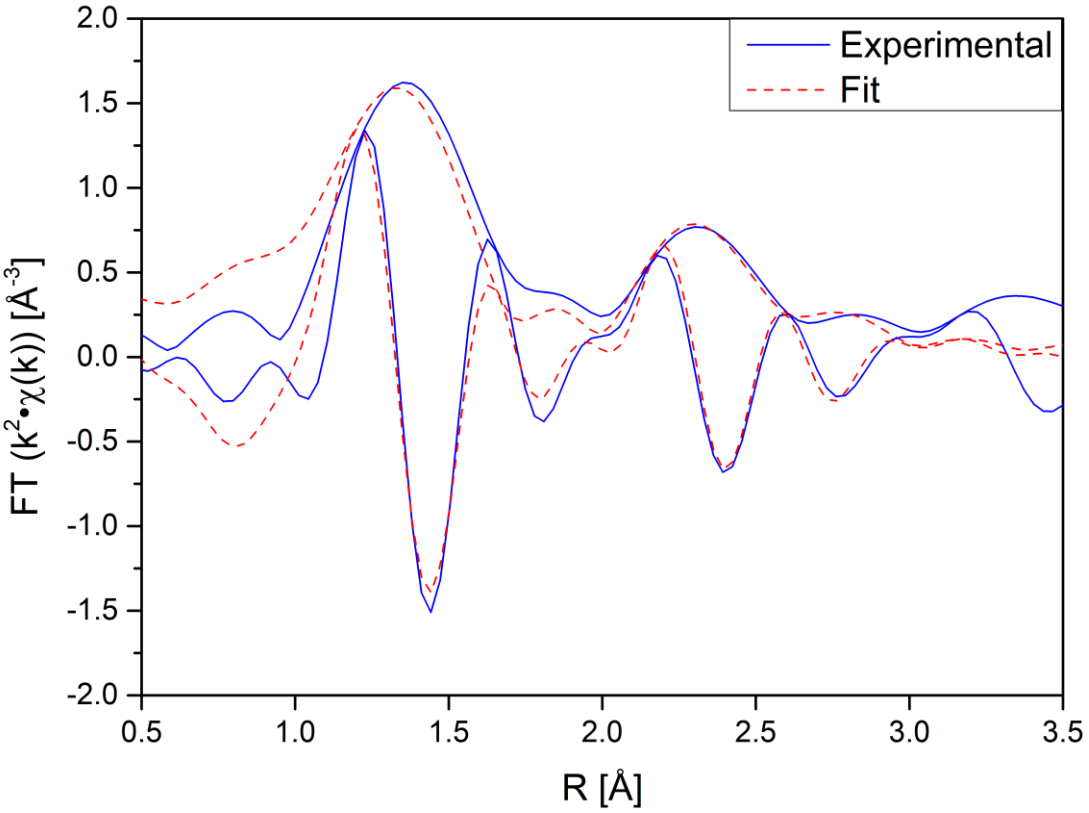


Figure S15. Experimental (solid blue) and fitted (dashed red) Co K-edge EXAFS spectrum of **[Co^{III}(TAML^{sq})]**.

[Co^{III}(TAML^{q})(NNs)(Y)]: Sample preparation was performed as described previously[2] in an argon filled glovebox to afford 4.0 mL of a toluene solution of **[Co^{III}(TAML^{q})(NNs)(Y)]** (5.0 mM). The experimental Co K-edge EXAFS data and our fitting model is shown in Table S3 and Figure S16. A fit was obtained by including a Co–N shell containing 6.1(4) atoms at a distance of 1.91(1) Å and a Co–C shell containing 8 atoms at a distance of 2.76(3) Å. A multiple scattering shell (arising from scattering within the ligand framework) was included to further improve the quality of the fit. The experimental data is in close agreement with a DFT-optimized structure of **[Co^{III}(TAML^{q})(NNs)(Y)]**. Consistent with XANES analysis as reported earlier[2], the coordination numbers indicate an octahedral coordination around cobalt in the solid state and clearly indicates the formation of a cobalt-nitrene bond, together with the coordination of a sixth unidentified ligand (as was described earlier).[2]

Table S3. Fitting parameters for the experimental Co K-edge EXAFS spectrum of **[Co^{III}(TAML^{q})(NNs)(Y)]** and the DFT calculated Co–N bond lengths for Y = vacant site and Y = NH_3. The experimental and simulated spectrum is shown in Figure S5. CN = coordination number, DW = Debye Waller factor, R = distance, Abs-Sc = Absorber Scatterer, MS = multiple scattering path.

Abs-Sc	**CN**	**R(Å)**	**DW (Å^{-2})**	**Co–N from DFT with Y = vacant site (Å)**	**Co–N from DFT with Y = NH_3 (Å)**
CoN	6.1(4)	1.91(1)	0.005(1)	1.860	1.892
CoC	8	2.76(3)	0.002(3)	1.859	1.885
CoNC (MS)	12	2.84(2)	0.011(3)	1.848	1.860
				1.867	1.856
				1.767	1.819
					2.21932
E_0=2(2) eV, Amp=0.95, R factor = 0.013, 2.7<k<10.6; 1.1<R<3; k^1, k^2 weighted fit					

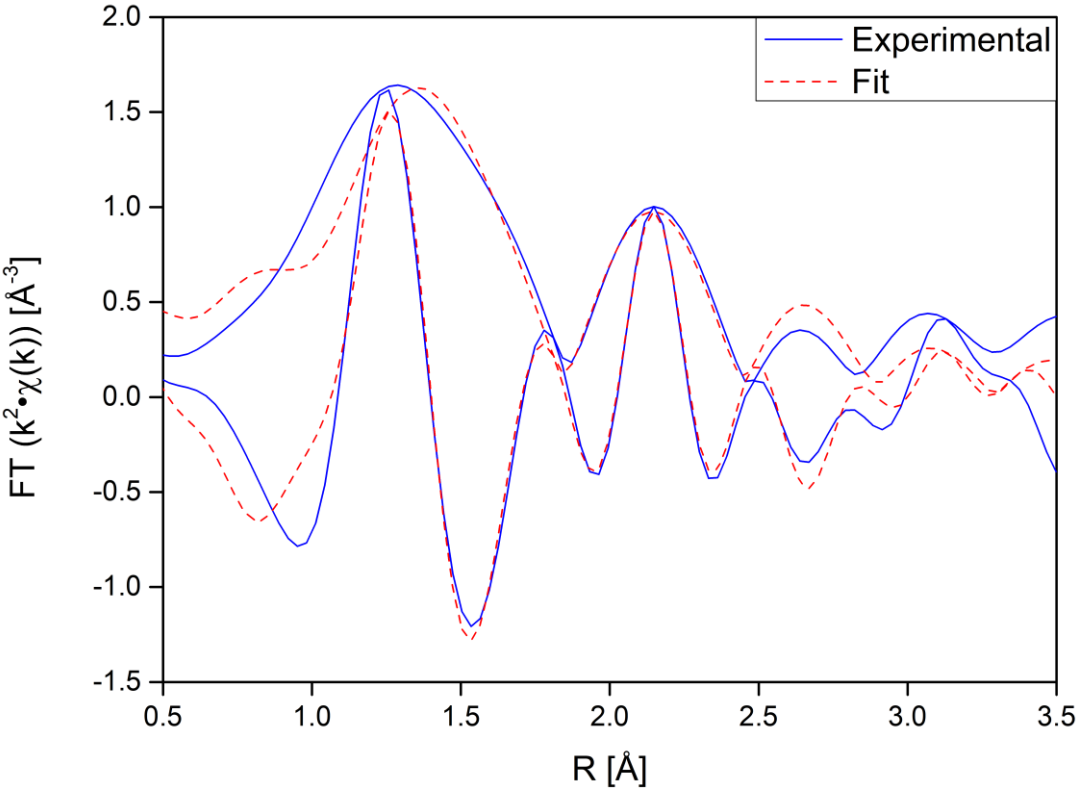


Figure S16. Experimental (solid blue) and fitted (dashed red) Co K-edge EXAFS spectrum of **[Co^{III}(TAML^{q})(NNs)]**.

UV-Vis titration for the formation of $PPh_4[Co^{III}(TAML^{q})(NTs)_2]$

A 75 µM solution of **$PPh_4[Co^{III}(TAML^{red})]$** in CH_2Cl_2 was prepared in a nitrogen filled glovebox and the UV-Vis spectrum was measured in a nitrogen filled 1.0 cm quartz cuvette that was closed with a Teflon screw-cap. 0.5, 1.0, 2.0 or 2.5 equivalent aliquots of the tosylnitrene precursor N-((2-methoxyphenyl)-λ^3-iodaneylidene)-4-methylbenzenesulfonamide (^{OMe}PhI=NTs) in CH_2Cl_2 (5.00 mM) were added, and the UV-Vis spectrum was measured after every addition. Upon addition of the nitrene precursor the band characteristic for **$PPh_4[Co^{III}(TAML^{red})]$** ($\lambda_{max}$ = 510 nm) decreases in intensity, whereas the absorbance above 700 nm and below 400 nm increases (Figure S17). Identical to the changes we observed in the characterization of **$PPh_4[Co^{III}(TAML^{q})(NNs)_2]$**.[2] Isosbestic points at 406 and 685 nm indicate clean conversion of **$PPh_4[Co^{III}(TAML^{red})]$** to **$PPh_4[Co^{III}(TAML^{q})(NTs)_2]$** as the sole reaction product, previously characterized by HRMS, XANES and magnetic moment (supported by NEVPT2-CASSCF calculations) as being the anionic bis-nitrene species. Reactivity studies (catalysis, single-turnover experiment) are also consistent with the formation of cobalt-nitrene bonds as the nitrene can be transferred to different substrates.

Consistent with our previous observations,[2] addition of a larger excess iminoiodinane and prolonged standing over time (especially in presence of a larger excess iminoiodinane) leads to degradation of the sample. This was observed after addition of 12.5 equivalents ^{OMe}PhI=NTs (Figure S18), which causes the loss of the isosbestic point at 685 nm, indicating follow-up reactivity.

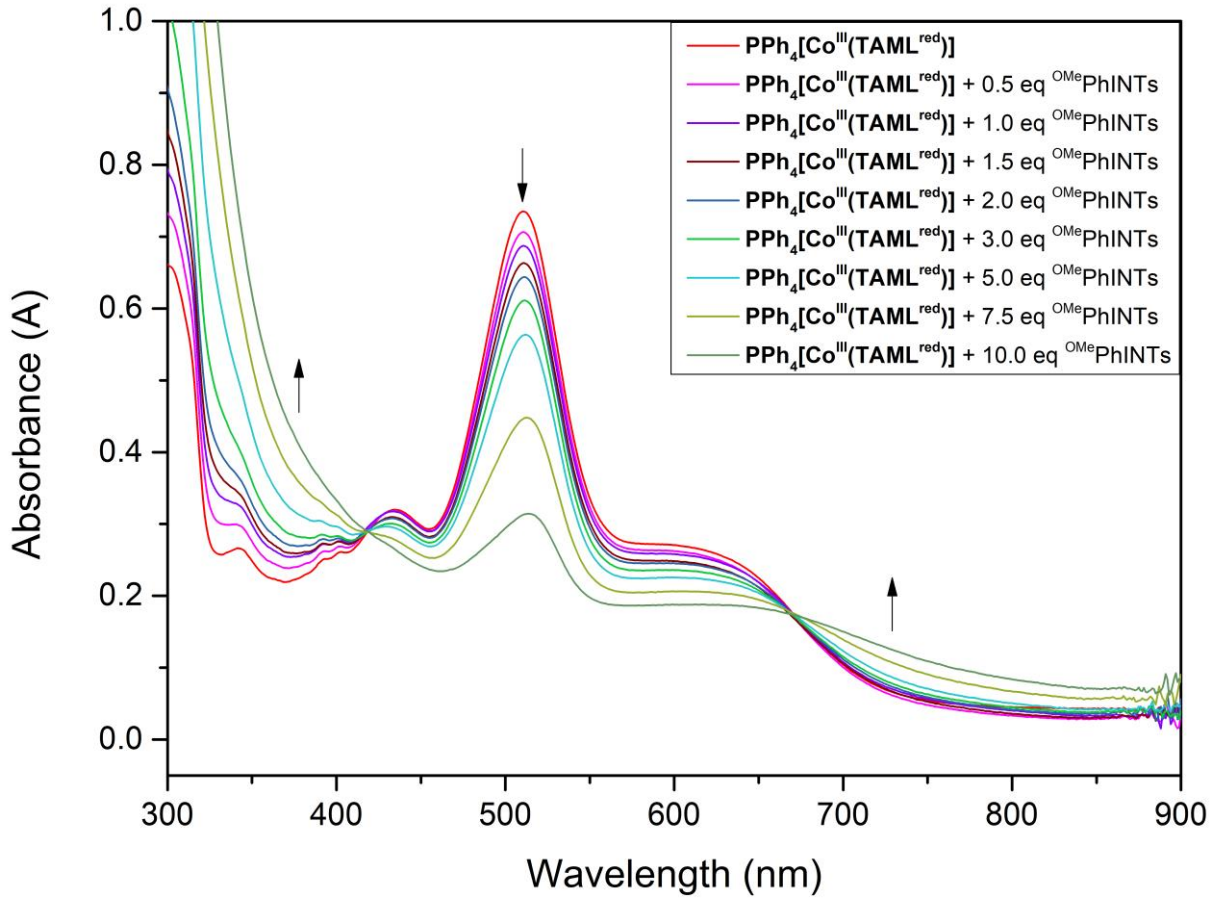


Figure S17. Additions of aliquots ^{OMe}PhINTs to **$PPh_4[Co^{III}(TAML^{red})]$** (75 µM in CH_2Cl_2).

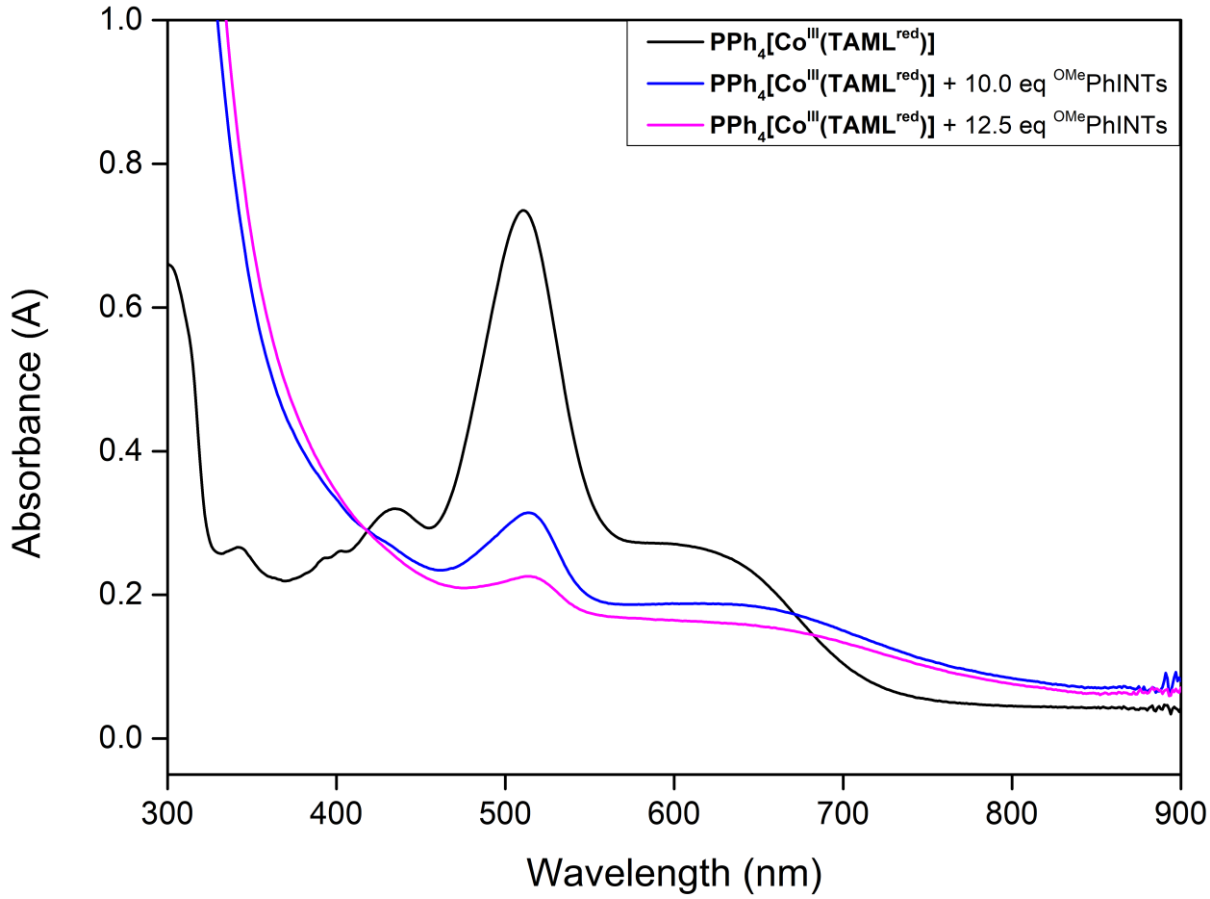


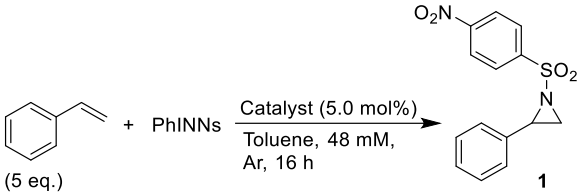
Figure S18. Additions of 10.0 and 12.5 equivalents ^{OMe}PhINTs to **PPh$_4$[Co^{III}(TAML^{red})]** (75 µM in CH_2Cl_2).

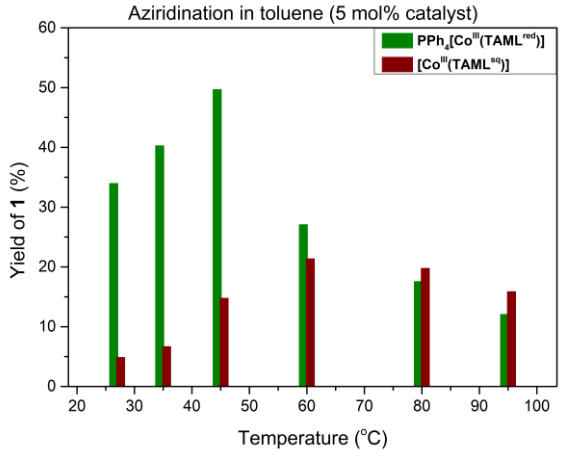
Catalytic aziridination reactions and mechanistic studies

Optimization studies

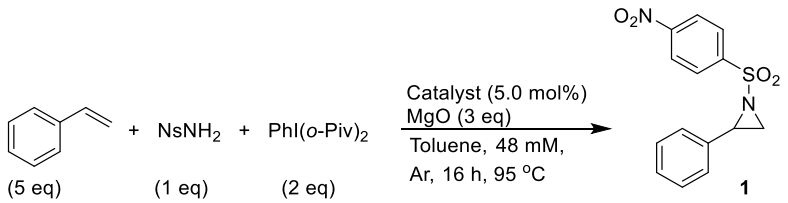
We started our investigations into the aziridination of styrenes with **$PPh_4[Co^{III}(TAML^{red})]$** and **$[Co^{III}(TAML^{sq})]$** by studying the formation of **1** from styrene (5 eq) and PhINNs (1 eq, 48 mM) with 5 mol% catalyst in toluene for 16 hours at various reaction temperatures (Scheme S1). The *in situ* formation of PhINNs from $NsNH_2$ (1 eq) and PhI(*o*-Piv)$_2$ (2 eq) in presence of MgO (3.0 eq) was also attempted in toluene at 95 °C for 16 hours, but only afforded 2% (for **$[Co^{III}(TAML^{sq})]$**) or 10% (**$PPh_4[Co^{III}(TAML^{red})]$**) of **1** (Scheme S2). These yields are significantly lower than when using pre-formed PhINNs, and we therefore focused on using PhINNs in further reactions.

Further optimization of the reaction conditions can be found in Table S4. The optimal conditions were set as in entries 7 and 12 for **$PPh_4[Co^{III}(TAML^{red})]$** and **$[Co^{III}(TAML^{sq})]$**. It should be noted that the conditions in entries 8 and 9 for **$PPh_4[Co^{III}(TAML^{red})]$** are synthetically also appealing due to the lower catalyst loading and the aerobic conditions; we therefore also performed the substrate screening under these conditions. **$[Co^{III}(TAML^{sq})]$** is not stable under atmospheric conditions, as it rapidly reacts with H_2O from the air.[1a] In addition, monitoring the yield of **1** under the optimal reactions conditions (Figure S19) demonstrated that the reaction already went to completion in 20 minutes for **$PPh_4[Co^{III}(TAML^{red})]$** and in 2 hours for **$[Co^{III}(TAML^{sq})]$**. Prolonged standing of the reaction mixtures under these conditions did not affect the yield of **1** for **$PPh_4[Co^{III}(TAML^{red})]$**, but led to a reduction (13%) in yield of **1** for **$[Co^{III}(TAML^{sq})]$**. This indicates that **$[Co^{III}(TAML^{sq})]$** is involved in a reaction with **1** to form unknown products.





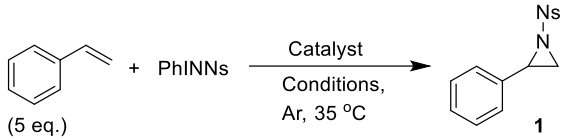
Scheme S1. Formation of **1** at various temperatures in toluene, catalyzed by **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$**. Reaction conditions: PhINNs (1.0 eq, 48 Mm), styrene (5.0 eq.) and catalyst (5.0 mol%) were reacted under an argon atmosphere for 16 h.



$PPh_4[Co^{III}(TAML^{red})]$: 10%
$[Co^{III}(TAML^{sq})]$: 2%

Scheme S2. Formation of **1** via *in situ* formation of PhINNs from $NsNH_2$ and PhI(*o*-Piv)$_2$.

Table S4. Optimization of the reaction conditions for the formation of **1**, catalyzed by **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$**.



Entry	Catalyst loading (mol%)	Solvent	Concentration (mM) – Time (h)	Yield
		$PPh_4[Co^{III}(TAML^{red})]$		
1	5.0	Toluene	48 – 16	40%
2	5.0	Benzene	48 – 16	41%
3	5.0	MeCN	48 – 16	18%
4	5.0	DCM	48 – 16	58%
5[a]	5.0	DCM	48 – 16	44%
6	5.0	DCM	24 – 16	77%
7	**5.0**	**DCM**	**24 – 2**	**76%**
8	2.5	DCM	24 – 2	64%
9[b]	2.5	DCM	24 – 2	67%
10[c]	-	DCM	24 – 2	0%
		$[Co^{III}(TAML^{sq})]$		
11	5.0	Toluene	48 – 16	7%
12	5.0	DCM	48 – 16	57%
13	**5.0**	**DCM**	**24 – 2**	**74%**
14	2.5	DCM	24 – 2	35%
15[b]	2.5	DCM	24 – 2	[d] -

[a] 1.0 eq. styrene was used. [b] aerobic conditions. [c] No catalyst added. [d] **$Co^{III}(TAML^{sq})$** is not stable under aerobic conditions

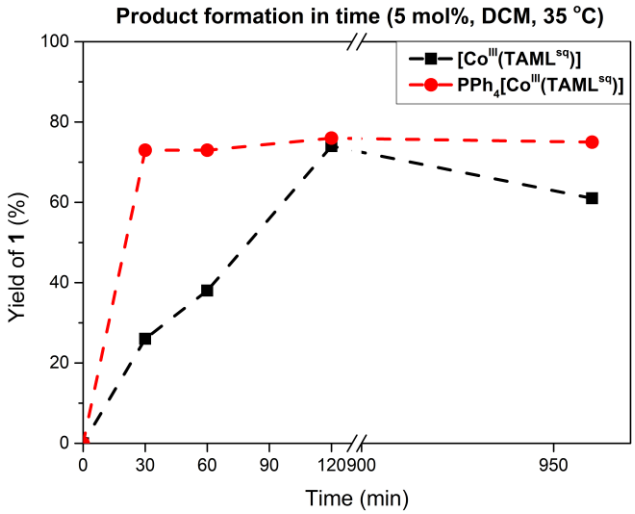


Figure S19. Formation of **1** at various times in DCM, catalyzed by **$PPh_4[Co^{III}(TAML^{red})]$** or **$[Co^{III}(TAML^{sq})]$**. Reaction conditions: PhINNs (1.0 eq, 24 Mm), styrene (5.0 eq.) and catalyst (5.0 mol%) were reacted under an argon atmosphere at 35 °C.

Standard procedure for the aziridination with ***PPh$_4$[Co^{III}(TAML^{red})]***

An oven-dried reaction tube was charged with iminoiodinane (96.0 µmol, 1.0 eq.) and filled with argon, followed by addition of DCM (1.0 mL).* All styrenes were filtered over basic alumina prior to use and sparged with argon in a vial and then added (480 µmol, 5.0 eq) to the tube under an argon flow. A solution of **PPh$_4$[Co^{III}(TAML^{red})]** (4.8 µmol, 5 mol%, *or* 2.4 µmol, 2.5 mol%)) in DCM (2.0 mL) and 1.0 mL extra DCM were then added. The reaction mixture was stirred at 35 °C for 2 hours and then cooled to r.t. 1,3,5-Trimethoxybenzene (8 µmol in 100 µL DCM) was added as an internal standard, the mixture was concentrated under reduced pressure and analyzed by ^{1}H NMR spectroscopy.

* Reactions under aerobic conditions were performed in flame-dried vials.

Standard procedure for the aziridination with ***[Co^{III}(TAML^{sq})]***

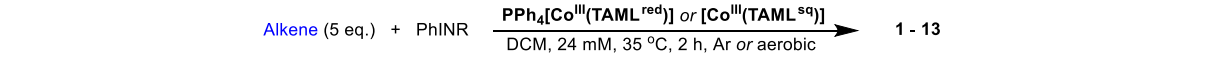
An oven-dried reaction tube was charged with iminoiodinane (96.0 µmol, 1.0 eq.) and filled with argon, followed by addition of DCM (1.0 mL). All styrenes were filtered over basic alumina prior to use and sparged with argon in a vial and then added (480 µmol, 5.0 eq) to the tube under an argon flow. A solution of **[Co^{III}(TAML^{sq})]*** (4.8 µmol, 5 mol% *or* 2.4 µmol, 2.5 mol%) in DCM (2.0 mL) and 1.0 mL extra DCM were then added. The reaction mixture was stirred at 35 °C for 2 hours and then cooled to r.t. 1,3,5-Trimethoxybenzene (8 µmol in 100 µL DCM) was added as an internal standard, the mixture was concentrated under reduced pressure and analyzed by ^{1}H NMR spectroscopy.

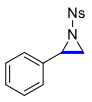
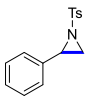
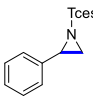
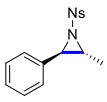
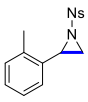
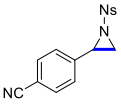
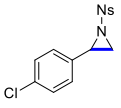
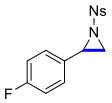
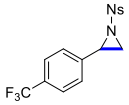
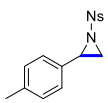
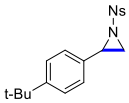
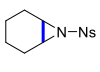
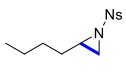
***[Co^{III}(TAML^{sq})]** was prepared freshly from **Li[Co^{III}(TAML^{red})]** and (Thi)BF$_4$ in MeCN according to a literature procedure,[2] followed by concentration under reduced pressure, extraction in CH_2Cl_2 and filtration. Unreacted **Li[Co^{III}(TAML^{red})]** is removed by this procedure as this complex is not soluble in CH_2Cl_2.

Substrate scope

The performed substrate scope and yields can be found in Table S5.

Table S5. Substrate scope for the aziridination of alkenes with iminoiodinanes and either **PPh$_4$[Co^{III}(TAML^{red})]** or **[Co^{III}(TAML^{sq})]** as the catalyst, using different catalyst loadings and under argon or aerobic conditions. Yields based on ^{1}H NMR integration using 1,3,5-trimethoxybenzene as an internal standard. [a] Reaction performed in duplicate, average of two yields.



Catalyst	Catalyst loading	 1	 2	 3	 4	 5	 6	 7
PPh$_4$[Co^{III}(TAML^{red})]	5.0 mol% Ar	76%	33%	43%	43%	73%	41%[a]	58%
	2.5 mol% Ar	64%	-	-	49%	70%	44%[a]	58%
	2.5 mol% aerobic	67%	-	-	32%	65%	44%	59%
[Co^{III}(TAML^{sq})]	5.0 mol% Ar	74%	25%	50%	50%	68%	54%	58%
	2.5 mol% Ar	35%	-	-	23%	40%	20%	28%
		 8	 9	 10	 11	 12a	 12b	 13
PPh$_4$[Co^{III}(TAML^{red})]	5.0 mol% Ar	63%	43%[a]	63%	59%	26%	9%	25%
	2.5 mol% Ar	57%	55%	67%	57%	29%	14%	21%
	2.5 mol% aerobic	61%	63%	66%	66%[a]	31%	8%	22%[a]
[Co^{III}(TAML^{sq})]	5.0 mol% Ar	59%	64%	69%	65%	21%	5%	27%
	2.5 mol% Ar	42%	14%	56%	45%	5%	7%	6%

ESI-HRMS⁻ analysis of nitrene formation at 35 °C.

[Co^{III}(TAML^{q})(NNs)(Y)] and **[Co^{III}(TAML^{q})(NNs)$_2$]$^{-}$** were prepared according to previously reported procedures, with the exception that the reactions were performed at 35 °C in CH_2Cl_2. Adduct Y was not detected in the HRMS-ESI^{-} analysis of the mono-nitrene adduct.

HRMS-ESI^{-} (*m*/*z*) calcd for **[Co^{III}(TAML^{q})(NNs)$_2$]$^{-}$** ($C_{31}H_{28}Cl_2Co_1N_8O_{12}S_2$): 896.9977, found 897.0005 [M^{-}] (Figure S20). The peak at *m*/*z* 894.9944 is attributed to minor decomposition or a side reaction of the nitrene-complex over time at 35 °C.

HRMS-ESI^{-} (*m*/*z*) calcd for **[Co^{III}(TAML^{q})(NNs)]** ($C_{25}H_{24}Cl_2Co_1N_6O_8S_1$): 697.0085, found 697.0096 [M^{-}] (Figure S21). The peak at *m*/*z* 694.9758 [M-2H]$^{-}$ is attributed to minor decomposition or a side reaction of the nitrene-complex over time at 35 °C.

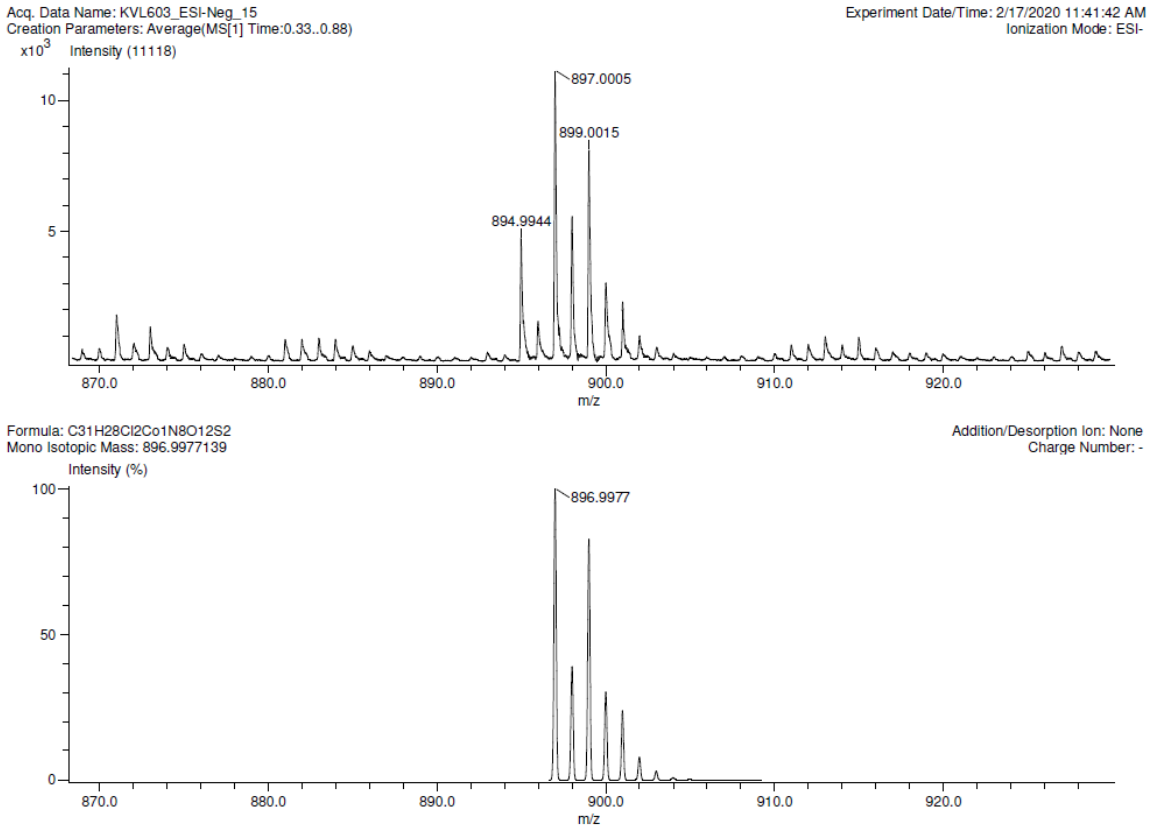


Figure S20. HRMS-ESI^{-} spectrum of **[Co^{III}(TAML^{q})(NNs)$_2$]$^{-}$** prepared at 35 °C (top) and simulation for [M]$^{-}$ (bottom).

