Supporting Information belonging to the paper:

[Co(TPP)]-Catalyzed Carbene Transfer from Acceptor-Acceptor Iodonium Ylides via *N*-enolate Carbene Radicals

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1. General Considerations

Chemicals and solvents

All reactions were carried out under argon using standard Schlenk techniques or under an inert atmosphere in a N_2-filled glovebox, unless noted otherwise. All chemicals were of commercial grade and used without further purification, unless noted otherwise. All solvents used were pre-dried using either a Solvent Purification System (SPS) from MBraun (MB SPS-800, with standard MBraun drying columns) or were dried and distilled from sodium (PhMe/pentane), sodium/benzophenone (THF/Et_2O) or CaH_2 (CH_2Cl_2, MeOH). All solvents were further dried/stored on activated 3 Å molecular sieves and degassed by sparging with argon unless mentioned otherwise.

NMR spectroscopy

NMR spectra (^1H and ^{13}C) were measured on a Bruker DRX 500, Bruker AMX 400, Bruker DRX 300 or on a Varian Mercury 300 spectrometer at RT unless noted otherwise. Chemical shifts were reported in ppm with respect to $SiMe_4$ by referencing the solvent peak to $SiMe_4$.[1] Individual peaks are reported as: chemical shift (in ppm) (multiplicity (s: singlet, d: doublet, t: triplet, q: quartet, m: multiplet), integration, coupling constant (in Hz).

EPR spectroscopy

EPR spectra were recorded on a Bruker EMX X-band spectrometer equipped with an ER 4112HV-CF100 He cryostat. Simulations of the EPR spectra were performed by iteration of the anisotropic g-values, hyperfine coupling interactions and line widths using EasySpin,[2a] via the cwEPR 3.2 GUI.[2b]

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 inert atmosphere using the solvent as a background. The cuvette was custom outfitted with an extra 10 mL round bottom flask for mixing purposes.

In-situ AT-IR spectroscopy (ReactIR)

Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FT-IR) spectra were recorded on a ReactIR 15 (Mettler-Toledo, 1400003) using a silicon probe (Mettler–Toledo, 14472000). Measurements were performed under inert atmosphere in a two-neck Schlenk flask using the solvent as background.

Cold-Electronspray-ionization MS (CSI-MS)

Mass spectra were collected on a HR-ToF Bruker Daltonik GmbH (Bremen, Germany) Impact II, an ESI-ToF MS capable of resolution of at least 40000 FWHM. Detection was in positive-ion mode and the source voltage was between 4 and 6 kV. The sample was introduced with a syringe pump at a flow rate of 18 µl/hr. The drying gas (N_2) was held between 0°C and –40°C and the spray gas was held between 10°C and –35°C. The machine was calibrated prior to every experiment via direct infusion of a TFA-Na solution, which provided a *m/z* range of singly charged peaks up to 3500 Da in both ion modes. Software acquisition Compass 2.0 for Otof series. Software processing m-mass and Compass 2.0.

Single-crystal X-ray diffraction

X-ray diffraction data of the *N*-enolate-alkyl adduct $\mathbf{I}^{\mathbf{E\text{-}A}}$ were measured on a Bruker D8 Quest Eco diffractometer using graphite monochromated (Triumph) Mo Kα radiation (λ = 0.71073 Å) and a CPAD Photon III C14 detector. The sample was cooled with N_2 to 100 K with a Cryostream 700 (Oxford Cryosystems). Intensity data were integrated using the SAINT software.[3] Absorption correction and scaling was executed with SADABS.[4] The structures were solved using intrinsic

phasing with the program SHELXT 2018/2.[5] The crystal structure contained two voids (total solvent accessible volume = 1404 Å^3), and the highly disordered, non-coordinating solvent molecules within (CD_2Cl_2 and C_5H_{10}) the asymmetric unit could not be refined reliably. Thus, the SQUEEZE[6] procedure in PLATON[7] (version 10421) was applied, accounting for 416 electrons per unit cell, congruent with the presence of 8 × CD_2Cl_2 (42 e$^-$/molecule) and 2 × C_5H_{10} (40 e$^-$/molecule) solvent molecules in the unit cell. Refinement in space group $P2_12_12_1$ was performed as an inversion twin, resulting in a twin fraction (Flack parameter[8]) of 0.079(9). Least-squares refinement was performed with SHELXL-2018/3.[9] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were introduced at calculated positions with a riding model. The crystal data for **I^{E-A}** is summarized as shown in Table S1. The X-ray crystallographic data for **I^{E-A}** was deposited at the Cambridge Crystallographic Data Centre (CCDC) under the deposition number CCDC 2091203.

Table S1. Crystal structure and determination data

Compound	***N*-enolate adduct I^{E-A}**
CCDC	2091203
Empirical formula	$C_{54}H_{41}CoN_4O_8$
Formula weight	932.84
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	$P2_1\ 2_1\ 2_1$
Unit cell dimensions	a = 15.2083(10) Å b = 18.0873(12) Å c = 19.7691(13) Å a = 90° b = 90° g = 90°
Volume	5438.0(6) Å^3
Z	4
Density (Calculated, does not contain contribution from disordered solvent molecules)	1.139 cm^{-3}
Absorption Coefficient	0.367 mm^{-1}
F(000)	1936
Theta range for data collection	2.6° to 33.1°
Index ranges	$-23 \le h \le 23$, $-27 \le k \le 27$, $-30 \le l \le 30$
Reflections collected	727966
Independent reflections	20785 [R_{int} = 0.054]
Observed data [I>2s(I)]	20455
Refinement method	Full-matrix least-squares on F^2
Data / parameters	20785 / 629
Goodness-of-fit on F^2	1.158
Final R indices [I>2s(I)]	R_1 = 0.0447, wR_2 = 0.1186
Largest diff. peak and hole	0.695 and -0.683 eA^{-3}

DFT calculations

DFT geometry optimizations were performed without simplifications on full atomic models using TURBOMOLE 7.4.1[10] coupled to the PQS Baker optimizer[11] via the BOpt package.[12] Unless mentioned otherwise, convergence criteria (scfconv = 7) were used on a m4 grid using Grimme's version 3 zero-damping dispersion correction.[13] For a description of the functional and basis sets used, see below. All minima, without imaginary frequencies, were characterized by calculating the analytical Hessian matrix. Energy output generated in Hartree units was converted to kcal·mol^{-1} by multiplication with 627.51.

Grimme's dispersion corrections were added to compensate for the underestimation of metal-ligand interactions from uncorrected DFT calculations. However, these dispersion corrections lead to an overestimation of association/dissociation energies to/from the non-solvated [Co(TPP)] catalyst. This is due to neglected dispersion interactions of the solvent with the free catalyst's binding sites. As such, a van der Waals π-complex between benzene and [Co(TPP)] was used, either in a 1:1 adduct for all *mono*-carbenoid species or a 2:1 benzene:[Co(TPP)] adduct for all *bis*-carbenoid species resp. These adducts were used as the energetic reference point in all calculations. Nevertheless, this simplified solvation model also leads to an erroneous cancelation of all translational entropy contributions to the computed free energies. This is due to a complete counterbalance of translational entropy contributions of association/dissociation steps which are accompanied by the opposite solvent dissociation/association resp. (Co-benzene + L ↔ Co-L + benzene). Since this is not representative of reality, where the translational entropy contributions of substrate/product association/dissociation cannot be discarded, an additional entropy correction of 25 cal·mol^{-1}·K^{-1} to all computed free energies of substrate/product association/dissociation is added. Moreover, to correct for the differences in reference volume between reactions in the gas phase and in solution, we applied a correction of +2.5 or −2.5 kcal·mol^{-1} for all associative or dissociative steps, respectively, whereby a non-gaseous molecule was released or added for other species than the above mentioned benzene adducts.

Geometric minima:

To decrease calculation times, the following approach was used:

1) All input structures were generated as protein database files (.pdb).
2) All individual components, such as the free catalyst were pre-optimized at the ri-DFT BP86[14]/def2-SVP[15] level of theory without imaginary frequencies as confirmed via an analytical Hessian matrix calculation.
3) Geometric variances of intermediates were selected on the basis of opposing dihedral angles (e.g. 0° vs. 180°) for bonds that were considered relevant. Variances of the tetraphenylporphyrin ligand were omitted due to its rigidity. All ester groups were locked in a *cis*-conformation (dihedral angle H_3**C–O–C=O** = 0°). The minima obtained from the optimization of individual components or *mono*-carbenoid structures were used to minimize the amount of dihedral angle variances for *bis*-carbenoid structures.
4) All intermediates of relevance and their geometric variances were pre-optimized at the ri-DFT BP86/def2-SVP level of theory *without* a following Hessian matrix calculation. On the basis of their SCF energy, the lowest intermediates within 10 kcal·mol^{-1} were selected for a follow-up Hessian matrix calculation.
5) Of the structures obtained from step 4, those lowest in energy in their respective geometrically distinct groups were selected for calculation at the BP86/def2-TZVP[15] level of theory. A geometrically distinct group here means any group that converges to the same general structure based on their respective dihedral angles.
6) Of the structures selected for calculation at the BP86/def2-TZVP level of theory, the lowest in energy was selected as the final geometrical ground state for that intermediate.

Transition states:

1) Using the structures obtained after step 6 of calculating the geometric minima, a 10-point drive was used pertaining the bond(s) of interest at the BP86/def2-SVP level of theory.
2) The highest point of the drive was selected and a single-point calculation with the corresponding Hessian matrix was performed to ascertain if said point was a suitable guess. If not, variations in step 1 were introduced until a suitable guess was found.
3) The corresponding structure was then optimized in a transition-state optimization at the BP86/def2-TZVP level and was checked for having one imaginary frequency in the desired reaction coordinate. This was further confirmed by following the intrinsic reaction coordinate.

In case of broken-symmetry solutions, corrected broken-symmetry energies were estimated from the energy (E_S) of the optimized single-determinant broken symmetry solution and the energy (E_{S+1}) from a separate unrestricted single-point calculation of the high spin-state at the same level of theory. The following approximate correction formula (6) was used:[16]

$$E = \frac{S_{S+1}^2 \cdot E_S - S_S^2 \cdot E_{S+1}}{S_{S+1}^2 - S_S^2}$$

EPR parameters were calculated with the ORCA 4.2.1[17] software package at the B3LYP[18]/ZORA-TZVPP[19] level using the coordinates from the structures optimized in TURBOMOLE as the input. Graphical representations of structures and visualization of orbitals were generated using IboView v20150427.[20] Spin density plots were generated using IQMol 2.9.2 (http://iqmol.org/).

TD-DFT calculations

TD-DFT calculations were performed with the standalone TURBOMOLE 7.5 program package[10] at the ri-(U)DFT b3-lyp, def2-TZVPP level, using a COSMO solvation model (DCM : ε = 8.93, refractive index 1.4244) and the Random Phase Approximation (RPA). For each computed spectrum 50 roots were evaluated.

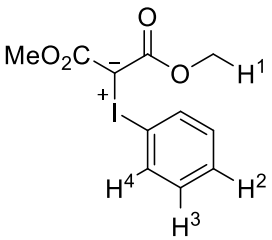
NEVPT2-CASSCF calculations

The ORCA 4.2.1 software package was used to perform NEVPT2-corrected CASSCF calculations. Input geometries were obtained at the BP86/def2-TZVP level of theory at the doublet spin surface, following the above described general protocol. To reduce computational costs, the def2-TZVP basis set was used in conjunction with the RIJCOSX[21] approximation and the def2-TZVP/C fitting basis set. Spin states were calculated for the doublet, quartet and sextet states. To correct the CASSCF energy values, *N*-electron valence state perturbed corrections (NEVPT2)[22] were performed on converged CASSCF wavefunctions together with the spin-orbit mean field method (SOMF).[23] Canonical orbitals were used for visualization using IboView with an isosurface of 80.0 and the energies reported in Hartree units. The energy states of individual spin states are reported in kcal·mol^{-1}. A general flow scheme to perform these calculations was reported by van Leest et al., and was used here accordingly.[24]

Abbreviations

For a list of used abbreviations for all compounds, see Table S15–Table S23 in section 14.

2. Synthesis and characterization of iodonium ylides



DMM•IY

DMM•IY was prepared according to a modified (scaled down) literature procedure[25] and spectroscopic data was in accordance with previously reported data. KOH (2.00 g; 36 mmol; 6 eq.) was finely powdered using a mortar and added to a flame dried 100 mL Schlenk flask right away. The solid was cycled three times with Ar/vacuum and to this was added dry MeCN (20 mL). While stirring, dimethylmalonate (693 µL; 6 mmol; 1 eq.) was added and the reaction mixture was stirred at 0°C for 5 min. To this, in one portion, was added diacetoxyiodobenzene (PIDA) (2.13 g; 6.6 mmol; 1.1 eq.) and the mixture was stirred for exactly 2 h at 0°C during which it gradually became yellow.

Workup: 10 mL water was added, and the mixture was stirred for 2 min, after which it was immediately filtered on a porosity sintered glass funnel (P3) until all solvent was removed. The reaction flask was washed with another 10 mL water and this rinse is used to slurry-wash the filter cake, after which all solvent was removed once again. Subsequently, the filter cake was slurry-washed twice with 10 mL Et_2O and dried on the filter for 10 min. Lastly, all solid material was scraped off and collected in a pill jar which was dried on high vacuum for 1–2 h at RT. Isolated yield: 1.93 g (76% yield).

^{1}H-NMR (400 MHz, DMSO-d_6): δ 7.73 (td, $^3J_{H-H}$ = 7.2, $^4J_{H-H}$ = 2.4 Hz, 2H, *H-4*, *o*-C**H**), 7.51 (tt, $^3J_{H-H}$ = 7.2, $^4J_{H-H}$ = 1.2 Hz, 1H, *H-2*, *p*-C**H**), 7.45 (tt, $^3J_{H-H}$ = 7.2, $^4J_{H-H}$ = 2.4 Hz, 2H, *H-3*, *m*-C**H**), 3.49 (s, 6H, *H-1*, OC**H**$_3$). The spectrum is in accordance with literature, except that the methyl peak is erroneously reported at 3.75 ppm which is its shift in $CDCl_3$ and not in DMSO-d_6 as also evident from the literature spectra[25].

Notes:

1) It is imperative that the temperature is kept at 0°C during the reaction AT ALL TIMES. Increase of temperature leads to decomposition as evident from the presence of iodobenzene in the ^{1}H-NMR spectrum of the product.

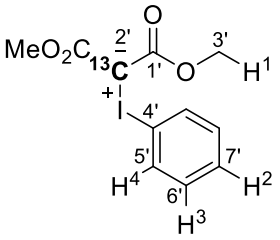
2) It is also imperative that the product is dried properly at room temperature or lower for it is far more unstable when wet.

3) Use a long, cylindrical Schlenk flask and do not stir too rapidly. Otherwise, solid material will accumulate above the solvent level leading to unreacted material that cannot be easily purified out. Do not stir too slowly either for the reaction will not proceed to completion. Around 600 rpm using a medium-sized, oval-shaped stir bean is generally the sweet spot.

4) The product can be stored for months at –20°C without any decomposition in a sealed, amber pill jar.

5) If iodobenzene impurities are present, the product can be purified by redissolving in a minimum of dichloromethane followed by precipitation with pentane. It can then be filtered off and washed with pentane to recollect the purified material. If in solution, the product is stable for at least several hours at –78°C in dichloromethane.

6) For further notes, the reader is kindly directed to the highly detailed *Organic Syntheses* procedure[25].



^{13}C-DMM•IY

^{13}C-DMM•IY was prepared according to a modified (scaled down) literature procedure[26] and spectroscopic data was in accordance with previously reported data from the *Organic Synthesis* paper.[25] KOH (119 mg; 2.1 mmol; 3.2 eq.) was finely powdered using a mortar and added to a flame dried 5 mL Schlenk flask right away in an ethanol bath actively cooled to −5°C. The solid was cycled three times with Ar/vacuum and to this was added dry MeOH (2 mL). While stirring, 2-^{13}C-diethylmalonate (100 µL; 105.4 mg; 0.65 mmol; 1 eq.) was added via a glass syringe, which was rinsed with the reaction mixture five times. Immediately after, in one portion, was added diacetoxyiodobenzene (PIDA) (203.5 mg; 0.63 mmol; 0.97 eq.) and the mixture was stirred for exactly 1 h at −5°C.

Workup: To the mixture at −5°C was added 2 mL ice-water (0°C) via a measuring cylinder with the Schlenk flask open to air. A white precipitate formed immediately. Without stirring, the mixture was kept at −5°C for 1–2 min after which it was vacuum filtered over a medium-porosity sintered glass filter (P3). It was slurry-washed with pipettes of ice-water five times to collect and wash all solid material. Between each washing, all solvent was removed entirely. Afterwards, it was slurry-washed with several pipettes of Et_2O once and washed once more with Et_2O with the vacuum on. It was dried on the filter for five minutes, after which it was collected in an amber pill jar and dried on high vacuum at 20°C for 5 min. Yield: 104.2 mg (48%). ^{1}H-NMR (400 MHz, DMSO-d_6): δ: 7.73 (d, $^3J_{H\text{-}H}$ = 7.5 Hz, 2H, *H-4*, *o*-C**H**), 7.51 (t, $^3J_{H\text{-}H}$ = 7.5 Hz, 1H, *H-2*, *p*-C**H**), 7.45 (t, $^3J_{H,H}$ = 8.5, 7.5 Hz, 2H, *H-3*, *m*-C**H**), 3.49 (s, 6H, *H-1*, OC**H$_3$**). ^{13}C-NMR (100 MHz, DMSO-d_6): 166.03 (2C, *C-1'*, **C**=O), 131.07 (2C, *C-5'*, *o*-**C**), 130.89 (2C, *C-6'*, *m*-**C**), 130.17 (1C, *C-7'*, *p*-**C**), 116.02 (1C, *C-4'*, *ipso*-**C**), 57.55 (broad, 1C, *C-2'*, ^{13}C-labeled ylidic carbon), 51.01 (2C, *C-3'*, O**C**H$_3$).

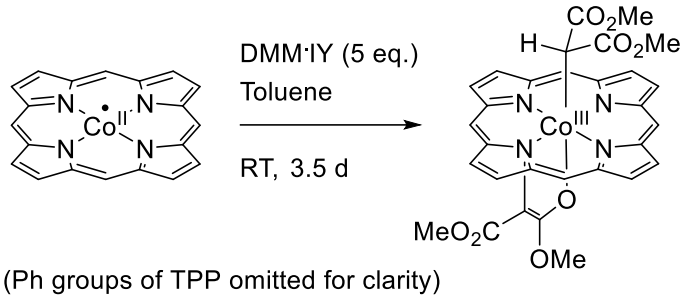
Notes:

1) The type of alcoholic solvent dictates the type of ester obtained as explained by Neilands.[26,27] Since DMM•IY was the focus of study, yet its ^{13}C-counterpart was not commercially available, we opted for the one-pot transesterification and ylidation of its ^{13}C-ethyl analogue.

2) The ^{1}H-NMR shows the product to be >95% pure with trace amounts of $PhI(OAc)_2$, Et_2O, some non-transesterified material and a small amount of decomposition into PhI and $(MeO_2C)_2C{=}C(CO_2Me)_2$.

2) The ^{13}C-NMR shows significantly more decomposition as a consequence of its longer measuring time. However, a broad singlet of the labeled ylidic carbon is clearly present in accordance with literature spectra as are the rest of the peaks[25]. The greatly increased integral is in accordance with the expected higher ^{13}C-content.

3. Isolation of mono-alkyl-mono-enolate species I^{E-A}



(Ph groups of TPP omitted for clarity)

To a flame-dried Schlenk flask was added [Co(TPP)] (15 mg; 22.3 µmol; 1 eq.) and DMM•IY (37.3 mg; 111.6 µmol; 5 eq.), which was subsequently cycled three times with Ar/vacuum (>1 min. vacuum). To this was added 10 mL toluene and the reaction mixture was stirred at room temperature for 3.5 days *in the dark*. Aliquots were taken to assess reaction completion and optimize purification methods. The remaining 7 mL was evaporated *in vacuo* and subsequently redissolved in a minimum volume of CH_2Cl_2 (not dry or degassed). The mixture was purified via column chromatography in the dark (SiO_2; 2:98 acetone: CH_2Cl_2). The third fraction (brown; R_f = 0.3 in CH_2Cl_2) was collected and evaporated at room temperature in the dark. After evaporation, a dark-brown solid was obtained. Yield: 12.8 mg (88%). NMR analysis shows the resulting spectra to be in agreement with the *mono*-alkyl-*mono*-enolate structure (Table S2 for detailed analysis).

The ^{1}H-NMR spectrum shows clear desymmetrization of the β-H pyrrole and o/m-phenyl signals, three $COOCH_3$ peaks in a 1:2:1 ratio and a distinct peak at −4.57 ppm that corresponds to the alkyl C–H peak. The large negative shift is due to the strong aromatic ring current exhibited by the porphyrin macrocycle that shifts the outer β–pyrrolic and o-phenyl peaks downfield and atoms near its center upfield. 2D ^{1}H^{1}H-COSY, ^{1}H^{13}C-HSQC and HMBC corroborate these findings.

Crystals suitable for X-ray diffraction were obtained via layering of a CD_2Cl_2 solution with cyclopentane in the dark. ^{1}H-NMR (CD_2Cl_2; 300 MHz): 8.78 (d, $^3J_{H-H}$ = 5.0 Hz, 2H, *H-2/3*, β-pyrrole); 8.72 (s, 2H, *H-4*, β-pyrrole); 8.69 (d, $^3J_{H-H}$ = 5.0 Hz, 2H, *H-2/3*, β-pyrrole), 8.38 (bs, 4H, *H-10*, *o*-Ph); 8.29 (s, 2H, *H-1*, β-pyrrole (*N*-enolate)); 8.21 (bs, 2H, *H-5/9*, *o*-Ph); 8.11 (bs, 2H, *H-5/9*, *o*-Ph); 7.89 (t, $^3J_{H-H}$ = 7.2 Hz, 4H, *H-7*, *p*-Ph); 7.83 (d, $^3J_{H-H}$ = 7.1 Hz, 2H, *H-6/8*, *m*-Ph); 7.77 (m, 6H, *H-6/8 & 10,11*, *m*-Ph); 3.19 (s, 3H, *H-12*, *N*-enolate O*CH*$_3$); 1.94 (s, 6H, *H-13*, alkyl ester O*CH*$_3$); 1.34 (s, 3H, *H-14*, *N*-enolate free ester O*CH*$_3$); −4.57 (s, 1H, *H-15*, alkyl C–*H*). ^{13}C-NMR (CD_2Cl_2; 75 MHz): 171.54 (2C, *C-21*, alkyl *C*=O); 169.01 (1C, *C-22*, *N*-enolate C=*C*-O); 164.66 (2C, *C-2*, α-pyrrole (*N*-enolate)); 162.49 (1C, *C-23*, *N*-enolate free ester *C*=O); 152.36 (2C, *C-4/7*, α-pyrrole); 148.98 (2C, *C-4/7*, α-pyrrole); 148.95 (2C, *C-9*, α-pyrrole); 141.93 (2C, *C-11/17*, *ipso*-Ph); 141.13 (2C, *C-11/17*, *ipso*-Ph); 137.26 (4C, *C-18*, *o*-Ph); 136.03 (2C, *C-10*, β-pyrrole); 134.64 (2C, *C-5/6*, β-pyrrole); 134.30 (2C, *C-5/6*, β-pyrrole); 133.70 (2C, *C-12/16*, *o*-Ph); 133.25 (2C, *C-12/16*, *o*-Ph); 128.76 (2C, *C-13/15*, *m*-Ph); 128.76 (2C, *C-14/20*, *p*-Ph); 128.70 (2C, *C-14/20*, *p*-Ph); 127.59 (6C, *C-13/15 & 19*, *m*-Ph); 127.44 (2C, *C-2*, β-pyrrole (*N*-enolate)); 126.10 (2C, *C-3*, *meso-C* (*N*-enolate)); 124.56 (2C, *C-8*, *meso-C*); 93.67 (1C, *C-24*, *N*-enolate *C*); 50.25 (1C, *C-25*, *N*-enolate O*C*H$_3$); 49.85 (1C, *C-26*, *N*-enolate free ester O*C*H$_3$); 49.46 (2C, *C-27*, alkyl ester O*C*H$_3$); 0.05 (1C, *C-28*, alkyl *C*–H). CSI$^+$-MS (*m/z*): calculated for $C_{54}H_{41}CoN_4O_8$: 932.22564, found 932.2258 [M$^+$] (error: 0.17 ppm). UV/Vis (DCM) λ_{max} (nm) (ε): 356 (37800), 455 (70000).

Table S2. Interpretation of 2D-NMR spectra for the *mono*-alkyl-*mono*-*N*-enolate species $\mathbf{I^{E-A}}$ in CD_2Cl_2.

COSY			**HSQC**			**HMBC**		
f1(ppm)	f2 (ppm)	Assignment	**f1(ppm)**	f2 (ppm)	Assignment	**f1(ppm)**	f2 (ppm)	Assignment
8.78	8.69	β-pyrrole	**171.54**	-		**171.54**	−4.57 1.94	Carbonyl (alkyl)
8.72		β-pyrrole	**169.01**	-		**169.01**	1.34 3.81	Carbonyl (alkyl dimer) + Carbonyl (*N*-enolate)
8.69	8.78	β-pyrrole	**164.66**	-		**167.32**	3.75	Carbonyl (alkyl dimer)
8.38	7.89	*meta*-Ph	**162.49**	-		**164.66**	8.29	α-pyrrole (*N*-enolate)
8.29		β-pyrrole	**152.36**	-		**162.49**	3.19	Carbonyl (*N*-enolate free ester)
8.21	7.77	*ortho*-Ph	**148.98**	-		**152.36**	8.78 8.69	α-pyrrole (*C*-4/7)
8.11	7.77	*ortho*-Ph	**148.95**	-		**148.98**	8.78 8.69	α-pyrrole (*C*-4/7)
7.89	8.38 7.83	*para*-Ph	**141.93**	-	*ipso*-Ph	**148.95**	8.72	α-pyrrole (*C*-9)
7.83	7.89 7.77	*ortho*-Ph	**141.13**	-	*ipso*-Ph	**141.93**		
7.77	8.21 8.11 7.83	*meta*-Ph + *ortho*-Ph	**137.26**	8.38	*ortho*-Ph	**141.13**		
4.52		Alkyl dimer (C−*H*)	**136.03**	8.72	β-pyrrole	**137.26**		
4.32		Alkyl dimer (C−*H*)	**134.64**	8.69	β-pyrrole	**136.03**	8.72	β-pyrrole (*C*-10)
3.81		Alkyl dimer (OC*H*$_3$)	**134.30**	8.78	β-pyrrole	**134.64**	8.78	β-pyrrole (*C*-5/6)
3.75		Alkyl dimer (OC*H*$_3$)	**133.70**	8.11	*ortho*-Ph	**134.30**	8.69	β-pyrrole (*C*-5/6)
3.19		N-enolate Ester OC*H*$_3$	**133.25**	8.21	*ortho*-Ph	**133.70**		
1.94		Alkyl OC*H*$_3$	**129.59**			**133.25**		
1.52		*H*$_2$O	**128.76**	7.89 7.83	*para*-Ph; *meta*-Ph	**129.59**		
1.34		N-enolate OC*H*$_3$	**128.70**	7.89	*para*-Ph	**128.76**		
1.27		Unknown	**127.59**	8.38 7.77	*meta*-Ph	**128.70**		
1.21		H-grease	**127.44**	-	β-pyrrole (N-enolate)	**127.59**		
0.09		Si-grease	**126.10**	-	*meso*	**127.44**	8.29	β-pyrrole (*N*-enolate) (*C*-2)
−4.57		Alkyl C−*H*	**124.55**	-	*meso*	**126.10**	8.29	*meso* (*N*-enolate)
			93.67	-	*N*-enolate C	**124.55**	8.72	*meso*
			54.07	3.81	Alkyl dimer (OC*H*$_3$)	**93.67**		*N*-enolate C
			53.42	3.75	Alkyl dimer (OC*H*$_3$)	**54.07**		O−*C*H$_3$ (alkyl dimer)
			50.25	1.34	O−C*H*$_3$ (*N*-enolate)	**53.42**		O−*C*H$_3$ (alkyl dimer)
			49.85	3.19	O−C*H*$_3$ (*N*-enolate free ester)	**50.25**		O−*C*H$_3$
			49.46	1.94	O−C*H*$_3$ (alkyl)	**49.85**		O−*C*H$_3$
			30.25	1.21	H-grease	**49.46**		O−*C*H$_3$
			14.45		Unknown	**30.25**		H-grease
			0.05	−4.57	Alkyl C−*H*	**14.45**		Unknown
						0.05		Alkyl *C*−H

Single-crystal X-ray diffraction analysis

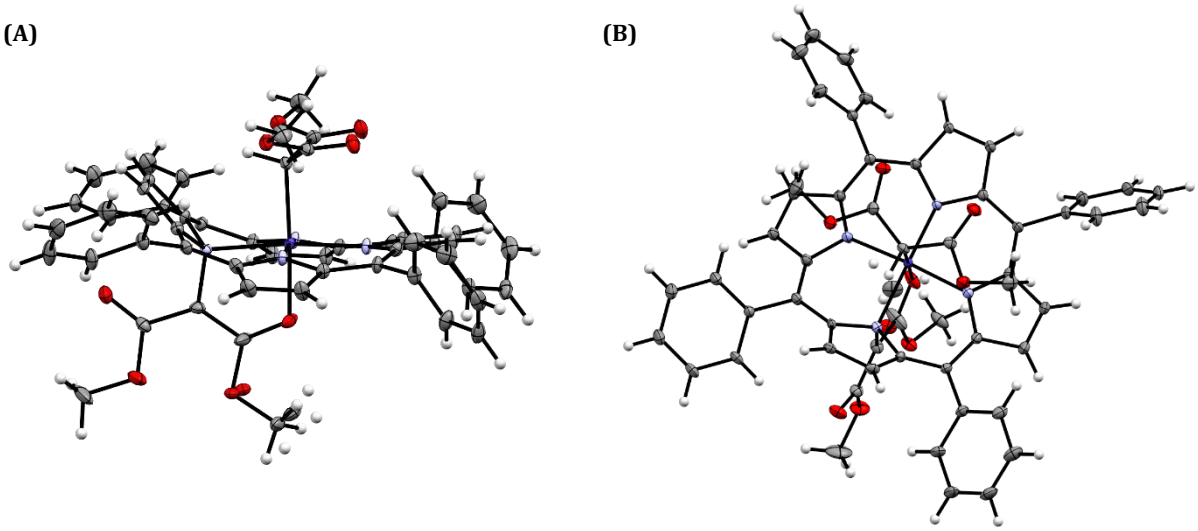


Figure S1. (A) 50% thermal ellipsoid probability plot (side view) of the SC–XRD measurement of the *mono*-alkyl-*mono*-*N*-enolate species $\mathbf{I}^{\mathbf{E\text{-}A}}$. (B) Top view.

Bond-length analysis

Functionalization of one of the porphyrin's pyrroles by the enolate moiety leads to alteration of the overall aromatic structure of the macrocycle. To ascertain the magnitude of these changes, a bond-length analysis as well as use of the harmonic oscillator model for aromaticity (HOMA) was used and compared to the [Co(TPP)(CH_2CO_2Et)] structure reported by Cenini and coworkers.[28] A comparison to the calculated structures obtained by DFT was performed as well (Table S3 & Figure S2).

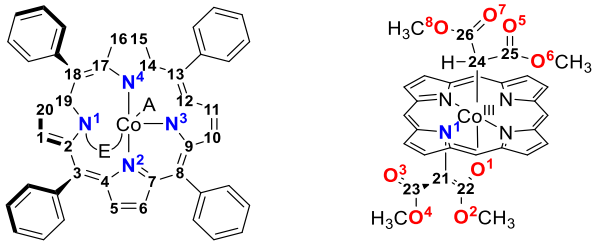


Figure S2. Numbering scheme for the bond-length analysis in Table S2.

Table S3. Selected bond lengths for relevant moieties of the *mono*-alkyl-*mono*-*N*-enolate species $\mathbf{I}^{\mathbf{E\text{-}A}}$ (experimental and calculated) and *mono*-alkyl species (calculated only).[a]: N–Co bond to which CH_2-moiety faces.

Bond	$\mathbf{I}^{\mathbf{E\text{-}A}}$ (experimental) (Å)	[Co(TPP)(CH_2CO_2Et)] (experimental) (Å)	$\mathbf{I}^{\mathbf{E\text{-}A}}$ (calculated) (Å)	[Co(TPP)(CH_2CO_2Et)] (calculated) (Å)
Alkyl				
Co1–C24	2.045(2)	2.012(4)	2.11361	1.98340
C24–C25	1.486(3)	1.438(7)	1.48594	1.48284
C24–C26	1.486(3)	-	1.48595	-
C25–O5	1.206(3)	1.202(5)	1.21802	1.22268
C25–O6	1.357(3)	1.364(4)	1.37680	1.36792
C26–O7	1.213(3)	-	1.21798	-
C26–O8	1.351(3)	-	1.37684	-
N-enolate				
N1–Co1	2.120(2)	1.952(3)	2.26796	1.96073
N1–C21	1.489(3)	-	1.48646	-
C21–C22	1.400(4)	-	1.40877	-
C21–C23	1.441(3)	-	1.44257	-
C22–O1	1.260(3)	-	1.27355	-
C22–O2	1.416(4)/1.359[(a)]	-	1.35140	-
C23–O3	1.217(3)	-	1.23869	-
C23–O4	1.356(3)	-	1.36831	-
O1–Co1	1.952(2)	-	2.02500	-

Porphyrin				
C1–C2	1.381(3)	1.430(5)	1.39858	1.43916
C2–N1	1.464(3)	1.389(3)	1.44517	1.38911
C2–C3	1.393(3)	1.385(4)	1.39768	1.39291
C3–C4	1.398(3)	1.382(4)	1.40605	1.39162
C4–N2	1.378(3)	1.385(4)	1.38682	1.38914
C4–C5	1.439(3)	1.421(4)	1.44478	1.43920
C5–C6	1.351(3)	1.331(5)	1.36363	1.36163
C6–C7	1.447(3)	1.429(4)	1.44382	1.44039
C7–N2	1.377(3)	1.385(3)	1.37644	1.38614
C7–C8	1.400(3)	1.384(4)	1.39922	1.39539
C8–C9	1.394(3)	1.372(3)	1.39667	1.39269
C9–N3	1.372(3)	1.389(3)	1.37528	1.39171
C9–C10	1.449(3)	1.430(5)	1.44437	1.44068
C10–C11	1.356(3)	1.335(4)	1.36140	1.36171
C11–C12	1.443(3)	1.419(4)	1.44432	1.43804
C12–N3	1.379(3)	1.382(3)	1.37536	1.38568
C12–C13	1.393(3)	1.387(3)	1.39662	1.39187
C13–C14	1.396(3)	1.378(4)	1.39916	1.38981
C14–N4	1.369(3)	1.383(4)	1.37636	1.38771
C14–C15	1.443(3)	1.425(3)	1.44378	1.43892
C15–C16	1.355(3)	1.332(5)	1.36357	1.36141
C16–C17	1.441(3)	1.428(3)	1.44480	1.44046
C17–N4	1.376(3)	1.382(3)	1.38685	1.38802
C17–C18	1.401(3)	1.391(4)	1.40600	1.39324
C18–C19	1.388(3)	1.383(4)	1.39776	1.39341
C19–N1	1.457(3)	1.382(4)	1.44521	1.38947
C19–C20	1.387(3)	1.427(5)	1.39854	1.43967
C20–C1	1.396(3)	1.335(4)	1.38963	1.36176

(a) Less accurate due to partial disorder.

Table S4. Selected bond angles and dihedral angles of the crystal structure of the *mono*-alkyl-*mono*-*N*-enolate $\mathbf{I^{E-A}}$ species.

N-enolate (N)		***Co(1)-Ligands***		***Dihedral angles***	
C2–N1–C19	101.80°	***N1 –Co1–N2***	88.69°	***C1–C2–C3–C4***	-145.98°
C2–N1–C21	111.95°	***N1 –Co1–N3***	173.90°	***C7–C8–C9–C10***	177.84°
C2–N1 –Co1	113.60°	***N1–Co1–N4***	88.55°	***C11–C12 –C13–C14***	-179.78°
C19–N1 –C21	114.30°	***N1–Co1–C24***	91.94°	***C17–C18 –C19 –C20***	148.48°
C19–N1 –Co1	112.90°	***N1–Co1 –O1***	85.41°		
C21–N1 –Co1	102.73°	***N2–Co1–N3***	91.32°		
		N2–Co1–N4	171.72°		
		N2–Co1–C24	93.23°		
		N2–Co1–O1	85.58°		
		N3–Co1–N4	90.60°		
		N3–Co1–C24	94.16°		
		N3–Co1–O1	88.51°		
		N4–Co1–C24	94.67°		
		C24–Co1–O1	177.11°		

Harmonic oscillator model for aromaticity (HOMA) analysis

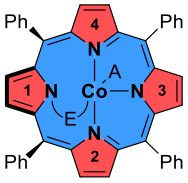


Figure S3. Numbering scheme for the HOMA analysis of the four pyrrolic rings (red; 1–4) and the macrocycle (blue).

Table S5. HOMA values for the four pyrrolic rings (red; 1–4) and the macrocycle (blue; 5).[a]: The HOMA values of the macrocycle are derived from the delocalization pathways derived from bond-length analysis (Table S3) of each species.

Ring	**I^{E-A}** (experimental)	[Co(TPP)(CH_2CO_2Et)] (experimental)	**I^{E-A}** (calculated)	[Co(TPP)(CH_2CO_2Et)] (calculated)
Pyrrole **1** (*N*-enolate)	0.45	0.68	0.65	0.69
Pyrrole **2**	0.60	0.69	0.64	0.69
Pyrrole **3**	0.58	0.71	0.62	0.69
Pyrrole **4**	0.62	0.69	0.64	0.68
Average	**0.56**	**0.69**	**0.64**	**0.69**
Porphyrin[a]	**0.91**	**0.97**	**0.89**	**0.99**

Bond-length analysis (Table S3) show that the experimental and calculated values (see Section 14 for further details) are in agreement. Some overestimation of delocalization effects in DFT explains the small differences between the experimental and calculated data. A bond-length analysis of the crystal structure of the *N*-enolate-alkyl species **I^{E-A}** shows that the aromaticity of the porphyrin is not lost, only altered as a result of pyrrole functionalization. A bond-length analysis performed on the non-functionalized *mono*-alkyl adduct [Co(TPP)(CH_2CO_2Et)] reported by Cenini and coworkers.[28] shows that the β-pyrrole C–C bonds are localized for all four pyrrole rings, with bond lengths along the inner periphery of the macrocycle even out to 1.384 ± 0.004 Å (1.391 ± 0.003 Å). The C–C backbone of the pyrrole rings is only moderately delocalized when comparing the respective bond lengths to 2,3-dihydropyrrole.[29] For the functionalized pyrrole ring in **I^{E-A}**, the C–N bonds lengthen and the C–C backbone shortens. The β-pyrrole C–C bonds of the other 3 pyrrole rings remain localized double bonds with only a small degree of delocalization. Delocalization now travels via the outer C–C periphery of the functionalized pyrrole-ring with an average bond length of 1.387 ± 0.010 Å (exp) and 1.392 ± 0.010 Å (calc.) (Figure S4).

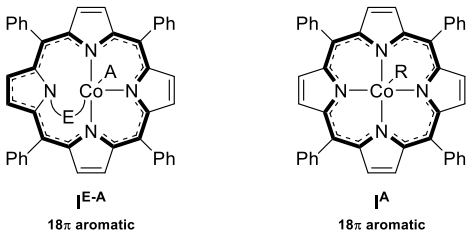


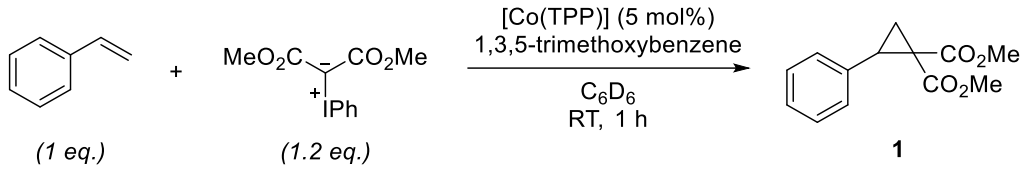
Figure S4. Aromatic delocalization pathway for the *mono*-alkyl-*mono*-*N*-enolate species **I^{E-A}** (E = (MeO_2C)C=C(OMe)–O; A = C(CO_2Me)) and **[**Co(TPP)(CH_2CO_2Et)**]** (R = CH_2CO_2Et), respectively.

A HOMA (Harmonic Oscillator Model for Aromaticity[30] confirms these findings (Table S5). For [Co(TPP)(CH_2CO_2Et)], the porphyrin has a HOMA value of 0.97, which is purely aromatic. The pyrroles have values around 0.69, indicating they do not exhibit significant local aromaticity and delocalize largely into the porphyrin macrocycle. For **I^{E-A}**, the overall aromaticity of the porphyrin is somewhat decreased to 0.91. Most striking is the *N*-enolate pyrrole with a HOMA value of 0.45, suggesting significant deviation from a standard aromatic pyrrole. The other pyrrole rings do not exhibit any significant local aromaticity either and the average HOMA value is decreased to 0.56, suggesting some decrease in overall conjugation. These values are in line with a functionalized, tilted pyrrole ring and the observed upfield shift of the β-pyrrole ^{1}H-NMR chemical shifts vs. [Co(TPP)(CH_2CO_2Et)].[31] This is most pronounced for the *N*-enolate pyrrole, shifting from 8.88 ppm in [Co(TPP)(CH_2CO_2Et)] to 8.29 ppm in **I^{E-A}** (vide supra).

4. Catalytic studies

Identification, yield determination and characterization of known products was performed using ^{1}H-NMR spectroscopy. All experiments were performed in duplo and yields were determined based on relative integrals with respect to 1,3,5-trimethoxybenzene as an internal standard.

General experimental method:



Scheme S1. General scheme for the [Co(TPP)]-catalyzed reaction of styrene and DMM•IY towards (**1**).

A 4 mL glass vial with a 10 mm Teflon-coated stir bean was flame-dried and to this, after cooling and open to air, was added DMM•IY (36.1 mg; 108 µmol; 1.2 eq.) and 1,3,5-trimethoxybenzene (5.0 mg; 30 µmol; 0.33 eq.). The vial was added to an Ar bucket, in which it was cycled three times with Ar/vacuum (vacuum ≥ 2 min.). To this was added styrene (10.3 µL; 9.4 mg; 90 µmol; 1 eq.), which was filtered over basic alumina, degassed and then added via a Gilson pipette (that was cycled beforehand >20 times rapidly in and out of the Ar bucket). Quickly afterwards, 1 mL of a stock solution of [Co(TPP)] in deuterated solvent (3.0 mg/mL) was added to the vial and the vial was sealed with a cap. The reaction mixture was then stirred at 400 RPM for 1 h in the center of the stirring plate. Afterwards, the reaction was quenched by cycling the mixture through a syringe in open air and filtering the mixture via a syringe filter (PTFE, hydrophobic, 0.45 µm) into an NMR tube. A ^{1}H-NMR spectrum was recorded and used for yield determination.

Sample spectrum:

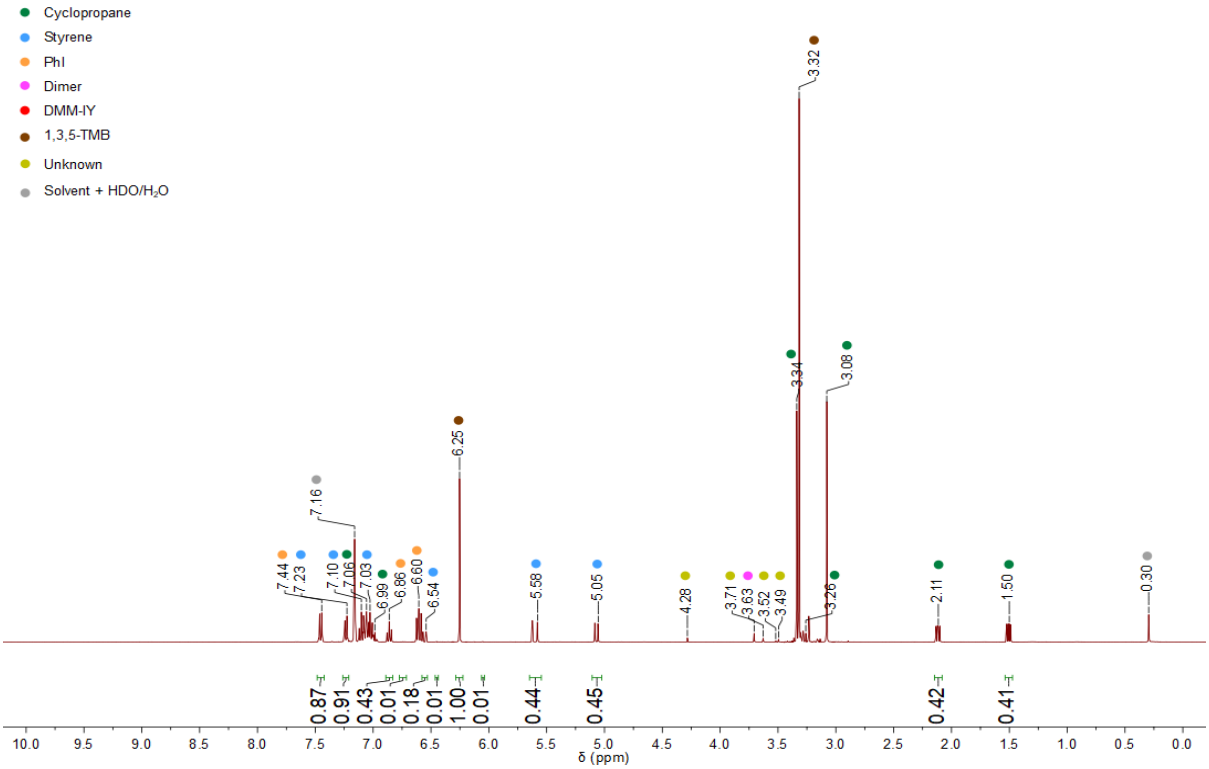
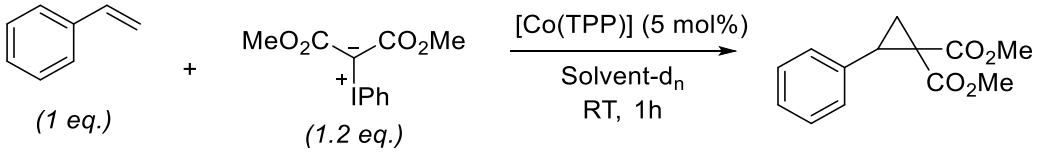


Figure S5. Sample ^{1}H-NMR spectrum of a catalytic mixture of DMM•IY, styrene and [Co(TPP)].

Optimization

We set out to screen numerous solvents under the initial conditions depicted in Scheme S2 and analyzed the samples directly with quantitative ^{1}H-NMR with respect to 1,3,5-trimethoxybenzene. Benzene-d_6, dichloromethane-d_2 and toluene-d_8 turned out to give near quantitative yields and, as such, were monitored over time (Figure S2).



Scheme S2. Initial reaction conditions.

Entry	Solvent	Yield (^{1}H-NMR)
1	**C_6D_6**	**99 ± 4%**
2	**Toluene-d_8**	**98 ± 5%**
3	**CD_2Cl_2**	**98 ± 1%**
4	$CDCl_3$	66 ± 4%
5	THF-d_8	58 ± 0%
6	DMSO-d_6	84 ± 1%
7[a]	CD_3OD	4%
8[a]	CD_3CN	31%

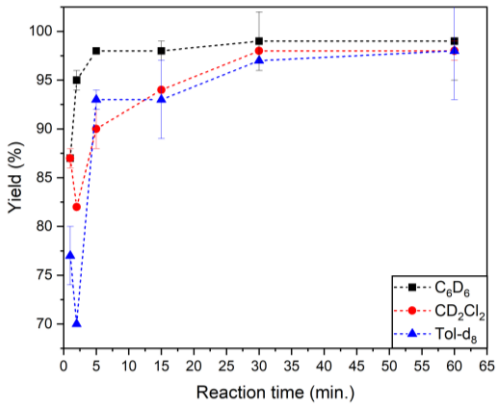
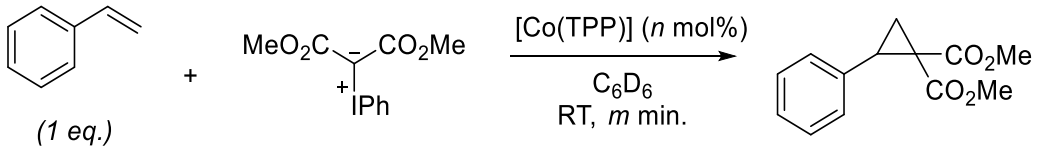


Figure S6. A: Solvent screening. [a] = single run experiment; catalyst only partially soluble. B: Reaction monitored over time by ^{1}H-NMR with respect to 1,3,5-trimethoxybenzene in C_6D_6, CD_2Cl_2 and toluene-d_8 at 1, 2, 5, 15, 30 and 60 min.

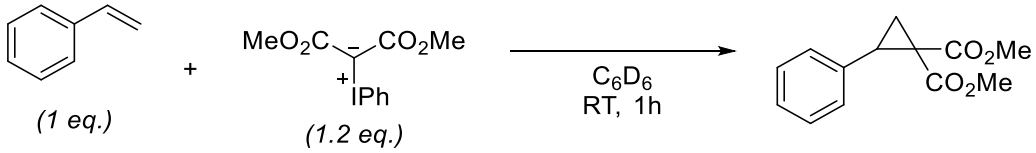


Scheme S3. Screening of catalyst loading and reaction time.

Table S6. Optimization of conditions. [a]: Different batch of DMM•IY was used.

Entry	DMM•IY (eq.)	Catalyst loading (mol%)	Temp. (°C)	Time (min.)	Yield (%)	T.O.N.
9	1	5.0	RT (20)	60	81 ± 4%	16
10	1.2	2.0	RT (20)	60	68 ± 2%	35
11	1.2	1.0	RT (20)	60	42 ± 3%	42
12 [a]	**1.2**	**2.5**	**RT (20)**	**5**	**99 ± 1%**	**40**
13 [a]	1.2	2.0	RT (20)	5	79 ± 1%	40
14 [a]	1.2	1.0	RT (20)	5	48 ± 1%	48
15 [a]	1.2	0.1	RT (20)	5	4 ± 1%	40

Control experiments

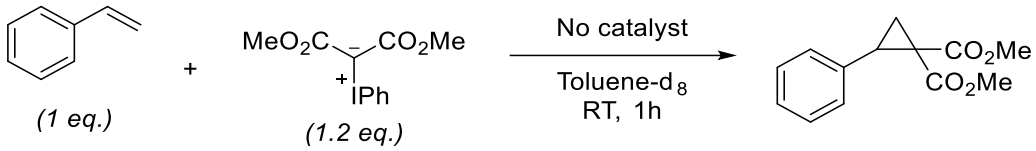


Scheme S4. Control experiments to verify the catalytic role of [Co(TPP)].

Table S7. Control experiments.

Entry	Catalyst	Additive/Alteration	Yield (%)
16	H_2(TPP)	-	0 ± 0%
17	$Co[OAc]_2 \bullet 4\ H_2O$	-	0 ± 0%
18	$Co[OAc]_2 \bullet 4\ H_2O + H_2$(TPP)	-	0 ± 0%
19	[Co(TPP)]	Aerobic	45 ± 2%
20	[Co(TPP)]	TEMPO (5 eq.)	0 ± 0%
21	[Co(TPP)]	$PhI(OAc)_2$ instead	0 ± 0%
22	[Co(TPP)]	DMM instead	0 ± 0%
23	[Co(TPP)]	$PhI(OAc)_2$, DMM & KOH	0 ± 0%
24	-	-	0 ± 0%
25	-	Dark	0 ± 0%
26	-	No 1,3,5-TMB	0 ± 0%
27	[Co(TPP)]	$DMM \cdot N_2$	0 ± 0%

Temperature dependence of the background reaction



Scheme S5. Screening of the temperature dependence of the background reaction.

Table S8. Thermal background control screening

Entry	Temperature (°C)	Yield (%)	Conversion Styrene (%)	Conversion Ylide (%)
28	–78	0 ± 0%	0 ± 0%	0 ± 0%
29	0	0 ± 0%	0 ± 0%	0 ± 0%
30	RT (20)	0 ± 0%	0 ± 0%	1 ± 1%
31	40	0 ± 0%	0 ± 0%	4 ± 0%
32	60	1 ± 1%	0 ± 0%	18 ± 0%
33	80	2 ± 0%	0 ± 0%	32 ± 0%

. The conversion of the ylide is determined by the ^{1}H-NMR integrals of iodobenzene vs. 1,3,5-trimethoxybenzene.

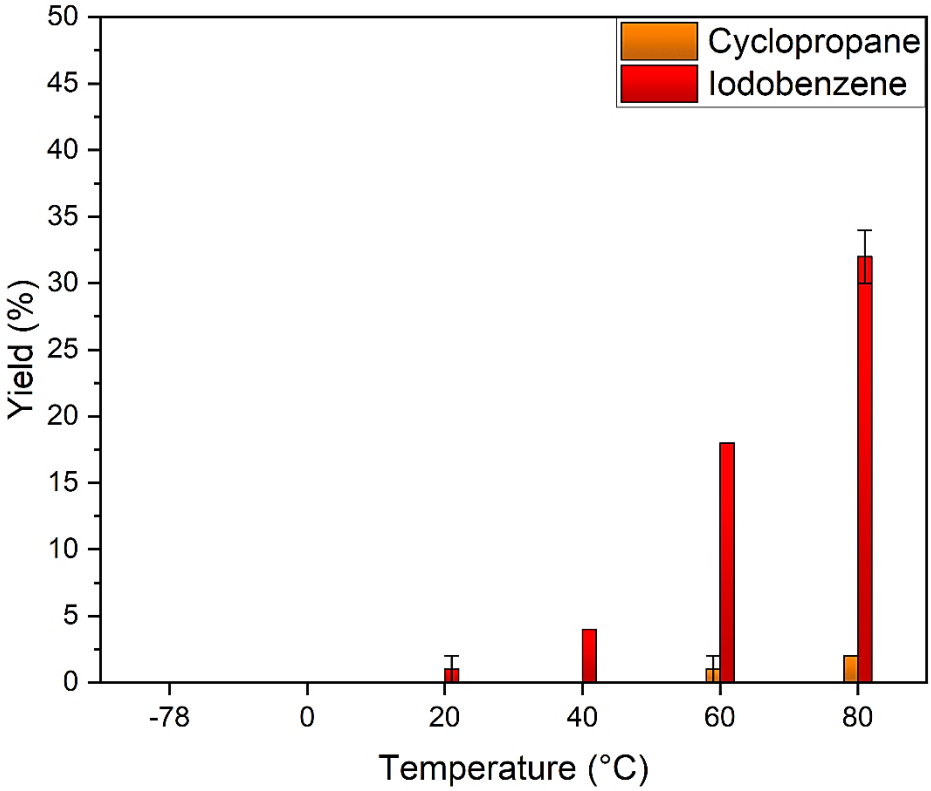


Figure S7. Background reaction of DMM•IY and styrene at various temperatures (°C). Iodobenzene was used as the reference point of conversion, since the thermally generated carbene leads to a wide variety of decomposition products (see NMR spectra; Background reaction).

5. EPR studies

Standard procedure for sample preparation (both RT and 40 K measurements)
To a quartz EPR tube was added 24 eq. of DMM•IY (14.4 mg) (^{13}C-DMM•IY: 14.5 mg). To facilitate sample preparation, the EPR sample holder was attached, and this was subsequently bubbled with Ar for at least 15 min. in a septum-sealed tube holder together with an EPR-tube cap. The following needs to be performed as quickly as possible: To the sample was added 400 µL of a 3 mg/mL stock solution of [Co(TPP)] in C_6H_6 (RT) or toluene (40 K). The septum was removed immediately afterwards, the EPR tube was closed with the cap and the sample was flash frozen in liq. N_2. The cap was secured with parafilm and the tube was kept in liquid nitrogen until measured. For measurements at RT, the sample was slowly thawed in the EPR cavity while continuously measuring EPR spectra until an isotropic signal was obtained.

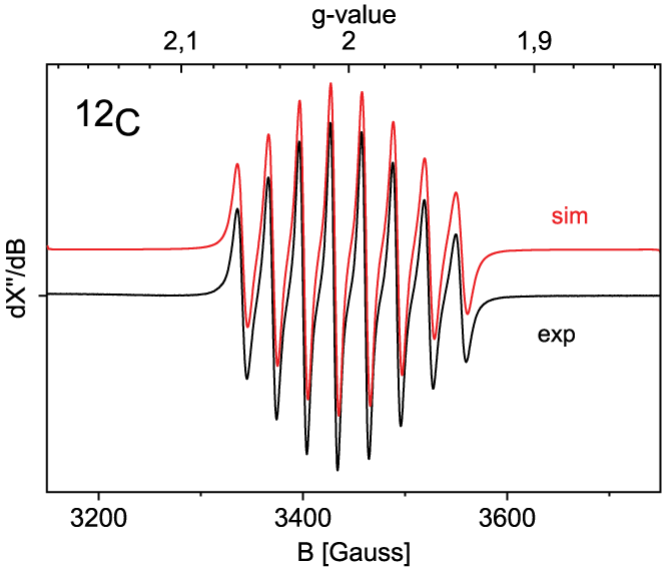


Figure S8. X-Band EPR spectrum of the $\mathbf{I^{E\text{-}T}}$ species in benzene at 293 K. Microwave freq. = 9.643412 GHz, Mod. Amp. = 1 Gauss, microwave power 20.00 mW. Simulation parameters (garlic): g_{11}= g_{22}= 1.996, g_{33} = 2.002 (g_{iso} = 1.998); $A^{59Co}{}_{11}$ = $A^{59Co}{}_{22}$ = *127 MHz*, $A^{59Co}{}_{33}$ =*3 MHz* ($A^{59Co}{}_{iso}$ = 85.6 MHz), logtcorr = –9.86. Note that only 8 resolved HFI lines are visible in this spectrum, in contrast to the 9 lines visible in Figure S5 obtained with the ^{13}C labeled carbene precursor.

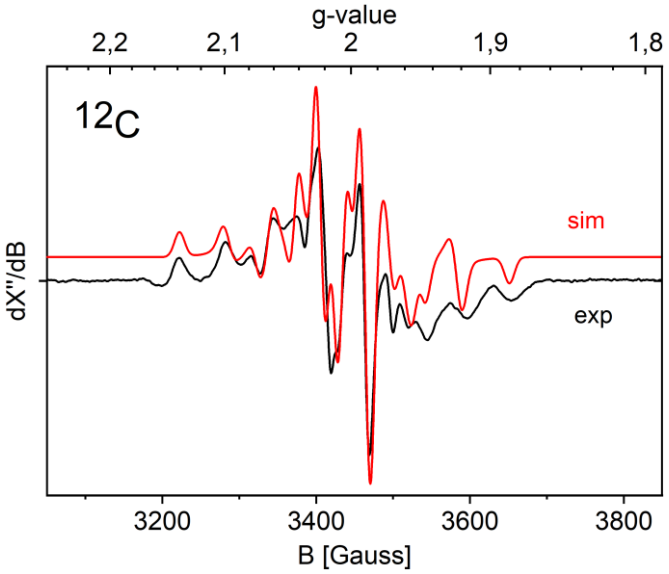


Figure S9. X-Band EPR spectrum of $\mathbf{I^{E\text{-}T}}$ species in toluene glass at 40 K. Microwave freq. = 9.643487 GHz, Mod. Amp. = 4 Gauss, microwave power 0.6325 mW. Simulated parameters (pepper): g_{11}= 1.997; g_{22}= 2.006; g_{33} = 2.008 (g_{av} = 2.004); $A^{59Co}{}_{11}$ = 21 MHz; $A^{59Co}{}_{22}$ = 173 MHz; $A^{59Co}{}_{33}$ = 103 MHz; $A^{59Co}{}_{avg}$ = 85 MHz Euler angles A^{59Co} tensor: [–50, 38, 73] (inspired by DFT).

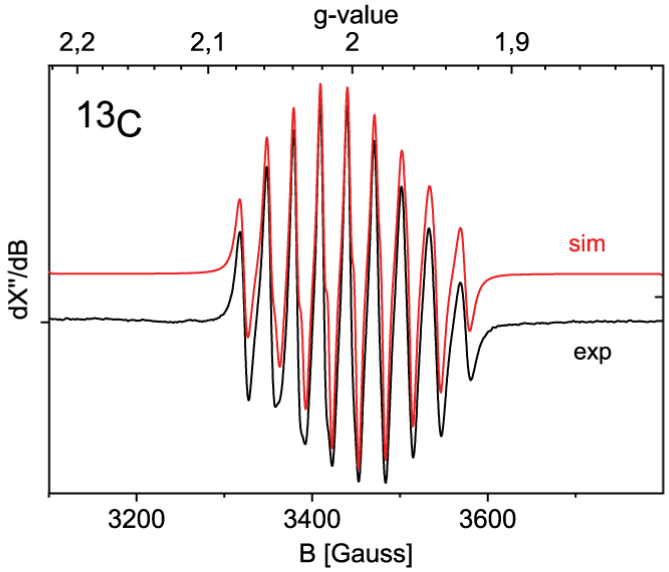


Figure S10. X-Band EPR spectrum of the ^{13}C-labeled $\mathbf{I}^{\mathbf{E\text{-}T}}$ species in benzene at 293 K. Microwave freq. = 9.644876 GHz, Mod. Amp. = 4 Gauss, microwave power 0.6325 mW. Simulation parameters (garlic): g_{11}= g_{22}= 1.997, g_{33} = 2.002 (g_{iso} = 1.998); $A^{59Co}{}_{11}$ = $A^{59Co}{}_{11}$ = *127 MHz*, $A^{59Co}{}_{33}$ =*3 MHz* ($A^{59Co}{}_{iso}$ = 85.6 MHz), additionally HFI with one single ^{13}C nucleaus: $A^{13C}{}_{11}$ = $A^{13C}{}_{22}$ = *107 MHz*, $A^{13C}{}_{33}$ = *100 MHz* ($A^{13C}{}_{iso}$ = 105 MHz), logtcorr = –9.86. Note that clearly 9 resolved HFI lines are visible in this spectrum, in contrast to the 8 lines visible in Figure S4 obtained with the unlabeled carbene precursor.

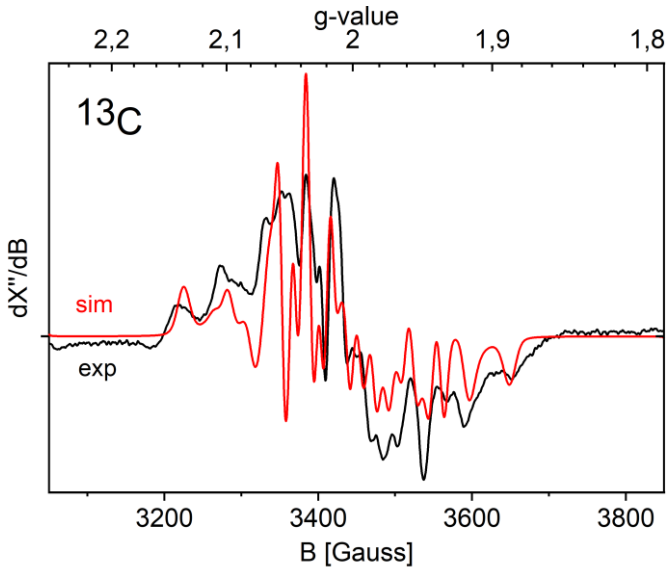


Figure S11. X-Band EPR spectrum of ^{13}C-labeled $\mathbf{I}^{\mathbf{E\text{-}T}}$ species in toluene glass at 40 K. Microwave freq. = 9.642937 GHz, Mod. Amp. = 4.000 Gauss, microwave power 0.6325 mW. Simulated parameters (pepper): g_{11}= 1.998; g_{22} = 2.004; g_{33} = 2.006 (g_{av} = 2.003); $A^{59Co}{}_{11}$ = 21 MHz; $A^{59Co}{}_{22}$ = 173 MHz; $A^{59Co}{}_{33}$ = 103 MHz; $A^{59Co}{}_{avg}$ = 85 MHz, Euler angles A^{59Co} tensor: [–32, 38, 73] (based on DFT); $A^{13C}{}_{11}$ = 260 MHz; $A^{13C}{}_{22}$ = 30 MHz; $A^{13C}{}_{33}$= 30 MHz; $A^{13C}{}_{avg}$ = 107 MHz, Euler angles A^{13C} tensor: [154, 44, –168] (based on DFT).

EPR parameters

Table S9. Experimental EPR parameters of species $\mathbf{I^{E-T}}$, $\mathbf{^{13}C\text{-}I^{E-T}}$, $\mathbf{I^{E}}$ and $\mathbf{I^{T}}$ derived from spectral simulations,[a],[b] compared to DFT-calculated EPR values (in parentheses).[c]

40 K					***RT*** [d]		
Exp. Species I^{E-T}			**Exp. Species I^{E}**	**Exp. Species I^{T}**	**Exp. Species I^{E-T}**		
	^{12}C	**^{13}C**	**^{12}C**	**^{12}C**		**^{12}C**	**^{13}C**
g_{11}	1.997 *(1.986)*	1.998 *(1.986)*	2.051 *(2.131)*	2.018 *(2.006)*	g_{11}	1.996 *(-)*	1.997 *(-)*
g_{22}	2.006 *(1.995)*	2.004 *(1.995)*	2.168 *(2.203)*	1.988 *(1.982)*	g_{22}	1.996 *(-)*	1.997 *(-)*
g_{33}	2.008 *(2.023)*	2.006 *(2.023)*	2.027 *(2.014)*	2.047 *(2.010)*	g_{33}	2.002 *(-)*	2.002 *(-)*
$\boldsymbol{g_{av}}$	***2.004 (2.001)***	***2.003 (2.001)***	**2.082** ***(2.116)***	**2.018** ***(1.999)***	$\mathbf{g_{iso}}$	***1.998 (2.001)***	***1.998 (2.001)***
$A^{59Co}{}_{11}$	21 *(20)*	21 *(20)*	−109 *(−50)*	15 *(−42)*	$A^{59Co}{}_{11}$	3 *(-)*	3 *(-)*
$A^{59Co}{}_{22}$	−173 *(−114)*	−173 *(−114)*	−124 *(−183)*	30 *(−56)*	$A^{59Co}{}_{22}$	127 *(-)*	127 *(-)*
$A^{59Co}{}_{33}$	−103 *(−67)*	−103 *(−67)*	390 *(297)*	135 *(−131)*	$A^{59Co}{}_{33}$	127 *(-)*	127 *(-)*
$\boldsymbol{A^{59Co}{}_{av}}$	***−85 (−53)***	***−85 (−53)***	52 *(21)*	60 *(−76)*	$A^{59Co}{}_{iso}$	***86 (−22)***	***86 (−22)***
Euler angles	−50, 38, 73 *(−32 38 73)*	−32, 38, 73 *(−32 38 73)*	0, 66, −70 *(0, 66, −70)*	−31, 39, 74 (−31, 39, 74)			
$A^{13C}{}_{11}$		260 (221)			$A^{59Co}{}_{11}$		107 *(-)*
$A^{13C}{}_{22}$		30 (32)			$A^{59Co}{}_{22}$		107 *(-)*
$A^{13C}{}_{33}$		30 (37)			$A^{59Co}{}_{33}$		100 *(-)*
$\mathbf{A^{13C}{}_{av}}$		**107 (97)**			$\boldsymbol{A^{13C}{}_{iso}}$		**105** ***(89)***
Euler angles		154, 44, −169 (154, 44, −169)					
					$log(t_{cor})$	−9.86	−9.86

[a] Spectral simulations performed with Easyspin,[2a] using the cwEPR plugin.[2b]
[b] Hyperfine couplings in MHz.
[c] Calculated with Orca 4.2.1 (B3LYP, ZORA-def2-TZVPP).
[d] Spectra in isotropic solution show a rooftop pattern due to slow tumbling at the EPR time scale, which was simulated assuming some remaining (axial) anisotropy on the tumbling time scale. Simulations assuming fully isotropic spectra yield identical g_{iso} and A_{iso} values, but without the observed rooftop line shape.

Table S10. DFT calculated EPR parameters of other species in the proposed catalytic cycle (not consisted with the experimental data).[a],[b]

Species	g_{11}	g_{22}	g_{33}	g_{iso}	$A^{59Co}{}_{11}$	$A^{59Co}{}_{22}$	$A^{59Co}{}_{33}$	$A^{59Co}{}_{iso}$	***Euler angles***	$A^{13C}{}_{11}$	$A^{13C}{}_{22}$	$A^{13C}{}_{33}$	$A^{13C}{}_{iso}$	***Euler angles***
B3LYP/ZORA-def2-TZVPP														
Mono-terminal carbene $\boldsymbol{I^{T}}$	*1.982*	*2.006*	*2.010*	*1.999*	*−56*	*−42*	*−131*	*−76*	*−31, 39, 74*	*224*	*42*	*35*	*100*	*−71, 34, 70*
Mono-enolate adduct $\boldsymbol{I^{E}}$	*2.014*	*2.131*	*2.203*	*2.116*	*−50*	*−183*	*297*	*21*	*0, 66, 70*	*4*	*7*	*4*	*5*	*99, −128, 0*
B3LYP/def2-TZVP														
Mono-bridging carbene $\boldsymbol{I^{B}}$	2.07	2.13	2.27	2.16	491	301	125	306	−127, 0, 103	−11	−15	−16	−14	−109, 0, 147
Bis-terminal carbene $\boldsymbol{I^{T\text{-}T}}$	1.98	1.98	1.98	1.98	−160	−156	8	−103	−118, 7, 104	16	18	158	64	−114, 29, 98
Mono-bridging-mono-terminal carbene $\boldsymbol{I^{B\text{-}T}}$	2.01	2.07	2.11	2.06	−59	246	515	234	−157, 7, 161	70	33	27	44	−7, 24, 12
Cis-bis-bridging carbene $\boldsymbol{c\text{-}I^{B\text{-}B}}$	1.98	2.01	2.04	2.01	47	25	3	25	5, 24, −4	0	0	0	0	0, 0, 0
Trans-bis-bridging carbene $\boldsymbol{t\text{-}I^{B\text{-}B}}$	2.02	2.24	2.27	2.18	802	562	439	601	175, 3, −175	0	0	0	0	0, 0, 0
Cis-bis-enolate adduct $\boldsymbol{c\text{-}I^{E\text{-}E}}$	2.02	2.05	2.14	2.07	−129	253	435	187	−6, 5, −1	−1	−1	2	0	−156, 42, 167
Trans-bis-enolate adduct $\boldsymbol{t\text{-}I^{E\text{-}E}}$	2.00	2.15	2.16	2.11	214	272	655	381	71, 1, −71	2	2	4	3	167, 41, −161

[a] Hyperfine couplings in MHz.
[b] Calculated with Orca 4.2.1.

Single-turnover EPR measurement (detection of mono-terminal carbene $\mathbf{I^T}$)

To a Schlenk flask containing DMM•IY (1.5 mg; 4.5 µmol; 2.0 eq.) was added 1 mL [Co(TPP)] stock solution (1.5 mg; 1.5 mg/mL; 2.23 µmol; 1 eq.) and stirred for 1 min. To this was added 1 mL 2.23 mM styrene stock solution (232 µg; 2.23 µmol; 1 eq.) and the mixture was stirred for 10 seconds after which a 400 µL aliquot was taken into an EPR tube. The sample was further prepared according to the general procedure (vide supra) and measured. The spectrum obtained under these conditions (Figure S12) is indicative for formation of *mono*-terminal carbene species $\mathbf{I^T}$ from species $\mathbf{I^{E-T}}$.[32]

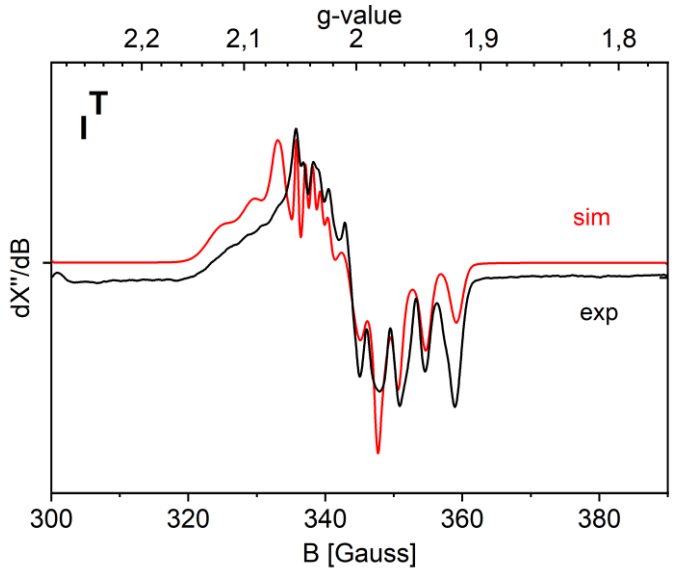


Figure S12. X-Band EPR spectrum of species $\mathbf{I^T}$ measured in a toluene-d_8 glass at 40 K. Microwave freq. = 9.644278 GHz, Mod. Amp. = 5 Gauss, microwave power 6.325 mW. Simulated parameters (pepper): g_{11}= 2.018; g_{22} = 1.988; g_{33} = 2.047 (g_{av} = 2.018); $A^{59Co}{}_{11}$ = 15 MHz; $A^{59Co}{}_{22}$ = 30 MHz; $A^{59Co}{}_{33}$ = 135 MHz; $A^{59Co}{}_{avg}$ = 60 MHz, Euler angles A^{59Co} tensor: [–31, 39, –74] (based on DFT).

Active species detection (dependent on the order of addition of reagents)
To a vial was added DMM•IY (36.1 mg; 108 µmol; 1.2 eq.), which was subsequently cycled three times with Ar/vacuum (vacuum >2 min.). To this was added styrene (9.37 mg; 10.3 µL; 90 µmol; 1 eq.), after which 1 mL of a 1.5 mg/mL stock solution of [Co(TPP)] in toluene-d_8 was added (1.5 mg; 2.25 µmol; 2.5 mol%) (Figure S13). For the reverse order, [Co(TPP)] was added first and stirred in absence of styrene for 3 min (Figure S15). All components combined were stirred for 20 seconds, after which a 400 µL aliquot was taken and frozen for EPR measurement according to the general procedure (vide supra).

When an aliquot was taken from the reaction in the order DMM•IY: Styrene: [Co(TPP)], flash frozen and measured, it revealed a spectrum (Figure S14) highly reminiscent of the previously detected *mono*-terminal carbene $\mathbf{I^T}$ (Figure S8). Additionally, the extra species matches well with that of [Co(TPP)] and as such, it can be concluded that the species detected in the reaction mixture is $\mathbf{I^T}$. In the reverse order (Figure S15), a species was detected that did not match with [Co(TPP)], the *mono*-terminal carbene $\mathbf{I^T}$ nor the *mono*-enolate-*mono*-terminal carbene $\mathbf{I^{E-T}}$. Based on the relatively high offset from g = 2.00 and the large ^{59}Co-HFIs, it can be concluded this is a cobalt-centered radical. We assign this spectrum to the *mono*-enolate adduct $\mathbf{I^E}$, present prior to its rearrangement to $\mathbf{I^T}$ (Figure S13).