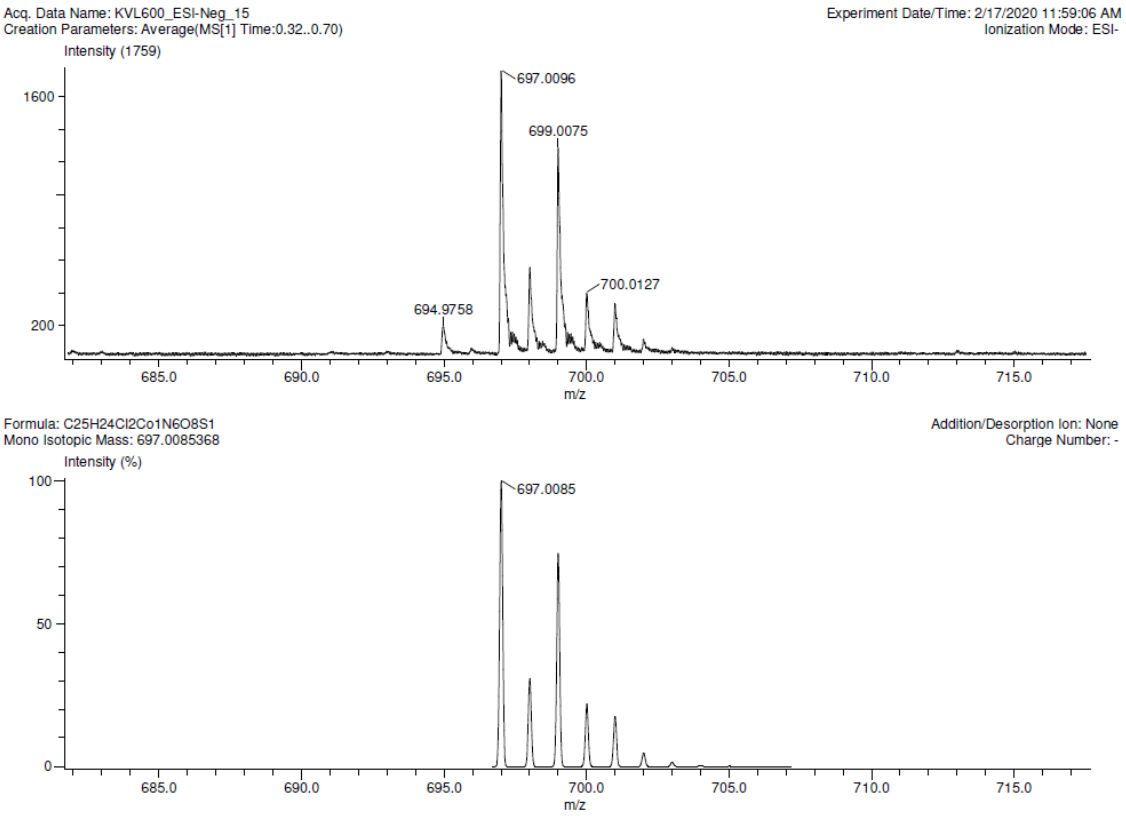


Figure S21. HRMS-ESI$^-$ spectrum of **[Co^{III}(TAML^q)(NNs)]** prepared at 35 ^{o}C and simulation for [M]$^-$ (bottom).

*Quantification of **[Co^{III}(TAML^{q})(NNs)(Y)]** formation from **[Co^{III}(TAML^{sq})]***

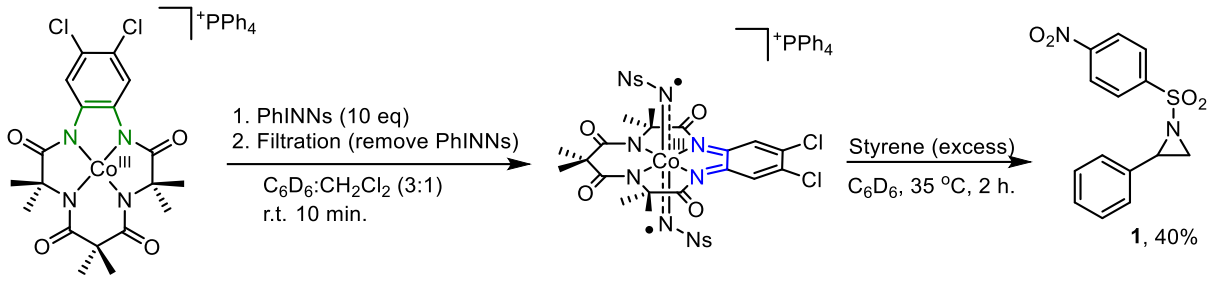
[Co^{III}(TAML^{sq})] and **[Co^{III}(TAML^{q})(NNs)(Y)]** were prepared according to previously reported methods with C_6D_6 as the solvent for **[Co^{III}(TAML^{q})(NNs)(Y)]** formation.[2] The X-Band EPR spectrum of **[Co^{III}(TAML^{sq})]** (in C_6D_6 at room temperature) was recorded with different modulation amplitudes and the double integral of the signal was calculated with Bruker's Xenon software. The spectrum of **[Co^{III}(TAML^{q})(NNs)(Y)]** (generated from the **[Co^{III}(TAML^{sq})]** solution, and used without further dilution) was then measured in the same EPR tube, filled to the same height and measured with the same settings, albeit at different modulation amplitudes. The results are summarized in Table S6. We noted that separate measurements (of the same sample and the same experimental settings) of the spectrum of **[Co^{III}(TAML^{q})(NNs)(Y)]** afforded slight variations in the double integrals. To correct for this experimental error, we measured four spectra at each modulation amplitude and then calculated the average double integral, which afforded 97-102% conversion of **[Co^{III}(TAML^{sq})]** to **[Co^{III}(TAML^{q})(NNs)(Y)]**. Of course conversions >100% are impossible, and only occur in our wildest dreams. However, taking the found experimental error into account, these experiments indicate the quantitative (>99%) formation of **[Co^{III}(TAML^{q})(NNs)(Y)]** from **[Co^{III}(TAML^{sq})]**. In addition, no **[Co^{III}(TAML^{sq})]** signal was present in the spectra of **[Co^{III}(TAML^{q})(NNs)(Y)]**, again consistent with quantitative conversion of the starting complex.

Table S6. Double integrals of the signals recorded for **[Co^{III}(TAML^{sq})]** and **[Co^{III}(TAML^{q})(NNs)(Y)]** at different modulation amplitudes (Mod. Amp.) in X-Band EPR at room temperature. The conversion is calculated from the average double integral for **[Co^{III}(TAML^{q})(NNs)(Y)]** with respect to **[Co(TAML^{sq})]**.

	[Co^{III}(TAML^{sq})]	**[Co^{III}(TAML^{q})(NNs)(Y)]**		
Mod. Amp.	Double integral	Double integral measurements	Average double integral	Conversion
4	29290	29739 25495 29882 28228	28336	97%
6	41218	42166 38668 44060 43276	42030	102%
8	55742	58324 52109 57790 56497	56180	101%

Single-turnover experiments with ***[Co^{III}(TAML^{q})(NNs)$_2$]$^{-}$*** and ***[Co^{III}(TAML^{q})(NNs)(Y)]***

[Co^{III}(TAML^{q})(NNs)$_2$]$^{-}$: **PPh$_4$[Co^{III}(TAML^{red})]** (6.29 mg; 7.5 µmol; 1.0 eq) and PhINNs (30.1 mg; 75 µmol; 10 eq) were suspended in C_6D_6 (1.5 mL) under argon and stirred for 10 minutes (Scheme S3). CH_2Cl_2 (0.5 mL) was added and the mixture was stirred for another minute and filtered over a syringe filter (FPTE, 0.45 µm) to remove the excess PhINNs. 1.35 mL of the resulting solution (5.0 µmol **[Co^{III}(TAML^{q})(NNs)$_2$]$^{-}$**) was then added to styrene (1.0 mL) at 35 °C under argon and stirred for 2 hours. Trimethoxybenzene (4.0 µmol) was then added as an internal standard for ^{1}H NMR analysis and the reaction mixture was concentrated under reduced pressure. ^{1}H NMR analysis (Figure S22) showed formation of aziridine **1** in 2.0 µmol, 40% yield.



Scheme S3. Single-turnover experiment with **[Co^{III}(TAML^{q})(NNs)$_2$]$^{-}$**.

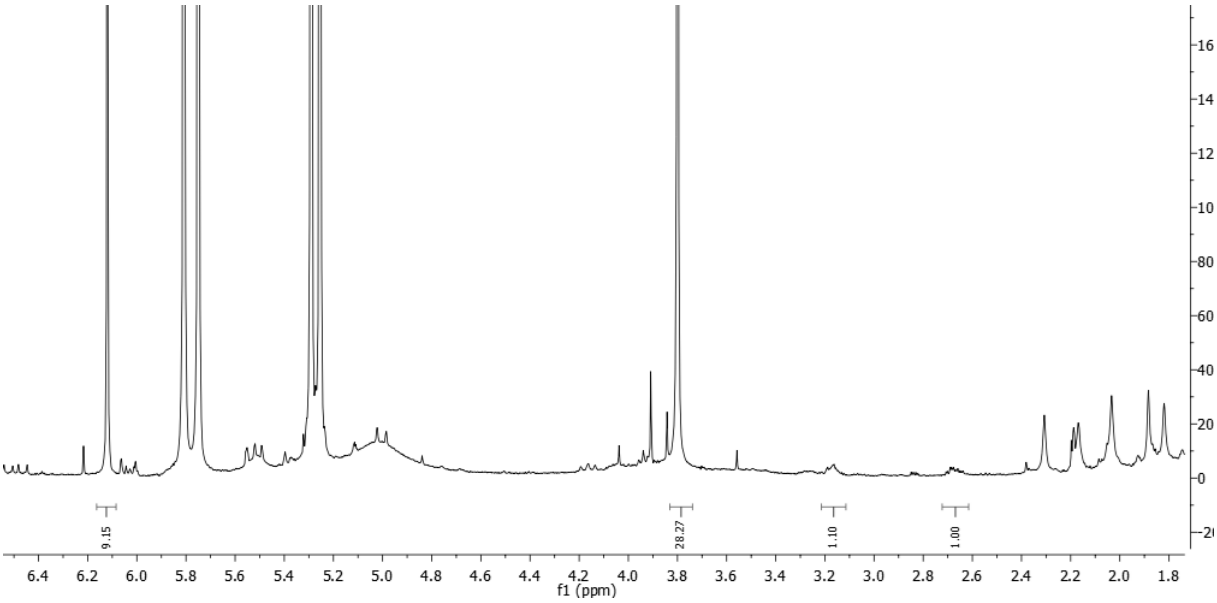
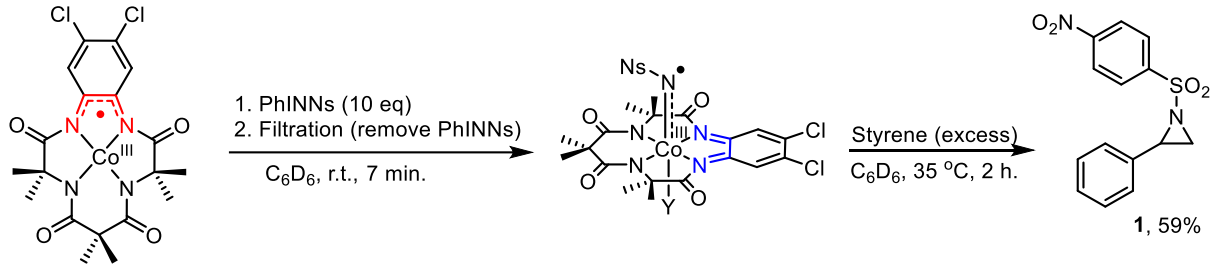


Figure S22. ^{1}H NMR analysis to determine the yield of **1** in the single-turnover experiment with **[Co^{III}(TAML^{q})(NNs)$_2$]$^{-}$**. 1,3,5-trimethoxybenzene (4.0 µmol) added as internal standard.

[Co^{III}(TAML^{q})(NNs)(Y)]: A solution of **[Co^{III}(TAML^{sq})]** (4.98 mg; 10.0 µmol) in C_6D_6 (2.0 mL) was prepared according to the previously reported method.[2] The **[Co^{III}(TAML^{sq})]** solution was added to PhINNs (40.4 mg; 100 µmol) and stirred for 7 minutes and filtered over a syringe filter (FPTE, 0.45 µm) to remove the excess PhINNs (Scheme S4). 1.00 mL of the resulting solution (5.0 µmol **[Co^{III}(TAML^{q})(NNs)(Y)]**) was then added to styrene (1.0 mL) at 35 °C under argon and stirred for 2 hours. Trimethoxybenzene (6.96 µmol) was then added as an internal standard for ^{1}H NMR analysis and the reaction mixture was concentrated under reduced pressure. ^{1}H NMR analysis (Figure S23) showed formation of aziridine **1** in 2.94 µmol; 59% yield.



Scheme S4. Single-turnover experiment with **[Co^{III}(TAML^{q})(NNs)(Y)]**.

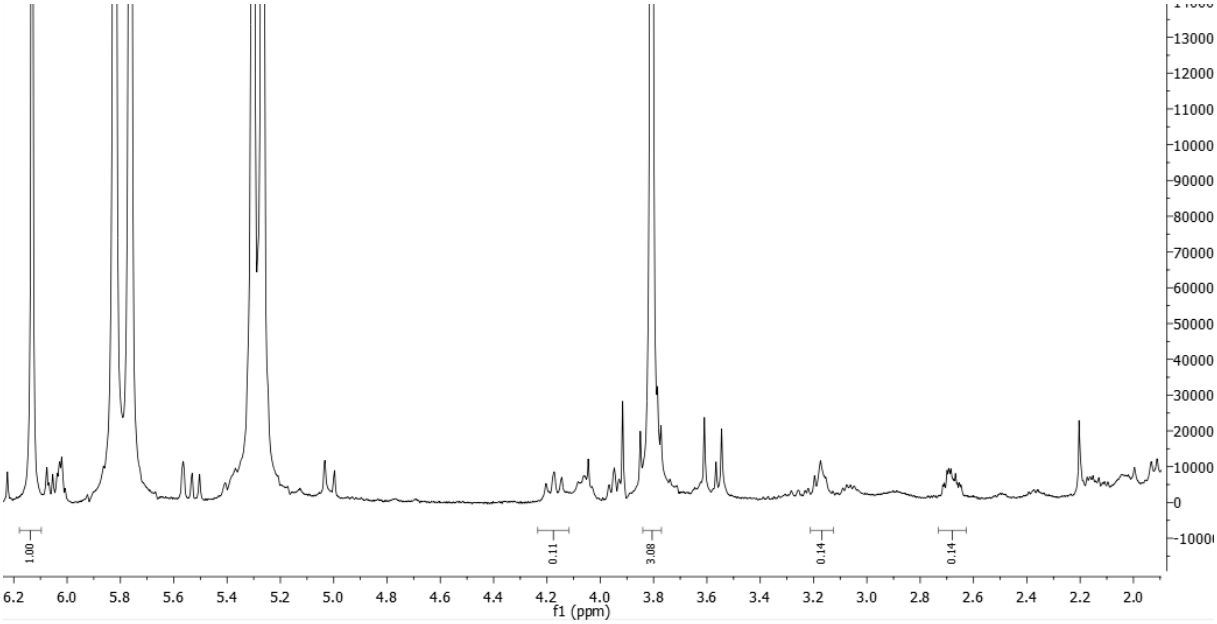


Figure S23. ^{1}H NMR analysis to determine the yield of **1** in the single-turnover experiment with **[Co^{III}(TAML^{q})(NNs)(Y)]**. 1,3,5-trimethoxybenzene (6.96 µmol) added as internal standard.

Spin trapping studies with TEMPO, PBN and DMPO

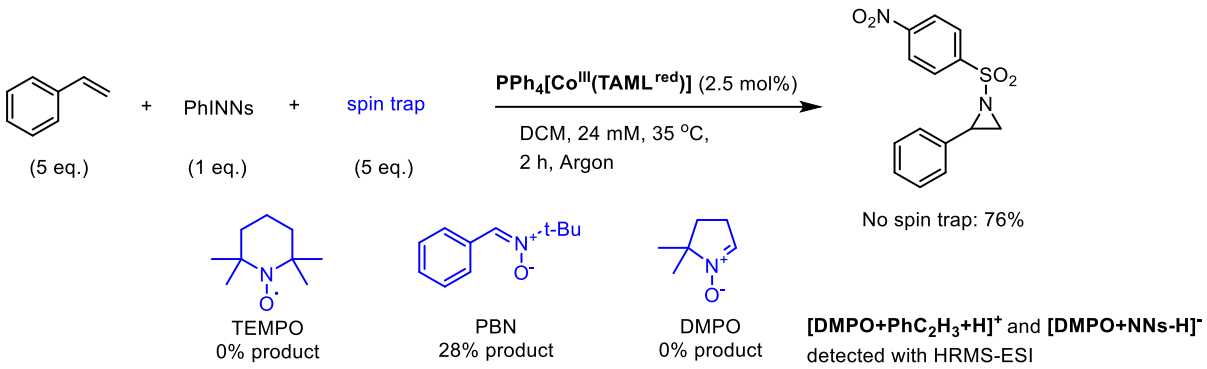
To probe the intermediacy of radical species in the reactions, five equivalents TEMPO, PBN or DMPO (with respect to PhINNs) were added under the standard conditions (entries 8 and 13, Table 1 in the main text) with styrene as the substrate. The results are summarized in Scheme S5 and Scheme S6.

The ESI- and FD-HRMS spectra are shown in Figure S24, Figure S25, Figure S26 and Figure S27 and an overview of the calculated and found adducts of DMPO with styrene and NNs can be found in Table S7.

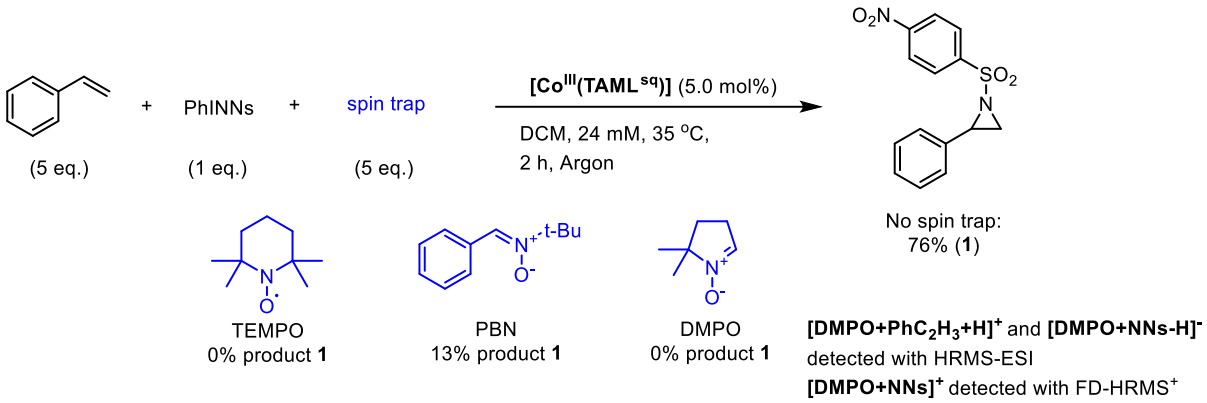
To investigate the formation of trapped radical adducts further, the reaction with **$PPh_4[Co^{III}(TAML^{red})]$** (Entry 8, Table 1 in the main text) was repeated in presence of 5 equivalents DMPO (with respect to PhINNs) and concentrated *in vacuo* after 75 minutes. The mixture was then dissolved in 0.3 mL toluene (under argon) and analyzed by X-Band EPR (Figure S28). A mixture of radicals was observed, and simulation of the experimental spectrum afforded satisfactory agreement with the presence of three radical species (components A, B and C, see Table S7). All these radical species showed coupling to an $I = 1$ nucleus (39-41 MHz or 13.9-14.6 Gauss), which we attribute to coupling with ^{14}N present in DMPO, as these coupling constants are close to those observed for DMPO-trapped radicals.[27] Unfortunately, NNs or styrene radical adducts with DMPO are unknown, and therefore we are unable to conclusively assign the observed EPR signals to specific DMPO adducts.

Adduct C does not show any further hyperfine coupling interactions (besides coupling with one ^{14}N nucleus), and its structure remains unknown. Adducts A and B show further hyperfine coupling with several other nuclei than one ^{14}N nucleus. Simulation afforded for component A; $A^{N}_{iso} = 41$ MHz (14.6 G) and $A^{H}_{iso} = 8.5$ MHz (3.0 G) and for component B $A^{N1}_{iso} = 40$ MHz (14.3 G), $A^{N2}_{iso} = 27$ MHz (9.6 G), $A^{H1}_{iso} = 8$ MHz (2.9 G) and $A^{H2}_{iso} = 5$ MHz (1.8 G). Based hereon, we tentatively propose that compound B is a [DMPO+NHNs]$^{\bullet}$ adduct, which would be consistent with the observed coupling with two different nitrogen and two different proton nuclei. The exact nature of component A remains unknown. We can rule out the formation of a 1-phenylethyl adduct of DMPO, as in this case the observed coupling to the ^{1}H nucleus would be much larger (20.49 G).[27a] A different spin adduct of DMPO with styrene (or NNs) can however not be ruled out, nor confirmed.

Concluding, the performed X-Band EPR studies clearly indicate that multiple radicals have formed adducts with DMPO, which is consistent with the HRMS analysis described above.



Scheme S5. Spin trapping studies for the **$PPh_4[Co^{III}(TAML^{red})]$** catalyzed formation of **1**.



Scheme S6. Spin trapping studies for the **$[Co^{III}(TAML^{sq})]$** catalyzed formation of **1**.

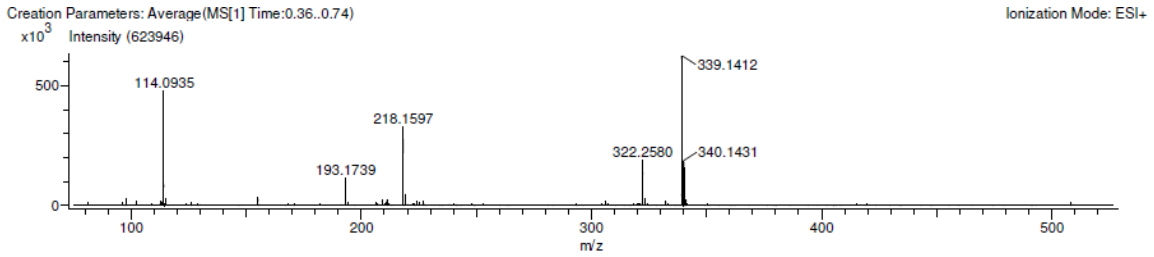


Figure S24. ESI-HRMS$^+$ of the **PPh$_4$[Co^{III}(TAML^{red})]** catalyzed formation of **1**, with addition and trapping by DMPO.

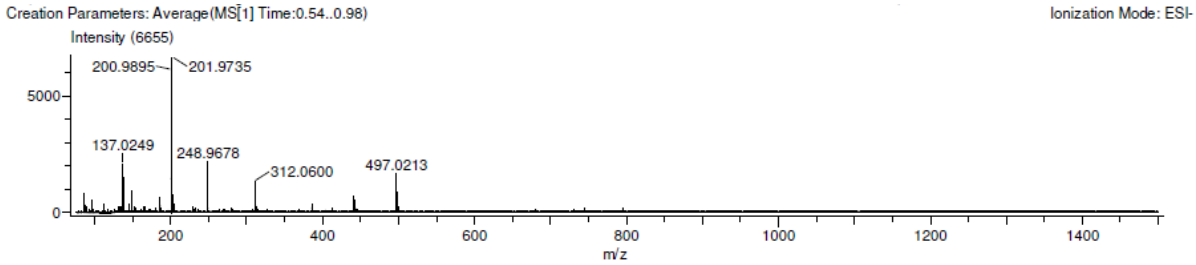


Figure S25. ESI-HRMS$^-$ of the **PPh$_4$[Co^{III}(TAML^{red})]** catalyzed formation of **1**, with addition and trapping by DMPO.

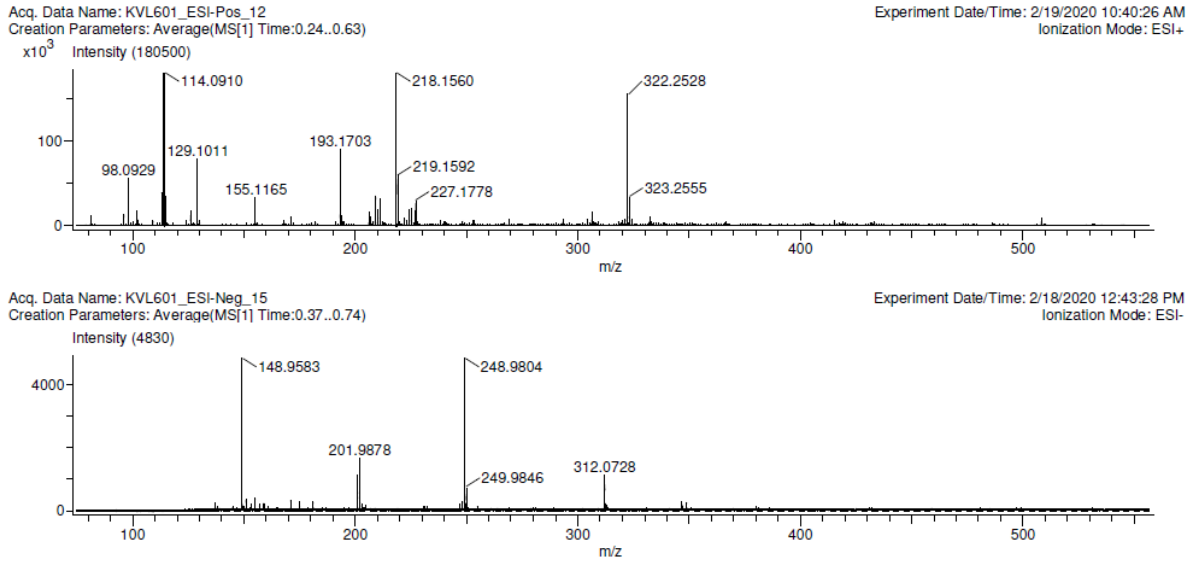


Figure S26. ESI-HRMS$^+$ (top) and ESI-HRMS$^-$ (bottom) of the **[Co^{III}(TAML^{sq})]** catalyzed formation of **1**, with addition and trapping by DMPO.

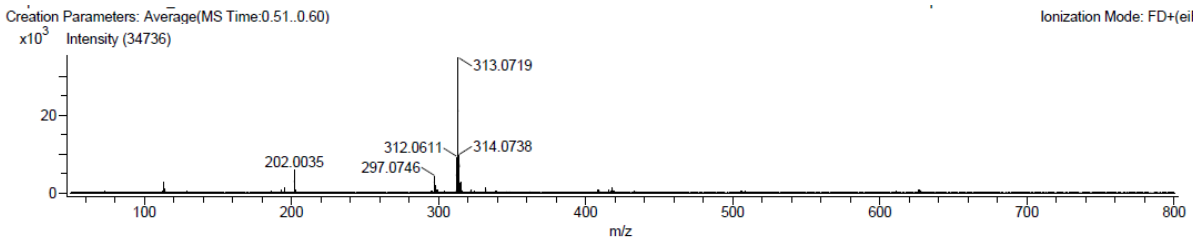


Figure S27. FD-HRMS$^+$ of the **[Co^{III}(TAML^{sq})]** catalyzed formation of **1**, with addition and trapping by DMPO.

Table S7. Calculated and found adducts of DMPO with styrene and NNs in ESI- and FD-HRMS.

Adduct	**Calculated *m/z***	**Found (PPh$_4$[Co^{III}(TAML^{red})])**	**Found ([Co^{III}(TAML^{sq})])**
[DMPO+styrene+H]$^+$	218.1545	218.1597 (Figure S24)	218.1560 (Figure S26 top)
[DMPO+NNs-H]$^-$	312.0654	312.0600 (Figure S25)	312.0728 (Figure S26 bottom)
[DMPO+NNs]$^+$	313.0732	-	313.0719 (Figure S27)

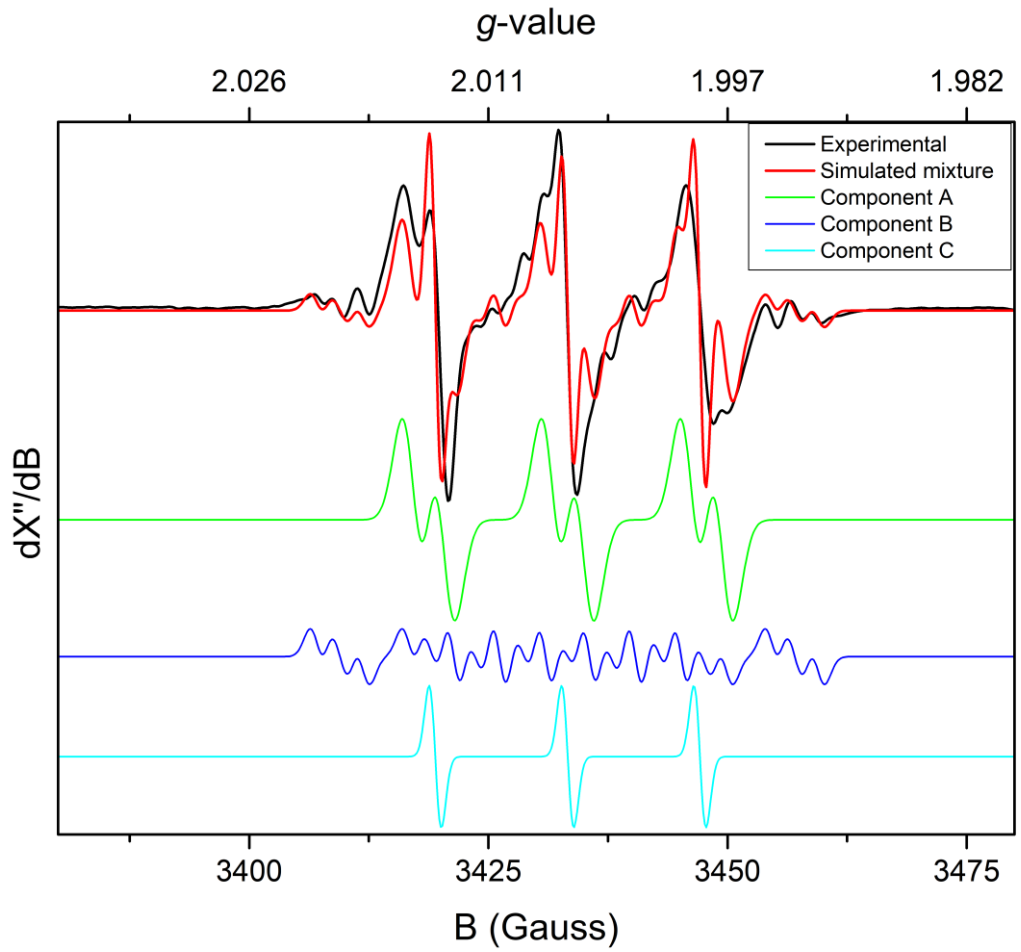


Figure S28. Experimental and simulated X-Band EPR spectrum of the DMPO trapping experiment with **$PPh_4[Co^{II}(TAML^{red})]$** as the catalyst. Microwave frequency 9.641092 GHz, modulation amplitude 1.499 G, power 0.6325 mW, room temperature, toluene.

Table S8. Simulated components for the X-Band EPR spectrum in Figure S28, with a 9.641092 GHz microwave frequency. Conversion from MHz to Gauss (G) was achieved by dividing the coupling in MHz by the product of g_e and a conversion factor of 1.4 MHz·G^{-1} (2.0037*1.4) = 2.80518.

Component and weight	**g_{iso}**	**Linewidth (W_{iso})**	**Hyperfine coupling interactions (A in MHz and G) and nuclear spin (I)**			
A (3.5)	2.00625	1.5	A^{N}_{iso} = 41 MHz / 14.6 G (I = 1)	A^{H}_{iso} = 8.5 MHz / 3.0 G (I = ½)		
B (2.0)	2.00625	1.0	A^{N1}_{iso} = 40 MHz / 14.3 G (I = 1)	A^{N2}_{iso} = 27 MHz / 9.6 G (I = 1)	A^{H1}_{iso} = 8 MHz / 2.9 G (I = ½)	A^{H1}_{iso} = 5 MHz / 1.8 G (I = ½)
C (1.0)	2.00625	0.75	A^{N}_{iso} = 39 MHz / 13.9 G (I = 1)			

Deactivation of ***PPh$_4$[Co^{III}(TAML^{red})]$^-$***

To study potential catalyst deactivation we added aliquots of PhINNs (48 µmol, 1 molar equiv.) after 30 and 60 minutes to five equivalents styrene under standard conditions with 2.5 mol% **PPh$_4$[Co^{III}(TAML^{red})]** under an aerobic atmosphere. In the first 30 minutes we observed 28 turn-over numbers (TONs) towards **1** (Figure S29). Addition of a second aliquot PhINNs led to 7 more TON, and addition of another equivalent PhINNs after 60 minutes afforded another 3 TON towards **1**. However, addition of another 2.5 mol% catalyst after 90 minutes led to 25 TON towards **1** for the new batch of catalyst, thus indicating that catalyst deactivation is occurring under these reaction conditions.

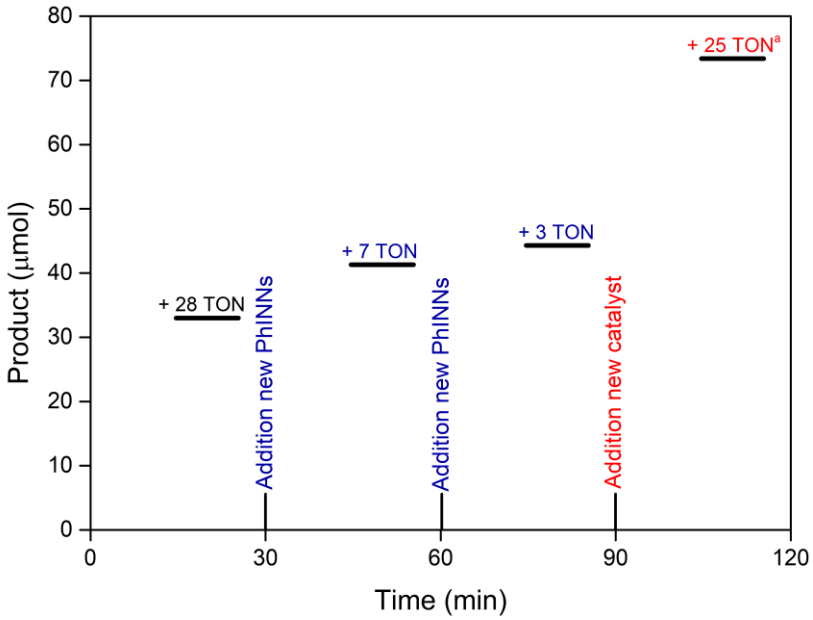


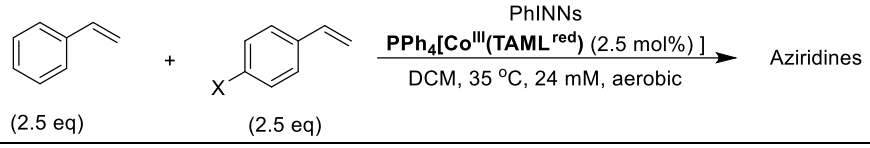
Figure S29. Deactivation study for **PPh$_4$[Co^{III}(TAML^{red})]** in the formation of **1** under aerobic conditions. [a] Addition of fresh 2.5 mol% catalyst.

Hammett plots

Hammett analysis was performed with intermolecular competition experiments under standard conditions for **PPh_4[Co^{III}($TAML^{red}$)]** (2.5 mol%, aerobic,Table S9 and Figure S30) and **[Co^{III}($TAML^{sq}$)]** (5.0 mol%, argon, Table S10 and Figure S31). Compared to the amount of PhINNs, 2.5 eq styrene and 2.5 eq of a *para*-functionalized (X = *t*Bu, F, Cl, CN, CF_3 or Me) styrene were present. Aliquots of the reactions were taken after 10 and 15 minutes for **PPh_4[Co^{III}($TAML^{red}$)]** and 30 and 60 minutes for **[Co^{III}($TAML^{sq}$)]**, to ensure that the conversion of PhINNs was below 50%, and the samples analyzed by ^{1}H NMR spectroscopy. The average ratio between the amount of *para*-functionalized-aziridine and **1** was then calculated, which is equal to k_x/k_H at conversion lower than 50%. Plotting $\log(k_x/k_H)$ versus $\rho^\bullet\sigma_{JJ}^\bullet + \rho^+\sigma^+ + C$ and applying multiple linear regression, we found linear correlations for **PPh_4[Co^{III}($TAML^{red}$)]** (R^2 = 0.99, $\rho_{JJ}^\bullet$ = 0.14, ρ^+ = −0.80, C = 0.01, $\rho^+/\rho^\bullet$ = 5.71, slope ρ = 1.00) and **[Co^{III}($TAML^{sq}$)]** (R^2 = 0.96, $\rho^\bullet$ = 0.14, ρ^+ = −1.21, $\rho^+/\rho^\bullet$ = 8.64, slope ρ = 1.00), which indicated that electronic effects dominate the reaction rate. In this formula, $\sigma_{JJ}^\bullet$ and σ^+ are reported in literature and $\rho^\bullet$ and ρ^+ are found by the multiple component linear regression.[28]

When using only the electronic (σ^+) parameter for the construction of the Hammett plots, linear correlations were found for **PPh_4[Co^{III}($TAML^{red}$)]** (ρ^+ = -0.78, R^2 = 0.98, Figure S32) and **[Co^{III}($TAML^{sq}$)]** (ρ^+ = -1.19, R^2 = 0.96, Figure S33). This can be expected for systems with unusually high $|\rho^+/\rho^\bullet|$ ratios, as electronic effects are more important than radical stabilization effects. The ρ^+ values are similar as observed for the Hammett plots in which radical stabilization ($\sigma_{JJ}^\bullet$) was included, however with a slightly lower R^2 value for **PPh_4[Co^{III}($TAML^{red}$)]**. In combination with the observed radical character of the reaction according to the spin trapping experiments and the importance of electronic effects (according to all four Hammett analysis plots) we argue that inclusion of the significant radical stabilization ($\rho^\bullet$ = 0.14) gives a more accurate description of the transition states.

Table S9. Hammett $\sigma_{JJ}^\bullet$ and σ^+ parameters for functionalized styrenes and obtained ratios for k_x and k_H in the **PPh_4[Co^{III}($TAML^{red}$)]** catalyzed aziridination. [a] Average over two or three measurements, see also Figure S30 for the error bars.



Entry	X	$\sigma_{JJ}^\bullet$	σ^+	$k_x : k_H$ [a]	$\log(k_x/k_H)$
1	*t*Bu	0.26	-0.256	1.89 : 1.00	0.28 ± 0.000
2	F	-0.02	-0.073	1.15 : 1.00	0.06 ± 0.000
3	Cl	0.22	0.114	1.03 : 1.00	0.01 ± 0.002
4	H	0	0	1.00 : 1.00	0.00 ± 0.000
5	CN	0.42	0.659	0.35 : 1.00	-0.46 ± 0.024
6	CF_3	-0.01	0.612	0.37 : 1.00	-0.43 ± 0.016
7	Me	0.15	-0.311	2.04 : 1.00	0.31 ± 0.037

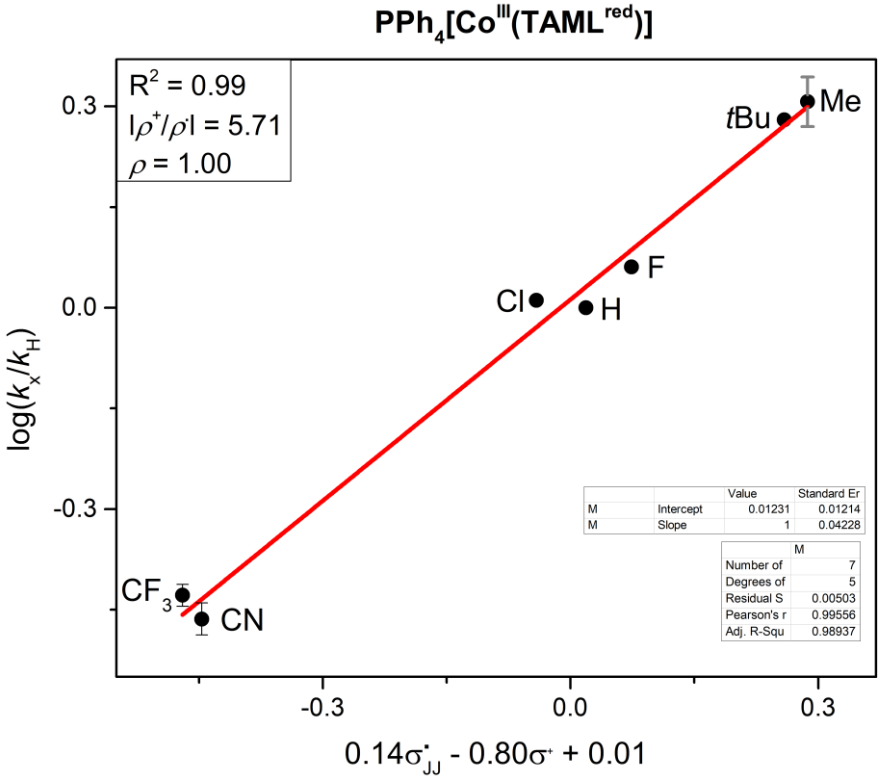
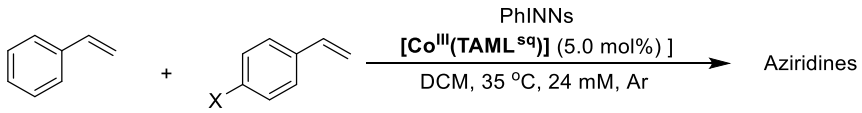


Figure S30. Hammett plot for **PPh$_4$[Co^{III}(TAML^{red})]** in the aziridination of styrene derivatives.

Table S10. Hammett $\sigma_{JJ}^{\bullet}$ and σ^{+} parameters for functionalized styrenes and obtained ratios for k_x and k_H in the **Co^{III}(TAML^{sq})** catalyzed aziridination. Average over two or three measurements, see also Figure S31 for the error bars.



Entry	X	$\sigma_{JJ}^{\bullet}$	σ^{+}	$k_x : k_H$ [a]	log(k_x/k_H)
1	*t*Bu	0.26	–0.256	2.5 : 1.0	0.40 ± 0.000
2	F	–0.02	–0.073	0.79 : 1.0	–0.10 ± 0.010
3	Cl	0.22	0.114	0.79 : 1.0	–0.10 ±0.000
4	H	0	0	1.00 : 1.00	0.00 ± 0.000
5	CN	0.42	0.659	0.14 : 1.0	–0.84 ± 0.081
6	CF_3	–0.01	0.612	0.21 : 1.0	–0.68 ± 0.020
7	Me	0.15	–0.311	2.50 : 1.0	0.40 ± 0.049

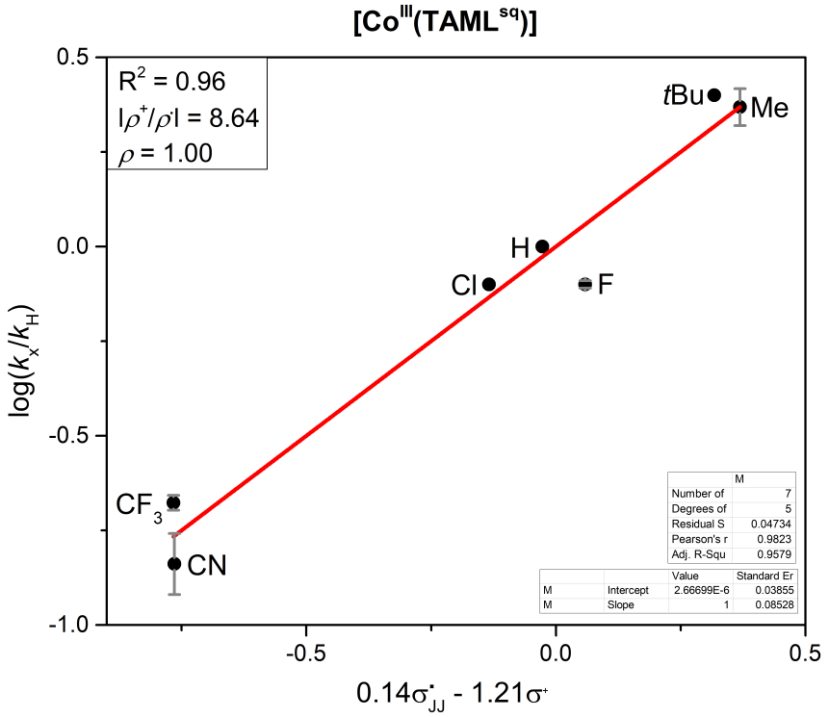


Figure S31. Hammett plot for **[Co^{III}(TAML^{sq})]** in the aziridination of styrene derivatives.

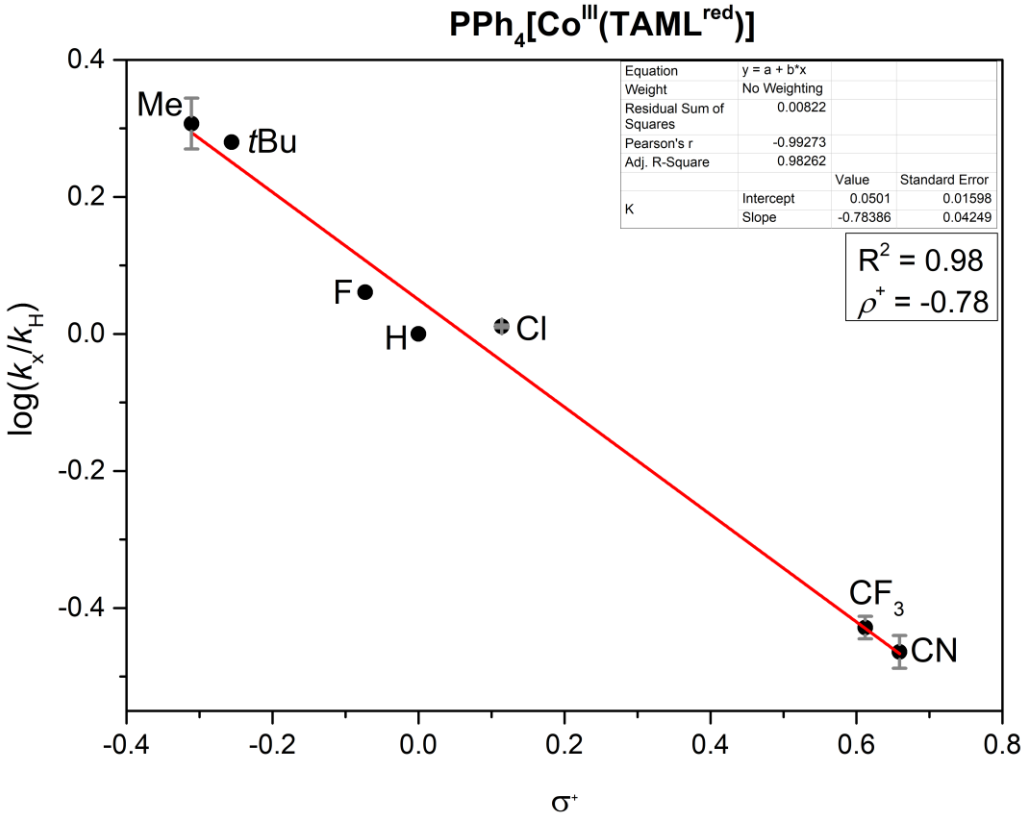


Figure S32. Electronic Hammett plot for **PPh$_4$[Co^{III}(TAML^{red})]** in the aziridination of styrene derivatives.

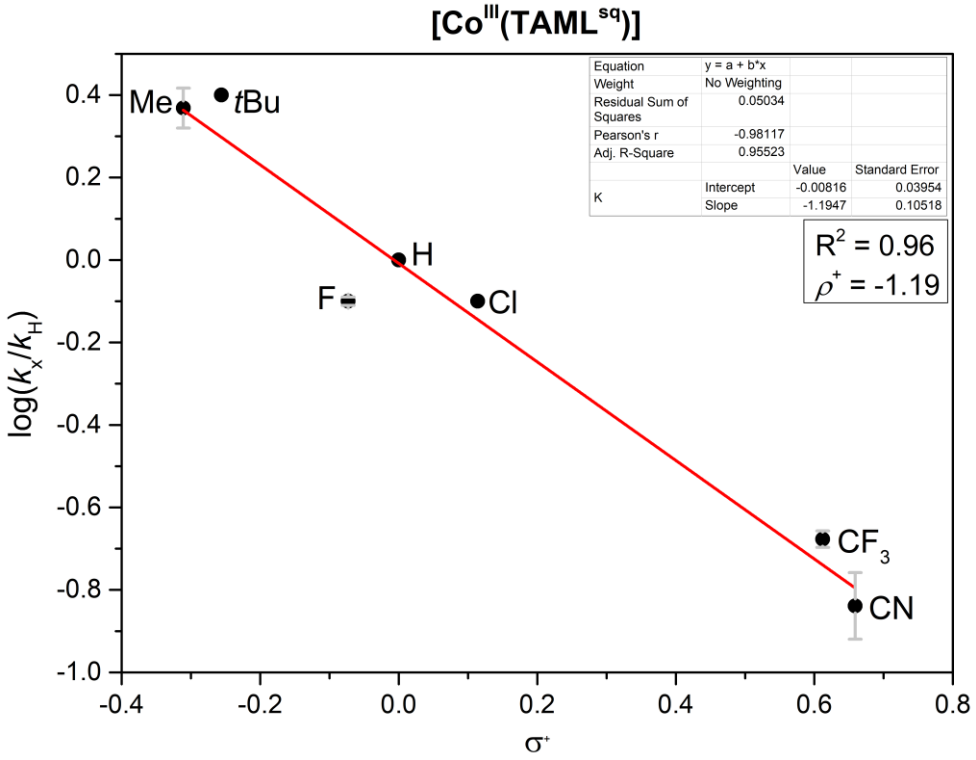


Figure S33. Electronic Hammett plot for **[Co^{III}(TAML^{sq})]** in the aziridination of styrene derivatives.

Complete Active Space Self Consistent Field Calculation

The NEVPT2 corrected CASSCF calculations was performed according to the methods described in the general considerations.

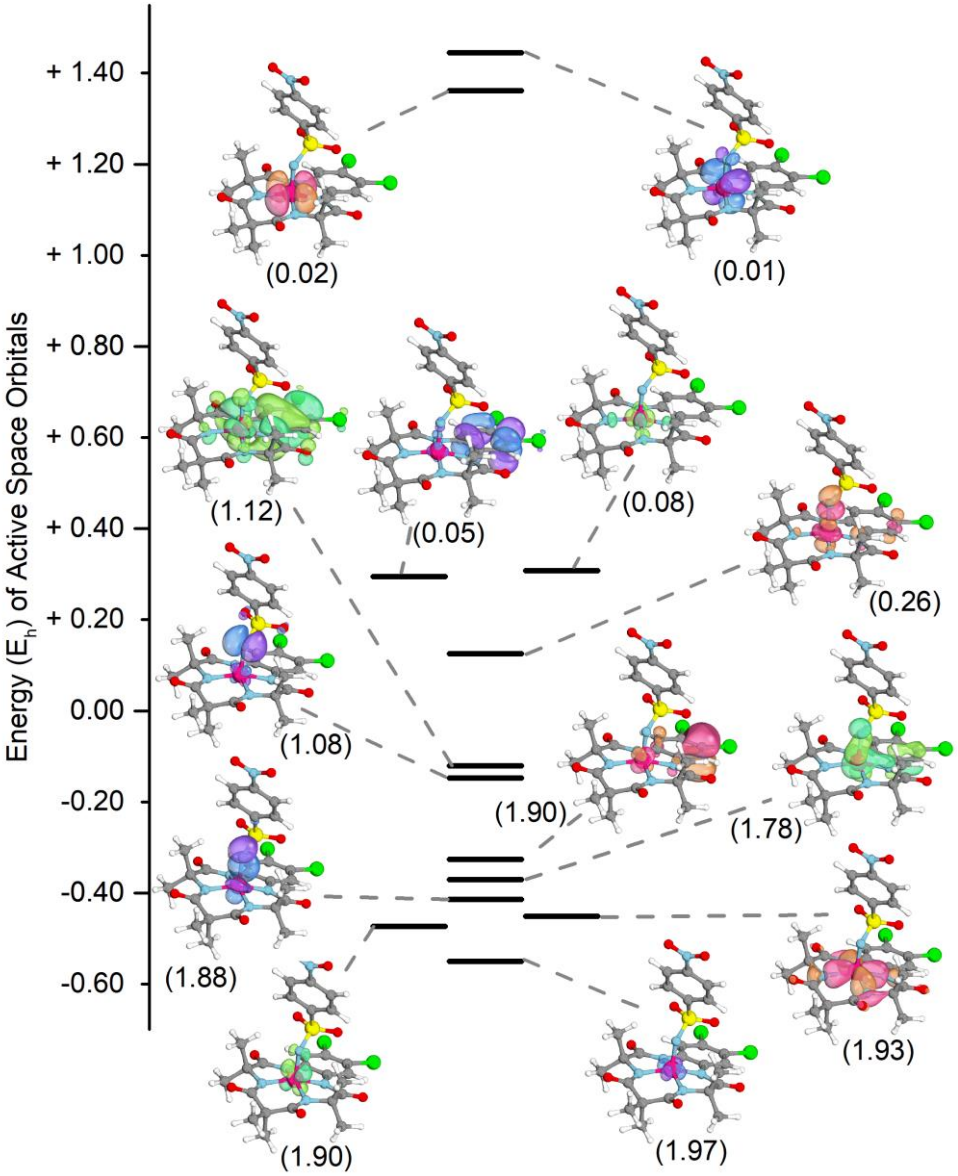
[Co^{III}(TAML^{sq})(NNs)]$^{-}$ NEVPT2-CASSCF(14,13)

The total and relative energies for the singlet, triplet and quintet spin state and their states and contributions for **[Co^{III}(TAML^{sq})(NNs)]$^{-}$** were obtained from NEVPT2 corrected CASSCF(14,13) calculations and are reported in Table S11. The triplet spin state is the most stable and has some multi-reference character in the L_{π}, d_{z^2}, N_{pz} manifold. A quantitative orbital analysis can be found in Scheme S7 and it can be seen that the two unpaired electrons reside in the ligand π-system and the nitrene N_{py} orbital. The most relevant active orbitals and an assignment (from Löwdin population analysis) of the electronic structure can be seen in Scheme S8.

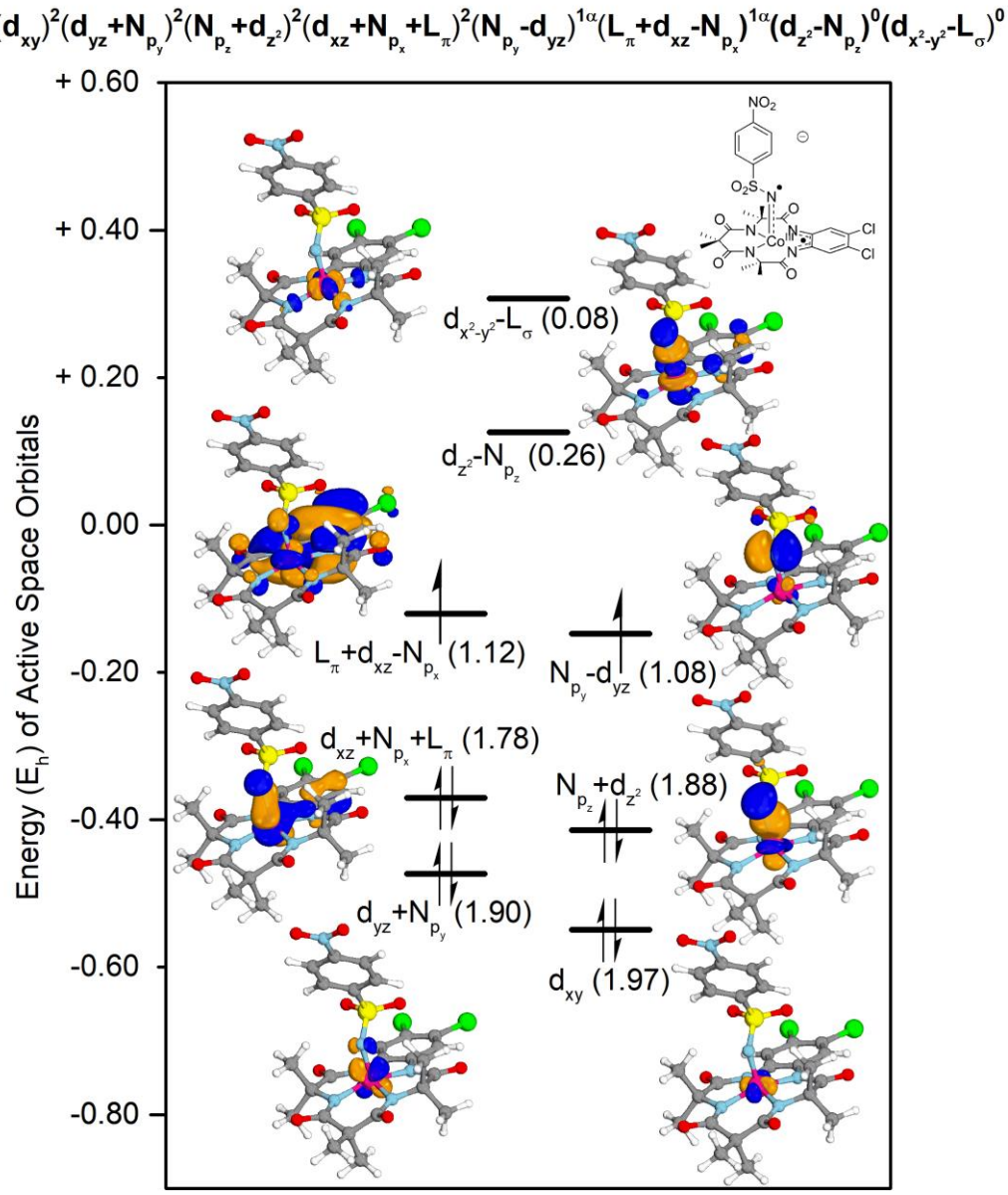
Table S11. Total and relative energies (NEVPT2 corrected) for multiple spin states and their states and contributions for the single-root NEVPT2-CASSCF(14,13) calculation on **Co^{III}(TAML^{sq})(NNs)]$^{-}$**.

Multiplicity	Total energy (kcal mol^{-1})	Relative energy (kcal mol^{-1})	Contribution : state
1 (singlet)	-2882104.561	+8.6	0.77260 : 2222221100000
			0.04116 : 2212122110000
			0.01634 : 2122221110000
			0.01161 : 2222201102000
			0.01022 : 2122221200000
			0.00914 : 2222021120000
			0.00734 : 2212222100000
			0.00553 : 2121221200100
			0.00508 : 2222121110000
			0.00482 : 2212122101000
			0.00475 : 2220221100200
			0.00467 : 2222201201000
			0.00459 : 2221122110000
			0.00448 : 2222201111000
			0.00411 : 2221121110100
			0.00401 : 2211222100100
			0.00362 : 2221221100100
			0.00351 : 1221221100110
			0.00308 : 2122121210000
			0.00300 : 2222211101000
3 (triplet)	-2882113.112	= 0.0	0.60834 : 2222221100000
			0.05518 : 2222121110000
			0.05106 : 2222121200000
			0.02531 : 2121222110000
			0.01625 : 2221221110000
			0.01528 : 2122222100000
			0.01481 : 2222211200000
			0.01333 : 2222211110000
			0.01316 : 2221221200000
			0.01017 : 2122122110000
			0.01015 : 2222221010000
			0.00995 : 2212121200100
			0.00927 : 2222201102000
			0.00636 : 2222021210000
			0.00573 : 2222021120000
			0.00531 : 2222121020000
			0.00412 : 2202221100200
			0.00410 : 2211221200100
			0.00395 : 2220221120000
			0.00374 : 2212121110100
			0.00353 : 2112222100100

			0.00332 : 2121122120000 0.00322 : 2222201111000 0.00302 : 2221121210000 0.00283 : 1212221100110 0.00265 : 2121222200000
5 (quintet)	-2882079.947	+33.2	0.83332 : 2222211110000 0.01400 : 1212212120000 0.01266 : 2212211120000 0.01003 : 2222011112000 0.00952 : 2022211110200 0.00939 : 2212211210000 0.00903 : 2122211110100 0.00578 : 2221111112000 0.00569 : 1122212110100 0.00568 : 1212212210000 0.00533 : 1222212110000 0.00397 : 2112211120100 0.00374 : 1122211110101 0.00308 : 0222211110200 0.00282 : 2112211210100 0.00270 : 2221211111000 0.00261 : 1222211110100



Scheme S7. Energies of active orbitals with their occupancies in parentheses obtained from NEVPT2-CASSCF(14,13) calculations on **[Co^{III}(TAML^{sq})(NNs)]**$^{-}$. Isosurface for canonical orbitals set at 80.0.



Scheme S8. Most relevant active orbitals, occupancies (in parenthesis) and assignment of the electronic structure of NEVPT2-corrected CASSCF(14,13) calculations on **[Co^{III}(TAML^{sq})(NNs)]$^-$**. Isosurface for canonical orbitals set at 80.0.

Density Functional Theory Calculations

All calculations were performed according to the methods described in the general considerations. The level of theory was BP86/def2-TZVP with Grimme's version 3 zero-damping dispersion corrections on an m4 grid, as this was previously shown to be the most accurate for the systems under investigation.[2]

The spin densities (red, positive α-spin density and blue negative β-spin density) and NPA charges (black) of **C**, **D**, **J**, $\mathbf{J^{NH_3}}$, **TS2**, **TS2'**, **TS4** and $\mathbf{TS4^{NH_3}}$ are depicted in Scheme S9.
The graphical representations and α and β spin occupations of the ligand-centered redox active orbital in **C**, **D**, **J**, $\mathbf{J^{NH_3}}$, **TS2**, **TS2', TS4** and $\mathbf{TS4^{NH_3}}$ are depicted in Table S14. From these occupations the TAML redox state can be assigned as follows: **C** ($TAML^{sq}$), **D** ($TAML^{q}$), **J** ($TAML^{q}$), $\mathbf{J^{NH_3}}$ ($TAML^{q}$), **TS2** ($TAML^{sq}$), **TS2'** ($TAML^{red}$) $\mathbf{TS4^{NH_3}}$ ($TAML^{sq}$) and **TS4** ($TAML^{sq}$). Herein *red* is double (αβ) filled, *sq* is mono (α) filled and *q* is empty. Moreover, the bond lengths of the redox active moiety in the TAML in **TS2'** indicate full aromaticity, consistent with the assigned $TAML^{red}$ state. For additional orbital analysis of **C** we refer to the CASSCF section in this supporting information. The CASSCF results of **D** and **J** were previously described.[2]

Absolute and relative energies for all DFT optimized structures with the BP86 functional

The relevant absolute energies for all compounds are reported in Table S12. The relative Gibbs free energies for all relevant intermediates are reported in Table S13. The barrierless steps from **B** → $\mathbf{[Co^{III}(TAML^{sq})(NNs)]^-}$**+PhI** and **I** → $\mathbf{[Co^{III}(TAML^{q})(NNs)]}$**+PhI** are truly barrierless, as was shown by stepwise elongation of the N-I bond from the nitrene intermediates (Figure S34 and Figure S35, respectively). Similarly, the barrierless transition from $\mathbf{TS4^{NH_3}}$ → $\mathbf{L^{NH_3}}$ was shown by stepwise elongation of the aziridine N-C(Ph) bond from the coordinated aziridine product (see Figure S36). A transition state was located for the conversion of $\mathbf{I^{NH_3}}$ to $\mathbf{J^{NH_3}}$**+PhI** ($\mathbf{TS5^{NH_3}}$), however this transition state was found to be of equal energy as $\mathbf{J^{NH_3}}$ within the DFT accuracy (ΔG^{o} = 0.4 kcal mol^{-1}) and therefore barrierless.

Table S12. Calculated $<s^2>$ and energies (in Hartree) for all relevant compounds in their described spin state.

Compound + spin state	**$<s^2>$**	**SCF** (Hartree)	**ZPE correction** (Hartree)	**Enthalpy correction 298K** (Hartree)	**Entropy correction 298K** (Hartree)	**ΔG^{o}_{298K}** (Hartree)
$\mathbf{[Co^{III}(TAML^{red})]^-}$ **(CH_2Cl_2) (A)** (Triplet)	2.0112	-4520.32285	0.39255	0.42842	0.32366	-4519.99919
$\mathbf{[Co^{III}(TAML^{sq})]}$ **(CH_2Cl_2) (H)**	0.9829	-4520.17726	0.39280	0.42873	0.32373	-4519.85353
$\mathbf{[Co^{III}(TAML^{sq})(NH_3)]}$	1.1059	-4656.79452	0.42469	0.54932	0.50358	-4656.36983
$\mathbf{[Co^{III}(TAML^{sq})(NH_3)]}$ **(CH_2Cl_2)** $\mathbf{(H^{NH_3})}$	1,3939	-4576.78333	0.43034	0.46893	0.35953	-4576.42380
$\mathbf{[Co^{III}(TAML^{red})]^-}$ (Triplet)	2.0112	-3560.45169	0.36334	0.39355	0.30505	-3560.14664
$\mathbf{[Co^{III}(TAML^{sq})]}$ (Doublet)	0.9656	-3560.30626	0.36357	0.39390	0.30453	-3560.00172
$\mathbf{[Co^{III}(TAML^{q})(NNs)]}$ (Doublet)	0.8274	-4600.19427	0.46717	0.50998	0.39150	-4599.80276
$\mathbf{[Co^{III}(TAML^{q})(NNs)]}$ **(CH_2Cl_2)** (**J**) (Doublet)	0.8247	-5560.07054	0.49681	0.54492	0.41454	-5559.65600
$\mathbf{[Co^{III}(TAML^{q})(NNs)(NH_3)]}$ **(CH_2Cl_2)** ($\mathbf{J^{NH_3}}$) (Doublet)	1.0430	-5616.66746	0.53373	0.58454	0.44956	-5616.21790
$\mathbf{[Co^{III}(TAML^{q})(NNs)]}$ **nitrene on other side** (Doublet)	0.7762	-4600.19171	0.46700	0.50989	0.39017	-4599.80154
$\mathbf{[Co^{III}(TAML^{sq})(NNs)]^-}$ (Triplet)	2.0119	-4600.35180	0.46728	0.50993	0.39198	-4599.95981
$\mathbf{[Co^{III}(TAML^{sq})(NNs)]^-}$ **(CH_2Cl_2) (C)** (Triplet)	2.0117	-5560.22788	0.49656	0.54472	0.41304	-5559.81485
$\mathbf{[Co^{III}(TAML^{q})(NNs_2)]^-}$	2.5010	-5640.20623	0.56876	0.62456	0.47452	-5639.73171

(Triplet)						
$[Co^{III}(TAML^{q})(NNs_2)]^{-}$ (CH_2Cl_2) (D) (Triplet)	2.5609	-6600,08151	0.59832	0.65948	0.49663	-6599,58488
B (Triplet)	2.0155	-5129.94635	0.55551	0.60623	0.46854	-5129.47780
TS1 (Triplet)	2.0236	-6169.82793	0.65802	0.72061	0.55568	-6169.27226
TS2 (Triplet)	2.1419	-5950.00605	0.70100	0.76377	0.60074	-5949.40531
E (Triplet)	2.0121	-5950.08751	0.70676	0.76908	0.60523	-5949.48228
TS2' (Triplet)	2.0209	-4910.14973	0.59937	0.64874	0.51937	-4909.63037
F (Triplet)	2.7854	-4910.17094	0.60137	0.65106	0.51997	-4909.65097
TS3' (Triplet)	2.1751	-4910.16529	0.60097	0.65035	0.51954	-4909.64576
G (Triplet)	2.0158	-4910.17915	0.60266	0.65249	0.51882	-4909.66034
I (Doublet)	1.0363	-5129.80207	0.55642	0.60704	0.46936	-5129.33271
I^{NH_3} (Doublet)	1.03920	-6089.67380	0.58572	0.64193	0.48921	-6089.18458
$TS5^{NH_3}$ (Doublet)	0.7601	-5186.42534	0.59483	0.64637	0.51156	-5185.91378
TS4 (Doublet)	0.8520	-4910.00333	0.59995	0.64947	0.51969	-4909.48364
$TS4^{NH_3}$ (Doublet)	1.25830	-4966.59619	0.63647	0.68901	0.55239	-4966.04380
K (Doublet)	1.1893	-4910.02506	0.60250	0.65211	0.52132	-4909.50374
TS5 (Doublet)	1.3512	-4910.02309	0.60209	0.65120	0.52164	-4909.50145
L (Doublet)	1.0044	-4910.03778	0.60319	0.65311	0.51887	-4909.51891
L^{NH_3} (Doublet)	1.12770	-4966.64258	0.55269	0.69273	0.63993	-4966.08989
NH_3 (CSS)	-	-56.58725	0.03334	0.03716	0.01427	-56.57298
DCM (CSS)	-	-959.85546	0.02825	0.03283	0.00205	-959.85341
PhI (CSS)	-	-529.60483	0.08733	0.09430	0.05615	-529.54868
PhINNs (CSS)	-	-1569.45945	0.19148	0.21078	0.14204	-1569.31742
Styrene (CSS)	-	-309.77710	0.12925	0.13718	0.09746	-309.67964
Cis-aziridine 1 (CSS)	-	-1349.70008	0.23756	0.25638	0.19045	-1349.50964
Trans-aziridine 1 (CSS)	-	-1349.70111	0.23705	0.25629	0.18627	-1349.51484

Calculations were performed at the BP86/def2-TZVP/disp3/m4-grid level of theory. Conversion from Hartree to kcal mol^{-1} can be achieved by multiplication with 627.503.

Table S13. Absolute and relative Gibbs free energies for all intermediates in the three catalytic cycles. See Table S12. [a] See general description of the computational methods for the applied correction.