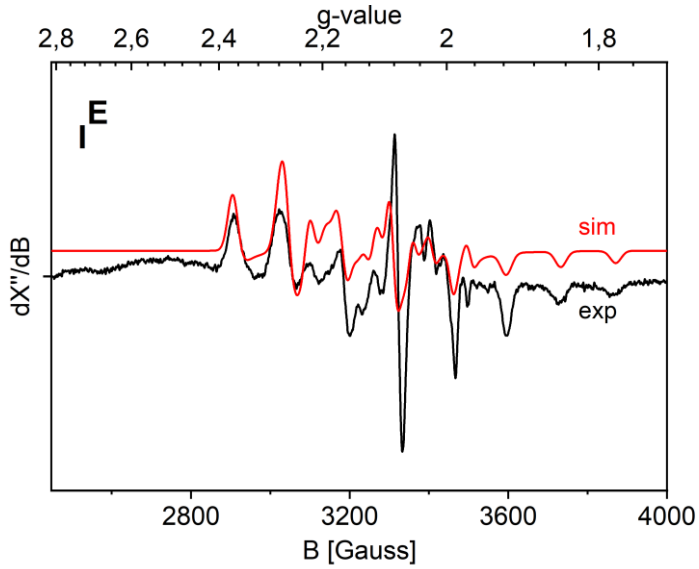


Figure S13. X-Band EPR spectrum of $\mathbf{I^E}$ species in toluene-d_8 glass at 40 K. Microwave freq. = 9.643446 GHz, Mod. Amp. = 4.000 Gauss, microwave power 0.6325 mW. Simulated parameters (pepper): g_{11}= 2.051; g_{22} = 2.168; g_{33} = 2.027 (g_{av} = 2.082); $A^{59Co}{}_{11}$ = –109 MHz; $A^{59Co}{}_{22}$ = –124 MHz; $A^{59Co}{}_{33}$ = 390 MHz; $A^{59Co}{}_{avg}$ = 52 MHz, Euler angles A^{59Co} tensor: [0, 66, –70] (based on DFT).

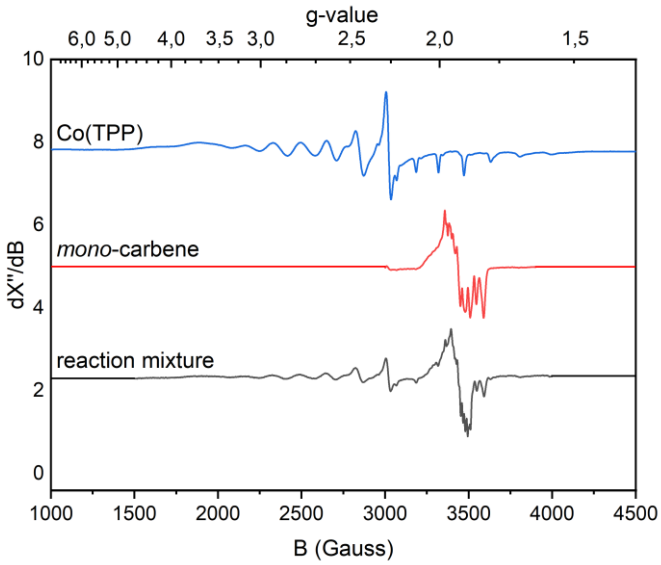


Figure S14. Comparison of the EPR spectrum obtained in toluene-d_8 glass at 40 K after reaction order DMM•IY: Styrene: [Co(TPP)] (black) with [Co(TPP)] (blue) and the *mono*-terminal carbene species $\mathbf{I^T}$ (red). Exp. data (black spectrum): Microwave freq. = 9.644508 GHz, Mod. Amp. = 4 Gauss, microwave power 6.325 mW.

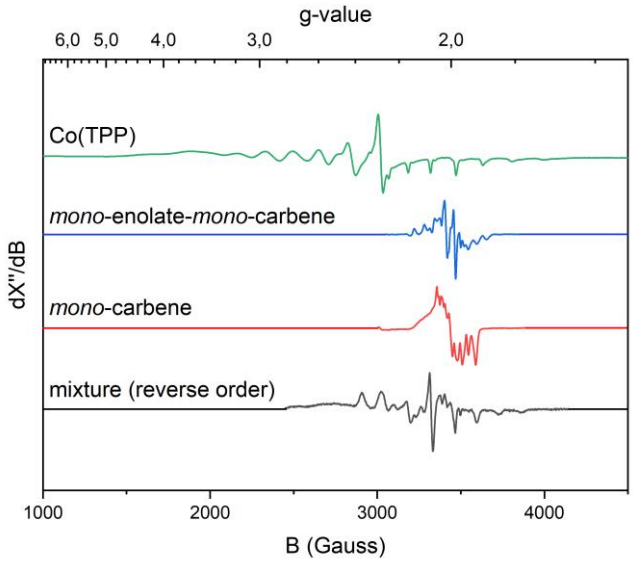


Figure S15. Comparison of the EPR spectrum obtained in toluene-d_8 glass at 40 K after reaction order DMM•IY: [Co(TPP)]: Styrene: (black) with [Co(TPP)] (green), *mono*-enolate-*mono*-terminal carbene (blue) and the *mono*-terminal carbene (red). Exp. data (black spectrum): Microwave freq. = 9.643446 GHz, Mod. Amp. = 4 Gauss, microwave power 0.6325 mW.

UV/Vis Studies

Procedure for titration of [Co(TPP)] with 0 to 20 eq. of DMM•IY (5 µM [Co(TPP)])
A stock solution of DMM•IY in CH_2Cl_2 was cooled to −78°C and kept in the dark at all times. A second stock solution of [Co(TPP)] (473 µg in 28.2 mL; 25 µM) in CH_2Cl_2 was kept at room temperature (20°C). To an inert UV/Vis cuvette was added 1 mL of [Co(TPP)] solution to the reaction flask and 0.2–4.0 mL of DMM•IY solution to the cuvette, which was supplemented to a total of 5.0 mL with pure CH_2Cl_2. Two stock solutions (12.5 µM (0–2.0 eq.); 25 µM (2.0–2.5 eq.) were used. Care was taken to ensure complete separation of both solutions. The setup was transported carefully to the UV/Vis spectrometer, where the solutions were mixed and measured as soon as possible.
To account for small weighing errors imposed by experimental constraints, we calibrated the relative concentrations based on a titration performed at a large volume scale, using a 5 µM solution of [Co(TPP)] with a 25 µM DMM•IY solution (1 mg/120 mL) in CH_2Cl_2. To ensure complete dissolution of DMM•IY, the solution was kept in the dark but at RT and used within 30 min. Decomposition was checked by repeating the experiment with the same equivalents.

Titration of [Co(TPP)] with DMM•IY (Figure S16) results in the clear transition to a single new species with absorption at 357 (29800) and 430 (70600) via isosbestic points at 383, 424 nm for the Soret peak and 518 and 542 for the Q band. The stark decrease of the Soret peak and its redshift as well as the collapse of the Q band are in line with porphyrin functionalization.[33] The absence of the Q band is a result of breaking the orbital degeneracy; the already forbidden transition of $S_0 \rightarrow S_1$ is no longer possible (as would be the case for a symmetric porphyrin macrocycle).

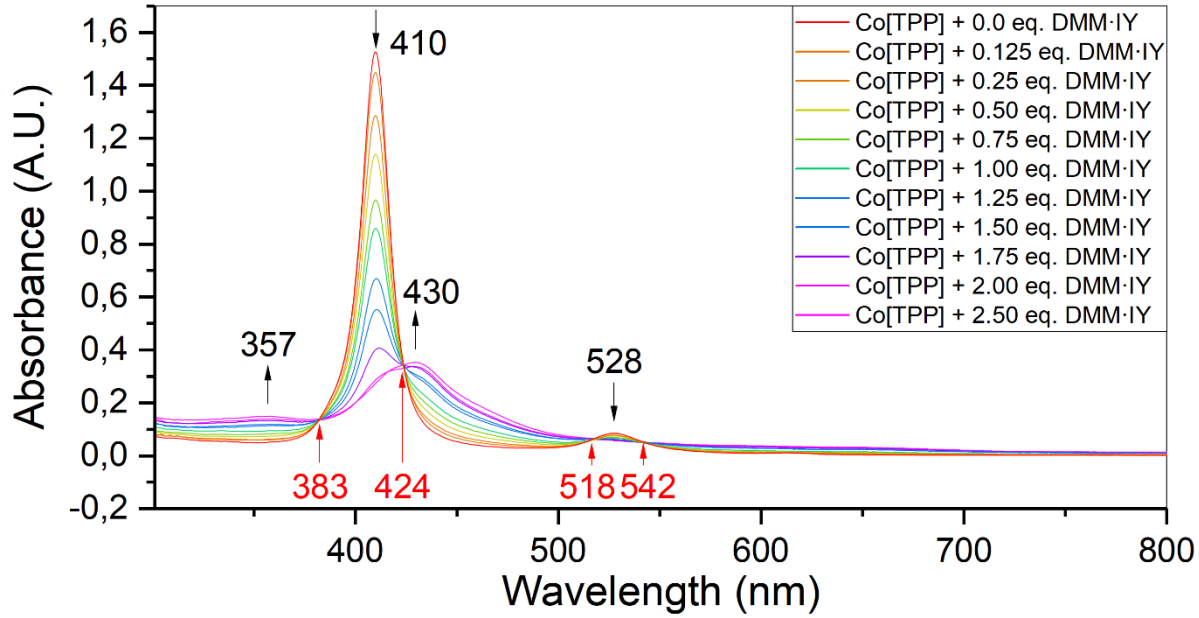


Figure S16. Titration of 5 µM [Co(TPP)] with 0 to 2.50 eq. of DMM·IY.

Procedure for sample preparation at 5 µM [Co(TPP)] with 20 eq. DMM•IY measured over time
A 125 µM stock solution of DMM•IY in the desired solvent (PhMe or CH_2Cl_2) was cooled to −78°C and kept in the dark at all times. A second 25 µM stock solution of [Co(TPP)] was kept at room temperature (20°C). To an inert UV/Vis cuvette (see Figure S18 & Figure S19) was added 1.0 mL of [Co(TPP)] solution to the reaction flask and 4.0 mL of DMM•IY solution to the cuvette. Care was taken to ensure complete separation of both solutions. The setup was transported carefully to the UV/Vis spectrometer, where the solutions were mixed, measured as soon as possible and

periodically for a set amount of time. For experiments carried out in the dark, the setup was wrapped in aluminum foil until the cuvette was inserted into the spectrometer.
Note: For experiments conducted in C_6H_6, the reaction was performed at catalytic concentrations (4.5 mM) and diluted down to UV/Vis concentrations (5 µM). This is due to the instability of the DMM•IY in solution at room temperature (20°C) (Figure S17).

After mixing DMM•IY and [Co(TPP)] in C_6H_6 (Figure S17), a gradual change from 420 to 458 can be observed for the first 13.5 min. After that, a second change occurs whereby the peak at 420 increases in intensity and a second species at 418 nm is formed slowly over the course of roughly 2 hours. Moreover, two new Q-bands arise at 529 and 609 respectively. The intensity of these peaks and their wavelengths are in line with that of a non-functionalized porphyrin.[34] Similarly, in toluene-h_8 (Figure S18), two species are detected. Initially, only one peak at 419 nm is present. This signal is assigned to the *N*-enolate-carbene radical species $\mathbf{I}^{\mathbf{E-T}}$ (see also EPR (Figure S8–Figure S11) and CSI$^+$-MS (Figure S34 & Figure S37) studies). The peak at 419 nm transitions slowly to 458 nm via a single isosbestic point at 441 nm over 45 min. A minor shoulder peak at 419 nm remains, like in C_6H_6. Additionally, a broad band around 295 nm arises. In CH_2Cl_2 (Figure S19), two species are detected. One at 418 nm and one at 430 nm at t = 0 min. The species at 430 nm is likely the same species at 420 nm in C_6H_6, but slightly shifted due to solvent effects (on the basis of UV/Vis titrations (Figure S16), EPR (Figure S8–Figure S11) and CSI$^+$-MS (Figure S27 & Figure S42). This species, at 430 nm, disappears gradually over time into a new species at 455 nm via a single isosbestic point at 441 nm. The minor species at 418 nm remains constant as does the slight Q-band at 525 nm. As in C_6H_6, it is likely this to be an non-functionalized porphyrin since its spectroscopic properties are quite similar to [Co(TPP)] (Soret peak: 410 nm; Q-band: 525 nm (CH_2Cl_2). On the basis of this spectroscopic evidence, it is concluded that the transition to the redshifted species at 458 (C_6H_6/toluene-h_8) or 455 (CH_2Cl_2) is the deactivation product $\mathbf{I}^{\mathbf{E-A}}$.

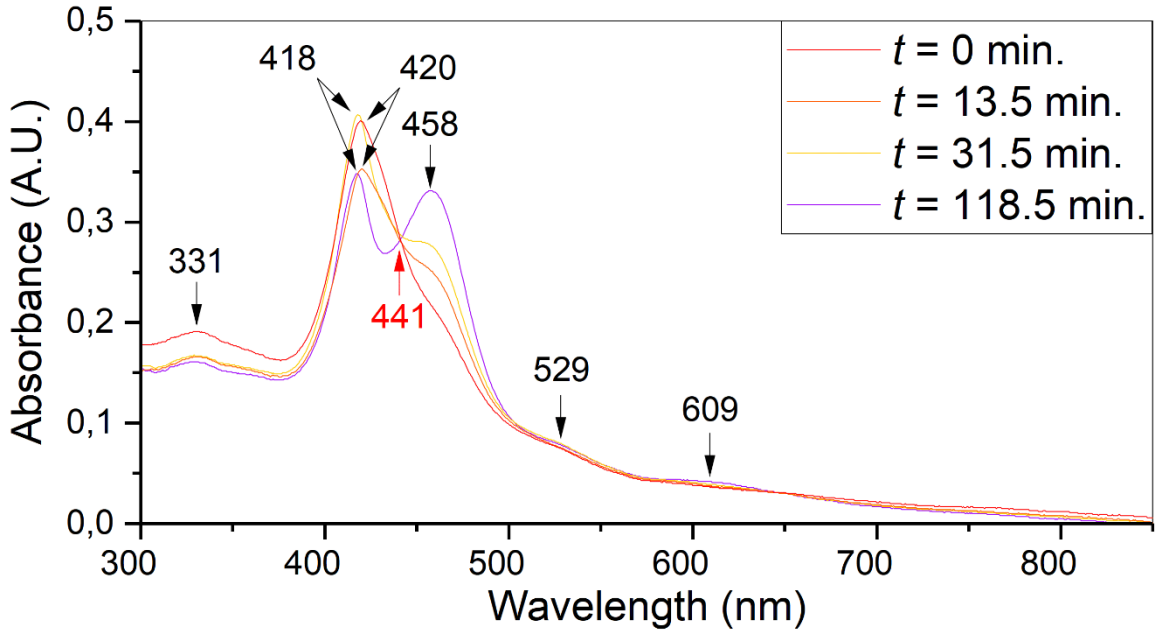


Figure S17. 24 eq. DMM•IY + 1 eq. [Co(TPP)] in C_6H_6 at ~5 µM followed over 2 h (1 scan/90 s). For clarity, only the endpoints of each successive change are shown.

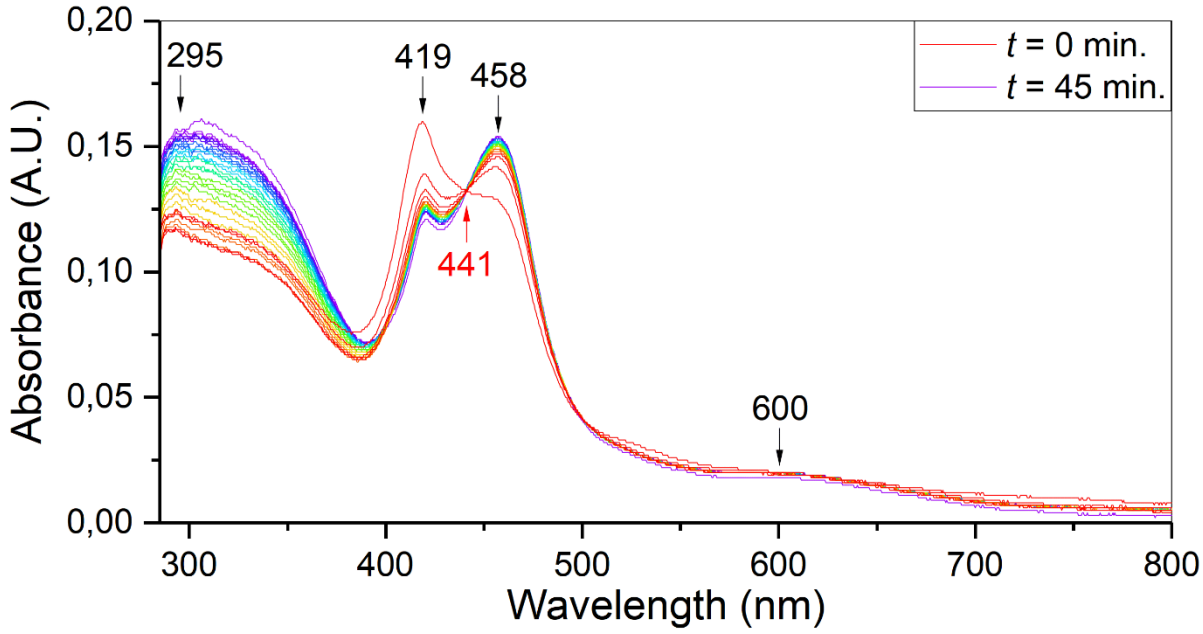


Figure S18. 20 eq. DMM•IY + 1 eq. [Co(TPP)] in toluene at 5 μM followed over 45 min (1 scan/90 s).

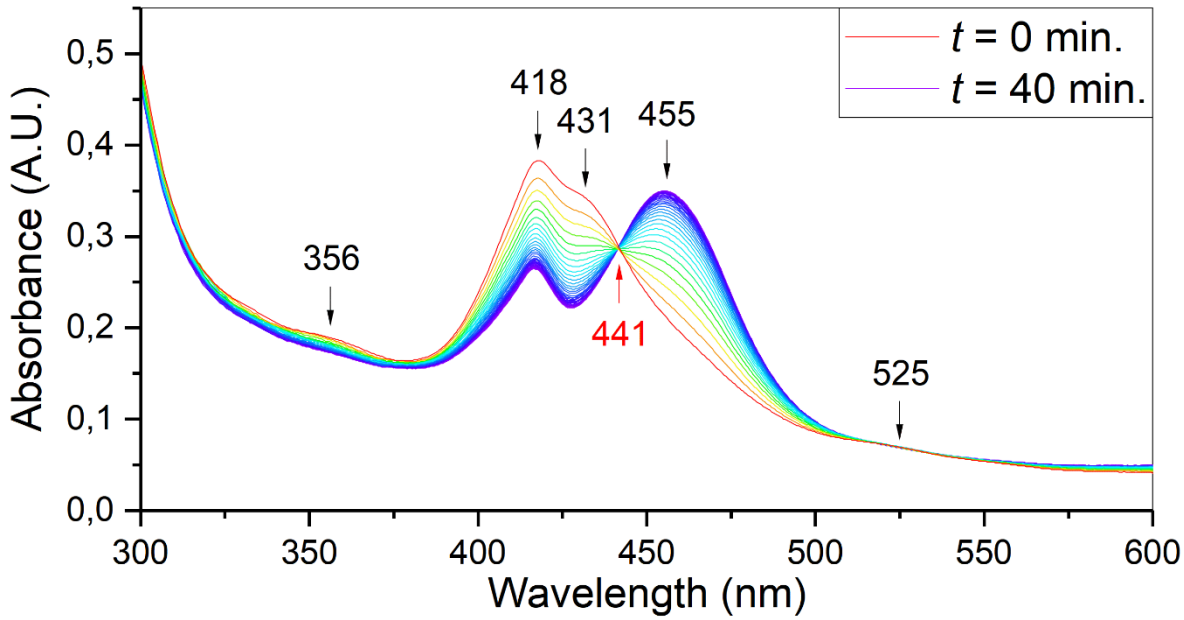


Figure S19. 20 eq. DMM•IY + 1 eq. [Co(TPP)] in CH_2Cl_2 at 5 μM followed over 40 min (1 scan/60 s).

In-situ IR studies

General procedure

To a flame-dried two-neck Schlenk flask was added the ReactIR probe and the flask was subsequently cycled three times with Ar/vacuum (vacuum >2 min.). Benzene was added via a septum on the other neck until the probe was submerged and a background spectrum was recorded. The solvent was removed followed by insertion of the ReactIR probe. Measurements were started prior to sample injection to ensure complete measurement. Subsequently, the sample was injected as a solution or a stock solution of [Co(TPP)] was added to solid DMM•IY in the reaction flask. Spectra were recorded for 15 min. at 15 second intervals.

Reaction components

DMM•IY (Suspension & Filtered)

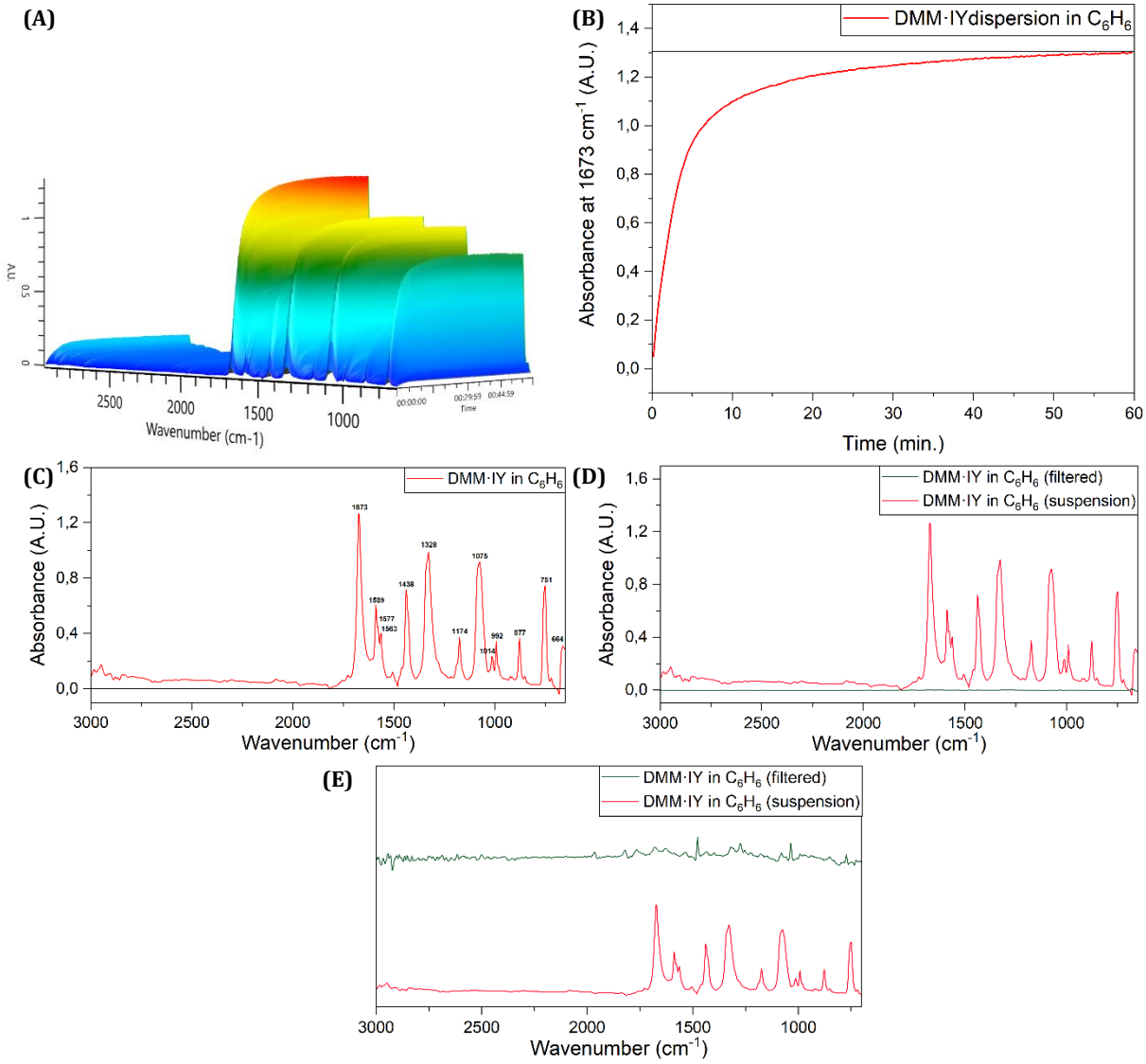


Figure S20. 3D-surface plot of the *in-situ* ATR-FT-IR spectrum of DMM•IY in suspension in C_6H_6 over time (1 h) (A). Trendline of the absorption intensity at 1673 cm^{-1} over time (B). *in-situ* ATR-FT-IR spectrum of DMM•IY in suspension in C_6H_6. (C). Comparison of *in-situ* ATR-FT-IR spectra between DMM•IY in suspension and after filtration (D). Comparison of normalized *in-situ* ATR-FT-IR spectra between DMM•IY in suspension and after filtration (E).

[Co(TPP)] & Styrene

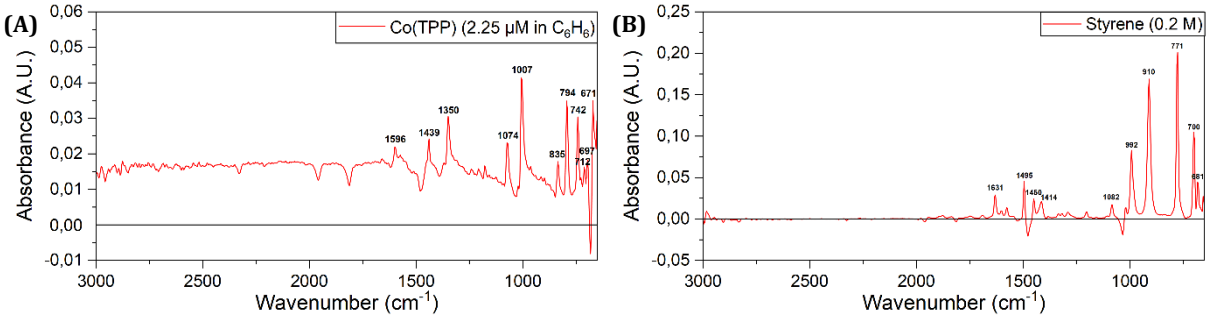


Figure S21. *in-situ* ATR-FT-IR spectra of [Co(TPP)] (2.25 µM) (A) and styrene (0.2 M) in C_6H_6 (B).

Formation of mono-enolate-mono-carbene radical $\boldsymbol{I^{E-T}}$

The measurement setup was prepared according to the general procedure. Additionally, to a separate flame-dried Schlenk flask was added DMM•IY (10.2 mg; 3.4 eq.; 30.5 µmol) followed by addition of a solution of [Co(TPP)] in C_6H_6 (4 mL; 1 eq.; 2.25 mM; 9 µmol). Measurements were started prior to transfer of the reaction mixture to ensure complete measurement. The reaction was stirred for 5 min., after which it was transferred entirely to a 10 mL syringe and filtered through a syringe filter (PTFE, hydrophobic, 0.45 µm). To supersaturate the solution for higher intensity (Figure S22A), [Co(TPP)] (50 mg; 1 eq.; 74 µmol) and DMM•IY (48 mg; 1.9 eq.; 144 µmol) were added to the measurement Schlenk flask and cycled three times with Ar/vacuum. Measurements were started prior to addition of 4 mL of C_6H_6 and the reaction was measured for 40 minutes (1 scan/min.).

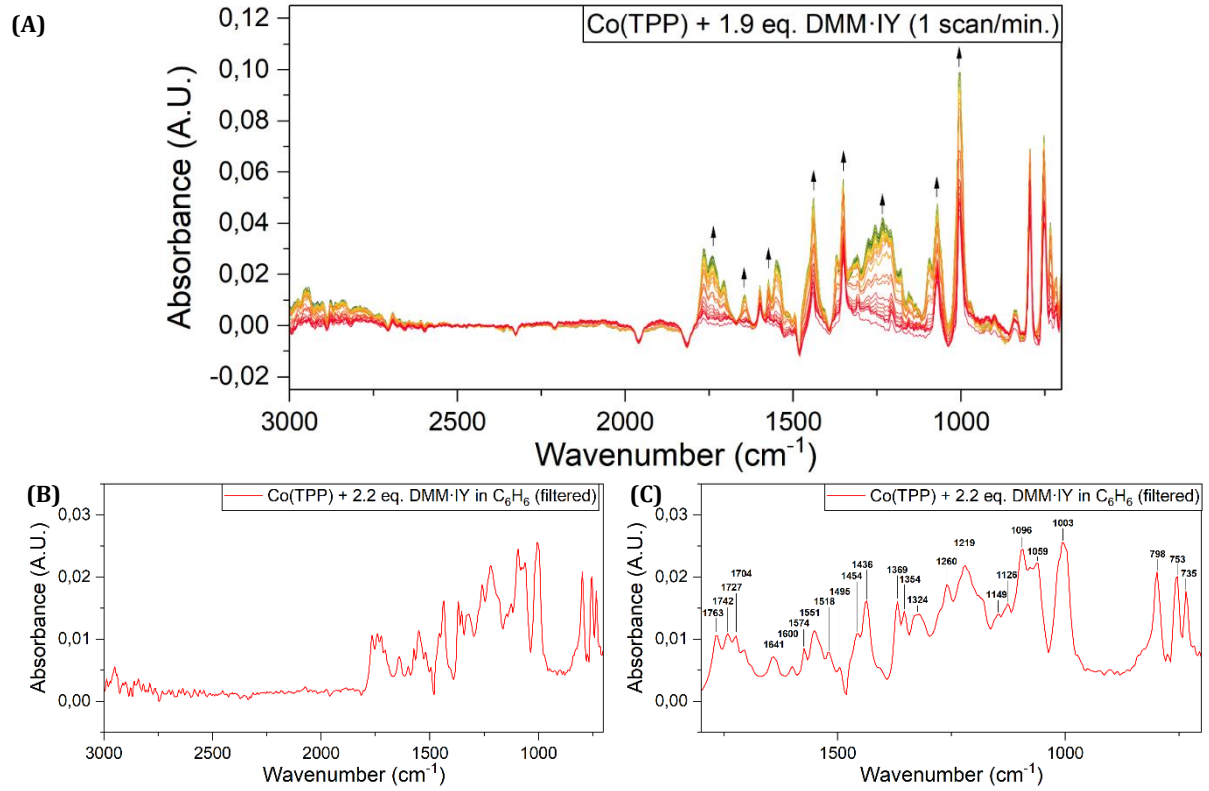


Figure S22. *in-situ* ATR-FT-IR spectrum of the reaction between [Co(TPP)] and DMM•IY at supersaturated concentration (vs. solubility of [Co(TPP)]) measured for 40 min (1 scan/min.) (A). *in-situ* ATR-FT-IR spectrum of a filtered solution of the reaction between [Co(TPP)] and an excess of DMM•IY (B). Zoomed in-spectrum of (B) with labeled peaks (C).

Reaction monitoring:
To a flame-dried two-neck Schlenk flask was added the ReactIR probe and the flask was subsequently cycled three times with Ar/vacuum (vacuum >2 min.). Benzene was added via a septum on the other neck until the probe was submerged and a background spectrum was recorded. The solvent was removed *in vacuo* and DMM•IY (82 mg; 24 eq.; 245 μmol), followed by insertion of the ReactIR probe. Subsequently, the flask was cycled three times with Ar/vacuum. Measurements were started at an interval of 15 seconds, after which styrene was added (23.2 μL; 20 eq.; 202.5 μmol) was added, followed by a stock solution of [Co(TPP)] (4.5 mL; 5 mol%.; 2.25 mM; 10.1 μmol). The reaction was monitored for 60 min. at 15 second intervals (Figure S23).

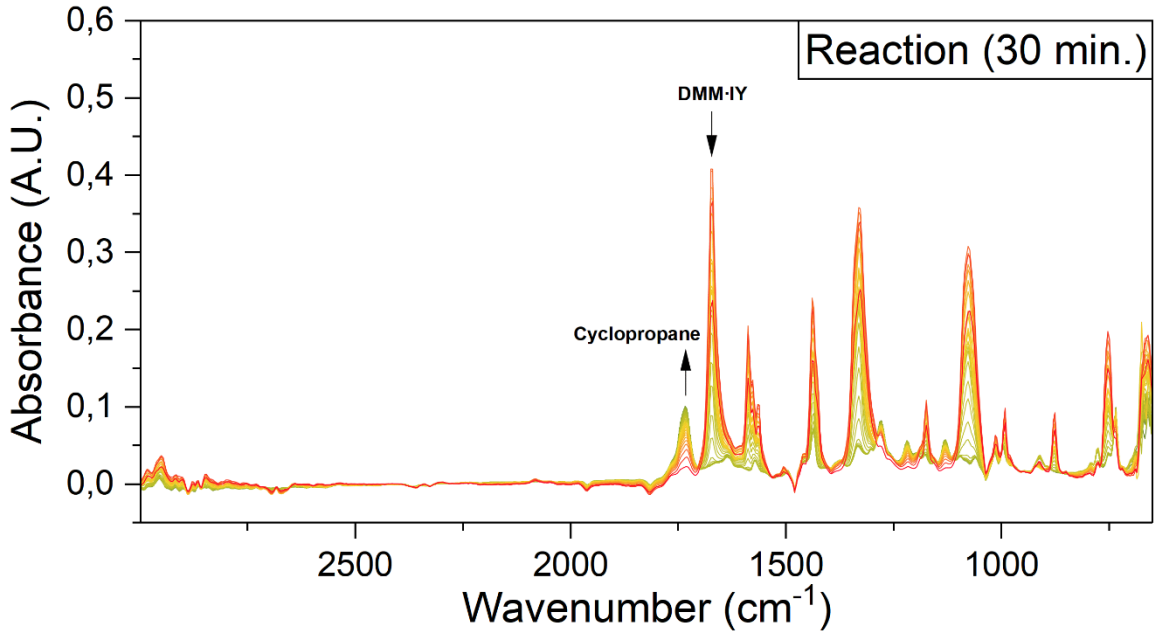


Figure S23. ATR-IR spectrum of the reaction between DMM•IY and styrene catalyzed by [Co(TPP)]. The reaction mixture was monitored for 30 min. (1 spectrum/15 s.) Assignments were based on literature reports.[25]

For further comparison, IR spectra were simulated from optimized geometries obtained via DFT calculations at the BP86/def2-TZVP/disp3 level of theory. To acquire an accurate scale factor, a calibration was made based on work by Ikeno et al.[35] and the reported complexes were calculated without simplifications at the BP86/def2-TZVP/disp3 level of theory (Figure S24 and Table S11). Subsequently, all relevant carbene intermediates ($\mathbf{I}^{T}$,$\mathbf{I}^{T-T}$,$\mathbf{I}^{B-T}$,$\mathbf{I}^{E-T}$,$\mathbf{I}^{E}$ and $\mathbf{I}^{B}$) and alkyl adducts ($\mathbf{I}^{A}$,$\mathbf{I}^{A-T}$,$\mathbf{I}^{A-B}$ and $\mathbf{I}^{E-A}$) were considered and $\mathbf{I}^{E-T}$ and $\mathbf{I}^{E-A}$ fit the data best (Figure S26A & B) (Table S12).

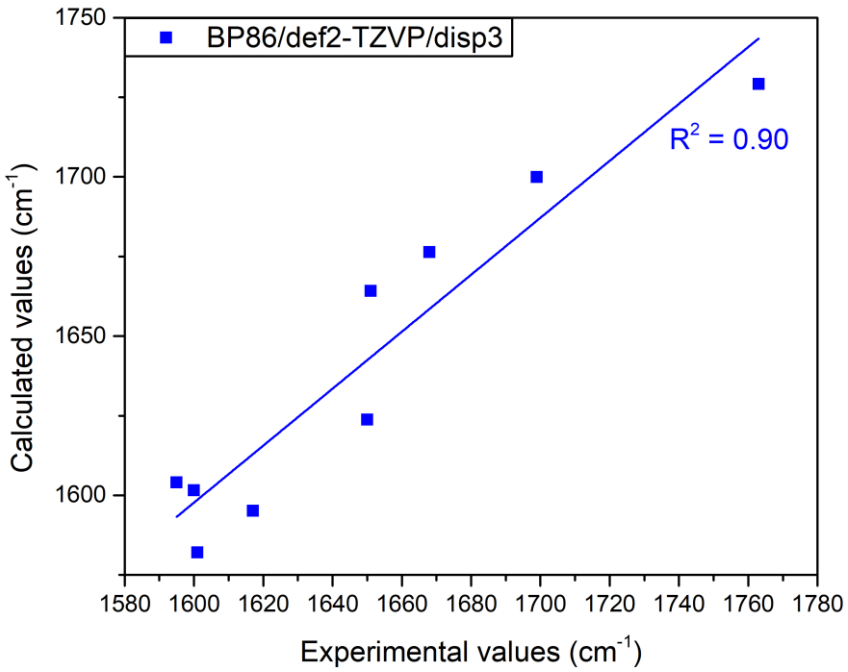


Figure S24. Correlation graph between experimental and calculated wavenumbers of C=O vibrations of metal carbene complexes with pendant ester groups.

Table S11. Experimental and calculated wavenumbers of C=O vibrations of metal carbene complexes with pendant ester groups.

Compound	**Experimental data (cm^{-1})**	**BP86/def2-TZVP/disp3[35]**
DMM•IY	1668	1676,4
DMM·N_2	1763	1729,2
Methyldiazoacetate	1699	1699,9
Co(Acacen)Cl(=$CHCO_2Et$)	1600	1601,6
Co(Acacen)MeIm(=$CHCO_2Et$)	1595	1604,1
Co(Salen)I(=$CHCO_2Et$)	1617	1595,1
Co(Salen)MeIm(=$CHCO_2Et$)	1601	1582,1
CuBox(=$CHCO_2Et$)	1650	1623,8
RuPyBox(=$CHCO_2Et$)	1651	1664,2
Scale Factor	**-**	**1,00 ±0,01**

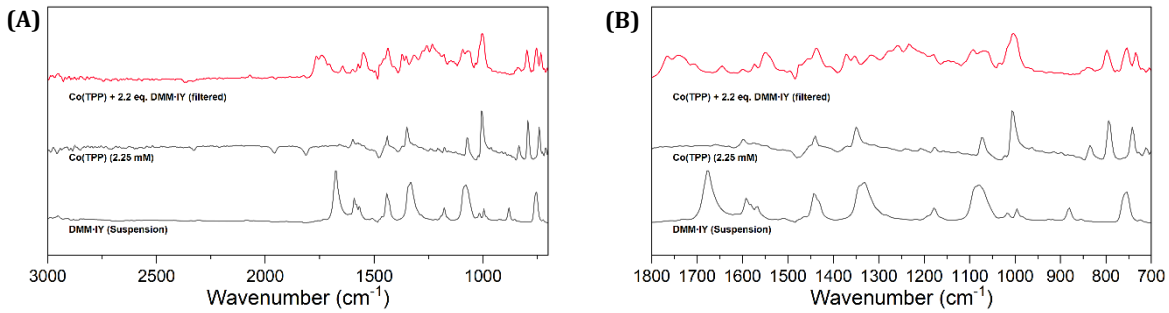


Figure S25. Comparison of *in-situ* ATR-FT-IR spectra of the reaction between [Co(TPP)] and 2.2 eq. DMM•IY after filtration at t = 0 h (red); [Co(TPP)] (2.25 mM) and DMM•IY in suspension (A). Zoomed-in version (B). All spectra are normalized.

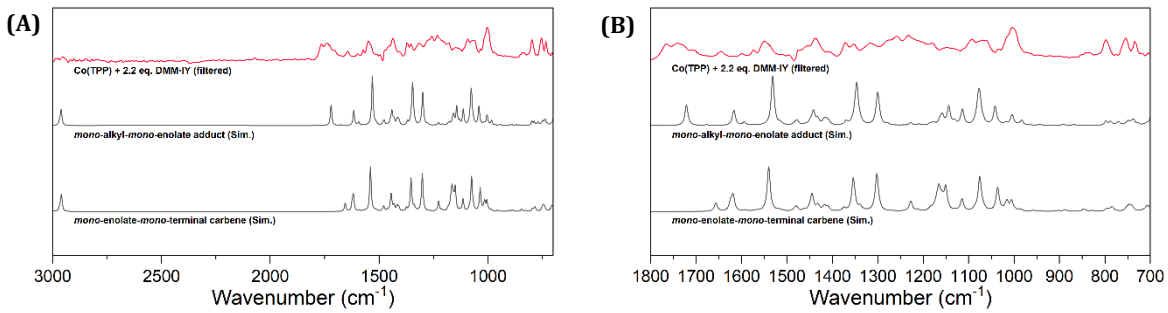


Figure S26. Comparison of *in-situ* ATR-FT-IR spectra of the reaction between [Co(TPP)] and 2.2 eq. DMM•IY after filtration at t = 0 h (orange); at t = 24 h (green); the *mono*-alkyl-*mono*-enolate adduct $\mathbf{I^{E-A}}$ simulated and the *N*-enolate-carbene radical $\mathbf{I^{E-T}}$ simulated (A). Zoomed-in version (B). All spectra are normalized. For the simulations, the scale factor was set at 1.00.

Table S12. Overview of experimental data of [Co(TPP)] and the reaction mixture of [Co(TPP)] & DMM•IY and a comparison with the most characteristic peaks in DFT-simulated IR spectral data for [Co(TPP)], the mono-enolate-mono-terminal carbene and the mono-alkyl-mono-enolate adduct (Scale factor for DFT = 1.00; based on Figure S24/Table S11).

Vibration mode	[Co(TPP)] (Exp.)	[Co(TPP)] + DMM·IY (Exp).	[Co(TPP)] (DFT)	*Mono*-enolate-*mono*-terminal carbene (DFT)	*Mono*-alkyl-*mono*-enolate adduct (DFT)
Ph flip + pyrrole flip	742	734 754	746.5 746.6	740.0 744.7 747.4 752.3	726.8 736.8 740.8 748.1 759.8
***β*-pyrrole scissor mode**	1071	1062 1094	1074 1074.3	1066.5 1070.5 1074.6 1078.1	1067.6 1073.7 1075.9 1077.7
***β*-pyrrole rocking mode**	1207	1177 1209	1197.6 1197.7	1175.7 1178.9 1191.1	1176.6 1176.8 1179.0 1193.4 1209.9
Porphyrin stretch	1350	1354 1368	1349.4	1339.2 1350.9 1351.7 1374.7	1339.4 1346.1 1350.1 1369.7
Enolate C=C stretch	N/A	1548	N/A	1540.0	1531.2
Carbonyl stretches	N/A	1573 1599 1644 1705 1738 1765	N/A	1618.3 1623.8 1656.1	1616.7 1721.0

Data interpretation:

From Figure S20 (D and E), it is clear that DMM•IY is practically insoluble in C_6H_6 as the overall absorbance is almost zero and no trace of the ylide's absorption peaks can be observed. It can therefore be concluded that the increased intensity over time seen in A and B is due to smaller particle distribution as a result of stirring. The detected wavelengths of DMM•IY are in accordance with reported literature.[25] Consequently, reliable kinetic measurements to determine reaction orders are not possible for this system as one of the reagents (DMM•IY) is only present as a suspension that gradually disperses over time. Such systems are highly dependent on particle size, solid-phase morphology and stirring speed.

Comparing the obtained spectra in Figure S22 with its separate components, it can be seen that no residual DMM•IY is left as its main absorption peaks are completely absent (Figure S25A). Deconvolution of the DFT simulated IR spectra, revealed the splitting of the porphyrin's β-pyrrolic

H-flipping, scissor, rocking and porphyrin stretching modes (742, 1071, 1207 and 1350 cm^{-1} resp.) into two distinct peaks (734/754; 1062/1094; 1177/1209; 1354/1368 cm^{-1} resp.) in agreement with desymmetrization of the porphyrin ring in $\mathbf{I^{E\text{-}T}}$ (Table S11). On top of that, various peaks can be observed in the carbonyl stretching region typical for metal-alkyl and metal-carbene species with pendant ester groups.[28] More specifically, two sets of peaks can be observed at 1573 and 1599 cm^{-1} and 1738 cm^{-1}. These are attributed to the metal-carbene and metal-alkyl species respectively. The additional peaks at 1705 and 1765 cm^{-1} are tentatively assigned to a free- and coordinated alkyl dimer ($CH(CO_2Me)_2$, respectively (Table S12) in accordance with literature[36] and observations in ^{1}H-NMR (Table S2 and Figure S59). The peak at 1644 cm^{-1} is attributed to the carbonyl stretching band of the free ester attached to the *N*-enolate carbene moiety as reported by Setsune and coworkers[37] and corroborated by our DFT results. The splitting of the porphyrin's β-pyrrolic and porphyrinic vibrational modes as well as the appearance of three distinct carbonyl peaks is in line with the conclusions derived from EPR studies (vide supra).A zoomed-in version paints an even clearer picture of this (Figure S25B). The splitting of the ligand vibrations as well as the appearance of multiple separate carbonyl stretches in two distinct regions is in agreement with desymmetrization of the porphyring ring in *N*-enolate-carbene radical $\mathbf{I^{E\text{-}T}}$ and its deactivated analogue, the *N*-enolate-alkyl speciest $\mathbf{I^{E\text{-}A}}$.

Additional temporal reaction monitoring clearly shows the decrease of signals belonging to DMM•IY and increase of the cyclopropane product **1** over time (Figure S23) in line with catalytic results and spectroscopic evidence. The high intensity of peaks belonging to DMM•IY obscures the faint signals that could belong to any catalytic relevant intermediate. This can also be seen from the difference in intensity between Figure S23 and Figure S22, conducted at equimolar concentrations of [Co(TPP)].

Coldspray ESI-MS$^+$ studies:

General procedure for measuring a coldspray ESI-MS sample:
To a 4 mL vial was added DMM•IY (18.0 mg; 24 eq.; 53.9 µmol). To a flame dried Schlenk flask was added [Co(TPP)] (15 mg; 22.3 µmol; 4.5 mM) and 5 mL dry C_6H_6 as a stock solution. In an Ar bucket were also added 2 empty vials (for filtration & dilution), 1 with ~2 mL C_6H_6 (for diluting) and a syringe equipped with syringe filter. This was bubbled with Ar for 10 min. Subsequently 500 µL [Co(TPP)] stock solution was added to the reaction vial, the mixture was stirred for 60 s and an aliquot was taken up with the syringe through the filter. This was added to the filtration vial, an aliquot was taken and diluted 100-1000x in the dilution vial. Lastly, the mixture was transferred to a glass syringe and taken for mass measurement. The mass spectra are in accordance with the free catalyst [Co(TPP)], a *bis*-carbenoid species and fragmentation to a *mono*-carbenoid species and a trace amount of dimer of *mono*-carbenoid species with one eq. of H_2O.

CSI-ESI$^+$ (*m/z*) calculated for $[Co(TPP)]^+$ ($C_{44}H_{28}CoN_4$): 671.16460 Da, found 671.1674 Da [M$^+$] (error: 4.17 ppm) (Figure S27).

CSI-ESI$^+$ (*m/z*) calculated for $[Co(TPP)(DMM\text{-}carbene)]^+$ ($C_{49}H_{34}CoN_4O_4$): 801.19121 Da, found 801.1942 Da [M$^+$] (error: 3.73 ppm) (Figure S27).

CSI-ESI$^+$ (*m/z*) calculated for $[Co(TPP)(DMM\text{-}carbene)_2]^+$ ($C_{54}H_{40}CoN_4O_8$): 931.21781 Da, found 931.2207 Da [M$^+$] (error: 3.10 ppm) (Figure S27).

CSI-ESI$^+$ (*m/z*) calculated for $[Co(TPP)(DMM\text{-}carbene)_2(+H)]^+$ ($C_{54}H_{41}CoN_4O_8$): 932.22564 Da, found 932.2258 Da [M$^+$] (error: 0.17 ppm) (Figure S27).

CSI-ESI$^+$ (*m/z*) calculated for $([Co(TPP)(DMM\text{-}carbene)_2(H_2O)]^+$ ($C_{98}H_{71}Co_2N_8O_9$): 1621.40080 Da, found 1621.3956 Da [M$^+$] (error: –3.21 ppm) (Figure S27).

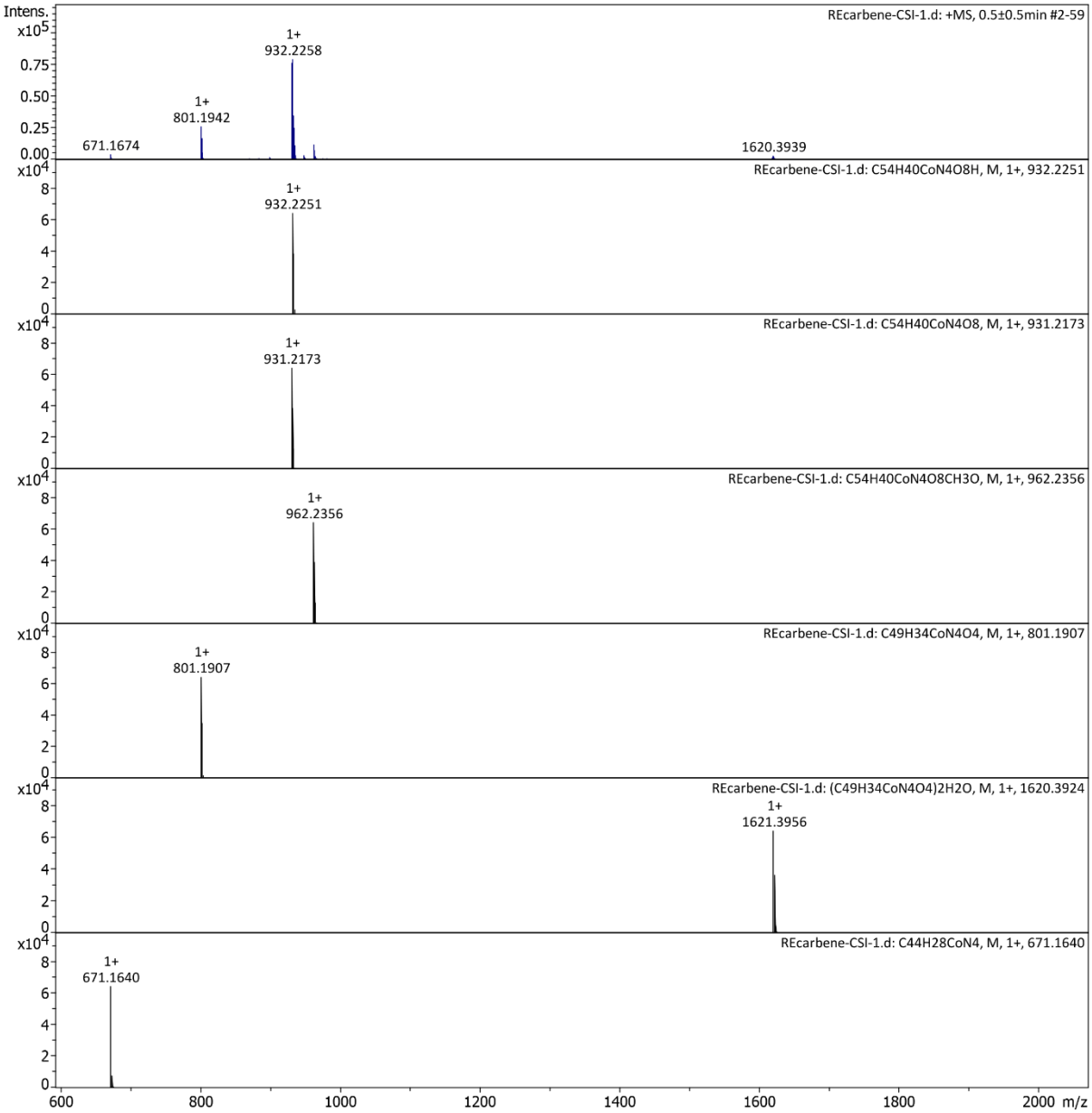


Figure S27. Coldspray ESI-MS$^+$ spectrum at 10°C (top) and simulations for different detected *mono*-cationic (fragmentation) species below. From top to bottom: $[Co(TPP)(DMM\text{-}carbene)_2(+H)]^+$ *m/z* = 932.2251 Da; $[Co(TPP)(DMM\text{-}carbene)_2]^+$ *m/z* = 931.2173 Da; $[Co(TPP)(DMM\text{-}carbene)_2(OMe)]^+$ *m/z* = 962.2356 Da; $[Co(TPP)(DMM\text{-}carbene)]^+$ *m/z* = 801.1907 Da, $[Co(TPP)(DMM\text{-}carbene)_2(H_2O)]^+$ *m/z* = 1621.3956 Da, $[Co(TPP)]^+$ *m/z* = 671.1640 Da.

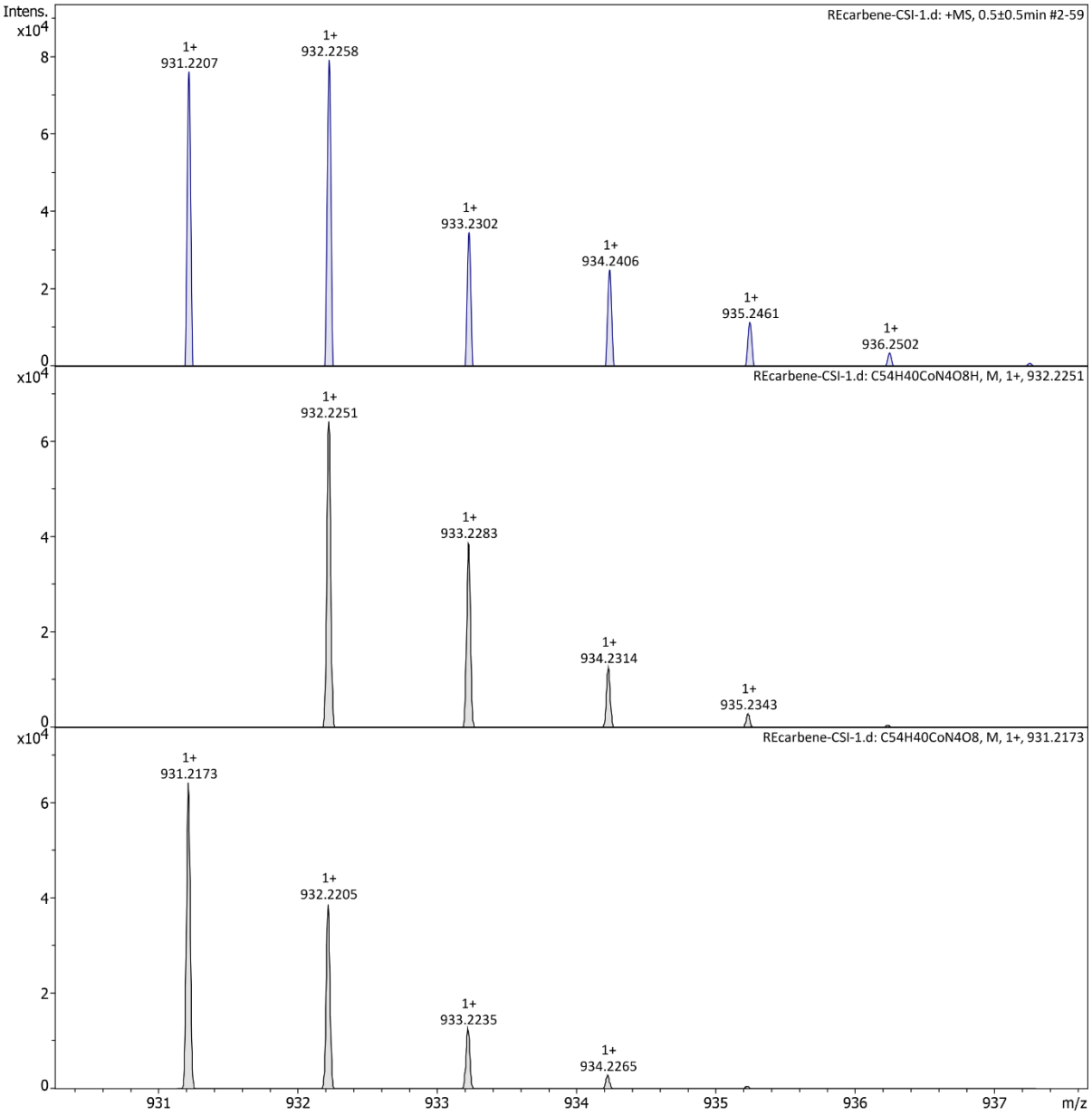


Figure S28. Zoomed-in view of the CSI-ESI⁺-MS spectrum of a *bis*-carbenoid species (top) and simulations of *mono*-cationic species below. From top to bottom: $[Co(TPP)(DMM\text{-}carbene)_2(+H)]^+$ m/z = 932.2251 Da ; $[Co(TPP)(DMM\text{-}carbene)_2]^+$ m/z = 931.2173 Da.

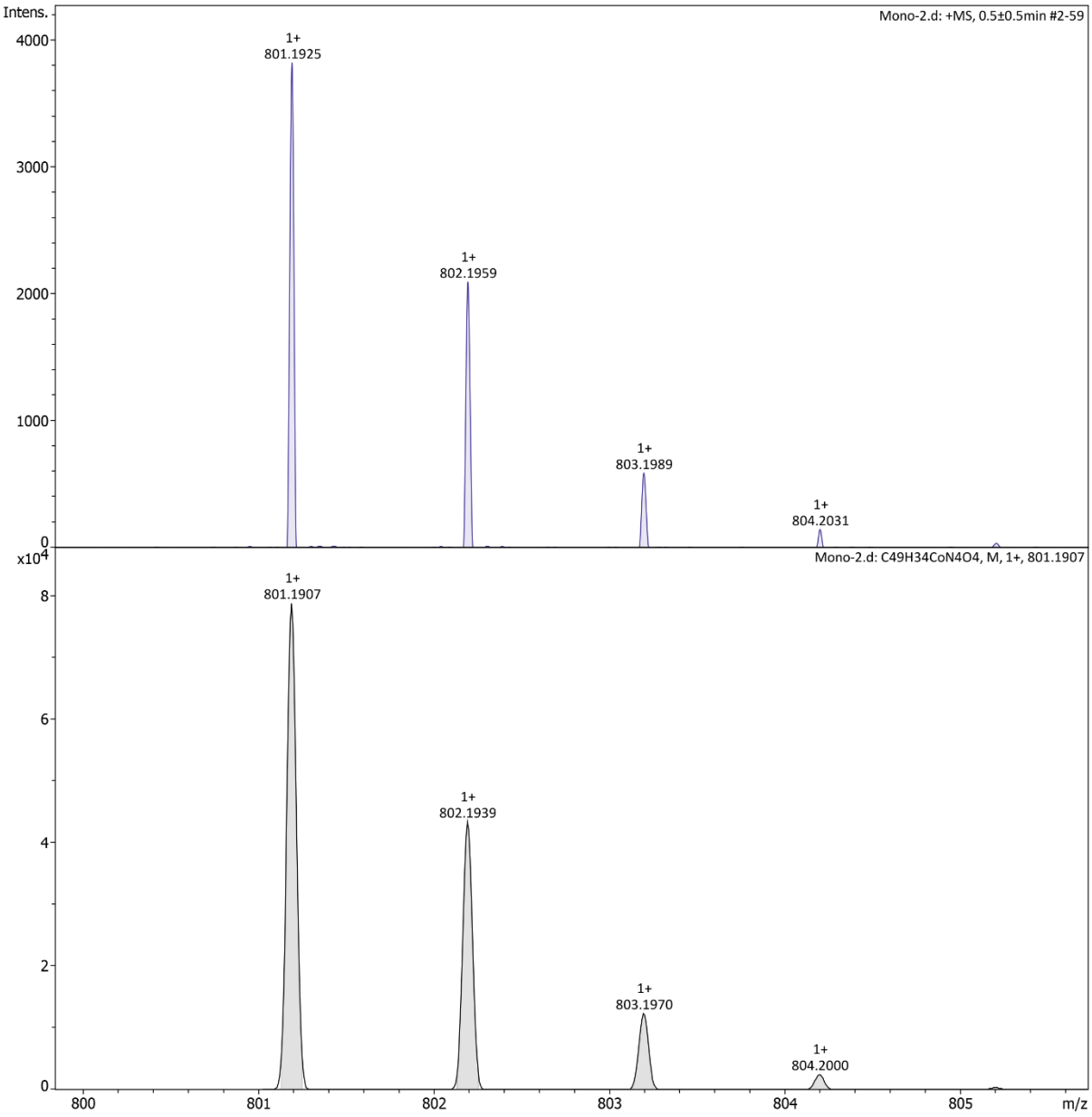
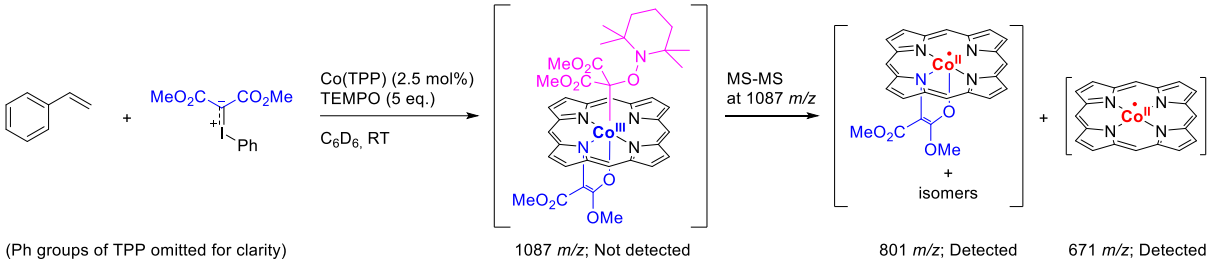


Figure S29. Zoomed-in view of the CSI-ESI$^+$-MS spectrum of a *mono*-carbenoid species (top) and simulation of $[M]^+$ below.

Trapping studies with TEMPO (A/B) and in-situ measurements (C)

Samples for mass analysis were obtained according to the general procedure described above.



Scheme S6. Detection of fragments of a *bis*-carbenoid TEMPO adduct via selective ionization (MS-MS) at 1087 ± 5 *m/z*.

As can be seen from spectra in Figure S30 and Figure S31, no TEMPO adduct can be found of either any *mono*-carbenoid (*m/z* = 957 Da) or *bis*-carbenoid species (*m/z* = 1087 Da) resp. Prominent peaks are that of free *mono*-carbenoid and *bis*-carbenoid adducts at *m/z* = 801 Da and *m/z* = 931 Da. Trapping species at *m/z* = 1087 ± 5 Da using MS-MS, followed by selective ionization clearly shows fragmentation to *m/z* = 801 Da and *m/z* = 671 Da (Figure S33). These correspond to *mono*-carbenoid and free [Co(TPP)] species resp. The proposed intermediate TEMPO adduct is a neutral Co^{III}-alkyl species that cannot be directly detected as such. Upon ionization, dissociation of the weak Co^{III}-alkyl bond likely occurs to produce a species at *m/z* = 801 Da and further ionization causes the remaining carbene fragment to dissociate into *m/z* = 671 Da. Since MS-MS analysis is highly selective within a ±5 *m/z* error margin and that no other isomers at *m/z* = 1087 Da could stem from the reaction, these data point to the presence of the TEMPO adduct of $\mathbf{I}^{\mathbf{E\text{-}T}}$, which fragments immediately upon ionization.

Reaction A (Figure S30): To a vial containing DMM•IY (9.4 mg; 1.5 eq.; 28.1 µmol) and TEMPO (23.8 mg; 8.4 eq.; 152 µmol) was added 1 mL [Co(TPP)] in C_6H_6 (1.5 mg/mL; 5 mol%; 2.25 µM). A CSI^+-MS sample was taken accordingly.

Reaction B (Figure S31): To a vial containing DMM•IY (9.4 mg; 1.5 eq.; 28.1 µmol) and TEMPO (20.8 mg; 7.5 eq.; 133 µmol) was added styrene (2.08 µL; 1.89 mg; 1 eq.; 18.2 µmol) followed by 1 mL [Co(TPP)] in C_6H_6 (1.5 mg/mL; 5 mol%; 2.25 µM). A CSI^+-MS sample was taken accordingly.

Reaction C (Figure S32): To a vial containing DMM•IY (10.2 mg; 1.7 eq.; 28.1 µmol) was added styrene (2.08 µL; 1.89 mg; 1 eq.; 18.2 µmol) followed by 1 mL [Co(TPP)] in C_6H_6 (1.5 mg/mL; 5 mol%; 2.25 µM). A CSI^+-MS sample was taken accordingly.

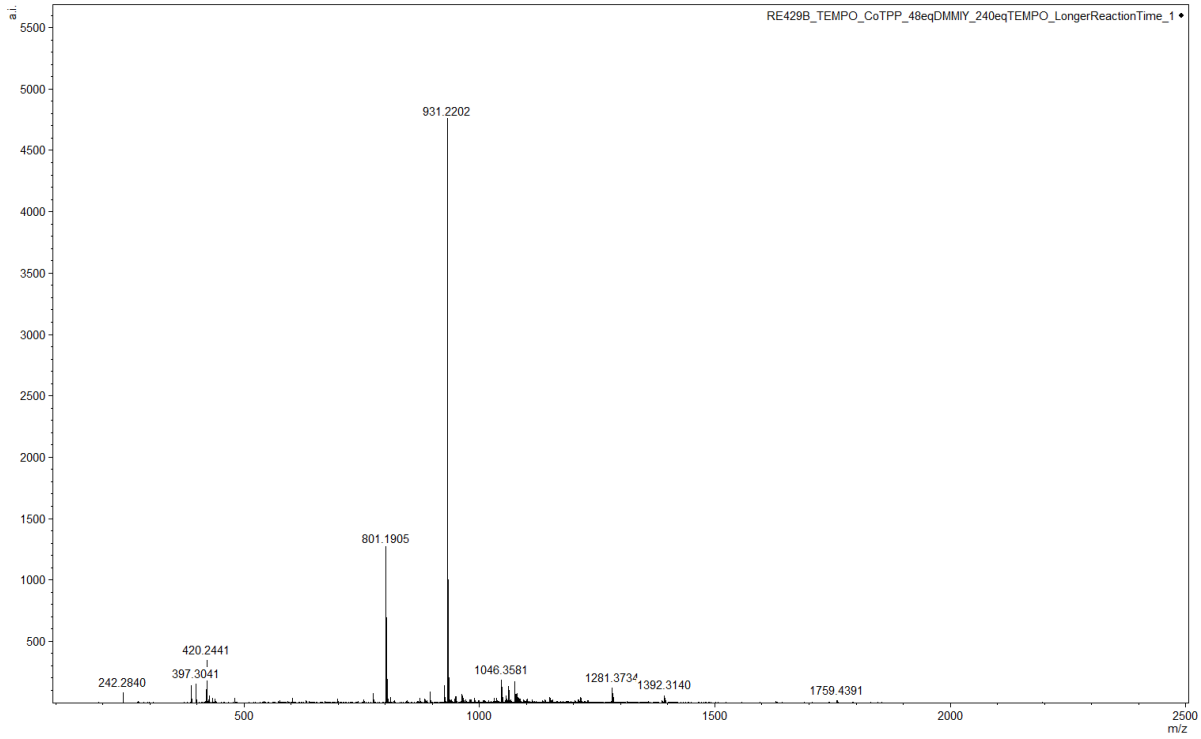


Figure S30. *A*: CSI-ESI⁺-MS spectrum of the reaction mixture of [Co(TPP)], DMM•IY and TEMPO at 10 °C.

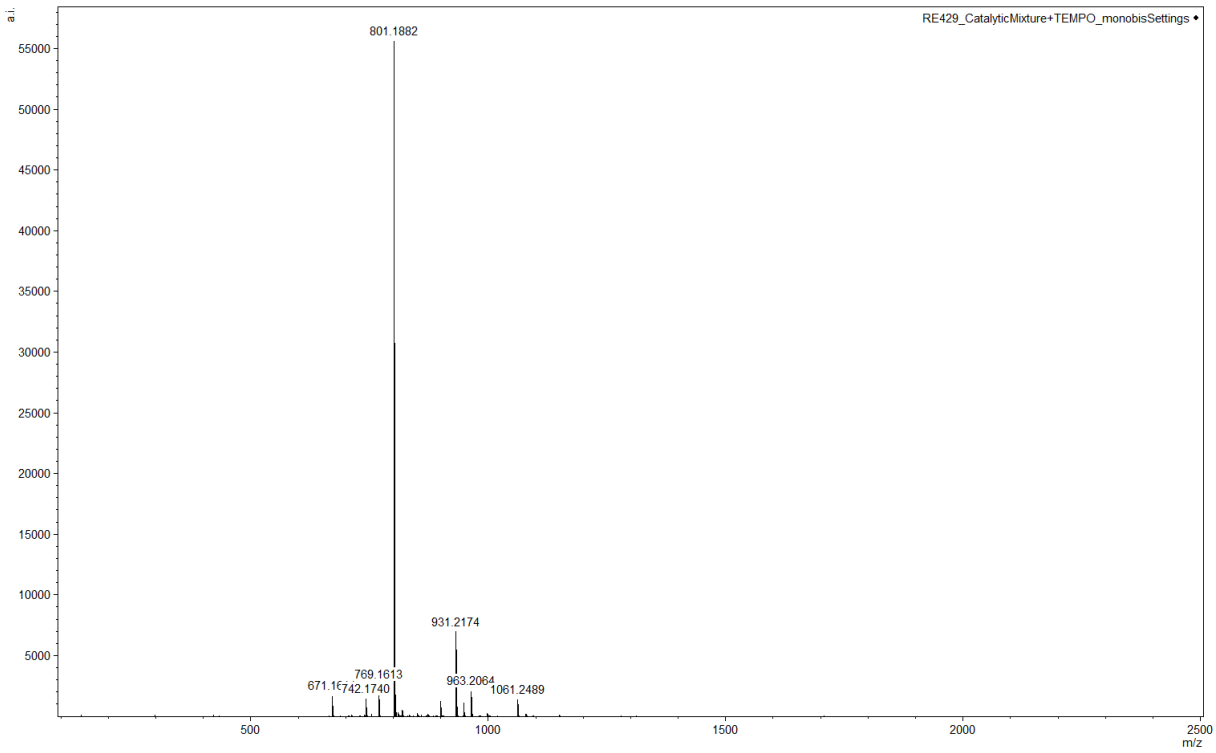


Figure S31. *B*: CSI-ESI⁺-MS spectrum of a catalytic mixture with TEMPO at 10°C.

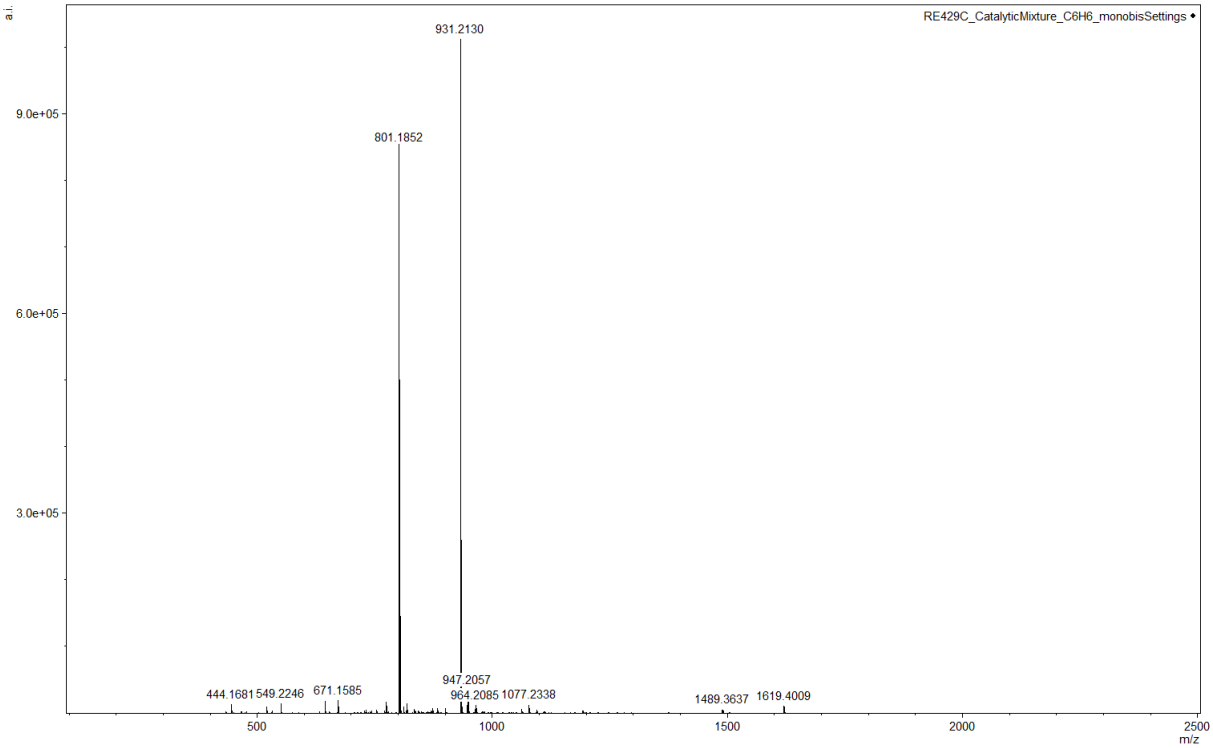


Figure S32. *C*: CSI-ESI$^+$-MS spectrum of a catalytic mixture at 10°C.

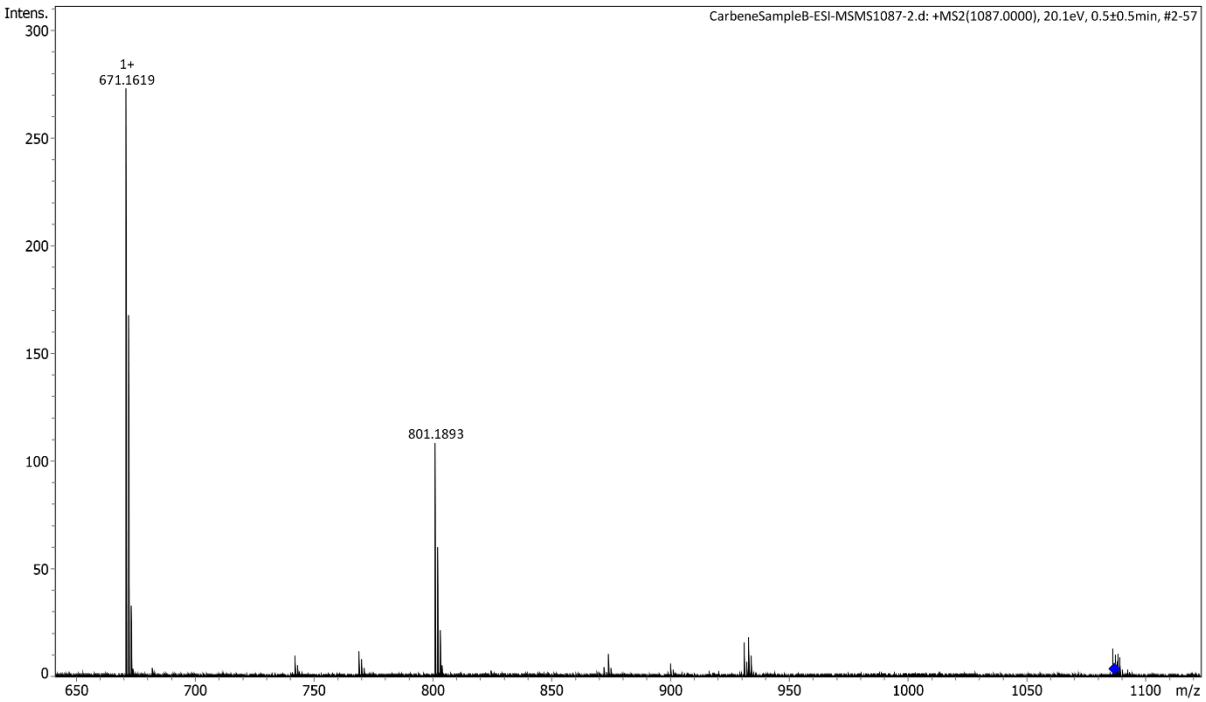


Figure S33. MS-MS spectrum of the fragmentation of the isolated 1087 ± 5 *m/z* in C_6H_6 of reaction B.

H/D labeling studies:
Samples for mass analysis were obtained according to the general procedure described above. Stock solutions were made at 1.5 mg/mL [Co(TPP)] in the desired solvent. 24 eq. of DMM•IY were used vs. [Co(TPP)] and reactions were run for at least >5 min. to ensure detectable deactivation products.