Intermediate	**Gibbs free energy of formation at 298K** (kcal mol^{-1})	**Correction applied** [a] (kcal mol^{-1})	**ΔG^{o}_{298K}** (kcal mol^{-1})
Anionic bis-nitrene cycle			
A	-5000140.733	0	= 0
B	-5000149.894	+7.9	-1.26
C	-5000170.175	0	-29.44
TS1	-5000166.034	+7.9	-17.40
D	-5000170.985	0	-30.25
TS2	-5000167.345	+7.9	-18.71
E	-5000215.644	+7.9	-74.91
1-cis	-5000208.616	0	-67.88
1-trans	-5000211.879	0	-71.15
Anionic mono-nitrene cycle			
A	-4015389.344	0	= 0
B	-4015398.505	+7.9	-1.26
C	-4015398.786	0	-29.44
TS2'	-4015412.066	+7.9	-14.82
F	-4015424.992	+7.9	-27.75
TS3'	-4015421.723	+7.9	-24.48
G	-4015430.872	+7.9	-33.63
1-cis	-4015427.785	0	-38.44

1-trans	-4015431.048	0	-41.70
Neutral mono-nitrene cycle (five coordinate)			
H	-4015297.942	0	= 0
I	-4015307.461	+7.9	-1.62
J	-4015319.107	0	-21.17
TS4	-4015320.613	+7.9	-14.77
K	-4015332.605	+7.9	-26.76
TS5	-4015331.168	+7.9	-25.32
L	-4015342.124	+7.9	-36.28
1-cis	-4015334.483	0	-38.44
1-trans	-4015339.646	0	-41.70
Neutral mono-nitrene cycle (six coordinate with NH_3 as axial donor)			
$\mathbf{H}^{NH_3}$	-4050795.956	0	+1.70 (with respect to **H**)
$\mathbf{I}^{NH_3}$	-4050813.796	+7.6	-8.24
$\mathbf{J}^{NH_3}$	-4050811.869	0	-14.21
$\mathbf{TS4}^{NH_3}$	-4050811.662	+7.9	-6.11
$\mathbf{L}^{NH_3}$	-4050840.584	+7.9	-35.03
1-cis	-4050834.397	0	-38.44
1-trans	-4050837.660	0	-41.70

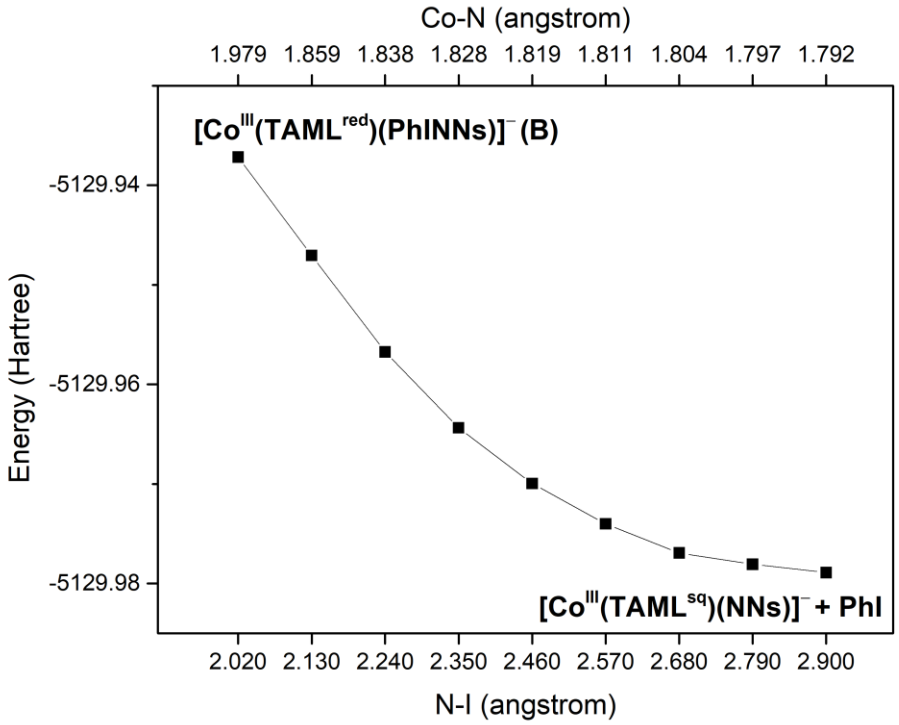


Figure S34. Energetic profile for the transition of **B** to **$[Co^{III}(TAML^{sq})(NNs)]^{-}$+PhI**.

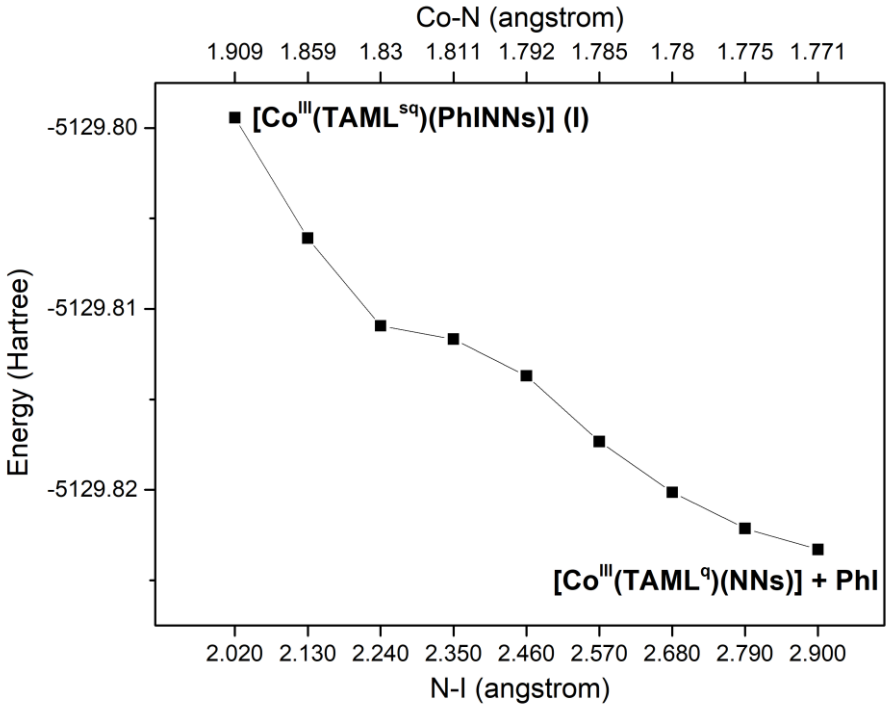


Figure S35. Energetic profile for the transition of **I** to **[Co^{III}(TAML^{q})(NNs)]+PhI**.

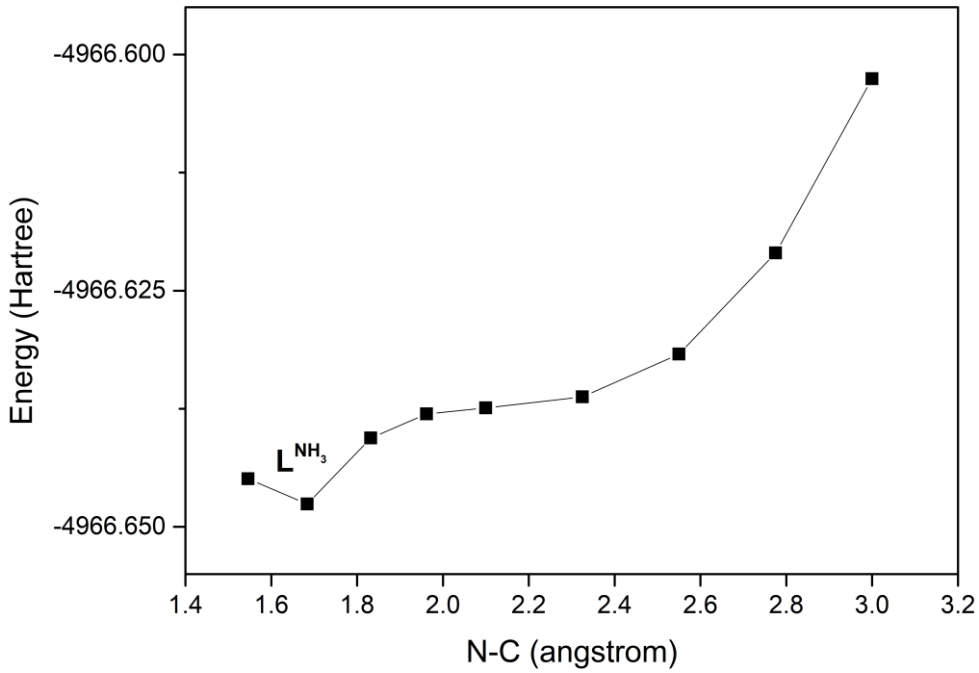
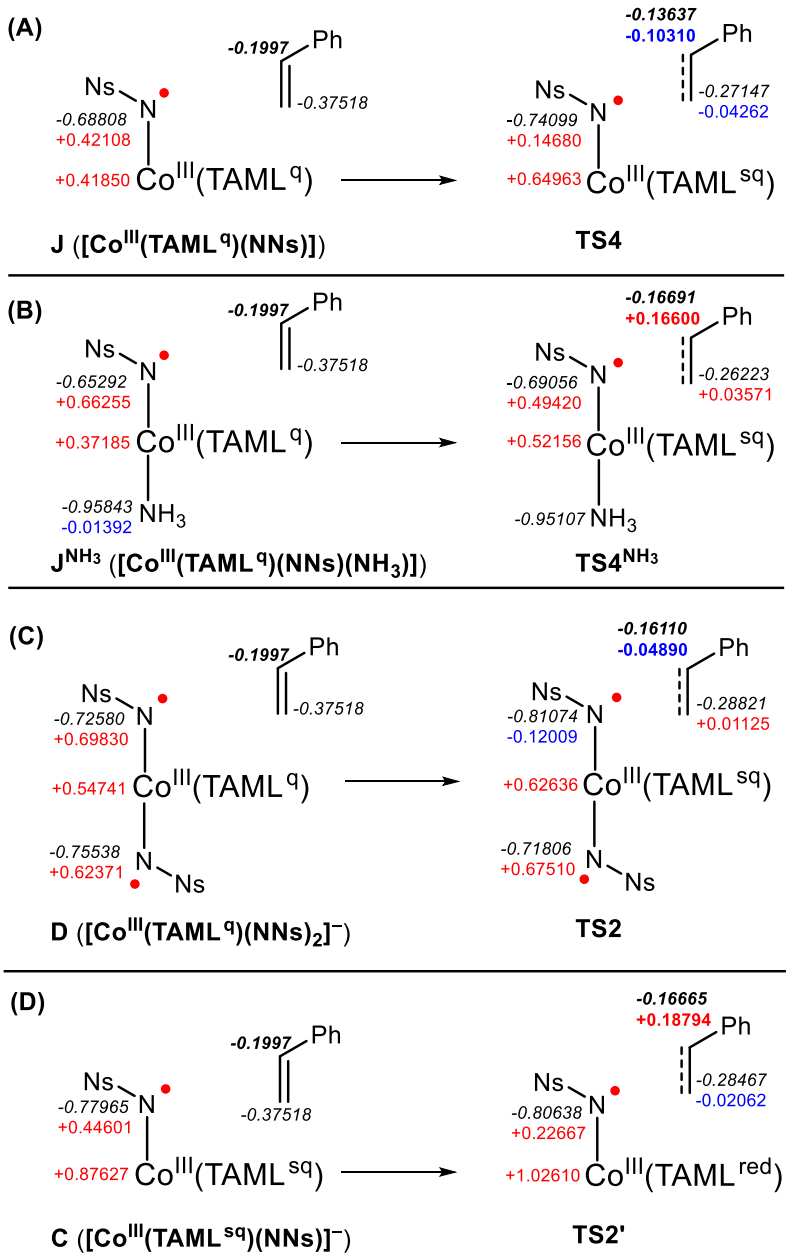
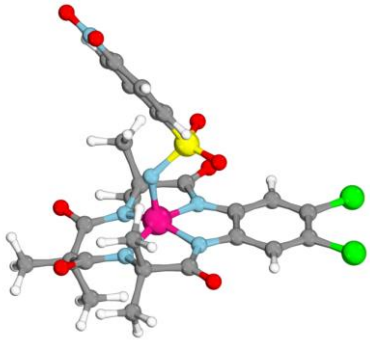
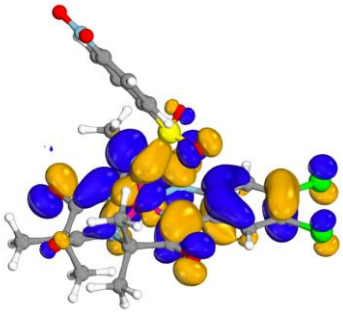
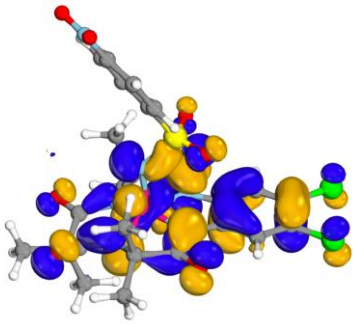
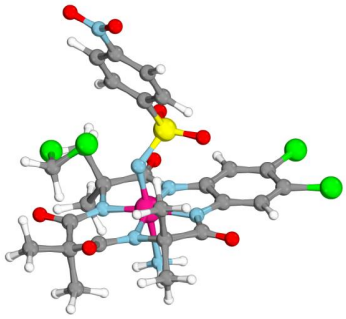
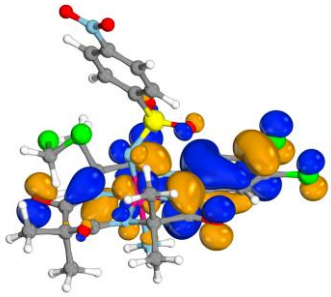
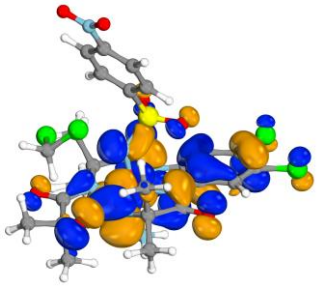
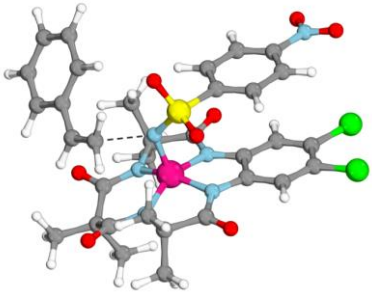
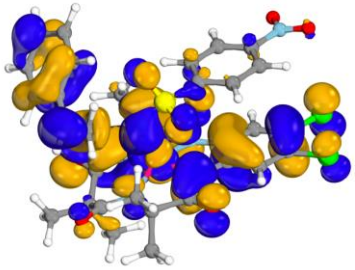
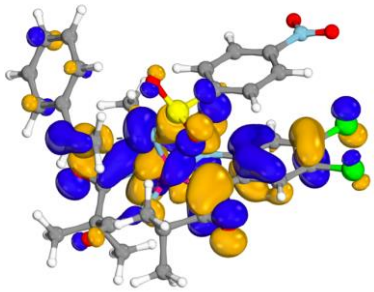
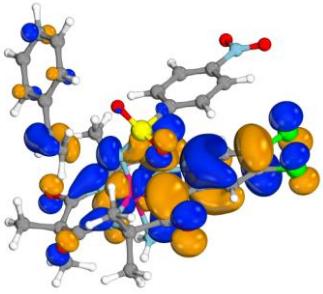
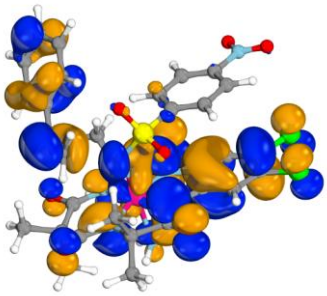


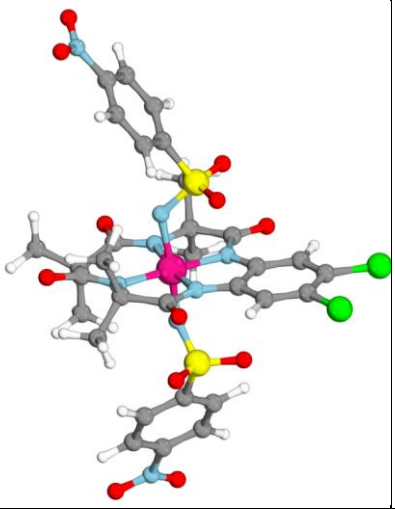
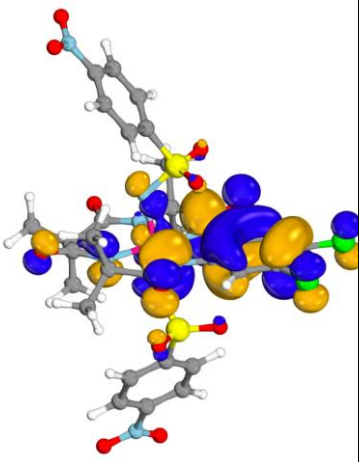
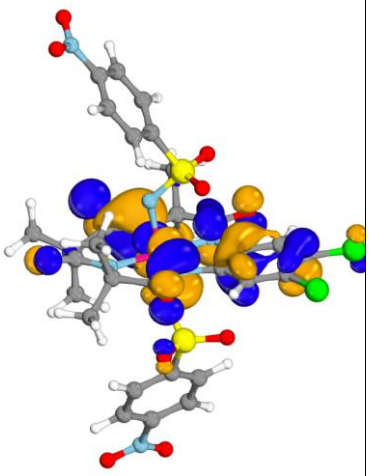
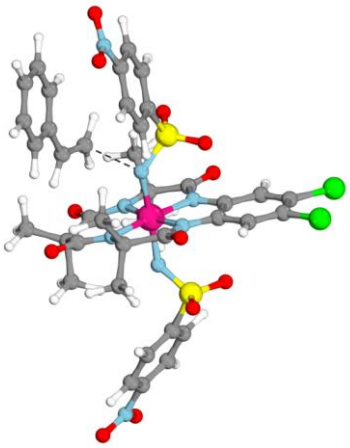
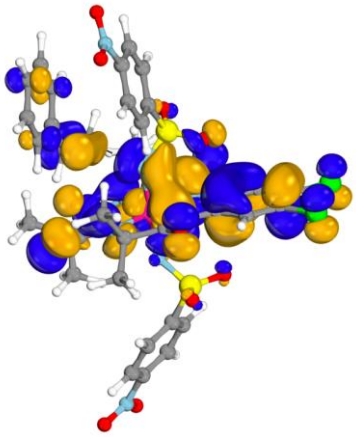
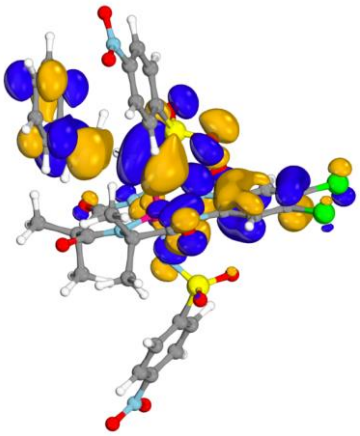
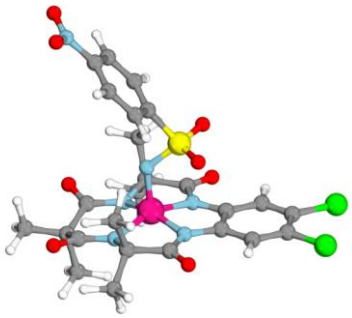
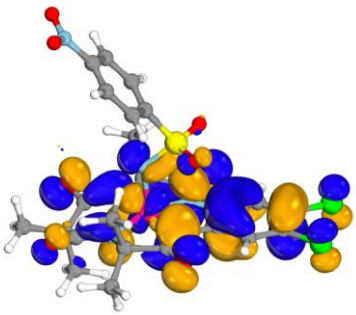
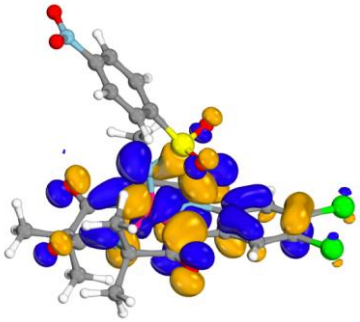
Figure S36. Energetic profile for the aziridine ring-opening starting from **L^{NH_3}**

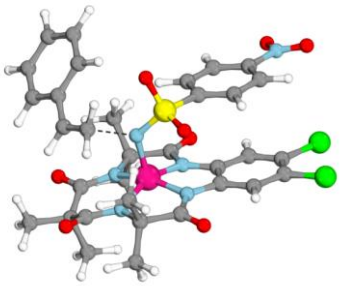
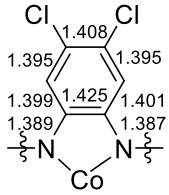
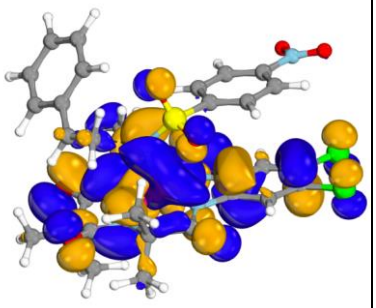
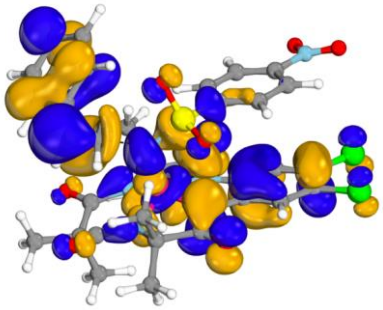


Scheme S9. NPA charges (black) and spin densities (red for α and blue for β).

Table S14. Graphical representations and α and β spin occupations of the ligand-centered redox active orbital in **C**, **D**, **J**, **J^{NH_3}** **TS2**, **TS2'**, **TS4** and **TS4^{NH_3}** and the assignment of the TAML oxidation state.

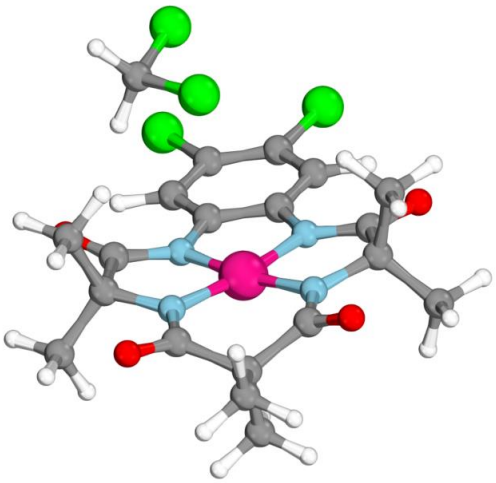
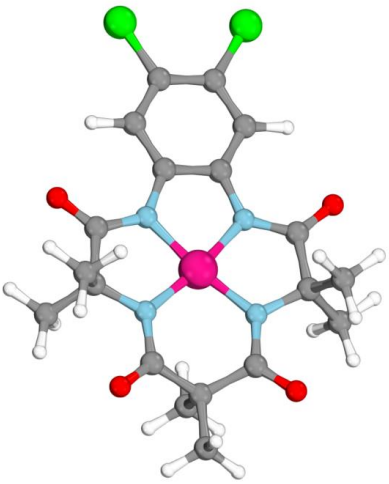
Complex and TAML oxidation state	**α spin orbital (occupation) [energy]**	**β spin orbital (occupation) [energy]**
J ($TAML^{q}$)	(0) [-0.2097 E_h]	(0) [-0.2049 E_h]
		
J^{NH_3} (+CH_2Cl_2) ($TAML^{q}$)	(0) [-0.2089 E_h]	(0) [-0.2089 E_h]
		
TS4 ($TAML^{sq}$)	(1) [-0.2145 E_h]	(0) [-0.1956 E_h]
		
TS4^{NH_3} ($TAML^{sq}$)	(0) [-0.2021 E_h]	(1) [-0.2108 E_h]
		

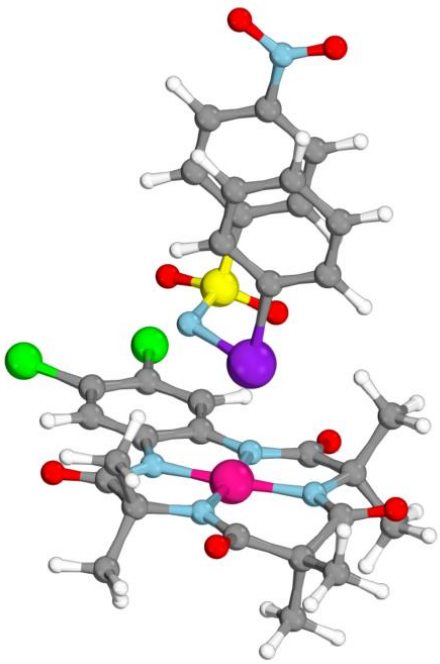
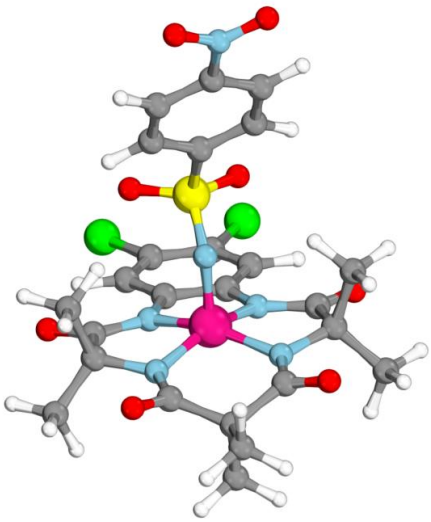
D (TAML^{q})	(0) [-0.1150 E_h]	(0) [-0.1128 E_h]
		
TS2 (TAML^{sq})	(1) [-0.1164 E_h]	(0) [-0.1032 E_h]
		
C (TAML^{sq})	(1) [-0.1055 E_h]	(0) [-0.0857 E_h]
		

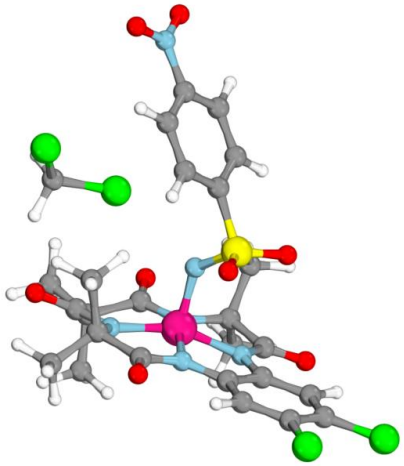
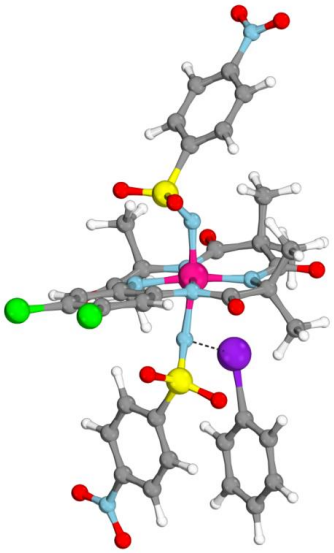
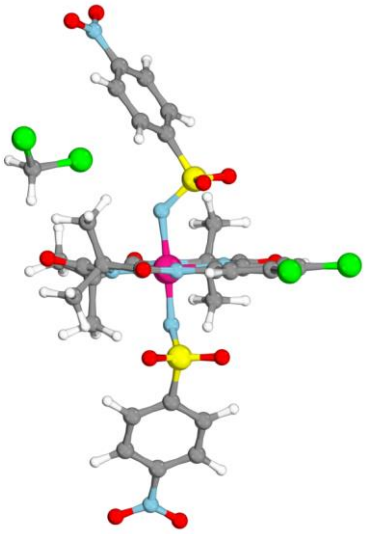
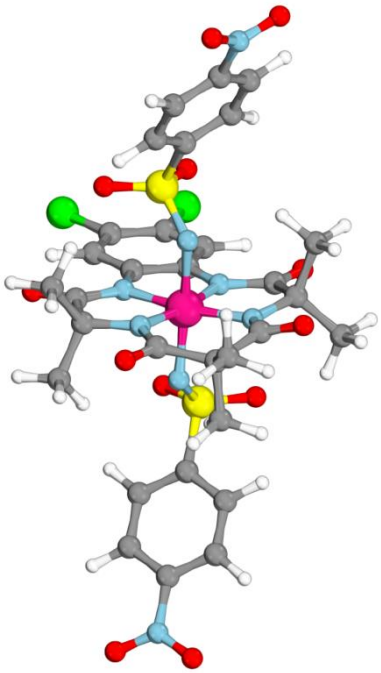
TS2' (TAML^{red})	(1) [-0.1207 E_h]	(1) [-0.0940 E_h]
 		

Graphical representations of complexes

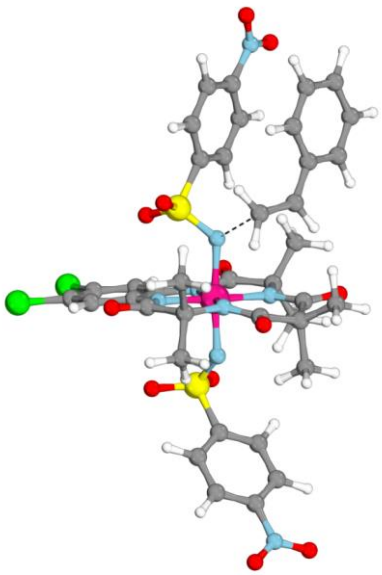
All relevant converged geometries (BP86/def2-TZVP/disp3) are depicted below.

$[Co^{III}(TAML^{red})]^{-}(CH_2Cl_2)$ (A)	$[Co^{III}(TAML^{red})]^{-}$
	

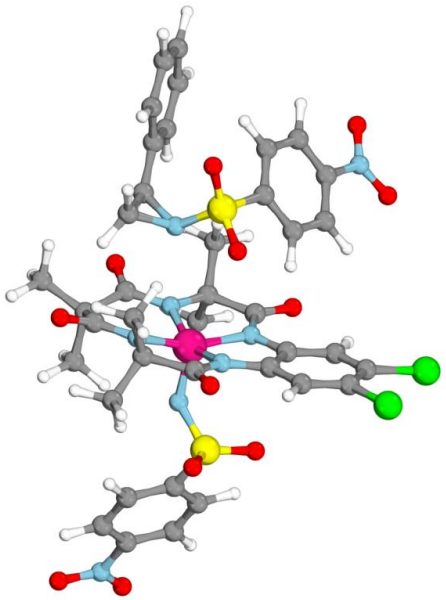
B	$[Co^{III}(TAML^{sq})(NNs)]^{-}$
	

C	TS1
	
$[Co^{III}(TAML^{q})(NNs)_2]^{-}$ (CH_2Cl_2) (D)	**$[Co^{III}(TAML^{q})(NNs)_2]^{-}$**
	

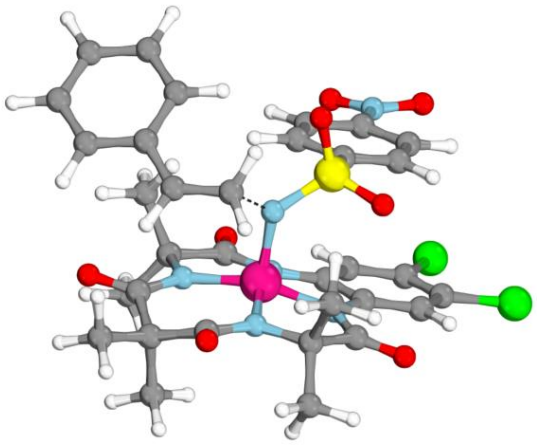
TS2



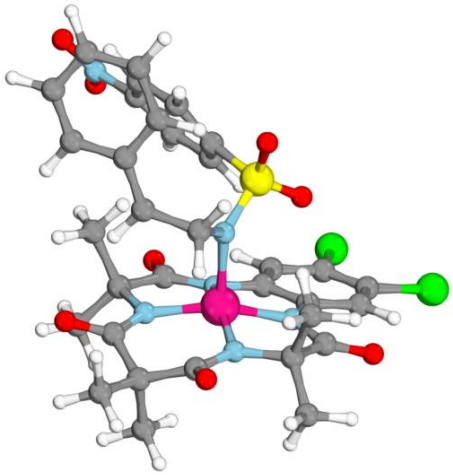
E



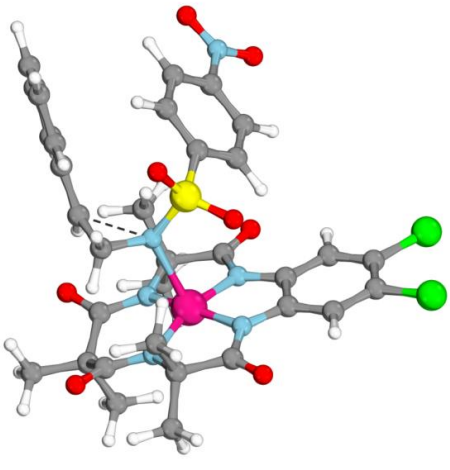
TS2’



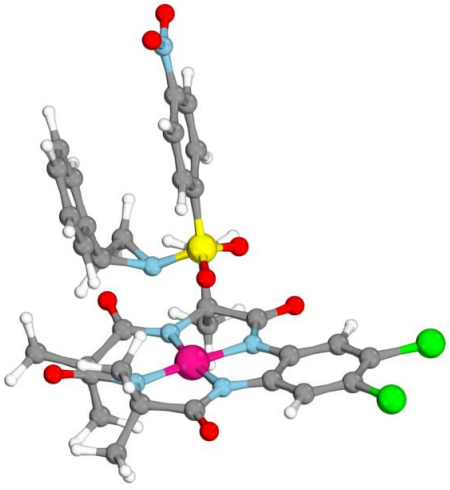
F

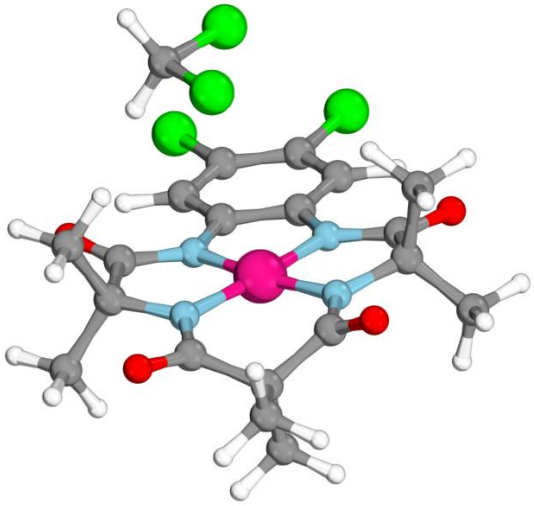
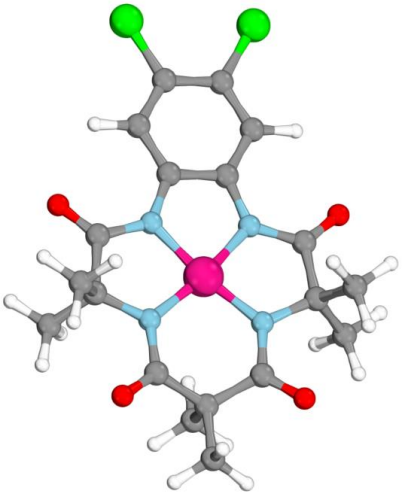


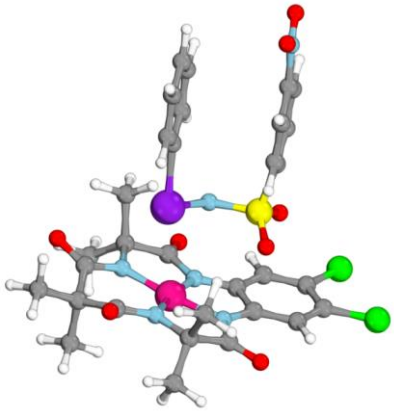
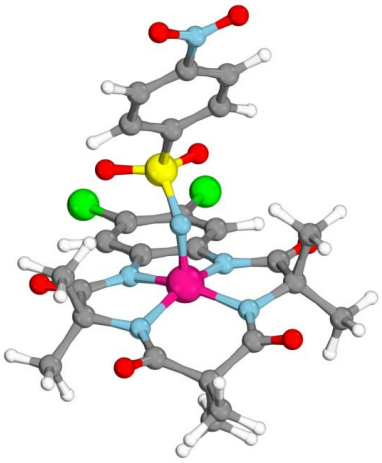
TS3’

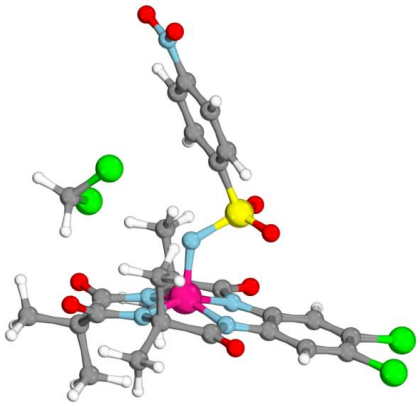
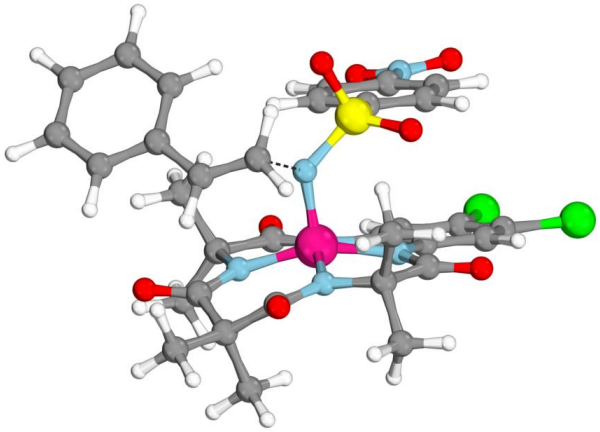


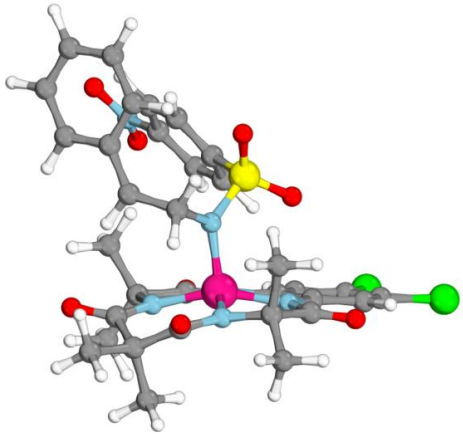
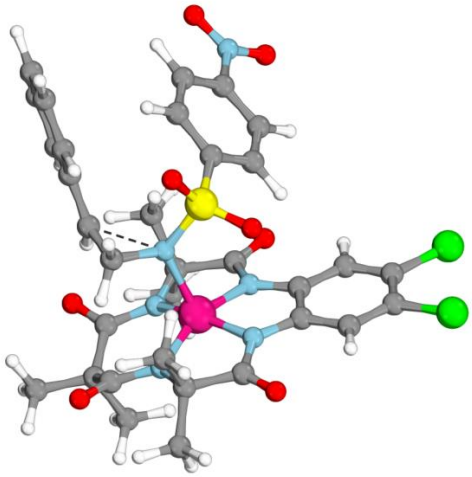
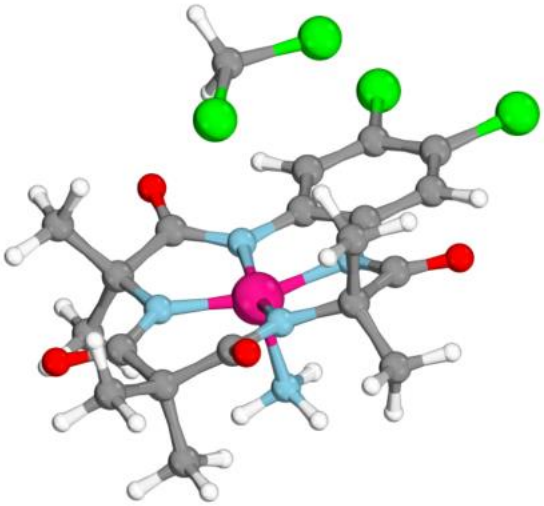
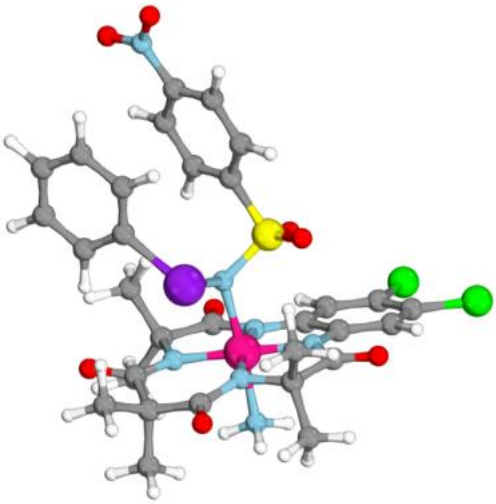
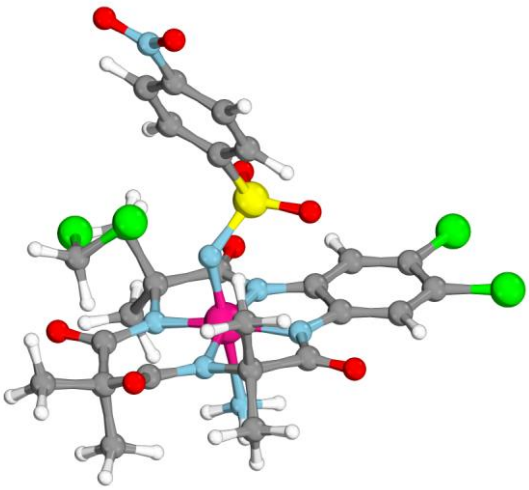
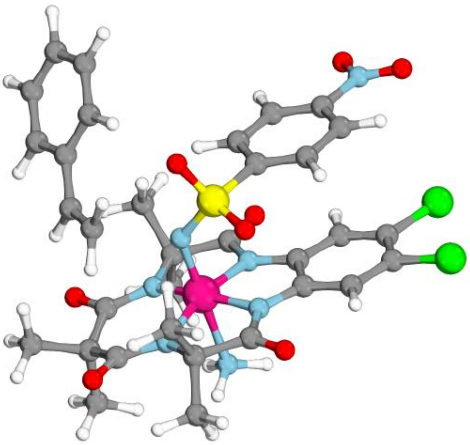
G

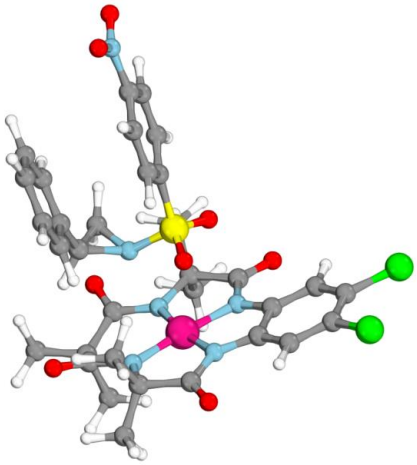
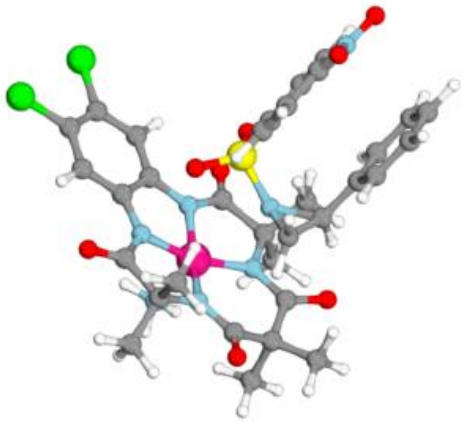
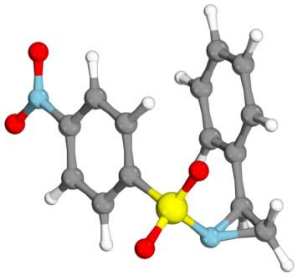
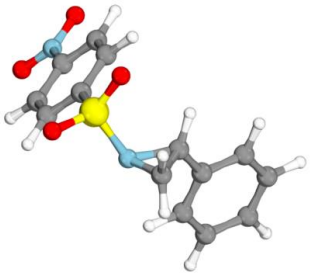


$[Co^{III}(TAML^{sq})]^{-}$ (CH_2Cl_2) (H)	$[Co^{III}(TAML^{sq})]$
	

I	$[Co^{III}(TAML^{q})(NNs)]$
	

$[Co^{III}(TAML^{q})(NNs)]$ (CH_2Cl_2) (J)	TS4
	

K	TS5
	
H^{NH_3}	I^{NH_3}
	
J^{NH_3}	$TS4^{NH_3}$
	

L	L^{NH_3}
	
Cis-aziridine 1	**Trans-aziridine 1**
	

List of xyz coordinates for all structures

$[Co^{III}(TAML^{red})]^{-}$ (CH_2Cl_2) (A)

55 atoms

Co	2.6491629	2.3745206	-0.0421946
Cl	8.4448543	5.7401529	0.7671961
O	5.6415505	1.7617190	2.4651533
O	0.9908164	-0.6123507	2.0353411
N	4.2805318	2.6017714	0.7784009
N	2.3994915	0.9384185	1.0749388
C	4.5937657	1.7581639	1.8152360
C	3.4226197	0.7960749	2.1448743
C	1.2873273	0.1394779	1.0954201
C	0.4328593	0.1121197	-0.2046062
C	5.0247895	3.6929512	0.3211100
C	6.2843959	4.1108353	0.7606090
C	6.8746220	5.2400496	0.1835495
C	2.8715611	1.2561778	3.5112966
C	3.9827442	-0.6328975	2.2165754
C	-0.8372132	-0.7059747	0.0544540
H	6.7912561	3.5596946	1.5475905
H	2.0731412	0.5800818	3.8362081
H	2.4665225	2.2747285	3.4227469
H	3.6870490	1.2631426	4.2475853
H	4.3103432	-0.9576800	1.2183862
H	3.2172700	-1.3248782	2.5838368
H	4.8515669	-0.6394569	2.8883622
H	-0.5686229	-1.7061864	0.4153556
H	-1.4248817	-0.7829937	-0.8681647
N	3.0891559	3.8899072	-0.9956396
N	1.0280081	2.4220680	-0.9136958
C	0.0298531	1.4940732	-0.7969630
C	1.2855870	-0.6038165	-1.2878387
C	4.3494739	4.4245245	-0.6992058
C	6.2173295	5.9496745	-0.8321506
C	2.0844999	4.4963328	-1.6976438
C	0.7768791	3.6669227	-1.6889694
O	-1.1260780	1.6606164	-1.2141214
H	0.7041006	-0.6979150	-2.2170472
H	1.5587335	-1.6119065	-0.9419710
C	4.9541045	5.5447733	-1.2757504
Cl	6.9323111	7.3668390	-1.5621562
O	2.1499546	5.6065305	-2.2427261
C	0.4104948	3.3656728	-3.1531809
C	-0.2917393	4.5474911	-1.0098676
H	4.4352153	6.1047008	-2.0483867
H	-0.5682430	2.8763239	-3.2051683
H	1.1665631	2.7037819	-3.6000050
H	0.3898312	4.3078955	-3.7177582
H	-0.0152962	4.7195903	0.0403429
H	-1.2651090	4.0470939	-1.0473460
H	-0.3408279	5.5153400	-1.5275953
H	2.2041776	-0.0422341	-1.4997787
H	-1.4635769	-0.2276955	0.8176025
H	2.6573128	6.4804087	-0.0236233
C	2.5546152	6.8108024	1.0146864
H	1.7565046	7.5491788	1.1307481
Cl	4.0944108	7.5783634	1.5069802
Cl	2.1382305	5.3909999	2.0209681

[$Co^{III}(TAML^{sq})$] (CH_2Cl_2) (H)

55 atoms

Co	2.5637873	2.4868912	0.0134014
Cl	8.4622119	5.6627721	0.5437238
O	5.6749118	1.7138608	2.2995931
O	0.9024492	-0.4344513	2.0734578
N	4.2326014	2.6731436	0.7453747
N	2.3652520	1.0315329	1.0765624
C	4.5855456	1.7632808	1.7537958
C	3.3906376	0.8646936	2.1431804
C	1.2330408	0.2275300	1.0917415
C	0.4387605	0.1431284	-0.2301378
C	4.9867426	3.7187986	0.2741336
C	6.2874317	4.0913280	0.6533207
C	6.8722181	5.1971167	0.0531688
C	2.8833604	1.4036805	3.5003604
C	3.8840029	-0.5847202	2.2560134
C	-0.8060467	-0.7221018	-0.0116764
H	6.8187792	3.5241733	1.4118029
H	2.0529985	0.7833828	3.8529069
H	2.5377575	2.4412093	3.3895908
H	3.7030948	1.3777247	4.2304975
H	4.1722934	-0.9689988	1.2676667
H	3.0996351	-1.2229604	2.6741620
H	4.7650751	-0.6098539	2.9095405
H	-0.5120541	-1.7103635	0.3611926
H	-1.3540500	-0.8317026	-0.9544023
N	3.0225067	3.9711188	-0.9583175
N	0.9897223	2.4872364	-0.9018523
C	0.0104264	1.5097475	-0.8211218
C	1.3627954	-0.5308565	-1.2853401
C	4.2783454	4.4805248	-0.7249497
C	6.1738708	5.9454700	-0.9433506
C	2.0028291	4.5582610	-1.7120005
C	0.7202291	3.7015809	-1.7264198
O	-1.1291318	1.6653402	-1.2573762
H	0.8137188	-0.6497849	-2.2296482
H	1.6641645	-1.5265335	-0.9311824
C	4.8892643	5.5895865	-1.3312941
Cl	6.9058236	7.3273421	-1.6758870
O	2.0864661	5.6515184	-2.2554997
C	0.4306930	3.3429414	-3.1966474
C	-0.4035816	4.5686027	-1.1225068
H	4.3556609	6.1692609	-2.0784822
H	-0.5286933	2.8216787	-3.2740186
H	1.2246801	2.6968395	-3.5968642
H	0.3939854	4.2655999	-3.7900954
H	-0.1952523	4.7727153	-0.0635832
H	-1.3612511	4.0465585	-1.2057014
H	-0.4492885	5.5209368	-1.6668878
H	2.2646873	0.0652410	-1.4721515
H	-1.4790716	-0.2673632	0.7244548
H	2.5189555	6.4792276	0.2485905
C	2.5010377	6.6369456	1.3316075
H	1.9281674	7.5272022	1.6034398
Cl	1.7024864	5.2229329	2.0893841
Cl	4.1803178	6.8600337	1.8937305

[$Co^{III}(TAML^{red})$]$^{-}$

50 atoms

Co	0.00000000	0.00000000	0.00000000
Cl	5.91572996	3.24889119	-0.21671688
O	3.69837564	-1.39281770	0.11496289
O	-0.89721875	-3.87637713	0.46127304
N	1.84121319	-0.00000000	-0.00000000
N	0.10130006	-1.83417955	0.08321454
C	2.47853102	-1.21061592	0.11031340
C	1.47162427	-2.37726475	0.28717294
C	-0.96842886	-2.68823629	0.11341613
C	-2.31088775	-2.13796554	-0.44631171
C	2.43165107	1.26628321	-0.06912997
C	3.79618126	1.56898599	-0.10565882
C	4.20081718	2.90689750	-0.16912990
C	1.66885021	-2.90061310	1.72518073
C	1.81421360	-3.45653377	-0.75261499
C	-3.42318480	-3.15381400	-0.16064899
H	4.52811552	0.76675420	-0.08245526
H	1.03627490	-3.77830844	1.89077779
H	1.39164114	-2.11751184	2.44578363
H	2.72666091	-3.15955525	1.87306752
H	1.61359804	-3.07885362	-1.76524381
H	1.21237618	-4.35546211	-0.58188554
H	2.88282206	-3.69848085	-0.67507433
H	-3.14700549	-4.13294344	-0.57079594
H	-4.36413559	-2.80975429	-0.60541919
N	0.15367748	1.83436104	-0.04534075
N	-1.82096675	0.25541064	0.03113656
C	-2.76270289	-0.73900409	0.06202965
C	-2.12426189	-2.00658277	-1.98376687
C	1.46544029	2.31545307	-0.09459288
C	3.25089839	3.93938912	-0.19340626
C	-1.00108668	2.57227350	0.01742018
C	-2.25246269	1.67077675	0.18345543
O	-3.94968385	-0.56022656	0.37129456
H	-3.06415631	-1.67006085	-2.44617413
H	-1.85353767	-2.98307262	-2.41169792
C	1.88255658	3.64900517	-0.15556673
Cl	3.73645542	5.61867917	-0.27438339
O	-1.08119365	3.80346649	-0.01019720
C	-3.26937155	2.07328798	-0.89729574
C	-2.79876282	1.94944388	1.60015257
H	1.14438948	4.44460727	-0.17120729
H	-4.21992415	1.55230050	-0.73950543
H	-2.88025746	1.81540336	-1.89219360
H	-3.42390770	3.15983842	-0.85309505
H	-2.06245752	1.62655504	2.35099631
H	-3.73213816	1.39782631	1.75397558
H	-2.97077331	3.02837493	1.71397790
H	-1.33328776	-1.28365266	-2.22086596
H	-3.57969736	-3.27018745	0.91894493

[$Co^{III}(TAML^{sq})$]

50 atoms

Co	0.00000000	0.00000000	0.00000000
Cl	5.91183043	3.19855482	0.07626219
O	3.67184872	-1.41981401	-0.09650990
O	-0.91283757	-3.82499388	0.52360897
N	1.83189220	-0.00000000	0.00000000
N	0.09300983	-1.81369079	0.05020869
C	2.46727401	-1.25030618	0.00429124
C	1.45808198	-2.40069155	0.19522297
C	-1.00026247	-2.66762829	0.11522708
C	-2.33472146	-2.14165930	-0.45610981
C	2.43935753	1.23180122	-0.00810088
C	3.81493412	1.52281790	0.01767415
C	4.22020960	2.85010104	0.02690732

C	1.71814258	-2.95271728	1.61393826
C	1.72675882	-3.46079223	-0.88483736
C	-3.45133684	-3.13280369	-0.11071600
H	4.54351411	0.71806148	0.03435599
H	1.09739317	-3.83656640	1.79031828
H	1.47707491	-2.19046017	2.36891408
H	2.77931038	-3.21898196	1.70386617
H	1.49581073	-3.05870410	-1.88094033
H	1.11220354	-4.34882399	-0.70431753
H	2.78817717	-3.73852289	-0.85880365
H	-3.18881921	-4.13361287	-0.47210980
H	-4.39406754	-2.80892206	-0.56602856
N	0.18540939	1.82217037	-0.05240710
N	-1.79881655	0.27073652	-0.04383765
C	-2.76626978	-0.72330713	-0.02093609
C	-2.14770554	-2.07873357	-2.00067330
C	1.47155876	2.30253844	-0.03510712
C	3.26136278	3.91062895	0.00300469
C	-0.99324076	2.57933082	-0.10128335
C	-2.25054564	1.69380095	0.00525896
O	-3.94551384	-0.49496091	0.24610404
H	-3.08850708	-1.76003731	-2.47184116
H	-1.88735016	-3.07565974	-2.38075525
C	1.90030670	3.64075683	-0.03182913
Cl	3.77943039	5.55873304	0.02630385
O	-1.03416839	3.79627239	-0.19584093
C	-3.16085849	2.03034102	-1.18918204
C	-2.91750957	2.05869427	1.35012327
H	1.17424379	4.44814188	-0.04937975
H	-4.11744426	1.50696371	-1.09542783
H	-2.67796435	1.73329376	-2.13114656
H	-3.33572850	3.11346675	-1.21225004
H	-2.27291869	1.76070661	2.18830936
H	-3.87935656	1.54561716	1.44138240
H	-3.06955509	3.14545604	1.38692028
H	-1.35382312	-1.37241500	-2.27704766
H	-3.60121629	-3.19205380	0.97473164

[Co^{III}($TAML^{q}$)(NNs)]

67 atoms

Cl	5.86235270	3.09074634	-1.15900557
O	3.64699355	-1.43658346	-0.38560091
O	-0.98127249	-3.82943762	-0.17457615
N	1.81196334	-0.02275419	-0.36133240
N	0.10042343	-1.82766342	-0.37241448
C	2.44288814	-1.28246774	-0.30921040
C	1.42860410	-2.42048212	-0.10741805
C	-1.00107420	-2.64461653	-0.50638313
C	-2.23328091	-2.03168825	-1.20046999
C	2.41393107	1.18936588	-0.53138177
C	3.77652104	1.45552209	-0.75894815
C	4.18501526	2.76776117	-0.91745698
C	1.56738101	-2.90322184	1.35387360
C	1.78666626	-3.53548843	-1.10564972
C	-3.38182339	-3.04412363	-1.18898945
H	4.49637829	0.64260426	-0.77568559
H	0.90937053	-3.76676580	1.50417671
H	1.27396996	-2.10475550	2.04665528
H	2.61014948	-3.18744196	1.54631806
H	1.60528482	-3.20012718	-2.13632503
H	1.18584405	-4.42769839	-0.90973122
H	2.85110584	-3.77491462	-0.99820448
H	-3.06178426	-3.97479767	-1.67144028
H	-4.24743059	-2.63336475	-1.72257293
N	0.18874673	1.82017290	-0.32497888
N	-1.77890128	0.30669823	-0.45081087
C	-2.71052787	-0.70912677	-0.58093192
C	-1.81012403	-1.71724630	-2.66383204
C	1.46245324	2.27373385	-0.48802243
C	3.24135766	3.84673446	-0.85701721
C	-0.99019637	2.58483256	-0.31650714
C	-2.23864424	1.69132066	-0.19286103
O	-3.89181597	-0.53463306	-0.28320658
H	-2.66849014	-1.31014438	-3.21699085
H	-1.48298172	-2.64173845	-3.15829656
C	1.89524326	3.60321056	-0.64577057
Cl	3.77152811	5.47943830	-1.02639983
O	-1.01729784	3.79677183	-0.40918798
C	-3.24350734	2.17295851	-1.25550684
C	-2.79613871	1.86405549	1.23641034
H	1.18052892	4.41861860	-0.58417391
H	-4.19916570	1.65550280	-1.13431825
H	-2.85493705	1.98254641	-2.26560503
H	-3.38965027	3.25334559	-1.13541514
H	-2.10003236	1.43931807	1.96864943
H	-3.75910980	1.34786626	1.31006032
H	-2.92102221	2.93414225	1.44725964
H	-0.99058668	-0.98876572	-2.69615233
H	-3.69089693	-3.27839525	-0.16429664
Co	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.76681635
S	0.88037563	1.05034012	2.66758455
O	2.31206854	0.83646762	2.43954954
O	0.36176248	2.41623726	2.60881897
H	-1.27866839	1.63110085	4.48535016
C	-0.68470749	0.83385328	4.92955367
C	0.92014519	-1.19589074	6.04011392
C	0.45098187	0.35817074	4.26326484
C	-1.02446910	0.28610094	6.16360043
C	-0.21686009	-0.72050708	6.69473317
C	1.25677848	-0.64877492	4.80472235
H	-1.89602545	0.62552806	6.71867228
H	2.14131896	-0.98208063	4.26413987
H	1.51973199	-1.97726781	6.50238607
N	-0.58094848	-1.30771581	8.01445607
O	0.15492615	-2.18827965	8.46689926
O	-1.59455340	-0.87732213	8.56839141

[Co^{III}($TAML^{q}$)(NNs)]

67 atoms

Co	2.3228155	3.2069426	-0.2052319
Cl	6.7221491	7.8894063	1.8558106
O	4.8659030	3.2321893	2.8401195
O	0.6586421	0.3438485	2.0461139
N	3.6258029	3.8395979	0.9809166
N	1.9430378	1.9870030	1.1283947
C	3.9423890	3.0265095	2.0727997
C	2.9123290	1.9054034	2.2550967
C	0.9249490	1.0478626	1.0708764
C	0.2515442	0.7470295	-0.2732029
C	4.0832080	5.1062083	0.7613916
C	5.1386455	5.7683300	1.4121744
C	5.4035077	7.0877407	1.0818965
C	2.2513482	2.1873975	3.6245231
C	3.6636966	0.5618926	2.2382551
C	-1.0453082	-0.0411859	-0.0216800

H	5.7440669	5.2405419	2.1421764
H	1.5901244	1.3621894	3.9001688
H	1.6659644	3.1164472	3.5821131
H	3.0447646	2.3033793	4.3742342
H	4.1092827	0.3945777	1.2494387
H	2.9804539	-0.2566329	2.4878926
H	4.4720675	0.6059127	2.9794157
H	-0.8259454	-0.9489706	0.5508460
H	-1.5013291	-0.3096719	-0.9804158
N	2.2972871	4.9835812	-0.7265402
N	0.6751640	3.0801479	-1.0974807
C	-0.0668642	1.9345956	-1.1966963
C	1.2646929	-0.1499515	-1.0458528
C	3.2916296	5.7872532	-0.2260077
C	4.6118132	7.7690150	0.1054531
C	1.3321092	5.3453917	-1.6719988
C	0.4213632	4.1770379	-2.0619566
O	-0.9447880	1.7922883	-2.0564468
H	0.8096067	-0.4625935	-1.9950471
H	1.4921237	-1.0420049	-0.4463422
C	3.5599890	7.1294118	-0.5372955
Cl	4.9572933	9.4072569	-0.3132443
O	1.2571653	6.4609113	-2.1621379
C	0.8561418	3.7594672	-3.4874420
C	-1.0284816	4.6928096	-2.0263335
H	2.9660047	7.6502295	-1.2811321
H	0.1849677	2.9744909	-3.8525739
H	1.8850064	3.3727479	-3.4708985
H	0.8061206	4.6320451	-4.1516065
H	-1.3378827	4.8904877	-0.9908045
H	-1.7060215	3.9571279	-2.4669172
H	-1.0773132	5.6323757	-2.5916804
H	2.1977268	0.3890287	-1.2614041
H	-1.7655549	0.5580986	0.5506193
N	3.3393824	2.4428930	-1.3981242
S	4.9801949	2.5631920	-1.4167664
O	5.3678583	3.9324624	-1.7527701
O	5.6015536	1.9077150	-0.2684108
C	5.2422929	1.5208777	-2.8514895
C	5.6044755	-0.0764660	-5.0519991
C	5.4173251	0.1446690	-2.6714486
C	5.2487370	2.1055149	-4.1223762
C	5.4356837	1.2960414	-5.2398363
C	5.6016274	-0.6671022	-3.7876916
H	5.4220573	-0.2744801	-1.6660552
H	5.1216143	3.1827007	-4.2236461
H	5.4533612	1.7069934	-6.2473950
H	5.7454951	-1.7418925	-3.6959960
N	5.7987256	-0.9442902	-6.2471960
O	5.9427195	-2.1532558	-6.0534157
O	5.8014878	-0.3967712	-7.3517395

[Co^{III}(TAML^{sq})(NNs)]$^{-}$

67 atoms

Cl	3.60628844	-5.64316688	-0.85985110
O	-1.14498320	-3.75579178	-0.49227461
O	-3.92792988	0.63374977	-0.04972282
N	0.12256161	-1.82170578	-0.35978693
N	-1.82719846	-0.23412533	-0.35274259
C	-1.06003207	-2.53949323	-0.35164734
C	-2.28481224	-1.62444890	-0.13466058
C	-2.73906015	0.78619401	-0.36215640
C	-2.26093518	2.14121159	-0.93571800
C	1.40346604	-2.32164697	-0.48206538
C	1.79279447	-3.66363352	-0.60069800
C	3.14495504	-3.96809824	-0.71362359
C	-2.76298316	-1.85570549	1.31548326
C	-3.35917588	-2.04138196	-1.15399507
C	-3.36084045	3.18911910	-0.73563537
H	1.04222994	-4.44755225	-0.59000230
H	-3.68535868	-1.28888703	1.48470175
H	-1.99352221	-1.51015109	2.01766162
H	-2.94024485	-2.92871760	1.47342298
H	-3.02793569	-1.79736649	-2.17355801
H	-4.29892363	-1.51950575	-0.94927873
H	-3.50579430	-3.12718243	-1.08530877
H	-4.29880465	2.83464847	-1.17957057
H	-3.06131648	4.13715667	-1.19825155
N	1.82595807	-0.03294702	-0.34580013
N	0.13962572	1.83518502	-0.36827292
C	-0.92337885	2.69584883	-0.38760966
C	-2.03502678	1.90692005	-2.45633775
C	2.38897565	-1.28764460	-0.47086431
C	4.12099716	-2.94466066	-0.69982025
C	2.48290678	1.18585250	-0.35641038
C	1.50645198	2.36593878	-0.16444086
O	-0.82712259	3.89884972	-0.10796297
H	-1.73633631	2.84992720	-2.93758401
H	-2.96775420	1.55518578	-2.92145194
C	3.75017855	-1.61030974	-0.57437264
Cl	5.81811151	-3.32362695	-0.82810959
O	3.69292992	1.32842396	-0.50004423
C	1.86616754	3.43406127	-1.21257367
C	1.71800373	2.89090354	1.27200901
H	4.49652629	-0.82276830	-0.54547257
H	1.29871237	4.35145617	-1.02871971
H	1.63508652	3.06559743	-2.22233681
H	2.94353786	3.63590056	-1.15271576
H	1.43223986	2.11608544	1.99412602
H	1.09720065	3.78080596	1.42489554
H	2.77927594	3.13625401	1.41556444
H	-1.25059157	1.15827931	-2.62187967
H	-3.53766284	3.37200804	0.33150601
Co	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.77996626
S	1.00864913	-0.87697696	2.68761829
O	0.82872314	-2.32571214	2.55058439
O	2.38209492	-0.36271614	2.68792043
H	1.45612955	1.38611860	4.42864753
C	0.68625852	0.77312668	4.89633790
C	-1.27159856	-0.87469260	6.06004421
C	0.26840072	-0.40387538	4.26521408
C	0.12365879	1.13413811	6.11662811
C	-0.84865332	0.30327400	6.68155403
C	-0.70514514	-1.22868879	4.83877374
H	0.42254832	2.04113215	6.63820013
H	-0.99727206	-2.14416657	4.32524321
H	-2.03014676	-1.49110211	6.53840400
N	-1.44280350	0.67878729	7.98211990
O	-2.29645438	-0.07395822	8.46779788
O	-1.05331911	1.72475223	8.51624500

[Co^{III}(TAML^{sq})(NNs)]$^{-}$ (CH_2Cl_2)

72 atoms

Cl	8.1657393	7.2869632	0.6554561
O	5.3440610	3.4873242	2.6256924

O	0.9500193	0.7560061	2.0965661
N	3.9928697	4.2002146	0.8861468
N	2.2365255	2.4086872	1.1666031
C	4.3017612	3.4144071	1.9825922
C	3.1734257	2.4129183	2.3147455
C	1.2019866	1.5267534	1.1499487
C	0.4114803	1.3748114	-0.1702627
C	4.7527649	5.2174176	0.3436634
C	6.0017519	5.6819221	0.7810468
C	6.6135441	6.7250700	0.0945718
C	2.4882123	2.9107913	3.6048951
C	3.8402184	1.0405947	2.5210677
C	-0.8438836	0.5338100	0.0869988
H	6.4688882	5.2365410	1.6536409
H	1.7998489	2.1440222	3.9760166
H	1.9182335	3.8228364	3.3908840
H	3.2499350	3.1286180	4.3659564
H	4.2621581	0.6786553	1.5725062
H	3.1083820	0.3144823	2.8869105
H	4.6571238	1.1540454	3.2455624
H	-0.5694387	-0.4122582	0.5676320
H	-1.3638438	0.3399405	-0.8583332
N	2.8964100	5.2422427	-1.0674047
N	0.9670809	3.6215356	-1.0872914
C	0.0004833	2.6698817	-0.9114030
C	1.3597514	0.6149240	-1.1405449
C	4.1190710	5.8198921	-0.7860307
C	5.9862979	7.3213945	-1.0242023
C	2.0402436	5.5503766	-2.1099506
C	0.7327206	4.7321914	-2.0387314
O	-1.1252943	2.7474606	-1.4221466
H	0.8441801	0.4262984	-2.0935793
H	1.6484163	-0.3500567	-0.6986489
C	4.7433774	6.8777983	-1.4631498
Cl	6.7449905	8.6368333	-1.8806784
O	2.2730579	6.3760088	-2.9875115
C	0.4284230	4.2163799	-3.4554779
C	-0.3629600	5.7004763	-1.5406566
H	4.2511413	7.3429954	-2.3114186
H	-0.5638852	3.7560798	-3.4858077
H	1.1791464	3.4715357	-3.7560772
H	0.4758260	5.0611657	-4.1549248
H	-0.1240674	6.0372238	-0.5240374
H	-1.3277885	5.1814715	-1.5363180
H	-0.4029643	6.5750596	-2.2045224
H	2.2650550	1.2030874	-1.3359296
H	-1.5380324	1.0714490	0.7457116
Co	2.2817538	4.0176391	0.1877030
N	1.3879701	5.0933457	1.2660974
S	1.8645211	6.5296922	1.8374309
O	3.0814461	6.4826814	2.6518402
O	1.7522642	7.5963748	0.8385652
H	-0.8445396	7.4464788	1.4365587
C	-0.7690149	7.1143818	2.4714188
C	-0.5012118	6.2359946	5.1276237
C	0.4620436	6.6637519	2.9617955
C	-1.8786689	7.1181823	3.3096415
C	-1.7287385	6.6729628	4.6259032
C	0.6052435	6.2339346	4.2841642
H	-2.8563714	7.4452336	2.9622318
H	1.5778475	5.8890225	4.6321591
H	-0.4348852	5.8897964	6.1561847
N	-2.9089108	6.6565658	5.5142251
O	-2.7469968	6.2958876	6.6861873
O	-3.9967197	7.0063989	5.0382237
C	-1.3217964	2.2414045	3.5923827
H	-0.5831221	1.4783201	3.3197747
H	-2.3510397	1.8756188	3.5429690
Cl	-1.0139730	2.7454899	5.2923119
Cl	-1.1405453	3.5815626	2.4328322