Reaction A (Toluene-H_8) (Figure S34–Figure S37): Several prominent peaks can be found at *m/z* = 931.2184 Da, *m/z* = 801.1899 Da and *m/z* = 671.16372 Da. These correspond to *bis*-carbenoid species, *mono*-carbenoid species and [Co(TPP)] respectively. From the isolated fragments around *m/z* = 931 Da by use of MS-MS (Figures S31 & S34), it can be seen that fragment *m/z* = 801 Da can originate from either *bis*-carbenoid species at *m/z* = 931 Da or its HAT product at *m/z* = 932 Da. When zoomed in on *m/z* = 931 Da, the isotopic pattern clearly reveals the presence of *m/z* = 932 Da as well as a good match with simulation. Additionally, the zoomed-in spectrum of *m/z* = 801 Da reveals the absence of the HAT product at *m/z* = 802 Da of a potential *mono*-carbenoid species, which strongly suggests that this signal indeed stems from a fragmentation process rather than a second radical species present in solution.

*Reaction B (*Toluene-D_8) (Figure S38–Figure S41): From Figures S35 and S36 the peak at *m/z* = 933 Da is striking and the isotopic pattern matches with the simulated pattern of the DAT product of a *bis*-carbenoid species. Selective ionization at *m/z* = 933 ± 5 Da via MS-MS further corroborates that the HAT or DAT-product fragments to a *mono*-carbenoid species at *m/z* = 801 Da. Additionally, fragmentation to *m/z* = 874 Da occurs in toluene-d_8 whereas it fragments to *m/z* = 872 Da in toluene suggesting the presence of deuterium in the former. The peak at *m/z* = 1029 Da cannot be fully explained, although it is most likely an adduct of a *bis*-carbenoid species with a partially-deuterated toluene molecule (Figure S34).

Reaction C/D (CH_2Cl_2/CD_2Cl_2) (Figure S42–Figure S47): In both the CH_2Cl_2 and CD_2Cl_2 the major species is exclusively the *bis*-carbenoid species at 931 *m/z*. From the isotopic pattern in both solvents, it can be clearly seen that there is no significant amount of HAT- or DAT-product resp. Selective ionization at *m/z* = 931 Da reveals fragmentation patters that signify the loss of a methoxy group and 2 protons (*m/z* = 899 Da), the loss of an ester group (*m/z* = 872 Da) and further similar fragmentation. Surprisingly, fragmentation to the mass of a *mono*-carbenoid species at *m/z* = 801 Da is largely suppressed in CH_2Cl_2/CD_2Cl_2 compared to toluene/toluene-d_8. This suggests that either the HAT- or DAT-product does not form or that its fragmentation pattern varies per solvent.

Reaction A (Spectra):

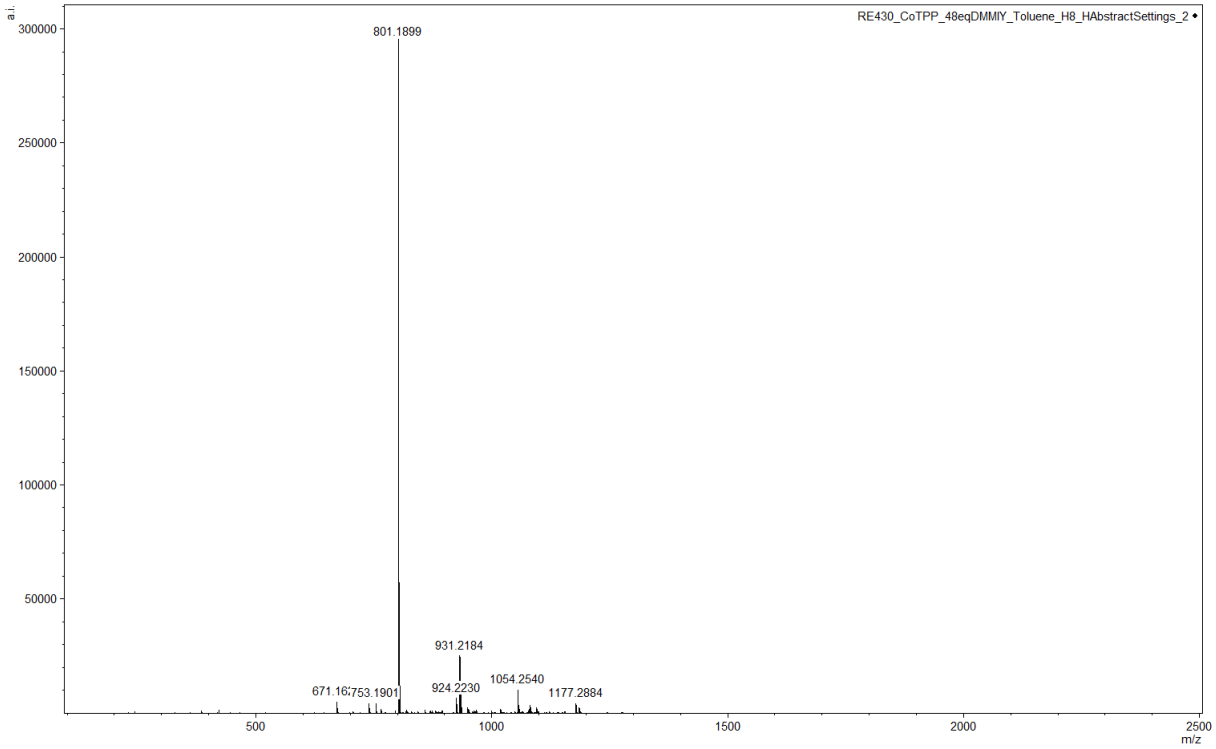


Figure S34. *A:* CSI-ESI$^+$-MS spectrum of the reaction of [Co(TPP)] and DMM•IY in toluene.

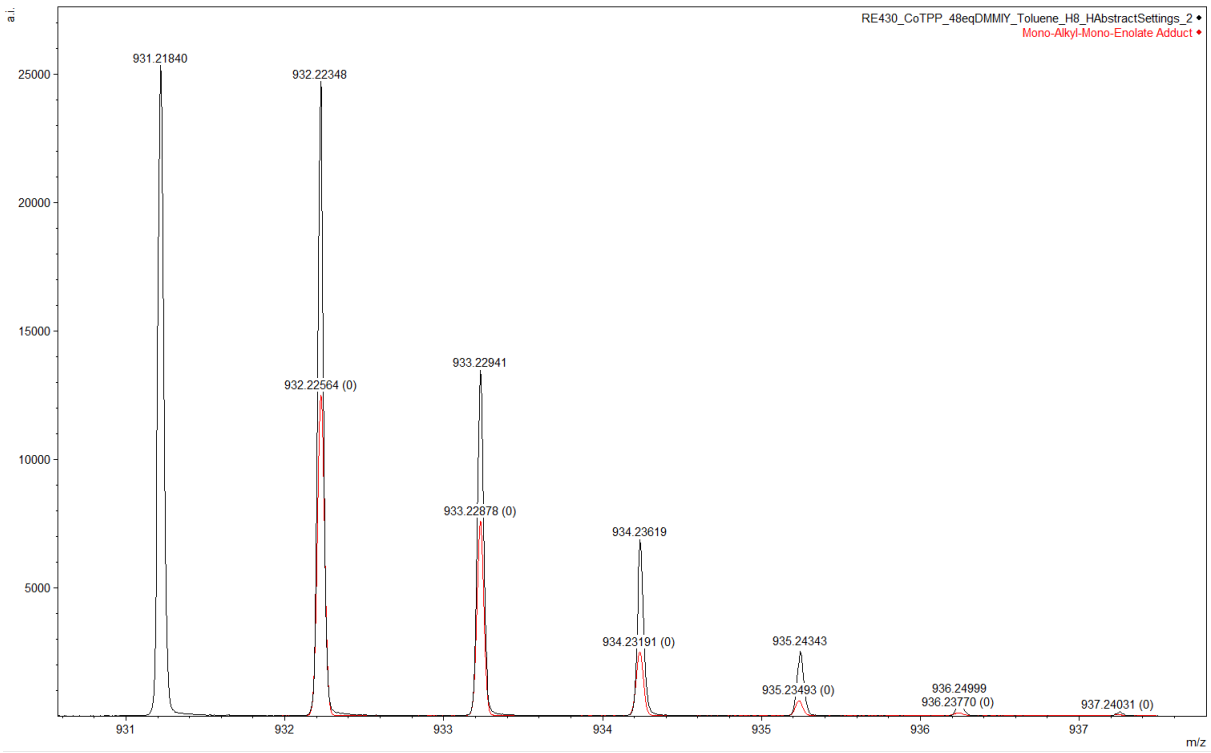


Figure S35. *A:* Zoomed-in view of the CSI-ESI$^+$-MS spectrum of the HAT product of the *bis*-carbenoid species (black) and simulation of [Co(TPP)(DMM-carbene)$_2$(+H)]$^+$ (red) in toluene.

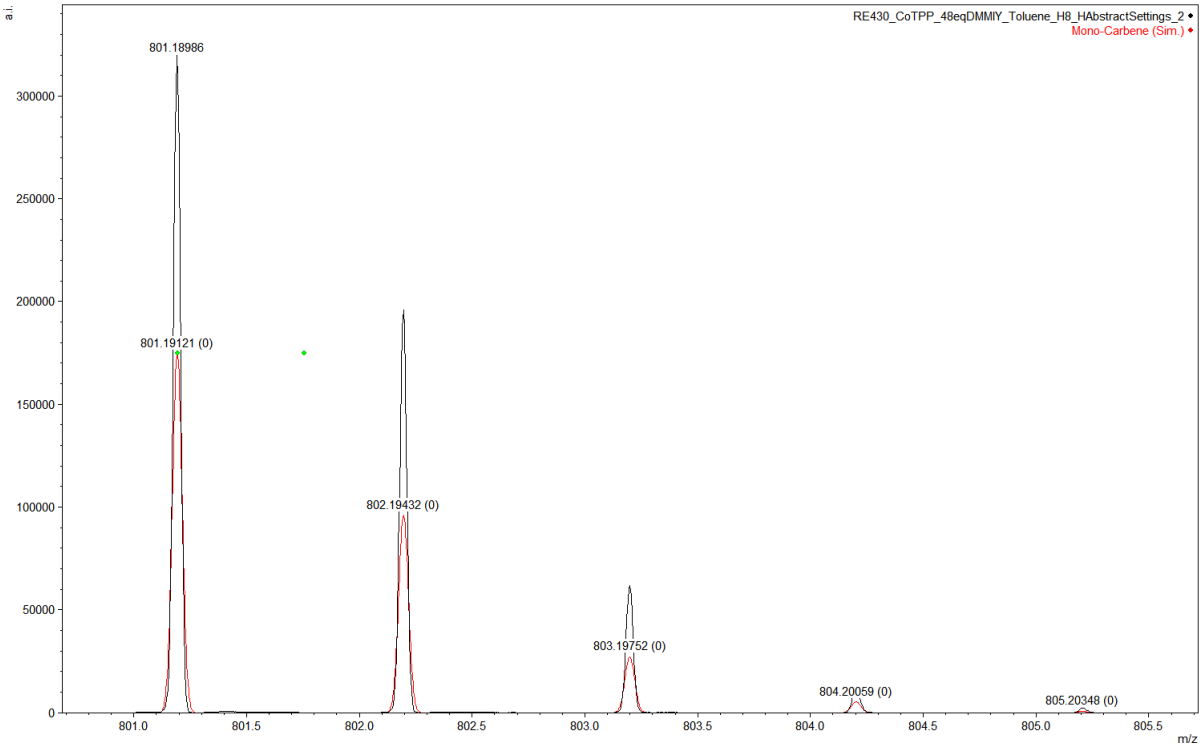


Figure S36. *A:* Zoomed-in view of the CSI-ESI⁺-MS spectrum of the peak at m/z = 801 Da (black) and simulation of [Co(TPP)(DMM-carbene)]⁺ (red) in toluene.

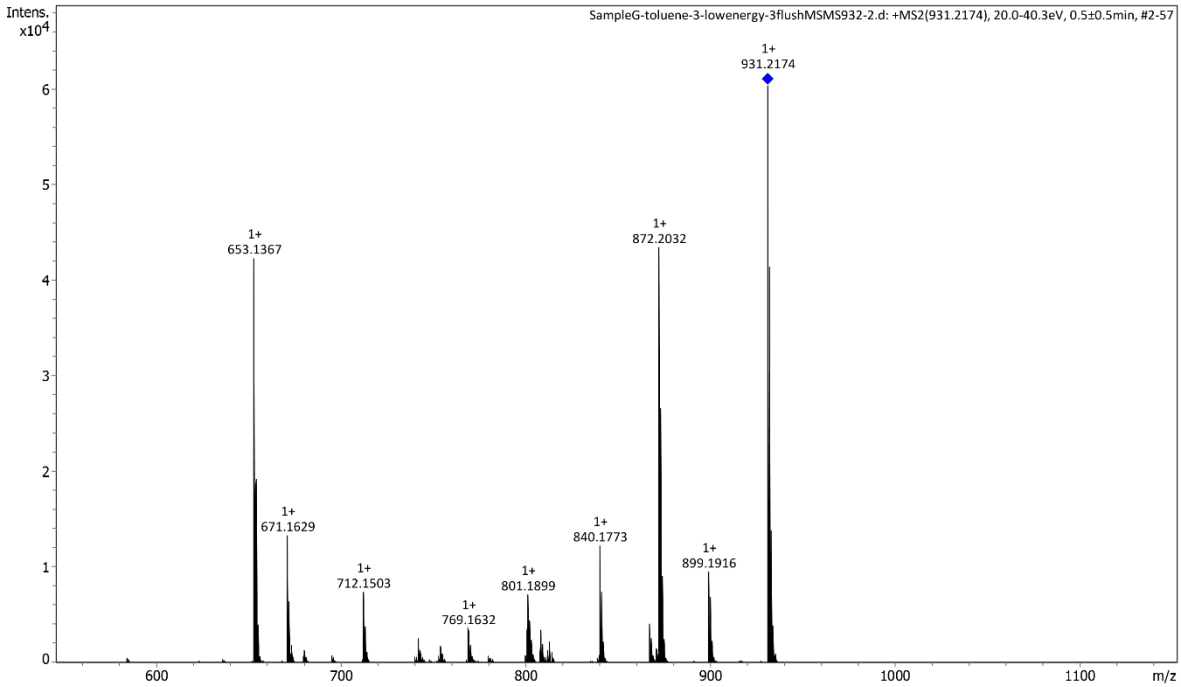


Figure S37. *A:*MS–MS spectrum of the fragmentation of the isolated *m/z* = 931 ± 5 Da in toluene.

Reaction B (Spectra):

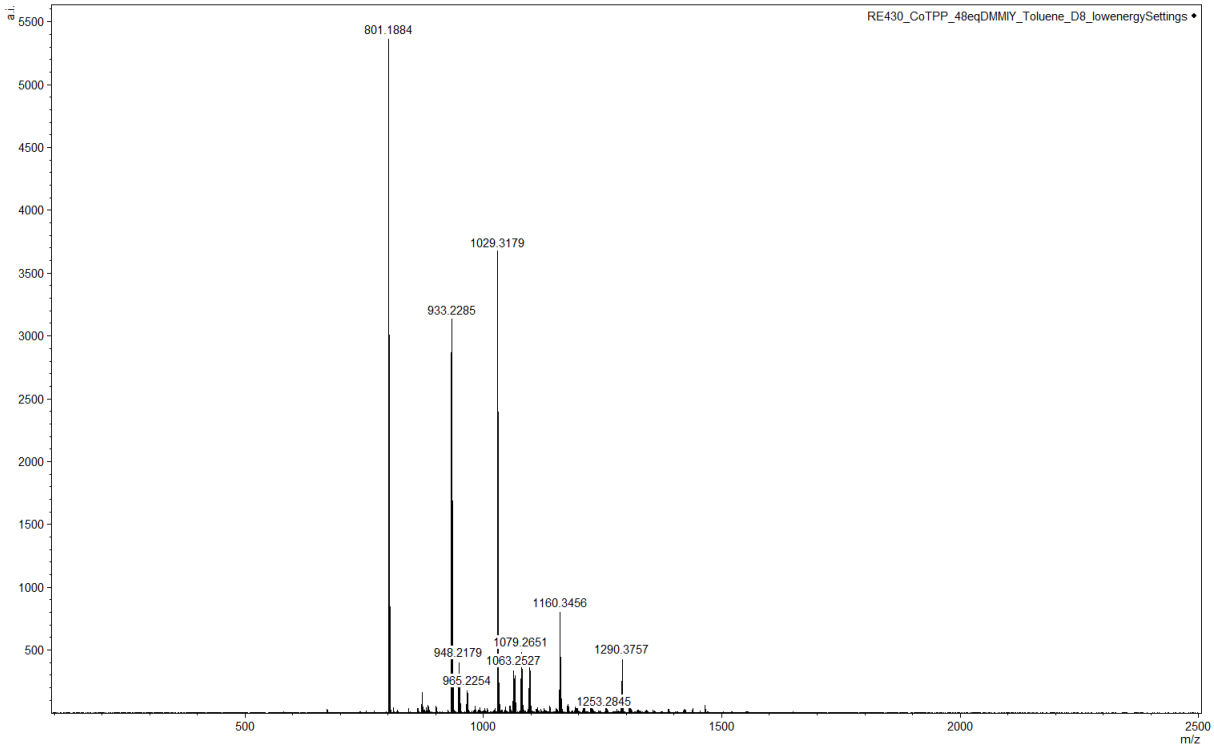


Figure S38. *B:* CSI-ESI$^+$-MS spectrum of the reaction of [Co(TPP)] and DMM•IY in toluene-d$_8$.

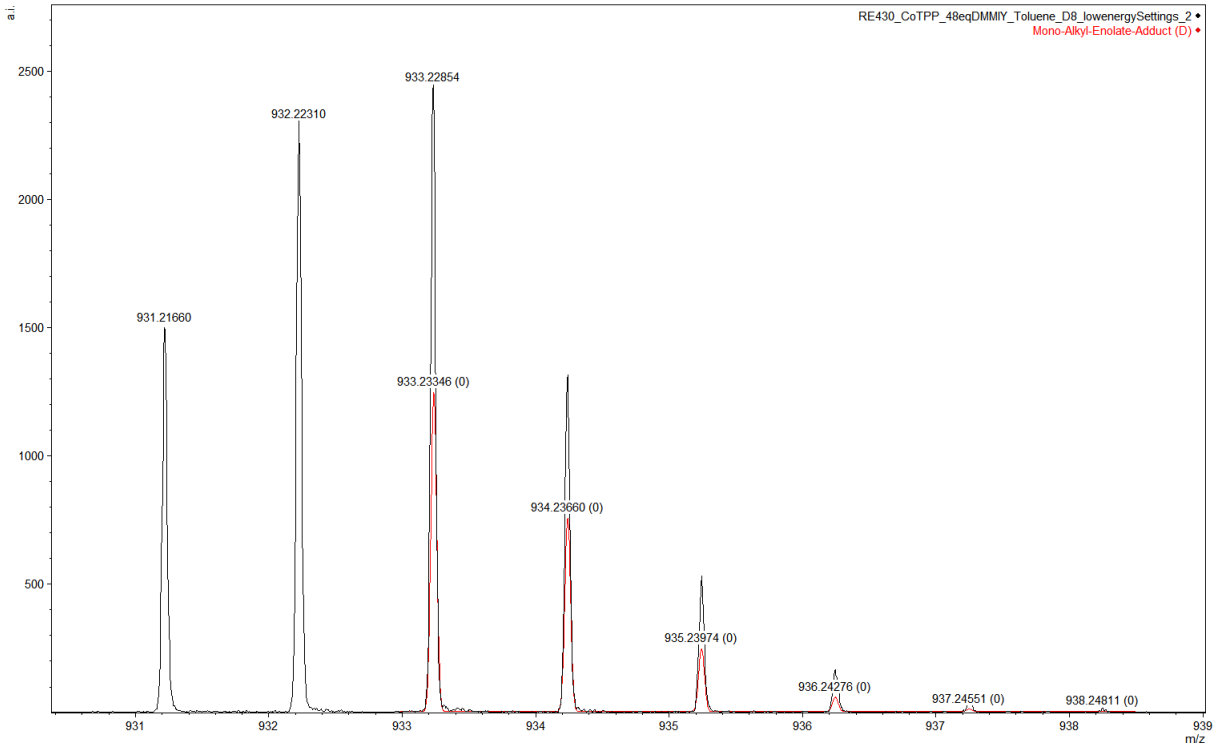


Figure S39. *B:* Zoomed-in view of the CSI-ESI$^+$-MS spectrum of the DAT product of the *bis*-carbenoid species (black) and simulation of [Co(TPP)(DMM-carbene)$_2$(+D)]$^+$ (red) in toluene-d$_8$.

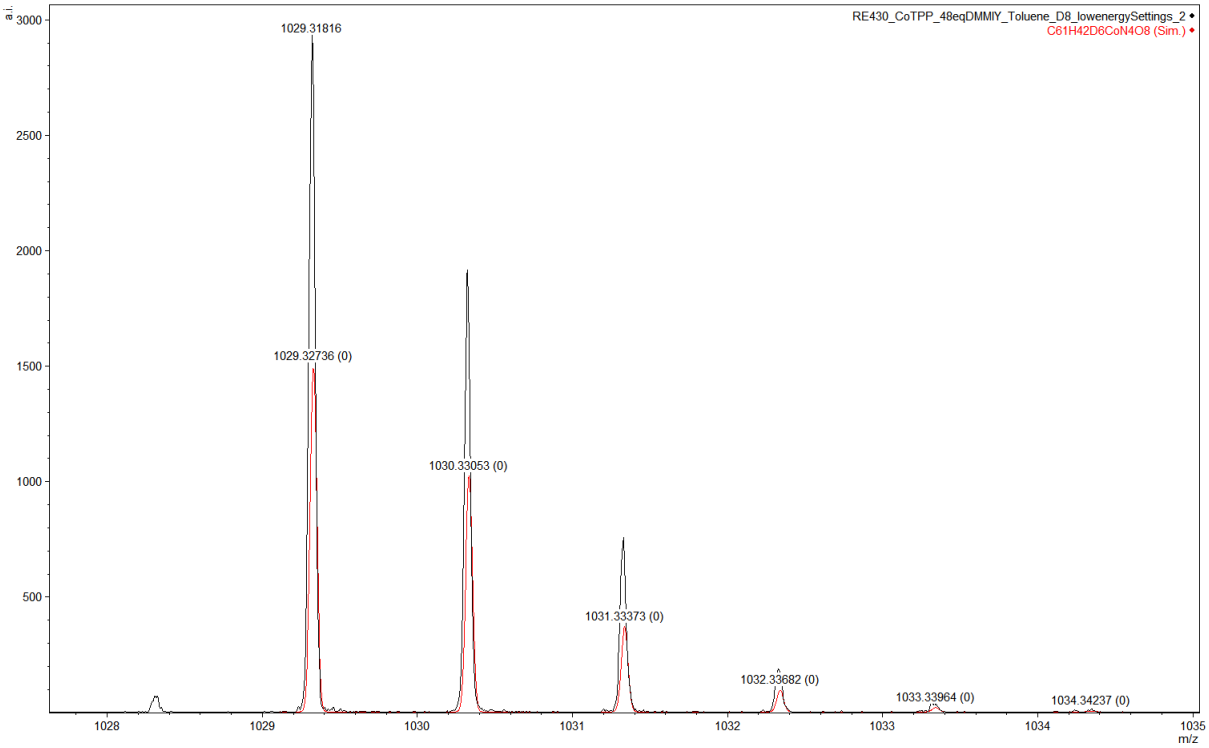


Figure S40. *B*:-Zoomed-in view of the CSI-ESI$^+$-MS spectrum of peak at m/z = 1029 Da (black) and simulation of $[Co(TPP)(DMM\text{-}carbene)_2(toluene\text{-}d_6)]^+$ (red) in toluene-d_8. To simulate the mass, a non-deuterated analog of $C_{61}H_{54}CoN_4O_8$ was used with a shift of –0.01 to compensate for the deuterium-proton mass difference.

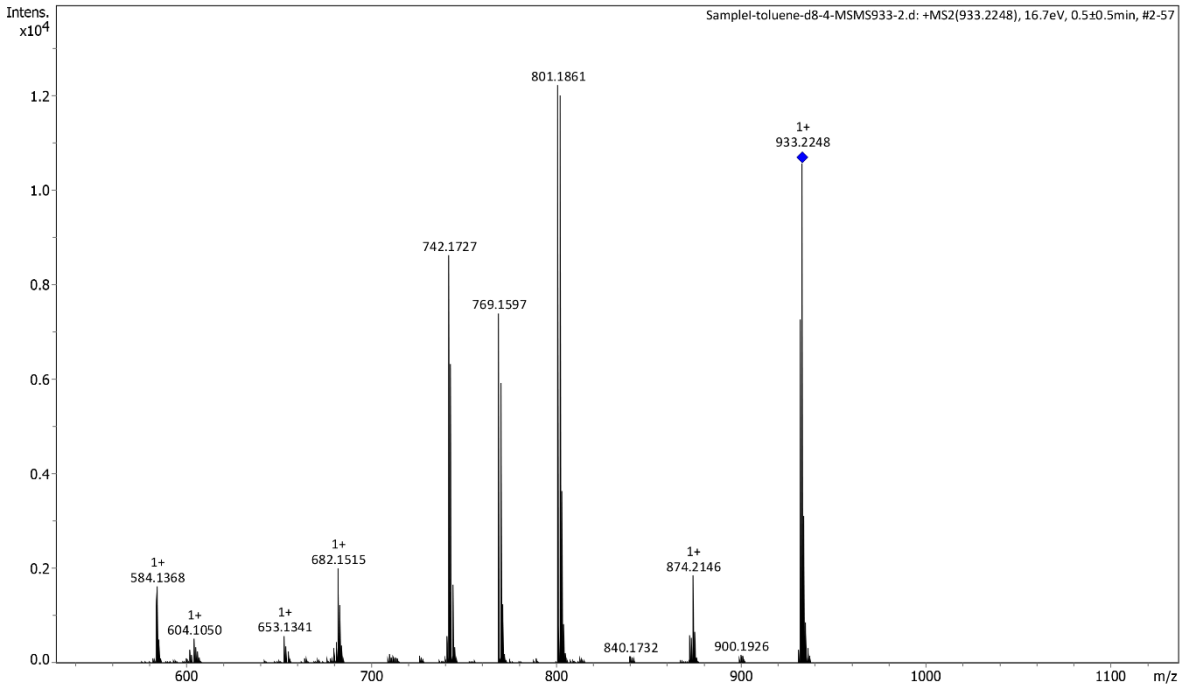


Figure S41. *B:* MS-MS spectrum of the fragmentation of the isolated peak at m/z = 933 ± 5 Da in toluene-d_8.

Reaction C (Spectra):

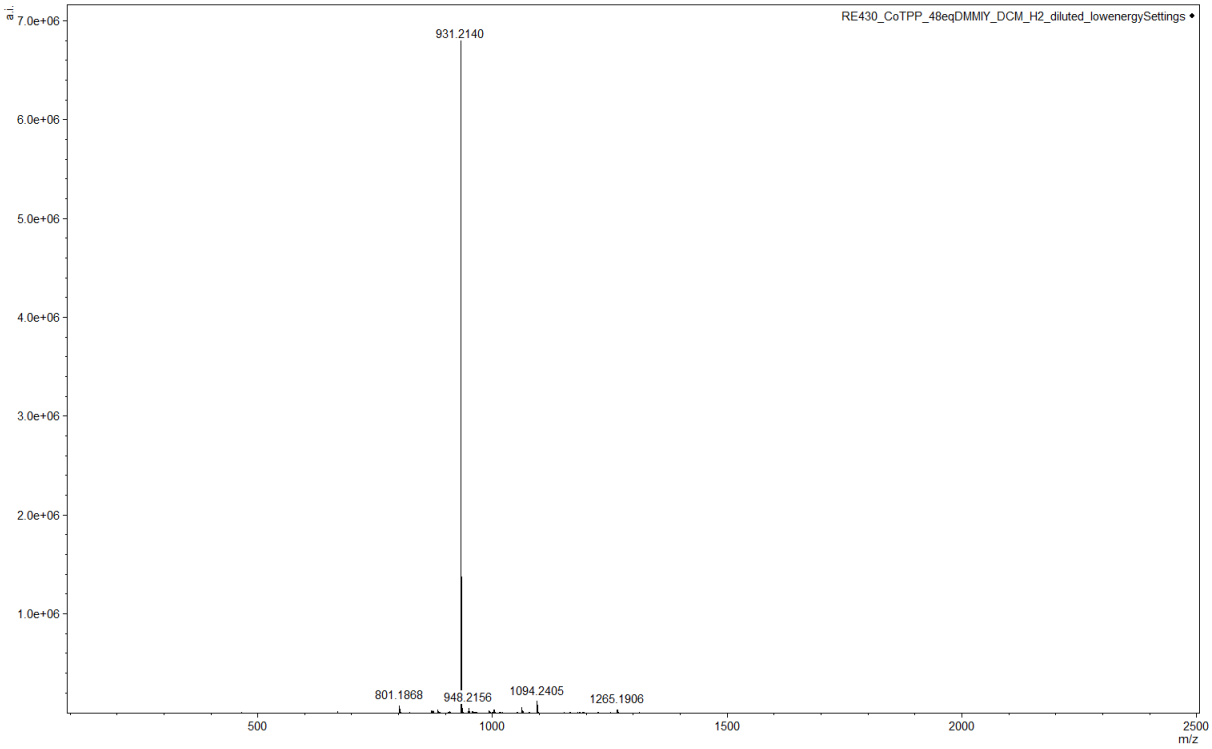


Figure S42. *C:* CSI-ESI$^+$-MS spectrum of the reaction of [Co(TPP)] and DMM•IY in CH_2Cl_2.

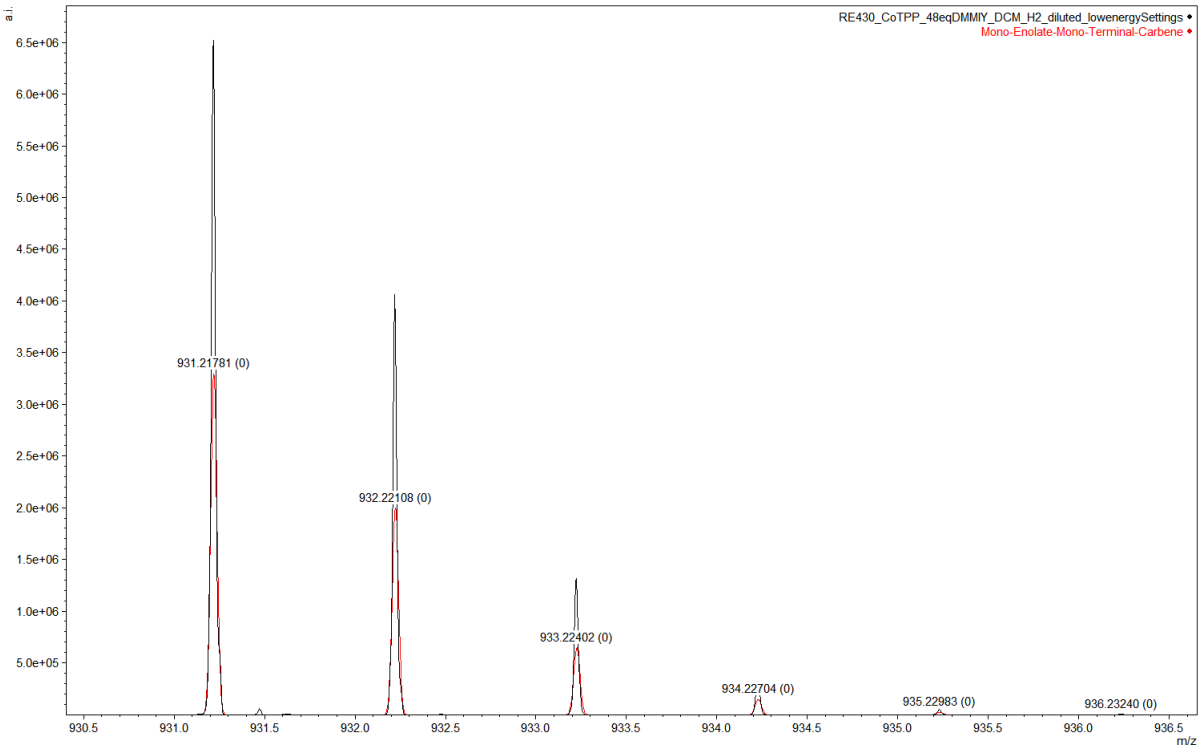


Figure S43. *C:* Zoomed-in view of the CSI-ESI$^+$-MS spectrum of the *bis*-carbenoid species (black) and simulation of [Co(TPP)(DMM-carbene)$_2$]$^+$ (red) in CH_2Cl_2.

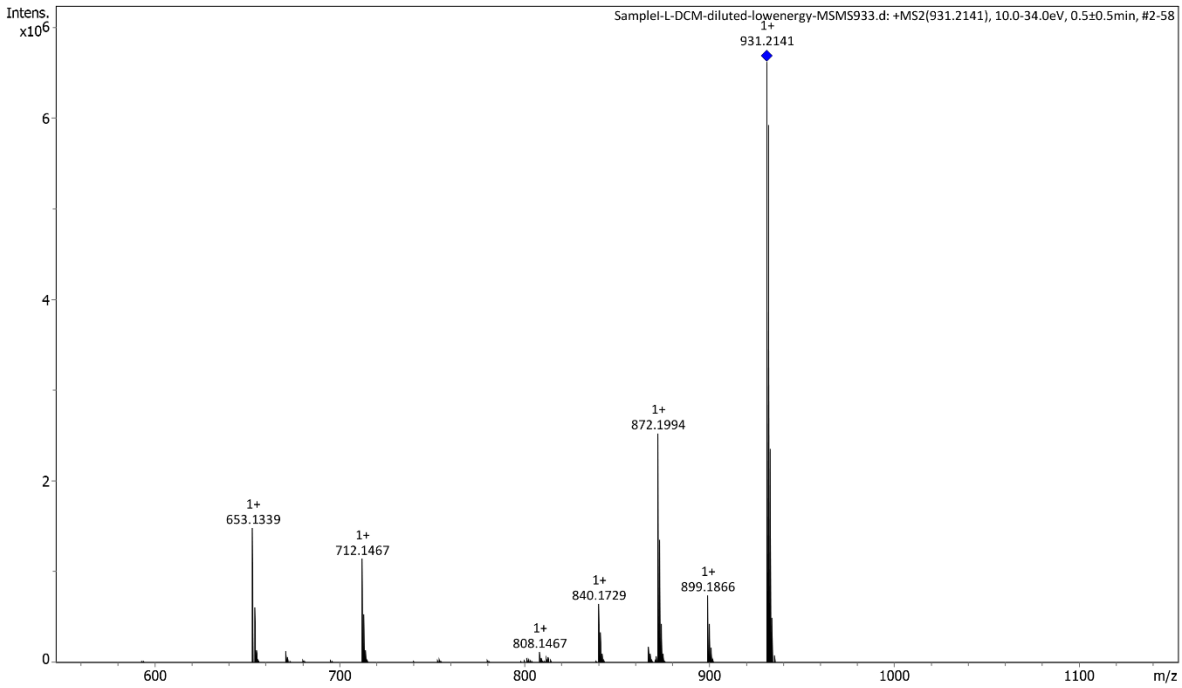


Figure S44. *C:* MS-MS spectrum of the fragmentation of the isolated peak at m/z = 931 ± 5 Da in CH_2Cl_2.

Reaction D (Spectra):

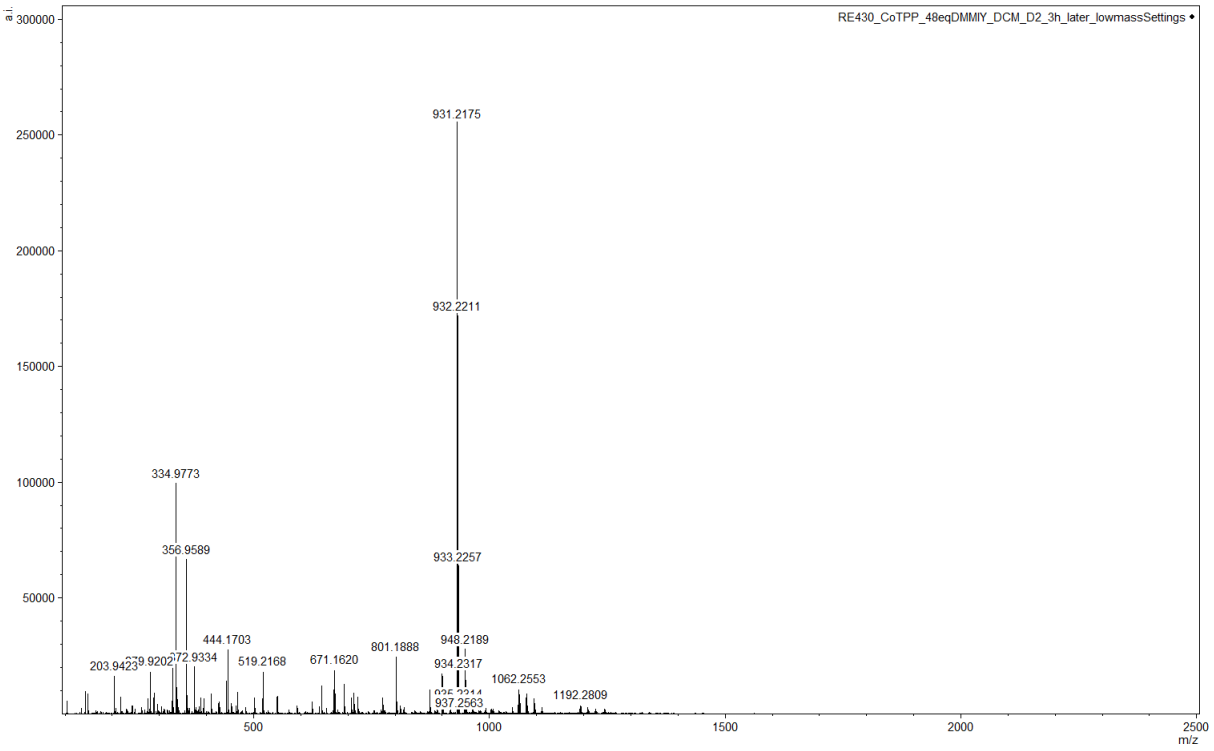


Figure S45. *D*: CSI-ESI$^+$-MS spectrum of the reaction of [Co(TPP)] and DMM•IY in CD_2Cl_2.

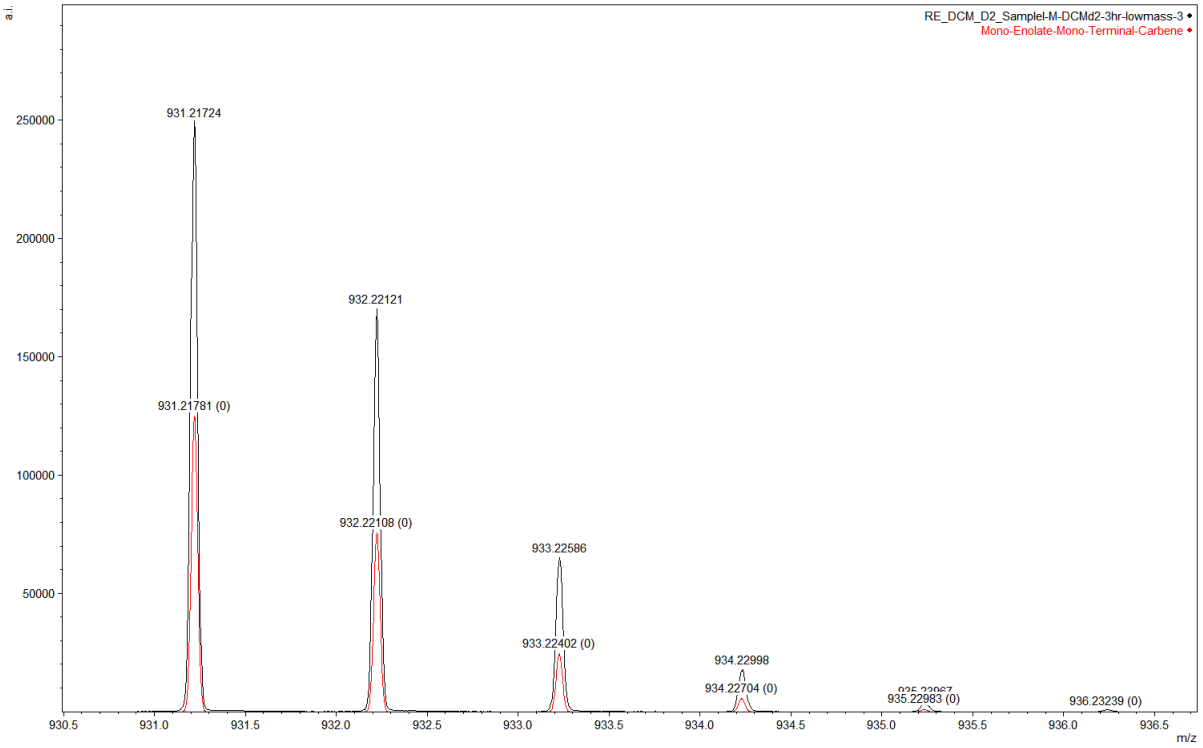


Figure S46. *D:* Zoomed-in view of the CSI-ESI$^+$-MS spectrum of the *bis*-carbenoid species (black) and simulation of $[Co(TPP)(DMM\text{-}carbene)_2]^+$ (red) in CD_2Cl_2.

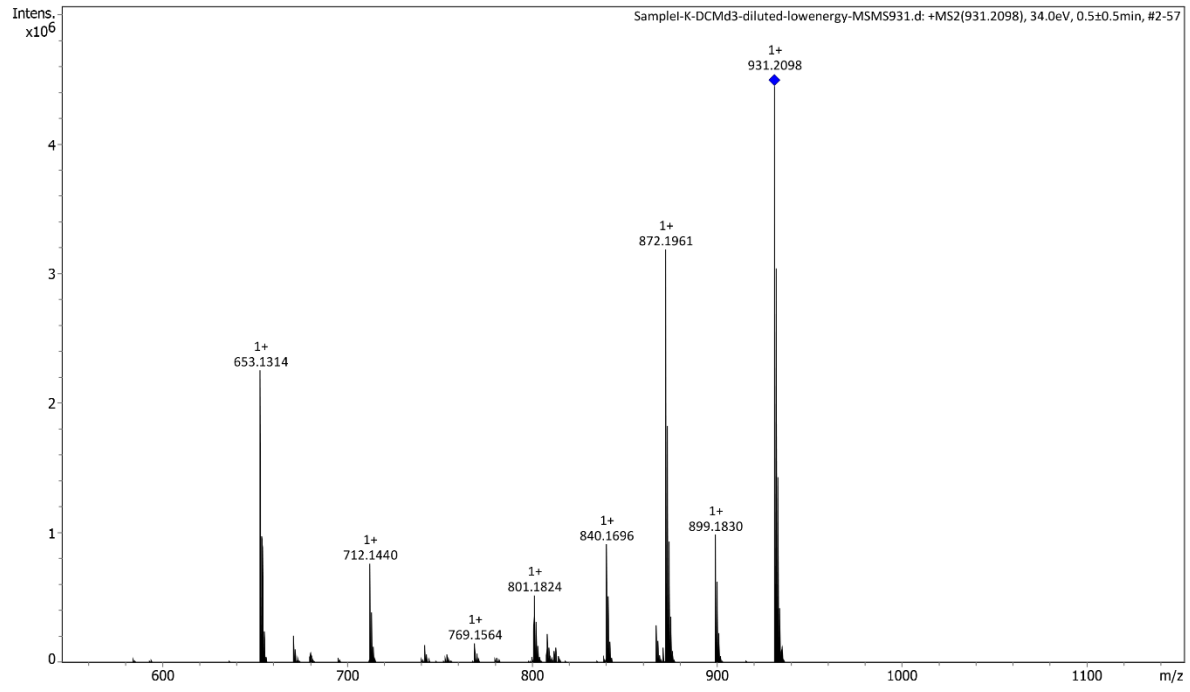


Figure S47. *D:* MS-MS spectrum of the fragmentation of the isolated peak at m/z = 931 ± 5 Da in CD_2Cl_2.

Spectroscopic studies of the HAT-induced catalyst deactivation reactions

Cobalt(III)–carbene radicals are known to deactivate rapidly through hydrogen–atom–transfer (HAT) from either the starting diazo reagent or the solvent.[28,38] Thus far, mechanistic studies of these deactivation processes have focused entirely on *mono*-substituted carbenes generated from diazo reagents. With *N*-enolate-carbene radical $\mathbf{I^{E-T}}$ in hand, we set out to study potential deactivation pathways of acceptor-acceptor carbene radicals generated from iodonium ylides. During X-band EPR spectroscopic measurements of $\mathbf{I^{E-T}}$ and excess of DMM•IY in C_6H_6, toluene-h_8 and toluene-d_8, we noticed that the rate of signal decay is strongly dependent on the solvent. Samples in toluene-h_8 turned EPR-silent within seconds. In toluene–d_8 this became a matter of minutes and in C_6H_6 the carbene radical could still be detected even after 1 day in solution. Notably, catalysis runs in non–deuterated toluene failed to produce any cyclopropane, whereas in toluene-d_8 cyclopropane **1** was obtained quantitatively. Solvent-based HAT-deactivation must be the dominant deactivation pathway of $\mathbf{I^{E-T}}$, and the stark difference between regular– and deuterated toluene hints at a strong kinetic isotope effect typical for radical-type HAT reactions.[39] Time–dependent UV/Vis studies in CH_2Cl_2 clearly show a clean transition of the *N*-enolate–carbene radical $\mathbf{I^{E-T}}$ species (430 nm) to a new species (455 nm) via a single isosbestic point at 441 nm within 30 min (Figure S19) The similarity of the obtained spectrum with that of $\mathbf{I^{E-T}}$ points to formation of a related *N*-enolate complex. A smaller peak at 418 nm was also detected that did not change over time (assigned to species $\mathbf{I^{A'}}$).

The peak at 455 nm matches closely to the data of a related *N*-enolate Co^{III} complex with a *trans* bromido ligand (synthesized from [Co^{III}(TPP)(Br)]), as reported by Mansuy and coworkers (458 nm).[33] In combination with the continued absence of any Q–band, this suggests that the *N*-enolate moiety is still intact. The apparent redshift from 430 to 455 nm can be attributed to conversion of the π-accepting carbene radical moiety to a σ-donating alkyl group.[33] Ergo, the peak at 455 can be attributed to the *N*-enolate–alkyl adduct $\mathbf{I^{E-A}}$. The same transition was found in toluene (Figure S18). Interestingly, in C_6H_6 (Figure S17), a slightly more diffuse isosbestic point was found around 441 nm, and over time the broad peak at 420 nm (attributed to $\mathbf{I^{E-T}}$ in C_6H_6) with a shoulder at 418 nm drops in intensity and converts to 458 nm over a period of 2 hours. The shoulder at 418 nm remains and appears as a clear peak after the reaction. The peak at 458 nm is again assigned to $\mathbf{I^{E-A}}$. It is likely that the smaller signal at 418 nm belongs to *mono*-alkyl-adduct $\mathbf{I^{A}}$, formed by HAT-induced deactivation of *mono*-terminal-carbene species $\mathbf{I^{T}}$. The significant blue shift of this and the appearance of a new Q-band at 612 suggest the presence of an unmodified (and non-oxidized) porphyrin macrocycle.[34] This minor species is already formed *during* the conversion of [Co(TPP)] to $\mathbf{I^{E-T}}$, suggesting that *mono*-terminal-carbene $\mathbf{I^{T}}$ undergoes HAT-induced deactivation more rapidly than the *N*-enolate-carbene radical $\mathbf{I^{E-T}}$. In toluene, similar results are obtained (Figure S18) The wavelengths and relative concentrations of $\mathbf{I^{A}}$ formed during formation of $\mathbf{I^{E-T}}$ vary a bit among the solvents, but overall similar HAT-induced deactivation processes are observed in CH_2Cl_2, benzene and toluene. Most likely the minor species $\mathbf{I^{A}}$ contains an unidentified 6th ligand L that blocks a follow-up reaction with excess iodonium ylide to produce $\mathbf{I^{E-A}}$, as this is not observed in the time-dependent UV/Vis studies.

To confirm that the solvent is a likely hydrogen atom source, isotopic labeling studies were performed using CSI^{+}-MS in deuterated and non-deuterated toluene (see Figure S34–Figure S41). When conducted in toluene-h_8, a clear signal at 932 *m/z* corresponding to $\mathbf{I^{E-A}}$ was observed. It was also found via MS-MS analysis that this species easily fragments to 801 *m/z*, in line with reported Co–C homolysis of Co^{III}-alkyl fragments,[40] thus matching the expected HAT-product. In toluene–d_8, a peak at 933 *m/z* was found instead, which is in line with formation of the DAT-product $\mathbf{D\text{-}I^{E-A}}$. Moreover, MS-MS analysis shows the fragmentation of $\mathbf{D\text{-}I^{E-A}}$ to produce the same peak at 801 *m/z* by loss of a deuterated alkyl fragment. This shows that the hydrogen atom source

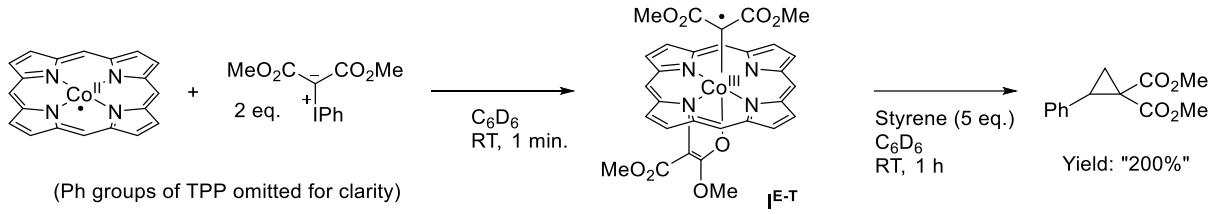
for deactivation of the carbene radicals in toluene is undoubtedly the solvent. However, for benzene and CH_2Cl_2 this is less clear (see Figure S27 and Figure S42–Figure S47). The C–H bond BDEs of benzene and CH_2Cl_2 are stronger, and as such we cannot exclude another hydrogen atom source being responsible for the observed HAT deactivation products in these solvents (e.g. trace impurities).

Deactivation through solvent-based HAT is further supported by the *in-situ* ATR-FT-IR measurements (Figure S22)showing signals at 1705, 1738 and 1765 cm^{-1}. DFT simulations of the IR spectra (Figure S24) show that these peaks correspond to Co^{III}-alkyl or free alkyl species, and they do not match with any of the Co^{III}-carbene radical species.

Single-turnover experiments:

To an oven-dried vial was added DMM•IY (15.05 mg; 45 µmol; 2 eq.) and 1,3,5-trimethoxybenzene (1.275 mg; 7.58 µmol; 0.34 eq.). The vial was added to an Ar bucket, in which it was cycled thrice with Ar/vacuum (vacuum ≥ 2 min.). To this was added a 5 mL solution of [Co(TPP)] in C_6D_6 (14.97 mg; 3.0 mg/mL; 4.5 µM; 1 eq.). The reaction mixture was stirred for 1 min at room temperature, after which styrene (12.8 µL; 11.63 mg; 111.67 µmol; 5 eq.) was added and the mixture was stirred for an additional hour at 400 RPM in the center of the stirring plate. Subsequently, the reaction was quenched by cycling the mixture through a syringe in open air followed by filtration through a syringe filter (PTFE, hydrophobic, 0.45 µm) into an NMR tube. A ^{1}H-NMR spectrum was recorded and used for yield determination vs. the internal standard (1,3,5-trimethoxybenzene).

Note: 200% yield means in this experiment that *N*-enolate-carbene radical species $\mathbf{I}^{\mathbf{E-T}}$ effectively transfers two carbene units to styrene instead of one expected.



Scheme S7. Single-turnover experiment with 2.0 eq. DMM•IY and 1.0 eq. [Co(TPP)].

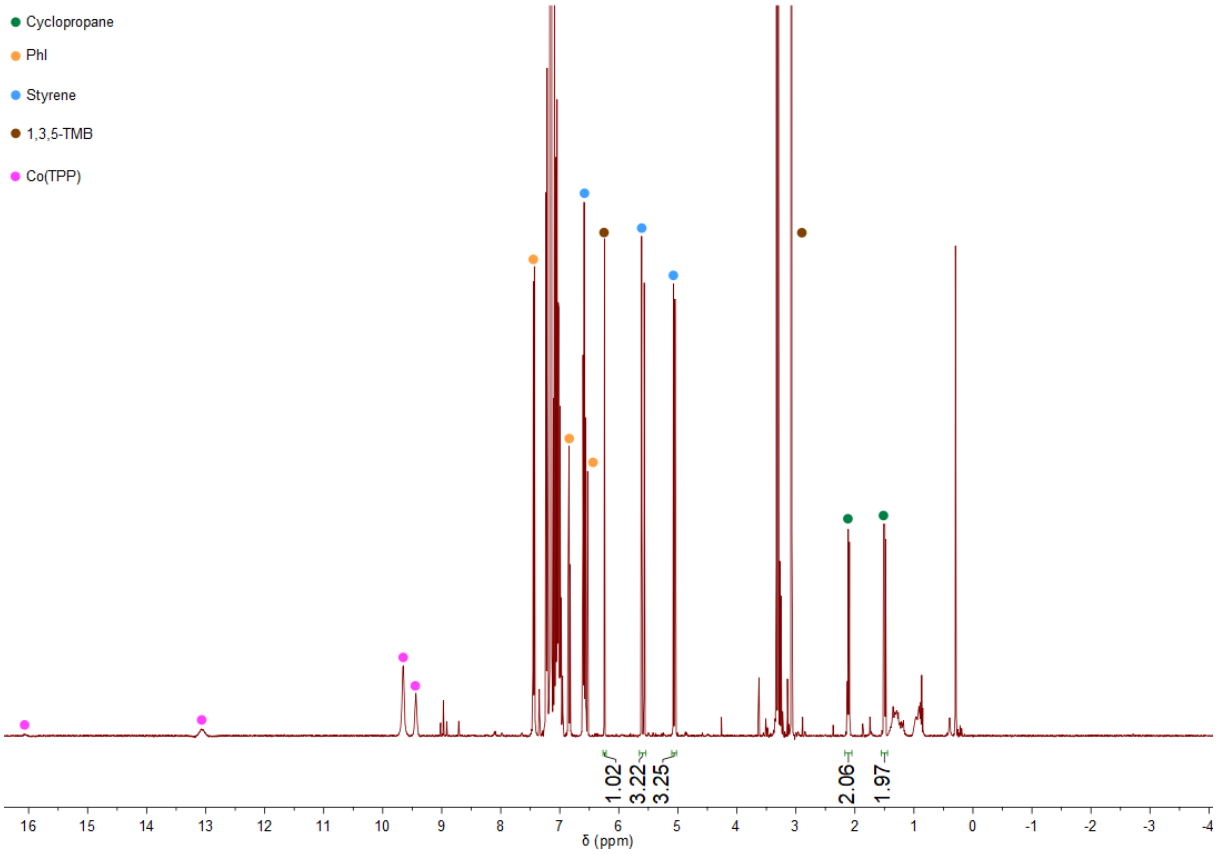


Figure S48. ^{1}H-NMR spectrum of a single-turnover experiment. Yields were determined with respect to the aryl proton peaks of 1,3,5-trimethoxybenzene as internal standard.

Carbene formation monitoring:

To check for the influence of the solid-state morphology of the iodonium ylide, two batches were synthesized. Batch A was made via the general protocol. Batch B was recrystallized from CH_2Cl_2/*n*-pentane. Reactions were carried out according by measuring the ylide in an oven-dried vial and adding a 1.5 mg/mL stock solution of [Co(TPP)] to the solid. The disappearance of [Co(TPP)] signals was followed over time with ^{1}H-NMR at intervals of 1, 2, 5, 10 and 15 min (Figure S49–Figure S50). To quench the reaction, samples were made by filtering the samples through a syringe filter (PTFE, hydrophobic, 0.45 µm) in open air into an NMR tube.

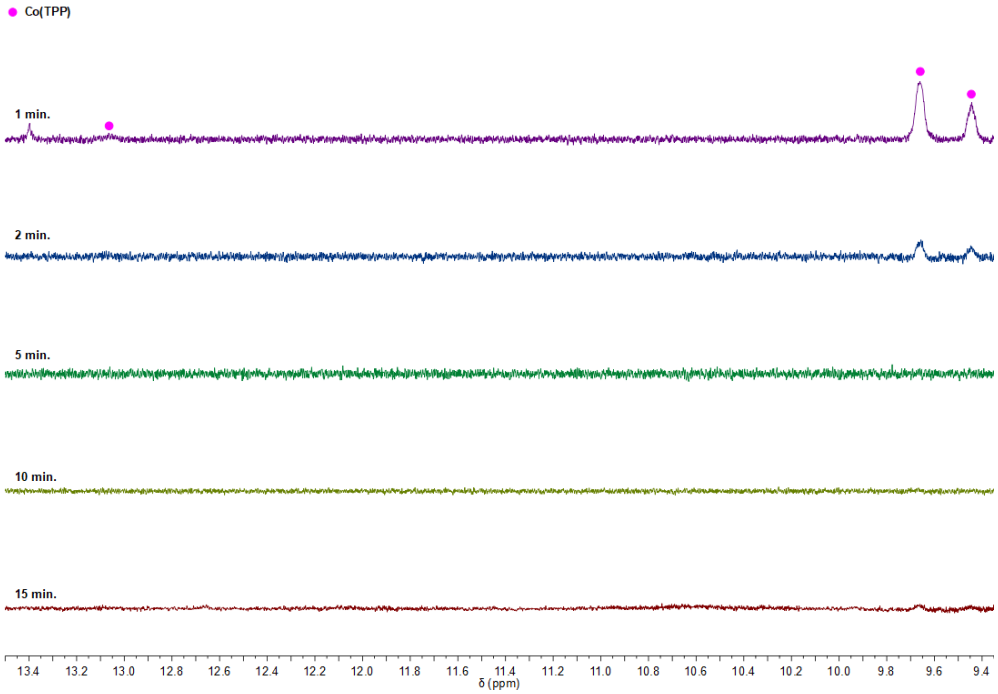


Figure S49. Disappearance of [Co(TPP)] signals (pink) of the reaction between DMM•IY (Batch A) and [Co(TPP)].

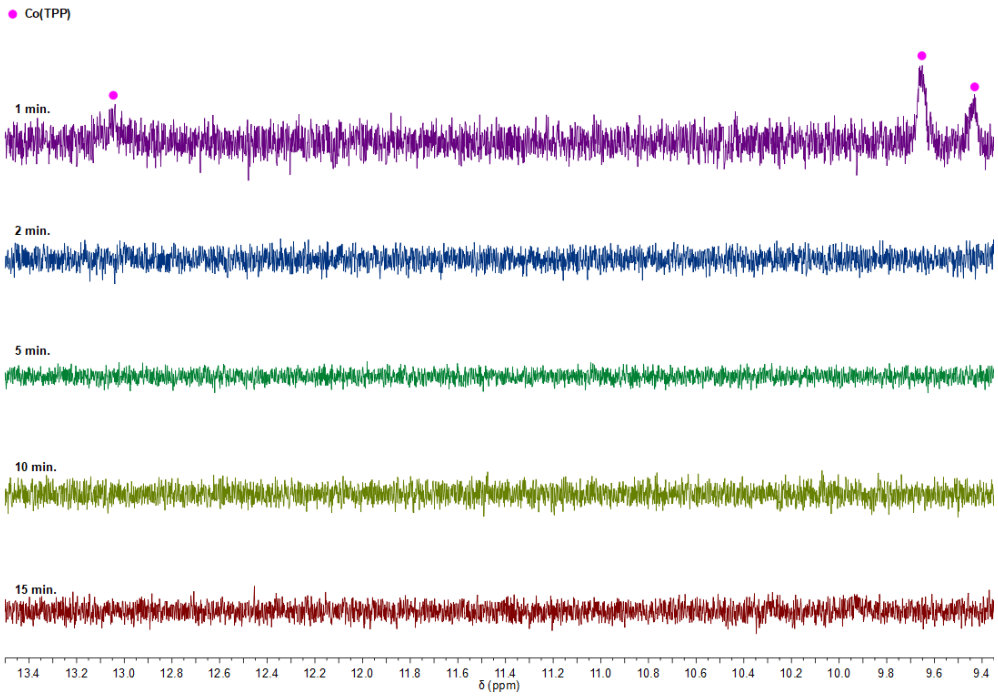


Figure S50. Disappearance of [Co(TPP)] signals (pink) of the reaction between DMM•IY (Batch B) and [Co(TPP)].

Control reactions with dimethyldiazomalonate (DMM·N_2):

To compare with the iodonium ylide DMM•IY, the diazo analogue was tested as a carbene precursor in duplo in the same fashion according to the general protocol (vide supra). At room temperature after 1 h (Figure S51), no conversion of either styrene nor any product formation was detected. Due to the overlap of the only proton signal of the diazo compound with the internal standard, the conversion of the diazo reagent could not be accurately determined. However, in addition to the absence of styrene conversion or product formation, no change in [Co(TPP)] signals was detected either. Ergo, it seems that under identical conditions to DMM•IY, the diazo analogue does not react. Additionally, the reaction was run for 60 h at 60°C to force the reaction to occur (Figure S52). However, even under these conditions, less than 10% product was observed. In contrast to the room temperature experiments, no signal belong to free [Co(TPP)] could be found. Instead, several diamagnetic signals could be found between 8 and 10 ppm, similar to literature data[28] for [Co(TPP)]-alkyl species. It is likely these belong to HAT-derived deactivation products of any carbene species produced during the reaction. These findings suggest that diazo reacts both sluggishly and the thereafter formed carbenes deactivate quickly under the reaction conditions. The reported yields are also in line with literature data[41] for similar reactions involving acceptor-acceptor diazo compounds and [Co(TPP)].

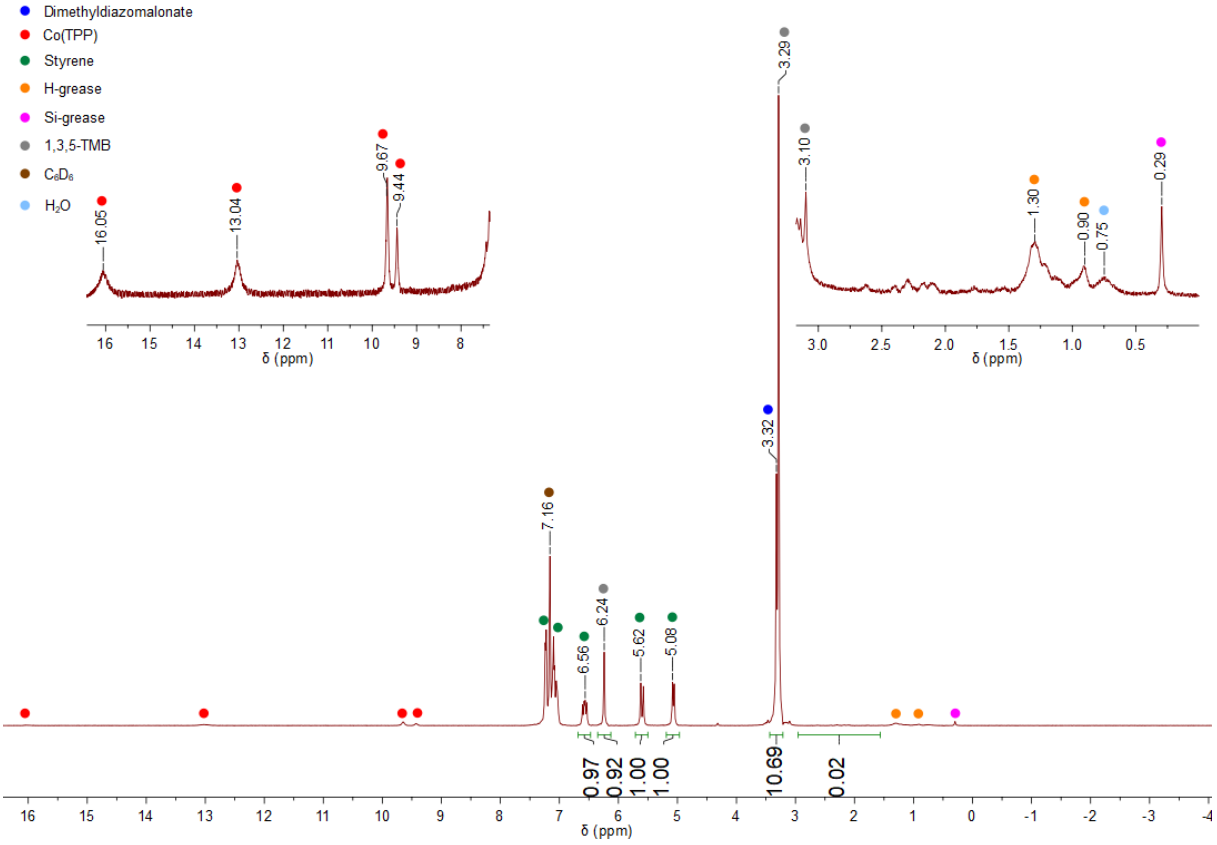


Figure S51. Control experiment for the [Co(TPP)]-catalyzed cyclopropanation with dimethyldiazomalonate (DMM·N_2) at RT for 1 h under standard conditions.

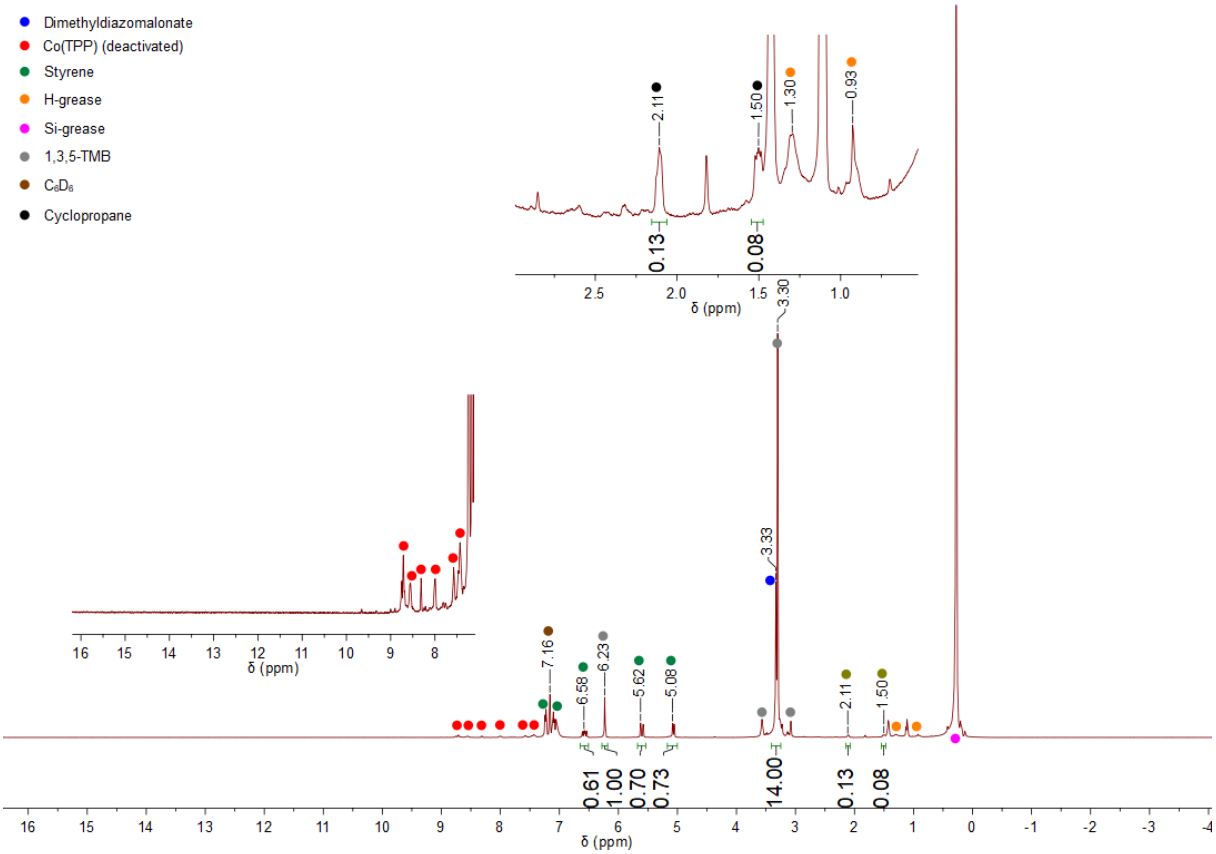
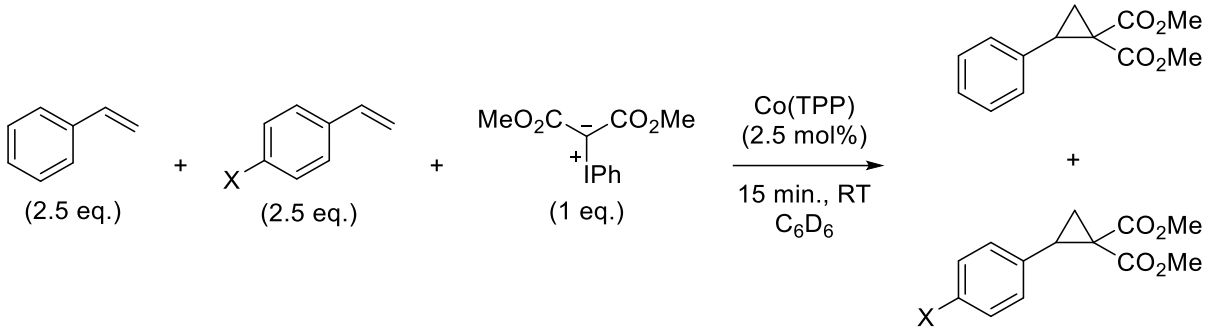


Figure S52. Control experiment for the [Co(TPP)]-catalyzed cyclopropanation with dimethyldiazomalonate (DMM·N_2) at 60°C for 60 h under otherwise standard conditions.

Hammett plots:



Scheme S8. Conditions for the intermolecular competition experiments to perform a Hammett analysis.

The Hammett analysis was performed via intermolecular competition between styrene and *para*-functionalized styrenes (X = *t*Bu, Me, F, Cl, CF_3 and NO_2) using the optimized conditions described in Table S6 (Scheme S10). To ensure complete and reliable conversion, the reaction time was extended from 5 to 15 min. All experiments were performed in duplo. Samples were analyzed via quantitative ^{1}H-NMR spectroscopy. The average ratio of *para*-functionalized vs. non-functionalized cyclopropane was determined, which can be equated to the ratio of k_H:k_x as the excess of styrenes prevents styrene conversions >50%. The resulting log(k_H:k_x) values were plotted against $\rho^{\bullet}\sigma_{JJ}^{\bullet}$, $\rho^{+}\sigma^{+}$ or $\rho^{-}\sigma^{-}$ or a combination and multiple linear regression was applied. The $\sigma_{JJ}^{\bullet}$ values were obtained from Jiang[42a] and the σ^{+}/σ^{-} values from Taft and coworkers.[42b] The best fits were obtained for $\{\rho^{\bullet}\sigma_{JJ}^{\bullet} + \rho^{-}\sigma^{-} + C\}$.

We suspected that the order of addition might influence whether the *mono*-terminal carbene or the *mono*-enolate-*mono*-terminal carbene is the dominant active species and as such we performed a Hammett analysis for both reactions with order of addition DMM•IY: Styrenes: [Co(TPP)] and order of addition DMM•IY: [Co(TPP)]: styrenes. The latter experiments were run for 3 min. prior to addition of styrenes.. The results are displayed in Table S13–Table S14. Blank control experiments on all functionalized styrenes showed no background reaction.

As can be seen in Figure S53–Figure S54, the reaction order has little effect on the Hammett parameters. Since EPR experiments do indicate that different intermediates (either the *mono*-terminal carbene radical $\mathbf{I^T}$ or the *N*-enolate-carbene radical $\mathbf{I^{E-T}}$) dominate upon changing the reaction order, these Hammett results suggests that both carbenes have very similar electronic properties. The necessary addition of $\sigma_{JJ}^{\bullet}$-values for an accurate fit supports the previously established radical character of these intermediates.

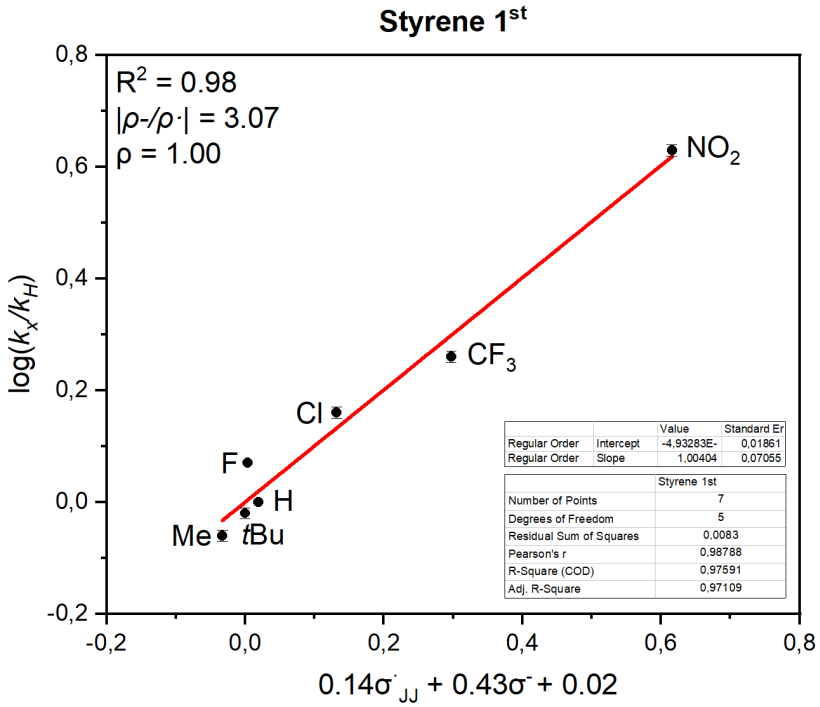


Figure S53. Hammett plot for the reaction in the order DMM•IY: Styrenes: [Co(TPP)].

Table S13. Hammett parameters ($\sigma_{JJ}^{\bullet}$, σ^{-} and σ^{+}) and the obtained $k_X:k_H$ and $\log(k_X:k_H)$ results for the reaction in the order DMM•IY: Styrenes: [Co(TPP)]. Error margins are shown for the $\log(k_X:k_H)$ values.

Entry	X	$\sigma_{JJ}^{\bullet}$	σ^{-}	σ^{+}	$k_X:k_H$	$\log(k_X:k_H)$
1	*t*Bu	0.26	−0.13	−0.26	0.95	−0.02 ± 0.01
2	Me	0.15	−0.17	−0.31	0.87	−0.06 ± 0.01
3	H	0	0	0	1.00	0.00 ± 0.00
4	F	−0.02	−0.03	−0.07	1.17	0.07 ± 0.00
5	Cl	0.22	0.19	0.11	1.44	0.16 ± 0.01
6	CF_3	−0.01	0.65	0.61	1.81	0.26 ± 0.01
7	NO_2	0.36	1.27	0.79	4.28	0.63 ± 0.01

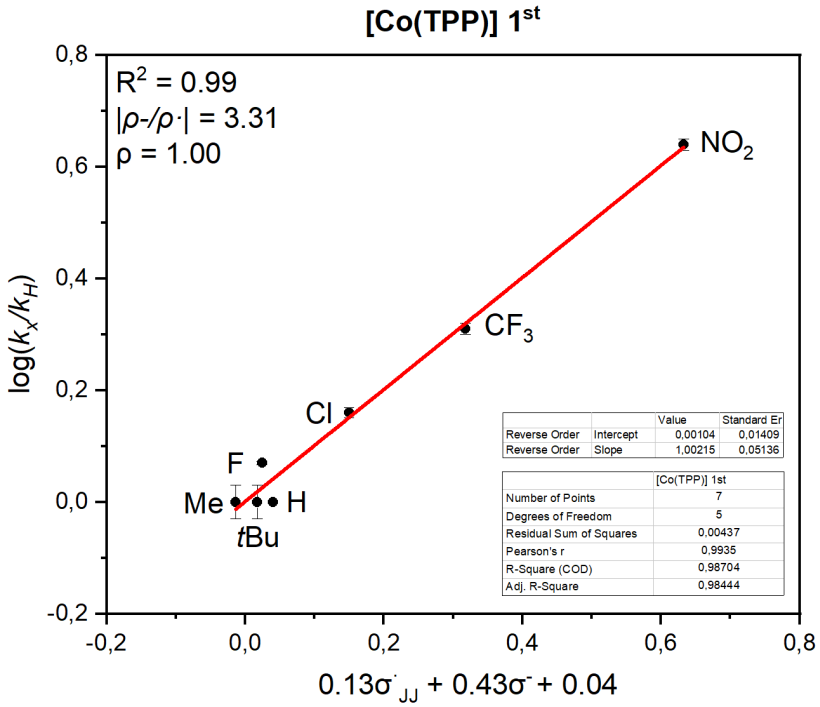


Figure S54. Hammett plot for the reaction in the order DMM•IY: [Co(TPP)]: Styrenes.