$[Co^{III}(TAML^{q})(NNS_2)]^{-}$

84 atoms

Cl	5.87098453	3.17790786	-0.76188406
O	3.68927528	-1.40630862	-0.18691703
O	-0.76840380	-3.81349011	1.01313317
N	1.84467067	-0.00145765	-0.17055782
N	0.13226769	-1.88746148	0.19681052
C	2.48733926	-1.24477193	-0.05522920
C	1.52093776	-2.37766657	0.35062658
C	-0.91483672	-2.66359629	0.55258173
C	-2.36041824	-2.18628798	0.23891337
C	2.41637611	1.21861458	-0.30755660
C	3.78728894	1.51152707	-0.45794697
C	4.18291292	2.82883914	-0.56720158
C	1.87483133	-2.68947532	1.82676873
C	1.79059511	-3.59214219	-0.55366921
C	-3.33547357	-3.03239139	1.07731729
H	4.50887701	0.70244443	-0.49271694
H	1.27218147	-3.53550330	2.17070307
H	1.65369472	-1.81685795	2.45546938
H	2.94418925	-2.92995833	1.89934670
H	1.52369785	-3.34861680	-1.58970794
H	1.19835507	-4.44386331	-0.20301001
H	2.86016375	-3.83778437	-0.51418715
H	-3.16428781	-4.09686775	0.88798553
H	-4.36704390	-2.76584336	0.82243541
N	0.17944717	1.85597866	-0.10552697
N	-1.84783905	0.28962220	0.27101258
C	-2.77556801	-0.69493995	0.39045447
C	-2.57017760	-2.50324007	-1.27024612
C	1.44579373	2.29951667	-0.27033417
C	3.22523877	3.89589485	-0.52272279
C	-1.00403985	2.59232112	-0.04262824
C	-2.26504073	1.70688021	0.12538124
O	-3.98980994	-0.44358933	0.49960299
H	-3.61362698	-2.29424839	-1.54505674
H	-2.35470451	-3.56595828	-1.45452402
C	1.87718753	3.63790869	-0.37488179
Cl	3.74725200	5.54508027	-0.65254068
O	-1.06344129	3.80741423	-0.15295606
C	-3.08169708	1.88963408	-1.17773942
C	-3.03444733	2.22971672	1.35231460
H	1.14914691	4.44231514	-0.33259531
H	-4.03521876	1.35806925	-1.08305976
H	-2.52097403	1.47623154	-2.02721100
H	-3.26347861	2.95944273	-1.34222016
H	-2.44546605	2.05382482	2.25990651
H	-3.99784815	1.71878126	1.42606982
H	-3.18388232	3.31171343	1.23968122
H	-1.90784820	-1.88391188	-1.88970826
H	-3.18193081	-2.85151525	2.14996329
N	-0.40187660	-0.13474964	-1.84117944
S	0.69663461	-0.15960152	-3.00235967
O	1.28048435	1.17540205	-3.19632599
O	1.61773892	-1.30011537	-2.93687687

C	-0.39049112	-0.47216790	-4.40278992
C	-2.11312310	-0.95678955	-6.49944702
C	-0.74909982	-1.79053217	-4.70756764
C	-0.88959502	0.60362283	-5.14567257
C	-1.75867308	0.36291312	-6.20538910
C	-1.62000193	-2.03845686	-5.76402579
H	-0.33865497	-2.60789191	-4.11603226
H	-0.58336429	1.61740317	-4.88696205
H	-2.16488800	1.17314803	-6.80757083
H	-1.92217392	-3.05003922	-6.02879401
Co	0.00000000	0.00000000	0.00000000
N	-0.00000000	-0.00000000	1.96048463
S	0.65730101	1.14363992	2.87329465
O	2.11451810	1.21280286	2.68732736
O	-0.09081141	2.40558933	2.85651715
H	-1.60810120	1.21332522	4.66086081
C	-0.84063114	0.60625440	5.14051873
C	1.18447506	-0.93210563	6.33487852
C	0.38837282	0.41490012	4.49944868
C	-1.06435220	0.02665047	6.38472538
C	-0.04631806	-0.73670763	6.96548687
C	1.40092803	-0.34754198	5.08991290
H	-2.00755087	0.15363551	6.91313248
H	2.35167713	-0.46802215	4.57123604
H	1.94877442	-1.53112085	6.82507467
N	-3.03163218	-1.21683633	-7.62719776
O	-3.33316640	-2.39194683	-7.86915936
O	-3.44704062	-0.24522027	-8.27124362
N	-0.27762154	-1.34770169	8.29062045
O	0.63817296	-2.01508376	8.78851061
O	-1.37384966	-1.15782309	8.83242118

B

79 atoms

Co	-0.4047375	0.1738483	0.3998018
Cl	4.9100708	4.2545649	1.0259531
O	2.8455757	-0.1889679	2.6044413
O	-1.7010675	-2.8069889	2.7194406
N	1.2227650	0.5879707	1.1319911
N	-0.4585054	-1.2312972	1.5892277
C	1.7245697	-0.2497847	2.1051551
C	0.6836054	-1.3079709	2.5422813
C	-1.4984345	-2.1173562	1.7102063
C	-2.3693004	-2.3438015	0.4435320
C	1.8263334	1.7369202	0.6215265
C	3.0169398	2.3302142	1.0492739
C	3.4331962	3.5220383	0.4568560
C	0.3097869	-0.9515584	3.9971156
C	1.3413694	-2.6956190	2.4707467
C	-3.5711746	-3.2196094	0.8149816
H	3.5879422	1.8790853	1.8545420
H	-0.4368471	-1.6574148	4.3751812
H	-0.0765501	0.0738859	4.0541729
H	1.2209059	-0.9961268	4.6092836
H	1.5604285	-2.9559327	1.4252633
H	0.6734701	-3.4533724	2.8967363
H	2.2850717	-2.6721211	3.0312120
H	-3.2257373	-4.1458744	1.2890925
H	-4.1553693	-3.4505094	-0.0831532
N	-0.1168562	1.6291062	-0.6811480
N	-1.9711728	-0.0846696	-0.5420467
C	-2.8747292	-1.0926025	-0.3307709
C	-1.4630403	-3.1140755	-0.5587928
C	1.0524578	2.3422414	-0.4091364
C	2.6686071	4.1212393	-0.5604896
C	-1.0672114	1.9238359	-1.6307226
C	-2.2686918	0.9485465	-1.5741376
O	-4.0185083	-1.1042815	-0.8069895
H	-2.0382047	-3.3643346	-1.4621316
H	-1.1060687	-4.0472279	-0.0988508
C	1.4799129	3.5353854	-0.9975426
Cl	3.1695087	5.6196450	-1.3013369
O	-1.0150956	2.8448970	-2.4458972
C	-2.4009939	0.2966439	-2.9624567
C	-3.5102089	1.8029821	-1.2490152
H	0.8819231	4.0037723	-1.7732634
H	-3.3041029	-0.3229165	-3.0036370
H	-1.5228468	-0.3322868	-3.1673548
H	-2.4538620	1.0855904	-3.7243148
H	-3.4108976	2.2647948	-0.2578389
H	-4.4114163	1.1823877	-1.2665541
H	-3.5843720	2.6066766	-1.9941585
H	-0.5959668	-2.5059274	-0.8456123
H	-4.2298325	-2.7025088	1.5245135
S	0.1974537	3.6737527	2.9978145
O	0.9682862	4.6974718	2.3008349
O	0.8655525	2.5088045	3.5761487
C	-0.6043826	4.5076029	4.3819219
C	-2.1117807	5.6987181	6.3608665
C	-0.9282398	3.7825988	5.5342689
C	-0.9930750	5.8463080	4.2416837
C	-1.7520256	6.4503106	5.2367724
C	-1.6936870	4.3776844	6.5321725
H	-0.5944274	2.7494591	5.6237414
H	-0.7071473	6.3900849	3.3415401
H	-2.0917499	7.4805135	5.1508131
H	-1.9980299	3.8298535	7.4211211
N	-1.0325985	3.3588777	1.9626662
I	-2.0660572	1.6748153	2.4167143
C	-3.4294070	2.6032938	3.8589407
C	-5.0755332	3.8089803	5.7332305
C	-3.8075540	3.9292767	3.6678834
C	-3.8593590	1.8606261	4.9566585
C	-4.6934797	2.4752115	5.8977141
C	-4.6346226	4.5321342	4.6199078
H	-3.4206972	4.4923738	2.8171584
H	-3.5337248	0.8283220	5.0980475
H	-5.0244546	1.9135611	6.7727682
H	-4.9168564	5.5793041	4.5010780
H	-5.6985481	4.2940094	6.4850805
N	-3.0039644	6.2988466	7.3664586
O	-3.4119369	7.4517235	7.1671581
O	-3.3185917	5.6133456	8.3486597

TS1

96 atoms

Cl	8.2009907	6.5517768	-0.4262897
O	5.2711322	2.5452484	1.1620089
O	0.2729290	1.2421731	1.9871955
N	3.7762335	3.9416376	0.0795861
N	1.6780652	2.4344130	0.6341879
C	4.1190780	2.8555202	0.8800001
C	2.8784881	2.1248085	1.4569235
C	0.4504730	2.0236840	1.0322815
C	-0.8171446	2.5507832	0.2938561
C	4.5560073	4.9061767	-0.4658999

C	5.9033687	5.1783912	-0.1614485
C	6.5440015	6.2074819	-0.8230070
C	2.7297453	2.7226907	2.8806694
C	3.1803106	0.6217764	1.5139552
C	-1.4115999	3.6473215	1.2248254
H	6.4172362	4.5830914	0.5872235
H	1.8820386	2.2422930	3.3816677
H	2.5586616	3.8048724	2.8150265
H	3.6524977	2.5453595	3.4497265
H	3.2782377	0.2168067	0.4981835
H	2.3646227	0.1029610	2.0271451
H	4.1275785	0.4627467	2.0457191
H	-1.5765983	3.2198107	2.2234052
H	-2.3701454	3.9917947	0.8124315
N	2.6029777	5.2354285	-1.7154095
N	0.3948505	3.8906270	-1.4836494
C	-0.7331483	3.2328504	-1.1034398
C	-1.8268301	1.3886582	0.2047905
C	3.8669648	5.6774065	-1.4811191
C	5.8574948	6.9821943	-1.8091930
C	1.7023027	5.6276789	-2.6861762
C	0.3369343	4.8978656	-2.5769154
O	-1.7681008	3.2429251	-1.7962500
H	-2.7809647	1.7574601	-0.1867047
H	-1.9658562	0.9516410	1.1996849
C	4.5392716	6.7226000	-2.1372111
Cl	6.6717220	8.2833887	-2.6213076
O	1.9287124	6.4708410	-3.5473945
C	0.0576289	4.2465308	-3.9435534
C	-0.6900338	5.9987774	-2.2310186
H	4.0207997	7.3028273	-2.8939916
H	-0.9498142	3.8188298	-3.9433908
H	0.7984502	3.4595088	-4.1350201
H	0.1493391	5.0103531	-4.7275579
H	-0.4633345	6.4124020	-1.2376284
H	-1.7004415	5.5762081	-2.2255627
H	-0.6220040	6.8022332	-2.9759882
H	-1.4703254	0.5972032	-0.4709556
H	-0.7240206	4.4986475	1.3062938
S	3.8123695	2.5302723	-3.0212156
O	3.0316148	2.5491755	-4.2628820
O	4.8524835	3.5583799	-2.8840034
Co	2.0050969	3.9085679	-0.5389877
N	1.3820772	5.0908051	0.6851743
S	2.0098185	6.4408343	1.2662041
O	3.1403609	6.2116870	2.1730335
O	2.1491868	7.5032157	0.2639584
H	-0.2450117	8.1778450	0.7992501
C	-0.3871340	7.7315928	1.7830279
C	-0.6808267	6.5471392	4.3147371
C	0.5869049	6.8636932	2.2878449
C	-1.5182667	8.0117065	2.5443845
C	-1.6498639	7.4138935	3.8002688
C	0.4475342	6.2731250	3.5494870
H	-2.2980222	8.6797643	2.1842049
H	1.2226990	5.6014784	3.9164683
H	-0.8265669	6.1022019	5.2969375
N	-2.8487291	7.7101794	4.6118466
O	-2.9432735	7.1722063	5.7220617
O	-3.6920557	8.4819539	4.1380915
N	2.9343871	2.4171326	-1.6638866
I	1.2972607	0.4438017	-1.8313491
C	4.7050291	0.9588844	-3.0470981
C	6.0077114	-1.4656961	-3.1219820
C	4.9051679	0.3238199	-4.2761912
C	5.1892265	0.4045256	-1.8566645
C	5.8449407	-0.8225476	-1.8912033
C	5.5625292	-0.9015648	-4.3184497
H	4.5046573	0.7751834	-5.1821633
H	5.0354202	0.9259212	-0.9125116
H	6.2155576	-1.2929500	-0.9827575
H	5.7026436	-1.4400490	-5.2525919
N	6.6326521	-2.8030196	-3.1565068
O	6.6469546	-3.4063599	-4.2383951
O	7.0964565	-3.2546314	-2.1031746
C	1.8372693	-0.6969021	-3.5196053
C	2.6113698	-2.1926120	-5.7292638
C	1.6041665	-0.1885910	-4.8019919
C	2.4622225	-1.9345698	-3.3254329
C	2.8429042	-2.6832501	-4.4404516
C	1.9970161	-0.9491700	-5.9058647
H	1.1584597	0.7957289	-4.9318991
H	2.6666100	-2.2985040	-2.3189176
H	3.3482784	-3.6393734	-4.2992007
H	1.8276620	-0.5569643	-6.9096992
H	2.9242687	-2.7756655	-6.5963451

TS2

100 atoms

Cl	7.2289704	7.5220038	1.5180817
O	4.2121440	3.5978670	3.0134953
O	0.5868000	0.2206086	1.3817599
N	3.4438932	4.0747430	0.8868651
N	1.7470833	2.0894525	0.8005518
C	3.4914935	3.3304826	2.0586918
C	2.5538844	2.0926402	2.0467705
C	0.8668513	1.1115122	0.5446984
C	0.2144981	0.9924085	-0.8636385
C	4.1510425	5.1699281	0.5261162
C	5.2461801	5.7345956	1.2100235
C	5.8670744	6.8467211	0.6782356
C	1.6844944	2.1677156	3.3158440
C	3.4773447	0.8550107	2.0951874
C	-1.1702147	0.3346914	-0.6926063
H	5.5901118	5.2836323	2.1357428
H	1.1566259	1.2184379	3.4515727
H	0.9504327	2.9745562	3.2103483
H	2.3264269	2.3701854	4.1839514
H	4.1246180	0.8352696	1.2103897
H	2.8584534	-0.0487735	2.1295896
H	4.1106107	0.9084213	2.9909193
H	-1.0696434	-0.5918610	-0.1174674
H	-1.6027204	0.1263547	-1.6770927
N	2.5847897	5.1542292	-1.2206859
N	0.7529432	3.3557786	-1.6240965
C	0.0338639	2.2136975	-1.8094037
C	1.1471201	0.0243964	-1.6469819
C	3.6773443	5.7737089	-0.7087883
C	5.4093737	7.4318235	-0.5459191
C	1.8545908	5.4601076	-2.3579715
C	0.7982584	4.3803742	-2.7026139
O	-0.7598504	2.0837990	-2.7595303
H	0.7002551	-0.2007307	-2.6253824
H	1.2638567	-0.9075004	-1.0765497
C	4.3314849	6.9054983	-1.2299628
Cl	6.2081522	8.8271686	-1.2009881

O	2.0317451	6.4533487	-3.0532259
C	1.2895254	3.7561827	-4.0310689
C	-0.5566244	5.0940504	-2.8594774
H	3.9739807	7.3544855	-2.1513619
H	0.5360453	3.0638017	-4.4189210
H	2.2257236	3.2074065	-3.8538597
H	1.4734387	4.5599708	-4.7559108
H	-0.8540679	5.5388932	-1.9010636
H	-1.3107805	4.3739408	-3.1926888
H	-0.4484480	5.9003254	-3.5973233
H	2.1328364	0.4834374	-1.8008401
H	-1.8561600	1.0018797	-0.1504230
N	3.2159259	2.5437319	-1.3410543
S	4.8100989	2.5425102	-1.4651667
O	5.2996831	3.7331445	-2.1706844
O	5.5124432	2.1406493	-0.2426959
C	4.9376571	1.1582615	-2.6092827
C	5.0277026	-0.9692035	-4.3582318
C	4.9535028	-0.1473322	-2.1041123
C	4.9691286	1.4022049	-3.9865185
C	5.0152809	0.3299066	-4.8726055
C	4.9971275	-1.2234437	-2.9841354
H	4.9295217	-0.3065439	-1.0266539
H	4.9613320	2.4304854	-4.3467458
H	5.0405117	0.4800605	-5.9500107
H	5.0067741	-2.2516686	-2.6284842
S	0.8167316	6.1662937	1.1161661
O	2.1074622	6.8490848	1.2942389
O	-0.0983601	6.7524339	0.1288677
H	-1.4387395	7.7485198	1.9590980
C	-1.0727672	7.2273308	2.8432668
C	-0.0913609	5.8278577	5.0719283
C	0.0056588	6.3463632	2.7189092
C	-1.6703194	7.4110439	4.0871160
C	-1.1811429	6.6953552	5.1807023
C	0.5118687	5.6637627	3.8300173
H	-2.5253648	8.0708867	4.2179104
H	1.3635580	4.9966207	3.7100610
H	0.2528528	5.2832101	5.9481242
N	5.0799020	-2.1101946	-5.2963095
O	5.0969333	-3.2512212	-4.8185893
O	5.1057270	-1.8619302	-6.5081202
N	-1.8716915	6.8164354	6.4782772
O	-1.3845118	6.2319970	7.4524424
O	-2.9146081	7.4834129	6.5186209
Co	2.0628670	3.6002955	-0.3150526
N	0.9874467	4.5590396	1.0128010
C	-1.2659721	3.9248601	0.8790806
H	-0.8807949	3.5670503	-0.0735629
H	-1.7089642	4.9201812	0.8609251
C	-1.4130539	3.0895840	1.9501194
H	-0.9263244	2.1118820	1.9119330
C	-2.1000628	3.3955349	3.1882031
C	-3.3247457	3.9615188	5.6670583
C	-3.0220262	4.4581800	3.3166445
C	-1.8387684	2.6006469	4.3295411
C	-2.4297309	2.8911823	5.5550906
C	-3.6277013	4.7322829	4.5379667
H	-3.2595863	5.0701319	2.4466626
H	-1.1370138	1.7703236	4.2388036
H	-2.1904266	2.2864571	6.4308325
H	-4.3213034	5.5693096	4.6259011
H	-3.7762094	4.2038370	6.6297158

$[Co^{III}(TAML^{q})(NNs)_2]^{-}$ (CH_2Cl_2)

89 atoms

Cl	7.9936617	7.4984758	0.8462443
O	5.3798542	3.4920226	2.6405357
O	0.9797263	0.7381728	2.1850179
N	4.0839637	4.1298321	0.8296366
N	2.3105199	2.2780975	1.1590552
C	4.3815441	3.3430836	1.9550410
C	3.2791182	2.3115805	2.2800483
C	1.2266449	1.4935853	1.2129438
C	0.3145507	1.3707560	-0.0416595
C	4.7441123	5.2192351	0.3749010
C	5.9638898	5.7416638	0.8534067
C	6.4877833	6.8709068	0.2598396
C	2.6262445	2.7898112	3.5987991
C	3.9678199	0.9468200	2.4691203
C	-1.0088946	0.7032148	0.3697053
H	6.4737404	5.2473004	1.6739446
H	1.9982847	1.9922226	4.0068022
H	1.9939080	3.6649367	3.4040666
H	3.4068330	3.0485054	4.3267235
H	4.4356958	0.6318704	1.5291323
H	3.2218020	0.2094793	2.7833652
H	4.7464085	1.0414390	3.2375529
H	-0.8016895	-0.2338469	0.8979041
H	-1.6146639	0.5054818	-0.5213293
N	2.8921249	5.2815573	-1.0492028
N	0.8956987	3.6246106	-1.0181673
C	-0.0248231	2.6251715	-0.8900434
C	1.0767424	0.4206650	-1.0099938
C	4.0561739	5.8797394	-0.7265053
C	5.8081634	7.5219290	-0.8251348
C	1.9646924	5.6171052	-2.0328293
C	0.7482360	4.6539234	-2.0801727
O	-1.0829078	2.6246000	-1.5420132
H	0.4459368	0.2020823	-1.8836721
H	1.3071309	-0.5200583	-0.4898885
C	4.6115207	7.0375833	-1.3108090
Cl	6.4836128	8.9454752	-1.5475579
O	2.0908715	6.5547390	-2.8066119
C	0.7922868	3.9816623	-3.4723772
C	-0.5189164	5.5121290	-1.9015277
H	4.0889037	7.5313427	-2.1242061
H	-0.1018261	3.3634691	-3.6066451
H	1.6869913	3.3485384	-3.5489511
H	0.8275726	4.7599657	-4.2458141
H	-0.5413899	5.9349524	-0.8903772
H	-1.4068137	4.8954343	-2.0674082
H	-0.4888477	6.3384255	-2.6242862
H	2.0107042	0.8855784	-1.3538242
H	-1.5843818	1.3581063	1.0362010
N	3.2952974	2.6871221	-1.4052154
S	4.8568847	2.3769081	-1.5398875
O	5.5765220	3.5459883	-2.0661682
O	5.4485282	1.6869142	-0.3880422
C	4.7709810	1.1596840	-2.8630339
C	4.5611160	-0.7016506	-4.8837040
C	4.5310534	-0.1813688	-2.5404674
C	4.9098381	1.5712807	-4.1926638
C	4.8058363	0.6333673	-5.2159051
C	4.4217560	-1.1232280	-3.5583527
H	4.4345602	-0.4723925	-1.4950525

H	5.1047383	2.6213784	-4.4081987
H	4.9104432	0.9147480	-6.2618378
H	4.2334831	-2.1737568	-3.3465675
Co	2.5026095	3.7370412	-0.0578626
N	1.4281457	4.7375101	1.2390140
S	1.5681239	6.3017672	1.5721271
O	2.8716680	6.6121656	2.1760766
O	1.1026885	7.1604821	0.4756773
H	-1.2100874	7.0890462	1.5528457
C	-0.9575504	6.8246281	2.5787927
C	-0.2370946	6.1325307	5.2041574
C	0.3518201	6.4419355	2.8879505
C	-1.9175424	6.8590082	3.5857628
C	-1.5439107	6.5061981	4.8838513
C	0.7192011	6.1069468	4.1950663
H	-2.9481082	7.1419084	3.3825712
H	1.7479892	5.8215789	4.4092453
H	0.0065733	5.8574437	6.2272529
N	4.4519531	-1.7006089	-5.9679922
O	4.2392562	-2.8771702	-5.6509174
O	4.5804169	-1.3053774	-7.1333254
N	-2.5644082	6.5230117	5.9518613
O	-2.2057046	6.2339079	7.0992971
O	-3.7227619	6.8275503	5.6402368
C	-1.0821710	2.0885084	4.0195291
H	-0.3100782	1.4557138	3.5621559
H	-2.0310113	1.5653795	4.1646660
Cl	-0.5124763	2.6224975	5.6390634
Cl	-1.3648924	3.4570284	2.9090143

E

100 atoms

Cl	7.5295302	8.7035613	1.3712848
O	6.4720540	3.7186414	1.3058476
O	2.7635772	0.1753228	0.5865172
N	4.5437890	4.5744071	0.3539763
N	3.2935113	2.3707300	0.2362563
C	5.3491857	3.5553745	0.8465082
C	4.6541494	2.1869931	0.8003416
C	2.4818112	1.2920193	0.1084408
C	1.1862802	1.4149569	-0.7279650
C	4.8150234	5.9267740	0.3985867
C	5.9903083	6.5543412	0.8383298
C	6.0610625	7.9429419	0.8240129
C	4.6267072	1.7005920	2.2666514
C	5.5034614	1.2655963	-0.0952771
C	0.2362595	0.2729177	-0.3327866
H	6.8299909	5.9555107	1.1757254
H	4.2088785	0.6912129	2.3181080
H	4.0306738	2.3894598	2.8788744
H	5.6552965	1.7063691	2.6507481
H	5.5142551	1.6570949	-1.1207377
H	5.0893350	0.2512918	-0.0805203
H	6.5351096	1.2540458	0.2809338
H	0.7514510	-0.6884060	-0.4336800
H	-0.6544982	0.2940414	-0.9701260
N	2.6286660	5.9235708	-0.3975409
N	1.0993843	3.9154437	-0.6386402
C	0.4052675	2.7455537	-0.6774562
C	1.6180138	1.2265374	-2.2113593
C	3.7124577	6.7093628	-0.0589787
C	4.9699014	8.7175095	0.3660603
C	1.3730225	6.3512056	-0.7473835
C	0.3817907	5.1849116	-0.9187674
O	-0.8374098	2.7060024	-0.7604454
H	0.7267622	1.2335709	-2.8551976
H	2.1246140	0.2564722	-2.3178436
C	3.8001597	8.1074469	-0.0792414
Cl	5.0541915	10.4559986	0.3364188
O	1.0340097	7.5295208	-0.8667515
C	-0.1067538	5.2055067	-2.3793262
C	-0.7636044	5.4639085	0.0774021
H	2.9685108	8.6992686	-0.4482361
H	-0.8845007	4.4457979	-2.5204851
H	0.7361216	4.9918809	-3.0516990
H	-0.5100095	6.1998021	-2.6137906
H	-0.4057590	5.3235096	1.1062657
H	-1.5978938	4.7828672	-0.1110090
H	-1.0865523	6.5067125	-0.0399490
H	2.2984587	2.0264828	-2.5319266
H	-0.0918036	0.3726077	0.7114418
N	1.3326489	3.5000607	2.7019851
S	1.9071762	4.5737555	3.8811251
O	1.5749663	4.1647645	5.2429220
O	3.2963513	4.8015034	3.5253631
H	2.4464764	6.7438702	2.0904296
C	1.4771551	6.9350274	2.5454818
C	-1.0096515	7.3854369	3.7730800
C	0.9641454	6.0438266	3.4901459
C	0.7354069	8.0617040	2.1956203
C	-0.5014475	8.2579806	2.8092118
C	-0.2600529	6.2680174	4.1278226
H	1.0907192	8.7553070	1.4379044
H	-0.6193629	5.5755532	4.8867081
H	-1.9767170	7.5856860	4.2288291
N	-1.3112459	9.4452523	2.4308143
O	-2.4573347	9.5253714	2.8894072
O	-0.7935597	10.2797756	1.6863979
C	1.2040373	2.0816970	3.1197597
H	1.6487361	1.3646577	2.4294654
H	1.3687948	1.8767102	4.1801433
C	-0.0268312	2.8229645	2.7480071
H	-0.3665448	2.7079084	1.7157177
C	-1.1299723	3.1926809	3.6766552
C	-3.2468210	4.0588361	5.3156013
C	-1.1155935	2.9316192	5.0550261
C	-2.2388530	3.8579072	3.1271904
C	-3.2876437	4.2915793	3.9383161
C	-2.1625043	3.3690336	5.8676917
H	-0.2679854	2.4181745	5.5032638
H	-2.2630759	4.0495378	2.0539932
H	-4.1317820	4.8208325	3.4943231
H	-2.1275776	3.1735984	6.9405026
H	-4.0595342	4.4050120	5.9561012
Co	2.9552622	4.0833051	-0.4595898
N	3.4668744	3.9182051	-2.1488614
S	4.8291246	4.5254201	-2.7670425
O	4.8575079	5.9891025	-2.8202072
O	6.0358809	3.8456145	-2.2853953
C	4.5283381	3.9254192	-4.4428349
C	4.0801168	3.0047778	-6.9987569
C	4.1750625	4.8327925	-5.4451507
C	4.6582799	2.5572213	-4.7126558
C	4.4293785	2.0882761	-6.0014795
C	3.9516782	4.3709013	-6.7405223
H	4.0856573	5.8899902	-5.1969337

H	4.9381970	1.8756781	-3.9101408
H	4.5159849	1.0325676	-6.2499131
H	3.6789114	5.0462274	-7.5489425
N	3.8419865	2.5111717	-8.3727786
O	3.5437555	3.3397465	-9.2414000
O	3.9552324	1.2967001	-8.5780135

TS2'

83 atoms

Cl	6.4197919	9.1135186	0.1617843
O	6.0351158	3.9961924	0.3396720
O	2.6550231	0.0056264	0.5669055
N	3.8055056	4.6161866	0.3019242
N	2.8687804	2.2736594	0.2925430
C	4.8401167	3.7114191	0.3884333
C	4.3322397	2.2602806	0.5270643
C	2.1881971	1.0946796	0.1948574
C	0.8447713	1.1190495	-0.5732217
C	3.9121239	5.9890198	0.1360414
C	5.0713049	6.7725843	0.2047779
C	4.9701349	8.1518046	0.0200001
C	4.7350542	1.7828193	1.9380592
C	5.0410991	1.4236691	-0.5554033
C	0.1593186	-0.2451264	-0.4397574
H	6.0283771	6.3045242	0.4134492
H	4.4230078	0.7413258	2.0736975
H	4.2835219	2.4214892	2.7054151
H	5.8261803	1.8662728	2.0363036
H	4.7047758	1.7354692	-1.5545374
H	4.8178410	0.3602556	-0.4173377
H	6.1228904	1.5939903	-0.4800993
H	0.8357148	-1.0372827	-0.7811866
H	-0.7654060	-0.2555363	-1.0282040
N	1.6064797	5.6860346	-0.0640343
N	0.3339143	3.5016291	-0.0608568
C	-0.1657464	2.2416086	-0.2344645
C	1.2221248	1.3596179	-2.0634036
C	2.6485766	6.6028135	-0.1035249
C	3.7257044	8.7523311	-0.2530143
C	0.2772217	5.9422410	-0.2829671
C	-0.5761532	4.6580358	-0.2701881
O	-1.3817308	1.9907506	-0.2740575
H	0.3162662	1.3305882	-2.6862668
H	1.9118059	0.5739809	-2.4049564
C	2.5647663	7.9818699	-0.3219038
Cl	3.5757413	10.4769425	-0.4479484
O	-0.2110679	7.0550906	-0.4909199
C	-1.2467890	4.5877435	-1.6592393
C	-1.6278187	4.8078019	0.8396484
H	1.5990041	8.4451561	-0.4981557
H	-1.9605121	3.7585485	-1.6949934
H	-0.4853220	4.4422221	-2.4390216
H	-1.7643933	5.5375279	-1.8462594
H	-1.1537423	4.7526137	1.8264325
H	-2.3611465	3.9988669	0.7742873
H	-2.1225974	5.7826676	0.7315082
H	1.7087474	2.3355402	-2.1843449
H	-0.0998957	-0.4614640	0.6053084
Co	2.0742333	3.9639543	0.4943101
N	1.8804535	3.9438265	2.3209236
S	2.6847352	4.9090545	3.3936381
O	2.1189465	4.6672175	4.7289196
O	4.1399766	4.8486802	3.2650402
H	4.2291575	7.3187115	3.1890800
C	3.1876550	7.5961224	3.0368028
C	0.4951067	8.2237062	2.5267448
C	2.2069252	6.6004195	3.0058198
C	2.8165924	8.9249926	2.8488121
C	1.4754067	9.2174710	2.5965244
C	0.8655443	6.9038576	2.7600669
H	3.5497679	9.7285097	2.8586294
H	0.1280493	6.1037125	2.7230747
H	-0.5301397	8.4905636	2.2822485
N	1.0810640	10.6269991	2.3846447
O	-0.0735307	10.8519974	2.0036998
O	1.9242731	11.5022433	2.6121122
C	1.3675754	2.2538105	3.2033268
H	2.1783156	1.6488308	2.8036189
H	1.5284875	2.6460186	4.2059431
C	0.0699971	1.9192185	2.8079261
H	-0.0486706	1.1808332	2.0146704
C	-1.1357399	2.5099859	3.3063444
C	-3.5515768	3.7178330	4.1299303
C	-1.1324412	3.5782718	4.2423379
C	-2.3838728	2.0664248	2.8013064
C	-3.5720737	2.6625761	3.2106038
C	-2.3247813	4.1685056	4.6412634
H	-0.1840592	3.9636568	4.6199641
H	-2.3918547	1.2835244	2.0419537
H	-4.5208630	2.3186994	2.7950659
H	-2.3027139	5.0001164	5.3479074
H	-4.4828632	4.1940049	4.4409012

F

83 atoms

Cl	7.6983346	8.2845730	-0.0440718
O	6.4336867	3.3616259	0.5648118
O	2.4623857	-0.0403140	0.4107871
N	4.3446994	4.3200456	0.2514751
N	3.0732021	2.1531933	0.1304002
C	5.2100066	3.2741303	0.4675984
C	4.4586132	1.9281879	0.6172731
C	2.2331272	1.0842181	-0.0552243
C	1.0043162	1.3068841	-0.9706287
C	4.6825299	5.6473958	0.0304785
C	5.9540341	6.2278075	0.1079682
C	6.1040683	7.5867181	-0.1694399
C	4.4920161	1.5796663	2.1208136
C	5.1987569	0.8741209	-0.2197058
C	0.1143198	0.0614142	-0.9243425
H	6.8079960	5.6216138	0.3941634
H	3.9680586	0.6316132	2.2884676
H	4.0124529	2.3768849	2.7039007
H	5.5380890	1.4929268	2.4449245
H	5.0794064	1.0897511	-1.2912592
H	4.8089249	-0.1273432	-0.0119773
H	6.2673844	0.9208857	0.0270219
H	0.7005124	-0.8277615	-1.1856639
H	-0.7239726	0.1765316	-1.6215188
N	2.3727901	5.7112695	-0.3569699
N	0.7947400	3.7473479	-0.5393199
C	0.1364299	2.5637016	-0.6924174
C	1.5687520	1.4992622	-2.4059501
C	3.5562131	6.4441972	-0.3316617
C	4.9940343	8.3723976	-0.5339668
C	1.1437850	6.1510970	-0.7921557

C	0.0840930	5.0256114	-0.8019143
O	-1.1018791	2.4700090	-0.7126439
H	0.7399963	1.6231439	-3.1182348
H	2.1551378	0.6162140	-2.6995165
C	3.7217239	7.8048350	-0.6207732
Cl	5.1634610	10.0741080	-0.8795517
O	0.8770583	7.3079263	-1.1217197
C	-0.5582574	5.0203822	-2.2014365
C	-0.9597621	5.3816062	0.2747343
H	2.8639509	8.4071245	-0.9044741
H	-1.3943810	4.3134481	-2.2317081
H	0.1852179	4.7308935	-2.9577950
H	-0.9164925	6.0322582	-2.4307939
H	-0.5062949	5.3536428	1.2722128
H	-1.7868394	4.6640764	0.2330360
H	-1.3347356	6.3970397	0.0884159
H	2.2131762	2.3859099	-2.4528894
H	-0.2983747	-0.0874210	0.0811382
Co	2.5108388	3.9306050	0.2067194
N	1.9680483	3.9779346	2.2128297
S	2.3785732	5.1501513	3.2795236
O	2.2588950	4.6602165	4.6551274
O	3.6268854	5.7537528	2.8336705
H	2.2466764	7.4879669	1.5797038
C	1.3153743	7.4421972	2.1388305
C	-1.0443304	7.3271937	3.6517417
C	1.1318045	6.4400253	3.0977534
C	0.3053929	8.3694583	1.9023596
C	-0.8686863	8.2908054	2.6549444
C	-0.0299533	6.4036624	3.8789914
H	0.4102139	9.1285647	1.1309987
H	-0.1358059	5.6523509	4.6572112
H	-1.9653373	7.3063962	4.2300796
N	-1.9543641	9.2580911	2.3985420
O	-3.0015764	9.1395601	3.0502547
O	-1.7622074	10.1347767	1.5479172
C	1.2615995	2.7772736	2.7556862
H	1.5493131	1.9370011	2.1117544
H	1.6242461	2.5517355	3.7664159
C	-0.2027586	3.0106408	2.7002415
H	-0.6461574	3.0385634	1.7045374
C	-1.0477967	3.3159007	3.7894615
C	-2.7961599	4.0581822	5.8950632
C	-0.6219105	3.2773881	5.1513093
C	-2.3917150	3.7240840	3.5325108
C	-3.2416087	4.0924879	4.5639041
C	-1.4847000	3.6427658	6.1751404
H	0.4080013	3.0103121	5.3823373
H	-2.7309519	3.7677143	2.4961426
H	-4.2571954	4.4215613	4.3375581
H	-1.1311124	3.6220709	7.2074519
H	-3.4630268	4.3557590	6.7053903

TS3'

83 atoms

Cl	7.5859891	8.4000033	0.1626656
O	6.4336675	3.4149394	0.5791859
O	2.5082489	-0.0514999	0.4112264
N	4.3352926	4.3325911	0.1928775
N	3.0972230	2.1458335	0.0787420
C	5.2149046	3.3072996	0.4404766
C	4.4822345	1.9500003	0.5799157
C	2.2704174	1.0630188	-0.0779146
C	1.0302830	1.2583324	-0.9891162
C	4.6466288	5.6781032	0.0176166
C	5.8947019	6.2903204	0.1689047
C	6.0163823	7.6645734	-0.0514431
C	4.5047422	1.6130581	2.0864693
C	5.2478928	0.9020231	-0.2408231
C	0.1547090	0.0043133	-0.9120918
H	6.7547929	5.6973654	0.4652354
H	3.9829995	0.6653860	2.2617628
H	4.0208979	2.4168318	2.6580112
H	5.5481284	1.5348786	2.4212180
H	5.1433854	1.1152797	-1.3143779
H	4.8631022	-0.1027805	-0.0379168
H	6.3119969	0.9587057	0.0231611
H	0.7465751	-0.8826102	-1.1689523
H	-0.6947672	0.1015339	-1.5984875
N	2.3504982	5.6888209	-0.4541034
N	0.7981824	3.7002258	-0.6215524
C	0.1483217	2.5134338	-0.7156683
C	1.5744691	1.4295893	-2.4336540
C	3.5135607	6.4543711	-0.3627718
C	4.9005276	8.4302341	-0.4302074
C	1.1090470	6.1176255	-0.8490201
C	0.0706463	4.9706803	-0.8715278
O	-1.0913345	2.3939718	-0.6862411
H	0.7353643	1.5308596	-3.1376011
H	2.1679007	0.5485272	-2.7198717
C	3.6490429	7.8287297	-0.5908775
Cl	5.0306703	10.1492308	-0.7091281
O	0.8050902	7.2808623	-1.1291442
C	-0.5739504	4.9563878	-2.2692930
C	-0.9807317	5.3096352	0.2046441
H	2.7852564	8.4160062	-0.8884426
H	-1.3826047	4.2168665	-2.3009167
H	0.1785057	4.6981443	-3.0279367
H	-0.9723058	5.9546658	-2.4933181
H	-0.5224981	5.2965638	1.2005895
H	-1.7929787	4.5747316	0.1637834
H	-1.3748142	6.3173707	0.0149033
H	2.2069061	2.3232202	-2.5046775
H	-0.2432389	-0.1355730	0.1006910
Co	2.5444874	3.9060561	0.0201272
N	1.6654227	3.9325162	2.2257270
S	2.1961514	5.0228984	3.3700103
O	2.0454361	4.5195837	4.7375376
O	3.4928743	5.5164444	2.9288293
H	2.1638755	7.2638754	1.5597400
C	1.2566030	7.3166209	2.1563297
C	-1.0439979	7.4451472	3.7569672
C	1.0374283	6.3815177	3.1722716
C	0.3065271	8.3025250	1.9086599
C	-0.8380312	8.3434546	2.7078806
C	-0.0914089	6.4597816	3.9959536
H	0.4345584	9.0097641	1.0928317
H	-0.2186811	5.7540244	4.8135780
H	-1.9423394	7.5204814	4.3655096
N	-1.8656875	9.3742732	2.4437191
O	-2.9057906	9.3382528	3.1158839
O	-1.6316857	10.2142624	1.5693147
C	1.2595018	2.5919352	2.7439907
H	1.5545060	1.8240434	2.0245720
H	1.6668043	2.3505322	3.7324605
C	-0.1578994	2.9729012	2.7010201

H	-0.5909784	3.0282098	1.7016645
C	-0.9820832	3.3683051	3.7928773
C	-2.6743109	4.2388989	5.8770718
C	-0.6094980	3.1952587	5.1522319
C	-2.2388607	3.9715049	3.5149807
C	-3.0691577	4.3999442	4.5418892
C	-1.4463884	3.6289512	6.1728157
H	0.3552795	2.7544295	5.3919775
H	-2.5292228	4.1171141	2.4738495
H	-4.0209996	4.8779669	4.3065037
H	-1.1379918	3.5033118	7.2116979
H	-3.3204037	4.5865318	6.6845226

G

83 atoms

Cl	7.7121674	7.5644512	1.7844217
O	5.6040124	2.8848619	2.2756468
O	1.1926886	0.2174288	1.2648764
N	4.1722871	3.8828021	0.7385912
N	2.5411579	1.9600198	0.5873569
C	4.5775136	2.8876842	1.5933076
C	3.5418449	1.7369796	1.6645498
C	1.5113105	1.0819973	0.4282607
C	0.7727318	1.1221402	-0.9410527
C	4.7719520	5.1314429	0.5513810
C	5.8854675	5.6485834	1.2194820
C	6.3200417	6.9445899	0.9252486
C	2.9409346	1.8287828	3.0828060
C	4.2679399	0.3999778	1.4560807
C	-0.4197746	0.1613004	-0.8898829
H	6.3978301	5.0459586	1.9638400
H	2.2097477	1.0272187	3.2339278
H	2.4661407	2.8089441	3.2127191
H	3.7541892	1.7435046	3.8168525
H	4.6608728	0.3411423	0.4310237
H	3.5753440	-0.4338687	1.6229660
H	5.1091393	0.3333661	2.1588986
H	-0.0781198	-0.8431577	-0.6124438
H	-0.9191291	0.1339476	-1.8657141
N	2.9887909	5.2583305	-0.9673586
N	1.1766521	3.5392208	-1.3645348
C	0.2762164	2.5174683	-1.4196998
C	1.7865285	0.6258811	-2.0076733
C	4.0923863	5.9194974	-0.4222288
C	5.6502253	7.7216112	-0.0335257
C	2.1021798	5.7528853	-1.8903782
C	0.8989598	4.8001997	-2.1053182
O	-0.8719556	2.6217589	-1.8878746
H	1.3003236	0.5833322	-2.9936152
H	2.1399877	-0.3829700	-1.7474776
C	4.5375045	7.2128505	-0.7104051
Cl	6.1770267	9.3457493	-0.4137471
O	2.1879317	6.8336457	-2.4773459
C	0.7598434	4.5293285	-3.6117965
C	-0.3296577	5.5601848	-1.5616128
H	4.0128780	7.8131152	-1.4479631
H	-0.1560408	3.9610291	-3.8113111
H	1.6250775	3.9534019	-3.9705084
H	0.7302992	5.4878834	-4.1469305
H	-0.1871221	5.7791879	-0.4953847
H	-1.2365043	4.9639070	-1.7082968
H	-0.4150708	6.5159667	-2.0966275
H	2.6502527	1.2996956	-2.0656904
H	-1.1554156	0.4850195	-0.1425707
Co	2.6713791	3.5843701	-0.2792513
S	1.0998550	5.6150436	2.5411886
O	2.2180094	5.2336501	3.3807607
O	1.2512001	6.4912569	1.3973652
H	-1.2702248	7.1546205	1.9425186
C	-1.2217535	7.0378217	3.0249665
C	-0.9876554	6.7950659	5.8157085
C	-0.1302997	6.3771494	3.6040929
C	-2.2203627	7.5555290	3.8449978
C	-2.0930064	7.4146898	5.2290215
C	0.0028493	6.2719292	4.9918314
H	-3.0896055	8.0653249	3.4345948
H	0.8693160	5.7621731	5.4079023
H	-0.9277127	6.7139316	6.8983327
N	-3.1704515	7.9263852	6.1024980
O	-3.0511159	7.7608444	7.3227495
O	-4.1355607	8.4829945	5.5644926
N	0.4751227	4.1945030	1.9396259
C	-0.8857091	3.9523132	1.4690329
C	-0.3396589	3.1472610	2.6087149
H	-0.9571512	3.5242326	0.4687317
H	-1.6383923	4.7089156	1.7058639
H	0.0619768	2.1562576	2.3733971
C	-0.8530471	3.2993102	4.0047956
C	-1.7525300	3.5701335	6.6552217
C	-0.0173904	2.9577306	5.0799579
C	-2.1509416	3.7545341	4.2747248
C	-2.5964780	3.8953320	5.5905057
C	-0.4631400	3.0958744	6.3948533
H	0.9923930	2.6017159	4.8760024
H	-2.8176944	4.0085091	3.4505623
H	-3.6034601	4.2675943	5.7842485
H	0.2020667	2.8363535	7.2198480
H	-2.0984138	3.6893712	7.6828749

I

79 atoms

Co	-0.2018878	0.1793654	0.3555671
Cl	5.1615253	4.1405329	0.9979707
O	3.0793139	-0.3146693	2.4768915
O	-1.5821488	-2.6944471	2.7406661
N	1.4659728	0.5229994	1.0254146
N	-0.2959433	-1.1928803	1.5596028
C	1.9524219	-0.3476845	2.0149696
C	0.8866134	-1.3713695	2.4559096
C	-1.3889016	-2.0286548	1.7216276
C	-2.3364282	-2.1733576	0.5065507
C	2.0781316	1.6529337	0.5584871
C	3.2832125	2.2262843	0.9975714
C	3.6981218	3.4200205	0.4323728
C	0.6092614	-1.0798796	3.9456268
C	1.4713474	-2.7833137	2.2716769
C	-3.5570545	-3.0015551	0.9196490
H	3.8609359	1.7492044	1.7828943
H	-0.1145258	-1.7986639	4.3394243
H	0.2374258	-0.0565714	4.0749420
H	1.5565290	-1.1624167	4.4948746
H	1.6436085	-2.9910819	1.2064664
H	0.7778086	-3.5290572	2.6765159
H	2.4284631	-2.8500605	2.8039596
H	-3.2340176	-3.9676496	1.3240390
H	-4.2094505	-3.1614737	0.0538164

N	0.1201512	1.6412303	-0.7027533
N	-1.8438518	0.0858704	-0.4369347
C	-2.8190826	-0.8473589	-0.1332399
C	-1.5387382	-2.9365441	-0.5902545
C	1.2915440	2.3052724	-0.4645731
C	2.9274538	4.0577023	-0.5943973
C	-0.9055736	2.0330349	-1.5771580
C	-2.1858556	1.1983373	-1.3711216
O	-4.0089195	-0.6958583	-0.4128246
H	-2.1858255	-3.1121154	-1.4608104
H	-1.2103268	-3.9095161	-0.1988697
C	1.7405042	3.5046406	-1.0429135
Cl	3.4585106	5.5494843	-1.2825761
O	-0.8202699	2.9394941	-2.3884783
C	-2.6313276	0.6530137	-2.7384718
C	-3.2293456	2.1768725	-0.7866779
H	1.1482797	3.9989208	-1.8066295
H	-3.6104357	0.1706951	-2.6509688
H	-1.9015703	-0.0774953	-3.1149831
H	-2.6949584	1.4847778	-3.4514265
H	-2.8626160	2.5975074	0.1594574
H	-4.1774331	1.6555402	-0.6251892
H	-3.3744599	3.0005959	-1.4981001
H	-0.6576734	-2.3680303	-0.9123591
H	-4.1413773	-2.4877292	1.6927717
S	-0.0792737	3.2455852	2.8602845
O	0.5361296	4.1338516	1.8783308
O	0.7345688	2.2288576	3.5250893
C	-0.7891627	4.2683067	4.1533331
C	-2.2696942	5.6645539	6.0010411
C	-0.9948280	3.7189867	5.4227670
C	-1.2642884	5.5440091	3.8264325
C	-2.0098756	6.2537971	4.7611741
C	-1.7512670	4.4205861	6.3576944
H	-0.5846278	2.7372570	5.6570067
H	-1.0651534	5.9536509	2.8365897
H	-2.4205835	7.2363308	4.5378612
H	-1.9708091	4.0088272	7.3402433
N	-1.3896539	2.6774701	2.0394246
I	-2.3687257	1.1711419	2.9665239
C	-3.7080474	2.3263048	4.1910222
C	-5.3213724	3.8862868	5.7948834
C	-4.1091473	3.5701538	3.7160523
C	-4.0855515	1.8307145	5.4373577
C	-4.9097919	2.6273650	6.2391101
C	-4.9222632	4.3547225	4.5398221
H	-3.7614156	3.9357240	2.7493649
H	-3.7354180	0.8619197	5.7951955
H	-5.2091173	2.2672513	7.2236453
H	-5.2306174	5.3439953	4.2007951
H	-5.9382649	4.5140047	6.4376628
N	-3.1819986	6.3518827	6.9431072
O	-3.6863254	7.4180893	6.5766082
O	-3.4095624	5.8024774	8.0255727

[Co^{III}(TAML^{q})(NNs)] (CH_2Cl_2) (J)

72 atoms

Cl	6.0183236	3.0166544	-1.1351295
O	3.6763842	-1.4485303	-0.3667848
O	-1.0187804	-3.6863721	0.1003992
N	1.8881676	0.0210736	-0.2910802
N	0.1248739	-1.7393802	-0.2308375
C	2.4810117	-1.2557829	-0.2466856
C	1.4435185	-2.3597188	0.0179532
C	-1.0027252	-2.5176856	-0.3043539
C	-2.2163541	-1.9155626	-1.0300718
C	2.5236340	1.2153260	-0.4693208
C	3.8897194	1.4418172	-0.7166058
C	4.3348360	2.7439285	-0.8709881
C	1.6190077	-2.7991680	1.4875050
C	1.7354921	-3.5146778	-0.9551971
C	-3.3980741	-2.8846676	-0.9373100
H	4.5840875	0.6085696	-0.7519189
H	0.9682462	-3.6576489	1.6835689
H	1.3416669	-1.9862937	2.1702927
H	2.6661698	-3.0802724	1.6614393
H	1.5409868	-3.2037638	-1.9910423
H	1.1085189	-4.3786085	-0.7165277
H	2.7935367	-3.7910347	-0.8662631
H	-3.1092560	-3.8651317	-1.3329862
H	-4.2493901	-2.4938299	-1.5061206
N	0.3222290	1.9098966	-0.2320418
N	-1.6863374	0.4423099	-0.3698504
C	-2.6558121	-0.5332899	-0.5220905
C	-1.7942161	-1.7216451	-2.5151787
C	1.6070483	2.3271815	-0.4070732
C	3.4260804	3.8496074	-0.7900673
C	-0.8352955	2.7054555	-0.2220383
C	-2.1099777	1.8462354	-0.1421429
O	-3.8474307	-0.2842331	-0.3415908
H	-2.6442838	-1.3325955	-3.0922567
H	-1.4941089	-2.6881516	-2.9432670
C	2.0762041	3.6442780	-0.5620213
Cl	4.0031567	5.4672623	-0.9549368
O	-0.8275838	3.9195496	-0.2954213
C	-3.0526454	2.3631589	-1.2458963
C	-2.7185225	2.0291309	1.2634705
H	1.3874345	4.4796328	-0.4840949
H	-4.0343038	1.8899831	-1.1615014
H	-2.6336082	2.1496404	-2.2390788
H	-3.1529423	3.4501917	-1.1362498
H	-2.0649419	1.5740881	2.0170166
H	-3.7015885	1.5477532	1.2954141
H	-2.8125300	3.1006748	1.4824635
H	-0.9543384	-1.0208464	-2.6008016
H	-3.7140517	-3.0105189	0.1051170
Co	0.0819305	0.0982815	0.0987663
N	0.1038211	0.1059556	1.8564894
S	0.9191247	1.2115098	2.7580516
O	2.3586489	1.0890477	2.5170053
O	0.3101957	2.5386555	2.6965075
H	-1.4643729	1.3076949	4.3723192
C	-0.7284374	0.7094761	4.9069974
C	1.2166024	-0.8114735	6.2548643
C	0.5400889	0.4989592	4.3554786
C	-1.0298225	0.1514519	6.1449469
C	-0.0506646	-0.5982479	6.7971750
C	1.5135568	-0.2590050	5.0109973
H	-2.0053608	0.2823449	6.6080418
H	2.4889831	-0.4030707	4.5483561
H	1.9432195	-1.4069576	6.8038324
N	-0.3768783	-1.2097443	8.1136975
O	0.4964450	-1.8909132	8.6565952
O	-1.5003935	-0.9986185	8.5762580
H	-1.5707567	-3.5973600	2.2132918
C	-1.9634256	-3.1109732	3.1122120

H	-2.7681870	-3.6834681	3.5807577
Cl	-0.6337858	-2.9603352	4.2993749
Cl	-2.6377675	-1.5311998	2.6121672

TS4

83 atoms

Cl	6.3916761	9.0987190	-0.1095701
O	5.9707686	4.0610758	0.5665129
O	2.5765680	0.0932119	0.6479926
N	3.7431906	4.6711881	0.4009142
N	2.8222171	2.3484528	0.4024734
C	4.7904534	3.7556073	0.5578403
C	4.2803440	2.3120160	0.6705621
C	2.1358528	1.1678165	0.2282757
C	0.8628772	1.2047912	-0.6355293
C	3.8707488	6.0128338	0.1395993
C	5.0440513	6.7860774	0.1303148
C	4.9536357	8.1386441	-0.1706250
C	4.6664260	1.8009313	2.0741623
C	5.0035368	1.4973860	-0.4225512
C	0.1954876	-0.1734402	-0.6219525
H	5.9978633	6.3327108	0.3807346
H	4.3656098	0.7530856	2.1763771
H	4.2066017	2.4134658	2.8567243
H	5.7555531	1.8880130	2.1836317
H	4.6986478	1.8391354	-1.4213428
H	4.7657380	0.4338746	-0.3168956
H	6.0853009	1.6448737	-0.3147461
H	0.9038494	-0.9356741	-0.9655896
H	-0.6873468	-0.1665882	-1.2711398
N	1.5752192	5.7116716	-0.0788057
N	0.3057181	3.5581998	-0.0647179
C	-0.1654332	2.2826556	-0.2495151
C	1.3256054	1.5484409	-2.0807387
C	2.6055575	6.6175758	-0.1601415
C	3.7000948	8.7332438	-0.4904265
C	0.2197471	5.9731755	-0.2681108
C	-0.6334935	4.6977009	-0.1879621
O	-1.3718108	2.0128751	-0.2162959
H	0.4595552	1.5478812	-2.7570080
H	2.0428471	0.7930573	-2.4307133
C	2.5341792	7.9777332	-0.4953853
Cl	3.5812502	10.4255424	-0.8132459
O	-0.2460863	7.0867046	-0.4612134
C	-1.4490451	4.6416972	-1.4954394
C	-1.5497101	4.8253663	1.0418126
H	1.5753184	8.4394577	-0.7085713
H	-2.1775865	3.8270645	-1.4560068
H	-0.7827200	4.4873564	-2.3558327
H	-1.9697514	5.5990435	-1.6230902
H	-0.9584577	4.7539758	1.9626866
H	-2.2787521	4.0091157	1.0418092
H	-2.0680833	5.7931451	1.0113975
H	1.8037504	2.5351617	-2.1160424
H	-0.1292618	-0.4540293	0.3881515
Co	2.0165045	4.0222898	0.5634972
N	1.7091845	4.0873482	2.3170372
S	2.5583877	4.9648699	3.4412544
O	1.8759958	4.7335019	4.7166989
O	4.0040245	4.7707448	3.3826928
H	4.3159864	7.2117949	3.1362594
C	3.3023199	7.5740445	2.9735223
C	0.6671121	8.4305092	2.4854596
C	2.2296198	6.6781415	3.0130034
C	3.0519024	8.9210504	2.7201237
C	1.7400641	9.3229945	2.4708129
C	0.9147902	7.0950686	2.7855648
H	3.8548623	9.6547931	2.6884220
H	0.0991215	6.3755379	2.8228467
H	-0.3347585	8.7861433	2.2557971
N	1.4775162	10.7530534	2.1603078
O	0.3410342	11.0529775	1.7865711
O	2.4120633	11.5456298	2.2971758
C	1.3291986	2.0745933	3.3222833
H	2.1977545	1.5732125	2.9062016
H	1.4564444	2.5793165	4.2762761
C	0.0795918	1.7419898	2.8481793
H	0.0205688	1.0244210	2.0269990
C	-1.1705697	2.2785446	3.3056065
C	-3.6544430	3.3591637	4.0555441
C	-1.2421576	3.3219946	4.2650044
C	-2.3735067	1.7959453	2.7331143
C	-3.6009784	2.3295358	3.1090408
C	-2.4713286	3.8519031	4.6291574
H	-0.3263109	3.7334787	4.6900173
H	-2.3196408	1.0242075	1.9652571
H	-4.5190094	1.9553782	2.6551721
H	-2.5171429	4.6605591	5.3595300
H	-4.6165032	3.7842435	4.3448017

K

83 atoms

Cl	7.6433326	8.2970947	0.0093630
O	6.4093653	3.3770033	0.6095706
O	2.4525083	-0.0055808	0.4718734
N	4.3215979	4.3281078	0.2563779
N	3.0666453	2.1739167	0.1657975
C	5.1961267	3.2742384	0.5135580
C	4.4396892	1.9408333	0.6723065
C	2.2193883	1.0977662	-0.0300326
C	1.0086594	1.3032569	-0.9548530
C	4.6644243	5.6378393	0.0485154
C	5.9366480	6.2264713	0.1448764
C	6.0762069	7.5786360	-0.1326095
C	4.4614024	1.6080077	2.1820372
C	5.1845923	0.8738962	-0.1472958
C	0.1333020	0.0474515	-0.9228073
H	6.7923944	5.6291723	0.4434940
H	3.9272076	0.6672607	2.3538411
H	3.9939352	2.4135388	2.7629729
H	5.5049396	1.5088532	2.5082187
H	5.0741894	1.0726483	-1.2223302
H	4.7953705	-0.1237896	0.0748601
H	6.2506630	0.9220071	0.1074726
H	0.7290210	-0.8333792	-1.1893613
H	-0.6997245	0.1574960	-1.6259998
N	2.3739264	5.6842689	-0.3616232
N	0.7829761	3.7375711	-0.5024165
C	0.1348097	2.5482233	-0.6607057
C	1.5805561	1.5185303	-2.3855245
C	3.5292752	6.4303743	-0.3282366
C	4.9515165	8.3645778	-0.5192677
C	1.1187494	6.1281924	-0.7894881
C	0.0719234	5.0043839	-0.7932171
O	-1.1013491	2.4531166	-0.6818177
H	0.7526032	1.6470525	-3.0964717

H	2.1680354	0.6406521	-2.6891809
C	3.6883214	7.7968296	-0.6194783
Cl	5.1290090	10.0504663	-0.8643689
O	0.8705612	7.2788141	-1.1212795
C	-0.5328996	4.9704358	-2.2133254
C	-1.0065698	5.3909291	0.2402144
H	2.8339458	8.3967805	-0.9164758
H	-1.3598313	4.2538229	-2.2505938
H	0.2316340	4.6770634	-2.9455224
H	-0.8996557	5.9725344	-2.4681607
H	-0.5859199	5.4130098	1.2523455
H	-1.8237666	4.6625659	0.1968715
H	-1.3898266	6.3916435	0.0010742
H	2.2218056	2.4079266	-2.4229847
H	-0.2856029	-0.1162106	0.0776287
Co	2.4986779	3.9385920	0.2491294
N	1.9450858	3.9425475	2.0813664
S	2.3659063	5.1408289	3.1737057
O	2.2449810	4.5839030	4.5162049
O	3.6174796	5.7194592	2.7186354
H	2.2264516	7.5152691	1.5284354
C	1.3043658	7.4570200	2.1003850
C	-1.0133134	7.3404275	3.6762599
C	1.1270501	6.4341632	3.0359928
C	0.2997921	8.4018278	1.9124164
C	-0.8536462	8.3151980	2.6908287
C	-0.0070107	6.3964119	3.8556017
H	0.3953638	9.1854423	1.1643561
H	-0.0941579	5.6406185	4.6312366
H	-1.9145892	7.3287679	4.2853023
N	-1.9462279	9.2988205	2.4732855
O	-2.9698858	9.1710370	3.1519808
O	-1.7635359	10.1760871	1.6268144
C	1.2317860	2.7458233	2.6376393
H	1.4677576	1.9003972	1.9834941
H	1.6299221	2.5097203	3.6302055
C	-0.2124914	3.0518481	2.6244992
H	-0.6765699	3.1165909	1.6407535
C	-1.0216982	3.3467852	3.7389842
C	-2.7074161	4.0404770	5.8899926
C	-0.5692417	3.2342744	5.0875769
C	-2.3551558	3.8036498	3.5129686
C	-3.1782428	4.1492657	4.5720932
C	-1.4058538	3.5758198	6.1388400
H	0.4518168	2.9170346	5.2900601
H	-2.7086737	3.8935844	2.4849469
H	-4.1890476	4.5111546	4.3820993
H	-1.0457689	3.4940851	7.1647856
H	-3.3540215	4.3177676	6.7232831

TS5

83 atoms

Cl	7.5913813	8.3027926	0.0595196
O	6.3900030	3.3810963	0.5585878
O	2.4394211	-0.0405238	0.4499163
N	4.2829827	4.3159621	0.2670991
N	3.0578946	2.1419975	0.1413320
C	5.1778641	3.2607900	0.4737095
C	4.4422974	1.9156267	0.6240421
C	2.2176468	1.0685849	-0.0489129
C	1.0098069	1.2803529	-0.9891716
C	4.6180724	5.6340115	0.0748195
C	5.8885367	6.2260257	0.1703169
C	6.0257840	7.5818253	-0.0941589
C	4.5085295	1.5664649	2.1282891
C	5.1805006	0.8669994	-0.2226315
C	0.1356073	0.0234400	-0.9778706
H	6.7467987	5.6291938	0.4623538
H	3.9720124	0.6289541	2.3109754
H	4.0715079	2.3730990	2.7325640
H	5.5599587	1.4542502	2.4236937
H	5.0562093	1.0866498	-1.2920415
H	4.7909116	-0.1344199	-0.0158110
H	6.2499130	0.9059468	0.0196352
H	0.7353624	-0.8526860	-1.2503441
H	-0.6932145	0.1390967	-1.6855342
N	2.3250704	5.6837605	-0.3436097
N	0.7705576	3.7177491	-0.5451286
C	0.1307482	2.5182079	-0.6906050
C	1.5983182	1.5074926	-2.4106841
C	3.4791624	6.4289727	-0.2961031
C	4.8999239	8.3676759	-0.4741930
C	1.0788299	6.1188743	-0.7861698
C	0.0380216	4.9827419	-0.8053180
O	-1.1054949	2.4166325	-0.6627705
H	0.7805277	1.6239910	-3.1356813
H	2.2052644	0.6401371	-2.7060260
C	3.6383595	7.7966682	-0.5810923
Cl	5.0717350	10.0583873	-0.8001214
O	0.8143071	7.2710443	-1.1067842
C	-0.5949189	4.9657297	-2.2097373
C	-1.0204159	5.3337594	0.2598942
H	2.7821328	8.3957168	-0.8755672
H	-1.4128011	4.2380938	-2.2435970
H	0.1582299	4.6954778	-2.9624892
H	-0.9816684	5.9659924	-2.4417216
H	-0.5753377	5.3373041	1.2620245
H	-1.8308047	4.5980073	0.2152403
H	-1.4181341	6.3364381	0.0543570
H	2.2269666	2.4062275	-2.4354593
H	-0.2896970	-0.1535348	0.0174639
Co	2.4763866	3.9079529	0.2084334
N	1.7692895	3.9362781	2.1987839
S	2.2529827	5.1271491	3.3138076
O	2.1253779	4.6064862	4.6698389
O	3.5244270	5.6393741	2.8336366
H	2.1776453	7.4194425	1.5683555
C	1.2561431	7.4154340	2.1435376
C	-1.0616703	7.4324444	3.7234737
C	1.0481715	6.4394344	3.1213574
C	0.2804429	8.3818128	1.9172617
C	-0.8734876	8.3600218	2.6993915
C	-0.0842006	6.4663474	3.9432744
H	0.3982021	9.1296948	1.1365589
H	-0.1915012	5.7479894	4.7516345
H	-1.9629133	7.4733401	4.3312686
N	-1.9386221	9.3662324	2.4423845
O	-2.9789472	9.2720414	3.1006706
O	-1.7166121	10.2245131	1.5869866
C	1.3863702	2.6201100	2.7849889
H	1.7013648	1.8048869	2.1319817
H	1.7766645	2.4609337	3.7945594
C	-0.0270992	3.0002127	2.6813911
H	-0.4416819	3.0002370	1.6734142
C	-0.8882971	3.3902711	3.7453858
C	-2.6742628	4.1662471	5.7716114

C	-0.5352108	3.2452897	5.1130440
C	-2.1687625	3.9154624	3.4253650
C	-3.0479997	4.2999323	4.4277861
C	-1.4228368	3.6303200	6.1088124
H	0.4444159	2.8574549	5.3818761
H	-2.4476182	4.0207872	2.3771600
H	-4.0239167	4.7110237	4.1691886
H	-1.1412209	3.5221371	7.1563475
H	-3.3616936	4.4756276	6.5599326

L

83 atoms

Cl	7.3499802	7.7014689	2.0848513
O	5.5704801	2.8736923	2.2504539
O	1.1836240	0.1991627	1.2048460
N	4.0997760	3.8931540	0.7637198
N	2.5428323	1.9346784	0.5489413
C	4.5353966	2.8594740	1.6057221
C	3.5170669	1.7026320	1.6527628
C	1.5182781	1.0298668	0.3557911
C	0.8349430	1.0491566	-1.0320310
C	4.6393005	5.1470023	0.6548032
C	5.6955888	5.7023880	1.3965328
C	6.0638544	7.0170476	1.1557766
C	2.8862948	1.7910567	3.0603623
C	4.2558315	0.3713930	1.4526466
C	-0.3230893	0.0472036	-1.0331418
H	6.2044463	5.1104570	2.1512099
H	2.1654191	0.9795296	3.1975388
H	2.3943144	2.7630863	3.1827586
H	3.6851930	1.7104852	3.8098447
H	4.6755271	0.3147814	0.4388307
H	3.5644674	-0.4651916	1.6031757
H	5.0772239	0.3008194	2.1769237
H	0.0456966	-0.9499976	-0.7661664
H	-0.7887146	0.0158235	-2.0248112
N	2.9437620	5.2363710	-0.9386998
N	1.1959747	3.4879848	-1.4043723
C	0.3061539	2.4351964	-1.4749073
C	1.9027145	0.6159812	-2.0762339
C	3.9590411	5.9364489	-0.3443725
C	5.3894937	7.8002303	0.1649867
C	2.0723193	5.7045707	-1.9323568
C	0.8902529	4.7396947	-2.1560622
O	-0.8408907	2.5491820	-1.9157196
H	1.4462367	0.5742686	-3.0749719
H	2.2810129	-0.3848707	-1.8254364
C	4.3498641	7.2657967	-0.5798499
Cl	5.8527343	9.4415067	-0.1155607
O	2.2025261	6.7573914	-2.5343004
C	0.7643255	4.4592683	-3.6619514
C	-0.3508426	5.4876737	-1.6186462
H	3.8348069	7.8628164	-1.3261859
H	-0.1435085	3.8799967	-3.8613112
H	1.6373080	3.8960187	-4.0200199
H	0.7160255	5.4127764	-4.2029934
H	-0.2226397	5.7100373	-0.5521121
H	-1.2477066	4.8809372	-1.7743850
H	-0.4478625	6.4381825	-2.1598542
H	2.7456485	1.3172680	-2.1005971
H	-1.0927543	0.3297831	-0.3050909
Co	2.6328594	3.5569926	-0.2791612
S	1.1140859	5.5793605	2.4579505
O	2.2799714	5.1865291	3.2277042
O	1.2347668	6.4260495	1.2834835
H	-1.2152211	7.1998931	1.9469959
C	-1.1255031	7.0805969	3.0261925
C	-0.7901562	6.8270041	5.8065678
C	-0.0371106	6.3836415	3.5656071
C	-2.0716849	7.6329685	3.8856240
C	-1.8937483	7.4828236	5.2611248
C	0.1509833	6.2711708	4.9458267
H	-2.9383910	8.1738063	3.5109342
H	1.0147864	5.7335586	5.3306987
H	-0.6924853	6.7435957	6.8863417
N	-2.9286146	8.0241729	6.1799200
O	-2.7823352	7.8155543	7.3872527
O	-3.8740591	8.6366109	5.6768786
N	0.4434761	4.1541333	1.9018138
C	-0.9409680	3.9557333	1.4718315
C	-0.4057384	3.1560182	2.6176169
H	-1.0544010	3.5071985	0.4843183
H	-1.6566084	4.7474518	1.7063633
H	-0.0466658	2.1469081	2.3934588
C	-0.8887654	3.3490998	4.0191828
C	-1.7414331	3.6762788	6.6769868
C	-0.0584246	2.9715800	5.0860452
C	-2.1597548	3.8683288	4.3003343
C	-2.5815744	4.0362622	5.6205680
C	-0.4801168	3.1380855	6.4054404
H	0.9281868	2.5585358	4.8766679
H	-2.8274112	4.1454221	3.4845044
H	-3.5687999	4.4519659	5.8246370
H	0.1785503	2.8463827	7.2244610
H	-2.0704224	3.8136052	7.7074911

[Co^{III}($TAML^{sq}$)(NH_3)]