Table S14. Hammett parameters ($\sigma_{JJ}^{\bullet}$, σ^{-} and σ^{+}) and the obtained $k_X:k_H$ and $\log(k_X:k_H)$ results for the reaction in the order DMM•IY: [Co(TPP)]: Styrenes. Error margins are shown for the $\log(k_X:k_H)$ values.

Entry	X	$\sigma_{JJ}^{\bullet}$	σ^{-}	σ^{+}	$k_X:k_H$	$\log(k_X:k_H)$
8	*t*Bu	0.26	−0.13	−0.26	1.00	0.00 ± 0.03
9	Me	0.15	−0.17	−0.31	1.00	0.00 ± 0.03
10	H	0	0	0	1.00	0.00 ± 0.00
11	F	−0.02	−0.03	−0.07	1.16	0.07 ± 0.00
12	Cl	0.22	0.19	0.11	1.46	0.16 ± 0.01
13	CF_3	−0.01	0.65	0.61	2.04	0.31 ± 0.01
14	NO_2	0.36	1.27	0.79	4.38	0.64 ± 0.01

Copies of the NMR spectra (Characterization):

Dimethylmalonate phenyliodonium ylide (DMM•IY) (^{1}H-NMR):

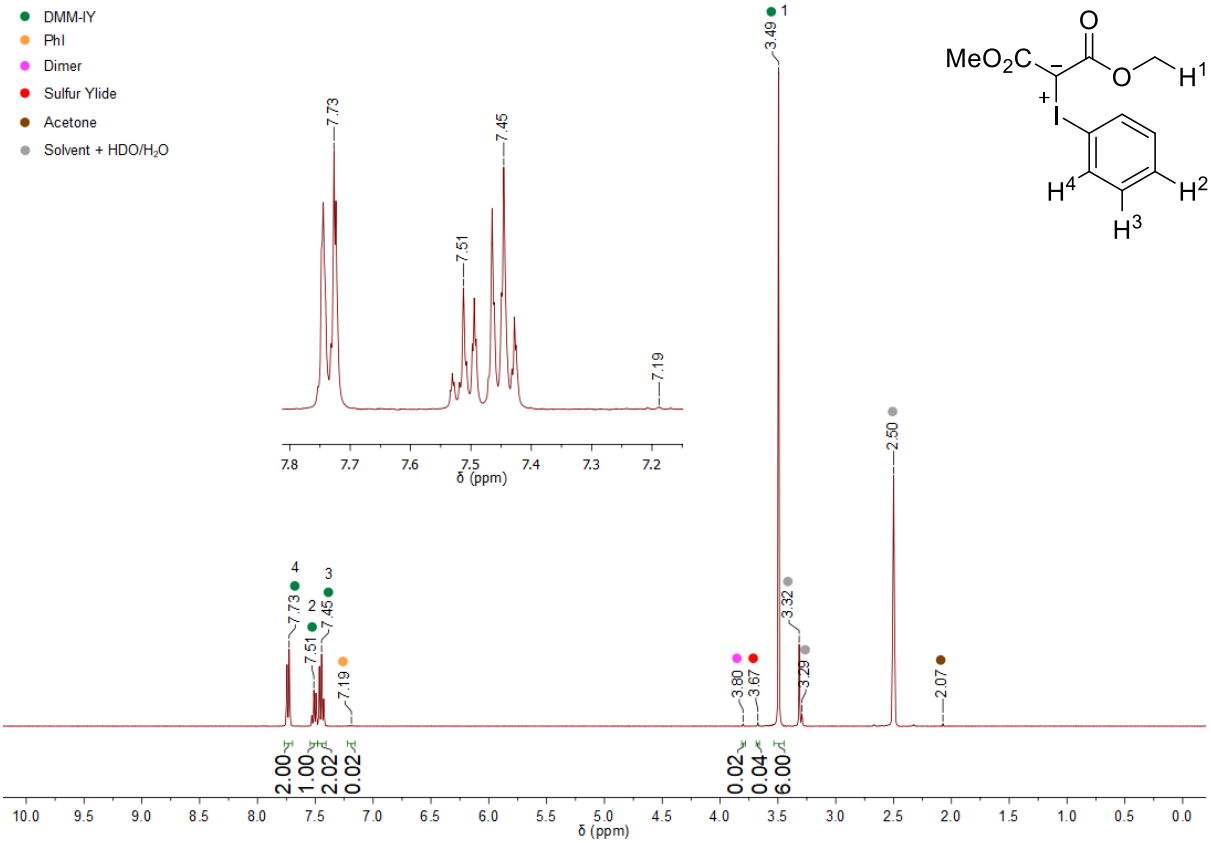


Figure S55. ^{1}H-NMR spectrum of dimethylmalonate phenyliodonium ylide (DMM•IY).

^{13}C-2-dimethylmalonate phenyliodonium ylide (^{13}C-DMM•IY) (^{1}H-NMR):

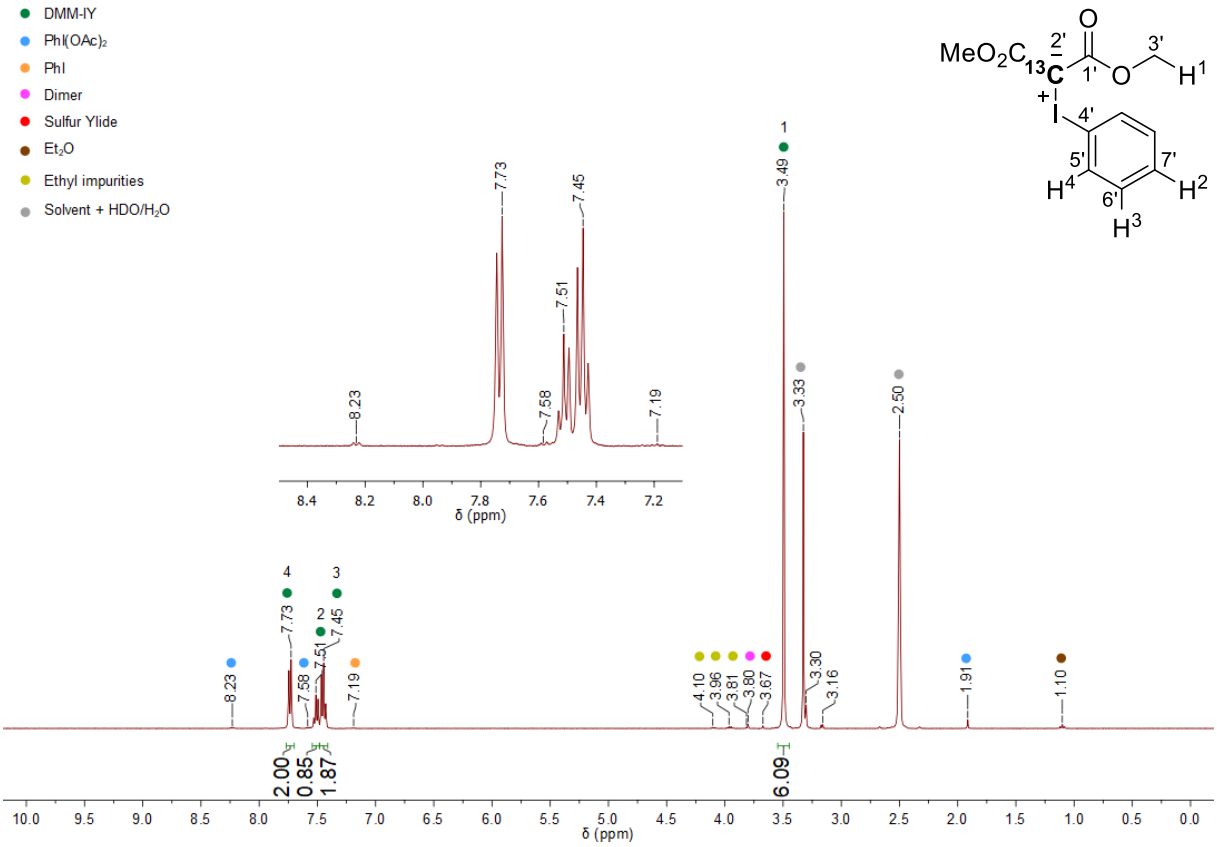


Figure S56. ^{1}H-NMR spectrum of ^{13}C-2-dimethylmalonate phenyliodonium ylide (^{13}C-DMM•IY).

^{13}C-2-dimethylmalonate phenyliodonium ylide (^{13}C-DMM•IY) (^{13}C-NMR):

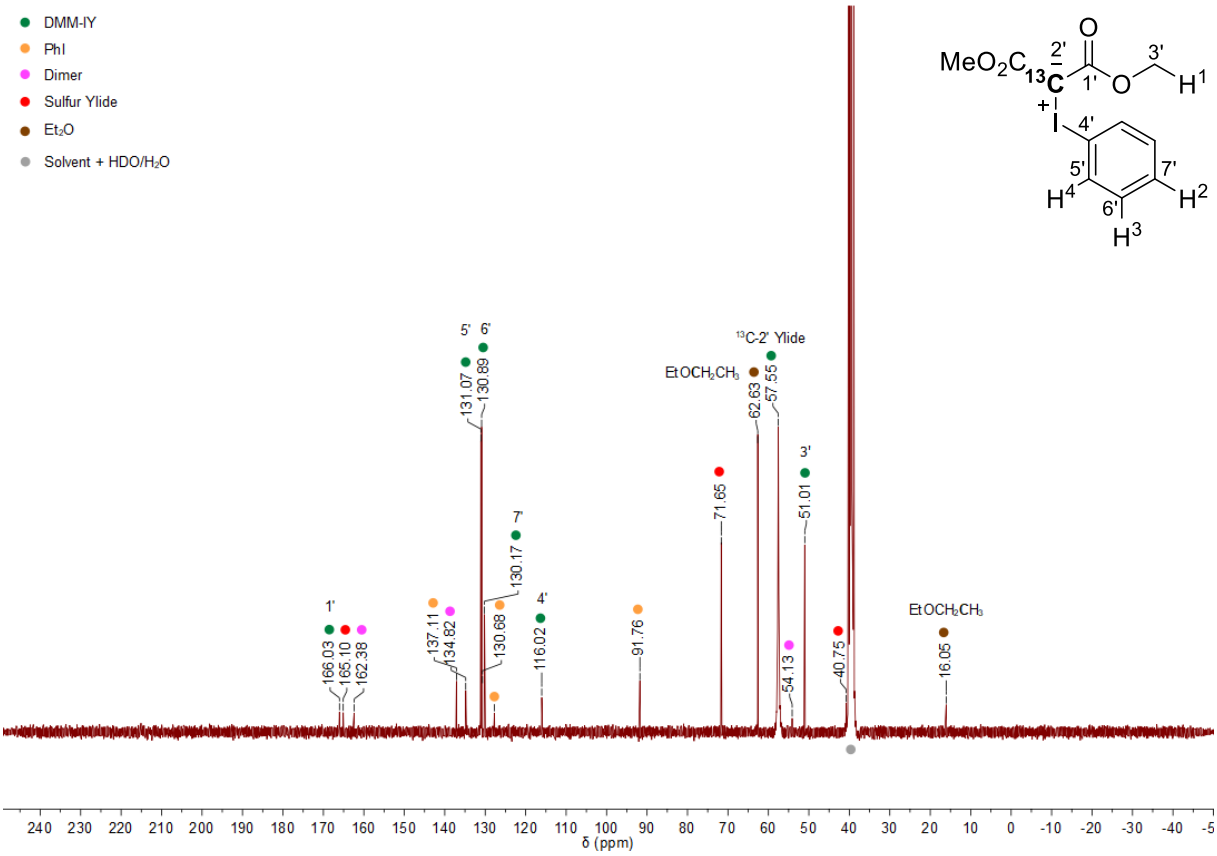


Figure S57. ^{13}C-NMR spectrum of ^{13}C-*2*-dimethylmalonate phenyliodonium ylide (^{13}C-DMM•IY).

Temperature dependence of the background reaction (full spectrum & zoom-ins):

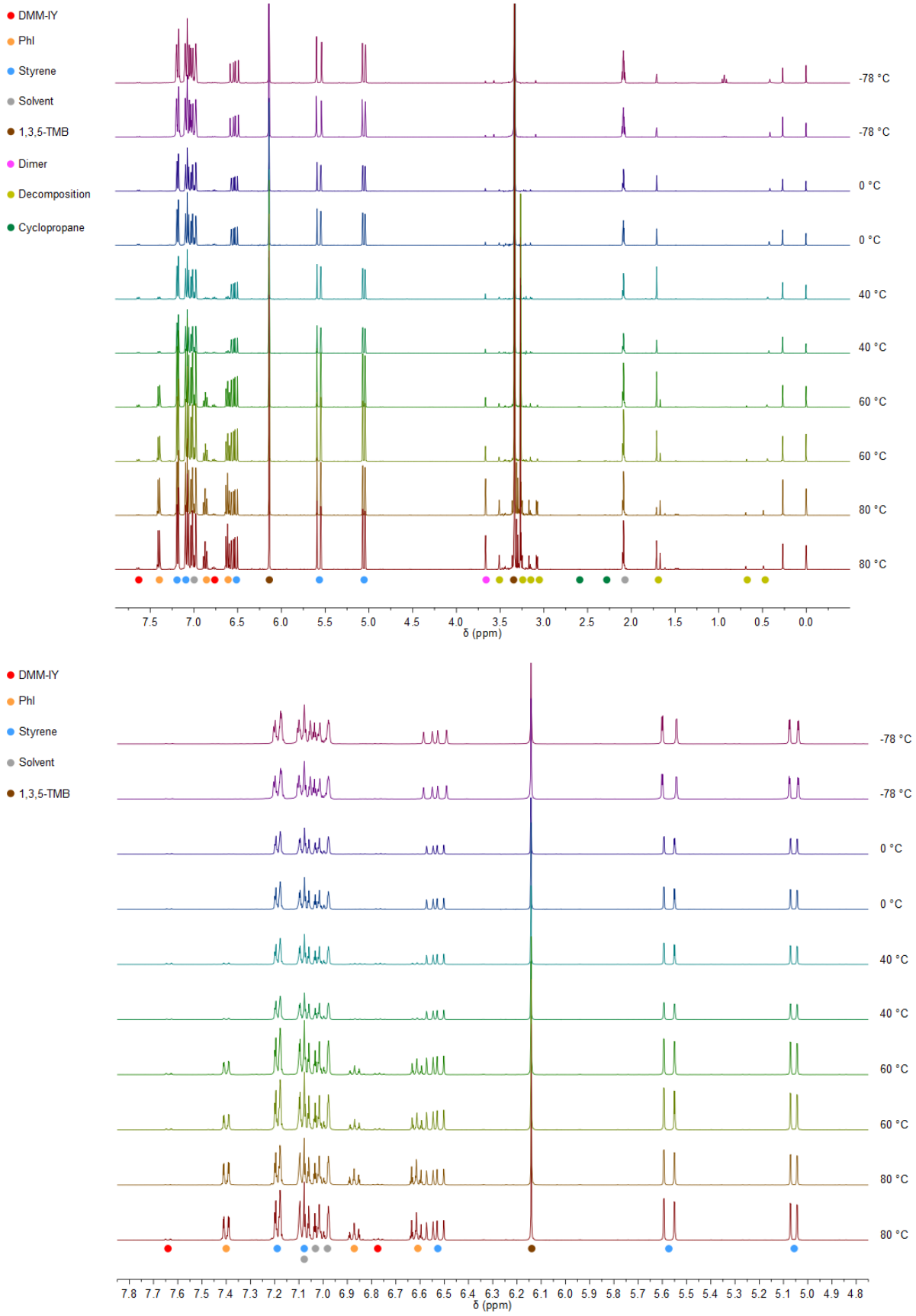
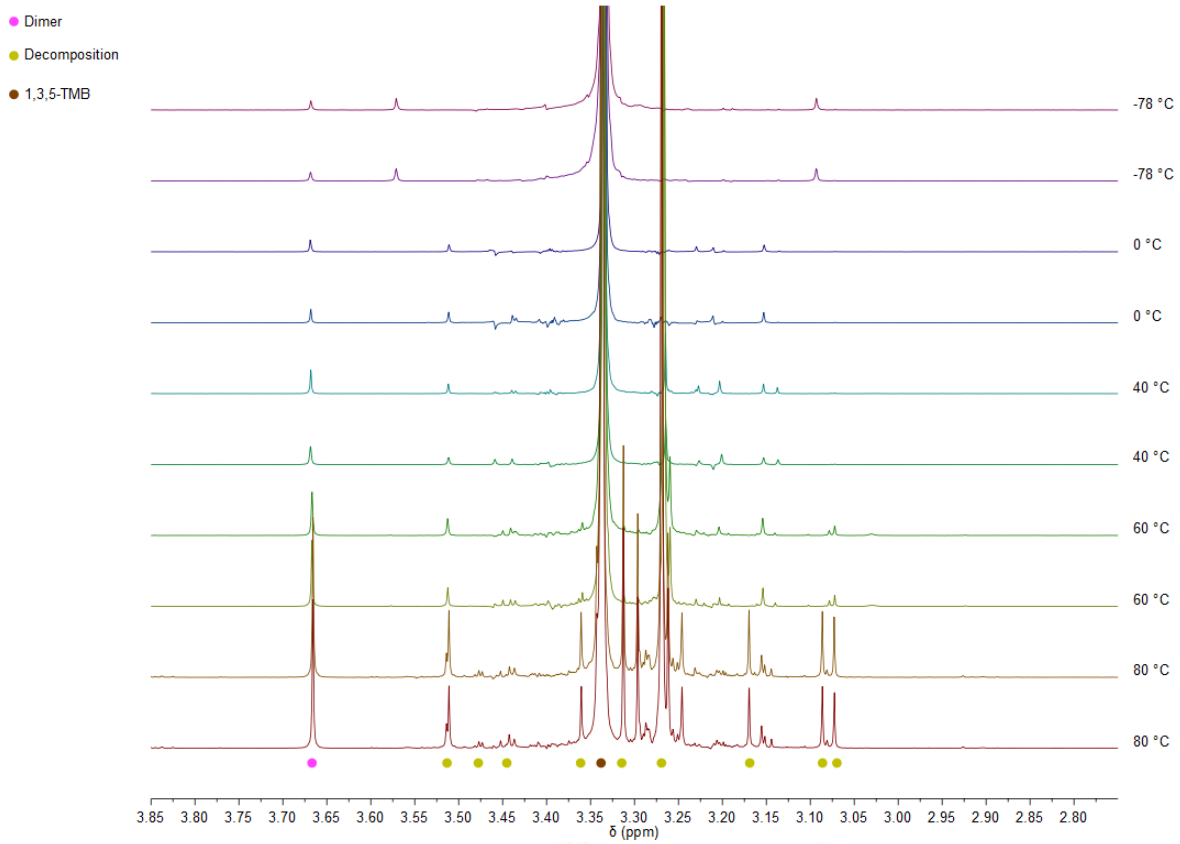


Figure S58. Temperature dependence of the background reaction (full spectrum & zoom-ins).



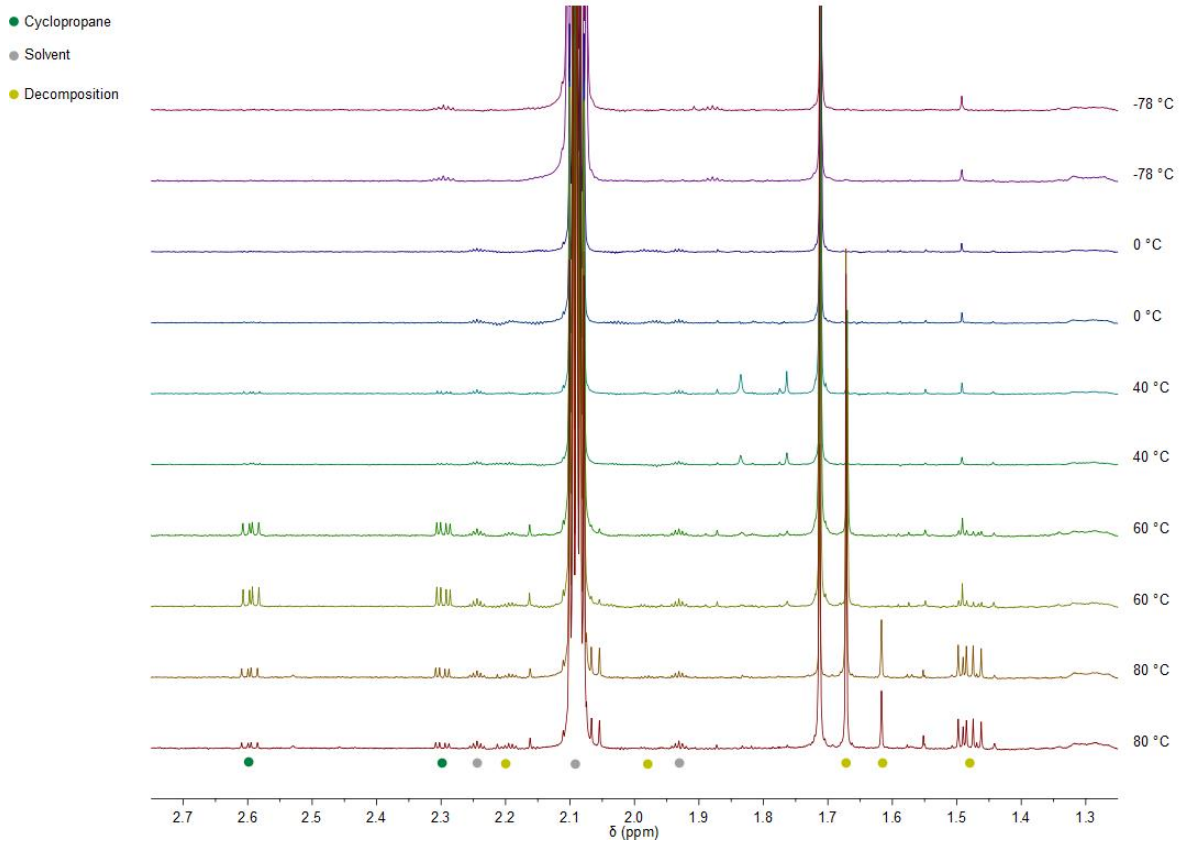


Figure S58, continued. Temperature dependence of the background reaction (full spectrum & zoom-ins).

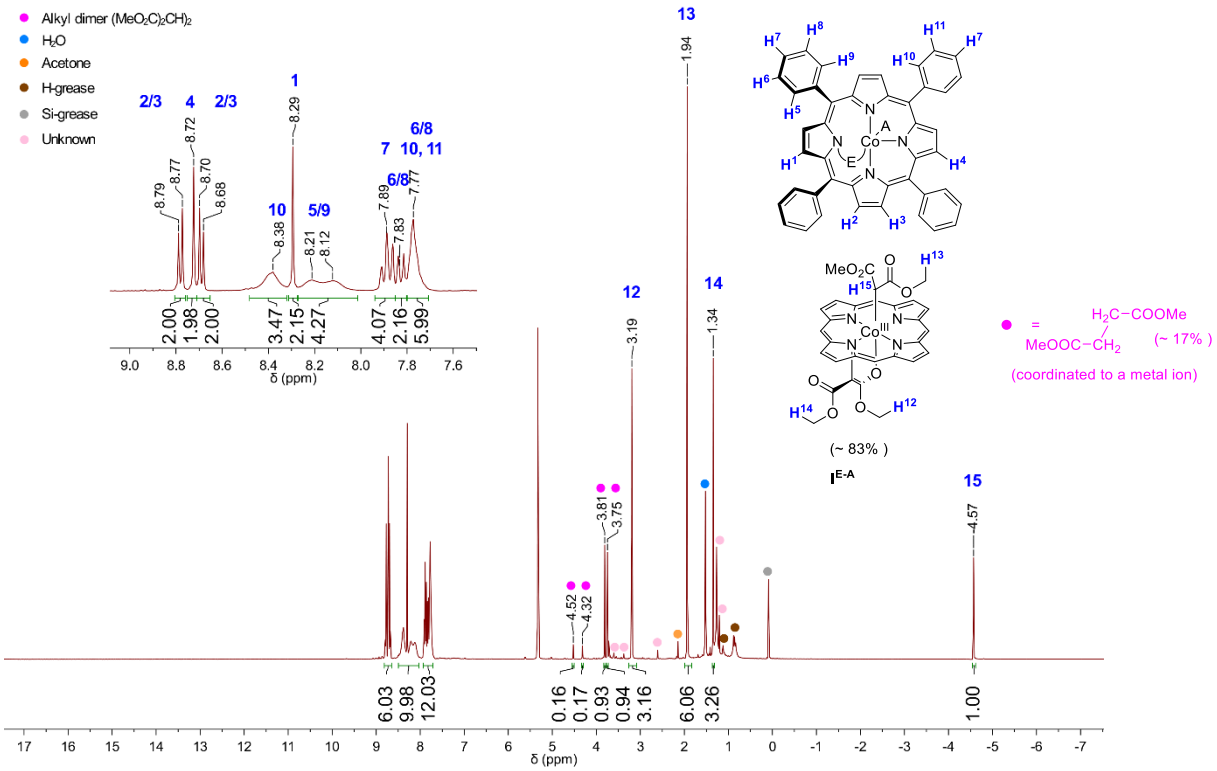


Figure S59. ^{1}H-NMR spectrum of $\mathbf{I}^{\mathbf{E\text{-}A}}$ in CD_2Cl_2.

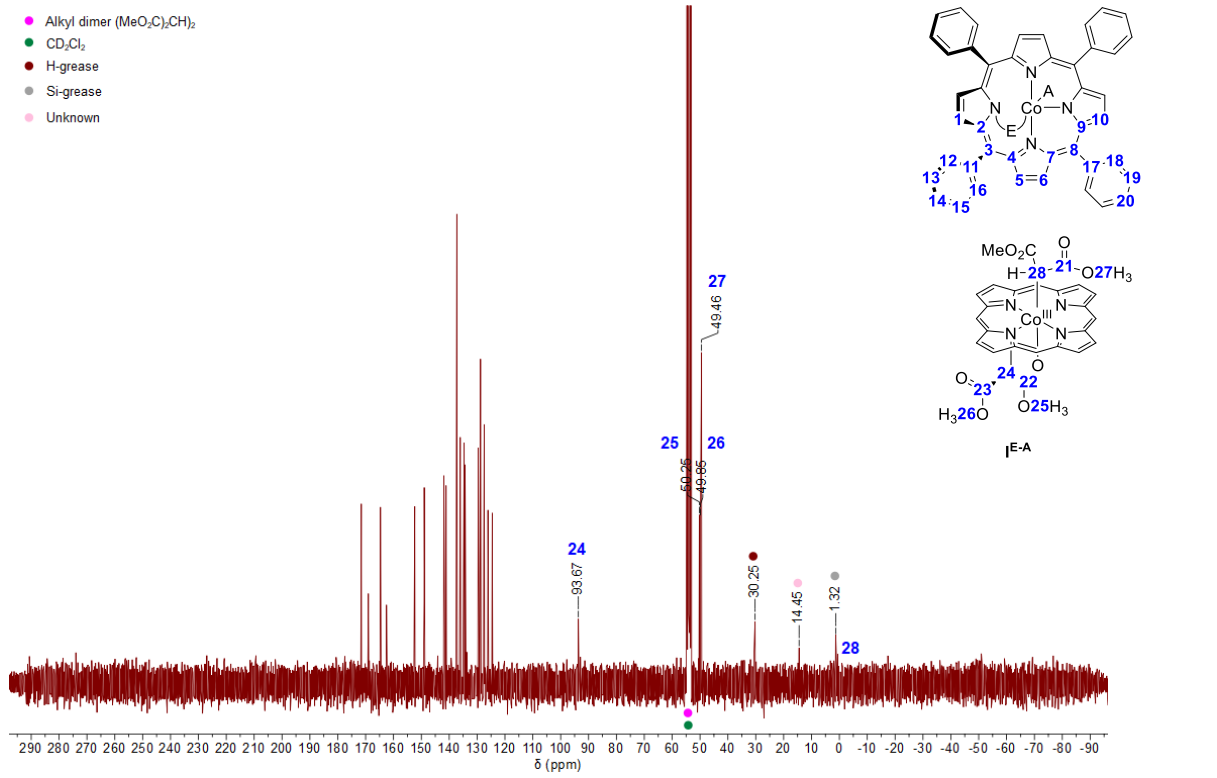


Figure S60. ^{13}C-NMR spectrum of $\mathbf{I}^{\mathbf{E\text{-}A}}$ in CD_2Cl_2.

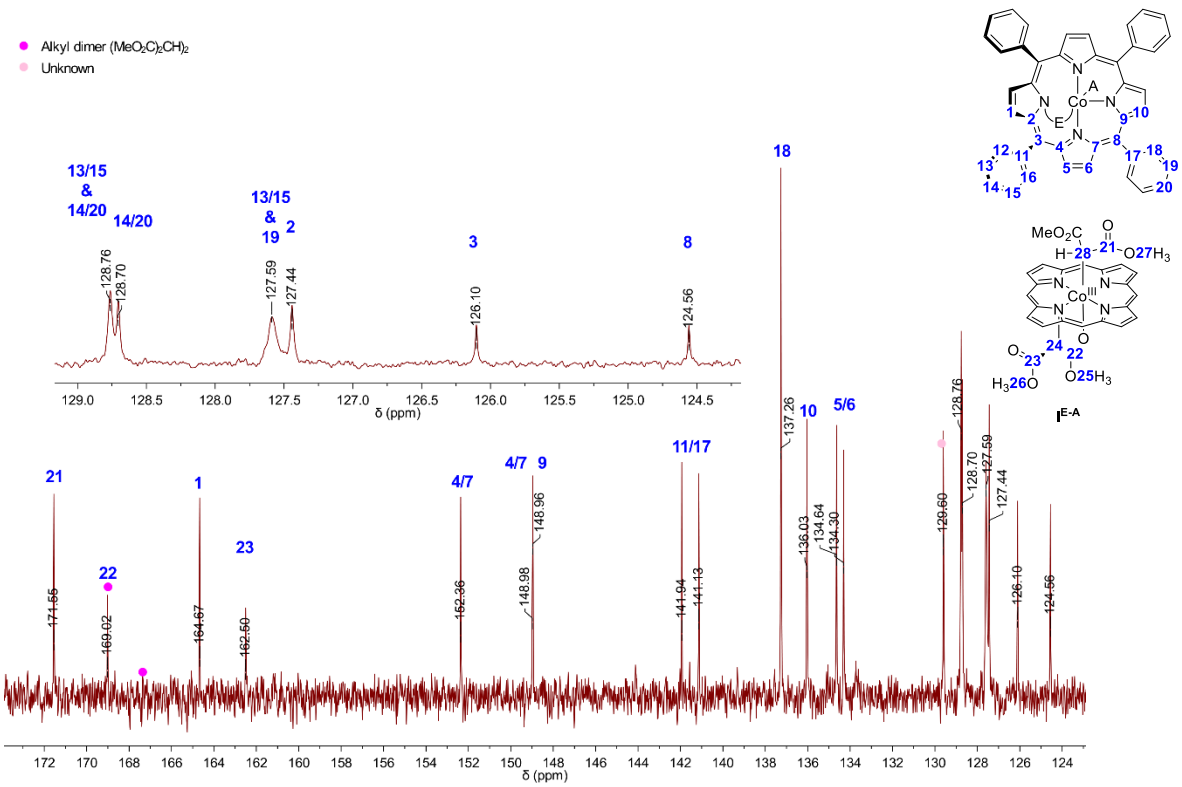


Figure S61. Zoom-in of ^{13}C-NMR spectrum of $\mathbf{I^{E-A}}$ in CD_2Cl_2.

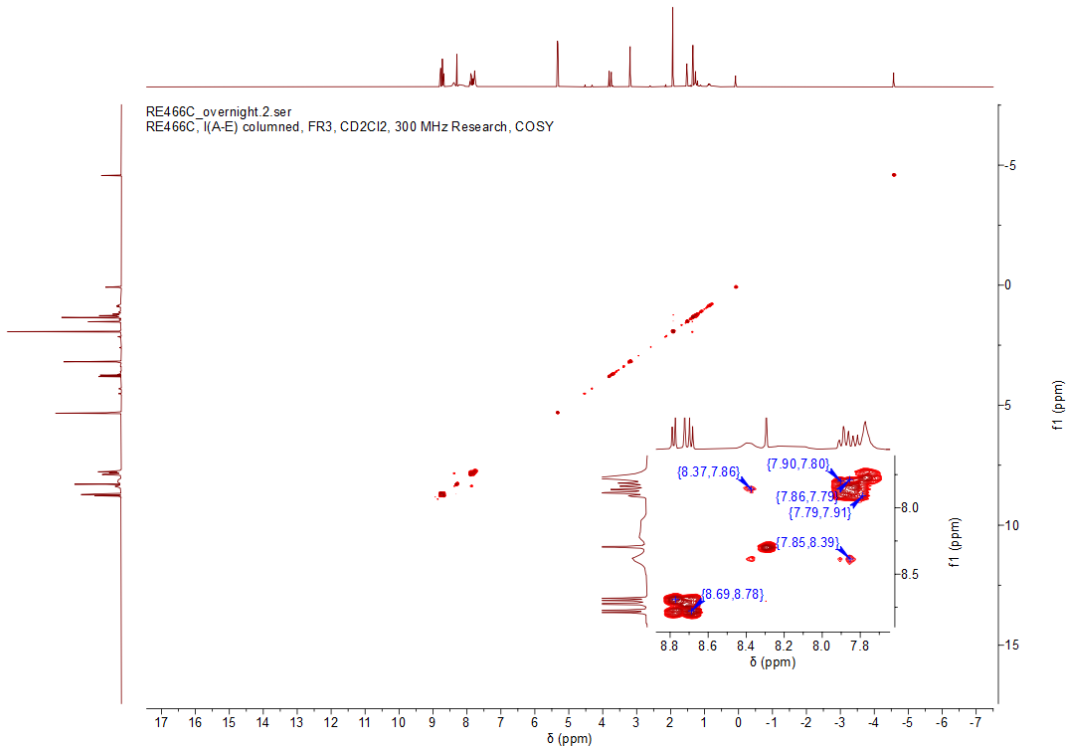


Figure S62. ^{1}H^{1}H-COSY NMR spectrum of $\mathbf{I^{E-A}}$ in CD_2Cl_2.

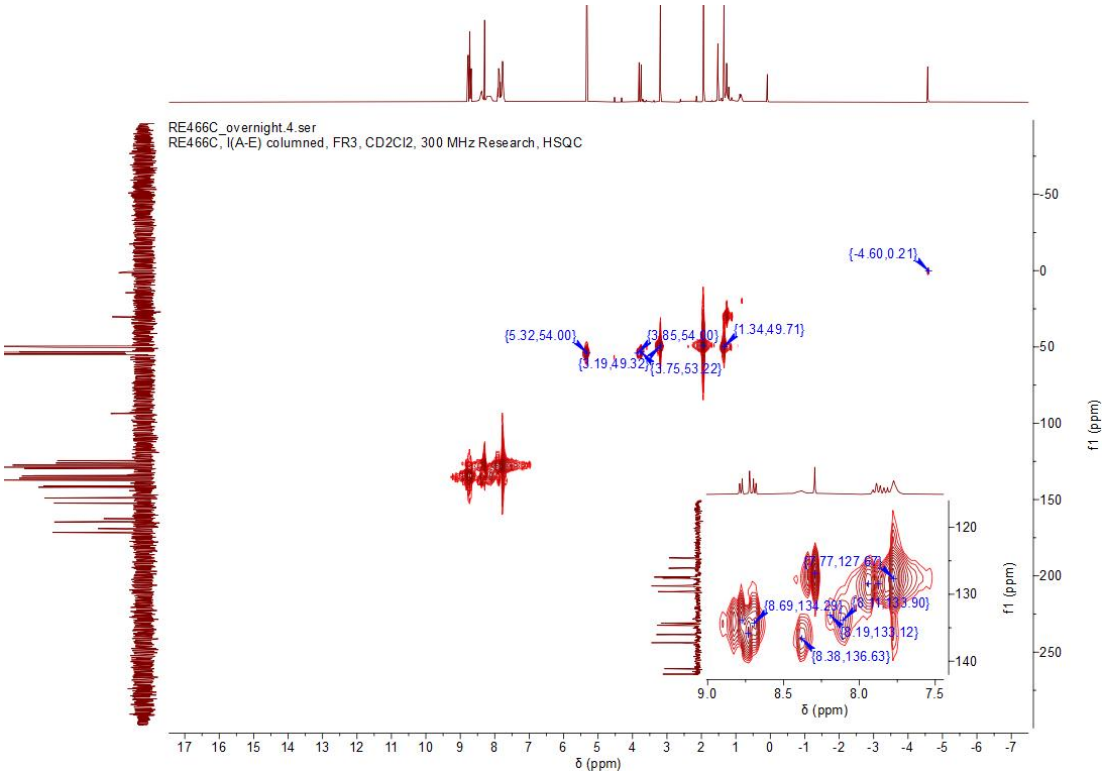


Figure S63. $^{1}H^{13}C$-HSQC NMR spectrum of $\mathbf{I^{E-A}}$ in CD_2Cl_2.

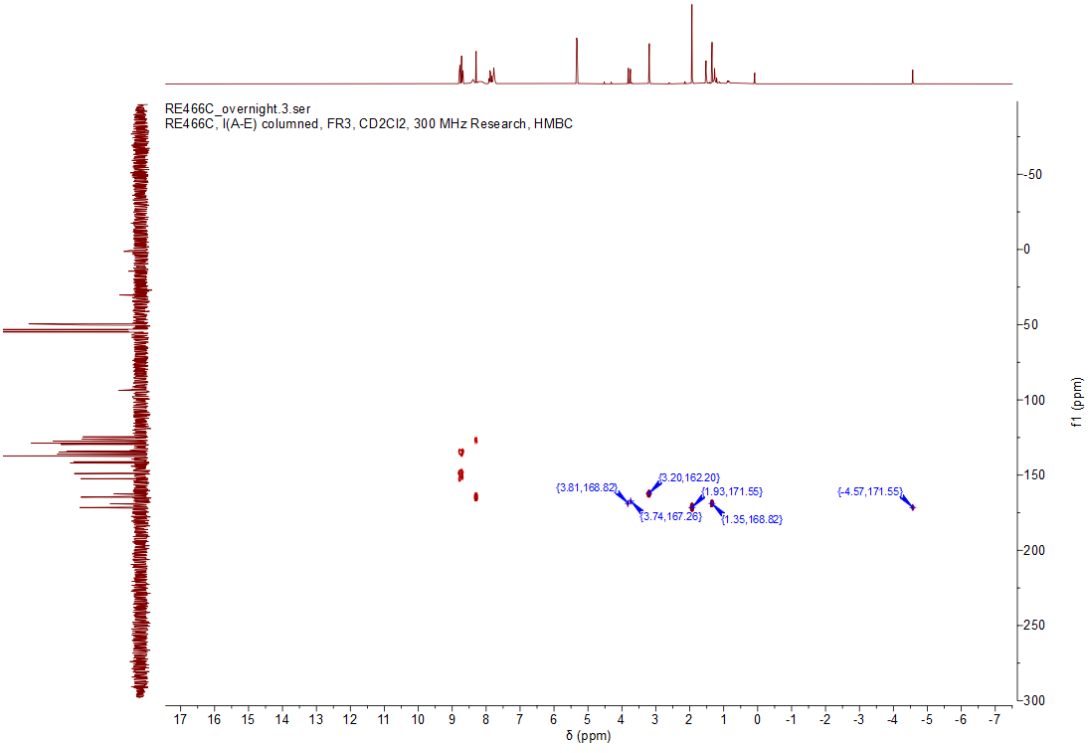


Figure S64. $^{1}H^{13}C$-HMBC NMR spectrum of $\mathbf{I^{E-A}}$ in CD_2Cl_2.

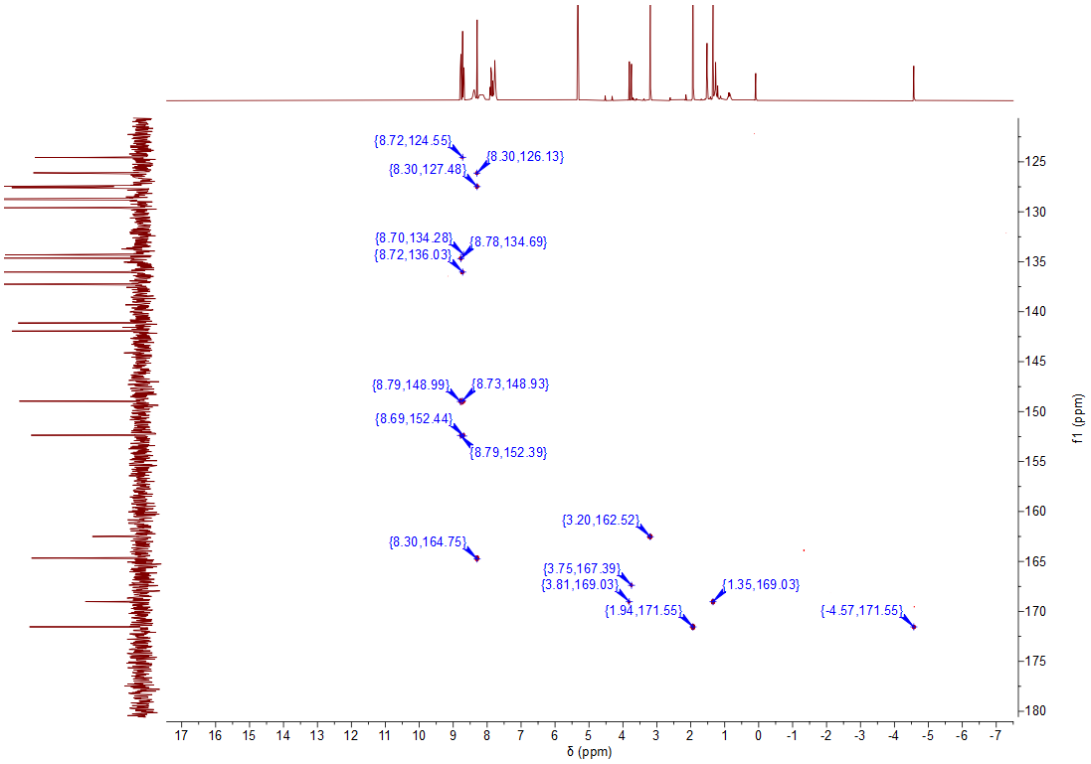


Figure S65. Zoom-in of $^{1}H^{13}C$-HMBC NMR spectrum of $\mathbf{I}^{\mathbf{E-A}}$ in CD_2Cl_2.

12. Density Functional Theory Calculations

Table S15. Calculated <s²> values, spin states and energies (in Hartree) of the reaction components.

Compound	Spin state	<s²>	SCF (Hartree)	ZPE correction (Hartree)	Enthalpy correction (Hartree)	Entropy correction (Hartree)	$\Delta G°_{298K}$ (Hartree)
Benzene	S = 0 [a]	-	−232.34386	0.09748	0.10296	0.06996	−232.27390
Toluene	S = 0 [a]	-	−271.67806	0.12397	0.13134	0.09225	−271.58581
Tolyl radical	S = ½	0.7662	−271.02744	0.11137	0.11816	0.08284	−270.94460
Styrene	S = 0 [a]	-	−309.77710	0.12925	0.13718	0.09746	−309.67964
Cyclopropane (**P**)	S = 0 [a]	-	−805.08864	0.24056	0.25827	0.19465	−804.89399
Iodobenzene	S = 0 [a]	-	−529.60482	0.08733	0.09431	0.05615	−529.54867
DMM•IY	S = 0 [a]	-	−1024.82718	0.19358	0.21212	0.14399	−1024.68319
N_2	S = 0 [a]	0.0000	−109.58042	0.00535	0.00866	−0.01373	−109.59415
DMM•N_2	S = 0 [a]	0.0000	−604.81956	0.11547	0.12831	0.07652	−604.74304
[Co(TPP)]	S = ½	0.7618	−3296.58022	0.58089	0.61935	0.51000	−3296.07022

[a] Closed-shell singlet

Table S16. Calculated <s²> values, spin states and energies (in Hartree) of the catalytic intermediates.

Compound	Spin state	<s²>	SCF (Hartree)	ZPE correction (Hartree)	Enthalpy correction (Hartree)	Entropy correction (Hartree)	$\Delta G°_{298K}$ (Hartree)
[Co(TPP)] *Mono*-Benzene (**[Co(TPP)]***)	S = ½	0.7627	−3528.95229	0.67960	0.72438	0.59955	−3528.35274
[Co(TPP)] *Bis*-Benzene (**[Co(TPP)]****)	S = ½	0.7634	−3761.32210	0.77825	0.82952	0.68883	−3760.63328
[Co(TPP)] *Mono* Iodonium Ylide (**I^{IY}**)	S = ½	0.7645	−4321.46088	0.77647	0.83367	0.68176	−4320.77911
[Co(TPP)] *Mono* Terminal Carbene (**I^{T}**)	S = ½	0.7556	−3791.85487	0.68738	0.73720	0.60049	−3791.25438
[Co(TPP)] *Mono* Benzene *Mono* Terminal Carbene (**I^{T*}**)	S = ½	0.7559	−4024.22493	0.78688	0.84274	0.69320	−4023.53172
[Co(TPP)] *Mono* Gamma Radical (**I^{G}**)	S = ½	0.7773	−4101.68419	0.82209	0.87856	0.72970	−4100.95449
[Co(TPP)] *Mono*-Iodonium Ylide *Mono*-Terminal Carbene (**I^{IY-T}**)	S = ½	0.7557	−4816.72588	0.88309	0.95177	0.77217	−4815.95372
[Co(TPP)] *Bis*-Terminal Carbene (**I^{T-T}**)	S = ½	0.8031	−4287.09624	0.79366	0.85504	0.69317	−4286.40306
[Co(TPP)] *Mono*-Bridged *Mono*-Terminal Carbene (**I^{B-T}**)	S = ½	0.7695	−4287.11683	0.79573	0.85603	0.69871	−4286.41812

[Co(TPP)] *Mono*-Enolate *Mono*-Terminal Carbene (**I$^{E–T}$**)	S = ½	0.7804	–4287.12549	0.79753	0.85709	0.70094	–4286.42455
[Co(TPP)] *Mono*-Enolate *Mono*-Gamma Radical (**I$^{E–G}$**)	S = ½	0.7649	–4596.94667	0.93139	0.99771	0.82968	–4596.11699
[Co(TPP)] *Mono* Enolate Adduct (**I^{E}**)	S = ½	0.7706	–3791.84445	0.68919	0.73789	0.60622	–3791.23823
[Co(TPP)] *Mono* Benzene *Mono* Enolate Adduct (**I^{E*}**)	S = ½	0.7707	–4024.21454	0.78804	0.84312	0.69677	–4023.51777
[Co(TPP)] *Mono*-Enolate *Mono*-Iodonium Ylide (**I$^{E–IY}$**)	S = ½	0.7695	–4816.71749	0.88511	0.95278	0.77730	–4815.94019
[Co(TPP)] *Mono* Bridging Carbene (**I^{B}**)	S = ½	0.7837	–3791.84280	0.68845	0.73759	0.60480	–3791.23800

Table S17. Calculated <s^2> values. spin states and energies (in Hartree) for bridging intermediates in deactivation pathways.

Compound	**Spin state**	**<s^2>**	**SCF (Hartree)**	**ZPE correction (Hartree)**	**Enthalpy correction (Hartree)**	**Entropy correction (Hartree)**	**ΔG°$_{298K}$ (Hartree)**
[Co(TPP)] *Bis-cis*-Bridged Carbene (***c*-I$^{B–B}$**)	S = ½	0.7624	–4287.09470	0.79505	0.85500	0.69837	–4286.39633
[Co(TPP)] *Bis-trans*-Bridged Carbene (***t*-I$^{B–B}$**)	S = ½	0.7955	–4287.10873	0.79662	0.85634	0.70071	–4286.40803
[Co(TPP)] *cis-Mono*-Bridged *Mono*-Enolate Carbene (***c*-I$^{B–E}$**)	S = ½	0.8776	–4287.10621	0.79724	0.85631	0.70401	–4286.40220
[Co(TPP)] *trans-Mono*-Bridged *Mono*-Enolate Carbene (***t*-I$^{B–E}$**)	S = ½	0.7804	–4287.11964	0.79785	0.85683	0.70458	–4286.41507
[Co(TPP)] *cis-Bis*-Enolate Adduct (***c*-I$^{E–E}$**)	S = ½	0.7681	–4287.12707	0.79864	0.85721	0.70548	–4286.42159
[Co(TPP)] *trans-Bis*-Enolate Adduct (***t*-I$^{E–E}$**)	S = ½	0.7677	–4287.12124	0.79909	0.85773	0.70503	–4286.41621

Table S18. Calculated <s^2> values, spin states and energies (in Hartree) for intermediates in HAT deactivation pathways.

Compound	**Spin state**	**<s^2>**	**SCF (Hartree)**	**ZPE correction (Hartree)**	**Enthalpy correction (Hartree)**	**Entropy correction (Hartree)**	**ΔG°$_{298K}$ (Hartree)**
[Co(TPP)] *Mono* Terminal Carbene Toluene Adduct (**I$^{T–Tol}$**)	S = ½	0.7557	–4063.55605	0.81442	0.87143	0.72222	–4062.83383
[Co(TPP)] *Mono* Alkyl Adduct (**I^{A}**)	S = 0 [a]	0.0000	–3791.84445	0.68919	0.73789	0.60622	–3791.23823
[Co(TPP)] *Mono* Alkyl Tolyl Radical Adduct (**I$^{A–Tol·}$**)	S = ½	0.7658	–4063.55918	0.81422	0.87087	0.72176	–4062.83742

[Co(TPP)] *Mono* Alkyl *Mono* Iodonium Ylide (**I^{A-IY}**)	S = 0 [a]	0.0000	– 4817.38396	0.89588	0.96452	0.78464	– 4816.59932
[Co(TPP)] *Bis*-Terminal Carbene Toluene Adduct (**I$^{T-T-Tol}$**)	S = ½	0.8035	– 4558.79356	0.91987	0.98899	0.81004	– 4557.98352
[Co(TPP)] *Mono*-Alkyl *Mono*-Terminal Carbene (**I^{A-T}**)	S = 0 [a]	0.0000	– 4287.76033	0.80727	0.86777	0.71181	– 4287.04851
[Co(TPP)] *Mono*-Alkyl *Mono*-Terminal Carbene Tolyl Radical (**I$^{A-T-Tol\cdot}$**)	S = ½	0.8079	– 4558.80645	0.92001	0.98830	0.81391	– 4557.99253
[Co(TPP)] *Mono*-Bridged *Mono*-Terminal Carbene Toluene Adduct (**I$^{B-T-Tol}$**)	S = ½	0.7693	– 4558.81499	0.92153	0.98981	0.81335	– 4558.00164
[Co(TPP)] *Mono*-Alkyl *Mono*-Bridged Carbene (**I^{A-B}**)	S = 0 [a]	0.0000	– 4287.77544	0.80893	0.86902	0.71245	– 4287.06299
[Co(TPP)] *Mono*-Alkyl *Mono*-Bridged Carbene Tolyl Radical (**I$^{A-B-Tol\cdot}$**)	S = ½	0.7659	– 4558.82219	0.92181	0.98958	0.81529	– 4558.00691
[Co(TPP)] *Mono*-Enolate *Mono*-Terminal Carbene Toluene Adduct (**I$^{E-T-Tol}$**)	S = ½	0.7715	– 4558.82531	0.92451	0.99133	0.82221	– 4558.00309
[Co(TPP)] *Mono*-Alkyl *Mono*-Enolate Adduct (**I^{E-A}**)	S = 0 [a]	0.0000	– 4287.78710	0.81041	0.86967	0.71672	– 4287.07038
[Co(TPP)] *Mono*-Alkyl *Mono*-Enolate Adduct Tolyl Radical (**I$^{E-A-Tol\cdot}$**)	S = ½	0.7657	– 4558.83110	0.92330	0.99013	0.81977	– 4558.01133

[a] Closed-shell singlet

Table S19. Calculated $<s^2>$ values, spin states and energies (in Hartree) for relevant diazo adducts.

Compound	**Spin state**	**$<s^2>$**	**SCF (Hartree)**	**ZPE correction (Hartree)**	**Enthalpy correction (Hartree)**	**Entropy correction (Hartree)**	**$\Delta G°_{298K}$ (Hartree)**
[Co(TPP)] Diazo Adduct (**I^{D}**)	S = ½	0.7619	–3901.43755	0.69762	0.74970	0.60930	–3900.82825
[Co(TPP)] *Mono*-Diazo *Mono*-Terminal Carbene Adduct (**I^{D-T}**)	S = ½	0.7558	–4396.71034	0.80504	0.86812	0.70230	–4396.00804
[Co(TPP)] *Mono*-Diazo *Mono*-Enolate Adduct (**I^{D-E}**)	S = ½	0.7735	–4396.70176	0.80651	0.86840	0.70906	–4395.99270

Table S20. Calculated <s^2> values, spin states and energies (in Hartree) for quartet state (S = 3/2) intermediates in the Bis-carbene cycle.

Compound	Spin state	<s^2>	SCF (Hartree)	ZPE correction (Hartree)	Enthalpy correction (Hartree)	Entropy correction (Hartree)	$\Delta G°_{298K}$ (Hartree)
[Co(TPP)] *Mono*-Enolate *Mono*-Terminal Carbene (**I^{E-T}**) (S = 3/2)	S = 3/2	3.7780	–4287.09552	0.79549	0.85530	0.69942	–4286.39609
[Co(TPP)] *Mono*-Enolate *Mono*-Gamma Radical (**I^{E-G}**) (S = 3/2)	S = 3/2	3.8175	–4596.09527	0.92931	0.99638	0.82543	–4596.09527
[Co(TPP)] Enolate (**I^{E}**) (S = 3/2)	S = 3/2	3.7637	3791.82726	0.68757	0.73683	0.60333	–3791.22393
[Co(TPP)] *Mono*-Enolate *Mono*-Iodonium Ylide (**I^{E-IY}**) (S = 3/2)	S =3/2	3.7649	–4816.70193	0.88316	0.95142	0.77433	–4815.92760

Table S21. Calculated <s^2> values, spin states and energies (in Hartree) for various coordination modes of DMM·IY and DMM·N_2.

Compound	Spin state	<s^2>	SCF (Hartree)	ZPE correction (Hartree)	Enthalpy correction (Hartree)	Entropy correction (Hartree)	$\Delta G°_{298K}$ (Hartree)
[Co(TPP)] *Mono* Iodonium Ylide Carbonyl Adduct (**I$^{IY(C=O)}$**)	S = ½	0.7668	–4321.45764	0.77621	0.83350	0.68014	–4320.77750
[Co(TPP)] *Mono* Iodonium Ylide Methoxy Adduct (**I$^{IY(C-OMe)}$**)	S = ½	0.7636	–4321.45487	0.77623	0.83364	0.67957	–4320.77530
[Co(TPP)] *Mono* Iodonium Ylide Iodine Adduct (**I$^{IY(IPh)}$**)	S = ½	0.7610	–4321.45288	0.77629	0.83372	0.68159	–4320.77129
[Co(TPP)] *Mono* Diazo Carbonyl Adduct (**I$^{D(C=O)}$**)	S = ½	0.7641	–3901.43555	0.69808	0.74959	0.61165	–3900.82931
[Co(TPP)] *Mono* Diazo Methoxy Adduct (**I$^{D(C-OMe)}$**)	S = ½	0.7630	–3901.43579	0.69817	0.74981	0.61157	–3900.82423
[Co(TPP)] *Mono* Diazo Nitrogen Adduct (**I$^{D(C=N=N)}$**)	S = ½	0.7652	–3901.43514	0.69773	0.74952	0.61059	–3900.82455

Table S22. Calculated <s^2> values, spin states and energies (in Hartree) for all transition states.

Compound	Spin state	<s^2>	SCF (Hartree)	ZPE correction (Hartree)	Enthalpy correction (Hartree)	Entropy correction (Hartree)	$\Delta G°_{298K}$ (Hartree)	Negative eigenvalue (cm^{-1})
TS1 (I^{IY}-I^{T})	S = ½	0.7670	–4321.45358	0.77521	0.83197	0.68057	–4320.77300	–129.72
TS2 (I^{T}-I^{G})	S = ½	0.7680	–4101.64695	0.81903	0.87580	0.72616	–4100.92079	–272.73
TS3 (I^{G}-**P**)	S = ½	0.8100	–4101.68212	0.82178	0.87780	0.73008	–4100.95204	–207.72
TS4 (I^{IY-T}-I^{T-T})	S = ½	0.7661	–4816.71357	0.88254	0.95020	0.77491	–4815.93866	–48.94
TS5 (I^{T-T}-I^{B-T})	S = ½	0.7570	–4287.08448	0.79364	0.85386	0.69499	–4286.38949	–102.92
TS6 (I^{B-T}-I^{E-T})	S = ½	0.7586	–4287.08940	0.79487	0.85420	0.70055	–4286.38885	–83.31
TS7 (I^{E-T}-I^{E-G})	S = ½	0.7906	–4596.90575	0.92912	0.99554	0.82676	–4596.07899	–228.19
TS8 (I^{E-G}-**P**)	S = ½	0.8005	–4596.93877	0.93034	0.99665	0.82799	–4596.11078	–243.27
TS9 (I^{E-IY}-I^{E-T})	S = ½	0.7780	–4816.71348	0.88451	0.95188	0.77774	–4815.93574	None
TS10 (I^{B}-I^{E})	S = ½	0.7734	–3791.80607	0.68729	0.73582	0.60455	–3791.20152	–88.64
TS11 (I^{T}-I^{B})	S = ½	0.7617	–3791.82393	0.68675	0.73561	0.60328	–3791.22065	–376.97
TS12 (I^{E-T}-I^{E-G}) (Q)	S = ½	3.7891	–4596.87548	0.92600	0.99334	0.81956	–4596.05592	–342.97
TS13 (I^{E-G}-**P**) (Q)	S = ½	3.8356	–4596.92028	0.92901	0.99543	0.82648	–4596.09380	–337.33
TS14 (I^{E-IY}-I^{E-T}) (Q)	S = ½	3.8134	–4816.68943	0.88228	0.94979	0.77597	–4815.91346	–60.94
TS15 (I^{B-T}-***c***-I^{B-B})	S = ½	0.8043	–4287.08464	0.79429	0.85394	0.69823	–4286.38641	–61.92
TS16 (I^{B-T}-***t***-I^{B-B})	S = ½	0.7686	–4287.08811	0.79482	0.85441	0.69864	–4286.38948	–135.71
TS17 (***c***-I^{B-B}-***c***-I^{B-E})	S = ½	0.8542	–4287.08066	0.79510	0.85415	0.70108	–4286.37958	–109.18
TS18 (***t***-I^{B-B}-***t***-I^{B-E})	S = ½	0.7946	–4287.06893	0.79573	0.85478	0.70091	–4286.36803	–399.99
TS19 (***c***-I^{B-E}-***c***-I^{E-E})	S = ½	0.8773	–4287.08409	0.79593	0.85452	0.70368	–4286.38041	–327.69
TS20 (***t***-I^{B-E}-***t***-I^{E-E})	S = ½	0.8063	–4287.07787	0.79580	0.85459	0.70246	–4286.38172	–129.72
TS21 (I^{E-T}-***c***-I^{B-E})	S = ½	0.7752	–4287.08418	0.79580	0.85459	0.70246	–4286.38172	–272.73
TS22 (I^{E-T}-***t***-I^{B-E})	S = ½	0.7648	–4287.10222	0.79619	0.85518	0.70193	–4286.40029	–207.72
TS23 (I^{T}-I^{A})	S = ½	0.7588	–4063.53134	0.80845	0.86499	0.71329	–4062.81805	–1487.84
TS24 (I^{T-T}-I^{A-T})	S = ½	0.7772	–4558.78486	0.91660	0.98392	0.81051	–4557.97435	–409.45
TS25 (I^{B-T}-I^{A-B})	S = ½	0.8816	–4558.79939	0.91702	0.98381	0.81383	–4557.98556	–1078.77
TS26 (I^{E-T}-I^{A-E})	S = ½	0.7674	–4558.80093	0.91935	0.98515	0.81826	–4557.98267	–1499.9
TS27 (I^{A-IY}-I^{A-T})	S = 0 [(a)]	0.0000	–4817.37433	0.89593	0.96343	0.78827	–4816.58606	–64.33
TS28 (I^{A-T}-I^{A-B})	S = 0 [(a)]	0.0000	–4287.75106	0.80666	0.86643	0.71136	–4287.03969	–230.46
TS29 (I^{A-B}-I^{E-A})	S = 0 [(a)]	0.0000	–4287.74165	0.80750	0.86661	0.71428	–4287.02736	–105.16
TS30 (I^{D}-I^{T})	S = ½	0.7738	–3901.40841	0.69443	0.74621	0.60670	–3900.80171	–409.89
TS31 (I^{D-T}-I^{T-T})	S = ½	0.7680	–4396.66012	0.80115	0.86411	0.70129	–4395.95884	–351.79
TS32 (I^{D-E}-I^{E-T})	S = ½	0.7787	–4396.66670	0.80512	0.86595	0.71108	–4395.95562	–378.5

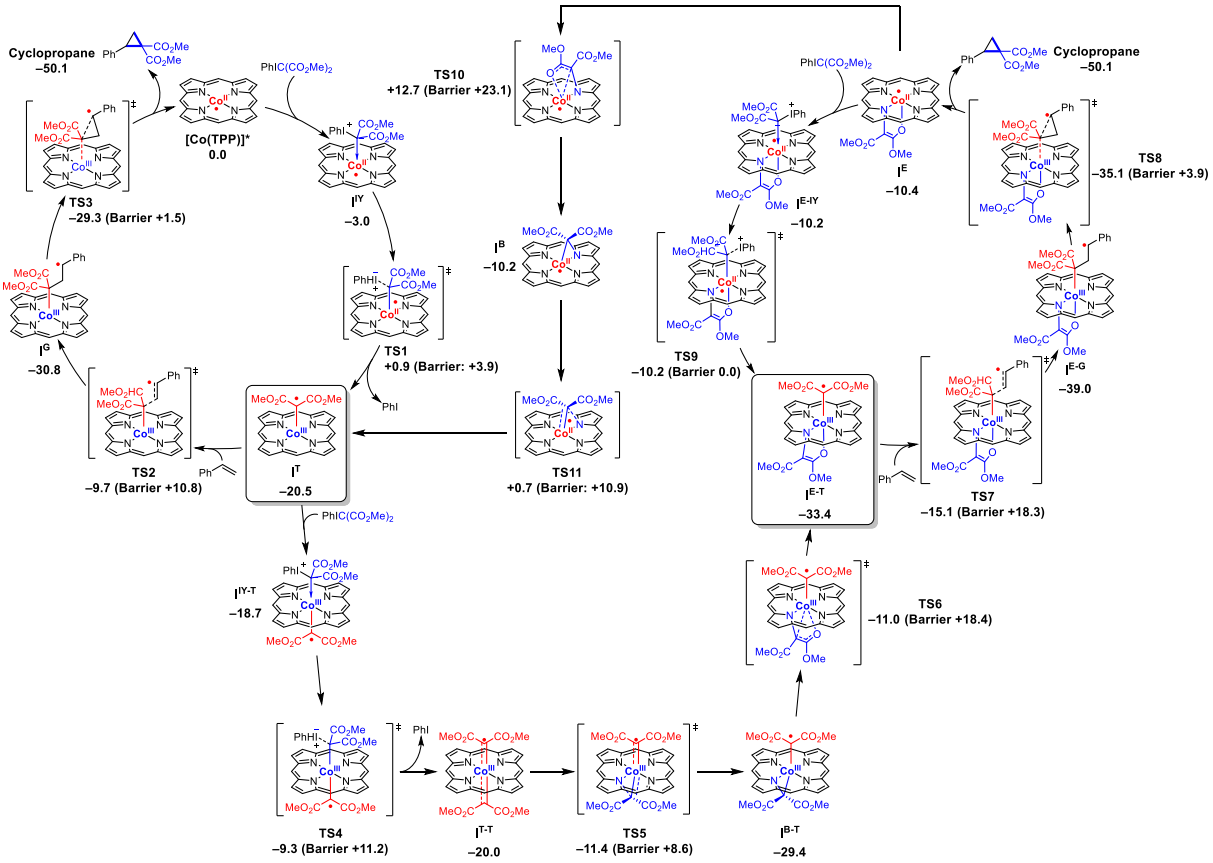
[(a)] Closed-shell singlet

Table S23. Calculated $<s^2>$ values, spin states, energies (in Hartree) and C=O stretch vibrations (in cm^{-1}) for metal-carbene complexes with pendant ester groups.

Compound	Spin State	$<s^2>$	SCF (Hartree)	ZPE correction (Hartree)	Enthalpy correction (Hartree)	Entropy correction (Hartree)	$\Delta G°_{298K}$ (Hartree)	C=O stretch (cm^{-1})
Co(Acacen)(Cl)($CHCO_2Et$)	S = 1	2.0126	–4147.83810	0.78515	0.84302	0.68897	–4147.14913	1601.6
Co(Acacen)(MeIm)($CHCO_2Et$)	S = ½	0.7564	–3953.26879	0.88365	0.94594	0.78323	–3952.48556	1604.1
Co(Salen)(I)($CHCO_2Et$)	S = 1	2.0120	–2982.90935	0.42071	0.45085	0.36012	–2982.54923	1580.0
Co(Salen(MeIm)($CHCO_2Et$)	S = ½	0.7557	–2950.72245	0.51844	0.55305	0.45277	–2950.26968	1582.1
Cu(Box)($CHCO_2Et$)	S = 0 [a]	0.0000	–2834.21122	0.50909	0.54165	0.44630	–2833.76492	1623.8
Ru(PyBox)($CHCO_2Et$)	S = 0 [a]	0.0000	–2259.87951	0.44287	0.47607	0.37954	–2259.49997	1664.2

[a] Closed-shell singlet.

Detailed description of the DFT-calculated catalytic mechanism



Scheme S9. Full catalytic cycle for the [Co(TPP)]-catalyzed reaction of DMM•IY and styrene. Free energies ($\Delta G°_{298K}$ in kcal·mol^{-1}) are reported relative to the *mono*- and *bis*-benzene adducts of [Co(TPP)] for 5- and 6-coordinate species, respectively. All calculations were performed at the BP86/def2-TZVP/disp3 (m4-grid) level of theory at the doublet spin surface (S = ½). Phenyl rings of the TPP ligand omitted for clarity.

To gain further insight into the mechanism of the metalloradical–catalyzed cyclopropanation of styrene with iodonium ylides we turned to density functional theory calculations. Reaction pathway calculations were performed at the BP86/def2-TZVP level of theory, using Grimme's D3 dispersion corrections ('zero' damping) at the doublet spin surface. This method has been properly benchmarked against experimental data for cobalt(II)-porphyrin systems.[43,44,45,46] Benzene adducts were used as reference points to correct for otherwise uncompensated dispersion interactions between the catalyst and the solvent (see page S3-S4). Reported energies are standard free energies at 298 K ($\Delta G°_{298K}$ in kcal·mol^{-1}). Based on the experimental results described in the main text and above, we envisioned two possible catalytic pathways: a "*mono*-carbene cycle" in which *mono*-carbene radical complex **I^{T}** is the key intermediate, and a "*bis*-carbene cycle" in which *N*-enolate–carbene radical **I^{E-T}** is the key carbene transfer intermediate. **[Co(TPP)]*** (the energetic reference point in Scheme S9) reacts with the iodonium ylide carbene precursor DMM•IY in order to generate the *mono*-iodonium ylide adduct **I^{IY}** in a slightly exergonic fashion ($\Delta G°$ = −3.0 kcal·mol^{-1}). Extrusion of iodobenzene occurs readily in **TS1** with a very low relative free energy barrier of only +3.9 kcal·mol^{-1}. Formation of the thus generated *mono*-terminal carbene **I^{T}** is significantly exergonic ($\Delta G°$ = −20.5 kcal·mol^{-1}). Addition of styrene to **I^{T}** proceeds in a stepwise fashion via **TS2** ($\Delta\Delta G‡$ = +10.8 kcal·mol^{-1}) to form the *mono*-γ-radical **I^{G}** ($\Delta G°$ = +30.8 kcal·mol^{-1}). Intermediate **I^{G}** subsequently proceeds to form the cyclopropane product **1** ($\Delta G°$ = +50.1 kcal·mol^{-1}) via an almost barrierless transition state **TS3** ($\Delta G‡$ = +1.5 kcal·mol^{-1}). This step is best described as a radical rebound reaction involving radical-attack on the cobalt-

carbon σ*-orbital leading to homolytic cleavage of the Co–C bond to produce the cyclopropane and regenerate **[Co(TPP)]***.

To ascertain the correct pathway towards the *mono*-enolate–*mono*-terminal carbene radical $\mathbf{I^{E-T}}$ on the basis of DFT, all possible *mono*- and *bis*-carbene structures involving terminal- or bridging carbenes or enolate adducts were considered (see Tables S16–S22). The *mono*-terminal carbene species $\mathbf{I^{T}}$ was found to be lower in energy ($\Delta G°$ = –20.5 kcal·mol^{-1}) than all other conceivable "*mono*–carbene species", including the *mono*–bridged carbene $\mathbf{I^{B}}$ ($\Delta G°$ = –10.2 kcal·mol^{-1}), the *mono*–enolate adduct $\mathbf{I^{E}}$ ($\Delta G°$ = –10.4 kcal·mol^{-1}) and the *mono*-iodonium ylide adduct $\mathbf{I^{IY}}$ ($\Delta G°$ = –3.0 kcal·mol^{-1}). The *mono*-terminal-carbene species $\mathbf{I^{T}}$ is also the starting point to enter into the "*bis*–carbene" cycle. Binding of a second molecule of DMM•IY to $\mathbf{I^{T}}$ to form $\mathbf{I^{IY-T}}$ ($\Delta G°$ = –18.7 kcal·mol^{-1}) is slightly endergonic ($\Delta\Delta G^{\circ}$ = +1.8 kcal·mol^{-1}). Subsequent iodobenzene extrusion to form $\mathbf{I^{T-T}}$ ($\Delta G°$ = –20.0 kcal·mol^{-1}) is slightly exergonic ($\Delta\Delta G^{\circ}$ = –1.3 kcal·mol^{-1}) and has a low **TS4** barrier ($\Delta G^{‡}$ = +11.2 kcal·mol^{-1}). Nucleophilic attack of a pyrrolic nitrogen onto one of the carbenes of $\mathbf{I^{T-T}}$ to afford *mono*-bridged-*mono*-terminal carbene radical $\mathbf{I^{B-T}}$ ($\Delta G°$ = –29.4 kcal·mol^{-1}) via **TS5** is again a low barrier process ($\Delta\Delta G^{‡}$ = +8.6 kcal·mol^{-1}). Subsequent breaking of the Co–C bond concomitant with coordination of the ester carbonyl group to the metal to form the *mono*-enolate-*mono*-terminal carbene radical $\mathbf{I^{E-T}}$ ($\Delta G°$ = –33.4 kcal·mol^{-1}) is exergonic ($\Delta\Delta G^{\circ}$ = –4.0 kcal·mol^{-1}). While this process has a significant **TS6** barrier ($\Delta G^{‡}$ = +18.4 kcal·mol^{-1}), this transition state is still readily accessible at RT, in good agreement with the experimental data (vide supra). Complex $\mathbf{I^{E-T}}$ is also thermodynamically most favorable among all conceivable "*bis*-carbene" complexes.

The *mono*-enolate-*mono*-terminal carbene radical complex $\mathbf{I^{E-T}}$ is the key carbene transfer intermediate in the "*bis*-carbene cycle". This cycle starts with the exergonic addition of styrene to $\mathbf{I^{E-T}}$ ($\Delta\Delta G°$ = –5.6 kcal·mol^{-1}) via **TS7** ($\Delta G^{‡}$ = +18.3 kcal·mol^{-1}) to generate the *N*-enolate-γ-radical $\mathbf{I^{E-G}}$. Similar to the *mono*-carbene cycle, $\mathbf{I^{E-G}}$ releases cyclopropane **1** ($\Delta G°$ = –50.1 kcal·mol^{-1}) via a low barrier (**TS8**: $\Delta G^{‡}$ = +3.9 kcal·mol^{-1}) and overall exergonic ($\Delta\Delta G°$ = –50.1 – 10.45 + 39.0 = –21.5 kcal·mol^{-1}) radical rebound step. This generates the *mono*-enolate adduct $\mathbf{I^{E}}$, which was experimentally detected. Subsequently, another equivalent of DMM•IY coordinates to $\mathbf{I^{E}}$ to afford *mono*-enolate-*mono*-iodonium ylide $\mathbf{I^{E-IY}}$ in an essentially thermoneutral reaction ($\Delta\Delta G°$ = +0.02 kcal·mol^{-1}). The latter proceeds to complete the "*bis*-carbene" cycle, regenerating $\mathbf{I^{E-T}}$ via barrierless release of iodobenzene in **TS9**.

The "*bis*-carbene cycle" is (re)connected to the "*mono*-carbene cycle" via intramolecular rearrangement of the *N*-enolate adduct $\mathbf{I^{E}}$ in **TS10** to the *mono*-bridging-carbene $\mathbf{I^{B}}$, followed by conversion of $\mathbf{I^{B}}$ to *mono*-terminal carbene radical $\mathbf{I^{T}}$ via **TS11**. The highest barrier of this process (**TS10**: $\Delta\Delta G^{‡}$ = +23.1 kcal·mol^{-1}) is readily accessible at RT, but should be relatively slow. It is in fact the highest barrier of the entire catalytic double–cycle, which directly explains why $\mathbf{I^{E}}$ is detectable with EPR in trapping experiments (Figure S13).

The barrier for styrene addition to the *mono*-carbene $\mathbf{I^{T}}$ is substantially lower than the barrier for styrene addition to the *N*-enolate-carbene radical $\mathbf{I^{E-T}}$ (+10.8 vs. +18.3 kcal·mol^{-1}). Conversely, activation of the iodonium ylide is barrierless for the "*bis*-carbene cycle", whereas this has a small barrier in the "*mono*-carbene cycle". Since styrene addition in **TS2** and **TS7** is the rate–determining step for both cycles, the "*mono*-carbene cycle" should be faster than the "*bis*-carbene cycle". Since the ylide is much less soluble than styrene, this implies that the *mono*-carbene cycle must be the dominant catalytic pathway under reaction conditions where all components are present before adding the catalyst. Experimentally, this is indeed what we observed, because $\mathbf{I^{T}}$ is detected as the resting state (Figure S12) when adding the catalyst to the premixed reagents.

However, formation of $\mathbf{I^{E-T}}$ from *mono*-carbene radical $\mathbf{I^{T}}$ is competitive with styrene addition to $\mathbf{I^{T}}$ at equimolar concentrations (+11.2 vs. +10.8 kcal·mol^{-1}), and hence both cycles are expected to be relevant. Experimentally we observed that in absence of styrene the reaction proceeds cleanly to $\mathbf{I^{E-T}}$ at RT, and the "*bis*-carbene cycle" is clearly connected to the "*mono*-carbene cycle" on the basis

of single turnover reactions and EPR measurements shown in Figure S12 & Figure S13. While accessible at RT, the computed barrier for formation of $\mathbf{I^T}$ from $\mathbf{I^E}$ is relatively high though (Scheme S9). Hence, in the presence of enough iodonium ylide DMM•IY the reaction should be largely trapped in the "*bis*-carbene cycle". Experimental detection of $\mathbf{I^E}$ with EPR spectroscopy for a reaction carried out by adding the reagents in the order {*(1)* DMM•IY, *(2)* [Co(TPP)], *(3)* styrene} (Figure S15) confirms this. The low solubility of DMM•IY has a significant influence on the (relative) rates though. Unfortunately this also prevents reliable kinetic studies to determine condition dependent kinetic reaction orders to gain more experimental information about the relative importance of the "*mono*-carbene" and "*bis*-carbene" cycles.

Experimentally, the reaction between [Co(TPP)] and DMM•IY proceeds cleanly towards $\mathbf{I^{E\text{-}T}}$ without detectable amounts of $\mathbf{I^T}$ (Figure S16). Computationally, the barrier for formation of $\mathbf{I^T}$ is lower than the barrier for formation of $\mathbf{I^{E\text{-}T}}$ (although both are very low), thus suggesting that $\mathbf{I^T}$ should be detectable in titrations. This apparent discrepancy can be explained by the heterogeneous nature of the reaction mixture (see Figure S20). Moreover, hypervalent iodine reagents are known to form polymeric/oligomeric linear $I^+–X^-$ chains,[47] and as such rapid and selective formation of "*bis*-carbene" species $\mathbf{I^{E\text{-}T}}$ may well be the result of a high local concentration of ylide leading to rapid conversion of $\mathbf{I^T}$ to $\mathbf{I^{E\text{-}T}}$.

Calculated UV/Vis spectra of catalytic intermediates (TD-DFT)

TD-DFT calculations were performed according to the procedure described in the general considerations. The free catalyst [Co(TPP)], the *N*-enolate-carbene radical $\mathbf{I}^{\mathbf{E\text{-}T}}$ and the *N*-enolate-alkyl species $\mathbf{I}^{\mathbf{E\text{-}A}}$ were calculated and are compared to the experimentally obtained UV/Vis spectra in Figure S66. The *mono*-terminal carbene $\mathbf{I}^{\mathbf{T}}$ was also computed, but does not match any of the observed experimental UV/Vis data. The closed-shell diamagnetic alkyl species $\mathbf{I}^{\mathbf{E\text{-}A}}$ best matches the computed values for the Soret peak at 456 (calc.) vs. 455 (exp.). The calculated Q-band features at 611 and 633 were not recorded in CH_2Cl_2 due to time window limitations, but similar features can be observed in the C_6H_6 and toluene spectra (Figure S17 & Figure S18). Two features in the calculated UV/Vis region at 336 and 385 nm are not experimentally observed, but are likely obscured by the broad absorption band. The [Co(TPP)] calculated values are in good agreement with the experimentally found values for the Soret peak at 410 nm (calc. 403 nm) and Q-band at 528 nm (calc. 533 nm). The calculated spectrum for carbene radical $\mathbf{I}^{\mathbf{E\text{-}T}}$ exhibits similar features as the experimental spectrum at comparable relative intensities. A weak transition can be found at near UV-wavelengths at 358 nm (calc. 380 nm), a red-shifted Soret peak at 429 nm (calc. 449 nm) and a significantly red-shifted weak Q-band at 600 nm (calc. 611 nm).

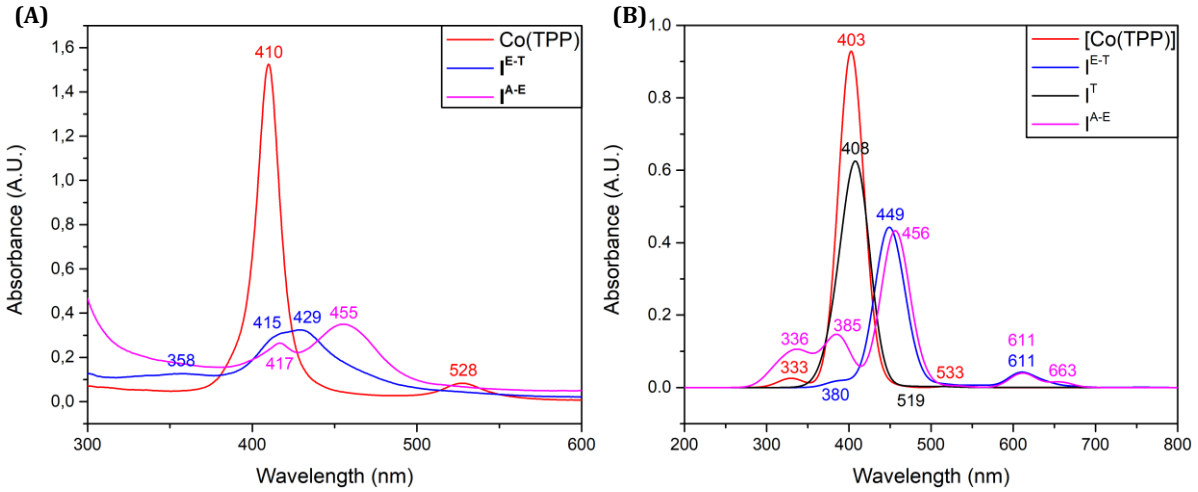


Figure S66. Graphical comparison of (A) experimentally obtained UV/Vis spectra (solvent: CH_2Cl_2) and (B) calculated spectra obtained with TD-DFT for [Co(TPP)] (red), $\mathbf{I}^{\mathbf{E\text{-}T}}$ (blue), $\mathbf{I}^{\mathbf{E\text{-}A}}$ (purple) and $\mathbf{I}^{\mathbf{T}}$ (black).

Complete Active Space Self Consistent Field (CASSCF) calculations:

All CASSCF and subsequent NEVPT2-corrected calculations were performed according to the procedure described in the general considerations. Energies are reported for the NEVPT2-corrected calculations in kcal·mol^{-1} in absolute values and relative to the ground spin state. States and their corresponding occupancies are ordered based on their relative contributions to the overall wavefunction. Orbitals were considered to be inactive on the basis of an occupance above 1.990 or below 0.010 and their preservation in the active space. Assigments are based on a Löwdin population analysis in combination with visual inspection using IboView.

[Co(TPP)]: CAS(13,10)
For comparison to the reaction intermediates, NEVPT2-corrected CASSCF calculations were performed for the free [Co(TPP)] catalyst. Since this complex has a well-established experimental doublet (S = ½) spin state,[48] only the doublet state was calculated for this system. [Co(TPP)] was found to have almost no multireference character (Table S24), which is in accordance with reported data.[48] As visualized in Figure S67, all metal d-orbitals were found to be correlated as were the four Gouterman porphyrin orbitals. The occupied a_{1u} and a_{2u} states were found to be non-degenerate as opposed to the free base [H_2(TPP)],[49] whereas the vacant e_g states are degenerate. As expected, the SOMO of the molecule is the Co(d_{z2}) orbital and the vacant metal-d orbital is the antibonding Co(d_{x2-y2}) in the porphyrin plane. The other metal d-orbitals were found to have an occupancy close to 2.00.

Table S24. Energies in kcal·mol^{-1} for the doublet spin state for [Co(TPP)] obtained with NEVPT2-CASSCF(13,10) calculations and the respective contribution of each state to the overall wavefunction.

Multiplicity	Energy (kcal·mol^{-1})	Relative energy (kcal·mol^{-1})	Contribution	State
2 (Doublet)	**–3290.55586516591**	**0.0**	**0.88809**	**2222221000**
			0.02874	2222111110
			0.00847	2222201200
			0.00847	2222201020
			0.00823	2202221002
			0.00823	2022221002
			0.00716	2211221011
			0.00716	2121221101
			0.00589	2222021200
			0.00589	2222021020
			0.00437	0222221002
			0.00414	2112222001

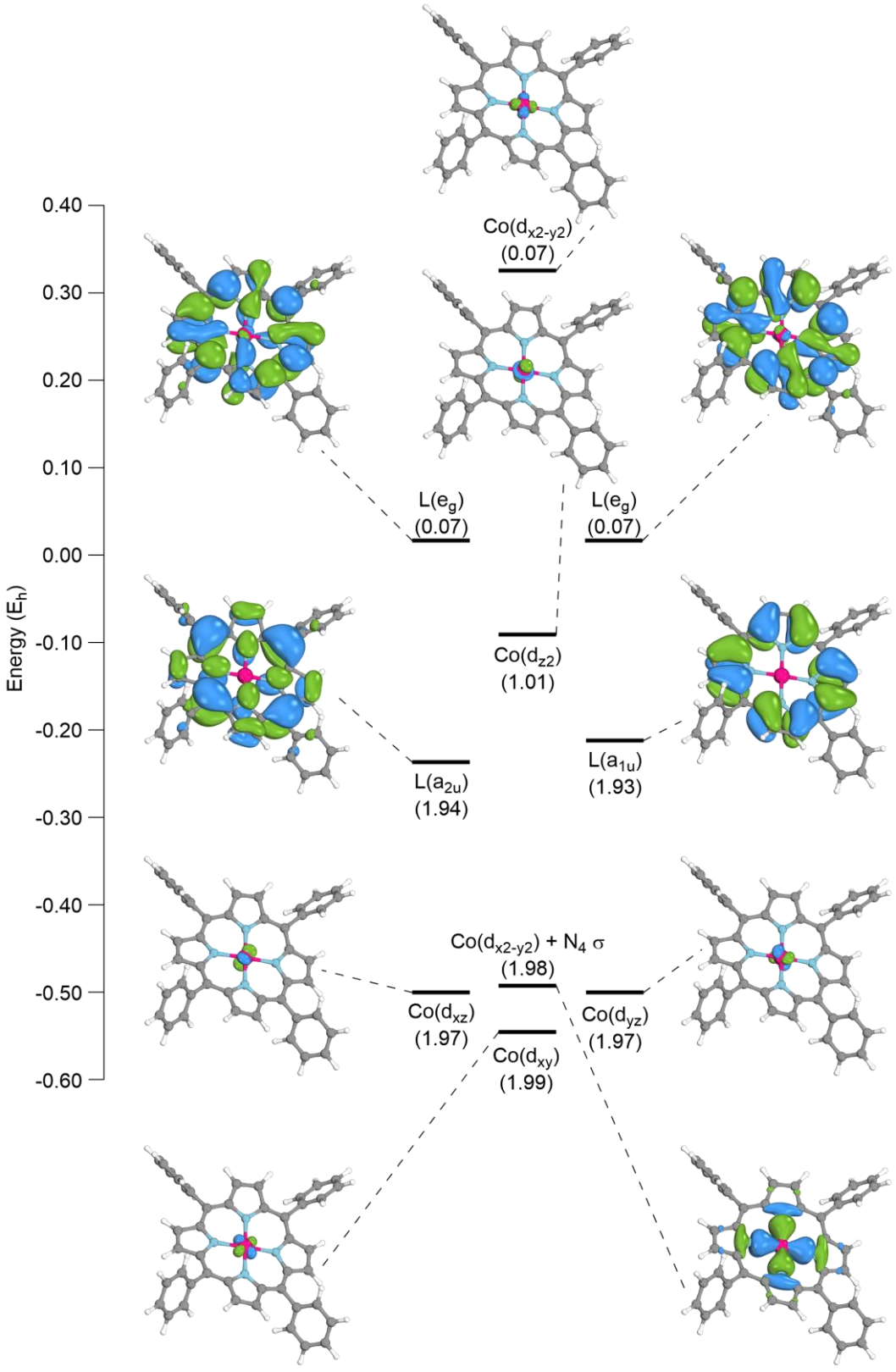


Figure S67. Energy diagram of the canonical molecular orbitals for the doublet spin state of [Co(TPP)] obtained with NEVPT2-CASSCF(13,10) calculations. Energies are in Hartree units. Occupancies depicted between parentheses. Isosurface set at 80.0 and generated using IboView.

***Mono*-Enolate Species $\mathbf{I^E}$:** CAS(13,10)

NEVPT2-corrected CASSCF(13,10) calculations show for the *mono*-enolate adduct $\mathbf{I^E}$ that all metal d–orbitals are correlated as well as the four Gouterman porphyrin orbitals. The MO centered on the *N*–enolate moiety was found to be entirely uncorrelated as well as any σ- or π- bonding interactions of the axial oxygen ligand. Furthermore, these calculations show that the doublet spin state (S = ½) is the spin ground state (Table S25). However, in contrast to [Co(TPP)], the quartet spin state (S = 3/2) is only +1.2 kcal·mol^{-1} higher in energy, despite the fact that neither spin state has significant multireference character. For the doublet state, when considering the symmetry of the porphyrin orbitals (Figure S68), the occupied a_{1u} and a_{2u}-orbitals are virtually degenerate whereas the vacant e_g-orbitals are split up. The e_g-orbitals are also lower in energy with respect to those in [Co(TPP)]. This is due to a decrease of symmetry of $\mathbf{I^E}$ with respect to [Co(TPP)]. Additionally, due to the axial carbonyl ligand, the Co(d_{z2}) is raised in energy. The remaining metal d-orbitals paint a similar picture as observed for [Co(TPP)]. Interestingly, when considering the quartet state, the Co(d_{yz}) is raised significantly in energy whereas the Co(d_{x2-y2}) is lowered significantly and both are singly occupied. In line with DFT calculations (Table S33), the spin density of the complex in the doublet spin state is concentrated almost entirely on cobalt, despite low lying vacant porphyrin orbitals. This purely cobalt-centered spin state change is in line with other high-spin Co(II)-tetraarylporphyrins.[50] We ascribe this to intermixing of the Co(d_{yz}) and Co(d_{x2-y2})-orbitals with the porphyrin LUMO orbitals in the quartet state, lowering the respective energy of the metal d-orbitals. Consequently, the antibonding interaction of the Co(d_{x2-y2}) AO with the N_4 σ LGO has a higher contribution of the N_4 σ LGO as a result of the lowering of the Co(d_{x2-y2}) orbital. The remaining metal d-orbitals and bonding Gouterman orbitals change only little in their energy and overall wavefunction (Figure S68). The active space was not conserved in the sextet spin state and as such as was not calculated.

Table S25. Energies in kcal·mol^{-1} for the doublet and quartet spin states for $\mathbf{I^E}$ obtained with NEVPT2-CASSCF(13,10) calculations and the respective contribution of each state to the overall wavefunction.

Multiplicity	Energy (kcal·mol^{-1})	Relative energy (kcal·mol^{-1})	Contribution	State
2 (Doublet)	**–2374948.883**	**0.0**	**0.86015**	**2222221000**
			0.02968	2222111110
			0.01831	2222220010
			0.00972	2022221002
			0.00940	2202221002
			0.00902	2222021200
			0.00808	2222201020
			0.00741	2222201200
			0.00711	2211221101
			0.00589	2222021020
			0.00453	0222221002
			0.00269	2212121101
4 (Quartet)	–2374947.647	+1.2	0.75765	2222211100
			0.06389	2222211001
			0.02802	2221111111
			0.02529	2112222100
			0.01344	1122222100
			0.01301	2222201110
			0.01046	1222211200
			0.00906	2220211120
			0.00801	2222011102
			0.00756	2221212100
			0.00714	2222011120
			0.00670	2212211200
			0.00642	2222210101
			0.00480	2220211102
			0.00339	2222121100
			0.00275	1222211101

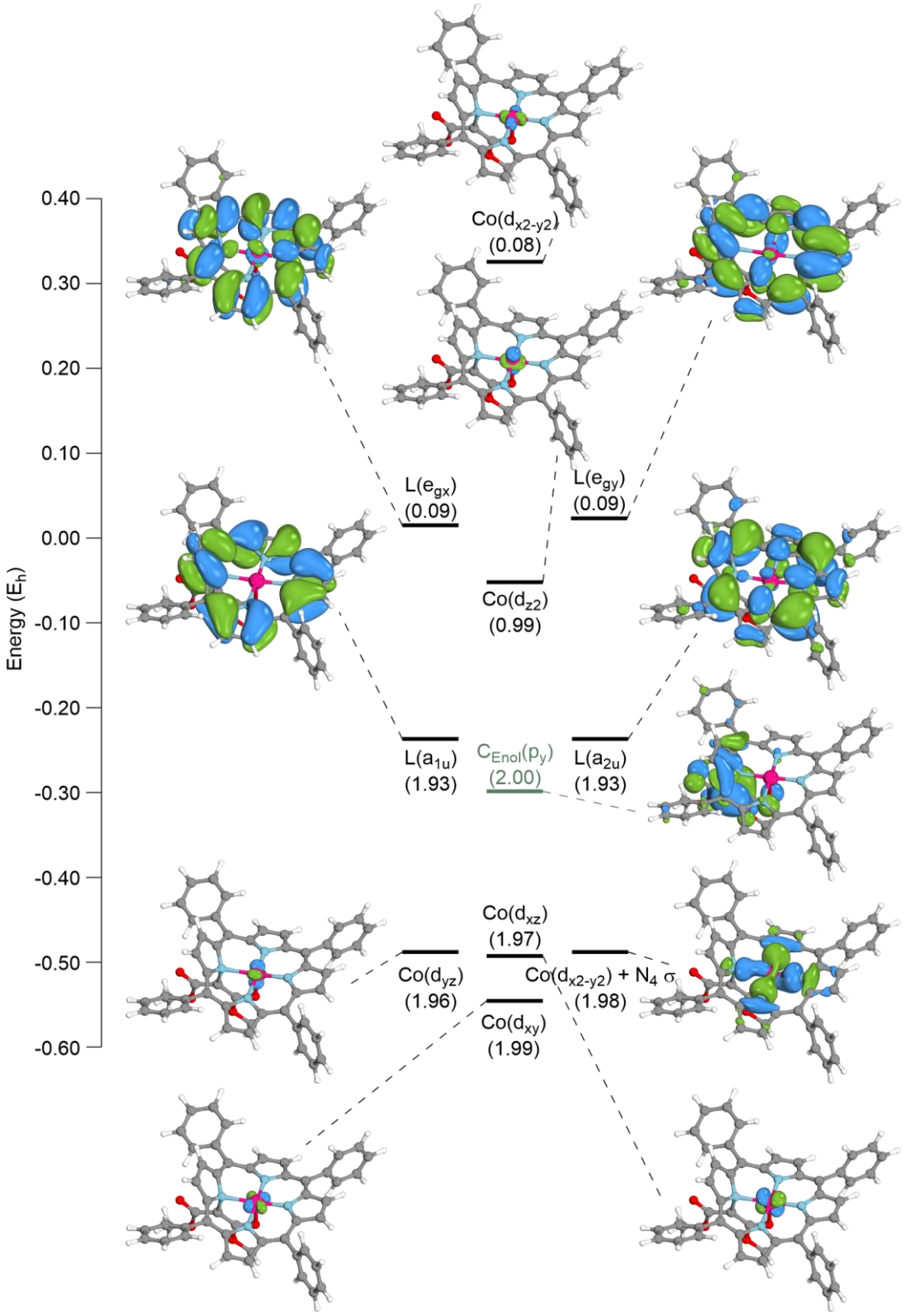


Figure S68. Energy diagram of the canonical molecular orbitals for the doublet spin state (S = ½) of **I^{E}** obtained with NEVPT2-CASSCF(13,10) calculations. Inactive orbitals are depicted in green. For clarity, the non-active MO of the enolate moiety is also visualized. Despite the breaking of degeneracy for the e_g-orbitals, the labeling is kept for clarity in comparison to unfunctionalized porphyrins. Energies are in Hartree units. Occupancies depicted between parentheses. Isosurface set at 80.0 and generated using IboView.

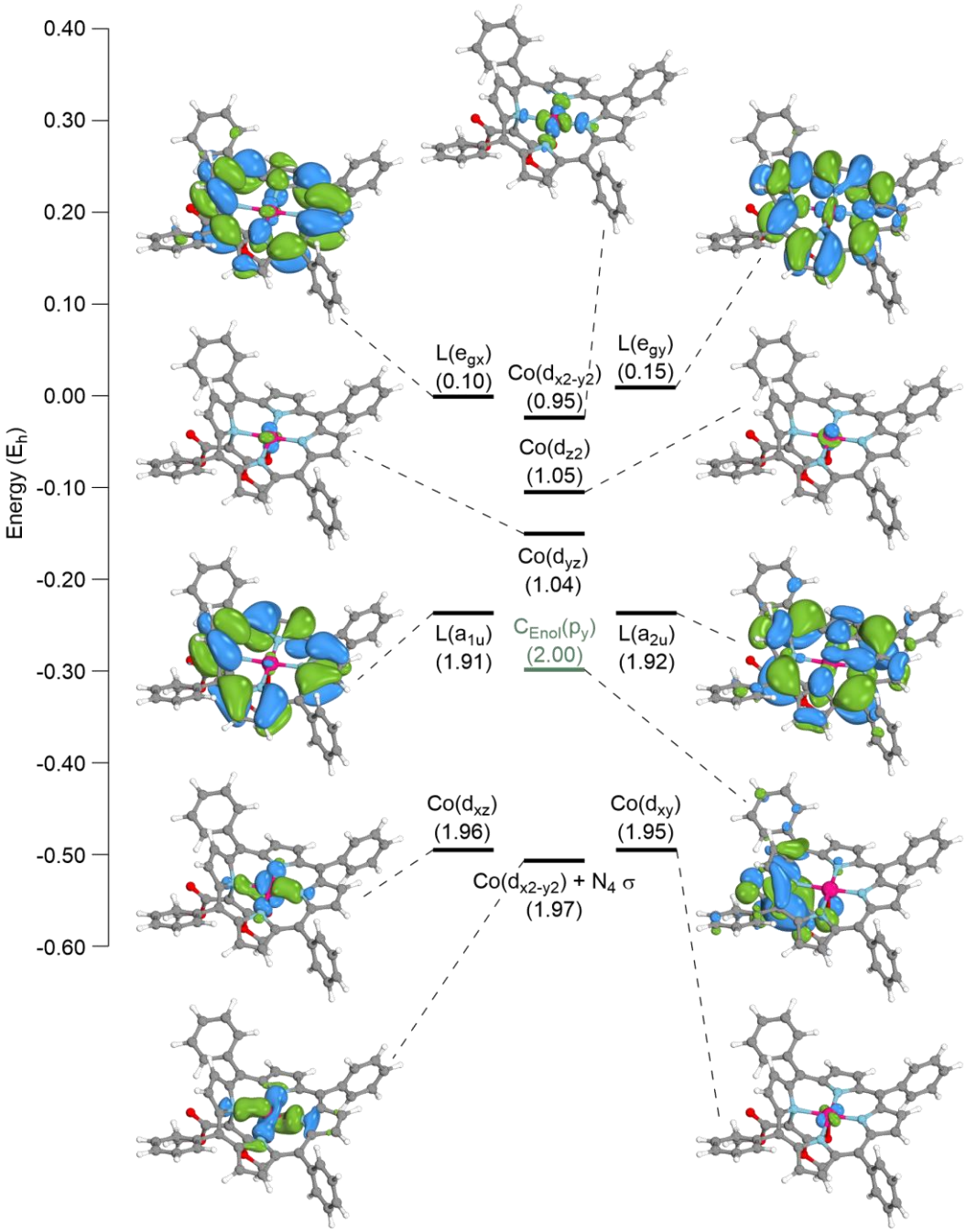


Figure S69. Energy diagram of the canonical molecular orbitals for the quartet spin state (S = 3/2) of **I^{E}** obtained with NEVPT2-CASSCF(13,10) calculations. Inactive orbitals are depicted in green. For clarity, the non-active MO of the enolate moiety is also visualized. Despite the breaking of degeneracy for the e_g-orbitals, the labeling is kept for clarity in comparison to unfunctionalized porphyrins. Energies are in Hartree units. Occupancies depicted between parentheses. Isosurface set at 80.0 and generated using IboView.

***Mono*-Terminal Carbene Radical Species I^T:** CAS(11,10)

In line with X-band EPR measurements, the *mono*-terminal carbene $\mathbf{I^T}$ was found to have negligible multireference character and the doublet spin state (S = ½) was found to be the ground state according to the NEVPT2-CASSCF(11,10) calculations. The quartet state (S = 3/2) is significantly higher in energy at +32.9 kcal·mol^{-1} relative to the ground state (Table S26). The Co(d_{yz})-orbital turned out to be uncorrelated. Apart from that, all other metal d-orbitals, the four Gouterman porphyrin orbitals and the carbene C(p_z) and C(p_x)-orbitals were found to be correlated (Figure S70). When considering the MOs, the Gouterman porphyrin orbitals are almost identical to those in the [Co(TPP)] complex, showing that the additional carbene moiety has little effect on the orbitals of the TPP ligand. The SOMO is located almost entirely on the carbene C(p_x) orbital (90.4%), with only a small component of the Co(d_{xz})-orbital (5.7%). This is more extreme than DFT predicts (based on QROs), with 77.6% electron density on the carbene and 17.3% on cobalt. The Co(d_{z2}) is raised significantly above the porphyrin e_g-orbitals, in line with the strong-field properties of the carbene radical ligand. However, the Co(d_{x2-y2}) remains the highest in energy. These results match closely to the previously reported NEVPT2-CASSCF results obtained for the [Co(TPP)(CHCOOEt] carbene radical complex.[51]

Table S26. Energies in kcal·mol^{-1} for the doublet, quartet and sextet spin states for $\mathbf{I^T}$ obtained with NEVPT2-CASSCF(11,10) calculations and the respective contribution of each state to the overall wavefunction.

Multiplicity	Energy (kcal·mol^{-1})	Relative energy (kcal·mol^{-1})	Contribution	Occupancy
2 (Doublet)	**–2374949.034**	**0.0**	**0.81910**	**2222210000**
			0.04515	2202210020
			0.02792	2221111100
			0.02030	2212210010
			0.00961	2222012000
			0.00912	2222010200
			0.00898	2112220010
			0.00782	2022210002
			0.00764	2122210001
			0.00595	2220212000
			0.00502	0222210002
			0.00493	2220210200
			0.00316	2211210020
4 (Quartet)	–2374916.134	+32.9	0.75178	2222111000
			0.05244	2022111002
			0.04158	2122111001
			0.02539	2211111110
			0.01682	2122201001
			0.01445	2212211000
			0.01279	2122021001
			0.00865	2220111200
			0.00833	2220111020
			0.00751	1122121001
			0.00540	2202111200
			0.00489	2112111002
			0.00449	2202111020
			0.00443	1122211001
6 (Sextet)	-2374871.578	+77.5	0.44878	2112211100
			0.25597	2112121100
			0.07001	2111212100
			0.05420	2111221100
			0.04543	2111122100
			0.02137	1112212100
			0.02026	2111111111
			0.01164	1112122100
			0.00560	2112011120
			0.00558	2112011102
			0.00387	1111222100
			0.00318	2112101102
			0.00318	2112101120
			0.00298	2110211120
			0.00273	2110211102
			0.00253	2111021111
			0.00252	2111201111

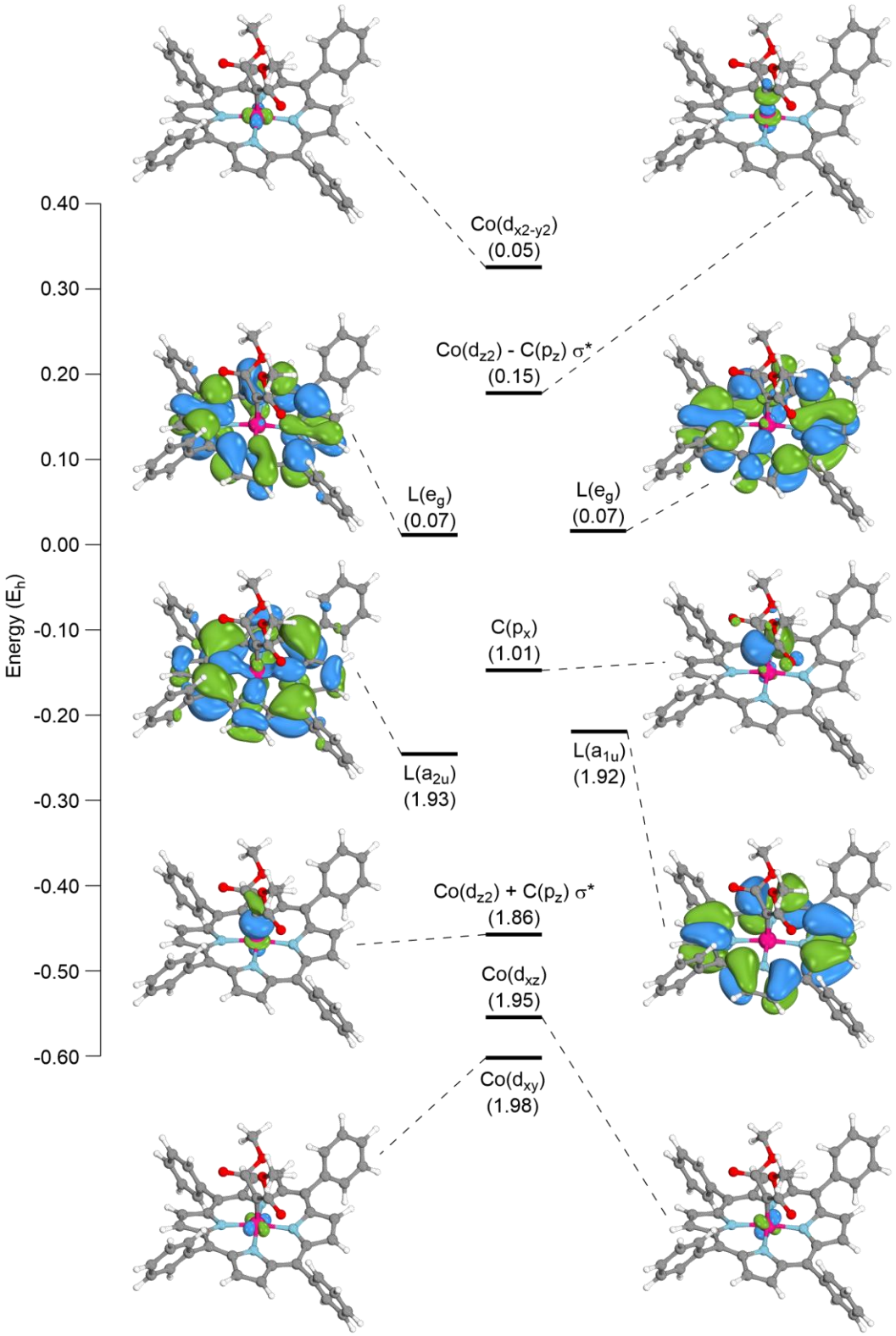


Figure S70. Energy diagram of the canonical molecular orbitals for the doublet spin state (S = ½) of $\mathbf{I^T}$ obtained with NEVPT2-CASSCF(11,10) calculations. Energies are in Hartree units. Occupancies depicted between parentheses. Isosurface set at 80.0 and generated using IboView.

***N*-Enolate-*C*arbene Radical Complex $\mathbf{I}^{\mathbf{E-T}}$:** CAS(10,11)

In agreement with the experimental X-band EPR sectra and DFT calculations, the spin ground state of the novel *N*-enolate-carbene radical $\mathbf{I}^{\mathbf{E-T}}$ is a doublet (S = ½), and the NEVPT2-CASSCF electronic structure reveals no significant multireference character (Table S27). The quartet (S = 3/2) and sextet (S = 5/2) spin states are well-separated from the ground state (+54.7 and 89.7 kcal·mol^{-1}, respectively). Electronically, there is little difference with the *mono*-terminal carbene $\mathbf{I}^{\mathbf{T}}$ in the energy levels and order of the correlated cobalt *d*-orbitals and carbene σ and π-orbitals. The SOMO is again entirely dominated by the carbene C(p_x) orbital (89.4%). However, due to the distortion of the porphyrin ring, the vacant e_g Gouterman orbitals are no longer degenerate. Additionally, the filled a_{1u} and a_{2u} Gouterman orbitals exhibit a certain degree of mixing, as can be seen in Figure S71, and are therefore almost degenerate as a result. The Co(d_{xy}), Co(d_{yz}) and the C_{enol}(p_y) were found to be uncorrelated. Any orbital centered on the axial oxygen ligand was also found to be uncorrelated, suggesting that the Co–O interaction is predominantly electrostatic in nature.

Table S27. Energies in kcal·mol^{-1} for the doublet, quartet and sextet spin states for $\mathbf{I}^{\mathbf{E-T}}$ obtained with NEVPT2-CASSCF(11,10) calculations and the respective contribution of each state to the overall wavefunction.

Multiplicity	Energy (kcal·mol^{-1})	Relative energy (kcal·mol^{-1})	Contribution	Occupancy
2 (Doublet)	**–2685052.779**	**0.0**	**0.84313**	**2222210000**
			0.03017	2221111100
			0.02245	2202210020
			0.01338	2212210010
			0.01091	2222010200
			0.00984	2112210011
			0.00882	1212220010
			0.00845	2220212000
			0.00776	2222012000
			0.00558	2220210200
			0.00302	2022210002
			0.00301	2221220000
4 (Quartet)	–2684998.046	+54.7	0.91112	2222111000
			0.02708	2220111200
			0.00589	2211211100
			0.00556	2211111101
			0.00508	2221111100
			0.00352	2022111020
			0.00335	2122120010
			0.00270	2122102010
6 (Sextet)	–2684963.040	+89.7	0.91967	2221111100
			0.02542	2201111120
			0.01466	2211111110
			0.00857	2111111111
			0.00825	1211121110
			0.00252	1211111111

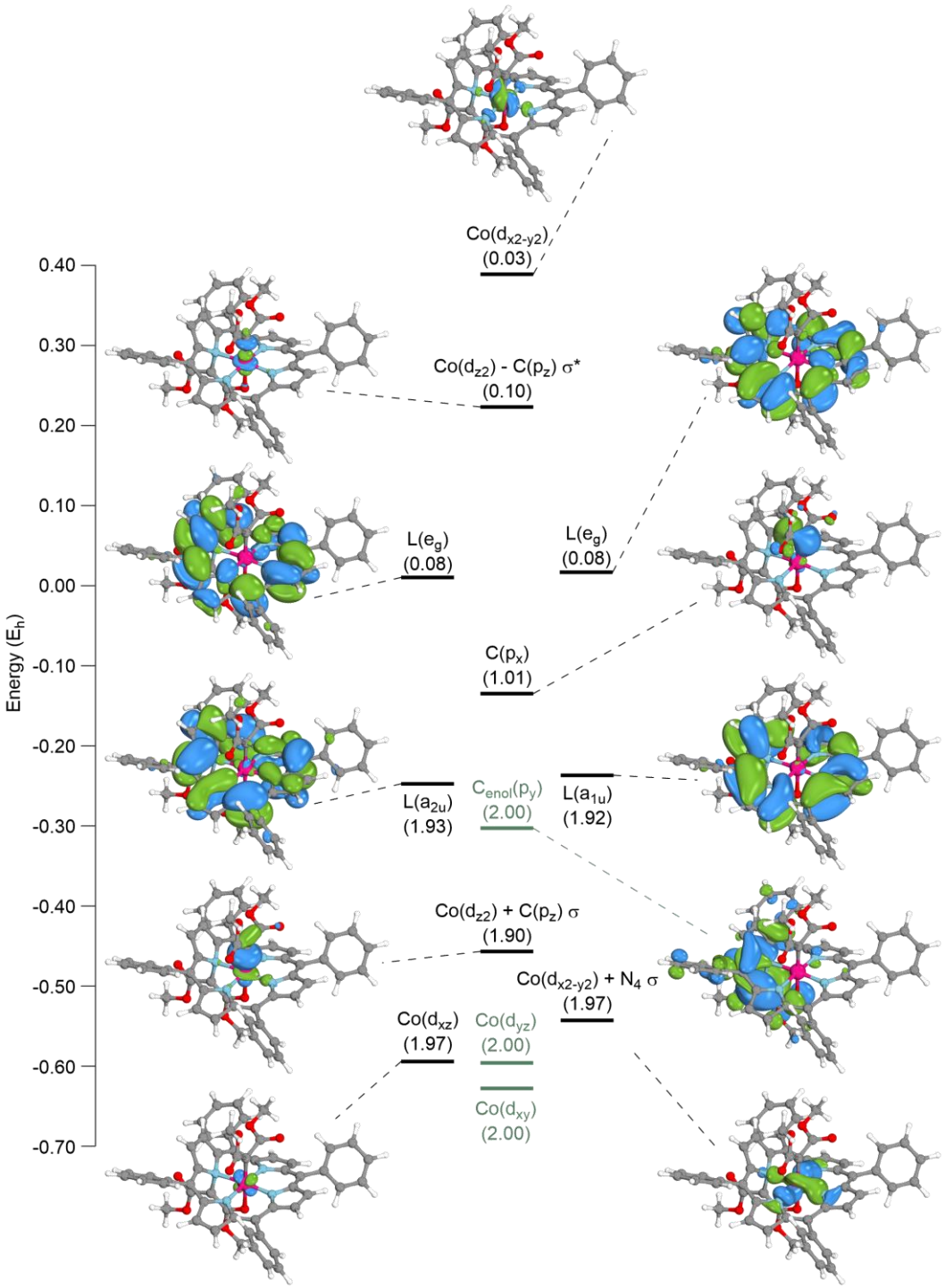
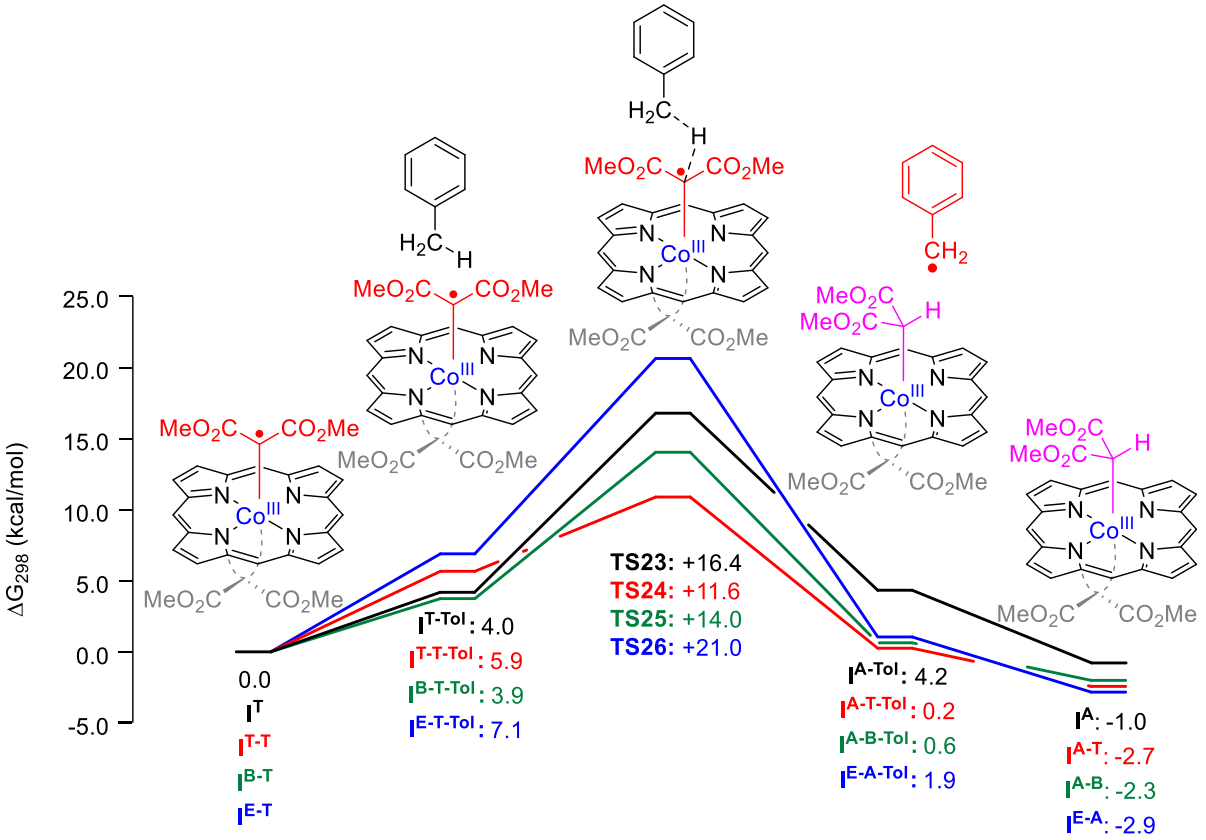


Figure S71. Energy diagram of the canonical molecular orbitals for the doublet spin state (S = ½) of $\mathbf{I^{E\text{-}T}}$ obtained with NEVPT2-CASSCF(11,10) calculations. Inactive orbitals are depicted in green. For clarity, the inactive MO of the enolate moiety is also visualized. Energies are in Hartree units. Despite the breaking of degeneracy for the e_g-orbitals, the labeling is kept for clarity in comparison to unfunctionalized porphyrins. Occupancies depicted between parentheses. Isosurface set at 80.0 and generated using IboView.

Deactivation via hydrogen-atom transfer (HAT):

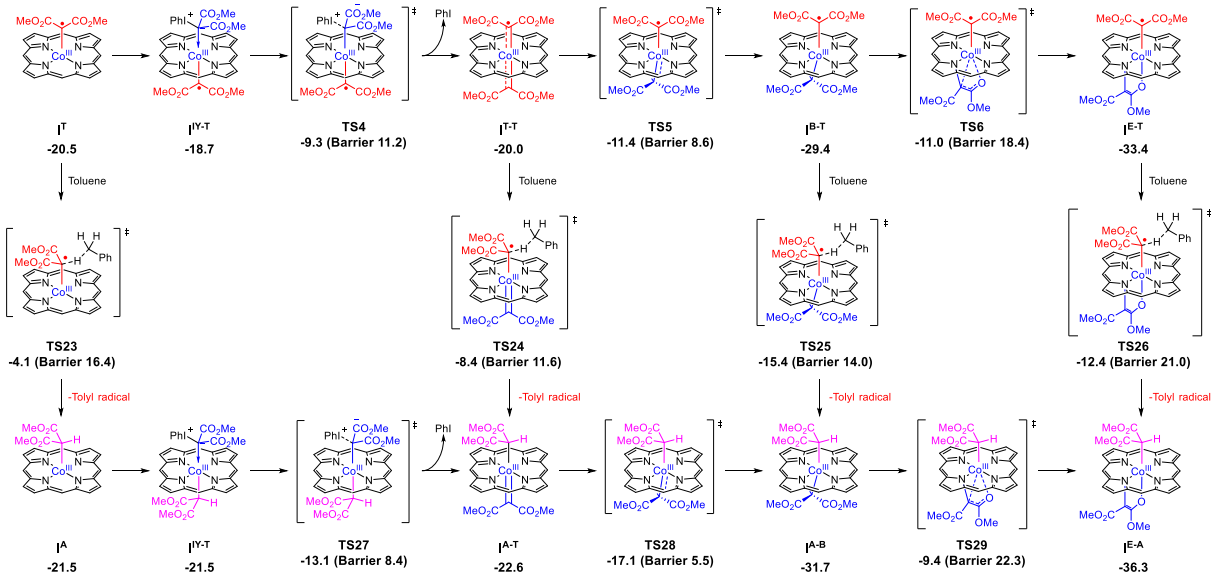
EPR, UV/Vis and H/D labeled CSI^{+}-MS studies have experimentally shown the formation of deactivated carbene radicals through hydrogen-atom transfer (HAT). DFT studies further corroborate these findings as shown in Scheme S10. The four carbene radicals (**I^{T}**, **I^{T-T}**, **I^{B-T}**, **I^{E-T}**) relevant in the catalytic cycle (Scheme S9) were investigated in HAT reactions with toluene. Approach of toluene to form a van-der-Waals adduct is, in all cases, endergonic. The relative heights of the HAT transition state barriers vary strongly among the different carbene radical complexes considered. The *N*-enolate-carbene radical species **I^{E-T}** has the highest HAT deactivation barrier (+21.0 kcal mol^{-1}), while HAT deactivation of *bis*-terminal carbene species **I^{T-T}** proceeds with a much lower barrier (+11.6 kcal mol^{-1}). The stability of the final alkyl species differs only marginally. The *mono*-terminal carbene **I^{T}** and the *mono*-bridging-*mono*-terminal carbene **I^{B-T}** have intermediate barriers.



Scheme S10. Schematic Gibbs free energy comparison ($\Delta G°_{298K}$ in kcal mol^{-1}) of the HAT reaction with toluene and the *mono*-terminal carbene (**I^{T}**; **black**), *bis*-terminal carbene (**I^{T-T}**; **red**), *mono*-bridged-*mono*-terminal carbene (**I^{B-T}**; **green**) and *mono*-enolate-*mono*-terminal carbene (**I^{E-T}**; **blue**) species.

Possible routes for formation of the final *N*-enolate-alkyl species $\mathbf{I}^{\mathbf{E-A}}$:

Aside from the direct formation of the *mono*-enolate-*mono*-terminal carbene $\mathbf{I}^{\mathbf{E-T}}$ described in the main text (main catalytic cycle) followed by HAT deactivation to from $\mathbf{I}^{\mathbf{E-A}}$, the latter deactivation product can in principle also be formed from the *mono*-alkyl adduct $\mathbf{I}^{\mathbf{A}}$ (Scheme S11). The UV/Vis data in Figure S17 indicate premature formation of the *mono*-alkyl adduct $\mathbf{I}^{\mathbf{A}}$ via HAT deactivation of $\mathbf{I}^{\mathbf{T}}$, suggesting that alternative routes for formation of $\mathbf{I}^{\mathbf{A-E}}$ might indeed be possible.

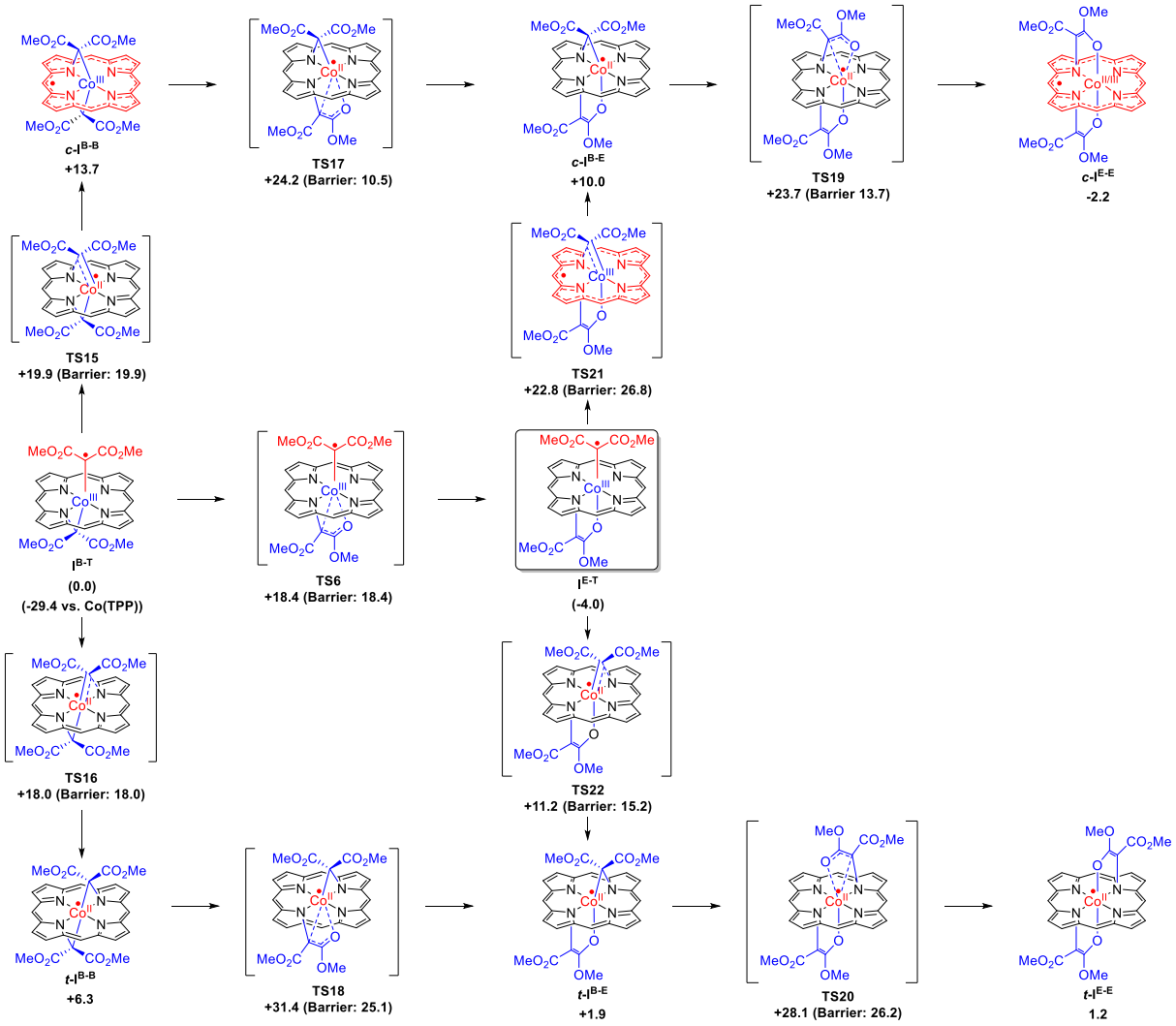


Scheme S11. Mechanistic overview of deactivation pathways via hydrogen atom transfer and enolate adduct formation by DFT ($\Delta G°_{298K}$ in kcal mol^{-1}) with the *mono*-terminal carbene $\mathbf{I}^{\mathbf{T}}$ as the starting point ([Co(TPP)] = 0.0 kcal mol^{-1}). Phenyl groups omitted for clarity.

Based on the relative barrier heights, it is conceivable that in toluene or in the presence of significant amounts of other HAT-donors with a comparable BDE, deactivation of $\mathbf{I}^{\mathbf{T}}$ via HAT to produce $\mathbf{I}^{\mathbf{A}}$ can readily occur before $\mathbf{I}^{\mathbf{E-T}}$ is formed. The iodonium ylide is poorly soluble and as such, competition with a readily available HAT-donor can overcome the lower barriers of carbene formation. However, experimentally conversion of $\mathbf{I}^{\mathbf{A}}$ to $\mathbf{I}^{\mathbf{E-A}}$ is not observed, and seems to be a very slow process. Since $\mathbf{I}^{\mathbf{A}}$ is experimentally detected (as a minor species) in reaction mixtures containing an excess of the iodonium ylide, this alternative pathway seems to be experimentally blocked. This suggests that $\mathbf{I}^{\mathbf{A}}$ contains an unidentified 6th ligand (Scheme 3) that prevents (or slows-down) subsequent reactions with DMM•IY.

Alternative 'bridging carbenes' as possible off-cycle species

Fischer-type carbene complexes are known to form catalytically inactive 'bridged carbenes' and enolate adducts with the surrounding ligand via nucleophilic attack of a ligand heteroatom lone pair onto the electrophilic carbene.[31] Despite being a reduced electrophilic/partially nucleophilic, one-electron reduced Fischer-type carbene, the 'carbene radical' species might be subject to similar deactivation pathways as previously investigated in our group.[32] Consequently, formation of alternative 'bridging carbene' species and *bis*-enolate species as possible off-cycle species, potentially providing alternative deactivation pathways, were also investigated (Scheme S12).



Scheme S12. Mechanistic overview of deactivation pathways via carbene bridging and enolate adduct formation by DFT ($\Delta G°_{298K}$ in kcal mol^{-1}) with the *mono*-bridged-*mono*-terminal carbene as the reference point. Phenyl groups omitted for clarity. Oxidation states of cobalt and the TPP ligand were determined on the basis of Mulliken spin densities. Free energies (298 K) in kcal mol^{-1}.

Starting from the *mono*-bridged-*mono*-terminal carbene (**I^{B-T}** ($\Delta G°$ = 0.0 kcal·mol^{-1}; $\Delta\Delta G^{[Co(TPP)]}$ = –29.4 kcal·mol^{-1}), further bridging of the terminal carbene to either a *cis*- or *trans*-conformation is comparable in energy for **TS15** ($\Delta G°$ = +19.9 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +19.9 kcal·mol^{-1}) and **TS16** ($\Delta G°$ = +18.0 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +18.0 kcal·mol^{-1}). The relative heights of these barriers are proportional to enolate adduct formation towards the catalytically active **I^{E-T}** ($\Delta G°$ = –4.0 kcal·mol-1) in **TS6** ($\Delta G°$ = +18.4 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +18.4 kcal·mol^{-1}). While the barriers for formation of ***c*-I^{B-B}** ($\Delta G°$ = +13.7 kcal·mol^{-1}) and ***t*-I^{B-B}** ($\Delta G°$ = +6.3 kcal·mol-1) are energetically similar, the relative ground states are not, with the *trans*-variant being far more stable than the *cis*-variant.

Enolate-adduct formation from ***c*-I^{B-B}** to ***c*-I^{B-E}** ($\Delta G°$ = +10.0 kcal·mol^{-1}) proceeds via a relatively low barrier in **TS17** ($\Delta G°$ = +24.2 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +10.5 kcal·mol^{-1}) whereas the barrier for transformation of ***t*-I^{B-B}** to ***t*-I^{B-E}** ($\Delta G°$ = +1.9 kcal·mol^{-1}) progresses via a significantly higher barrier in **TS18** ($\Delta G°$ = +31.4 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +25.1 kcal·mol^{-1}). Formation of ***c*-I^{B-E}** and ***t*-I^{B-E}** can also occur via bridging of the *mono*-terminal carbene over a pyrrole group of the porphyrin in **I^{E-T}** via **TS21** ($\Delta G°$ = +22.8 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +26.8 kcal·mol^{-1}) and **TS22** ($\Delta G°$ = +11.2 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +15.2 kcal·mol^{-1}), respectively. *bis*-enolate adduct formation from ***c*-I^{B-E}** to ***c*-I^{E-E}** ($\Delta G°$ = **–** 2.2 kcal·mol^{-1}) and ***t*-I^{B-E}** to ***t*-I^{E-E}** ($\Delta G°$ = +1.2 kcal·mol^{-1}) occurs via the highest barriers in **TS20** ($\Delta G°$ = +28.1 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +26.2 kcal·mol^{-1}) and **TS19** ($\Delta G°$ = +23.7 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +13.7 kcal·mol^{-1}), respectively.

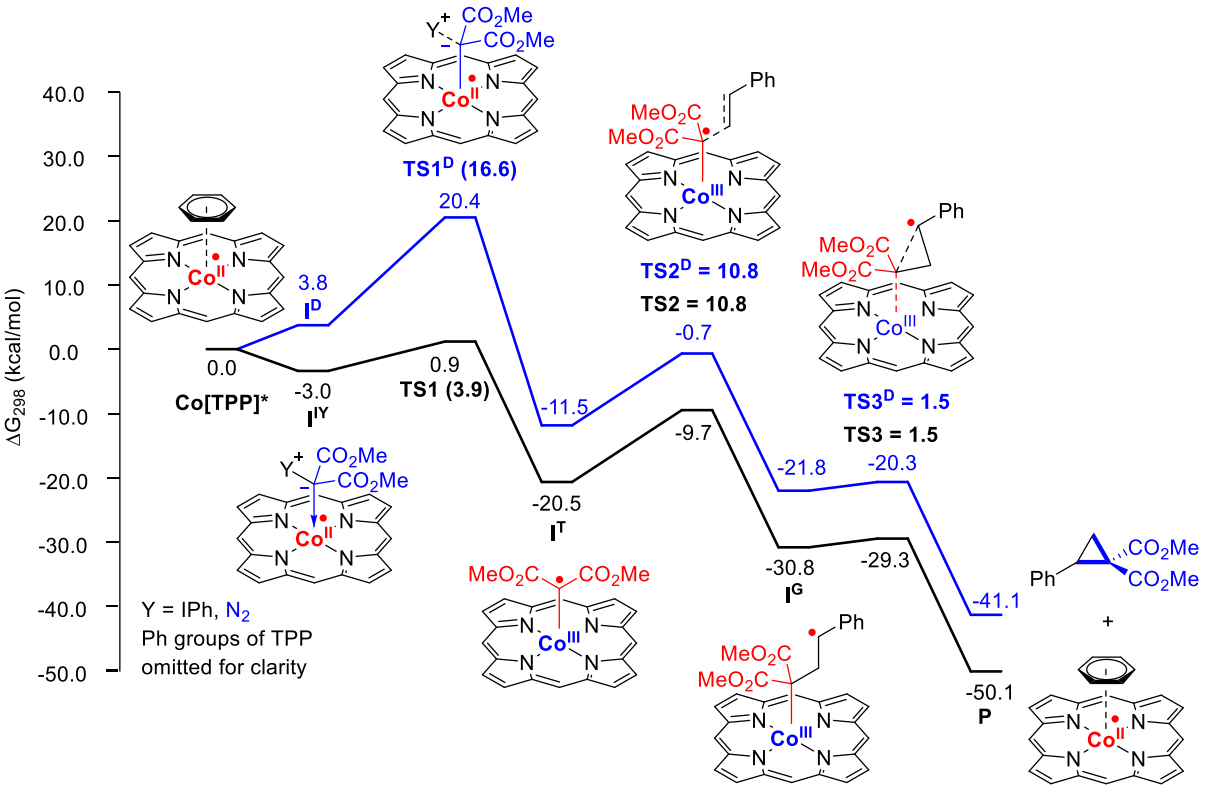
Interestingly, the *cis-bis-enolate* adduct ***c*-I^{E-E}** is more stable than its *trans* congener as opposed to the other *bis*-bridged intermediates and is even more stable than the *mono*-bridged-*mono*-terminal carbene. However, the most stable intermediate is, still, the catalytically active **I^{E-T}**. Since all reported processes are reversible intramolecular reactions with barriers accessible at room temperature, even if the alternative 'bridging carbenes' and *Bis*-enolates are formed, regeneration of the more stable catalytically active **I^{E-T}** species should be easy. Therefore, it can be concluded, on the basis of these computational studies, that formation of alternative off-cyle species or catalyst deactivation via formation of *bis*-enolate species should not play a significant role during catalysis.

Note: The oxidation state of the ***c*-I^{E-E}** species could not be clearly discerned from the Mulliken spin density and would require investigation of more accurate multireference methods. This is beyond the scope of the present paper, since this intermediate does not play an active role in the overall catalytic reaction anyway.

Comparison between diazo compound and iodonium ylide reactivity:

When comparing the reaction pathways using DFT calculations (Scheme S13), it became evident why the diazo compound DMM·N_2 is a much less suitable carbene precursor than iodonium ylide DMM•IY in experimental carbene transfer reactions (see Table S7). Coordination of the diazo compound in **I^{D}** is endergonic ($\Delta G°$ = 3.8 kcal·mol^{-1}) with respect to **[Co(TPP)]*** ($\Delta G°$ = 0.0 kcal·mol^{-1}) whereas binding of the ylide **I^{IY}** is exergonic ($\Delta G°$ = **–**3.0 kcal·mol^{-1}). However, the most profound difference is the much higher barrier for extrusion of N_2 in **TS1^{D}** ($\Delta G°$ = +20.4 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +16.6 kcal·mol^{-1}) compared the barrier for extrusion of IPh in **TS1** ($\Delta G°$ = +0.9 kcal·mol^{-1}; $\Delta\Delta G^{‡}$ = +3.9 kcal·mol^{-1}). This significant difference largely explains the difference in carbene transfer efficiency. The high **TS1^{D}** barrier for formation of *mono*-carbene radical **I^{T}** from **[Co(TPP)]*** and DMM·N_2 (+20.4 kcal·mol^{-1}) points to a low intrinsic reactivity of **[Co(TPP)]*** towards DMM·N_2. This is further supported by favorable coordination of the ester carbonyl groups for DMM·N_2 versus the central carbon, as opposed to DMM•IY (vide infra). Furthermore, the experimental **TS1^{D}** barrier might well be higher than computed, and additional active site blocking effects and competing catalyst deactivation processes might play a role (vide infra).

Formation of the terminal carbene **I^{T}** from the diazo compound is 9 kcal·mol^{-1} less exergonic than its formation from DMM•IY. This is a direct result of a different thermodynamic driving force for N_2 versus IPh extrusion from the different carbene precursors. Clearly, the driving force for carbene formation from DMM•IY is stronger. Since all intermediates formed from **I^{T}** are identical in the next steps, all subsequent barriers are equal and the intermediates are only offset by the same thermodynamic +9 kcal·mol^{-1} energy difference.

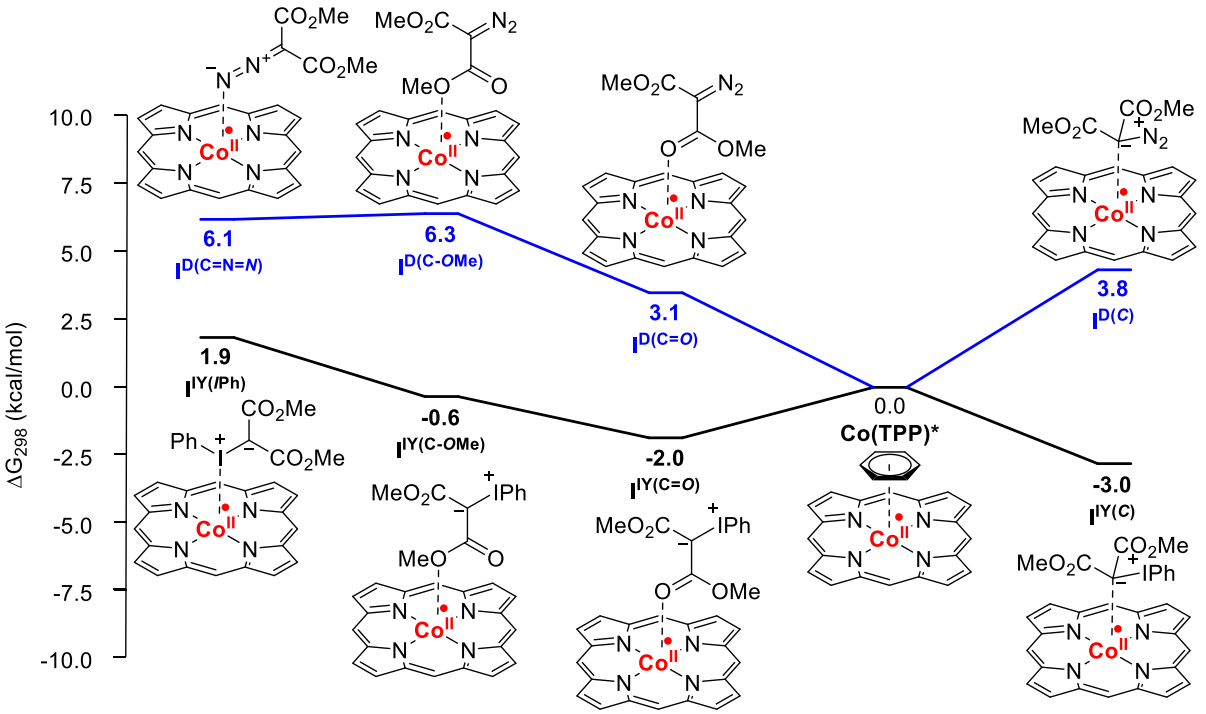


Scheme S13. Schematic Gibbs free energy comparison of the *mono*-carbenoid pathway towards the cyclopropanation of styrene from either dimethyldiazomalonate or its iodonium ylide analogue.

Potential barrier-increasing active site blocking effects by the diazo compound were also computationally explored by considering various coordination modes of both the ylide and the diazo reagent (Scheme S14). Coordination of the central carbon to form the carbenoid iodonium

ylide adduct $\mathbf{I}^{\mathbf{IY(}\mathit{C}\mathbf{)}}$ ($\Delta G°$ = –3.0 kcal·mol^{-1}) is exergonic, whereas formation of the analogous diazo adduct $\mathbf{I}^{\mathbf{D(}\mathit{C}\mathbf{)}}$ ($\Delta G°$ = +3.8 kcal·mol^{-1}) from the benzene adduct is endergonic. Furthermore, binding via the carbonyl moiety ($\mathbf{I}^{\mathbf{D(C=}\mathit{O}\mathbf{)}}$: $\Delta G°$ = +3.1 kcal·mol^{-1}) is less endergonic than formation the C-bound diazo compound ($\mathbf{I}^{\mathbf{D(C)}}$: $\Delta G°$ = +3.8 kcal·mol^{-1}). In contrast, for DMM•IY the C-bound coordination mode ($\mathbf{I}^{\mathbf{IY(C)}}$: $\Delta G°$ = –3.0 kcal·mol^{-1}) is favored over the carbonyl binding mode ($\mathbf{I}^{\mathbf{IY(C=}\mathit{O}\mathbf{)}}$: $\Delta G°$ = –2.0 kcal·mol^{-1}). Binding via the ether linkage in $\mathbf{I}^{\mathbf{D(C-}\mathit{O}\mathbf{Me)}}$ ($\Delta G°$ = +6.3 kcal·mol^{-1}) and in $\mathbf{I}^{\mathbf{IY(C-}\mathit{O}\mathbf{Me)}}$ ($\Delta G°$ = –0.6 kcal·mol^{-1}) is less favorable than via the carbonyl group for both adducts. Terminal nitrogen coordination in $\mathbf{I}^{\mathbf{D(C=N=}\mathit{N}\mathbf{)}}$ ($\Delta G°$ = +6.1 kcal·mol^{-1}) is comparably unfavorable for both systems. Iodine coordination in $\mathbf{I}^{\mathbf{IY(}\mathit{I}\mathbf{Ph)}}$ ($\Delta G°$ = +6.1 kcal·mol^{-1}) is the least favorable adduct for DMM•IY.

This comparison shows that coordination of the iodonium ylide to **[Co(TPP)]*** is favorable with the desired productive central carbon coordination mode as the energetic minimum. In contrast, all diazo adducts are uphill in energy with coordination of the more sterically accessible carbonyl group being the least unfavorable. Hence, the combination of a much higher transition state for formation of the *mono* carbene radical complex from DMM·N_2 than from DMM•IY, a relatively low barrier for deactivation of the *mono*-carbene species via HAT (**TS24**; Scheme S11) and an unfavorable coordination mode of DMM·N_2 as the most stable adduct supports the absence of detectable catalytic turnover in the reaction flask when using diazo compound DMM·N_2 as the carbene precursor. In contrast, for DMM•IY the desired coordination mode is favorable and PhI loss has a low barrier, thus explaining the much higher efficiency of DMM•IY as a carbene precursor in the [Co(TPP)-catalyzed cyclopropanation reactions.



Scheme S14. Comparison of the free Gibbs energy difference of various binding modes (carbonyl, ether, terminal nitrogen or iodine) for the diazo and the ylide respectively.

When considering electronic differences, the DFT HOMO's and LUMO's show that the diazo compound and the iodonium ylide share many similarities (Figure S72). Both have the largest lobe centered on the carbenoid carbon in the HOMO (**A** and **C**). Interestingly, the aryl ring delocalizes some of the electron density in the ylide. The LUMO is centered on the leaving group in both the N–N π^* orbital (**D**) and the I–C_{Ar} π^* orbital (**C**) for the diazo compound and the iodonium ylide, respectively. In the latter case the carbenoid carbon also contributes slightly to this orbital.

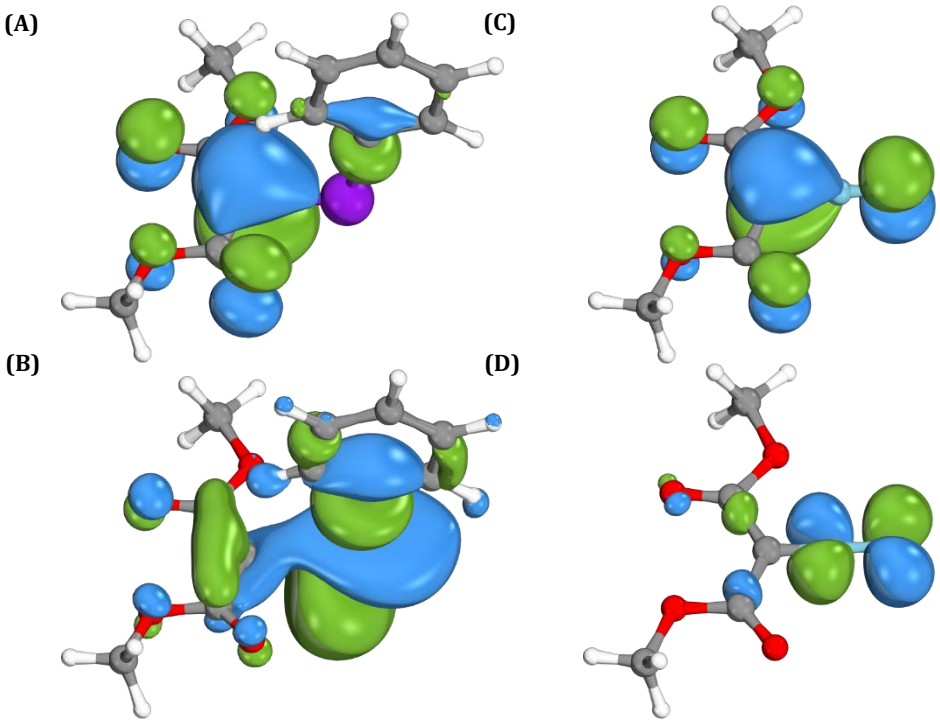


Figure S72. Frontier orbitals for **DMM·IY** (HOMO (**A**, top left) and LUMO (**B**, bottom left)) and **DMM·N₂** (HOMO (**C**, top right) and LUMO (**D**, bottom right)). Pictures are generated using IboView.

After forming an adduct with the catalyst, significant differences arise (Figure S73). The diazo compound only seems to form a Van der Waals adduct $\mathbf{I^D}$ as is evident from the frontier orbitals being entirely separated into two entities, [Co(TPP)] and DMM·N_2. The HOMO and SOMO are centered on [Co(TPP)] whereas the LUMO is centered on DMM·N_2 and is virtually identical to that of the unbound diazo. On the other hand, the DMM•IY adduct $\mathbf{I^{IY}}$ has a SOMO that has a significant component in the ylidic carbon, signifying (weak) coordination rather than a pure Van der Waals interaction. The HOMO and LUMO of this adduct are centered on the cobalt and ligand, respectively.

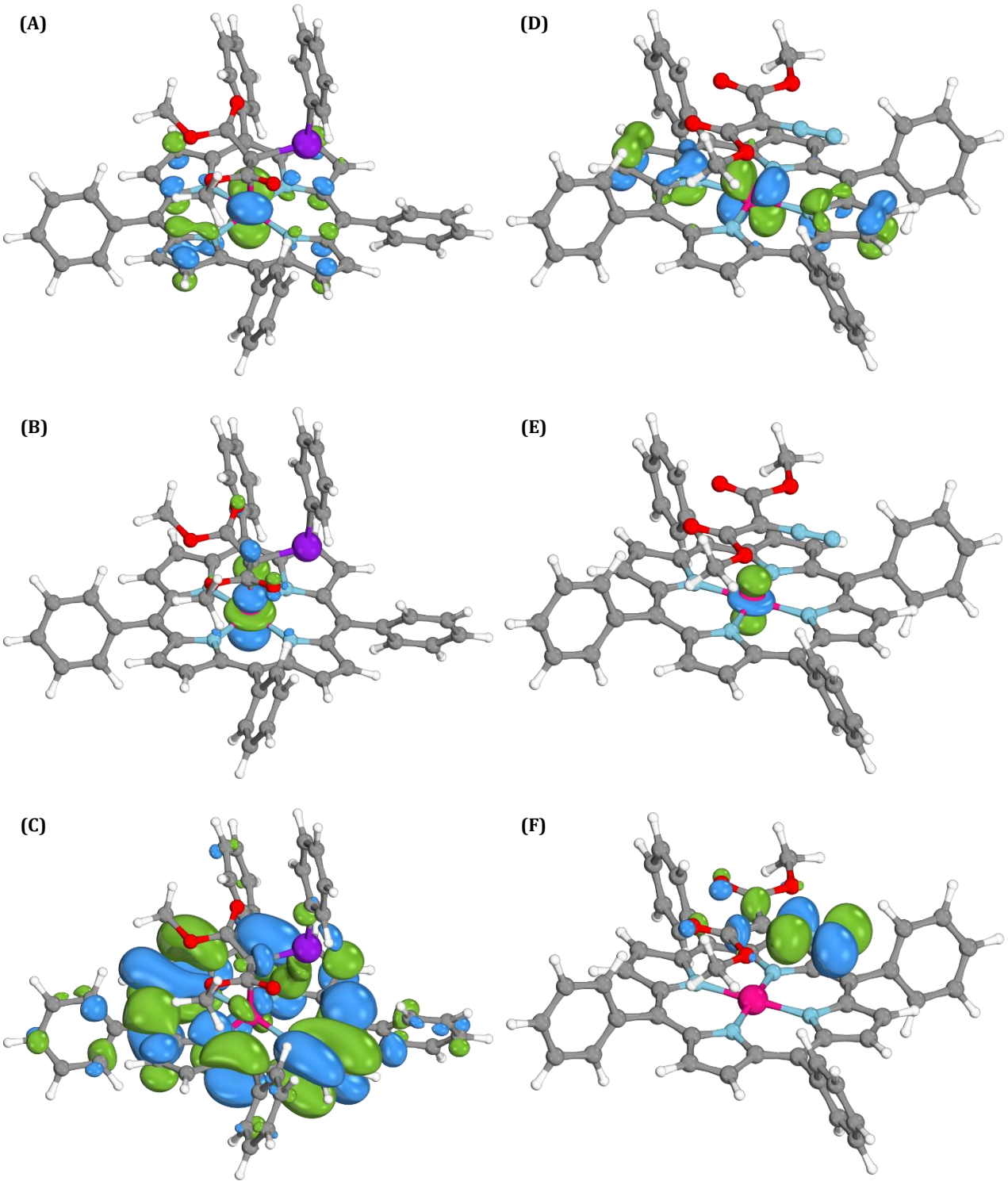


Figure S73. Frontier orbitals for $\mathbf{I^{IY}}$ (HOMO (**A**, top left), SOMO (**B**, middle left) and LUMO (**C**, bottom left)) and $\mathbf{I^{D}}$ (HOMO (**D**, top right), SOMO (**E**, middle right) and LUMO (**F**, bottom right)) based on QROs (BP86/def2-TZVP; Orca 4.2.1). Pictures are generated using IboView.

The transition state geometries reveal additional key differences (Figure S74). The HOMO of both **TS1** and $\mathbf{TS1^{D}}$ is centered on the Co-d_{yz} orbital. The SOMO is a mix of the Co-d_{z2} orbital and the ylidic fragment with a large contribution on the carbenoid carbon in **TS1**, whereas in $\mathbf{TS1^{D}}$ the overlap is mostly between the d_{z2} and the LUMO of DMM·N_2. The LUMO paints a picture similar to the SOMO, with a significant contribution from the Co-d_{z2} orbital. However, for **TS1** it resides also largely on the C–I π^* orbital, which is also the LUMO for DMM•IY, whereas for $\mathbf{TS1^{D}}$ it resides

largely in an orbital similar to the LUMO+1 rather than the LUMO. Consequently, injection of electrons from the HOMO and SOMO of [Co(TPP)] into the substrate located virtual orbitals is more favorable for DMM•IY than for DMM·N_2.