71 atoms

Cl	6.1612735	3.2937338	-0.6592151
O	3.8733206	-1.2905081	-0.4963330
O	-0.6801557	-3.6985313	0.1015578
N	2.0701259	0.1557961	-0.3796771
N	0.2890868	-1.6940705	-0.3596686
C	2.6726900	-1.1056053	-0.3725800
C	1.6551315	-2.2491061	-0.1493141
C	-0.7996866	-2.5006316	-0.1973432
C	-2.2240209	-1.9656630	-0.5015625
C	2.6678199	1.3740653	-0.4587312
C	4.0467276	1.6493331	-0.5462785
C	4.4689074	2.9661683	-0.5847427
C	1.8778943	-2.7299732	1.3027861
C	1.9769619	-3.3615764	-1.1628861
C	-3.2243387	-2.8006669	0.3222756
H	4.7619884	0.8325244	-0.5506880
H	1.2543914	-3.6086031	1.4955284
H	1.6029420	-1.9345917	2.0063963
H	2.9370561	-2.9823576	1.4433541
H	1.7894592	-3.0163910	-2.1906656
H	1.3546639	-4.2388480	-0.9651589
H	3.0377661	-3.6289290	-1.0786439
H	-3.0665580	-3.8671185	0.1312573
H	-4.2490307	-2.5200799	0.0579333
N	0.4229906	2.0296539	-0.3819503
N	-1.6460549	0.5006560	-0.4264947
C	-2.5934505	-0.4670450	-0.3109301
C	-2.4556669	-2.2566280	-2.0116847

C	1.7103476	2.4667607	-0.4346841
C	3.5233412	4.0463707	-0.5427297
C	-0.7499935	2.7924959	-0.3887696
C	-2.0291885	1.9316440	-0.2697672
O	-3.7936674	-0.1910992	-0.1473823
H	-2.3107779	-3.3279107	-2.2062769
H	-1.7610598	-1.6942278	-2.6505611
C	2.1634368	3.7997108	-0.4699523
Cl	4.0700813	5.6821572	-0.5662083
O	-0.7699664	4.0087873	-0.4895197
C	-2.9747557	2.3805919	-1.4012666
C	-2.6356413	2.2368415	1.1166194
H	1.4481909	4.6152019	-0.4228916
H	-3.9286072	1.8514624	-1.3169647
H	-2.5333612	2.1667671	-2.3866250
H	-3.1387335	3.4629158	-1.3273969
H	-1.9722586	1.8596255	1.9031993
H	-3.6149651	1.7560465	1.2022536
H	-2.7386666	3.3231712	1.2358126
H	-3.4819068	-1.9771004	-2.2851684
H	-3.0834094	-2.6197194	1.3960632
N	0.0573825	0.0958780	1.5626214
S	0.9399354	1.0250176	2.5732676
O	2.3763942	0.7655572	2.4316170
O	0.4792401	2.4150984	2.5589561
H	-1.3806090	1.4945876	4.2237054
C	-0.7908819	0.7137463	4.7021628
C	0.7925050	-1.2670874	5.9189101
C	0.4110767	0.2921053	4.1237573
C	-1.2108141	0.1360904	5.8968653
C	-0.4122514	-0.8476276	6.4829848
C	1.2081803	-0.6883112	4.7218379
H	-2.1389774	0.4338368	6.3806771
H	2.1489861	-0.9790043	4.2560628
H	1.3835446	-2.0313689	6.4195783
N	-0.8595853	-1.4670471	7.7597163
O	-0.1297453	-2.3248713	8.2627806
O	-1.9319596	-1.0836701	8.2334613
Co	0.2155864	0.1859004	-0.2578135
N	0.2295441	0.1678097	-2.4286964
H	0.8940758	0.8155583	-2.8587532
H	-0.7190016	0.4101219	-2.7254816
H	0.4397014	-0.7848198	-2.7355417

[Co^{III}(TAML^{q})(NNs)(NH_3)] (CH_2Cl_2) (H^{NH_3})

59 atoms

Cl	8.3822408	5.8895918	0.7885116
O	5.7323942	1.7486946	2.2743647
O	0.9898830	-0.3913407	2.1277818
N	4.3284193	2.6509503	0.6610041
N	2.4208198	1.0031436	1.0049975
C	4.6588408	1.7700365	1.6828688
C	3.4779201	0.8434086	2.0430352
C	1.2568768	0.2829557	1.1261342
C	0.3017661	0.2258355	-0.0929890
C	5.0408017	3.7603080	0.2483179
C	6.3008034	4.1865112	0.6990091
C	6.8317337	5.3748931	0.2099079
C	2.9993072	1.3454401	3.4276139
C	3.9916560	-0.6029810	2.1110697
C	-1.0670356	-0.2918778	0.3827553
H	6.8420561	3.5963897	1.4327298
H	2.2057442	0.6946790	3.8056552
H	2.6177996	2.3723711	3.3428534
H	3.8529968	1.3420062	4.1180833
H	4.2883636	-0.9537452	1.1110922
H	3.2112503	-1.2639115	2.5015362
H	4.8732707	-0.6384275	2.7638875
H	-0.9438457	-1.2465032	0.9052158
H	-1.7362155	-0.4163118	-0.4750110
N	3.0844177	3.9995700	-1.0232211
N	1.0519897	2.4610265	-1.0007151
C	0.0638948	1.5084902	-0.9330119
C	0.9164967	-0.8188187	-1.0644166
C	4.3175960	4.5463079	-0.7138429
C	6.1175860	6.1502905	-0.7410891
C	2.0348117	4.6168659	-1.6647598
C	0.8144986	3.6810736	-1.8331158
O	-0.9868265	1.5971323	-1.5799167
H	1.0108252	-1.7883614	-0.5564897
H	1.9151329	-0.5146585	-1.4038948
C	4.8702321	5.7387382	-1.2025336
Cl	6.7726673	7.6338583	-1.3477640
O	2.0386966	5.7837430	-2.0581651
C	0.7353025	3.3355084	-3.3351629
C	-0.4289898	4.4628442	-1.3719147
H	4.3171099	6.3437856	-1.9149643
H	-0.1423445	2.7109295	-3.5306028
H	1.6398776	2.7968628	-3.6587645
H	0.6677487	4.2639842	-3.9175016
H	-0.3864534	4.6251271	-0.2867285
H	-1.3405710	3.9117000	-1.6179566
H	-0.4330092	5.4392643	-1.8727411
H	0.2647564	-0.9373729	-1.9406740
H	-1.5280955	0.4180553	1.0815176
H	2.3813951	6.3805831	0.3669112
C	2.3029805	6.3631455	1.4587588
H	1.6776378	7.1760697	1.8372039
Cl	1.5261555	4.8170719	1.9359023
Cl	3.9387338	6.5502854	2.1455598
Co	2.7539863	2.3133502	-0.2725316
N	3.7302997	1.3268278	-1.7836606
H	4.5255548	1.8880474	-2.1032592
H	3.0923217	1.1775926	-2.5694991
H	4.0757371	0.4209639	-1.4573808

I^{NH_3}

83 atoms

Cl	5.9659219	3.3784281	0.1321046
O	3.3418874	-0.3647806	2.4670399
O	-1.1478370	-3.0041595	2.4000704
N	1.6822140	0.6946736	1.2452207
N	-0.1833190	-1.0152000	1.8058227
C	2.1847997	-0.2973559	2.0672808
C	1.1382527	-1.3934277	2.4045046
C	-1.2004369	-1.9329383	1.7766644
C	-2.4904623	-1.6612685	0.9288451
C	2.3703607	1.6916725	0.5969725
C	3.7419773	1.9795085	0.7044478
C	4.2751536	3.0349314	-0.0217760
C	1.0701268	-1.5094075	3.9370562
C	1.6983546	-2.6980594	1.7930498
C	-3.6967894	-2.2080823	1.7213135
H	4.3655742	1.3882584	1.3685854
H	0.3277455	-2.2646982	4.2184265
H	0.8246637	-0.5359182	4.3844673

H	2.0562094	-1.8000976	4.3215661
H	1.7476723	-2.6344398	0.6943484
H	1.0678110	-3.5487619	2.0668287
H	2.7206691	-2.8515109	2.1606523
H	-3.4873918	-3.2298588	2.0542910
H	-4.5923605	-2.1890280	1.0919141
N	0.2165447	2.1005151	-0.2584729
N	-1.8779575	0.6305063	0.0817903
C	-2.8620311	-0.2335870	0.4091111
C	-2.3426461	-2.5395240	-0.3446598
C	1.5300349	2.4943523	-0.2651987
C	3.4476784	3.8248196	-0.8722457
C	-0.8537789	2.6447738	-0.9307344
C	-2.1786917	1.8674466	-0.6952069
O	-4.0727370	0.0091436	0.2159176
H	-3.2596550	-2.4710420	-0.9453703
H	-2.1806337	-3.5855404	-0.0522288
C	2.0909744	3.5573394	-0.9931461
Cl	4.1151801	5.1449213	-1.7728613
O	-0.8037001	3.6406210	-1.6502209
C	-2.7404243	1.5050973	-2.0833449
C	-3.1296819	2.8398054	0.0295016
H	1.4557938	4.1696298	-1.6266199
H	-3.7004557	0.9894641	-1.9706424
H	-2.0453865	0.8474038	-2.6281025
H	-2.8741081	2.4197999	-2.6745252
H	-2.7996687	2.9694773	1.0668742
H	-4.1487104	2.4406623	0.0252288
H	-3.1112509	3.8108435	-0.4831407
H	-1.5026695	-2.2253901	-0.9780759
H	-3.9073991	-1.5924331	2.6069832
S	0.2361809	2.6852821	3.1835454
O	0.8501855	3.5591142	2.1935778
O	1.0753081	1.9752796	4.1413953
C	-0.8842548	3.7382797	4.1168681
C	-2.5637716	5.3993036	5.5132944
C	-0.7454074	3.8342210	5.5026552
C	-1.8328399	4.4944895	3.4186724
C	-2.6906421	5.3296018	4.1242572
C	-1.5938497	4.6833906	6.2132359
H	0.0151706	3.2409172	6.0092808
H	-1.9001137	4.4157647	2.3349048
H	-3.4633426	5.9088311	3.6237693
H	-1.5307809	4.7789496	7.2954256
N	-0.8240634	1.7075181	2.3024521
I	-1.8995502	0.4642452	3.6727917
C	-3.5935433	1.6933201	4.0122151
C	-5.8386119	3.2297650	4.4777663
C	-4.5355572	1.8208423	2.9891101
C	-3.7632542	2.2698322	5.2731075
C	-4.9037068	3.0428208	5.4999384
C	-5.6582275	2.6159798	3.2340631
H	-4.4126035	1.3104751	2.0320585
H	-3.0146140	2.1458476	6.0536740
H	-5.0476656	3.5144426	6.4727239
H	-6.3995495	2.7417114	2.4443573
H	-6.7154532	3.8527756	4.6556133
N	-3.5371144	6.2198254	6.2773023
O	-4.4073965	6.8156060	5.6372623
O	-3.4297750	6.2352415	7.5070058
Co	-0.1214246	0.5790220	0.7842106
N	0.4280380	-0.4786589	-0.8216080
H	1.2882698	-0.1095246	-1.2386021
H	-0.3335786	-0.4191076	-1.5034615
H	0.5731220	-1.4599894	-0.5691690

TS5^{NH_3} (equal energy as **J^{NH_3}** within the DFT error, and therefore considered as barrierless)

83 atoms

Cl	5.9944221	3.3515455	0.0463267
O	3.3846843	-0.3946815	2.3706464
O	-1.1684192	-2.8833638	2.5212929
N	1.7001010	0.7305471	1.2481305
N	-0.1604330	-0.9748616	1.7947088
C	2.2127877	-0.2893403	2.0301002
C	1.1489039	-1.3524225	2.4082683
C	-1.2139926	-1.8538869	1.8308020
C	-2.4920132	-1.6134447	0.9725889
C	2.3901467	1.7025653	0.5684786
C	3.7657407	1.9793830	0.6592430
C	4.3020744	3.0159093	-0.0901098
C	1.0851397	-1.3894099	3.9478287
C	1.6754523	-2.6971310	1.8596938
C	-3.7061260	-2.1572896	1.7537305
H	4.3888513	1.3957829	1.3303482
H	0.3391804	-2.1241844	4.2700006
H	0.8512296	-0.3915008	4.3420420
H	2.0722137	-1.6711203	4.3371373
H	1.7074785	-2.6927656	0.7591326
H	1.0347672	-3.5199481	2.1886821
H	2.6998932	-2.8484009	2.2217369
H	-3.4947030	-3.1713435	2.1086152
H	-4.5883685	-2.1608249	1.1054204
N	0.2397407	2.0938633	-0.3050771
N	-1.8678496	0.6529079	0.0835001
C	-2.8562513	-0.1974199	0.4326262
C	-2.3204013	-2.5105014	-0.2866065
C	1.5505909	2.4909407	-0.3080060
C	3.4726970	3.7974282	-0.9487194
C	-0.8389920	2.6394763	-0.9662392
C	-2.1689244	1.8843698	-0.6982052
O	-4.0632922	0.0472286	0.2294031
H	-3.2265490	-2.4482065	-0.9039562
H	-2.1687715	-3.5531393	0.0232790
C	2.1130556	3.5381535	-1.0562415
Cl	4.1427170	5.0947421	-1.8759936
O	-0.7783040	3.6172371	-1.7074926
C	-2.7494357	1.5125877	-2.0772443
C	-3.1047583	2.8705643	0.0287198
H	1.4784816	4.1423191	-1.6978761
H	-3.7142861	1.0105536	-1.9487639
H	-2.0679406	0.8412478	-2.6219535
H	-2.8785488	2.4236622	-2.6750335
H	-2.7722594	2.9937962	1.0654157
H	-4.1279762	2.4816320	0.0280779
H	-3.0783001	3.8410771	-0.4847504
H	-1.4678017	-2.2083706	-0.9073290
H	-3.9362982	-1.5269061	2.6219928
S	0.2711675	2.7102767	3.0543047
O	0.8388923	3.6640308	2.0994600
O	1.1677433	2.0103181	3.9686346
C	-0.8782829	3.6748446	4.0456145
C	-2.5706958	5.2416005	5.5326552
C	-0.7423840	3.6914793	5.4350383
C	-1.8348975	4.4590393	3.3918173
C	-2.6978760	5.2485987	4.1429539

C	-1.5983494	4.4904103	6.1917015
H	0.0235351	3.0777688	5.9076317
H	-1.8997411	4.4455073	2.3055493
H	-3.4752817	5.8487597	3.6757262
H	-1.5394011	4.5208061	7.2777928
N	-0.7763409	1.7529910	2.1671536
I	-2.0038305	0.3754303	4.0010417
C	-3.6727459	1.6516406	4.1629342
C	-5.8688360	3.3195186	4.3951263
C	-4.4981953	1.8320287	3.0503325
C	-3.9359230	2.2565078	5.3953816
C	-5.0513483	3.0893082	5.5051228
C	-5.5946834	2.6883251	3.1777788
H	-4.3080441	1.3163176	2.1089409
H	-3.2790085	2.0986702	6.2490526
H	-5.2648465	3.5747142	6.4582818
H	-6.2402332	2.8508491	2.3140400
H	-6.7239822	3.9899285	4.4827895
N	-3.5526130	6.0059164	6.3396977
O	-4.3698465	6.7051057	5.7355780
O	-3.5092933	5.8721342	7.5668737
Co	-0.1252774	0.6381005	0.8452401
N	0.4551166	-0.4885934	-0.8417453
H	1.2952476	-0.1063306	-1.2837119
H	-0.3287960	-0.4348896	-1.4966693
H	0.6206969	-1.4671697	-0.5964911

J^{NH_3}

76 atoms

Cl	6.1244967	3.1456161	-0.6789418
O	3.7595274	-1.4157987	-0.4009156
O	-0.9098348	-3.6514246	0.2398323
N	1.9912687	0.0742999	-0.3181703
N	0.1770025	-1.7361858	-0.3432492
C	2.5631557	-1.2003323	-0.2846556
C	1.5126417	-2.3120282	-0.0321025
C	-0.9496858	-2.4995060	-0.2251169
C	-2.2834330	-1.9585948	-0.7961492
C	2.6045783	1.2837029	-0.4109890
C	3.9851975	1.5367525	-0.5238748
C	4.4283823	2.8466539	-0.5726677
C	1.6695516	-2.7139638	1.4520815
C	1.8376306	-3.4907930	-0.9633205
C	-3.4402164	-2.8593348	-0.3301342
H	4.6867034	0.7079134	-0.5373555
H	1.0440636	-3.5864696	1.6635851
H	1.3486739	-1.8949834	2.1072171
H	2.7226174	-2.9500347	1.6549174
H	1.7045882	-3.2024155	-2.0163214
H	1.1778460	-4.3347265	-0.7396542
H	2.8829646	-3.7897173	-0.8164518
H	-3.1954760	-3.9097337	-0.5224590
H	-4.3563367	-2.5876598	-0.8657517
N	0.3693994	1.9808984	-0.3091369
N	-1.7093427	0.4787715	-0.4476646
C	-2.6756161	-0.4815299	-0.5027631
C	-2.1885904	-2.1060244	-2.3412525
C	1.6647963	2.3934000	-0.3749448
C	3.5021940	3.9422735	-0.5147092
C	-0.7971606	2.7565081	-0.2739995
C	-2.0887069	1.9013328	-0.2310425
O	-3.8809310	-0.2070196	-0.4115685
H	-2.0880322	-3.1689693	-2.6010617
H	-1.3292505	-1.5782580	-2.7632065
C	2.1395746	3.7181026	-0.4181489
Cl	4.0754630	5.5689439	-0.5467904
O	-0.8002444	3.9754172	-0.3043032
C	-2.9831949	2.4296021	-1.3716859
C	-2.7523891	2.1173202	1.1436065
H	1.4382877	4.5447795	-0.3546996
H	-3.9489449	1.9170233	-1.3547271
H	-2.5063806	2.2617006	-2.3494272
H	-3.1287839	3.5092991	-1.2424833
H	-2.1390433	1.6609213	1.9284192
H	-3.7450680	1.6552779	1.1417135
H	-2.8371775	3.1926966	1.3461591
H	-3.1059492	-1.7171895	-2.8041660
H	-3.6374763	-2.7307840	0.7389407
N	0.0112562	0.0638155	1.6120608
S	0.8275718	1.0874946	2.5956354
O	2.2774529	0.9884481	2.3968142
O	0.2166183	2.4188011	2.5856782
H	-1.5050143	1.2215350	4.2903543
C	-0.7669528	0.5990518	4.7927380
C	1.1883856	-0.9686400	6.0669561
C	0.4664526	0.3464845	4.1851550
C	-1.0302978	0.0583947	6.0473437
C	-0.0467884	-0.7154083	6.6627675
C	1.4455259	-0.4325806	4.8075051
H	-1.9803172	0.2224846	6.5510700
H	2.3992674	-0.6012968	4.3099032
H	1.9222944	-1.5796407	6.5883036
N	-0.3314497	-1.3060066	7.9970896
O	0.5510553	-1.9948893	8.5156182
O	-1.4331263	-1.0727020	8.5005983
H	-1.8671273	-3.4788414	2.2061855
C	-2.1406479	-3.0486002	3.1752987
H	-2.9451041	-3.5982745	3.6708851
Cl	-0.6969808	-3.1191927	4.2287365
Cl	-2.7191852	-1.3785558	2.8892671
Co	0.1362155	0.1428526	-0.2013042
N	0.2709527	0.2275509	-2.4149062
H	0.9129435	0.9551933	-2.7373796
H	-0.6668966	0.4321180	-2.7666093
H	0.5805567	-0.6743255	-2.7821749

TS4^{NH_3}

87 atoms

Cl	6.3531024	9.2330589	0.5449324
O	6.1598484	4.1019616	0.5457709
O	3.0123712	-0.0117749	0.2115715
N	3.9393594	4.6678621	0.2623449
N	3.0808200	2.2553534	0.0889525
C	4.9857940	3.7732711	0.4508614
C	4.5148275	2.2975690	0.4831748
C	2.4437489	1.0620116	-0.0500599
C	1.0150417	0.9839682	-0.6476578
C	3.9864820	6.0326151	0.1848853
C	5.1151361	6.8550906	0.3564385
C	4.9712794	8.2320029	0.2625867
C	4.7392664	1.7658975	1.9129884
C	5.3992388	1.5445631	-0.5310817
C	0.3212364	-0.2604977	-0.0523045
H	6.0757300	6.4062000	0.5912688
H	4.5684025	0.6842405	1.9249073
H	4.0546720	2.2509350	2.6172957

H	5.7671176	1.9908716	2.2257334
H	5.2239664	1.9134845	-1.5534655
H	5.1805919	0.4735335	-0.4987847
H	6.4530881	1.7216602	-0.2827880
H	0.9220977	-1.1526113	-0.2565140
H	-0.6747187	-0.3703803	-0.4938353
N	1.6871827	5.7046860	-0.1601418
N	0.4746017	3.4442537	-0.3632423
C	0.0260245	2.1797005	-0.5694046
C	1.2170721	0.7249988	-2.1688437
C	2.6965180	6.6281483	-0.0800866
C	3.7030781	8.8156729	-0.0323361
C	0.3518558	5.9117149	-0.4299985
C	-0.4523526	4.5978052	-0.5570648
O	-1.1777655	1.9354851	-0.7751772
H	0.2403632	0.5552377	-2.6406564
H	1.8461524	-0.1639697	-2.3082942
C	2.5796943	8.0204201	-0.2153261
Cl	3.5126603	10.5297743	-0.0940197
O	-0.1643580	7.0166291	-0.5767287
C	-1.0592895	4.6143458	-1.9773635
C	-1.5620734	4.6417270	0.5048104
H	1.6064345	8.4640964	-0.4020467
H	-1.7078737	3.7452171	-2.1201507
H	-0.2707318	4.6003719	-2.7453280
H	-1.6356570	5.5390916	-2.1061783
H	-1.1282171	4.5750477	1.5086804
H	-2.2424401	3.7959554	0.3660361
H	-2.1141293	5.5862889	0.4152899
H	1.7012654	1.5705556	-2.6748991
H	0.2126618	-0.1776134	1.0368402
N	1.9088495	3.9186856	1.9313152
S	2.6294169	4.7656984	3.1381913
O	2.0739749	4.2818647	4.4010992
O	4.0859520	4.7916506	3.0112502
H	4.0446022	7.2611979	3.2951570
C	2.9947495	7.4970991	3.1295187
C	0.2818192	8.0353147	2.6114080
C	2.0651786	6.4622328	2.9827989
C	2.5604123	8.8171449	3.0380320
C	1.2147764	9.0630175	2.7641293
C	0.7116380	6.7193750	2.7474896
H	3.2490199	9.6531678	3.1431393
H	0.0088083	5.8932511	2.6482604
H	-0.7535733	8.2750212	2.3802491
N	0.7616118	10.4703109	2.6147332
O	-0.4104558	10.6583449	2.2789748
O	1.5863409	11.3610679	2.8355097
C	0.8560785	2.0174087	2.8474835
H	1.4691313	1.4188196	2.1785214
H	1.3016447	2.2837435	3.8013026
C	-0.4878584	2.1589250	2.6111541
H	-0.8991602	1.7365007	1.6919453
C	-1.4494113	2.8298626	3.4541775
C	-3.4105374	4.1693216	4.9684292
C	-1.0842928	3.6125759	4.5772310
C	-2.8217620	2.7384126	3.1139291
C	-3.7896154	3.3948461	3.8643411
C	-2.0565969	4.2757879	5.3164105
H	-0.0337202	3.7235695	4.8410328
H	-3.1087741	2.1479118	2.2417786
H	-4.8417105	3.3125171	3.5893450
H	-1.7608938	4.8851928	6.1713449
H	-4.1676822	4.6917001	5.5547019
Co	2.2259924	3.9364995	0.1601873
N	2.6466650	3.9669488	-2.0473342
H	3.0746810	4.8440490	-2.3508128
H	1.7730521	3.8235407	-2.5567452
H	3.2824719	3.1918945	-2.2442705

L^{NH_3}

87 atoms

Cl	7.3621115	7.8065059	2.1254981
O	5.5586602	3.0002865	2.3832348
O	1.3758098	0.1284628	1.2461218
N	4.1479922	3.9589031	0.8057051
N	2.5926772	1.9448349	0.5753035
C	4.5648548	2.9501831	1.6693569
C	3.5945920	1.7456605	1.6664787
C	1.5695384	1.0529284	0.4386426
C	0.6656287	1.1219434	-0.8246762
C	4.6788145	5.2220184	0.6789148
C	5.7238808	5.7930914	1.4254281
C	6.0784559	7.1142875	1.1904437
C	2.9618748	1.7772637	3.0758596
C	4.4019864	0.4582997	1.4429174
C	-0.6515957	0.3906397	-0.5088797
H	6.2340200	5.2058063	2.1829677
H	2.2691947	0.9390860	3.1949900
H	2.4384337	2.7304861	3.2155181
H	3.7642494	1.7138757	3.8226232
H	4.8419594	0.4451693	0.4335643
H	3.7505319	-0.4151768	1.5546898
H	5.2207002	0.4087687	2.1724166
H	-0.4413850	-0.6195583	-0.1431894
H	-1.2783006	0.3470399	-1.4053033
N	2.9689955	5.3055875	-0.9168292
N	1.2129528	3.5111686	-1.4101535
C	0.3117258	2.4923899	-1.4729865
C	1.4208517	0.3221883	-1.9215654
C	3.9940752	6.0037578	-0.3208281
C	5.4024219	7.8872314	0.2020301
C	2.0783962	5.7772701	-1.8762597
C	0.9451875	4.7680153	-2.1717118
O	-0.7688741	2.5854581	-2.0815588
H	0.8040411	0.2645151	-2.8288320
H	1.6284463	-0.6959212	-1.5645287
C	4.3725863	7.3381314	-0.5494383
Cl	5.8493389	9.5362970	-0.0851741
O	2.1466042	6.8723508	-2.4206797
C	0.9170131	4.5083825	-3.6874855
C	-0.3430894	5.4825258	-1.7023723
H	3.8501641	7.9301094	-1.2947236
H	0.0546103	3.8845413	-3.9446348
H	1.8354658	3.9933709	-4.0106013
H	0.8592613	5.4663043	-4.2203167
H	-0.2718354	5.7070093	-0.6305807
H	-1.2146433	4.8524782	-1.9024125
H	-0.4324462	6.4325728	-2.2451055
H	2.3764704	0.7963386	-2.1815022
H	-1.2136258	0.9211408	0.2723637
S	1.1443086	5.5700307	2.4119789
O	2.3076809	5.1884470	3.1901659
O	1.2550044	6.4309908	1.2482195
H	-1.2049580	7.1619080	1.8978596
C	-1.1253633	7.0291262	2.9763037

C	-0.8139010	6.7456040	5.7565634
C	-0.0326970	6.3405751	3.5177826
C	-2.0888717	7.5555182	3.8328748
C	-1.9227015	7.3901095	5.2080990
C	0.1438584	6.2148224	4.8983957
H	-2.9602473	8.0872131	3.4560353
H	1.0123603	5.6860877	5.2850032
H	-0.7255375	6.6500964	6.8361008
N	-2.9762975	7.9004925	6.1228845
O	-2.8342037	7.6868903	7.3299343
O	-3.9328027	8.4939386	5.6175921
N	0.5039336	4.1368617	1.8329735
C	-0.8755165	3.9297948	1.3924449
C	-0.3418705	3.1246731	2.5346225
H	-0.9806354	3.4910385	0.4000598
H	-1.5994076	4.7132427	1.6293494
H	0.0279563	2.1202180	2.3071365
C	-0.8465745	3.2974946	3.9316658
C	-1.7514463	3.5807819	6.5779340
C	-0.0312723	2.9169400	5.0088926
C	-2.1293997	3.7962968	4.1967391
C	-2.5772559	3.9423820	5.5108763
C	-0.4786430	3.0622574	6.3223355
H	0.9634688	2.5177599	4.8130527
H	-2.7860626	4.0748907	3.3725894
H	-3.5737255	4.3423629	5.7015562
H	0.1694033	2.7692354	7.1492520
H	-2.1004098	3.7016552	7.6039170
Co	2.7964731	3.5222402	-0.4036266
N	4.0414252	2.8207016	-1.8454912
H	4.8483923	3.4412544	-1.9560656
H	3.5339462	2.7649035	-2.7326198
H	4.3668097	1.8861442	-1.5851261

NH_3

4 atoms

H	-0.0082234	-0.0140388	0.0109513
N	0.0168309	0.0290408	1.0319465
H	-0.9541823	-0.0143855	1.3485163
H	0.4645748	-0.8336166	1.3485859

DCM

5 atoms

C	-0.0038736	-0.0067291	1.0848155
H	1.0304545	-0.0263496	1.4386244
H	-0.5376021	0.8795483	1.4384666
Cl	0.0258819	0.0453891	-0.7026419
Cl	-0.8368607	-1.4488587	1.7367353

PhI

12 atoms

I	-0.5140288	0.0820415	3.1735726
C	-1.5631793	-0.9726835	4.6815585
C	-2.9433165	-2.3602801	6.6641686
C	-1.0188099	-2.1501258	5.2013236
C	-2.7878004	-0.4791665	5.1393384
C	-3.4740366	-1.1816880	6.1343588
C	-1.7179601	-2.8405256	6.1958180
H	-0.0634679	-2.5262207	4.8370932
H	-3.2033546	0.4396735	4.7272000
H	-4.4304942	-0.7990950	6.4935384
H	-1.2957544	-3.7602907	6.6032359
H	-3.4837974	-2.9036390	7.4397941

PhINNs

29 atoms

S	2.5271184	0.2362746	1.9840691
O	3.6414139	-0.4376807	1.3325360
O	2.5367051	1.6819888	2.1834545
C	1.0389238	-0.1447840	1.0443289
C	-1.3699418	-0.9046309	-0.0450437
C	-0.0424429	0.7409374	1.0840592
C	0.9387006	-1.3836389	0.3994789
C	-0.2773888	-1.7695694	-0.1534034
C	-1.2649322	0.3568809	0.5390550
H	0.0776847	1.7113422	1.5643652
H	1.8082566	-2.0391038	0.3609957
H	-0.4046623	-2.7363554	-0.6364009
H	-2.1406353	1.0001865	0.5886218
N	2.3432688	-0.6619017	3.3694239
I	1.0531606	0.1673643	4.6786676
C	-0.8314993	-0.6137738	3.9788856
C	-3.1808603	-1.5980620	2.9232133
C	-0.8075525	-1.8580987	3.3593020
C	-1.9845463	0.1592439	4.0910088
C	-3.1725514	-0.3542496	3.5592667
C	-2.0036459	-2.3451662	2.8230716
H	0.1266839	-2.4114150	3.2559868
H	-1.9667931	1.1463418	4.5537656
H	-4.0868288	0.2364545	3.6230557
H	-2.0066087	-3.3065077	2.3086364
H	-4.1029203	-1.9765752	2.4823510
N	-2.6991620	-1.3693286	-0.4987497
O	-2.7876268	-2.5254910	-0.9255570
O	-3.6493175	-0.5866824	-0.3924445

Styrene

16 atoms

H	0.0000000	0.1328321	-0.0216110
C	0.0000000	0.0777735	1.0677645
C	0.0000000	-0.0191232	3.8580464
C	0.0000000	-1.1784985	1.7066002
C	0.0000000	1.2570578	1.8077011
C	0.0000000	1.2162688	3.2074376
C	0.0000000	-1.2000415	3.1143992
H	0.0000000	2.2183413	1.2914085
H	0.0000000	2.1423630	3.7836925
H	0.0000000	-2.1634580	3.6293319
H	0.0000000	-0.0645168	4.9481064
C	0.0000000	-2.4527164	0.9757638
H	0.0000000	-3.3426465	1.6143346
C	0.0000000	-2.6337850	-0.3543682
H	0.0000000	-3.6357869	-0.7825893
H	0.0000000	-1.8030637	-1.0620183

Cis-aziridine 1

33 atoms

H	-0.0492434	2.0240977	1.1737276
C	-0.0169390	1.2868573	1.9773815
C	-0.9219191	0.1108865	1.9495140
H	0.2935621	1.6685708	2.9525380
N	0.5449531	-0.0229641	1.5732227
S	1.6848401	-0.7220664	2.6418557
O	2.9106095	-0.8108188	1.8746476
O	1.6873474	-0.0695703	3.9460727
C	0.9947053	-2.3628426	2.8292625

C	-0.1881414	-4.8200379	3.1028075
C	0.7835708	-3.1444728	1.6883801
C	0.6475867	-2.8091183	4.1047462
C	0.0467776	-4.0577618	4.2456603
C	0.1774660	-4.3898940	1.8257275
H	1.0805803	-2.7722631	0.7085879
H	0.8117928	-2.1641299	4.9656220
H	-0.2622772	-4.4337422	5.2182402
H	-0.0196672	-5.0279771	0.9666839
N	-0.8752747	-6.1307106	3.2464891
O	-1.0412160	-6.8029993	2.2254381
O	-1.2438767	-6.4600610	4.3769132
H	-1.5092749	-0.0253527	1.0374763
C	-1.5397856	-0.5429232	3.1381336
C	-2.7066930	-1.9353883	5.2847888
C	-2.3343549	-1.6792943	2.9111169
C	-1.3534588	-0.1022186	4.4562191
C	-1.9321616	-0.7963945	5.5203109
C	-2.9099968	-2.3745661	3.9735105
H	-2.4821483	-2.0320507	1.8883998
H	-0.7346402	0.7698776	4.6583283
H	-1.7751830	-0.4437197	6.5404395
H	-3.5115938	-3.2631637	3.7796257
H	-3.1529463	-2.4777877	6.1191318

Trans-aziridine 1

33 atoms

H	0.2029794	1.6122761	0.8432062
C	0.1107566	1.0848012	1.7937992
C	-1.0238603	0.1297494	2.0017037
H	0.5008614	1.5977664	2.6760729
H	-1.3264321	0.0257817	3.0483321
N	0.3415452	-0.3697752	1.6803575
S	1.2075621	-1.1026558	2.9468788
O	2.6069573	-1.0436954	2.5750058
O	0.7676462	-0.6188503	4.2503756
C	0.5997406	-2.7719779	2.7259738
C	-0.3584978	-5.3129073	2.3462330
C	1.1507819	-3.5607991	1.7116031
C	-0.4181773	-3.2445907	3.5575729
C	-0.9069476	-4.5359230	3.3654532
C	0.6649609	-4.8510441	1.5173405
H	1.9535456	-3.1633949	1.0918243
H	-0.8091928	-2.6076940	4.3498741
H	-1.6987787	-4.9465190	3.9886861
H	1.0627188	-5.5012531	0.7408247
N	-0.8837125	-6.6914993	2.1352720
O	-0.3781601	-7.3597766	1.2309612
O	-1.7907888	-7.0738713	2.8777317
C	-2.0891832	-0.1229481	0.9946345
C	-4.1438893	-0.5483146	-0.8708197
C	-3.4323027	-0.0731758	1.3927744
C	-1.7833723	-0.3958783	-0.3465769
C	-2.8055039	-0.6074829	-1.2720678
C	-4.4548175	-0.2813302	0.4645946
H	-3.6782380	0.1312252	2.4372858
H	-0.7382405	-0.4614143	-0.6523197
H	-2.5566952	-0.8241001	-2.3117489
H	-5.4960797	-0.2400798	0.7871045
H	-4.9411855	-0.7156489	-1.5959433

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