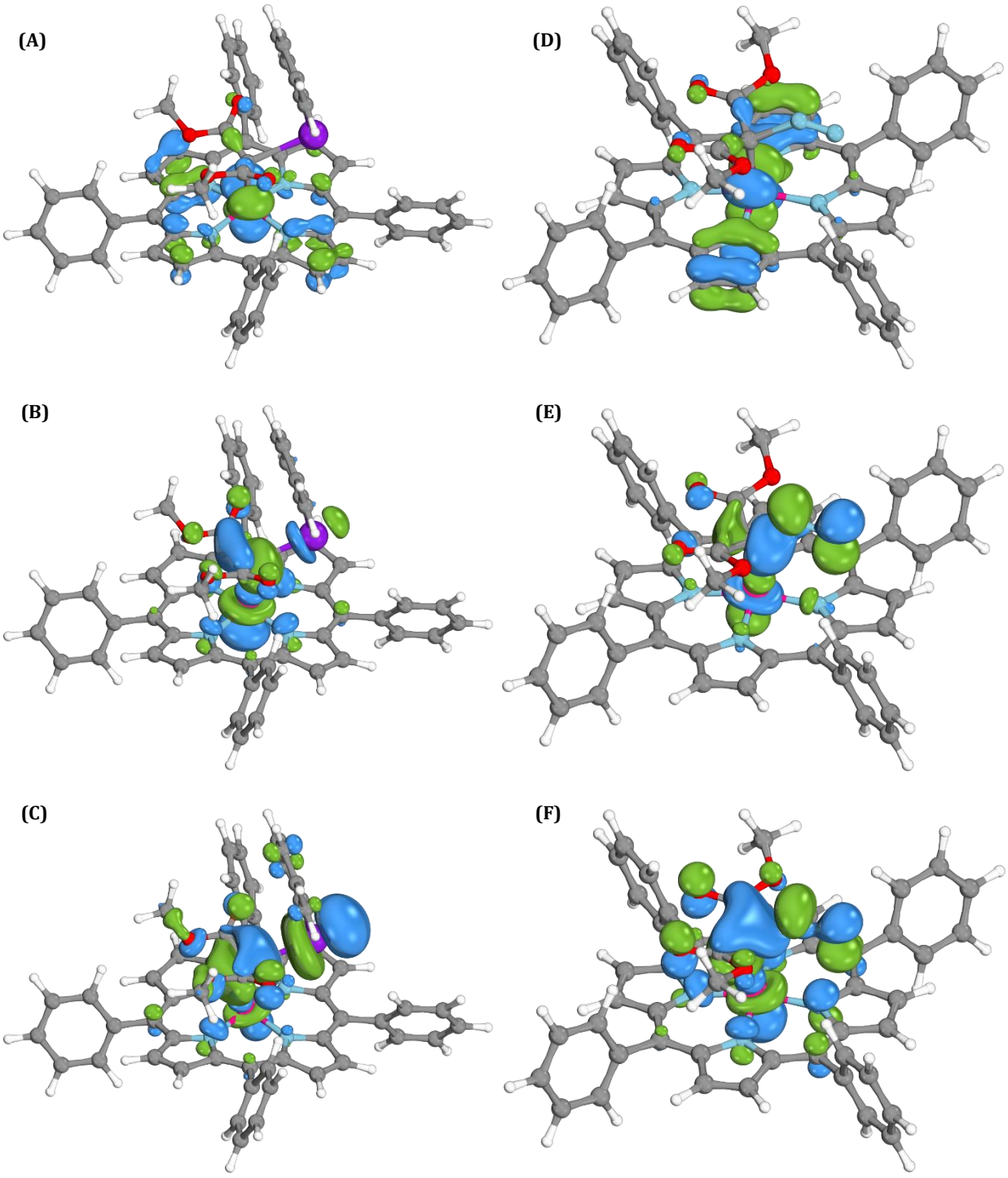


Figure S74. Frontier orbitals for **TS1** (HOMO (**A**, top left), SOMO (**B**, middle left) and LUMO (**C**, bottom left)) and **TS1^D** (HOMO (**D**, top right), SOMO (**E**, middle right) and LUMO (**F**, bottom right)) based on QROs (BP86/def2-TZVP; Orca 4.2.1). Pictures are generated using IboView.

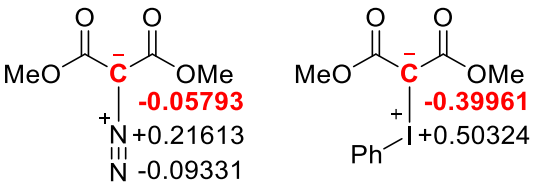


Table S28. Comparison of the Mulliken charge population of DMM·N_2 vs. DMM·IY. Only atoms of interest are listed.

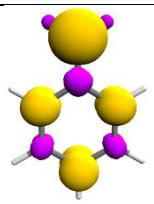
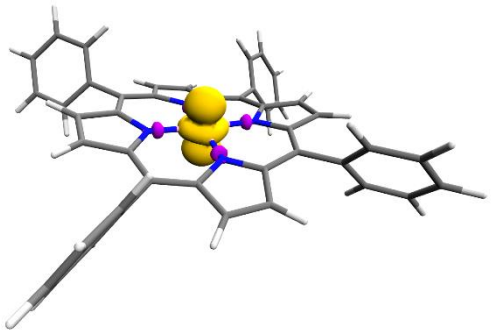
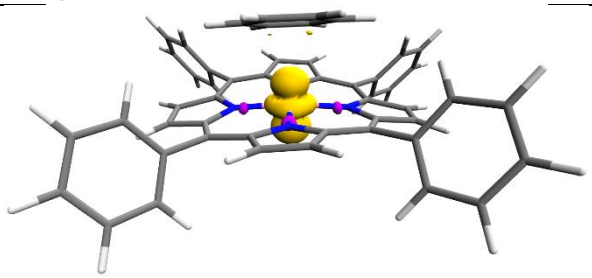
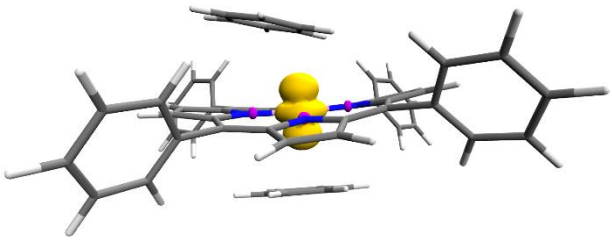
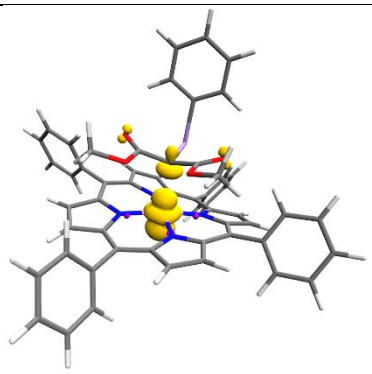
Atom (Group)	Mulliken Charge Population (DMM•N_2)	Mulliken Charge Population(DMM•IY)
C (**C**=O)	+0.26305	+0.30298
C (Ylidic)	**–0.05793**	**–0.39961**
C (**C**=O)	+0.30072	+0.30381
O (C=**O**)	–0.32393	–0.30391
O (C=**O**)	–0.27070	–0.36762
O (**O**Me)	–0.24397	–0.26217
O (**O**Me)	–0.17635	–0.18594
N (C=**N**=N)	**+0.21613**	N/A
N (C=N=**N**)	**–0.09331**	N/A
I (C–**I**–Ph)	N/A	**+0.50324**

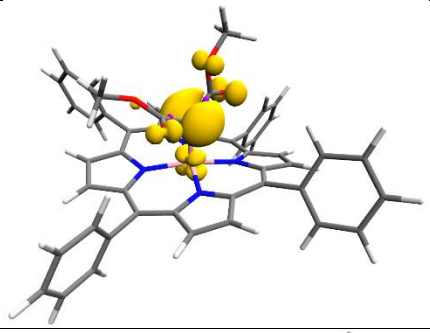
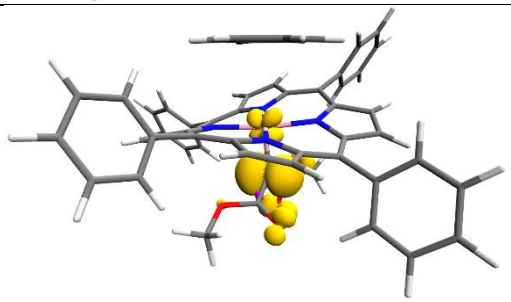
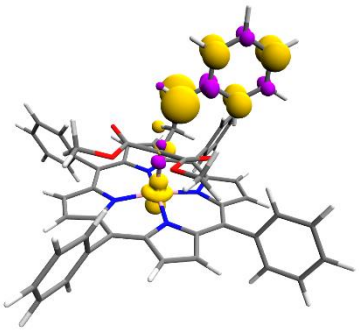
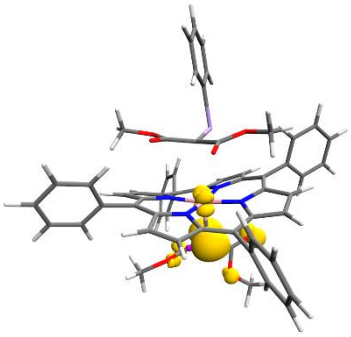
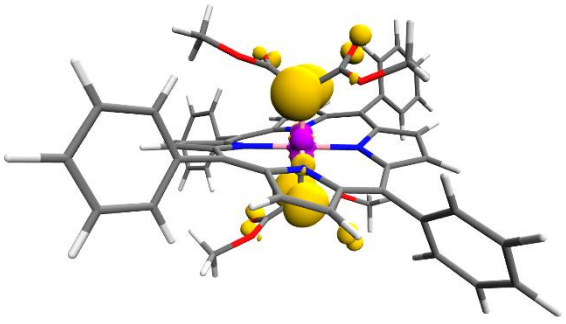
The most striking difference can be seen from the Mulliken charge population on the ylidic carbons and their respective leaving group moieties (Table S28, vide supra). The diazo compound has a largely delocalized negative charge, with minor negative charge on the ylidic carbon. The central nitrogen is slightly positive. However, the ylide has a large negative charge accumulated on the ylidic carbon and the iodine is significantly more positive. As such, the often drawn double C=I bond is largely polarized and has a strong ylidic character, as is evident from these values and the HOMO/LUMO graphical representations (Figure S72, vide supra).

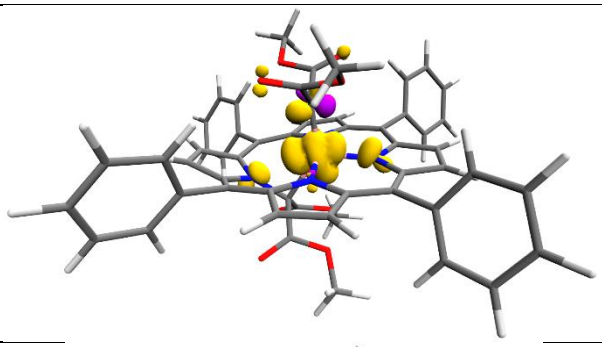
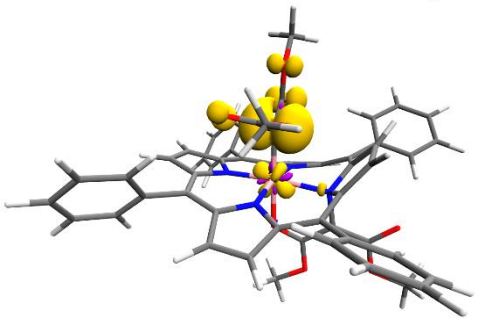
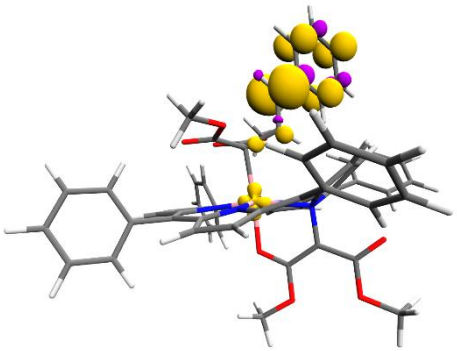
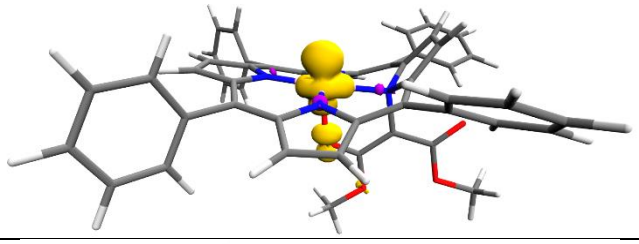
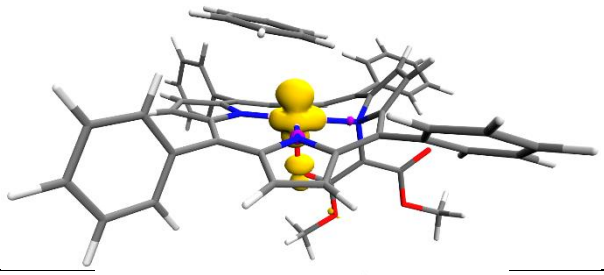
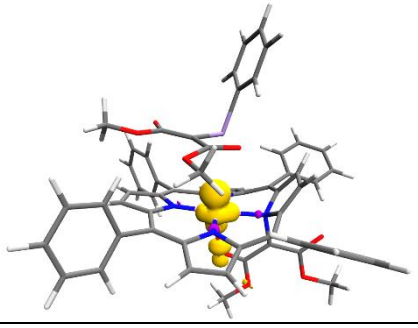
Ergo, the differences in reactivity can be attributed to the fact that the negative charge of the ylidic carbon in DMM•IY coordinates readily to cobalt, whereas the much lower negative charge of the corresponding carbon atom of DMM•N_2 does not. Moreover, the high positive charge of iodine in DMM•IY makes the iodobenzene a much better leaving group than N_2 in DMM·N_2.

Mulliken spin density plots:

Table S29. Spin density plots for miscellaneous reaction components and catalytic intermediates (isovalue: 0.004; α: yellow; β: purple).

Structure	Mulliken spin density	Plots
Tolyl radical	*C*H$_2$: +0.77 Ph: +0.33	
[Co(TPP)]	Co: +1.17 TPP: –0.12	
[Co(TPP)] *Mono*-Benzene (**[Co(TPP)]***)	Co: +1.10 TPP: –0.08	
[Co(TPP)] *Bis*-Benzene (**[Co(TPP)]****)	Co: +1.12 TPP: –0.09	
[Co(TPP)] *Mono* Iodonium Ylide (**I^{IV}**)	Co: +0.98 TPP: –0.05 C (Carbene): +0.07	

[Co(TPP)] *Mono* Terminal Carbene (**I^{T}**)	Co: +0.15 TPP: 0 C (Carbene): +0.69	
[Co(TPP)] *Mono* Benzene *Mono* Terminal Carbene (**I^{T*}**)	Co: +0.14 TPP: –0.01 C (Carbene): +0.72	
[Co(TPP)] *Mono* Gamma Radical (**I^{G}**)	Co: +0.27 TPP: 0 C (Carbene): 0 Styryl: +0.77	
[Co(TPP)] *Mono*-Iodonium Ylide *Mono*-Terminal Carbene (**I^{IY-T}**)	Co: +0.13 TPP: 0 C^{IY} (Carbene): 0 C^{T} (Carbene): +0.72	
[Co(TPP)] *Bis*-Terminal Carbene (**I^{T-T}**)	Co: –0.18 TPP: +0.01 C^{T} (Carbene): +0.54 C^{T} (Carbene): +0.52	

[Co(TPP)] *Mono*-Bridged *Mono*-Terminal Carbene (**I$^{B–T}$**)	Co: +0.85 TPP: +0.10 C^{B} (Carbene): –0.03 C^{T} (Carbene): +0.04	
[Co(TPP)] *Mono*-Enolate *Mono*-Terminal Carbene (**I$^{E–T}$**)	Co: +0.11 TPP: 0 C^{E} (Carbene): 0 C^{T} (Carbene): +0.75	
[Co(TPP)] *Mono*-Enolate *Mono*-Gamma Radical (**I$^{E–G}$**)	Co: +0.07 TPP: 0 C^{E} (Carbene): 0 C^{G} (Carbene): +0.03 Styryl: +0.90	
[Co(TPP)] *Mono* Enolate Adduct (**I^{E}**)	Co: +0.99 TPP: –0.08 C (Carbene): 0	
[Co(TPP)] *Mono* Benzene *Mono* Enolate Adduct (**I^{E*}**)	Co: +0.97 TPP: –0.08 C (Carbene): 0	
[Co(TPP)] *Mono*-Enolate *Mono*-Iodonium Ylide (**I$^{E–IY}$**)	Co: +0.97 TPP: –0.07 C^{E} (Carbene): 0 C^{IY} (Carbene): 0	

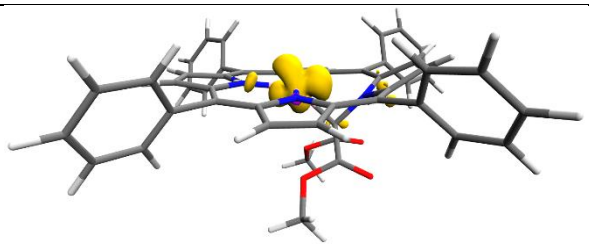
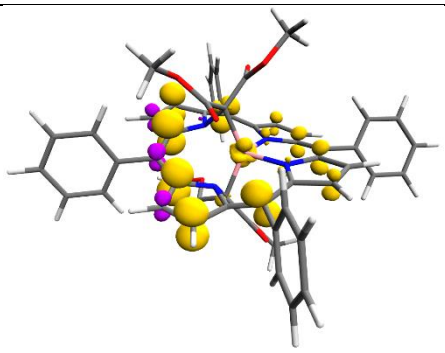
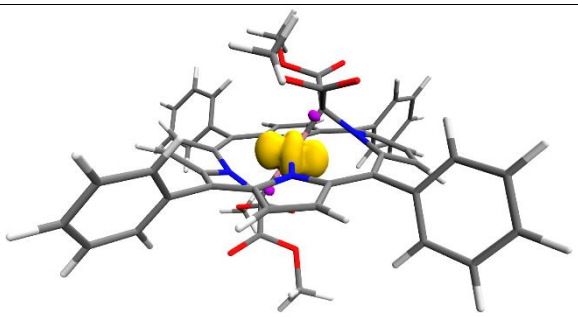
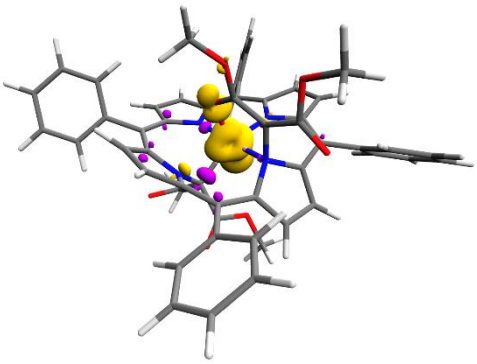
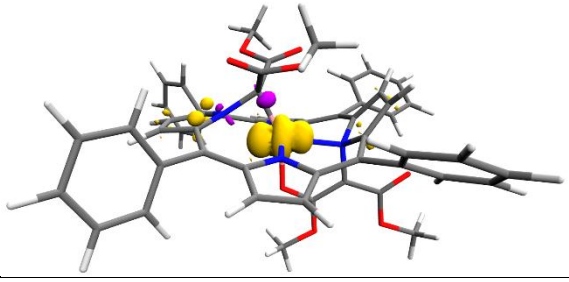
[Co(TPP)] *Mono* Bridging Carbene (**I**^{B})	Co: +0.92 TPP: +0.06 C (Carbene): +0.01	

Table S30. Spin density plots for bridging intermediates in deactivation pathways (isovalue: 0.004; α: yellow; β: purple).

Structure	**Mulliken spin density**	**Plots**
[Co(TPP)] *Bis-cis*-Bridged Carbene (***c*-I**$^{B-B}$)	Co: +0.07 TPP: +0.89 C^{B} (Carbene): +0.02 C^{B} (Carbene): +0.02	
[Co(TPP)] *Bis-trans*-Bridged Carbene (***t*-I**$^{B-B}$)	Co: +1.09 TPP: –0.01 C^{B} (Carbene): –0.04 C^{B} (Carbene): –0.03	
[Co(TPP)] *cis-Mono*-Bridged *Mono*-Enolate Carbene (***c*-I**$^{B-E}$)	Co: +1.19 TPP: –0.21 C^{B} (Carbene): –0.08 C^{E} (Carbene): 0	
[Co(TPP)] *trans-Mono*-Bridged *Mono*-Enolate Carbene (***t*-I**$^{B-E}$)	Co: +0.87 TPP: +0.21 C^{B} (Carbene): –0.05 C^{E} (Carbene): 0	

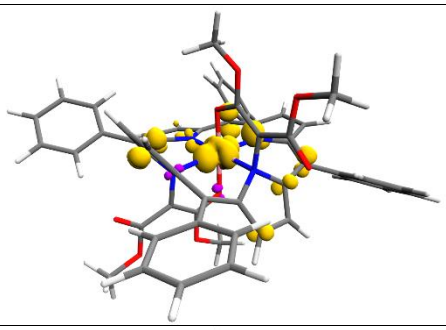
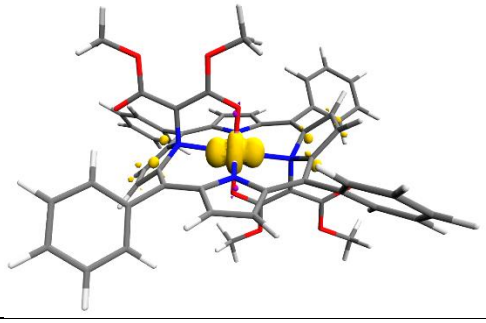
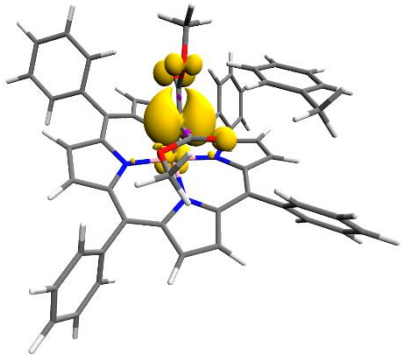
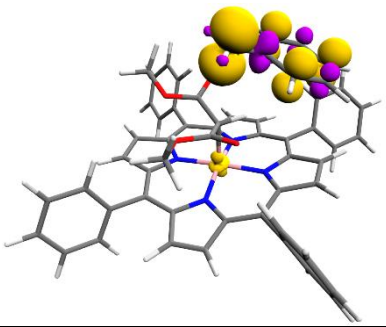
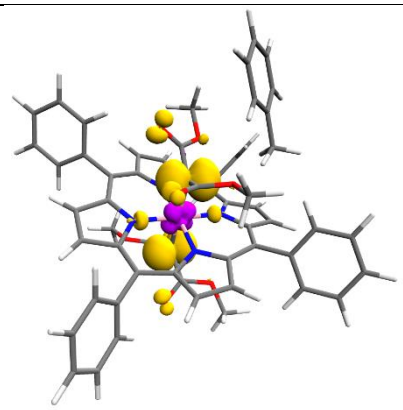
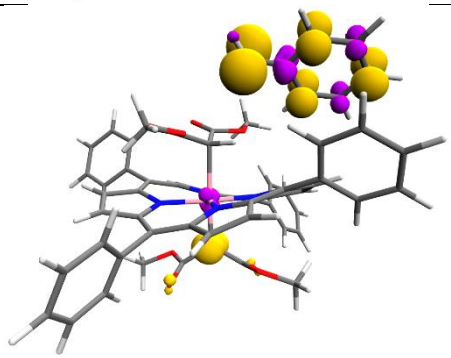
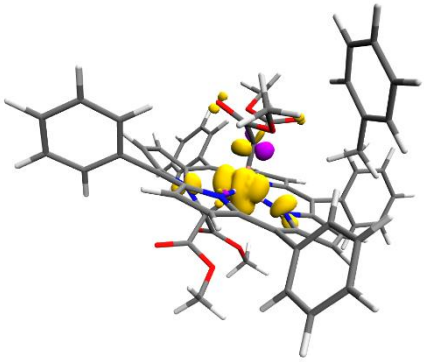
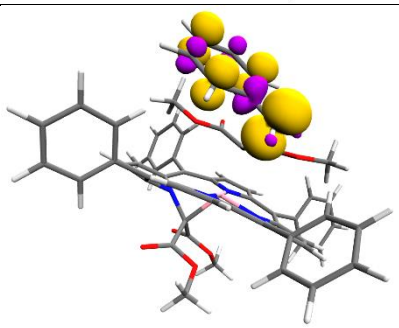
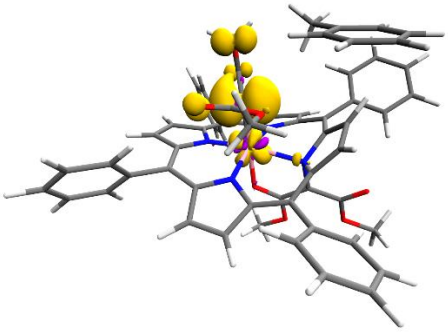
[Co(TPP)] *cis-Bis*-Enolate Adduct (***c*-I^{E-E}**)	Co: +0.49 TPP: +0.55 C^{E} (Carbene): 0 C^{E} (Carbene): 0	
[Co(TPP)] *trans-Bis*-Enolate Adduct (***t*-I^{E-E}**)	Co: +0.81 TPP: +0.21 C^{E} (Carbene): 0 C^{E} (Carbene): 0	

Table S31. Spin density plots for intermediates in HAT deactivation pathways (isovalue: 0.004; α: yellow; β: purple).

Structure	**Mulliken spin density**	**Plots**
[Co(TPP)] *Mono* Terminal Carbene Toluene Adduct (**I^{T-Tol}**)	Co: +0.14 TPP: 0 C (Carbene): +0.70 *C*H$_3$: 0 Ph: 0	
[Co(TPP)] *Mono* Alkyl Tolyl Radical Adduct (**I$^{A-Tol\cdot}$**)	Co: +0.04 TPP: 0 C (Carbene): 0 *C*H$_2$: +0.73 Ph: +0.22	

[Co(TPP)] *Bis*-Terminal Carbene Toluene Adduct (**I**$^{\mathbf{T\text{–}T\text{–}Tol}}$)	Co: –0.20 TPP: +0.01 C^{T} (Carbene): +0.58 C^{T} (Carbene): +0.51 *C*H_2: 0 Ph: 0	
[Co(TPP)] *Mono*-Alkyl *Mono*-Terminal Carbene Tolyl Radical (**I**$^{\mathbf{A\text{–}T\text{–}Tol\cdot}}$)	Co: –0.06 TPP: –0.02 C^{T} (Carbene): +0.20 *C*H_2: +0.70 Ph: +0.26	
[Co(TPP)] *Mono*-Bridged *Mono*-Terminal Carbene Toluene Adduct (**I**$^{\mathbf{B\text{–}T\text{–}Tol}}$)	Co: +0.85 TPP: +0.10 C^{B} (Carbene): –0.03 C^{T} (Carbene): +0.03 *C*H_2: 0 Ph: 0	
[Co(TPP)] *Mono*-Alkyl *Mono*-Bridged Carbene Tolyl Radical (**I**$^{\mathbf{A\text{–}B\text{–}Tol\cdot}}$)	Co: 0 TPP: +0.01 C^{B} (Carbene): 0 *C*H_2: +0.76 Ph: +0.28	
[Co(TPP)] *Mono*-Enolate *Mono*-Terminal Carbene Toluene Adduct (**I**$^{\mathbf{E\text{–}T\text{–}Tol}}$)	Co: +0.18 TPP: +0.01 C^{E} (Carbene): 0 C^{T} (Carbene): +0.69 *C*H_2: 0 Ph: 0	

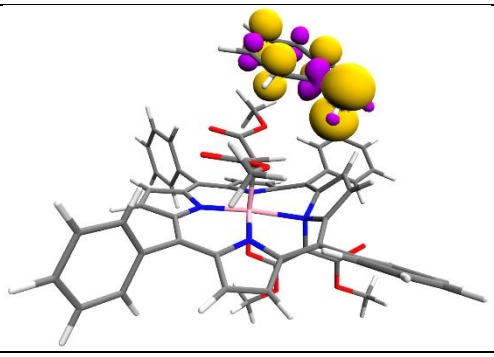
[Co(TPP)] *Mono*-Alkyl *Mono*-Enolate Adduct Tolyl Radical (**I**$^{\mathbf{A-E-Tol\cdot}}$)	Co: 0 TPP: 0 C (Carbene): 0 *C*H_2: +0.76 Ph: +0.28	

Table S32. Spin density plots for relevant diazo adducts (isovalue: 0.004; α: yellow; β: purple).

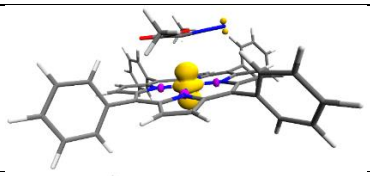
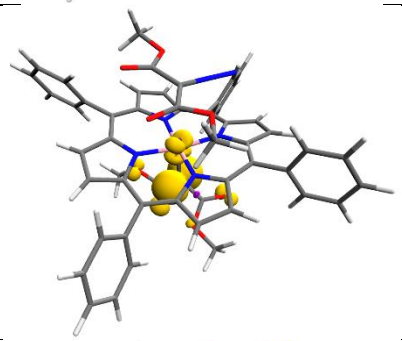
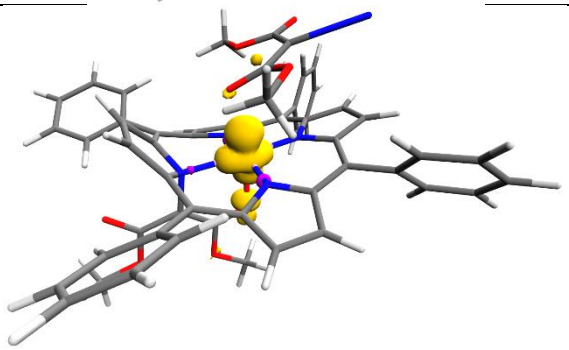
Structure	**Mulliken spin density**	**Plots**
[Co(TPP)] Diazo Adduct (**I**$^{\mathbf{D}}$)	Co: +1.13 TPP: –0.20 C (Carbene): 0.01	
[Co(TPP)] *Mono*-Diazo *Mono*-Terminal Carbene Adduct (**I**$^{\mathbf{D-T}}$)	Co: +0.15 TPP: –0.01 C^{D} (Carbene): 0 C^{T} (Carbene): +0.72	
[Co(TPP)] *Mono*-Diazo *Mono*-Enolate Adduct (**I**$^{\mathbf{D-E}}$)	Co: +0.98 TPP: –0.08 C^{D} (Carbene): 0 C^{E} (Carbene): 0	

Table S33. Spin density plots for quartet intermediates in the *bis*-carbenoid cycle (isovalue: 0.004; α: yellow; β: purple).

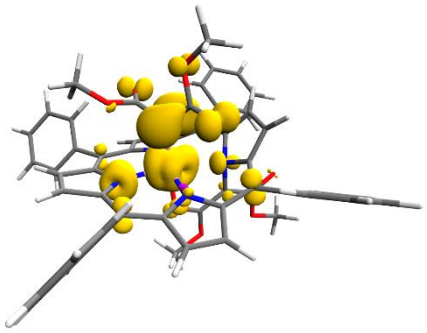
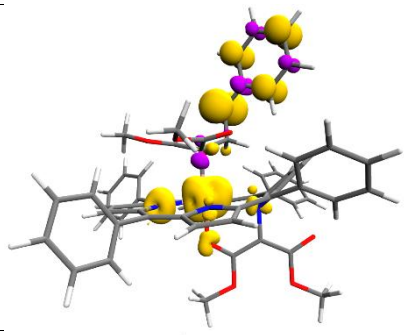
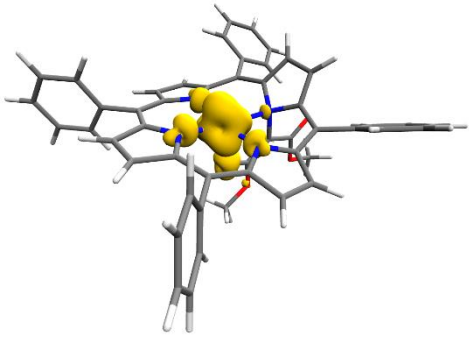
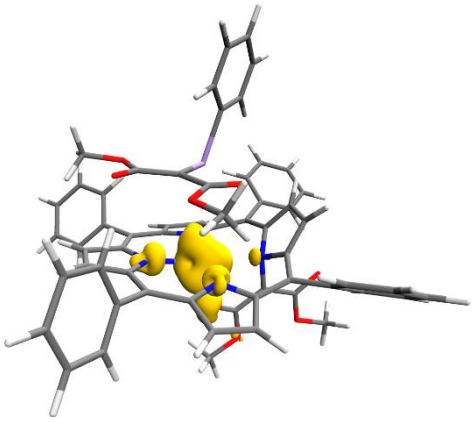
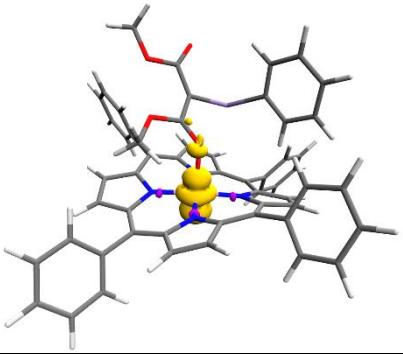
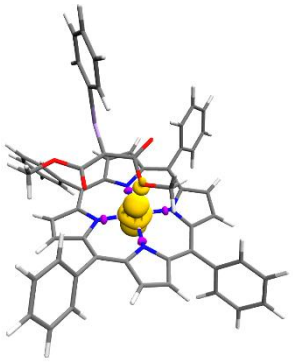
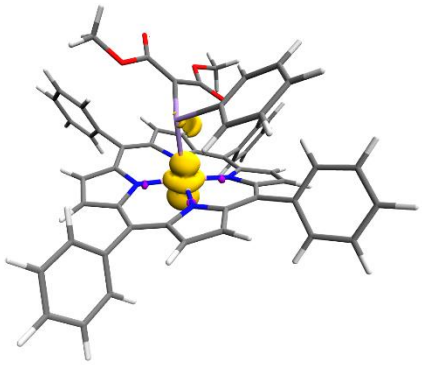
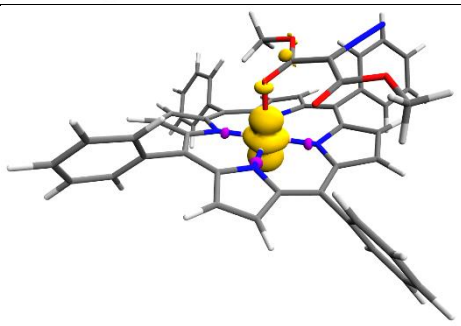
Structure	**Mulliken spin density**	**Plots**
[Co(TPP)] *Mono*-Enolate *Mono*-Terminal Carbene (**I^{E-T}**) (S = 3/2)	Co: +1.58 TPP: +0.46 C^{E} (Carbene): +0.04 C^{T} (Carbene): +0.65	
[Co(TPP)] *Mono*-Enolate *Mono*-Gamma Radical (**I^{E-G}**) (S = 3/2)	Co: +1.88 TPP: 0.31 C^{E} (Carbene): +0.02 C^{G} (Carbene): –0.04 Styryl: +0.78	
[Co(TPP)] Enolate (**I^{E}**) (S = 3/2)	Co: +2.57 TPP: +0.23 C (Carbene): 0	
[Co(TPP)] *Mono*-Enolate *Mono*-Iodonium Ylide (**I^{E-IY}**) (S = 3/2)	Co: +2.57 TPP: +0.26 C^{E} (Carbene): +0.01 C^{T} (Carbene): 0	

Table S34. Spin density plots for various coordination modes of DMM•IY and DMM•N_2 (isovalue: 0.004; α: yellow; β: purple).

Structure	Mulliken spin density	Plots
[Co(TPP)] *Mono* Iodonium Ylide Carbonyl Adduct (**$I^{IY(C=O)}$**)	Co: +1.09 TPP: –0.07 C (Carbene): +0.01	
[Co(TPP)] *Mono* Iodonium Ylide Methoxy Adduct (**$I^{IY(C-OMe)}$**)	Co: +1.13 TPP: –0.09 C (Carbene): 0	
[Co(TPP)] *Mono* Iodonium Ylide Iodine Adduct (**$I^{IY(IPh)}$**)	Co: +1.00 TPP: –0.06 C (Carbene): 0	
[Co(TPP)] *Mono* Diazo Carbonyl Adduct (**$I^{D(C=O)}$**)	Co: +1.11 TPP: –0.16 C (Carbene): +0.02	

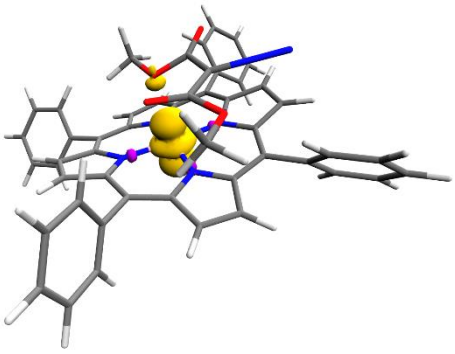
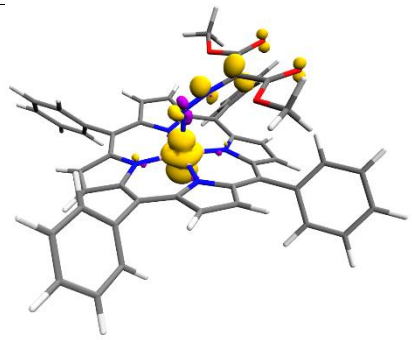
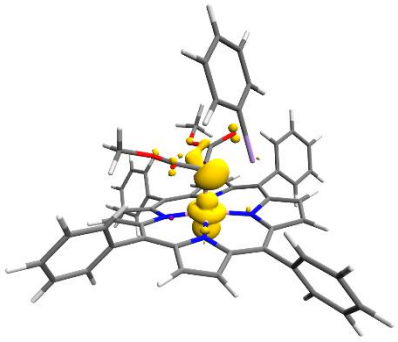
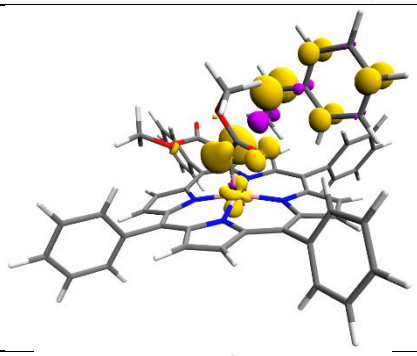
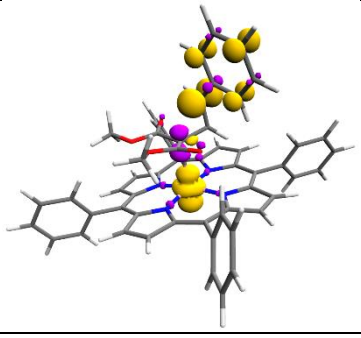
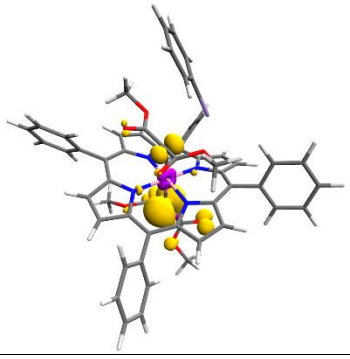
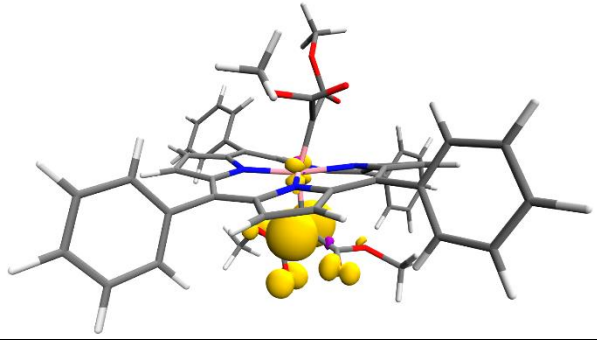
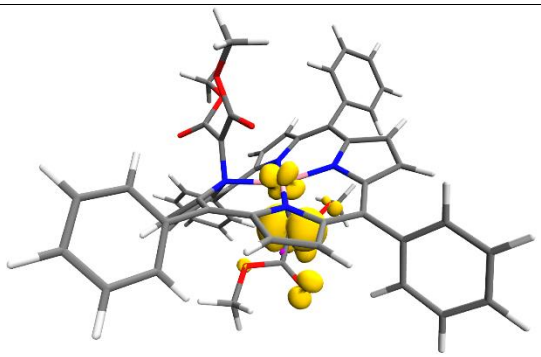
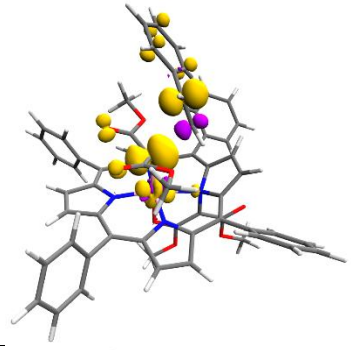
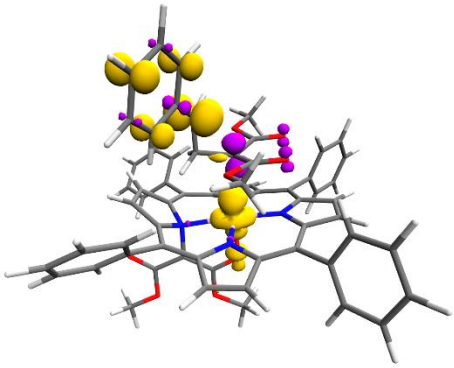
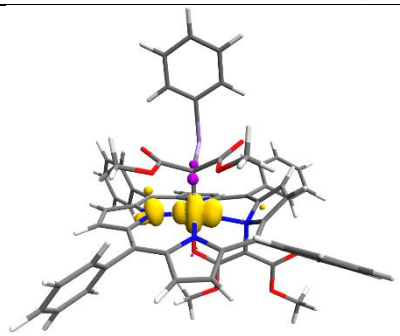
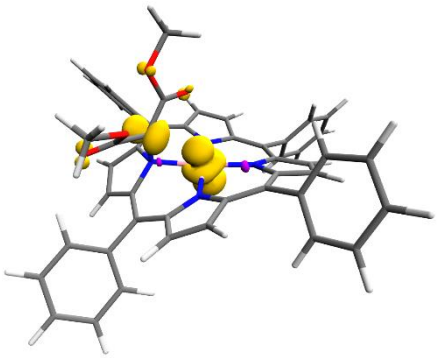
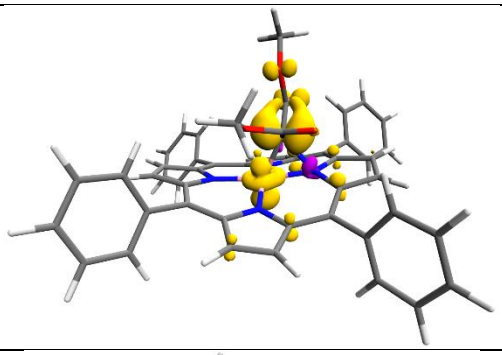
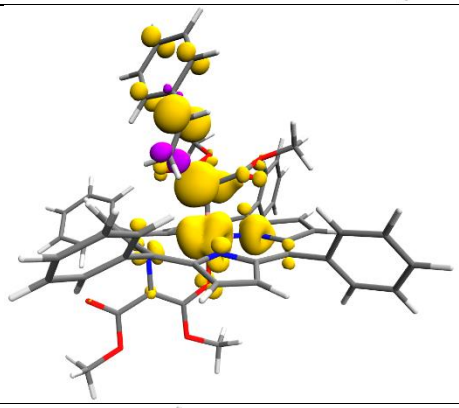
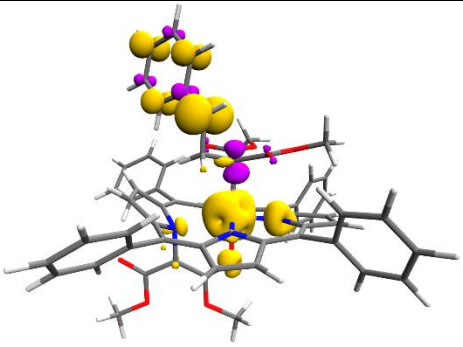
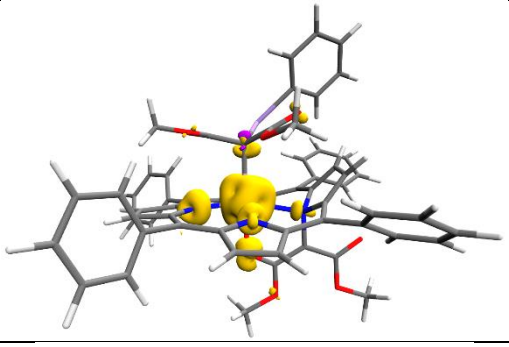
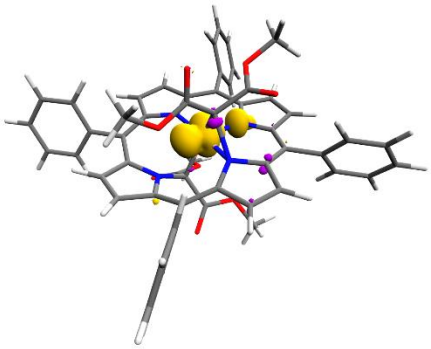
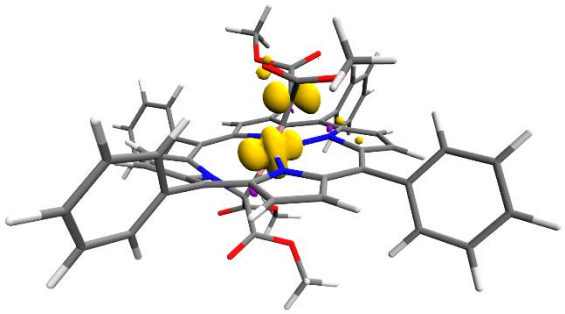
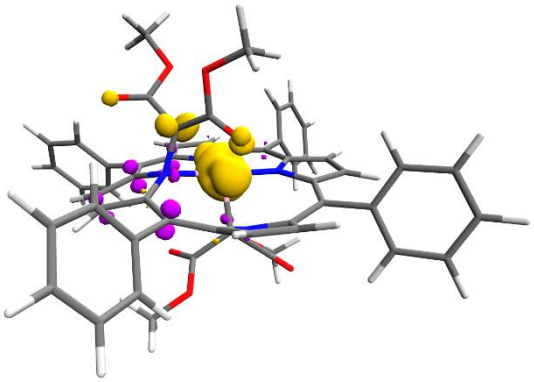
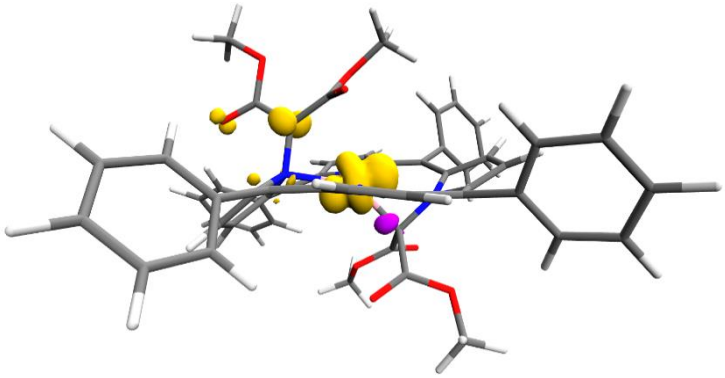
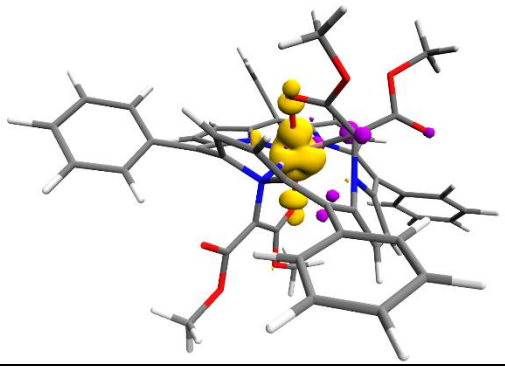
[Co(TPP)] *Mono* Diazo Methoxy Adduct ($\mathbf{I^{D(C\text{-}\mathit{O}Me)}}$)	Co: +1.15 TPP: –0.16 C (Carbene): 0	
[Co(TPP)] *Mono* Diazo Nitrogen Adduct ($\mathbf{I^{D(C=N=\mathit{N})}}$)	Co: +0.92 TPP: –0.02 C (Carbene): +0.09	

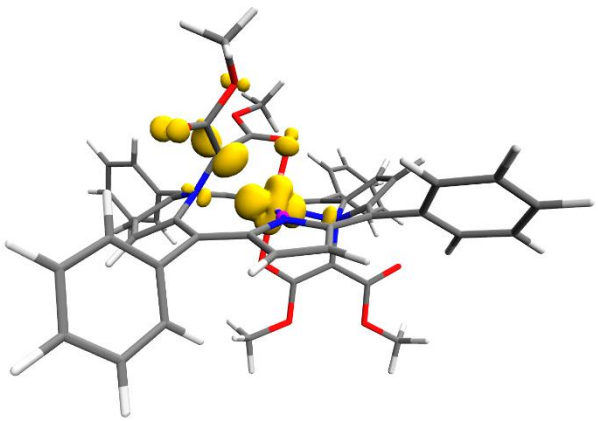
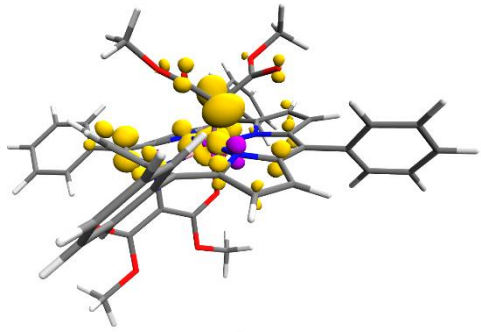
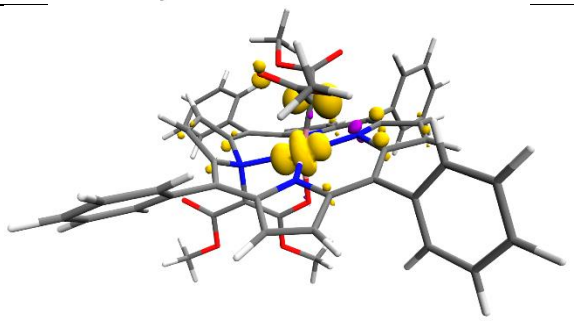
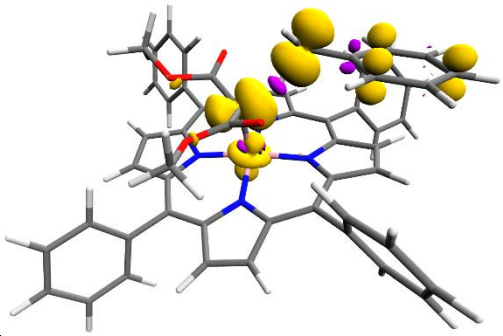
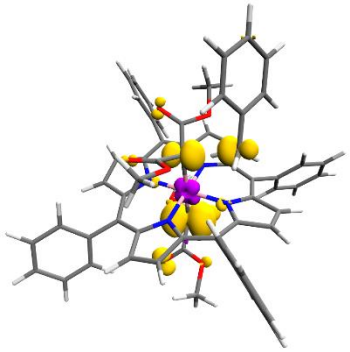
Table S35. Spin density plots for all transition states (isovalue: 0.004; α: yellow; β: purple).

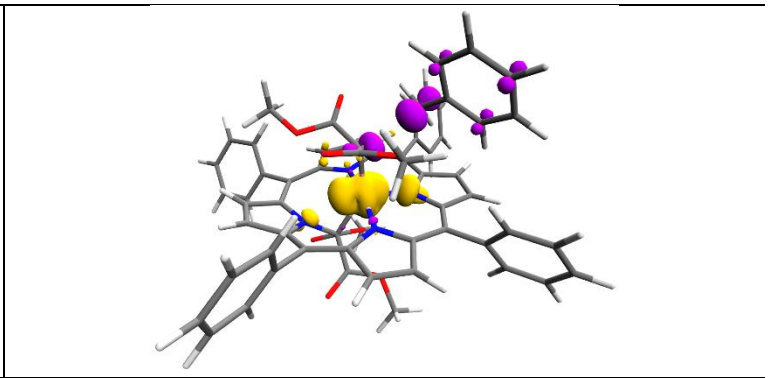
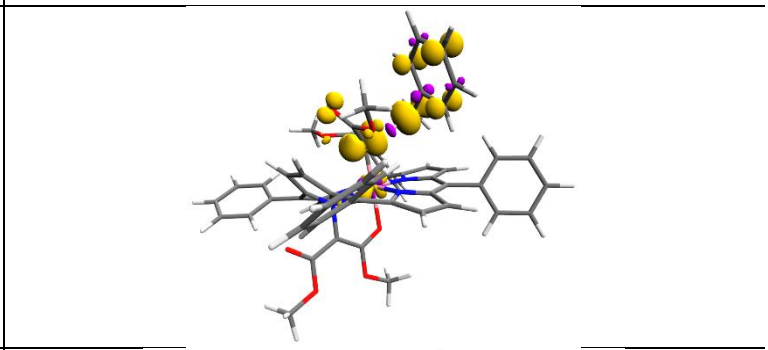
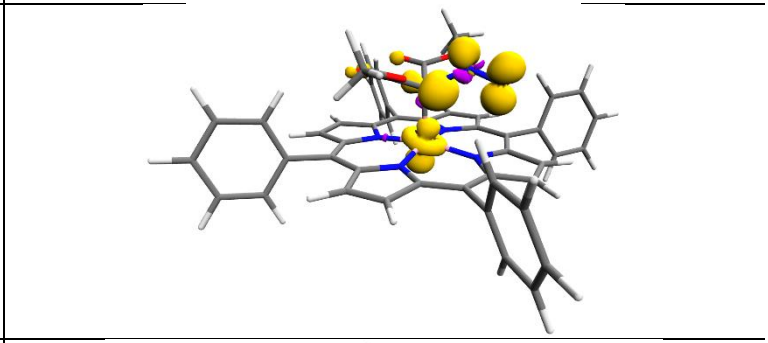
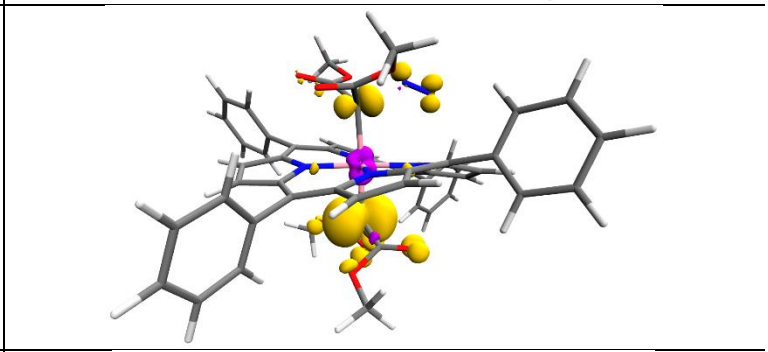
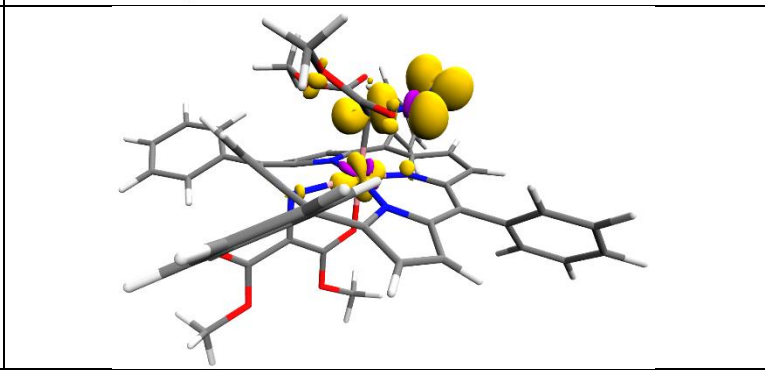
Structure	Mulliken spin density	Plots
TS1 (I^{IY}-I^{T})	Co: +0.70 TPP: –0.02 C (Carbene): +0.22	
TS2 (I^{T}-I^{G})	Co: +0.15 TPP: +0.43 C (Carbene): Styrene: +0.35	
TS3 (I^{G}-P)	Co: +0.81 TPP: –0.09 C (Carbene): –0.09 Styrene: +0.44	
TS4 ($I^{IY–T}$-$I^{T–T}$)	Co: –0.08 TPP: –0.01 C^{IY--T} (Carbene): +0.11 C^{T} (Carbene): +0.78	
TS5 ($I^{T–T}$-$I^{B–T}$)	Co: 0 TPP: 0 C^{T--B} (Carbene): 0 C^{T} (Carbene): +0.83	

TS6 (I^{B-T}-I^{E-T})	Co: +0.18 TPP: –0.02 C^{B--E} (Carbene): –0.02 C^{T} (Carbene): +0.69	
TS7 (I^{E-T}-I^{E-G})	Co: +0.24 TPP: +0.02 C^{T--G} (Carbene): +0.45 C^{E} (Carbene): 0 Styrene: +0.25	
TS8 (I^{E-G}-P)	Co: +0.67 TPP: –0.03 C^{G--P} (Carbene): –0.10 C^{E} (Carbene): 0 Styrene: +0.43	
TS9 (I^{E-IY}-I^{E-T})	Co: +0.87 TPP: +0.21 C^{IY--E} (Carbene): –0.04 C^{E} (Carbene): 0	
TS10 (I^{B}-I^{E})	Co: +0.96 TPP: –0.09 C (Carbene): +0.11	

TS11 (**I^{T}-I^{B}**)	Co: +0.43 TPP: +0.13 C (Carbene): +0.33	
TS12 (**I^{E-T}-I^{E-G}**) (S = 3/2)	Co: +1.62 TPP: +0.42 C^{T--G} (Carbene): +0.49 C^{E} (Carbene): +0.03 Styrene: +0.31	
TS13 (**I^{E-G}-P**) (S = 3/2)	Co: +2.15 TPP: +0.27 C^{G--P} (Carbene): –0.11 C^{E} (Carbene): +0.03 Styrene: +0.62	
TS14 (**I^{E-IY}-I^{E-T}**) (S = 3/2)	Co: +2.55 TPP: +0.30 C^{IY--E} (Carbene): 0 C^{E} (Carbene): 0	
TS15 (**I^{B-T}-*c*-I^{B-B}**)	Co: +1.02 TPP: +0.05 C^{T--B} (Carbene): –0.03 C^{B} (Carbene): –0.03	

TS16 (**I**$^{B-T}$-***t***-**I**$^{B-B}$)	Co: +0.82 TPP: +0.10 C^{T-B} (Carbene): +0.13 C^{B} (Carbene): –0.05	
TS17 (***c***-**I**$^{B-B}$-***c***-**I**$^{B-E}$)	Co: +1.03 TPP: –0.14 C^{B-E} (Carbene): +0.08 C^{B} (Carbene): –0.03	
TS18 (***t***-**I**$^{B-B}$-***t***-**I**$^{B-E}$)	Co: +0.92 TPP: +0.03 C^{B-E} (Carbene): +0.08 C^{B} (Carbene): –0.05	
TS19 (***c***-**I**$^{B-E}$-***c***-**I**$^{E-E}$)	Co: +1.09 TPP: –0.11 C^{B-E} (Carbene): –0.06 C^{E} (Carbene): 0	

TS20 (***t*-I$^{B–E}$-*t*-I$^{E–E}$**)	Co: +0.91 TPP: –0.07 C^{B--E} (Carbene): +0.12 C^{E} (Carbene): 0	
TS21 (I$^{E–T}$-*c*-I$^{B–E}$)	Co: +0.26 TPP: +0.49 C^{T--B} (Carbene): +0.20 C^{E} (Carbene): 0	
TS22 (I$^{E–T}$-*t*-I$^{B–E}$)	Co: +0.62 TPP: +0.26 C^{T--B} (Carbene): +0.13 C^{E} (Carbene): 0	
TS23 (I^{T}-I^{A})	Co: +0.21 TPP: –0.04 C (Carbene): +0.37 *C*H$_3$: +0.33 Ph: +0.14	
TS24 (I$^{T–T}$-I$^{A–T}$)	Co: –0.12 TPP: 0 C^{T--A} (Carbene): +0.18 C^{T} (Carbene): +0.71 *C*H$_3$: +0.11 Ph: +0.05	

TS25 (I^{B-T}-I^{A-B})	Co: +1.10 TPP: C^{T-A} (Carbene): –0.05 C^{B} (Carbene): –0.03 *C*H_3: –0.15 Ph: –0.06	
TS26 (I^{E-T}-I^{E-A})	Co: +0.05 TPP: +0.01 C^{T-A} (Carbene): +0.39 C^{E} (Carbene): 0 *C*H_3: +0.38 Ph: +0.17	
TS30 (I^{D}-I^{T})	Co: +0.49 TPP: –0.02 C (Carbene): +0.24	
TS31 (I^{D-T}-I^{T-T})	Co: –0.07 TPP: –0.03 C^{D-T} (Carbene): +0.10 C^{T} (Carbene): +0.80	
TS32 (I^{D-E}-I^{E-T})	Co: +0.18 TPP: +0.02 C^{D-T} (Carbene): +0.23 C^{E} (Carbene): 0	

Graphical representation of all DFT structures

(BP86/def2-TZVP)

Table S36. Graphical representation of miscellaneous reaction components.

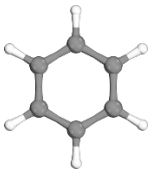
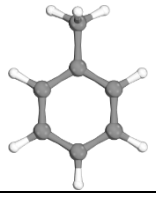
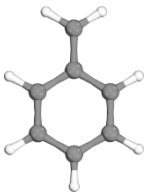
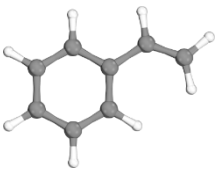
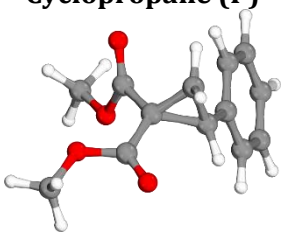
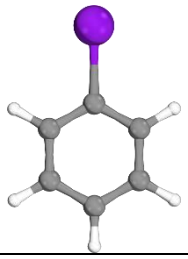
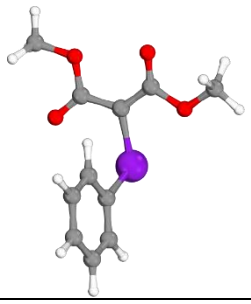
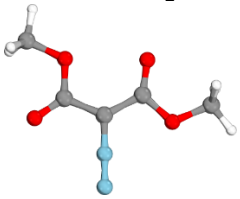
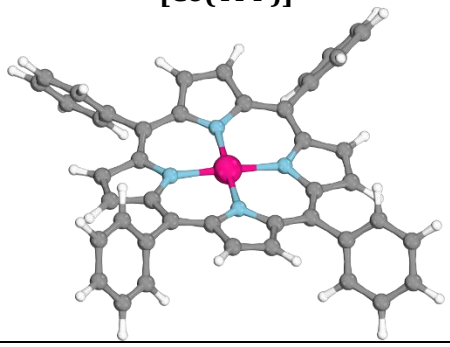
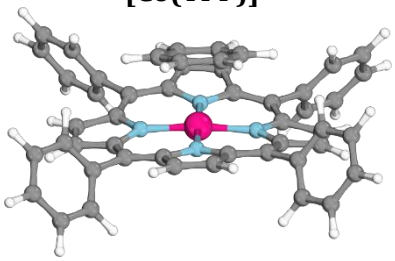
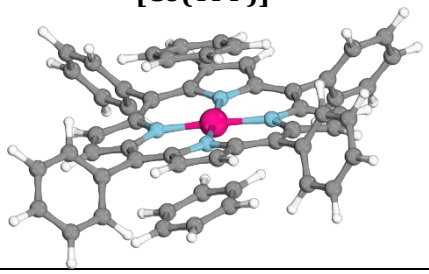
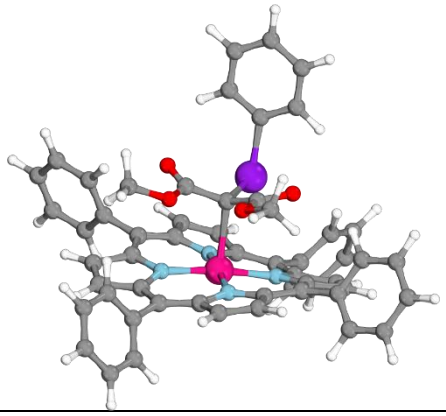
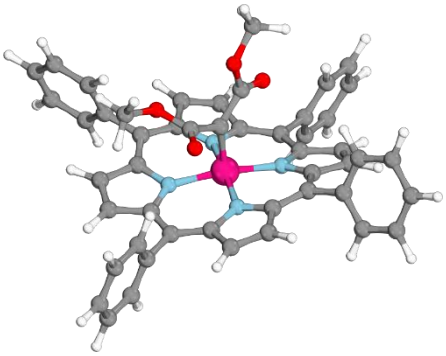
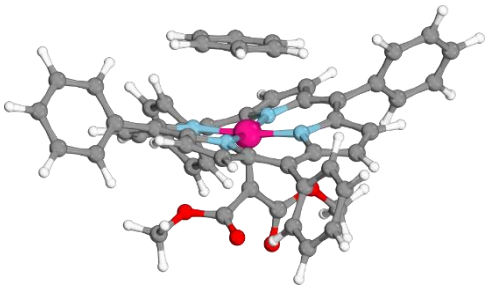
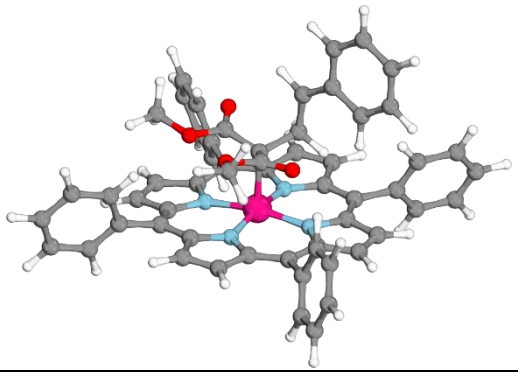
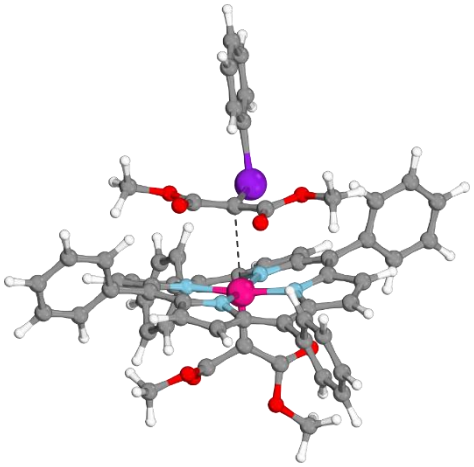
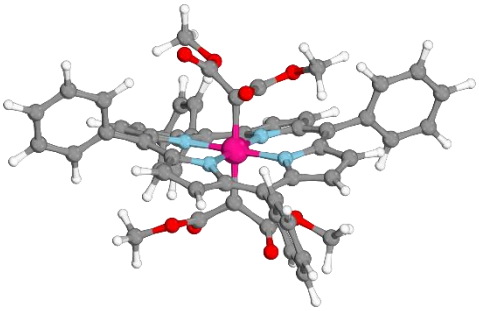
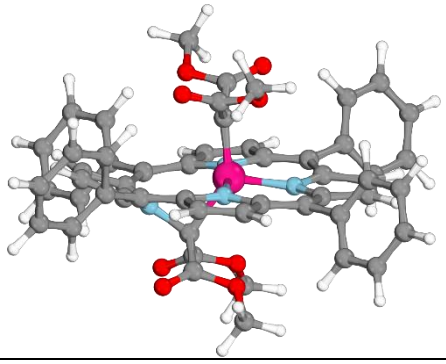
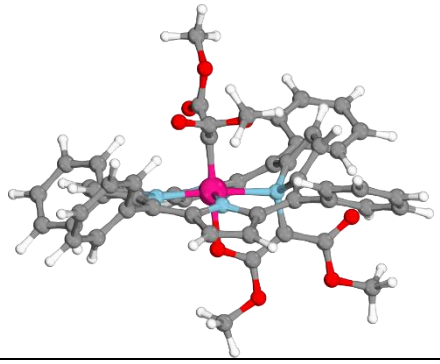
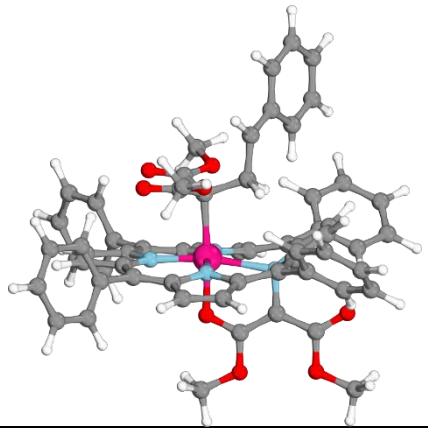
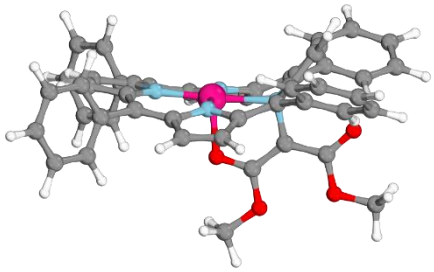
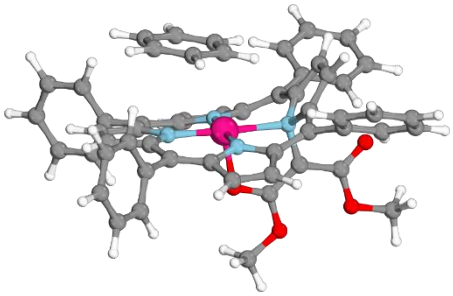
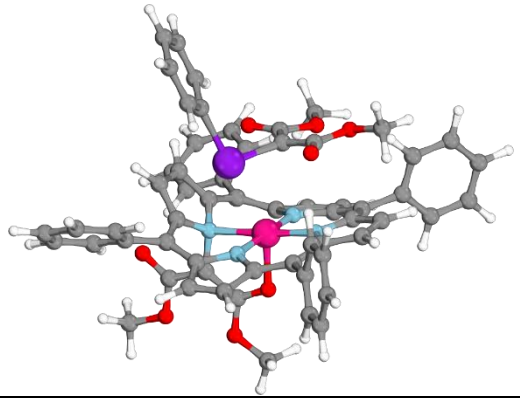
Benzene 	**Toluene** 
Tolyl radical 	**Styrene** 
Cyclopropane (P) 	**Iodobenzene** 
DMM•IY 	**N_2** 
DMM·N_2 	**[Co(TPP)]** 

Table S37. Graphical representation of catalytic intermediates.

[Co(TPP)]*	**[Co(TPP)]****
	
I^{IY}	**I^{T}**
	
I^{T*}	**I^{G}**
	
I^{IY-T}	**I^{T-T}**
	

$^{B-T}$	$^{E-T}$
	
$^{E-G}$	^{E}
	
^{E*}	$^{E-IY}$
	

^{B}

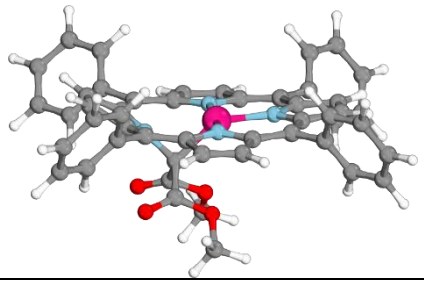


Table S38. Graphical representation of bridging intermediates in deactivation pathways.

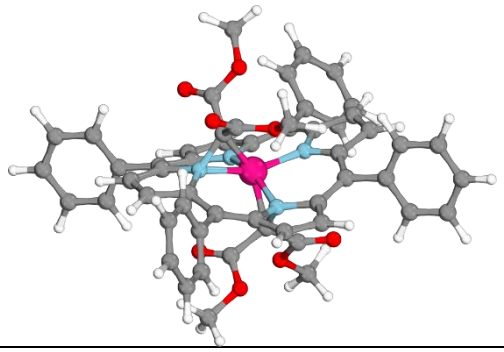
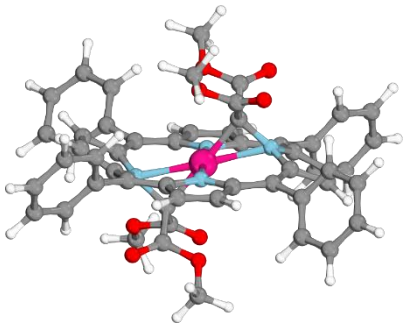
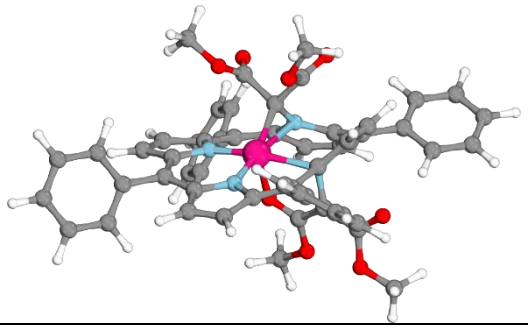
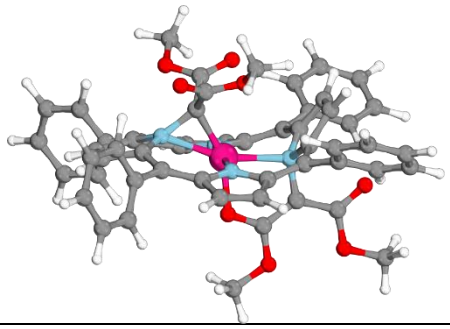
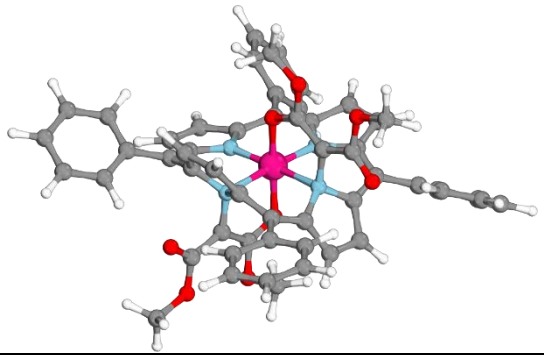
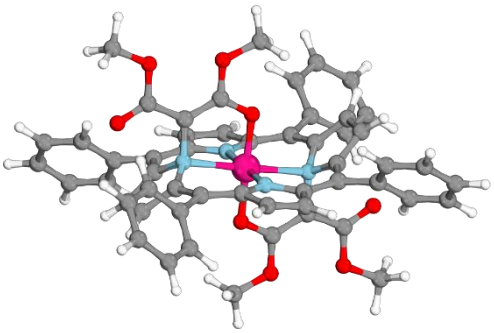
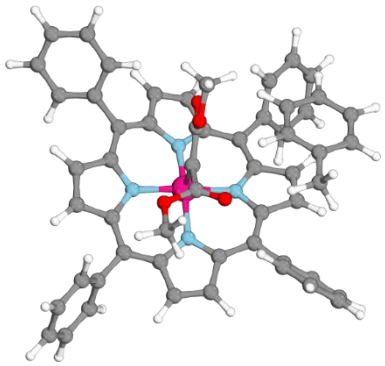
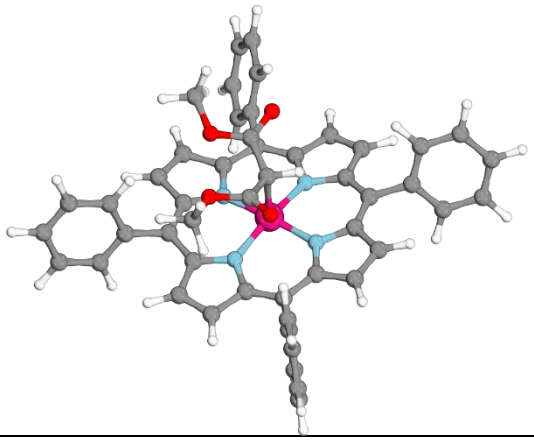
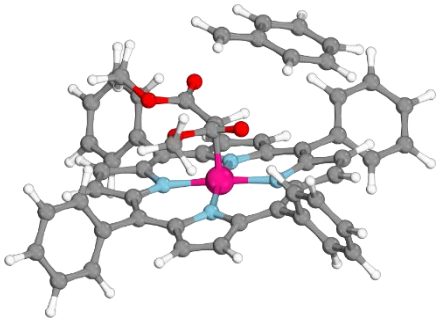
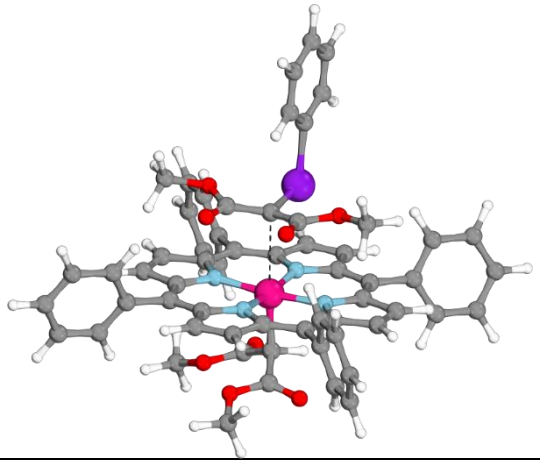
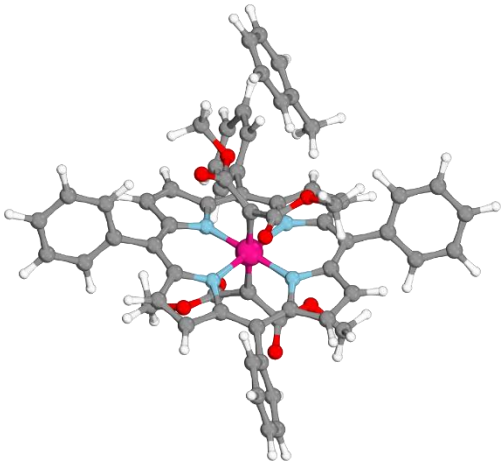
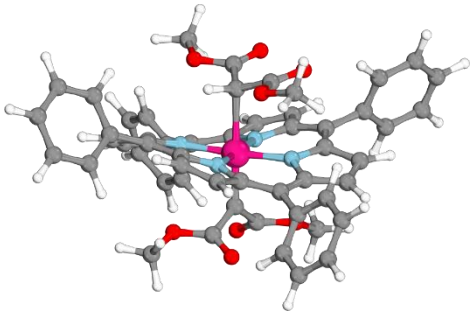
***c*-I^{B-B}** 	***t*-I^{B-B}** 
***c*-I^{B-E}** 	***t*-I^{B-E}** 
***c*-I^{E-E}** 	***t*-I^{E-E}** 

Table S39. Graphical representation of intermediates in HAT deactivation pathways.

$^{T-Tol}$ 	^{A} 
$^{A-Tol\cdot}$ 	$^{A-IY}$ 
$^{T-T-Tol}$ 	$^{A-T}$ 

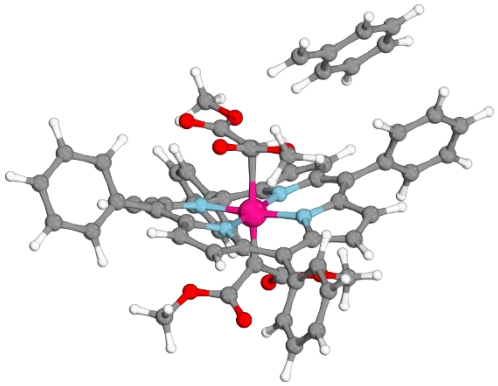
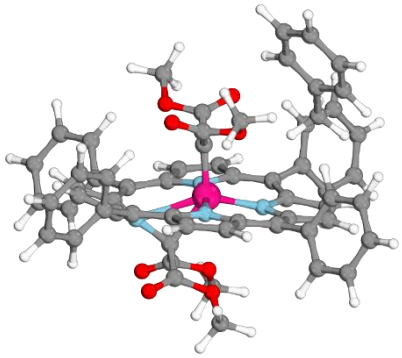
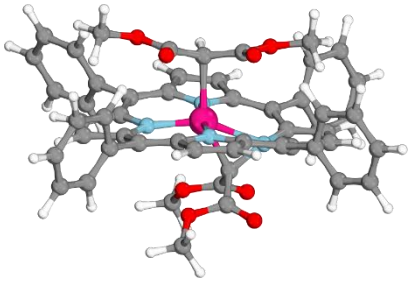
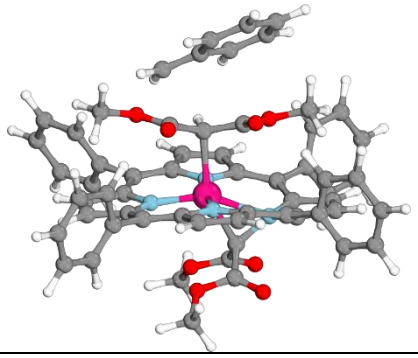
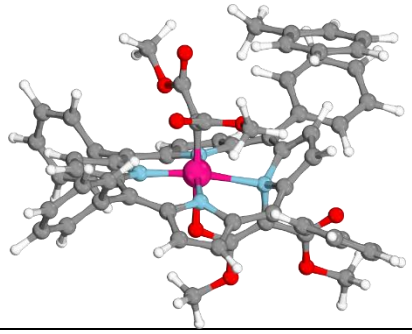
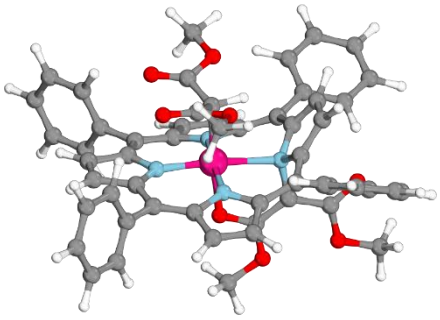
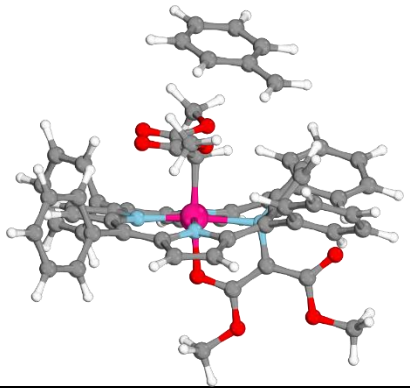
[A–T–Tol· 	**[B–T–Tol** 
[A–B 	**[A–B–Tol·** 
[E–T–Tol 	**[E–A** 
[E–A–Tol· 	

Table S40. Graphical representation of quartet intermediates in the *bis*-carbenoid cycle.

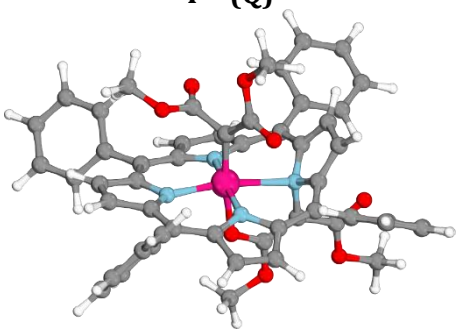
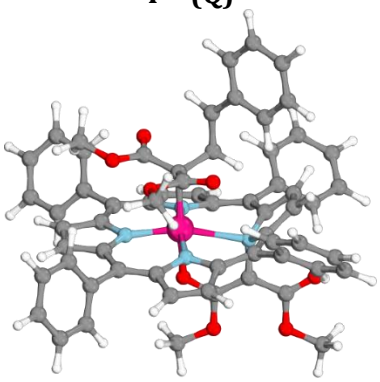
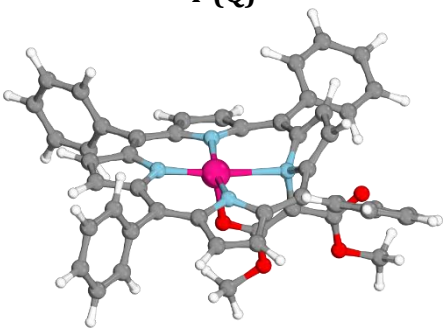
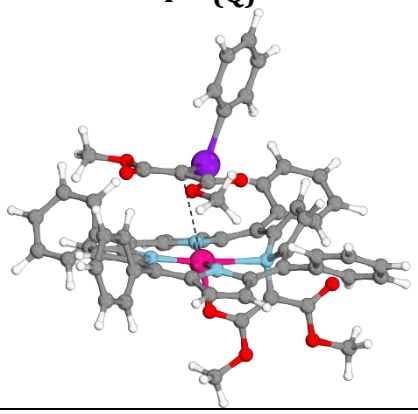
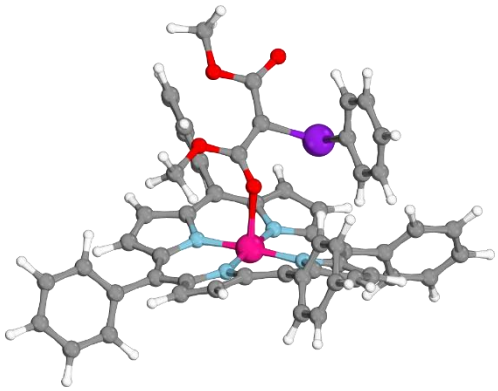
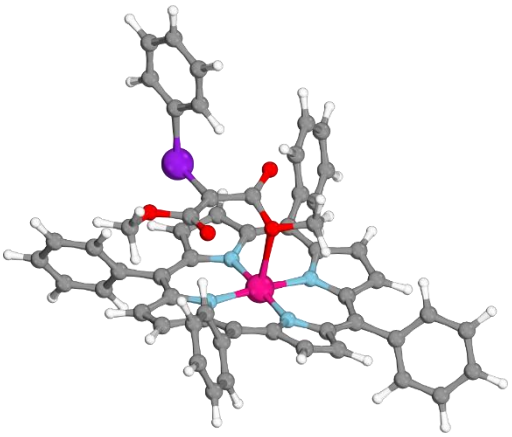
$\mathbf{I^{E-T}(Q)}$ 	$\mathbf{I^{E-G}(Q)}$ 
$\mathbf{I^{E}(Q)}$ 	$\mathbf{I^{E-IY}(Q)}$ 

Table S41. Graphical representation of various coordination modes of DMM·IY and DMM·N_2.

$\mathbf{I^{IY(C=}}\mathbf{\textit{O}}\mathbf{)}$ 	$\mathbf{I^{IY(}}\mathbf{\textit{O}}\mathbf{Me)}$ 

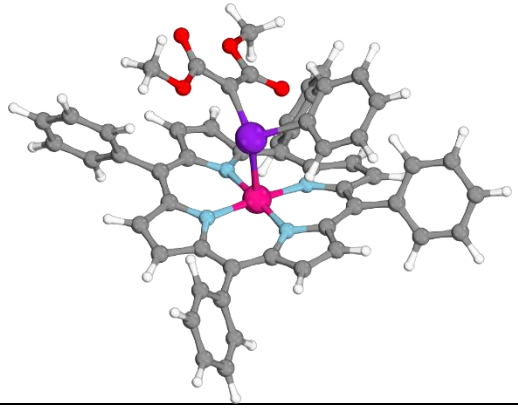
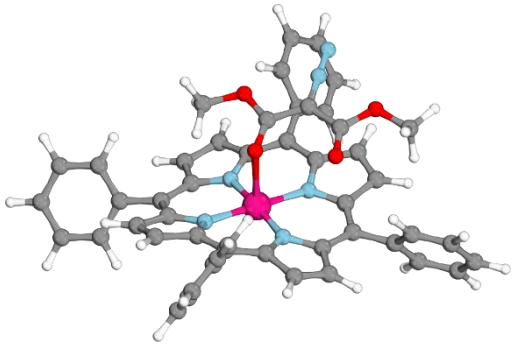
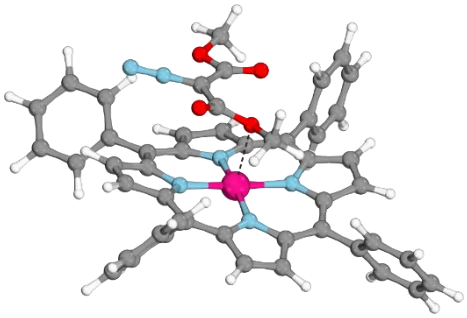
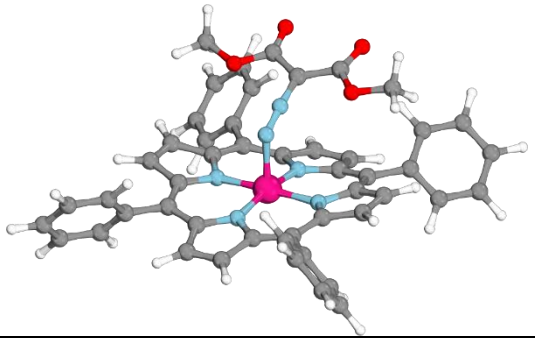
I^{IY}(*I*Ph) 	**I^{D}(C=*O*)** 
I^{D}(*O*Me) 	**I^{D}(C=N=*N*)** 

Table S42. Graphical representation of *bis*-carbenoid diazo adducts.

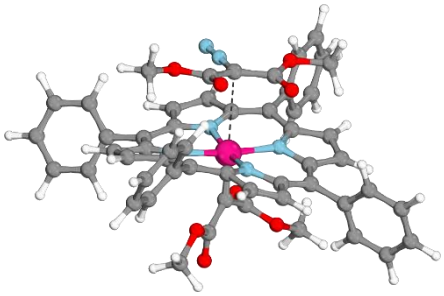
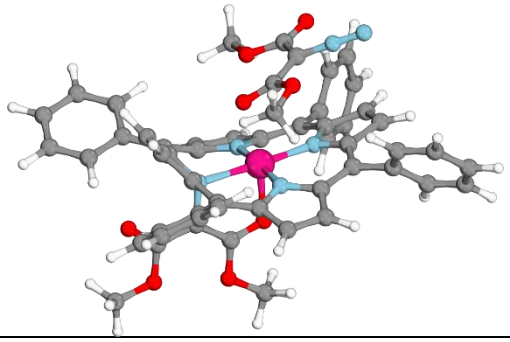
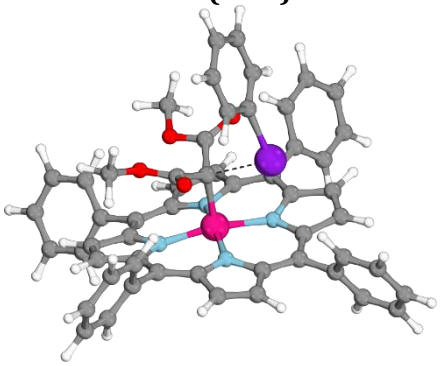
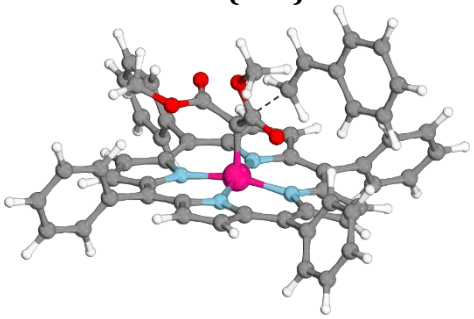
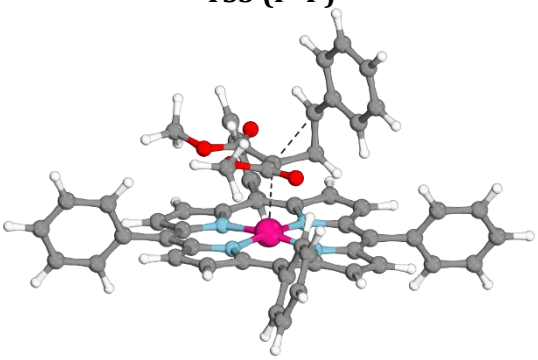
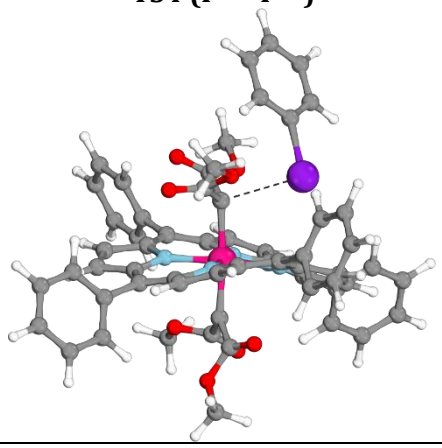
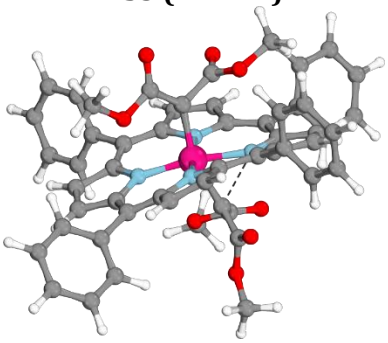
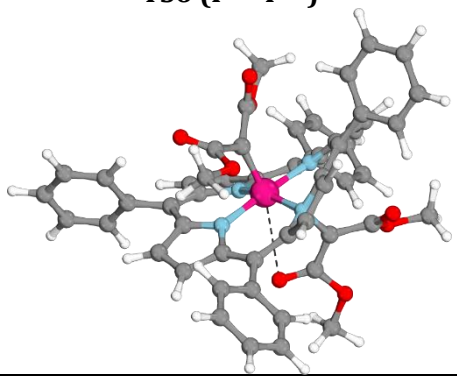
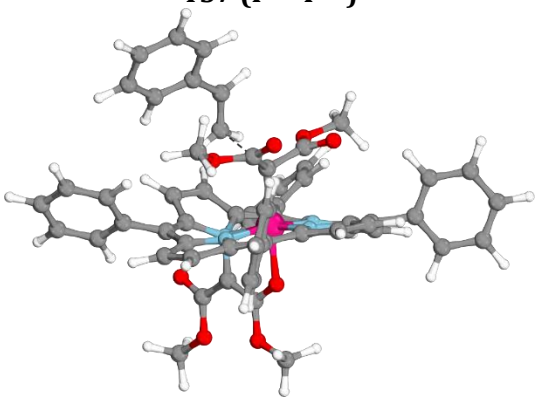
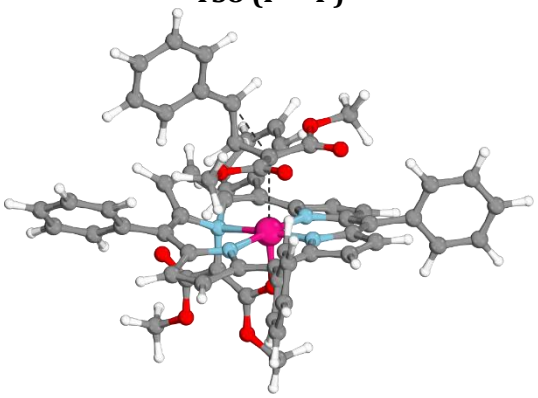
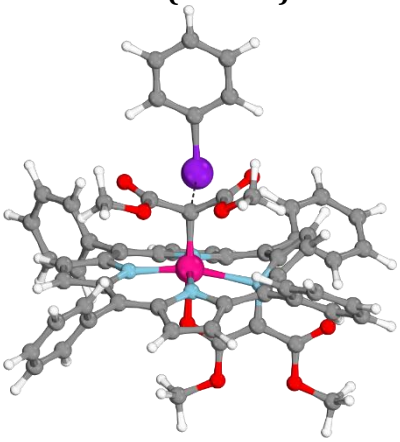
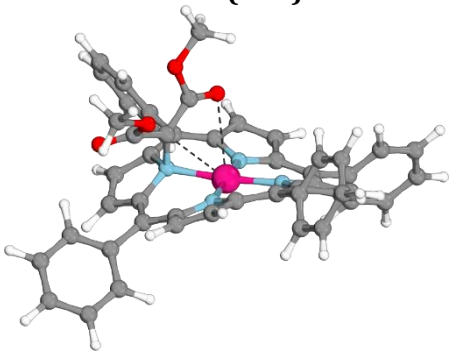
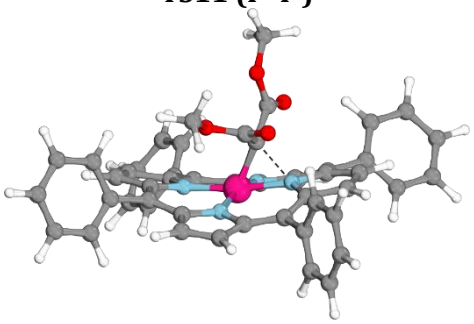
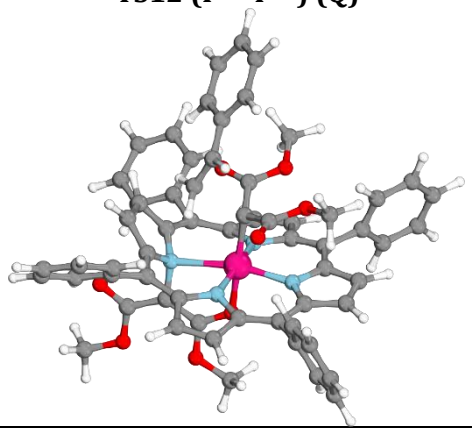
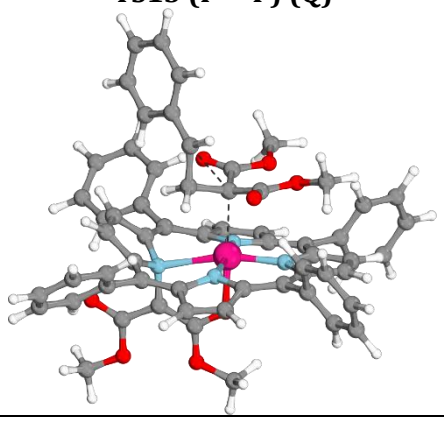
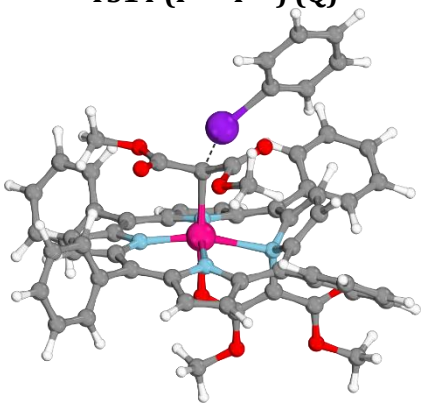
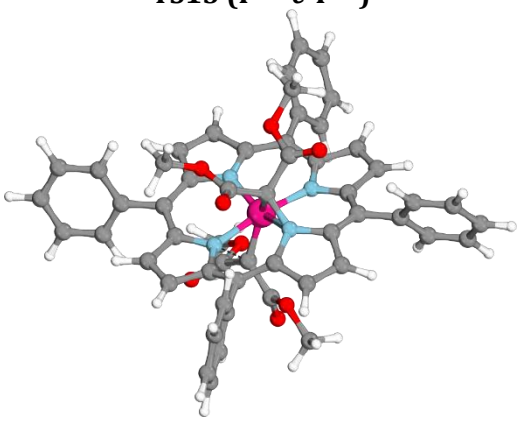
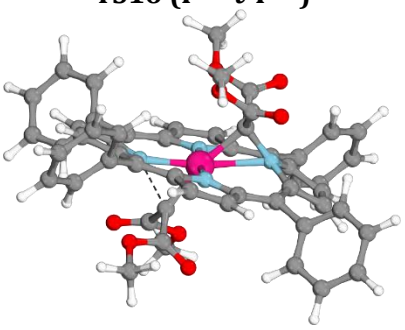
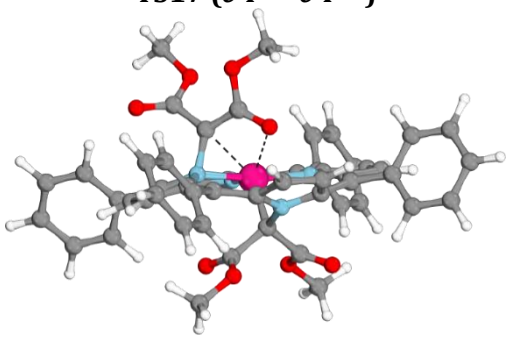
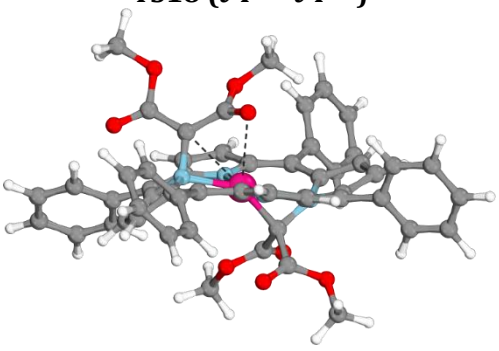
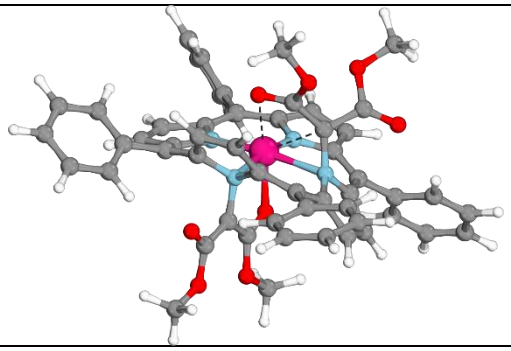
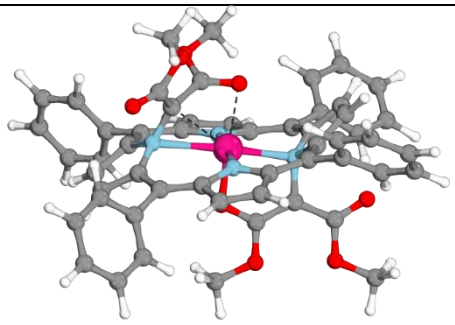
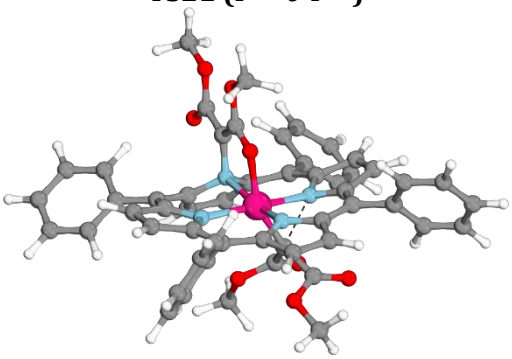
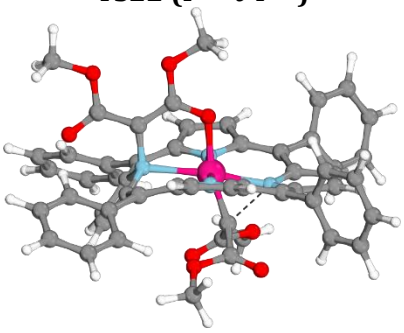
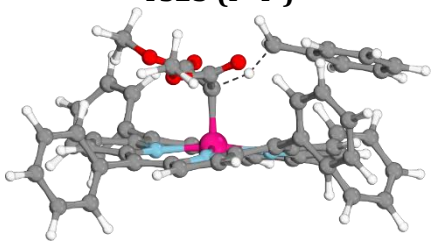
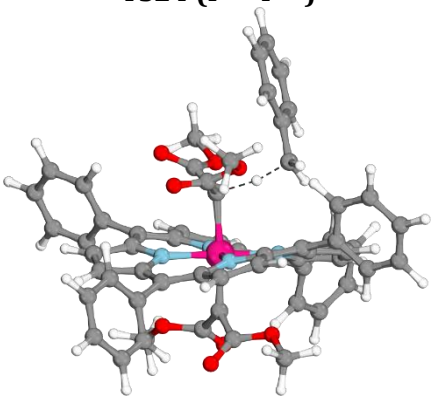
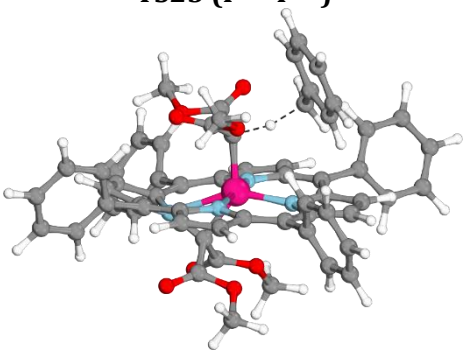
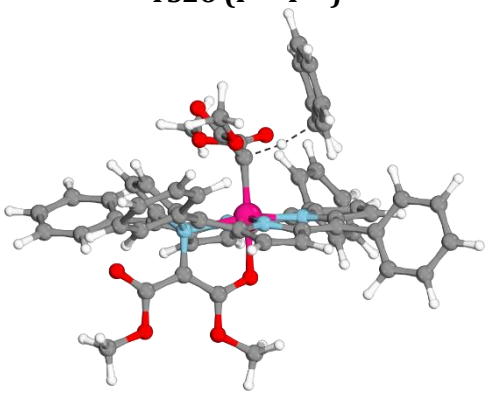
I^{D-T} 	**I^{D-E}** 

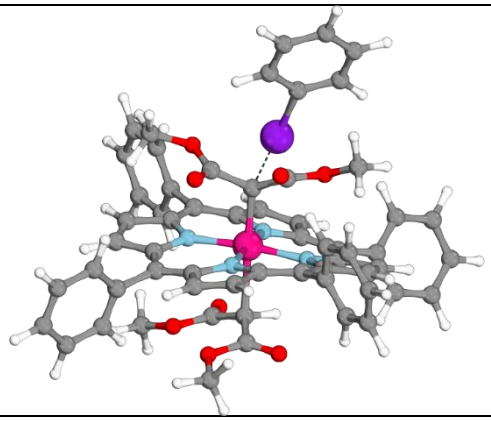
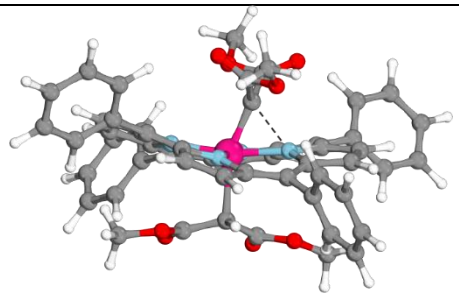
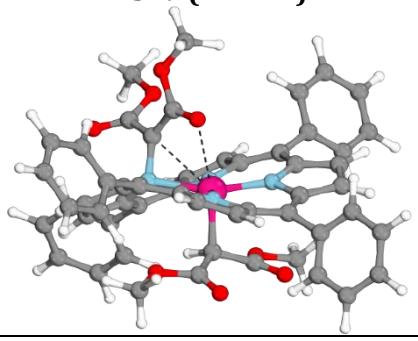
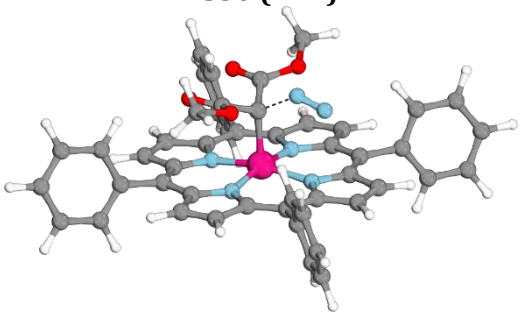
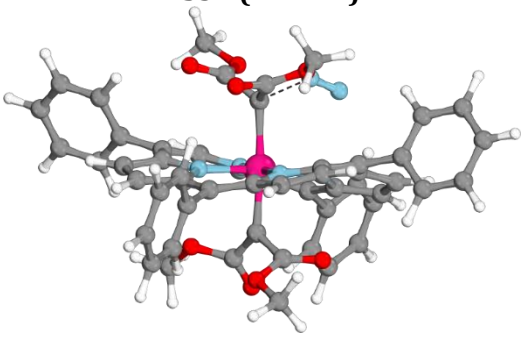
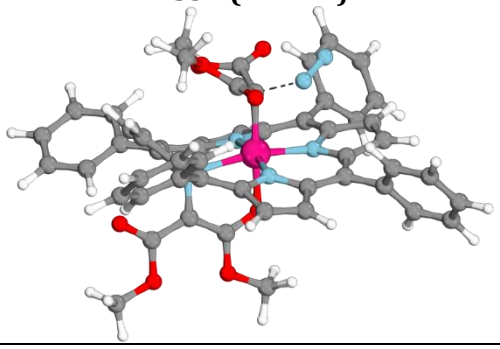
Table S43. Graphical representation of all transition states.

TS1 (I^{IY}-I^{T}) 	**TS2 (I^{T}-I^{G})** 

TS3 (I^{G}-P) 	**TS4 (I^{IY-T}-I^{T-T})** 
TS5 (I^{T-T}-I^{B-T}) 	**TS6 (I^{B-T}-I^{E-T})** 
TS7 (I^{E-T}-I^{E-G}) 	**TS8 (I^{E-G}-P)** 
TS9 (I^{E-IY}-I^{E-T}) 	**TS10 (I^{E}-I^{B})** 

TS11 (I^{B}-I^{T})	**TS12 (I^{E-T}-I^{E-G}) (Q)**
	
TS13 (I^{E-G}-P) (Q)	**TS14 (I^{E-IY}-I^{E-T}) (Q)**
	
TS15 (I^{B-T}-*c*-I^{B-B})	**TS16 (I^{B-T}-*t*-I^{B-B})**
	
TS17 (*c*-I^{B-B}-*c*-I^{B-E})	**TS18 (*t*-I^{B-B}-*t*-I^{B-E})**
	
TS19 (*c*-I^{B-E}-*c*-I^{E-E})	**TS20 (*t*-I^{B-E}-*t*-I^{E-E})**

	
TS21 (I^{E-T}-*c*-I^{B-E})	**TS22 (I^{E-T}-*t*-I^{B-E})**
	
TS23 (I^{T}-I^{A})	**TS24 (I^{T-T}-I^{A-T})**
	
TS25 (I^{B-T}-I^{A-B})	**TS26 (I^{E-T}-I^{E-A})**
	
TS27 (I^{A-IY}-I^{A-T})	**TS28 (I^{A-T}-I^{A-B})**

	
TS29 (I^{A-B}-I^{E-A}) 	**TS30 (I^{D}-I^{T})** 
TS31 (I^{D-T}-I^{T-T}) 	**TS32 (I^{D-E}-I^{E-T})** 

List of xyz coordinates for all reported structures:

Benzene:
12 atoms

H	0.0000000	0.0000000	–0.0271599
C	0.0000000	0.0000000	1.0639436
C	0.0000000	0.0000000	3.8600564
C	0.0000000	–1.2107550	1.7629670
C	0.0000000	1.2107550	1.7629670
C	0.0000000	1.2107550	3.1610330
C	0.0000000	–1.2107550	3.1610330
H	0.0000000	–2.1556927	1.2174264
H	0.0000000	2.1556927	1.2174264
H	0.0000000	2.1556927	3.7065736
H	0.0000000	–2.1556927	3.7065736
H	0.0000000	0.0000000	4.9511599

Toluene:
15 atoms

C	–0.0177326	0.0002821	1.0514749
C	0.0112942	0.0000478	3.8739519
C	–0.0104550	–1.2032317	1.7722827
C	–0.0146252	1.2035642	1.7724529
C	0.0005764	1.2066687	3.1693273
C	0.0047712	–1.2065522	3.1690204
H	–0.0191162	–2.1513696	1.2296907
H	–0.0265591	2.1517891	1.2300879
H	–0.0000059	2.1550716	3.7091570
H	0.0075018	–2.1550308	3.7087011
H	0.0200613	–0.0000650	4.9647697
C	0.0010406	–0.0000371	–0.4568020
H	1.0355547	–0.0141070	–0.8357151
H	–0.4848261	0.8963137	–0.8663059
H	–0.5084802	–0.8833438	–0.8660933

Tolyl radical:
14 atoms

C	–0.1352124	–0.0000000	1.0385733
C	0.0535338	–0.0000000	3.8707509
C	–0.0854911	–1.2196419	1.7819475
C	–0.0854913	1.2196418	1.7819475
C	0.0066760	1.2132778	3.1654750
C	0.0066758	–1.2132778	3.1654751
H	–0.1216228	–2.1665880	1.2396349
H	–0.1216237	2.1665879	1.2396349
H	0.0429469	2.1583828	3.7097982
H	0.0429470	–2.1583829	3.7097983
H	0.1259145	0.0000001	4.9587234
C	–0.2292741	0.0000001	–0.3639676
H	–0.2669881	0.9330904	–0.9253958
H	–0.2669905	–0.9330902	–0.9253958

Styrene:
16 atoms

H	1.3587538	0.3400343	0.2221206
C	0.7880445	0.2441703	1.1486822
C	–0.6672153	0.0069091	3.5088988
C	0.1160489	–0.9641512	1.4146782
C	0.7355070	1.3153268	2.0416785
C	0.0068944	1.2014928	3.2273600
C	–0.6139082	–1.0602683	2.6163815
H	1.2646854	2.2409488	1.8102741
H	–0.0376547	2.0356691	3.9286984
H	–1.1477193	–1.9810118	2.8552239
H	–1.2395066	–0.0904145	4.4328161
C	0.2035064	–2.0569540	0.4368340
H	0.8078876	–1.8279334	–0.4475135
C	–0.3654291	–3.2705043	0.5121671
H	–0.2280694	–4.0026645	–0.2831039
H	–0.9828254	–3.5806491	1.3568041

Cyclopropane:
31 atoms

H	0.0040647	0.3804787	0.0095243
C	–0.0131732	0.1367433	1.0739586
C	–1.4461089	0.2989574	1.6574813
C	–0.8267659	–1.0655845	1.4283128
H	–1.2382880	–1.6479372	0.6053905
H	–0.5894451	–1.6206461	2.3349961
C	1.1637078	0.6257568	1.8433391
C	3.3729730	1.6817279	3.2411343
C	1.5352020	0.1074417	3.0943798
C	1.9225591	1.6783202	1.3046100
C	3.0177550	2.2004376	1.9928490
C	2.6269067	0.6343963	3.7873225
H	0.9618435	–0.7038163	3.5424265
H	1.6445549	2.0917748	0.3329559
H	3.5944742	3.0159737	1.5538759
H	2.8975983	0.2186757	4.7589847
H	4.2282528	2.0882717	3.7824450
C	–2.4970071	0.7191748	0.6805356
O	–2.4351658	0.5229392	–0.5199700
O	–3.5523837	1.3032547	1.2982491
C	–1.5191369	0.7864510	3.0795687
O	–1.5687272	0.0741721	4.0640116
O	–1.4432405	2.1357875	3.1208312
C	–1.4234097	2.7024365	4.4506642
H	–0.5438534	2.3406329	5.0001291
H	–2.3321754	2.4252417	5.0012881
H	–1.3710292	3.7855886	4.3042006
C	–4.6237290	1.7137772	0.4174886
H	–5.0356916	0.8469462	–0.1162024
H	–4.2580858	2.4445409	–0.3160628
H	–5.3784756	2.1630848	1.0702820

Iodobenzene:
12 atoms

H	0.0000000	0.0003161	–0.0328243
C	0.0000000	0.0001603	1.0566093
C	0.0000000	0.0020352	3.8559266
C	0.0000000	–1.2061477	1.7632789
C	0.0000000	1.2033705	1.7672296
C	0.0000000	1.2171670	3.1645771
C	0.0000000	–1.2093581	3.1602270
H	0.0000000	–2.1471254	1.2111386
H	0.0000000	2.1607329	3.7091561
H	0.0000000	–2.1537130	3.7054379
H	0.0000000	0.0097338	4.9469003
I	0.0000000	3.0378284	0.7083430

DMM·IY:
27 atoms

C	–0.8223579	0.1530157	0.7874939
C	0.1977728	1.1666876	0.5932229
C	–1.2162575	–0.5275767	2.0184733
O	0.8851930	1.6529924	1.4783002
O	–1.9743007	–1.4953470	2.0740267
O	0.3399133	1.5362370	–0.7332722
O	–0.6452300	0.0226132	3.1238873
C	–0.9834078	–0.6398770	4.3597335
H	–0.4331589	–0.0940965	5.1334140
H	–0.6767352	–1.6948655	4.3362247
H	–2.0653085	–0.5923891	4.5459568
C	1.3568137	2.5293781	–0.9616348
H	1.3437708	2.7155736	–2.0410398
H	2.3428748	2.1600733	–0.6467971
H	1.1347594	3.4526872	–0.4086807
I	–1.8422414	–0.5651627	–0.8386291
C	–0.6284024	–2.2813248	–1.4013666
C	0.9488747	–4.4440259	–2.0532797
C	–0.9777201	–3.0426662	–2.5119674
C	0.4724284	–2.5570479	–0.6051197
C	1.2684602	–3.6565173	–0.9434734
C	–0.1693063	–4.1389238	–2.8343481
H	–1.8515401	–2.8045448	–3.1204435
H	0.7028971	–1.9282574	0.2586378
H	2.1390718	–3.8948145	–0.3311765
H	–0.4197822	–4.7524376	–3.7007804
H	1.5729191	–5.3003832	–2.3103619

N_2:
2 atoms

N	0.0000000	–1.9611573	0.5102107
N	0.0000000	–3.0308427	0.2427893

DMM·N_2:
17 atoms

C	–2.2084474	0.3848575	4.6984784
C	–3.1591165	1.0989663	5.5796424
C	–4.4032189	0.6070606	6.2047731
O	–1.2028665	0.9071702	4.2434423
O	–4.8573959	–0.5114659	6.0882998
O	–4.9825630	1.6006636	6.9453075
O	–2.5926732	–0.8860271	4.4717343
C	–1.6998961	–1.6364337	3.6144003
H	–0.6991478	–1.6991385	4.0620894
H	–1.6216429	–1.1591602	2.6285940
H	–2.1538753	–2.6284540	3.5328705
C	–6.2127671	1.2206987	7.6036267
H	–6.0361569	0.3894112	8.2990016
H	–6.9662359	0.9163865	6.8651107
H	–6.5383588	2.1152067	8.1435034
N	–2.8132164	2.3542756	5.8212334
N	–2.5124216	3.4259826	6.0238922

[Co(TPP)]:
77 atoms

C	3.1833135	3.5542293	–5.4023809
C	2.6435664	3.4155885	–6.6451684
C	1.4502493	2.6228693	–6.4987821
C	2.3061682	2.8718868	–4.4861534
N	1.2686854	2.2561783	–5.1738484
C	2.4394900	2.9227745	–3.0991617
C	1.5385652	2.2909198	–2.2411798
N	0.5346488	1.4132918	–2.6216787
C	–0.0525259	1.0027428	–1.4320937
C	1.5317406	2.4788237	–0.8135000
C	0.5347778	1.6963241	–0.3146390
C	–1.0013505	–0.0114242	–1.3062380
C	–1.5097693	–0.6956555	–2.4112145
N	–1.2956836	–0.3635179	–3.7404073
C	–2.6547396	–2.2423848	–3.5816803
C	–2.3395420	–1.8683513	–2.3105277
C	–1.6949213	–0.2631409	–6.6569247
N	–0.7249799	0.6500755	–6.2720119
C	–0.4266744	1.3637274	–7.4252612
C	–1.2778065	0.9473476	–8.5099860
C	–2.0497556	–0.0713350	–8.0393597
C	0.6140939	2.2814866	–7.5624499
C	–2.2678787	–1.2388119	–5.8401930
C	–2.0432454	–1.2828195	–4.4646610
H	4.0908121	4.0757154	–5.1178842
H	3.0193226	3.7965985	–7.5887738
H	2.1994924	3.1431341	–0.2753752
H	0.2201009	1.5853795	0.7173817
H	–3.2526189	–3.0876638	–3.9048846
H	–2.6227277	–2.3458800	–1.3786290
H	–1.2716826	1.3825321	–9.5034727
H	–2.8085350	–0.6398979	–8.5663218
Co	–0.0544154	0.9890160	–4.4519503
C	3.5526163	3.7137000	–2.5029113
C	5.6512360	5.1970768	–1.3551747
C	4.5642583	3.0733945	–1.7691203
C	3.6065526	5.1092646	–2.6495892
C	4.6470167	5.8454459	–2.0797114
C	5.6067457	3.8085784	–1.2015431
H	4.5260135	1.9895634	–1.6509098
H	2.8181878	5.6129409	–3.2107210
H	4.6701336	6.9298878	–2.1972632
H	6.3885300	3.2945828	–0.6403006
H	6.4646147	5.7720587	–0.9105133
C	0.8783613	2.8883043	–8.8973403
C	1.3918849	4.0497818	–11.4092170
C	0.7134573	4.2686954	–9.0951515
C	1.3081889	2.0993090	–9.9765981
C	1.5636382	2.6752313	–11.2225110
C	0.9659679	4.8449237	–10.3415972
H	0.3811657	4.8863633	–8.2595121
H	1.4469241	1.0278023	–9.8260731
H	1.9034483	2.0488660	–12.0486813
H	0.8262223	5.9180577	–10.4800077
H	1.5906191	4.4997888	–12.3828247
C	–3.1851833	–2.2355930	–6.4605371
C	–4.9109850	–4.1117618	–7.6540389
C	–4.5522379	–2.2562373	–6.1400983
C	–2.6970513	–3.1673119	–7.3909129
C	–3.5523815	–4.0993534	–7.9817008
C	–5.4086127	–3.1863493	–6.7322971
H	–4.9387018	–1.5290007	–5.4247721
H	–1.6360220	–3.1549022	–7.6442855
H	–3.1553762	–4.8206682	–8.6975226
H	–6.4692603	–3.1845467	–6.4768121
H	–5.5798474	–4.8389453	–8.1163588
C	–1.4593475	–0.4164686	0.0523757
C	–2.3431355	–1.1963479	2.6086938
C	–0.5700138	–0.9962348	0.9716531
C	–2.7991210	–0.2368571	0.4328508
C	–3.2374756	–0.6218491	1.7012871
C	–1.0081403	–1.3834222	2.2394701
H	0.4698211	–1.1470508	0.6784911
H	–3.4945753	0.2116571	–0.2779638
H	–4.2804253	–0.4693159	1.9827062
H	–0.3054268	–1.8382586	2.9391210
H	–2.6854585	–1.4985586	3.5993343

[Co(TPP)] *Mono*-Benzene ([Co(TPP)]*):
89 atoms

C	3.0751977	3.5123014	–5.2890721
C	2.5929933	3.3267033	–6.5486997
C	1.3903483	2.5422480	–6.4251883
C	2.1601325	2.8555714	–4.3903824
N	1.1502125	2.2234880	–5.0985693
C	2.2678525	2.9068109	–3.0023433
C	1.3638203	2.2629751	–2.1582963
N	0.3707056	1.3815033	–2.5536852
C	–0.1908083	0.9208376	–1.3718034
C	1.3668915	2.4133208	–0.7251564
C	0.3940291	1.5938298	–0.2387271
C	–1.1150859	–0.1181818	–1.2632176
C	–1.6471016	–0.7659871	–2.3791847
N	–1.4589450	–0.3908466	–3.7005196
C	–2.8364528	–2.2594039	–3.5751170
C	–2.4863664	–1.9345733	–2.2994656
C	–1.8549840	–0.2384179	–6.6197088

N	–0.8607561	0.6425720	–6.2239970
C	–0.4895455	1.3073692	–7.3828023
C	–1.3268759	0.9068857	–8.4856553
C	–2.1662766	–0.0568997	–8.0152760
C	0.5969355	2.1719580	–7.5103214
C	–2.4559267	–1.2058191	–5.8130055
C	–2.2287565	–1.2789312	–4.4385031
H	3.9694158	4.0444364	–4.9830673
H	3.0111842	3.6743034	–7.4872797
H	2.0242435	3.0788565	–0.1755801
H	0.0912728	1.4475853	0.7925483
H	–3.4543164	–3.0844737	–3.9129176
H	–2.7566460	–2.4401630	–1.3785484
H	–1.2699026	1.3188321	–9.4875397
H	–2.9401504	–0.5960627	–8.5512134
Co	–0.1601978	0.9232166	–4.3994088
C	3.3965226	3.6634147	–2.3926048
C	5.5489562	5.0629011	–1.2387877
C	4.3967255	2.9805788	–1.6816921
C	3.4898037	5.0588793	–2.5142405
C	4.5572394	5.7534448	–1.9412874
C	5.4656051	3.6734928	–1.1102829
H	4.3268628	1.8961633	–1.5841861
H	2.7123102	5.5950267	–3.0602909
H	4.6118202	6.8387046	–2.0397442
H	6.2371615	3.1266071	–0.5661087
H	6.3829593	5.6057059	–0.7917502
C	0.9516941	2.6884378	–8.8620059
C	1.6415733	3.6633250	–11.4111770
C	0.8548469	4.0582161	–9.1549738
C	1.4009207	1.8151307	–9.8658175
C	1.7437508	2.2978013	–11.1302428
C	1.1958255	4.5419935	–10.4197059
H	0.5059074	4.7410275	–8.3789239
H	1.4818144	0.7503731	–9.6418375
H	2.0961424	1.6060155	–11.8969114
H	1.1090602	5.6085974	–10.6325300
H	1.9085906	4.0412407	–12.3990594
C	–3.3880573	–2.1812794	–6.4453635
C	–5.1402681	–4.0241685	–7.6531167
C	–4.7550683	–2.1861938	–6.1239299
C	–2.9135191	–3.1127356	–7.3831770
C	–3.7816624	–4.0278745	–7.9815668
C	–5.6244547	–3.0998061	–6.7231095
H	–5.1308461	–1.4604373	–5.4012613
H	–1.8524038	–3.1132368	–7.6372324
H	–3.3949006	–4.7485377	–8.7037413
H	–6.6848470	–3.0860130	–6.4664261
H	–5.8193737	–4.7383088	–8.1209548
C	–1.5311788	–0.5782931	0.0917522
C	–2.3305128	–1.4562232	2.6445011
C	–0.6083059	–1.1757582	0.9655392
C	–2.8615268	–0.4298959	0.5164434
C	–3.2581098	–0.8639916	1.7828095
C	–1.0041871	–1.6115628	2.2315447
H	0.4253199	–1.2996640	0.6390677
H	–3.5827810	0.0335844	–0.1582367
H	–4.2945217	–0.7356093	2.0988013
H	–0.2753116	–2.0788560	2.8955352
H	–2.6401981	–1.7962973	3.6336881
H	4.6783761	0.5904572	–4.3965541
C	3.7585098	0.0513008	–4.6267161
C	1.3633805	–1.2621296	–5.2244561
C	2.9536989	–0.4263295	–3.5937474
C	3.3720237	–0.1307303	–5.9611557
C	2.1820729	–0.7919444	–6.2601718
C	1.7486748	–1.0767928	–3.8891362
H	3.2382022	–0.2641957	–2.5536493
H	3.9922554	0.2677948	–6.7646403
H	1.8651531	–0.9130662	–7.2964852
H	1.1104880	–1.4428811	–3.0853443
H	0.4306460	–1.7772473	–5.4526448

[Co(TPP)] *Bis*-Benzene ([Co(TPP)]):**

101 atoms

C	2.9476357	3.1902758	–4.9879975
C	2.4677296	3.0241172	–6.2511169
C	1.2781029	2.2164988	–6.1434953
C	2.0417246	2.4996905	–4.1032026
N	1.0461466	1.8642415	–4.8259087
C	2.1418100	2.5349158	–2.7135191
C	1.2482623	1.8622188	–1.8796782
N	0.2609752	0.9820712	–2.2897645
C	–0.3092436	0.5092312	–1.1177394
C	1.2471290	1.9911639	–0.4436696
C	0.2737345	1.1633531	0.0276500
C	–1.2568703	–0.5110204	–1.0291664
C	–1.7953097	–1.1350311	–2.1557202
N	–1.5880783	–0.7524091	–3.4707143
C	–3.0583736	–2.5493799	–3.3719805
C	–2.6879331	–2.2658614	–2.0923635
C	–1.9935433	–0.5297823	–6.3890805
N	–0.9785101	0.3185343	–5.9830559
C	–0.5925630	0.9916437	–7.1289601
C	–1.4289200	0.6176579	–8.2426338
C	–2.2932540	–0.3298409	–7.7857463
C	0.4862956	1.8660389	–7.2349082
C	–2.6373408	–1.4745997	–5.5909958
C	–2.4042421	–1.5842422	–4.2203887
H	3.8345735	3.7279834	–4.6707018
H	2.8798846	3.3966093	–7.1829286
H	1.9029144	2.6473157	0.1188060
H	–0.0301543	1.0001453	1.0560617
H	–3.7156633	–3.3377957	–3.7228797
H	–2.9774512	–2.7752942	–1.1794378
H	–1.3551079	1.0364715	–9.2405421
H	–3.0751483	–0.8474171	–8.3311601
Co	–0.3146249	0.6031508	–4.1445699
C	3.2454984	3.3165812	–2.0889771
C	5.3434805	4.7711777	–0.9023734
C	4.2574038	2.6588447	–1.3708154
C	3.3000961	4.7150781	–2.2013112
C	4.3403678	5.4370166	–1.6126719
C	5.2988989	3.3791325	–0.7828661
H	4.2184499	1.5722670	–1.2795347
H	2.5138662	5.2321791	–2.7534168
H	4.3645525	6.5240062	–1.7046989
H	6.0796810	2.8513806	–0.2328452
H	6.1561812	5.3351308	–0.4424897
C	0.8171859	2.4406948	–8.5683434
C	1.4425320	3.5366832	–11.0836097
C	0.6500084	3.8129796	–8.8124903
C	1.3039573	1.6258564	–9.6025780
C	1.6150624	2.1690928	–10.8507907
C	0.9588604	4.3575036	–10.0606774
H	0.2723649	4.4490554	–8.0104389
H	1.4385328	0.5595161	–9.4147911
H	1.9974458	1.5232388	–11.6427496
H	0.8180647	5.4252050	–10.2360312
H	1.6848544	3.9614325	–12.0587421
C	–3.6380548	–2.3787002	–6.2246080
C	–5.5311570	–4.0766244	–7.4312105
C	–5.0010759	–2.2738570	–5.9040637
C	–3.2383732	–3.3461381	–7.1602817
C	–4.1768641	–4.1895641	–7.7583829
C	–5.9408600	–3.1154529	–6.5025258
H	–5.3166511	–1.5207062	–5.1804168
H	–2.1804142	–3.4312904	–7.4131400
H	–3.8485601	–4.9399287	–8.4792840
H	–6.9969043	–3.0173694	–6.2460694
H	–6.2647416	–4.7350423	–7.8985052
C	–1.7048255	–0.9656974	0.3176906
C	–2.5665418	–1.8257270	2.8562374
C	–0.8146109	–1.5994800	1.1995537
C	–3.0340878	–0.7715505	0.7272189
C	–3.4619254	–1.1969157	1.9863114
C	–1.2415413	–2.0263418	2.4586349
H	0.2180514	–1.7582564	0.8852745
H	–3.7302886	–0.2798373	0.0460681
H	–4.4969833	–1.0329377	2.2901832
H	–0.5379370	–2.5219520	3.1293880
H	–2.9002631	–2.1588680	3.8399419
H	4.5284495	0.2624099	–4.5863045
C	3.6046054	–0.3037610	–4.7103962
C	1.1969009	–1.6870923	–5.0348160
C	2.9041604	–0.7509503	–3.5899728
C	3.1043541	–0.5493269	–5.9950270
C	1.9072391	–1.2463710	–6.1578467
C	1.6938300	–1.4364390	–3.7491602
H	3.2761544	–0.5354081	–2.5878037
H	3.6406495	–0.1735895	–6.8674048
H	1.4996720	–1.4153500	–7.1553369
H	1.1300308	–1.7669609	–2.8768870
H	0.2503939	–2.2133824	–5.1564903
H	–1.0303960	4.3419276	–5.5884854
C	–1.7748308	3.6285176	–5.2333957
C	–3.6368298	1.7416353	–4.3356826
C	–1.6912957	3.1310037	–3.9274731
C	–2.7773051	3.1730390	–6.0895447
C	–3.7081844	2.2280617	–5.6409305
C	–2.6247503	2.1882968	–3.4775848
H	–0.8954188	3.4649210	–3.2621644
H	–2.8210127	3.5323322	–7.1184528
H	–4.4734486	1.8543475	–6.3222041
H	–2.5519488	1.7961174	–2.4633520
H	–4.3423417	0.9845518	–3.9915474

[Co(TPP)] Iodonium Ylide (I^{IY}):

104 atoms

C	3.1652426	3.5877491	–4.8193793
C	2.6059576	3.5937042	–6.0607596
C	1.4049765	2.7991923	–5.9844484
C	2.2897832	2.8194274	–3.9692925
N	1.2255217	2.3170329	–4.7007460
C	2.4745167	2.6585763	–2.5958992
C	1.5221834	2.0424711	–1.7823702
N	0.3974650	1.3652534	–2.2188668
C	–0.2957676	1.0287434	–1.0614440
C	1.5289658	2.1395339	–0.3451187
C	0.3881402	1.5422200	0.0990714
C	–1.4368474	0.2278951	–1.0028167
C	–1.9974346	–0.3632476	–2.1395692
N	–1.5895135	–0.1418594	–3.4508449
C	–3.1800444	–1.8328449	–3.3767819
C	–2.9877161	–1.4065945	–2.0938329
C	–1.7303474	–0.0712677	–6.3824790
N	–0.7876613	0.8336631	–5.9263313
C	–0.4449730	1.5919442	–7.0348368
C	–1.2405549	1.2043842	–8.1737622
C	–2.0109763	0.1514703	–7.7787979
C	0.5901090	2.5254450	–7.0846520
C	–2.3925816	–1.0280073	–5.6123272
C	–2.3505753	–1.0165619	–4.2202456
H	4.0864258	4.0606150	–4.4968330
H	2.9754906	4.0717123	–6.9617277
H	2.2940023	2.6441501	0.2353759
H	0.0310581	1.4531095	1.1193460
H	–3.8418957	–2.6158167	–3.7311407
H	–3.4530304	–1.7772268	–1.1865361
H	–1.2015727	1.6787244	–9.1484107
H	–2.7354362	–0.4110600	–8.3585178
Co	–0.1044780	1.0056938	–4.0911188
C	3.7025789	3.1969147	–1.9482459
C	6.0314024	4.1579358	–0.6981715
C	4.6206573	2.3048603	–1.3677768
C	3.9623484	4.5750018	–1.8859035
C	5.1190476	5.0521792	–1.2658712
C	5.7778711	2.7842103	–0.7503882
H	4.4150592	1.2349563	–1.4271997
H	3.2425853	5.2706256	–2.3197836
H	5.3045520	6.1264107	–1.2195685
H	6.4861378	2.0804004	–0.3101550
H	6.9348102	4.5314054	–0.2138096
C	0.8812435	3.2200214	–8.3698905
C	1.4487673	4.5502733	–10.7863349
C	0.7114147	4.6096152	–8.4802908
C	1.3437920	2.5090588	–9.4886647
C	1.6250955	3.1672297	–10.6872115
C	0.9913622	5.2693954	–9.6786175
H	0.3541230	5.1679426	–7.6138894
H	1.4853051	1.4313043	–9.4048693
H	1.9889118	2.5990608	–11.5447422
H	0.8475904	6.3486829	–9.7482980
H	1.6679658	5.0654942	–11.7225307
C	–3.2140002	–2.0503298	–6.3178741
C	–4.7153415	–3.9849965	–7.6964313
C	–4.6162352	–2.0331769	–6.2666946
C	–2.5701009	–3.0460374	–7.0705107
C	–3.3185560	–4.0075589	–7.7529228
C	–5.3625823	–2.9946341	–6.9519651
H	–5.1169377	–1.2519422	–5.6926707
H	–1.4792772	–3.0583716	–7.0916753
H	–2.8078132	–4.7807074	–8.3294771
H	–6.4525276	–2.9659266	–6.9095286
H	–5.2984317	–4.7355502	–8.2322295
C	–2.0318395	–0.1021099	0.3224787
C	–3.1814412	–0.7574259	2.8070380
C	–1.3265055	–0.8789705	1.2558285
C	–3.3238361	0.3373318	0.6514970
C	–3.8938725	0.0138149	1.8845402
C	–1.8956209	–1.2037912	2.4885970
H	–0.3241298	–1.2279745	1.0022915
H	–3.8773436	0.9383212	–0.0714797
H	–4.8967748	0.3686026	2.1268186
H	–1.3354349	–1.8119968	3.2004616
H	–3.6268275	–1.0106178	3.7701091
C	1.5183759	–0.8577346	–4.3582531
I	0.7643283	–2.0491062	–2.7834927
C	1.1783691	–1.4815196	–5.6539714
O	0.4793694	–2.4846368	–5.7963182
O	1.7009524	–0.8044686	–6.7045314
C	2.8681124	–0.3756804	–3.9972191
O	3.3844011	–0.4837610	–2.8844869
O	3.4995420	0.2197733	–5.0376152
C	1.3664139	–1.3463831	–7.9982935
H	0.2932045	–1.2254506	–8.1967492
H	1.6345906	–2.4098766	–8.0599037
H	1.9546995	–0.7598887	–8.7117985
C	4.8405271	0.6726428	–4.7583893
H	5.4827264	–0.1740370	–4.4777892
H	4.8428621	1.4111984	–3.9473154
H	5.1821962	1.1327518	–5.6906658
C	2.1172103	–3.6886913	–2.8786414
C	3.9056218	–5.7840351	–3.0829203
C	1.8102423	–4.7506276	–3.7318074
C	3.2991196	–3.6345657	–2.1377802
C	4.1953437	–4.7019085	–2.2465394
C	2.7214461	–5.8064514	–3.8258160
H	0.8985310	–4.7350806	–4.3276999
H	3.5253471	–2.7662150	–1.5211535
H	5.1263261	–4.6799913	–1.6785986
H	2.5032009	–6.6454601	–4.4877058

H	4.6113167	–6.6119523	–3.1624385

[Co(TPP)] Terminal Carbene (I^T):

92 atoms

C	3.2006538	4.1014902	–4.7223984
C	2.5492056	4.1162253	–5.9175209
C	1.4059889	3.2518158	–5.7833440
C	2.4197147	3.2868388	–3.8299041
N	1.3110559	2.7728307	–4.4870773
C	2.6972112	3.1216030	–2.4758450
C	1.7893541	2.5095625	–1.6122712
N	0.6350930	1.8472126	–1.9905403
C	0.0075747	1.5027900	–0.8023258
C	1.8658080	2.6116290	–0.1780721
C	0.7421081	2.0253259	0.3203912
C	–1.0964078	0.6668242	–0.6807638
C	–1.6431393	0.0064455	–1.7782436
N	–1.3009417	0.2144350	–3.1020172
C	–2.7417238	–1.5972853	–2.9176387
C	–2.5628217	–1.0949152	–1.6633687
C	–1.4668239	0.1112526	–6.0225319
N	–0.6617849	1.1578481	–5.6012505
C	–0.3528336	1.8656257	–6.7537555
C	–1.0277823	1.2917128	–7.8885262
C	–1.6971196	0.1913808	–7.4386421
C	0.5983429	2.8777189	–6.8533596
C	–2.0261331	–0.8623475	–5.1989420
C	–1.9839964	–0.7636869	–3.8120678
H	4.1200429	4.6090579	–4.4521521
H	2.8238296	4.6390092	–6.8271541
H	2.6628486	3.1123760	0.3613796
H	0.4327722	1.9337052	1.3558731
H	–3.3473436	–2.4429006	–3.2257336
H	–2.9824220	–1.4495009	–0.7279462
H	–0.9676919	1.6790978	–8.9001209
H	–2.3118612	–0.5031510	–8.0017191
Co	0.1076925	1.3762659	–3.8083697
C	3.9497737	3.6836748	–1.8987022
C	6.3132485	4.7044035	–0.7689895
C	4.9415174	2.8163314	–1.4147303
C	4.1536493	5.0689987	–1.8021902
C	5.3277735	5.5757888	–1.2415008
C	6.1165800	3.3234795	–0.8564908
H	4.7821702	1.7396209	–1.4861722
H	3.3776918	5.7460714	–2.1621465
H	5.4701778	6.6549193	–1.1677119
H	6.8817356	2.6372080	–0.4908811
H	7.2305594	5.1007104	–0.3315355
C	0.8766571	3.4475135	–8.2029387
C	1.4063337	4.4613739	–10.7662218
C	0.0164772	4.3886226	–8.7842832
C	2.0036370	3.0138172	–8.9187221
C	2.2665730	3.5197053	–10.1930767
C	0.2811917	4.8943231	–10.0597597
H	–0.8618216	4.7214342	–8.2292210
H	2.6638655	2.2760211	–8.4590832
H	3.1441886	3.1749171	–10.7418427
H	–0.3925915	5.6300681	–10.5011517
H	1.6123613	4.8564393	–11.7618921
C	–2.7176282	–2.0163564	–5.8380999
C	–3.9597370	–4.2056956	–7.0830810
C	–4.1157949	–2.1201621	–5.8612662
C	–1.9472129	–3.0195024	–6.4460292
C	–2.5652412	–4.1089824	–7.0629852
C	–4.7333231	–3.2090925	–6.4813589
H	–4.7149316	–1.3364966	–5.3951584
H	–0.8600675	–2.9336239	–6.4144333
H	–1.9562142	–4.8865009	–7.5266723
H	–5.8220738	–3.2768870	–6.4978408
H	–4.4428495	–5.0557962	–7.5666994
C	–1.6102584	0.3275240	0.6758085
C	–2.5839677	–0.3575779	3.2194196
C	–0.8546375	–0.4922830	1.5288895
C	–2.8608874	0.7928242	1.1066708
C	–3.3437617	0.4546472	2.3732871
C	–1.3396809	–0.8320037	2.7931310
H	0.1082709	–0.8667883	1.1787867
H	–3.4514021	1.4241056	0.4408922
H	–4.3154181	0.8280610	2.6999586
H	–0.7464399	–1.4745994	3.4454762
H	–2.9618482	–0.6229441	4.2077211
C	1.3376147	0.0025524	–4.0407554
C	1.8679221	–0.1614004	–5.4187042
O	2.6934436	0.5603593	–5.9526312
O	1.2792991	–1.2124631	–6.0616857
C	1.7254401	–0.9276501	–2.9992663
O	1.2684756	–1.0374889	–1.8657249
O	2.7542096	–1.7409583	–3.4525038
C	1.6641244	–1.3572700	–7.4473107
H	2.7392645	–1.5650882	–7.5319772
H	1.0747949	–2.1979061	–7.8284550
H	1.4237589	–0.4413682	–8.0043883
C	3.1934753	–2.7264486	–2.5037256
H	3.9956665	–3.2793310	–3.0047916
H	2.3699522	–3.4024057	–2.2313905
H	3.5684443	–2.2487370	–1.5869041

[Co(TPP)] *Mono* Benzene *Mono* Terminal Carbene (I^{T*}):

104 atoms

C	3.2498398	3.8021737	–5.0492274
C	2.5502395	3.8329998	–6.2205154
C	1.3794152	3.0135330	–6.0351808
C	2.4702379	3.0271058	–4.1192070
N	1.3461316	2.5185784	–4.7493807
C	2.7146883	2.9449296	–2.7500415
C	1.7708010	2.4135668	–1.8687684
N	0.6568495	1.6790526	–2.2253131
C	–0.0004612	1.3933308	–1.0374607
C	1.7849237	2.6392976	–0.4485679
C	0.6653249	2.0476666	0.0597181
C	–1.0699491	0.5097598	–0.9035328
C	–1.5341721	–0.2482738	–1.9812080
N	–1.1779067	–0.0800747	–3.3031731
C	–2.4568857	–1.9980673	–3.0654179
C	–2.3568709	–1.4222933	–1.8331670
C	–1.3299672	–0.2371017	–6.2060015
N	–0.5658101	0.8409481	–5.8068276
C	–0.4203220	1.6371872	–6.9327965
C	–1.1947299	1.0932697	–8.0202024
C	–1.7112858	–0.0929047	–7.5872159
C	0.4727420	2.7020046	–7.0529127
C	–1.8000733	–1.2576247	–5.3736992
C	–1.7616158	–1.1359179	–3.9857855
H	4.1959488	4.2796046	–4.8184660
H	2.8117664	4.3343014	–7.1464620
H	2.5415270	3.2142609	0.0749290
H	0.3184343	2.0431046	1.0870411
H	–2.9715992	–2.9126309	–3.3391156
H	–2.7655036	–1.7740116	–0.8915728
H	–1.3112720	1.5577931	–8.9931309
H	–2.3408523	–0.7916381	–8.1283307
Co	0.1716531	1.1370910	–4.0342014
C	3.9768227	3.4834127	–2.1779981
C	6.3690636	4.4257216	–1.0519939
C	4.8891291	2.5861418	–1.5981692
C	4.2715642	4.8552033	–2.1821217
C	5.4614093	5.3237681	–1.6209154
C	6.0799224	3.0579077	–1.0425708
H	4.6515171	1.5209998	–1.6064280
H	3.5541972	5.5529294	–2.6168300
H	5.6772506	6.3932430	–1.6227986
H	6.7866660	2.3524337	–0.6032503
H	7.2991509	4.7921828	–0.6152394
C	0.5565327	3.4699029	–8.3245415
C	0.7434818	4.9736258	–10.6981322
C	0.2842515	4.8482010	–8.3246199
C	0.9323521	2.8595626	–9.5323706
C	1.0251206	3.6046401	–10.7091785
C	0.3733986	5.5935285	–9.5015429
H	–0.0009548	5.3312396	–7.3887958
H	1.1603640	1.7931536	–9.5388409
H	1.3257042	3.1152219	–11.6367031
H	0.1506103	6.6612728	–9.4838375
H	0.8156065	5.5555057	–11.6178518
C	–2.4465976	–2.4380396	–6.0076085
C	–3.6258205	–4.6642631	–7.2566424
C	–3.8231730	–2.6823339	–5.8795363
C	–1.6701778	–3.3196013	–6.7768942
C	–2.2553180	–4.4268371	–7.3937598
C	–4.4084881	–3.7877607	–6.4997928
H	–4.4337277	–1.9891112	–5.2993303
H	–0.6000010	–3.1324545	–6.8756004
H	–1.6373583	–5.1081189	–7.9802034
H	–5.4807354	–3.9610704	–6.3970574
H	–4.0833455	–5.5284226	–7.7399799
C	–1.6963439	0.3003924	0.4293859
C	–2.9371488	–0.0906655	2.9276129
C	–0.9759855	–0.2279188	1.5130720
C	–3.0511260	0.6215692	0.6169646
C	–3.6661942	0.4307964	1.8554138
C	–1.5907457	–0.4217336	2.7513128
H	0.0713589	–0.4957501	1.3735091
H	–3.6187652	1.0255152	–0.2220138
H	–4.7173597	0.6929531	1.9835749
H	–1.0170796	–0.8397573	3.5797816
H	–3.4169232	–0.2418789	3.8953984
C	1.5056516	–0.1728678	–4.1386158
C	2.2257727	–0.6350361	–5.3105890
O	2.8677598	–1.6882021	–5.3087653
O	2.1312399	0.1622471	–6.4123281
C	2.0332735	–0.6828598	–2.8472729
O	3.1373220	–0.3856559	–2.4143994
O	1.1547885	–1.4623623	–2.1728953
C	2.8216301	–0.3234546	–7.5742832
H	3.8808660	–0.5129125	–7.3526085
H	2.3642261	–1.2546454	–7.9391701
H	2.7216803	0.4719972	–8.3210784
C	1.5741033	–1.8428753	–0.8462810
H	1.8315249	–0.9479732	–0.2617944
H	2.4485145	–2.5061460	–0.8905757
H	0.7133409	–2.3592201	–0.4089689
H	–0.5641159	5.1539514	–1.2238405
C	–1.0945957	4.5884434	–1.9907145
C	–2.3991223	3.0710188	–3.9438198
C	–2.0943477	3.6827474	–1.6216386
C	–0.7578694	4.7462492	–3.3366512
C	–1.4172357	3.9951783	–4.3131610
C	–2.7423810	2.9220202	–2.5964014
H	–2.3431546	3.5444466	–0.5685497
H	0.0376566	5.4340235	–3.6264335
H	–1.1426296	4.0978997	–5.3623524
H	–3.4957065	2.1877986	–2.3095591
H	–2.8805428	2.4568611	–4.7049350

[Co(TPP)] Gamma Radical (I^G):

108 atoms

C	4.1464414	0.1337702	–2.8345494
C	3.7645858	–0.1968663	–4.0981555
C	2.6834633	–1.1383765	–3.9736312
C	3.3007608	–0.6097542	–1.9361417
N	2.3870604	–1.3818239	–2.6419158
C	3.4263789	–0.5541775	–0.5508948
C	2.5747225	–1.2455985	0.3055777
N	1.5233818	–2.0662838	–0.0835119
C	1.0121830	–2.5630975	1.1075428
C	2.7241467	–1.2482681	1.7375294
C	1.7597318	–2.0709531	2.2339171
C	–0.0911424	–3.3975445	1.2316749
C	–0.8288309	–3.8331061	0.1371477
N	–0.4976731	–3.6387543	–1.1964903
C	–2.3882258	–4.9843509	–1.0033060
C	–2.0181449	–4.6330902	0.2596579
C	–0.5533370	–3.9309451	–4.1273311
N	0.4275935	–3.0286237	–3.7472440
C	0.9707075	–2.5777315	–4.9434770
C	0.3062279	–3.1836070	–6.0672475
C	–0.6324686	–4.0296709	–5.5610819
C	2.0482497	–1.7089732	–5.0698467
C	–1.4192271	–4.6054110	–3.2726384
C	–1.4367804	–4.3827758	–1.8997313
H	4.9175308	0.8290987	–2.5206633
H	4.1568257	0.1680748	–5.0413886
H	3.4815128	–0.6925640	2.2797834
H	1.5548352	–2.3269145	3.2679404
H	–3.2218905	–5.6058359	–1.3112313
H	–2.4886722	–4.8952089	1.2013796
H	0.5406011	–2.9767904	–7.1060886
H	–1.3410546	–4.6507478	–6.0984766
Co	1.0842585	–2.6837934	–1.9162485
C	4.5641882	0.2134428	0.0307615
C	6.7351382	1.6180106	1.1310955
C	5.8722399	–0.2797092	–0.1000370
C	4.3567972	1.4176889	0.7187485
C	5.4362550	2.1164552	1.2646978
C	6.9503964	0.4176231	0.4477010
H	6.0366315	–1.2198233	–0.6298709
H	3.3410917	1.8028569	0.8203413
H	5.2619842	3.0545835	1.7936704
H	7.9604357	0.0186381	0.3439059
H	7.5774933	2.1631858	1.5591209
C	2.6059196	–1.4519644	–6.4282195
C	3.6985083	–1.0283155	–8.9781997
C	1.9809625	–0.5802764	–7.3302558
C	3.7857334	–2.1097347	–6.8116749
C	4.3258541	–1.8992262	–8.0820246
C	2.5263064	–0.3680279	–8.5991127
H	1.0663865	–0.0674839	–7.0283486
H	4.2606698	–2.7848640	–6.0975102
H	5.2403109	–2.4183321	–8.3734904
H	2.0359151	0.3173622	–9.2920234
H	4.1228944	–0.8628916	–9.9694644
C	–2.2988627	–5.6576958	–3.8525385
C	–3.8715147	–7.7161368	–4.9419078
C	–3.6904633	–5.5151019	–3.9441593
C	–1.7017046	–6.8399268	–4.3218234
C	–2.4833351	–7.8630296	–4.8608904
C	–4.4718735	–6.5394463	–4.4853152
H	–4.1555862	–4.5924533	–3.5938564
H	–0.6166442	–6.9372623	–4.2525355
H	–2.0076538	–8.7782372	–5.2169834
H	–5.5535506	–6.4153118	–4.5554597
H	–4.4832795	–8.5149736	–5.3632842
C	–0.4733782	–3.8951556	2.5839761
C	–1.1726239	–4.8919935	5.1112571
C	–0.1189009	–5.2024212	2.9516554
C	–1.1761425	–3.0914663	3.4918053
C	–1.5259104	–3.5889510	4.7499559
C	–0.4670288	–5.6960057	4.2106779
H	0.4434126	–5.8093905	2.2396166
H	–1.4491217	–2.0753056	3.2030774
H	–2.0771748	–2.9575106	5.4483508

H	–0.1826633	–6.7113573	4.4911454
H	–1.4452017	–5.2794845	6.0939649
C	2.4653859	–4.3252297	–1.8769978
C	2.8696745	–4.5254779	–3.3210294
O	3.7637539	–3.8771391	–3.8495943
O	2.1850422	–5.4790842	–3.9994764
C	1.7404688	–5.4138072	–1.1193839
O	1.8812021	–5.5792606	0.0874488
O	0.9224643	–6.1979711	–1.8598411
C	2.6118097	–5.6657313	–5.3656054
H	2.5480026	–4.7256860	–5.9272398
H	3.6456217	–6.0369604	–5.3970211
H	1.9189971	–6.4033605	–5.7833033
C	0.2180669	–7.2108931	–1.1107019
H	–0.4835933	–7.6581505	–1.8224460
H	–0.3278668	–6.7642464	–0.2709773
H	0.9222281	–7.9633483	–0.7289183
C	3.6932002	–3.8662852	–1.0618274
H	3.3754977	–3.7181553	–0.0236531
H	4.0591281	–2.9188042	–1.4569570
C	4.7295915	–4.9258850	–1.1229688
H	4.4864061	–5.8677771	–0.6236584
C	5.9874109	–4.8213406	–1.7600747
C	8.5582302	–4.6598003	–2.9424788
C	6.4016765	–3.6552526	–2.4717194
C	6.9118836	–5.9061741	–1.6826788
C	8.1702961	–5.8229079	–2.2588748
C	7.6631440	–3.5842940	–3.0447795
H	5.7016473	–2.8317934	–2.6037537
H	6.6132397	–6.8103517	–1.1478766
H	8.8602722	–6.6646646	–2.1815091
H	7.9551693	–2.6850798	–3.5896274
H	9.5472874	–4.5959735	–3.3978749

[Co(TPP)] *Mono*-Iodonium Ylide *Mono*-Terminal Carbene (I^{IY-T}):

119 atoms

C	2.5178946	3.6656624	–5.3019145
C	1.9599748	3.6507116	–6.5458185
C	0.8624880	2.7198761	–6.5016845
C	1.7222940	2.7925195	–4.4761215
N	0.7158649	2.2128213	–5.2239313
C	1.8603407	2.6896478	–3.0929244
C	0.8922742	2.0760142	–2.3029158
N	–0.2261520	1.4099349	–2.7738828
C	–0.9549629	1.0701850	–1.6523961
C	0.8694011	2.1330895	–0.8644036
C	–0.2899390	1.5429385	–0.4643244
C	–2.0985719	0.2701241	–1.6206492
C	–2.5419807	–0.4202840	–2.7484072
N	–1.9902697	–0.3223250	–4.0169530
C	–3.5965253	–1.9883569	–3.9811202
C	–3.5797332	–1.4196785	–2.7415927
C	–1.7138165	–0.6429045	–6.9418575
N	–1.0426916	0.4832092	–6.4831332
C	–0.6280682	1.1604038	–7.6216918
C	–1.0892855	0.4777795	–8.7973426
C	–1.7088795	–0.6670701	–8.3782955
C	0.1710900	2.3008481	–7.6320789
C	–2.4158598	–1.5344653	–6.1332625
C	–2.6153762	–1.2966044	–4.7729977
H	3.3664602	4.2421406	–4.9488313
H	2.2683044	4.1943379	–7.4326949
H	1.6391571	2.5883173	–0.2509823
H	–0.6620947	1.4076493	0.5452267
H	–4.2375303	–2.7816375	–4.3509676
H	–4.2095461	–1.6525401	–1.8902943
H	–0.9179766	0.8165056	–9.8136156
H	–2.1459679	–1.4533022	–8.9844888
Co	–0.5421786	0.8559580	–4.6177165
C	3.0049073	3.3873880	–2.4449316
C	5.1690396	4.7309102	–1.2617749
C	4.3089044	2.8879384	–2.5764364
C	2.7959488	4.5715690	–1.7203573
C	3.8725553	5.2379853	–1.1318051
C	5.3847035	3.5551621	–1.9859463
H	4.4697803	1.9697003	–3.1430567
H	1.7814042	4.9640956	–1.6349724
H	3.6987422	6.1597155	–0.5744561
H	6.3938011	3.1536363	–2.0900307
H	6.0095313	5.2520608	–0.8012386
C	0.3634131	3.0486530	–8.9044959
C	0.6959250	4.5138296	–11.2747539
C	–0.3151891	4.2629214	–9.0890476
C	1.2137002	2.5765201	–9.9143463
C	1.3776932	3.3066061	–11.0941460
C	–0.1502844	4.9912283	–10.2696086
H	–0.9724899	4.6222073	–8.2949988
H	1.7498976	1.6397970	–9.7565286
H	2.0453459	2.9344524	–11.8726499
H	–0.6840319	5.9332124	–10.4049165
H	0.8267553	5.0830626	–12.1961301
C	–3.0135325	–2.7628098	–6.7225223
C	–4.0995518	–5.1294463	–7.7721957
C	–4.0993331	–2.7138131	–7.6093620
C	–2.4794433	–4.0102768	–6.3594488
C	–3.0200478	–5.1853052	–6.8853722
C	–4.6395424	–3.8912302	–8.1316531
H	–4.5251852	–1.7452031	–7.8761589
H	–1.6339411	–4.0353553	–5.6694269
H	–2.5937219	–6.1490735	–6.6028947
H	–5.4883627	–3.8418784	–8.8154890
H	–4.5213628	–6.0489204	–8.1806694
C	–2.8074554	0.1017765	–0.3213118
C	–4.1386982	–0.1631764	2.1445609
C	–2.8834553	–1.1446515	0.3217392
C	–3.4013771	1.2183301	0.2933775
C	–4.0635375	1.0825320	1.5151178
C	–3.5441984	–1.2767283	1.5445143
H	–2.4106619	–2.0117340	–0.1395420
H	–3.3489420	2.1819541	–0.2135871
H	–4.5256748	1.9570712	1.9757486
H	–3.5876269	–2.2513787	2.0330857
H	–4.6548552	–0.2660143	3.1001835
C	–2.6205351	3.0958185	–4.5841726
C	0.7222339	–0.5220493	–4.6266251
C	–3.5030411	2.6900305	–3.4991175
O	–3.4238811	3.0846358	–2.3449094
O	–4.4873968	1.8188031	–3.9113352
C	–1.6411928	4.1643261	–4.4262299
O	–1.1201993	4.4733732	–3.3680045
O	–1.3431471	4.8075900	–5.6121781
C	–5.4388332	1.4624298	–2.8919079
H	–4.9370136	1.0149302	–2.0248649
H	–6.1059117	0.7329297	–3.3621681
H	–6.0000470	2.3483316	–2.5616050
C	–0.3682350	5.8611215	–5.4830264
H	–0.8077789	6.7258838	–4.9656364
H	–0.0850862	6.1265465	–6.5073258
H	0.5105489	5.5131066	–4.9275324
C	1.8063225	–0.6346945	–5.5950447
O	1.9485074	–0.0370156	–6.6554183
O	2.7434420	–1.5466317	–5.1446106
C	0.4421422	–1.6972364	–3.7738815
O	0.1380657	–2.7947014	–4.2253262
O	0.5111664	–1.4353455	–2.4459239
C	3.8228132	–1.7928870	–6.0613872
H	4.4663490	–2.5279500	–5.5657482
H	4.3793782	–0.8675805	–6.2693379
H	3.4428051	–2.1931246	–7.0124918
C	0.0955310	–2.5188753	–1.5903048
H	0.7833476	–3.3710346	–1.6786120
H	–0.9178398	–2.8469697	–1.8628633
H	0.1118610	–2.1073060	–0.5758720
I	–3.2970157	2.6722964	–6.5056858
C	–4.9641005	4.0375416	–6.6485794
C	–7.0972670	5.7883252	–6.8171793
C	–5.1466037	4.9666005	–5.6310965
C	–5.8144557	3.9533896	–7.7492539
C	–6.8900628	4.8444744	–7.8268023
C	–6.2289083	5.8476127	–5.7236594
H	–4.4626446	5.0022573	–4.7810182
H	–5.6570393	3.2131473	–8.5354148
H	–7.5675197	4.7936334	–8.6802847
H	–6.3882696	6.5822246	–4.9332584
H	–7.9391720	6.4782165	–6.8823071

[Co(TPP)] *Bis*-Terminal Carbene (I^{T-T}):

107 atoms

C	3.0351912	3.9526884	–4.8418625
C	2.3869948	4.0291921	–6.0433105
C	1.2697249	3.1207486	–5.9808607
C	2.2773725	3.0521574	–4.0105970
N	1.2182723	2.5426753	–4.7326968
C	2.5189274	2.8155821	–2.6559462
C	1.5998494	2.1520846	–1.8371995
N	0.4716981	1.4892430	–2.2500357
C	–0.2154392	1.1174679	–1.1180388
C	1.6250641	2.2054967	–0.3955932
C	0.4807658	1.6095568	0.0464690
C	–1.3376258	0.2857482	–1.0830858
C	–1.8033797	–0.3883040	–2.2165024
N	–1.3667942	–0.1956866	–3.5090907
C	–2.8385272	–1.9636673	–3.4624537
C	–2.7416979	–1.4815044	–2.1860508
C	–1.3624377	–0.2127374	–6.4698746
N	–0.6156640	0.8448023	–6.0058987
C	–0.3589825	1.6605736	–7.0839442
C	–0.9865304	1.1093469	–8.2605264
C	–1.5598118	–0.0727181	–7.8920603
C	0.4715613	2.7847424	–7.0789847
C	–1.9544458	–1.2062559	–5.6861447
C	–1.9978514	–1.1379778	–4.2916322
H	3.9389186	4.4662264	–4.5316374
H	2.6571286	4.6113218	–6.9181136
H	2.4082858	2.6791907	0.1870385
H	0.1372841	1.4892933	1.0680902
H	–3.4429124	–2.7877470	–3.8275876
H	–3.2375975	–1.8397598	–1.2900472
H	–0.9673028	1.5666964	–9.2437376
H	–2.0991017	–0.7795587	–8.5136646
Co	–0.0727328	1.1687044	–4.1199496
C	3.7665961	3.3355804	–2.0340350
C	6.1375232	4.2493932	–0.8383397
C	4.7600917	2.4248894	–1.6412376
C	3.9729001	4.7066772	–1.8206071
C	5.1518396	5.1616156	–1.2259569
C	5.9387801	2.8815794	–1.0479775
H	4.5983511	1.3616633	–1.8241065
H	3.1961318	5.4129684	–2.1177850
H	5.2983185	6.2298997	–1.0593146
H	6.7070165	2.1655871	–0.7524003
H	7.0582888	4.6042977	–0.3732608
C	0.5803282	3.6337480	–8.2957342
C	0.7958260	5.3057201	–10.5438510
C	0.1040086	4.9543787	–8.2483172
C	1.1698796	3.1636412	–9.4793830
C	1.2762539	3.9940958	–10.5970938
C	0.2103887	5.7826874	–9.3673119
H	–0.3581750	5.3101052	–7.3260287
H	1.5526328	2.1423755	–9.5127298
H	1.7420210	3.6182645	–11.5093670
H	–0.1700012	6.8042660	–9.3211799
H	0.8792492	5.9545656	–11.4168390
C	–2.6457707	–2.3469010	–6.3507696
C	–3.9271574	–4.5397195	–7.5570051
C	–3.8896943	–2.1883305	–6.9794061
C	–2.0514821	–3.6177955	–6.3343162
C	–2.6872703	–4.7072395	–6.9336624
C	–4.5264567	–3.2770970	–7.5795430
H	–4.3544049	–1.2014946	–6.9908691
H	–1.0782752	–3.7324315	–5.8555694
H	–2.2111341	–5.6888232	–6.9181910
H	–5.4953235	–3.1399995	–8.0621288
H	–4.4247499	–5.3902958	–8.0247882
C	–2.0321730	0.0333600	0.2080142
C	–3.4064930	–0.4414787	2.6097725
C	–1.4280664	–0.7042344	1.2376854
C	–3.3343529	0.5265997	0.3899278
C	–4.0151362	0.2908923	1.5861557
C	–2.1122437	–0.9393079	2.4323714
H	–0.4228107	–1.1003880	1.0864346
H	–3.7926472	1.1036129	–0.4150026
H	–5.0236259	0.6850384	1.7207592
H	–1.6352561	–1.5186741	3.2243816
H	–3.9399200	–0.6254450	3.5434802
C	1.2923286	–0.2015743	–4.2563629
C	–1.4324894	2.5197303	–3.9746656
C	–2.8488349	2.1775239	–3.7934300
O	–3.4029784	2.3284157	–2.7109248
O	–3.4261905	1.6336978	–4.8813742
C	–1.0864159	3.9482910	–4.0282121
O	–1.3307968	4.6325548	–5.0143278
O	–0.4253969	4.3806374	–2.9380735
C	2.5725394	0.0336676	–4.9331005
O	3.6376198	0.0975489	–4.3319148
O	2.4331656	0.2318383	–6.2630497
C	1.2024467	–1.3900881	–3.3902081
O	1.5269765	–1.3635075	–2.2151533
O	0.6911812	–2.4767370	–4.0166506
C	3.6361690	0.6541412	–6.9478122
H	3.9873171	1.6065099	–6.5291627
H	3.3395228	0.7812101	–7.9934119
H	4.4260025	–0.1029846	–6.8539491
C	0.4080246	–3.5961364	–3.1380452
H	–0.3155301	–3.2915300	–2.3701762
H	1.3284301	–3.9548232	–2.6594526
H	–0.0229599	–4.3691403	–3.7820052
C	–4.7593916	1.1086017	–4.6717531
H	–5.1037867	0.7970824	–5.6624109
H	–5.4219505	1.8768203	–4.2525271
H	–4.7118255	0.2478325	–3.9905076
C	0.1160661	5.7196112	–3.0348620
H	–0.6775806	6.4496944	–3.2409234
H	0.8671413	5.7551152	–3.8364265
H	0.5781867	5.9105274	–2.0614708

[Co(TPP)] *Mono*-Bridged *Mono*-Terminal Carbene (I^{B-T}):

107 atoms

C	–1.4109443	1.6354808	–3.1361120
C	–1.5969113	1.9239972	–4.4603890
C	–0.7882406	1.0337926	–5.2375794
C	–0.4932465	0.5429041	–3.0430055
N	–0.0125400	0.2796779	–4.3333558
C	–0.3585303	–0.2725635	–1.9143103
C	–0.0200865	–1.6420588	–1.9077769
N	0.1576033	–2.4955632	–2.9888401
C	0.5044443	–3.7247706	–2.4616440
C	0.2166202	–2.3718905	–0.6824412
C	0.5244652	–3.6558254	–1.0222717
C	0.9050419	–4.8581072	–3.1814015

C	1.1163705	–4.8782388	–4.5643180
N	0.8499755	–3.8348032	–5.4197533
C	1.6299439	–5.6328569	–6.6301113
C	1.6105391	–6.0072021	–5.3174099
C	0.2625472	–2.3097909	–7.9130131
N	–0.1048896	–1.5462753	–6.8177276
C	–0.5870202	–0.3506168	–7.3184020
C	–0.5609488	–0.3880005	–8.7607999
C	–0.0305144	–1.5909958	–9.1275518
C	–0.9792234	0.7976708	–6.5988558
C	0.8397225	–3.5836589	–7.8723983
C	1.1098737	–4.2864493	–6.6924435
H	–1.9589112	2.0317165	–2.2885647
H	–2.3275090	2.5981451	–4.8926532
H	0.1944399	–1.9348200	0.3095848
H	0.7927224	–4.4772122	–0.3666191
H	1.9489068	–6.2164352	–7.4873425
H	1.9001001	–6.9611842	–4.8897545
H	–0.8666741	0.4306526	–9.4028340
H	0.1601150	–1.9603288	–10.1293219
Co	–0.0295193	–2.1627649	–4.9344349
C	1.1649510	–0.5138824	–4.6300645
C	1.9437636	–0.0489913	–5.8465656
C	2.1771530	–0.5626337	–3.4903131
O	2.3596476	0.3191828	–2.6695912
O	1.8759535	1.0497709	–6.3654509
O	2.7724075	–1.0315900	–6.2799337
O	2.8997639	–1.7015903	–3.5374757
C	3.5015852	–0.7132441	–7.4814339
H	4.1101887	0.1916801	–7.3492292
H	4.1362708	–1.5848983	–7.6715676
H	2.7991552	–0.5556546	–8.3130134
C	3.8876404	–1.8355048	–2.4942745
H	4.3988682	–2.7802377	–2.7028811
H	3.3922114	–1.8722159	–1.5143479
H	4.5945222	–0.9950923	–2.5111948
C	–1.7829342	–2.6400026	–4.9293268
C	–0.6513347	0.3953984	–0.6189075
C	–1.1761053	1.7326914	1.7968558
C	–1.6631133	–0.0583890	0.2428908
C	0.0920441	1.5320786	–0.2568294
C	–0.1668080	2.1920414	0.9453364
C	–1.9247489	0.6062570	1.4415811
H	–2.2482477	–0.9319941	–0.0433884
H	0.8848727	1.8699656	–0.9253813
H	0.4248059	3.0664583	1.2202916
H	–2.7205924	0.2491543	2.0969531
H	–1.3805108	2.2516529	2.7343750
C	1.1464385	–4.2513415	–9.1703287
C	1.7068961	–5.5092924	–11.6214298
C	2.2053929	–3.8052952	–9.9749862
C	0.3714998	–5.3360535	–9.6087908
C	0.6498016	–5.9608494	–10.8262539
C	2.4843169	–4.4299691	–11.1924668
H	2.8085747	–2.9620385	–9.6356711
H	–0.4513173	–5.6833539	–8.9821286
H	0.0371597	–6.8012025	–11.1560361
H	3.3135361	–4.0747563	–11.8060342
H	1.9245740	–5.9973812	–12.5722928
C	–1.7185159	1.8465870	–7.3495993
C	–3.1174937	3.8286284	–8.7568834
C	–1.2008300	3.1481005	–7.4431279
C	–2.9468435	1.5464105	–7.9617074
C	–3.6419606	2.5357163	–8.6590136
C	–1.8958923	4.1324316	–8.1480694
H	–0.2422548	3.3673928	–6.9707914
H	–3.3520511	0.5387572	–7.8561944
H	–4.6016607	2.2988362	–9.1209916
H	–1.4807693	5.1383838	–8.2259018
H	–3.6617069	4.5994748	–9.3046319
C	1.1040003	–6.1196568	–2.4147530
C	1.4143324	–8.4946374	–0.9494598
C	–0.0158567	–6.7716896	–1.8739898
C	2.3787758	–6.6690586	–2.2144971
C	2.5331026	–7.8499460	–1.4846193
C	0.1404680	–7.9532882	–1.1470024
H	–1.0043923	–6.3419203	–2.0454444
H	3.2490441	–6.1584884	–2.6297477
H	3.5302381	–8.2646139	–1.3292025
H	–0.7368850	–8.4557649	–0.7369814
H	1.5353043	–9.4170515	–0.3797746
C	–2.4122888	–3.2593515	–3.7490684
O	–2.4133329	–4.4707137	–3.5757989
O	–2.9441188	–2.3656458	–2.8826276
C	–2.6268484	–2.4832380	–6.1295624
O	–3.3305746	–1.5011700	–6.3223487
O	–2.4931700	–3.5083241	–7.0033476
C	–3.4675054	–2.9434261	–1.6624639
H	–4.1681930	–3.7588376	–1.8837618
H	–3.9803262	–2.1229864	–1.1505203
H	–2.6393376	–3.3292713	–1.0508929
C	–3.1722464	–3.3231365	–8.2693318
H	–2.9510086	–4.2247420	–8.8489575
H	–2.7759964	–2.4339084	–8.7778958
H	–4.2542104	–3.2113532	–8.1188809

[Co(TPP)] *Mono*-Enolate *Mono*-Terminal Carbene (I^{E-T}):

107 atoms

C	1.7505485	4.2242480	–5.2501085
C	1.1540950	3.9904600	–6.4801008
C	0.9952993	2.6108560	–6.6439626
C	1.9380072	2.9992822	–4.6061838
N	1.4529195	1.9241845	–5.4457662
C	2.4131018	2.7781988	–3.3094378
C	1.8188540	1.7997767	–2.4959929
N	0.6011988	1.1899383	–2.7731030
C	0.1675395	0.6466445	–1.5882626
C	2.2008109	1.5131146	–1.1335566
C	1.1649619	0.8318761	–0.5626208
C	–1.0732808	0.0305756	–1.3843219
C	–1.8807129	–0.3968263	–2.4415036
N	–1.5213941	–0.3600975	–3.7708398
C	–3.5005514	–1.5144789	–3.5434080
C	–3.1396821	–1.0841515	–2.2994407
C	–1.4713069	–0.8367248	–6.6808341
N	–0.6552919	0.2221674	–6.3656376
C	–0.1209499	0.6609813	–7.5580169
C	–0.5067172	–0.2287954	–8.6269972
C	–1.3388564	–1.1609603	–8.0837835
C	0.4930342	1.9127927	–7.7345769
C	–2.4144376	–1.4016518	–5.8180789
C	–2.4740742	–1.0764881	–4.4576248
H	1.9693987	5.1844001	–4.7950008
H	0.8116719	4.7278582	–7.1986836
H	3.1412647	1.8070869	–0.6799138
H	1.0805746	0.4590312	0.4529791
H	–4.3826220	–2.0770904	–3.8300224
H	–3.6658928	–1.2217281	–1.3610871
H	–0.1705945	–0.1374079	–9.6544805
H	–1.8299953	–1.9938929	–8.5754114
Co	–0.1823772	0.8051966	–4.5559141
C	3.4255594	3.7268396	–2.8048803
C	5.3843174	5.5639642	–1.9548907
C	4.5070785	4.0665104	–3.6450315
C	3.3350117	4.3417784	–1.5408822
C	4.3068131	5.2493028	–1.1206993
C	5.4771118	4.9728639	–3.2187308
H	4.5732422	3.6050573	–4.6328014
H	2.4809970	4.1233539	–0.9004655
H	4.2158174	5.7238647	–0.1424761
H	6.3124258	5.2163891	–3.8767231
H	6.1437108	6.2736057	–1.6234798
C	0.5357508	2.5604874	–9.0584451
C	0.6477478	3.8283080	–11.5615544
C	–0.6038521	2.6113882	–9.8832073
C	1.7299145	3.1653058	–9.4982297
C	1.7821357	3.7900154	–10.7441299
C	–0.5451995	3.2417909	–11.1257864
H	–1.5375203	2.1788457	–9.5213751
H	2.6109088	3.1188810	–8.8540030
H	2.7149229	4.2440914	–11.0818348
H	–1.4371215	3.2865529	–11.7525331
H	0.6912453	4.3189425	–12.5350838
C	–3.4272687	–2.3343779	–6.3762488
C	–5.3576384	–4.0806385	–7.4387917
C	–4.3127472	–1.8968529	–7.3761152
C	–3.5259747	–3.6568705	–5.9133103
C	–4.4819634	–4.5247046	–6.4438215
C	–5.2718022	–2.7641482	–7.9011960
H	–4.2466371	–0.8640117	–7.7207031
H	–2.8379148	–4.0002915	–5.1395823
H	–4.5403757	–5.5522700	–6.0820213
H	–5.9588859	–2.4084564	–8.6703213
H	–6.1060582	–4.7585107	–7.8514625
C	–1.5341757	–0.1614293	0.0141244
C	–2.3942100	–0.4585573	2.6715446
C	–1.7254420	–1.4400281	0.5612014
C	–1.7820374	0.9676301	0.8126941
C	–2.2124033	0.8183998	2.1318852
C	–2.1497550	–1.5869888	1.8833556
H	–1.5259950	–2.3172062	–0.0559983
H	–1.6624479	1.9565194	0.3678782
H	–2.4136843	1.7024165	2.7387882
H	–2.2854201	–2.5858261	2.3007183
H	–2.7280420	–0.5744758	3.7036386
C	2.4815660	0.8740944	–5.6926505
C	3.6595774	1.3272357	–6.3873160
O	3.8478288	2.4967987	–6.7488268
O	4.5849973	0.3499358	–6.6383669
C	2.1911301	–0.4091720	–5.1935464
O	3.1140870	–1.3830643	–5.3508219
O	1.1087892	–0.7060127	–4.5967497
C	5.7550673	0.8073284	–7.3365486
H	5.4930381	1.2273294	–8.3183337
H	6.3830738	–0.0823161	–7.4567475
H	6.2872787	1.5767677	–6.7587993
C	2.7376459	–2.6776476	–4.8413711
H	3.5893070	–3.3268807	–5.0706336
H	1.8282334	–3.0466625	–5.3354768
H	2.5633668	–2.6402613	–3.7570518
C	–1.3970780	2.2558661	–4.5112255
C	–1.4498685	2.9787241	–3.2181156
O	–2.2046560	2.6860642	–2.3021669
O	–0.5219711	3.9679932	–3.1240685
C	–2.4183683	2.5964037	–5.4921120
O	–2.7846383	1.9659240	–6.4796212
O	–2.9771811	3.8278027	–5.1802488
C	–0.3809051	4.5445417	–1.8099713
H	–0.0779104	3.7679636	–1.0914614
H	–1.3229645	4.9988425	–1.4747796
H	0.4050458	5.3009663	–1.9064950
C	–4.0057885	4.2644807	–6.0828699
H	–3.6144332	4.3610029	–7.1062801
H	–4.8433540	3.5520233	–6.0956945
H	–4.3355972	5.2380917	–5.7039676

[Co(TPP)] *Mono*-Enolate *Mono*-Gamma Radical (I^{E-G}):

123 atoms

C	1.0331009	4.2279611	–4.8144647
C	0.5852660	4.0548604	–6.1087200
C	0.0264745	2.7686888	–6.2227392
C	0.7677491	3.0556628	–4.0855879
N	0.1604621	2.0643675	–4.9576122
C	0.9687892	2.8458398	–2.7283302
C	0.2026215	1.9346442	–1.9726917
N	–0.9979196	1.3495712	–2.3359847
C	–1.4717829	0.7227080	–1.1991369
C	0.5039579	1.6181412	–0.5956926
C	–0.5405899	0.8917317	–0.1107758
C	–2.6973433	0.0639128	–1.0818291
C	–3.5261573	–0.2108199	–2.1719583
N	–3.2581032	0.0952355	–3.4834032
C	–5.2106949	–1.1234124	–3.3578040
C	–4.7540624	–0.9636452	–2.0853999
C	–3.3336711	0.0297744	–6.4474914
N	–2.2963443	0.8433449	–6.0328998
C	–1.6443102	1.2413170	–7.1858196
C	–2.2517402	0.6098740	–8.3343347
C	–3.3085140	–0.1194447	–7.8817958
C	–0.6587914	2.2440469	–7.3085281
C	–4.3189526	–0.5186805	–5.6233403
C	–4.2624580	–0.4714897	–4.2284249
H	1.4418885	5.1331270	–4.3779682
H	0.5607382	4.7992719	–6.8974443
H	1.4086409	1.9190305	–0.0786998
H	–0.6747381	0.4909018	0.8880248
H	–6.0942432	–1.6529053	–3.6970726
H	–5.1844542	–1.3345942	–1.1617052
H	–1.9008730	0.7204625	–9.3546431
H	–4.0101304	–0.7142816	–8.4562676
Co	–1.8010292	1.1763357	–4.1418386
C	1.9810511	3.7031130	–2.0692339
C	3.9310741	5.3496265	–0.8892469
C	3.2641138	3.8137644	–2.6393768
C	1.6863523	4.4427479	–0.9095782
C	2.6549853	5.2579455	–0.3241416
C	4.2305028	4.6286387	–2.0493275
H	3.4868422	3.2521737	–3.5494080
H	0.6832495	4.3851344	–0.4850798
H	2.4102573	5.8334814	0.5697813
H	5.2233115	4.6985672	–2.4960313
H	4.6878233	5.9871179	–0.4297500
C	–0.4077919	2.8833393	–8.6216633
C	0.1160183	4.1747150	–11.0642076
C	–1.4627750	3.3736585	–9.4129604
C	0.9154665	3.0596028	–9.0680349
C	1.1723027	3.6975823	–10.2818981
C	–1.2018038	4.0135718	–10.6244032
H	–2.4874453	3.2693696	–9.0541271
H	1.7343567	2.6914935	–8.4464068
H	2.2022173	3.8212160	–10.6195897
H	–2.0296751	4.3970019	–11.2228160
H	0.3189548	4.6755284	–12.0118615
C	–5.5219392	–1.1333577	–6.2522088
C	–7.8281474	–2.2205171	–7.4258421
C	–6.7462150	–0.4484519	–6.1755371
C	–5.4656692	–2.3687775	–6.9132732
C	–6.6137831	–2.9089840	–7.4978350
C	–7.8910699	–0.9915872	–6.7622058
H	–6.7759864	0.5090448	–5.6522203
H	–4.5170754	–2.9060408	–6.9600819
H	–6.5603399	–3.8732117	–8.0056550
H	–8.8366512	–0.4505468	–6.7006998
H	–8.7242423	–2.6432343	–7.8825343
C	–3.1820341	–0.3135956	0.2757501
C	–4.1408743	–0.9600559	2.8330019
C	–2.6208453	–1.3786592	0.9945914
C	–4.2343015	0.4227198	0.8448156
C	–4.7079355	0.0991937	2.1180003
C	–3.0979930	–1.6994388	2.2678325

H	–1.8122717	–1.9576809	0.5456063
H	–4.6661766	1.2439619	0.2699002
H	–5.5240395	0.6781595	2.5531955
H	–2.6578436	–2.5333259	2.8167836
H	–4.5135139	–1.2119093	3.8269407
C	1.0038146	0.8339758	–5.0856848
C	2.3497774	1.0379064	–5.5758982
O	2.8325022	2.1337081	–5.8810761
O	3.0902960	–0.1113282	–5.6841120
C	0.4081768	–0.3807734	–4.7094012
O	1.1290072	–1.5190613	–4.8088865
O	–0.7818813	–0.4895257	–4.2728801
C	4.4299252	0.0918483	–6.1622209
H	4.8779878	–0.9076739	–6.1920290
H	4.9988830	0.7466200	–5.4862745
H	4.4312230	0.5427526	–7.1651491
C	0.4487366	–2.7222941	–4.4004637
H	1.1824675	–3.5214071	–4.5507780
H	–0.4449674	–2.9000233	–5.0145810
H	0.1488694	–2.6689410	–3.3446587
C	–3.0712366	2.9561909	–3.9408204
C	–4.2622939	2.7066353	–4.8271319
O	–5.3177216	2.1748011	–4.5324443
O	–4.0179567	3.1662942	–6.0961026
C	–5.0910331	2.9946052	–7.0341576
H	–4.7850703	3.5529301	–7.9260172
H	–6.0307287	3.3985416	–6.6338272
H	–5.2277171	1.9304154	–7.2740859
C	–2.2182387	4.1373361	–4.4240575
H	–1.8147351	3.8888595	–5.4037380
H	–1.3741636	4.2504972	–3.7344095
C	–2.9846117	5.4121931	–4.4980862
C	–3.4263628	3.0350487	–2.4837134
O	–4.3352058	2.4706088	–1.9022938
O	–2.5516539	3.8595108	–1.8089756
C	–2.7476522	3.9019111	–0.3851750
H	–3.7640883	4.2371055	–0.1359787
H	–2.5805768	2.9095599	0.0571751
H	–2.0041902	4.6135374	–0.0095001
H	–3.4148005	5.7835813	–3.5637898
C	–3.2181667	6.1563451	–5.6780512
C	–3.7131630	7.7053641	–8.0122352
C	–3.9872211	7.3584679	–5.6296851
C	–2.7102692	5.7669645	–6.9554763
C	–2.9525589	6.5277154	–8.0889609
C	–4.2277584	8.1107850	–6.7706090
H	–4.3925824	7.6808195	–4.6680354
H	–2.1344825	4.8473554	–7.0465510
H	–2.5430288	6.1999956	–9.0466938
H	–4.8222105	9.0234878	–6.7008207
H	–3.9025649	8.2991201	–8.9072420

[Co(TPP)] Enolate (I^E):

92 atoms

C	1.9138888	4.1457324	–5.2169769
C	1.4669224	3.8665576	–6.5040859
C	1.3104049	2.4846022	–6.6275131
C	2.0404329	2.9412178	–4.5222723
N	1.6435198	1.8393831	–5.3741768
C	2.4375408	2.7445797	–3.1944699
C	1.8372189	1.7392881	–2.4233309
N	0.6396508	1.1099303	–2.7582742
C	0.2004633	0.5146870	–1.5926153
C	2.1976521	1.4205960	–1.0617099
C	1.1752522	0.6875201	–0.5398817
C	–1.0583566	–0.0662024	–1.4208181
C	–1.9370800	–0.2959082	–2.4854351
N	–1.6209182	–0.1299789	–3.8203606
C	–3.6469836	–1.2333287	–3.6189542
C	–3.2180181	–0.9478209	–2.3562301
C	–1.5538560	–0.6232817	–6.7271449
N	–0.6020313	0.3135733	–6.3769446
C	0.0691756	0.6185140	–7.5594663
C	–0.3996001	–0.2339093	–8.6265813
C	–1.4182723	–0.9829020	–8.1202755
C	0.8662129	1.7581301	–7.7382035
C	–2.5802458	–1.0667073	–5.8894213
C	–2.6310986	–0.7554527	–4.5258259
H	2.0951843	5.1211494	–4.7768049
H	1.2232277	4.5765030	–7.2881006
H	3.1098837	1.7447978	–0.5723033
H	1.0739805	0.2982376	0.4678495
H	–4.5479292	–1.7576157	–3.9200760
H	–3.6958656	–1.1907482	–1.4128517
H	–0.0054368	–0.2316013	–9.6372612
H	–2.0366267	–1.7108229	–8.6350899
Co	–0.0431035	0.7263392	–4.5495643
C	3.3960951	3.7121409	–2.6247532
C	5.2487232	5.5789688	–1.6215616
C	4.5339896	4.0700404	–3.3773716
C	3.1933761	4.3232843	–1.3720053
C	4.1132096	5.2462770	–0.8757617
C	5.4518189	4.9915284	–2.8741175
H	4.6861371	3.6086012	–4.3555417
H	2.2928517	4.0891249	–0.8035909
H	3.9362697	5.7189815	0.0914826
H	6.3333718	5.2495699	–3.4627893
H	5.9676499	6.3004571	–1.2306442
C	1.1622909	2.3136831	–9.0735490
C	1.7924142	3.4191281	–11.5843713
C	0.1786621	2.4285322	–10.0751145
C	2.4643993	2.7829028	–9.3450754
C	2.7732305	3.3252782	–10.5921740
C	0.4930519	2.9746823	–11.3189653
H	–0.8419558	2.1113232	–9.8592152
H	3.2258165	2.7069777	–8.5657648
H	3.7878736	3.6732505	–10.7914945
H	–0.2827776	3.0667619	–12.0804663
H	2.0364268	3.8449096	–12.5587385
C	–3.6546552	–1.9269491	–6.4634647
C	–5.6819183	–3.5521372	–7.5391947
C	–4.9406487	–1.4110495	–6.6839541
C	–3.3976615	–3.2680763	–6.7867872
C	–4.4037392	–4.0744933	–7.3231957
C	–5.9479361	–2.2185812	–7.2168195
H	–5.1435473	–0.3684352	–6.4348160
H	–2.4006343	–3.6737422	–6.6090836
H	–4.1895882	–5.1160585	–7.5672335
H	–6.9424413	–1.8026982	–7.3850404
H	–6.4682577	–4.1824336	–7.9565361
C	–1.4752021	–0.4851300	–0.0515500
C	–2.2668287	–1.2782840	2.5275027
C	–0.9247751	–1.6309737	0.5426811
C	–2.4288662	0.2568789	0.6614529
C	–2.8231722	–0.1378028	1.9419221
C	–1.3161409	–2.0235504	1.8245234
H	–0.1891285	–2.2141050	–0.0131727
H	–2.8582008	1.1486608	0.2024077
H	–3.5639436	0.4506093	2.4853820
H	–0.8813614	–2.9182020	2.2726663
H	–2.5737548	–1.5857939	3.5280309
C	2.6905116	0.7829564	–5.5074454
C	3.9457056	1.2419758	–6.0444235
O	4.1760391	2.4138779	–6.3779697
O	4.9076673	0.2745283	–6.1719525
C	2.3405521	–0.5231453	–5.0982778
O	3.2808407	–1.4915888	–5.2112439
O	1.2076896	–0.8465020	–4.6333861
C	6.1538367	0.7463162	–6.7087217
H	6.8024875	–0.1360582	–6.7448521
H	6.5967967	1.5210599	–6.0661552
H	6.0205467	1.1649444	–7.7168602
C	2.8668863	–2.8010948	–4.7795024
H	3.7416110	–3.4399222	–4.9427134
H	2.0126107	–3.1614932	–5.3696549
H	2.5865060	–2.7979698	–3.7168085

[Co(TPP)] *Mono* Benzene *Mono* Enolate Adduct ($I^{E'}$):

104 atoms

C	0.6301979	–3.5266004	–2.0918761
C	–0.7586867	–3.5084765	–2.1243569
C	–1.2173661	–2.7913402	–1.0151914
C	1.0549231	–2.8184629	–0.9636421
N	–0.0920036	–2.3085033	–0.2450679
C	2.3673498	–2.5475845	–0.5626448
C	2.6928795	–1.3183887	0.0300374
N	1.8818827	–0.1867923	–0.0038774
C	2.7121718	0.8701350	0.3095772
C	4.0148090	–0.9631258	0.4934982
C	4.0365302	0.3907483	0.6353232
C	2.3610910	2.2195951	0.2230573
C	1.0485165	2.6517683	0.0123054
N	–0.0577938	1.8317367	–0.0266114
C	–0.7198567	4.0497810	–0.0323017
C	0.6428718	4.0379824	–0.0201402
C	–2.8517932	0.9170310	0.2352525
N	–2.0312858	–0.1516974	–0.0642292
C	–2.8638106	–1.2675818	–0.0732700
C	–4.1941337	–0.8932155	0.3489912
C	–4.1949827	0.4585938	0.5106019
C	–2.5394611	–2.4962503	–0.6678908
C	–2.4747712	2.2606708	0.1700214
C	–1.1502461	2.6707677	–0.0092001
H	1.3032118	–3.9569846	–2.8265776
H	–1.4075154	–3.9220032	–2.8898202
H	4.8209374	–1.6689781	0.6622894
H	4.8680039	1.0209212	0.9328782
H	–1.3851833	4.9066339	–0.0216196
H	1.3229032	4.8829962	0.0025341
H	–5.0187735	–1.5857472	0.4791803
H	–5.0243002	1.1004259	0.7885384
Co	–0.0733285	–0.1143928	–0.0907782
C	3.3941645	–3.5493093	–0.9163299
C	5.2809727	–5.5241887	–1.5970347
C	3.1299134	–4.9116831	–0.6657477
C	4.6095913	–3.1986057	–1.5349199
C	5.5443863	–4.1779211	–1.8691364
C	4.0696254	–5.8863405	–0.9999879
H	2.1803584	–5.1881729	–0.2021949
H	4.8036414	–2.1529498	–1.7754529
H	6.4770709	–3.8908424	–2.3568486
H	3.8555725	–6.9351199	–0.7894979
H	6.0142476	–6.2885261	–1.8582631
C	–3.5724802	–3.4711762	–1.0742350
C	–5.4743845	–5.3940467	–1.8540795
C	–4.7532095	–3.0855910	–1.7375333
C	–3.3502554	–4.8417826	–0.8280852
C	–4.2974521	–5.7906197	–1.2118079
C	–5.6956280	–4.0391846	–2.1209994
H	–4.9134286	–2.0330359	–1.9728894
H	–2.4277803	–5.1448096	–0.3279194
H	–4.1166129	–6.8462315	–1.0043291
H	–6.6007594	–3.7252305	–2.6428216
H	–6.2135353	–6.1382670	–2.1538985
C	–3.5287799	3.3083604	0.2852258
C	–5.5098897	5.2946600	0.4753263
C	–3.9272847	4.0301418	–0.8502597
C	–4.1331522	3.5963007	1.5179737
C	–5.1187103	4.5814927	1.6118355
C	–4.9103117	5.0174099	–0.7563888
H	–3.4563672	3.8071071	–1.8089511
H	–3.8186427	3.0432040	2.4041387
H	–5.5778198	4.7969756	2.5777385
H	–5.2116551	5.5685849	–1.6483884
H	–6.2783808	6.0651248	0.5495365
C	3.4300788	3.2500505	0.3560443
C	5.4377164	5.2058647	0.5784142
C	4.0008698	3.5465350	1.6026102
C	3.8754650	3.9477297	–0.7769396
C	4.8718166	4.9198982	–0.6671319
C	4.9996772	4.5166169	1.7125750
H	3.6496348	3.0123729	2.4865820
H	3.4305016	3.7180944	–1.7464004
H	5.2096787	5.4525500	–1.5572800
H	5.4324083	4.7391671	2.6889855
H	6.2164556	5.9646309	0.6651754
C	–0.1280353	–2.7271515	1.1879409
C	–0.1536113	–4.1522469	1.3971390
O	–0.1444676	–4.9933061	0.4859246
O	–0.1908292	–4.5429360	2.7103391
C	–0.1306071	–1.7014539	2.1605447
O	–0.1599173	–2.0731012	3.4635343
O	–0.1070493	–0.4645159	1.8961389
C	–0.2162721	–5.9660754	2.9034110
H	–0.2440381	–6.1071874	3.9896606
H	0.6792185	–6.4423108	2.4783767
H	–1.1042245	–6.4160454	2.4361377
C	–0.1622223	–0.9878903	4.4092911
H	–0.1876483	–1.4718994	5.3916355
H	–1.0441458	–0.3460470	4.2743888
H	0.7420747	–0.3715063	4.3080457
H	1.2540395	3.4134896	–3.2898232
C	0.6906477	2.4817344	–3.2252965
C	–0.7681802	0.1082890	–3.0052020
C	1.3606303	1.2649831	–3.0937416
C	–0.7080982	2.5140169	–3.2471401
C	–1.4375095	1.3293853	–3.1385444
C	0.6315298	0.0760325	–2.9814844
H	2.4499321	1.2393854	–3.0464526
H	–1.2256478	3.4707364	–3.3282590
H	–2.5278336	1.3542280	–3.1271744
H	1.1496256	–0.8758562	–2.8702410
H	–1.3326748	–0.8186501	–2.9095491

[Co(TPP)] *Mono*-Enolate *Mono*-Iodonium Ylide (I^{E-IY}):

119 atoms

C	2.4356407	4.7929535	–5.3649886
C	1.8143037	4.6598892	–6.5692916
C	1.0783248	3.4189514	–6.5282023
C	2.0752467	3.6384829	–4.5762197
N	1.2270272	2.8203136	–5.2951085
C	2.6108456	3.3467344	–3.3185138
C	2.2470913	2.2124174	–2.5874867
N	1.1851459	1.3823800	–2.9056733
C	1.0195498	0.5487967	–1.7973364
C	2.8115670	1.8346201	–1.3152131
C	2.0713390	0.7912419	–0.8420852
C	–0.1533612	–0.1728020	–1.5267550
C	–1.1015275	–0.3867558	–2.5302485
N	–0.7280246	–0.5411116	–3.9208778
C	–3.0396567	–0.6454504	–3.6642978
C	–2.4934631	–0.4325601	–2.4065745
C	–1.2281880	–0.1849686	–6.8287627
N	–0.4481164	0.9014235	–6.4311027
C	–0.1457962	1.5814165	–7.5926385
C	–0.6530537	0.8672333	–8.7402846
C	–1.2819244	–0.2468102	–8.2703423
C	0.4541330	2.8434124	–7.6365200
C	–2.0948971	–0.8818949	–5.9752079
C	–1.9973512	–0.7263025	–4.5894544

H	3.0970581	5.5854706	–5.0328803
H	1.8627933	5.3208399	–7.4277413
H	3.6605521	2.3203453	–0.8461599
H	2.2008196	0.2421140	0.0846149
H	–4.0895375	–0.6661449	–3.9353058
H	–3.0246841	–0.2632469	–1.4753927
H	–0.5395454	1.1872611	–9.7704747
H	–1.7755145	–1.0283685	–8.8378473
Co	0.3629713	1.2004215	–4.6821599
C	3.5503624	4.3274327	–2.7064839
C	5.2767891	6.2070483	–1.5364058
C	4.9107382	4.0318548	–2.5354623
C	3.0606186	5.5773970	–2.2917537
C	3.9228033	6.5095206	–1.7104316
C	5.7690799	4.9665907	–1.9516880
H	5.2923732	3.0663036	–2.8712097
H	2.0029409	5.8068626	–2.4401110
H	3.5326713	7.4769942	–1.3904279
H	6.8265016	4.7276793	–1.8282937
H	5.9478793	6.9373700	–1.0819915
C	0.3649756	3.6495805	–8.8846955
C	0.1299300	5.2293141	–11.1950494
C	–0.4639966	4.7849349	–8.8878887
C	1.0792150	3.3198463	–10.0453021
C	0.9606773	4.1053012	–11.1946905
C	–0.5794625	5.5673865	–10.0383691
H	–1.0090165	5.0344626	–7.9751960
H	1.7380396	2.4501578	–10.0370463
H	1.5256318	3.8423915	–12.0902979
H	–1.2293909	6.4440478	–10.0322061
H	0.0393144	5.8421604	–12.0929778
C	–3.2381707	–1.6720219	–6.4756702
C	–5.4247882	–3.2249234	–7.3313993
C	–4.0926317	–1.2095427	–7.4947096
C	–3.5145591	–2.9170682	–5.8737899
C	–4.5951700	–3.6860914	–6.3048058
C	–5.1740109	–1.9807231	–7.9189604
H	–3.9205872	–0.2254702	–7.9308143
H	–2.8673295	–3.2682430	–5.0671298
H	–4.7889538	–4.6524920	–5.8370421
H	–5.8331229	–1.6027381	–8.7019475
H	–6.2705360	–3.8273518	–7.6661929
C	–0.5145686	–0.5968906	–0.1586678
C	–1.2903428	–1.4415650	2.4110781
C	–1.0552710	–1.8835109	0.0399875
C	–0.3874760	0.2632100	0.9489086
C	–0.7713642	–0.1566536	2.2221065
C	–1.4335830	–2.2997641	1.3161900
H	–1.1677454	–2.5453656	–0.8217017
H	–0.0041186	1.2733923	0.7986401
H	–0.6771016	0.5254755	3.0683697
H	–1.8403594	–3.3022232	1.4571223
H	–1.5890476	–1.7693271	3.4078384
C	0.2387914	–1.6531461	–4.1598775
C	–0.2097928	–2.9488501	–3.7177891
O	–1.3068925	–3.1642029	–3.1823581
O	0.6803280	–3.9698839	–3.9288355
C	1.4592462	–1.3175234	–4.7862543
O	2.3421197	–2.3166851	–5.0244135
O	1.7804741	–0.1445049	–5.1400104
C	0.2212630	–5.2559467	–3.4835976
H	0.0231413	–5.2561024	–2.4018227
H	1.0355813	–5.9492388	–3.7222809
H	–0.6998942	–5.5533191	–4.0055903
C	3.5689185	–1.9118890	–5.6604840
H	4.1155150	–1.1863327	–5.0418794
H	3.3757796	–1.4627236	–6.6447710
H	4.1471481	–2.8359914	–5.7679709
C	–1.5728971	4.0905802	–4.1385562
C	–2.4217197	3.2976580	–5.0050148
O	–3.1213016	2.3466517	–4.6394114
O	–2.3765487	3.6925673	–6.3112967
C	–0.8771557	5.3497814	–4.2998795
O	–0.2131593	5.9199654	–3.4307789
O	–1.0404775	5.8898906	–5.5490730
C	–0.3808139	7.1557504	–5.7382112
H	0.6915925	7.0723607	–5.5196628
H	–0.8206831	7.9261182	–5.0892022
H	–0.5381217	7.4048930	–6.7937505
C	–3.2048121	2.9174029	–7.1994567
H	–4.2697642	3.0727880	–6.9753682
H	–2.9720840	1.8489507	–7.1108676
H	–2.9610642	3.2787113	–8.2043521
I	–1.3220979	3.2458161	–2.2811129
C	–3.0957453	3.8838983	–1.2432846
C	–5.3976316	4.6632395	0.0705839
C	–2.9832188	4.7226803	–0.1355195
C	–4.3245438	3.4227969	–1.7184608
C	–5.4826198	3.8288495	–1.0488477
C	–4.1540864	5.1084659	0.5265031
H	–2.0103757	5.0823351	0.2003304
H	–4.3657644	2.7806225	–2.5994272
H	–6.4551847	3.4859933	–1.4049347
H	–4.0892477	5.7667837	1.3939303
H	–6.3068049	4.9717373	0.5881583

[Co(TPP)] Bridging Carbene (I^{B}):

92 atoms

C	2.9193434	4.1195743	–5.0538464
C	2.4744313	3.8963552	–6.3192252
C	1.3245965	3.0306711	–6.2183050
C	2.0600652	3.3839944	–4.1548436
N	1.0926017	2.6831019	–4.8948100
C	2.2314240	3.4428323	–2.7616462
C	1.5526778	2.6538138	–1.8220711
N	0.8768375	1.4618209	–2.1053716
C	0.0568421	1.1579428	–1.0129988
C	1.2423794	3.0175038	–0.4832314
C	0.3317641	2.1070727	0.0092189
C	–0.9880915	0.2231838	–1.0198476
C	–1.6145084	–0.2938762	–2.1661712
N	–1.4745390	0.1101073	–3.5048241
C	–3.0258305	–1.6153998	–3.3410740
C	–2.5688502	–1.3754592	–2.0830909
C	–1.9792206	0.2966308	–6.4489505
N	–0.9388461	1.1269552	–6.0801241
C	–0.5242301	1.7572000	–7.2371571
C	–1.3586244	1.3574738	–8.3416531
C	–2.2595940	0.4527811	–7.8535328
C	0.5631194	2.6333580	–7.3237200
C	–2.6425373	–0.5837290	–5.5873189
C	–2.3703696	–0.6750218	–4.2172657
H	3.7754447	4.7078644	–4.7426906
H	2.8855784	4.2762005	–7.2483325
H	1.5956845	3.9261788	–0.0079537
H	–0.1915801	2.1392547	0.9586802
H	–3.7410889	–2.3659901	–3.6597599
H	–2.8257018	–1.9001143	–1.1695954
H	–1.2705422	1.7323111	–9.3560751
H	–3.0526177	–0.0571326	–8.3905533
Co	–0.1672149	1.3125162	–4.3118239
C	3.1772304	4.4364365	–2.1897328
C	4.9692362	6.2724866	–1.0437565
C	4.2220946	3.9906921	–1.3618283
C	3.0385408	5.8135924	–2.4308208
C	3.9277491	6.7251375	–1.8598382
C	5.1144267	4.9036829	–0.7980876
H	4.3302603	2.9189055	–1.1913166
H	2.2196380	6.1615895	–3.0619746
H	3.8031683	7.7928505	–2.0464130
H	5.9291693	4.5445099	–0.1676314
H	5.6648939	6.9857071	–0.5992717
C	0.9279193	3.1658329	–8.6675856
C	1.6098237	4.1626797	–11.2102617
C	0.7805746	4.5301864	–8.9648780
C	1.4203568	2.3083616	–9.6645448
C	1.7598454	2.8025526	–10.9256311
C	1.1183683	5.0249908	–10.2260566
H	0.3936149	5.1999305	–8.1955194
H	1.5373983	1.2476347	–9.4379144
H	2.1466800	2.1234878	–11.6870139
H	0.9923186	6.0869358	–10.4422027
H	1.8741827	4.5490990	–12.1954991
C	–3.6928479	–1.4703650	–6.1645853
C	–5.6717567	–3.1435060	–7.2639245
C	–5.0421912	–1.3121361	–5.8099364
C	–3.3506027	–2.4785850	–7.0800005
C	–4.3317026	–3.3096252	–7.6246422
C	–6.0241148	–2.1414633	–6.3553834
H	–5.3142686	–0.5270375	–5.1030193
H	–2.3033776	–2.6058128	–7.3580109
H	–4.0477888	–4.0920177	–8.3301081
H	–7.0687006	–2.0010226	–6.0734663
H	–6.4386899	–3.7919017	–7.6897078
C	–1.4663929	–0.2033188	0.3210846
C	–2.3031128	–0.9872370	2.8865968
C	–0.5546791	–0.7775757	1.2237507
C	–2.8002030	–0.0207451	0.7230935
C	–3.2147736	–0.4088369	1.9978734
C	–0.9734071	–1.1714037	2.4954298
H	0.4755887	–0.9275054	0.8988010
H	–3.5051680	0.4382730	0.0285956
H	–4.2510459	–0.2527259	2.3013234
H	–0.2594108	–1.6280642	3.1824157
H	–2.6285095	–1.2919034	3.8823257
C	1.2185771	0.5363232	–3.1882828
C	2.6873366	0.6355349	–3.6268190
O	2.8204164	0.2721600	–4.9190057
O	3.6204019	0.9216073	–2.9001366
C	1.1123166	–0.9400967	–2.7790907
O	0.8477004	–1.7099737	–3.8549118
O	1.3153210	–1.3775409	–1.6620053
H	–0.0952968	–3.3097103	–2.8967197
C	0.7488304	–3.1241811	–3.5748680
H	1.6737382	–3.4977921	–3.1149340
H	0.5744342	–3.5975648	–4.5458902
H	4.1091801	–0.0400307	–6.4541895
C	4.1755063	0.3101381	–5.4196254
H	4.8306435	–0.3407552	–4.8249141
H	4.5557568	1.3401395	–5.3833698

[Co(TPP)] *Bis-cis*-Bridged Carbene (c-$I^{B–B}$):

107 atoms

C	–1.4809907	1.6882483	–3.2544558
C	–1.3427103	2.0242831	–4.5733013
C	–0.7256708	0.9012769	–5.2229107
C	–0.9585101	0.3569074	–3.1032554
N	–0.5756161	–0.1447179	–4.3177392
C	–0.7183270	–0.2519785	–1.8504895
C	–0.0660989	–1.4445215	–1.6803795
N	0.3830189	–2.3272783	–2.7719430
C	0.3209245	–3.6675017	–2.1640869
C	0.0032349	–2.1834997	–0.4706597
C	0.2217044	–3.5093835	–0.7668371
C	0.2134476	–4.8635610	–2.8641028
C	0.0071242	–5.0037365	–4.2336559
N	–0.2484623	–3.9026613	–5.1792783
C	0.2874771	–5.8697953	–6.3203069
C	0.2058990	–6.1820447	–4.9818951
C	0.7771982	–2.3274916	–7.5568387
N	0.3955886	–1.4835567	–6.5477610
C	0.4066198	–0.2057246	–7.0983367
C	0.9330259	–0.2538933	–8.4332205
C	1.1504449	–1.5734057	–8.7232345
C	–0.1885887	0.9135386	–6.5110942
C	0.6720553	–3.7376093	–7.5305791
C	0.1751679	–4.4632333	–6.4754184
H	–1.8647150	2.2961448	–2.4421433
H	–1.5951296	2.9609050	–5.0580356
H	–0.2404155	–1.7654573	0.5001940
H	0.1925362	–4.3413151	–0.0707264
H	0.5588304	–6.5425653	–7.1266681
H	0.3962459	–7.1517318	–4.5336568
H	1.0701029	0.6061106	–9.0792887
H	1.4932532	–2.0050108	–9.6572595
Co	–0.0086337	–1.9508840	–4.7127688
C	1.5968675	–2.0305813	–3.5810954
C	–1.5271893	–3.1554543	–5.0218341
C	1.0736071	–4.4936411	–8.7477287
C	1.8076677	–5.9404054	–11.0413174
C	0.1030743	–5.1730246	–9.5004378
C	2.4137515	–4.5392655	–9.1618445
C	2.7789096	–5.2598020	–10.3009922
C	0.4693342	–5.8925814	–10.6395763
H	–0.9384213	–5.1141896	–9.1813040
H	3.1657482	–3.9969826	–8.5861854
H	3.8247250	–5.2916302	–10.6102524
H	–0.2944219	–6.4119431	–11.2204463
H	2.0928139	–6.5025464	–11.9316304
C	0.3773675	–6.1191512	–2.0752174
C	0.7151782	–8.4794275	–0.5940665
C	–0.6494648	–7.0731420	–2.0152359
C	1.5799146	–6.3605679	–1.3916624
C	1.7452292	–7.5358990	–0.6562983
C	–0.4825432	–8.2459106	–1.2764421
H	–1.5747784	–6.8879905	–2.5612036
H	2.3776529	–5.6188962	–1.4545352
H	2.6855077	–7.7177556	–0.1337819
H	–1.2904291	–8.9776629	–1.2306290
H	0.8460844	–9.3958764	–0.0170540
C	–1.1547452	0.4724731	–0.6250756
C	–1.9635716	1.8418190	1.6850697
C	–2.5144987	0.5550286	–0.2919121
C	–0.2027872	1.0814987	0.2057131
C	–0.6070524	1.7628320	1.3561069
C	–2.9159029	1.2368715	0.8589604
H	–3.2474497	0.0728968	–0.9402606
H	0.8503115	1.0184987	–0.0722025
H	0.1391713	2.2380074	1.9947961
H	–3.9753171	1.2920730	1.1142309
H	–2.2786475	2.3744908	2.5835504
C	–0.2560476	2.1778280	–7.2951679
C	–0.3795012	4.5677016	–8.7714602
C	0.4508514	3.3150284	–6.8731587
C	–1.0263624	2.2543473	–8.4662877
C	–1.0902279	3.4420466	–9.1972780
C	0.3923076	4.5004396	–7.6081678
H	1.0480804	3.2583240	–5.9622848
H	–1.5770327	1.3724912	–8.7960108
H	–1.6993372	3.4887891	–10.1011494
H	0.9530837	5.3736536	–7.2717645
H	–0.4275413	5.4948181	–9.3442134
C	2.3029619	–0.7428203	–3.4015279
O	2.0263221	0.1820757	–2.6570471
O	3.3697176	–0.7143327	–4.2624367
C	2.5671934	–3.1918591	–3.7351310
O	3.1822408	–3.6913369	–2.8098732
O	2.6791342	–3.5946469	–5.0170119
C	3.5644153	–4.7142005	–5.2358561
H	3.2492074	–5.5668771	–4.6194959
H	4.5984798	–4.4433807	–4.9838399
H	3.4644875	–4.9531352	–6.2992546

C	–2.3766495	–3.4823630	–3.8033351
O	–2.9062971	–4.7338164	–3.9155987
O	–2.6162392	–2.7409489	–2.8747349
H	–4.6131371	–4.4528509	–2.7288861
C	–3.7472144	–5.1237678	–2.8057257
H	–4.0677713	–6.1472521	–3.0261212
H	–3.1806839	–5.0836773	–1.8651168
C	–2.3557033	–2.8721796	–6.2145077
O	–2.1342798	–3.1537893	–7.3805639
O	–3.4698832	–2.1822080	–5.8148266
C	–4.3425617	–1.7773998	–6.8863598
H	–5.1638075	–1.2386520	–6.4029159
H	–4.7206335	–2.6511759	–7.4355185
H	–3.8106750	–1.1201587	–7.5880602
C	4.1223332	0.5135229	–4.2436673
H	4.9244310	0.3734874	–4.9754772
H	4.5374018	0.7031441	–3.2440343
H	3.4832105	1.3601130	–4.5302048

[Co(TPP)] *Bis-trans*-Bridged Carbene (*t*-I$^{B–B}$):

107 atoms

C	–1.1703352	1.7055202	–3.3206504
C	–1.0596374	2.0597751	–4.6448937
C	–0.3203905	1.0455831	–5.3171008
C	–0.5028646	0.4615196	–3.1347646
N	0.1187578	0.1260090	–4.3499914
C	–0.6952965	–0.3793825	–2.0273066
C	–0.5845797	–1.7799624	–2.0141408
N	–0.3339595	–2.6296557	–3.0856400
C	–0.2701574	–3.9113962	–2.5451839
C	–0.7063122	–2.5500889	–0.7944073
C	–0.5137045	–3.8547588	–1.1185147
C	0.0222064	–5.1105608	–3.2170722
C	0.1414710	–5.2608406	–4.6099685
N	–0.3619566	–4.3860559	–5.5860552
C	1.0650344	–5.8543687	–6.5939115
C	0.9805029	–6.2031759	–5.2642808
C	0.1680567	–2.4671252	–7.9526621
N	–0.0352355	–1.6197288	–6.8660827
C	–0.1265621	–0.3373876	–7.3992416
C	–0.0003563	–0.3958088	–8.8412222
C	0.1810774	–1.6985839	–9.1796466
C	–0.2948365	0.8757969	–6.7112523
C	0.3704100	–3.8551116	–7.9300681
C	0.2855713	–4.6832032	–6.7965389
H	–1.7729496	2.1845001	–2.5569518
H	–1.5543655	2.8804466	–5.1525611
H	–0.8921947	–2.1302997	0.1876133
H	–0.5476977	–4.7144688	–0.4586912
H	1.7073365	–6.2885079	–7.3523516
H	1.5424670	–6.9725872	–4.7463099
H	–0.0211953	0.4648111	–9.5002336
H	0.2971517	–2.1179236	–10.1726891
Co	–0.1731306	–2.1403883	–4.9792501
C	1.2280628	–0.8234089	–4.5154384
C	–1.5329071	–3.4993981	–5.4360896
C	–2.3494904	–3.3517505	–6.7075142
O	–2.4350156	–4.1671370	–7.6106919
O	–3.0234153	–2.1793447	–6.6931496
C	–2.5571053	–3.8690084	–4.3759890
O	–3.2651874	–3.0665576	–3.8032605
O	–2.6675367	–5.2192614	–4.1944150
C	–3.8540556	–1.9460284	–7.8492022
H	–3.2291267	–1.8707070	–8.7502589
H	–4.3637693	–0.9980085	–7.6503931
H	–4.5814684	–2.7583348	–7.9828876
C	–3.5393753	–5.6016971	–3.1085271
H	–3.1586400	–5.1904003	–2.1625195
H	–3.5196061	–6.6960014	–3.0861700
H	–4.5591492	–5.2324665	–3.2781024
C	0.7835577	–4.5411791	–9.1815823
C	1.5482011	–5.9052877	–11.5151030
C	0.0034549	–5.6006895	–9.6746076
C	1.9549184	–4.1791855	–9.8674367
C	2.3351883	–4.8579346	–11.0259086
C	0.3818103	–6.2731912	–10.8374197
H	–0.9100451	–5.8658365	–9.1409792
H	2.5683002	–3.3667967	–9.4747105
H	3.2518924	–4.5736960	–11.5447936
H	–0.2385422	–7.0857445	–11.2184839
H	1.8450602	–6.4345246	–12.4216796
C	0.3087121	–6.3301421	–2.4194152
C	0.8508220	–8.6753136	–0.9602440
C	–0.3870090	–7.5214559	–2.6911927
C	1.2930175	–6.3384265	–1.4154619
C	1.5609564	–7.5007959	–0.6919936
C	–0.1224614	–8.6823587	–1.9638161
H	–1.1396132	–7.5180989	–3.4803940
H	1.8540419	–5.4239465	–1.2185303
H	2.3337445	–7.4929456	0.0780336
H	–0.6786846	–9.5956737	–2.1800299
H	1.0601960	–9.5833569	–0.3932962
C	–1.1210848	0.3106558	–0.7802442
C	–1.8985667	1.6713801	1.5484937
C	–2.3669131	0.0487528	–0.1870113
C	–0.2720697	1.2671205	–0.1997615
C	–0.6579900	1.9386151	0.9614773
C	–2.7528496	0.7272419	0.9700924
H	–3.0312931	–0.6812310	–0.6518462
H	0.6956733	1.4565683	–0.6659839
H	0.0134448	2.6716080	1.4111891
H	–3.7270243	0.5239848	1.4173533
H	–2.2011210	2.2000950	2.4535632
C	–0.5287114	2.1150145	–7.4995414
C	–0.9495669	4.4950653	–8.9301060
C	0.3583093	3.1953250	–7.3594641
C	–1.6322532	2.2438765	–8.3587153
C	–1.8418096	3.4271751	–9.0684184
C	0.1505180	4.3752750	–8.0754480
H	1.2169598	3.0811577	–6.6966892
H	–2.3286217	1.4095079	–8.4542937
H	–2.7079050	3.5192477	–9.7254249
H	0.8520368	5.2038506	–7.9678420
H	–1.1133043	5.4194449	–9.4857603
C	2.2213120	–0.4294414	–5.5903802
O	2.4448244	0.7023022	–5.9853718
O	2.8677158	–1.5231180	–6.0644003
C	2.0273943	–1.0670895	–3.2516768
O	2.1294473	–0.3072224	–2.3037728
O	2.6527535	–2.2697370	–3.3098317
C	3.8054097	–1.2542440	–7.1258672
H	3.2739098	–0.8554464	–8.0019600
H	4.2621289	–2.2218184	–7.3583856
H	4.5678430	–0.5294673	–6.8089225
C	3.3991504	–2.6154652	–2.1262604
H	4.1674516	–1.8615601	–1.9055461
H	3.8583641	–3.5843922	–2.3481404
H	2.7193803	–2.6955316	–1.2654265

[Co(TPP)] *cis-Mono*-Bridged *Mono*-Enolate Carbene (*c*-I$^{B–E}$):

107 atoms

C	2.0820328	4.4424009	–5.0509454
C	1.6047661	4.2563554	–6.3486135
C	1.1651568	2.9436244	–6.4872789
C	1.9838175	3.2373745	–4.3553611
N	1.3995462	2.2332802	–5.2201680
C	2.3762918	3.0080482	–3.0164771
C	1.7421537	2.0912945	–2.1674944
N	0.5737030	1.4082977	–2.4706833
C	0.0877078	0.9020516	–1.2821531
C	2.0573306	1.8919514	–0.7638468
C	1.0271601	1.1923441	–0.2141917
C	–1.1527632	0.2698047	–1.1310926
C	–2.0130185	–0.0437865	–2.2086668
N	–1.7445895	0.2235740	–3.5295617
C	–3.5059277	–1.2420635	–3.4024933
C	–3.1588098	–0.9136850	–2.1204921
C	–1.8550780	–0.1127880	–6.6899889
N	–1.2850970	1.1507787	–6.5767079
C	–0.3524145	1.3269644	–7.6012324
C	–0.4824186	0.2020154	–8.4813311
C	–1.3832554	–0.6704326	–7.9268272
C	0.6243297	2.3375256	–7.6484368
C	–2.5811110	–0.7957034	–5.6992213
C	–2.5978619	–0.5614471	–4.2966511
H	2.4340348	5.3701459	–4.6118788
H	1.5060994	5.0067999	–7.1268218
H	2.9449595	2.2668882	–0.2658703
H	0.9012155	0.9016630	0.8234820
H	–4.3174483	–1.8865720	–3.7224445
H	–3.6019619	–1.2713752	–1.1974005
H	0.1429151	0.0512748	–9.3545102
H	–1.6371279	–1.6666778	–8.2722008
Co	–0.3526630	1.3558760	–4.1534939
C	3.4296908	3.9137293	–2.4955067
C	5.4498622	5.6453391	–1.5759890
C	4.6366048	4.0500033	–3.2095123
C	3.2432413	4.6797426	–1.3297434
C	4.2458282	5.5362325	–0.8736068
C	5.6380271	4.9036209	–2.7463824
H	4.7711408	3.4806597	–4.1314720
H	2.2942201	4.6149101	–0.7962844
H	4.0814824	6.1299282	0.0269178
H	6.5718068	4.9896106	–3.3040437
H	6.2339201	6.3139352	–1.2175677
C	1.1287602	2.7785928	–8.9556625
C	2.0967794	3.6031785	–11.4634807
C	0.2560595	2.9040413	–10.0559336
C	2.4965123	3.0804637	–9.1309947
C	2.9703649	3.4886898	–10.3762937
C	0.7385209	3.3107850	–11.2981652
H	–0.8071428	2.7105125	–9.9101908
H	3.1785675	2.9683844	–8.2852364
H	4.0315528	3.7082957	–10.5028918
H	0.0502728	3.4160357	–12.1380869
H	2.4725614	3.9229058	–12.4365686
C	–3.3739536	–1.9466356	–6.2050195
C	–4.8541862	–4.1025704	–7.2328894
C	–4.3357428	–1.7373230	–7.2085116
C	–3.1598449	–3.2511841	–5.7275106
C	–3.8929601	–4.3215513	–6.2407117
C	–5.0745539	–2.8082615	–7.7134456
H	–4.5039077	–0.7204913	–7.5653592
H	–2.4027056	–3.4152004	–4.9597113
H	–3.7090805	–5.3311706	–5.8704302
H	–5.8276946	–2.6311690	–8.4826068
H	–5.4287632	–4.9398714	–7.6315194
C	–1.5781079	–0.1537878	0.2315114
C	–2.4063766	–0.9544198	2.7998722
C	–0.8693727	–1.1394772	0.9374115
C	–2.7117780	0.4199978	0.8299005
C	–3.1222712	0.0239613	2.1040882
C	–1.2791858	–1.5353590	2.2120446
H	0.0028034	–1.6001114	0.4712625
H	–3.2663761	1.1852440	0.2848397
H	–4.0015960	0.4844092	2.5570355
H	–0.7200298	–2.3060078	2.7447580
H	–2.7268305	–1.2643456	3.7953748
C	2.2698878	1.0393303	–5.4245113
C	3.6203553	1.3012256	–5.8511177
O	4.0783791	2.4204315	–6.1192145
O	4.4109879	0.1826703	–5.9171733
C	1.6219480	–0.2057137	–5.3312257
O	2.2761308	–1.3186987	–5.7377790
O	0.4354766	–0.3364696	–4.9061966
C	5.7516704	0.4298181	–6.3691656
H	5.7570806	0.8799737	–7.3724406
H	6.2338877	–0.5538663	–6.3895369
H	6.2852850	1.1031565	–5.6826218
C	1.5075140	–2.5349253	–5.6547379
H	0.6014115	–2.4688707	–6.2746714
H	1.2128727	–2.7486744	–4.6178645
H	2.1758402	–3.3162243	–6.0322671
C	–1.6208494	2.0754395	–5.5291164
C	–1.4394248	3.5567043	–5.8787193
O	–1.6901488	4.0756574	–6.9481006
O	–1.0970193	4.2387347	–4.7594526
C	–3.1316692	2.0587343	–5.2161228
O	–4.0098037	1.6773993	–5.9635562
O	–3.3647717	2.6094737	–4.0021266
C	–1.1191676	5.6761788	–4.8868479
H	–0.4521079	5.9997547	–5.6961859
H	–0.7705172	6.0576431	–3.9223702
H	–2.1400830	6.0220277	–5.1004207
C	–4.7534707	2.6255913	–3.6056982
H	–4.7713334	3.1366843	–2.6381461
H	–5.1226745	1.5955881	–3.5063759
H	–5.3654800	3.1611513	–4.3438699

[Co(TPP)] *trans-Mono*-Bridged *Mono*-Enolate Carbene (*t*-I$^{B–E}$):

107 atoms

C	1.6234920	4.3127543	–4.9584871
C	1.1465652	4.0503966	–6.2327657
C	1.0674449	2.6586024	–6.3931376
C	1.8387013	3.0876252	–4.3085100
N	1.4994189	2.0147242	–5.1905072
C	2.2087501	2.8885000	–2.9673216
C	1.6143516	1.8892167	–2.1789572
N	0.4528613	1.2022501	–2.5241059
C	–0.0488799	0.6823850	–1.3494054
C	1.9148341	1.6548148	–0.7850258
C	0.8825898	0.9307049	–0.2680835
C	–1.3193050	0.1008860	–1.1676148
C	–2.2688273	–0.1458979	–2.1653609
N	–2.2270872	0.2888896	–3.5221411
C	–3.6566357	–1.5012011	–3.3449116
C	–3.2400954	–1.1826840	–2.0761603
C	–1.8122244	–0.4875228	–6.4866778
N	–0.8187505	0.4068083	–6.1470913
C	–0.2260714	0.8020543	–7.3431930
C	–0.7781005	0.0318935	–8.4316858
C	–1.7645083	–0.7520677	–7.9093751
C	0.5601403	1.9559013	–7.4972057
C	–2.8219575	–0.9761108	–5.6307538
C	–2.9717614	–0.6669787	–4.2748548
H	1.7321038	5.2809406	–4.4807686
H	0.7891679	4.7655394	–6.9657513
H	2.7976480	2.0188854	–0.2705307
H	0.7398626	0.6201891	0.7610738
H	–4.2726593	–2.3452641	–3.6347330
H	–3.4617894	–1.7205066	–1.1608479
H	–0.4575747	0.1002229	–9.4656811
H	–2.4307343	–1.4206064	–8.4433748
Co	–0.1946743	0.8434516	–4.3362454
C	3.1120170	3.9059417	–2.3909305
C	4.8504245	5.8892648	–1.4067199
C	4.2518761	4.2916214	–3.1266045
C	2.8469796	4.5508612	–1.1673514
C	3.7099532	5.5318349	–0.6801755

C	5.1143039	5.2695537	–2.6320825
H	4.4461278	3.8112872	–4.0882563
H	1.9419913	4.2962375	–0.6154428
H	3.4844741	6.0299122	0.2640057
H	5.9978919	5.5492067	–3.2075382
H	5.5248305	6.6562458	–1.0231801
C	0.7623186	2.5855932	–8.8177158
C	1.2217230	3.8436343	–11.2914975
C	–0.2905200	2.7722067	–9.7335552
C	2.0456656	3.0657691	–9.1505566
C	2.2706595	3.6821761	–10.3811984
C	–0.0608125	3.3941955	–10.9599309
H	–1.2966714	2.4562212	–9.4577808
H	2.8577462	2.9438477	–8.4302977
H	3.2711938	4.0384623	–10.6304913
H	–0.8890061	3.5438324	–11.6541799
H	1.3992482	4.3292941	–12.2521733
C	–3.8155592	–1.9325849	–6.1916277
C	–5.7255731	–3.7180369	–7.2317030
C	–5.1830776	–1.6113187	–6.1702539
C	–3.4204567	–3.1678210	–6.7310449
C	–4.3682333	–4.0526816	–7.2478369
C	–6.1305573	–2.4952423	–6.6887195
H	–5.4904855	–0.6589582	–5.7361626
H	–2.3618272	–3.4307378	–6.7321027
H	–4.0462774	–5.0113785	–7.6570130
H	–7.1881074	–2.2278687	–6.6703478
H	–6.4652613	–4.4101990	–7.6360664
C	–1.7042601	–0.3379026	0.2031832
C	–2.4932798	–1.1353802	2.7774276
C	–1.0242291	–1.3709705	0.8667335
C	–2.7887105	0.2875247	0.8394585
C	–3.1772840	–0.1079151	2.1207746
C	–1.4171897	–1.7671932	2.1466614
H	–0.1910875	–1.8661368	0.3657050
H	–3.3066082	1.0919435	0.3152526
H	–4.0157353	0.3904601	2.6095798
H	–0.8859933	–2.5762400	2.6502079
H	–2.7990615	–1.4451797	3.7777257
C	2.5419391	0.9781103	–5.3584380
C	3.7784035	1.4590450	–5.9210306
O	3.9862911	2.6384757	–6.2377359
O	4.7422043	0.4993215	–6.0924435
C	2.2067970	–0.3252186	–4.9478030
O	3.1359297	–1.2997586	–5.0773393
O	1.0769637	–0.6408351	–4.4579441
C	5.9708279	0.9884325	–6.6540341
H	5.8073941	1.4243703	–7.6503046
H	6.6239755	0.1113911	–6.7237168
H	6.4259654	1.7547265	–6.0099009
C	2.7241282	–2.6071298	–4.6376262
H	1.8565884	–2.9631508	–5.2109584
H	2.4655088	–2.6030310	–3.5693903
H	3.5917939	–3.2507316	–4.8183615
C	–1.8827543	1.6725878	–3.9363736
C	–2.5556845	2.2920181	–5.1417563
O	–2.0989251	3.2435716	–5.7456509
O	–3.7426305	1.7099841	–5.4640292
C	–1.9120687	2.6875596	–2.8070667
O	–2.6028320	2.6228047	–1.8049292
O	–1.0639333	3.7038606	–3.0703924
C	–4.2826333	2.1280258	–6.7380128
H	–5.2056297	1.5536925	–6.8674469
H	–3.5686645	1.8882237	–7.5388157
H	–4.4868588	3.2063810	–6.7413300
C	–0.9594761	4.6968732	–2.0317989
H	–0.1902830	5.3940056	–2.3789681
H	–0.6528599	4.2230470	–1.0886346
H	–1.9173319	5.2131687	–1.8807534

[Co(TPP)] *cis*-*Bis*-Enolate Adduct (*c*-I^{E-E}):

107 atoms

C	3.1529156	2.5877667	–5.6610051
C	2.6257153	2.4136998	–6.9457556
C	1.2354090	2.4813933	–6.8775750
C	2.0993612	2.7620899	–4.7718658
N	0.8397086	2.6678993	–5.5131706
C	2.0974432	3.0510313	–3.3888643
C	1.1098607	2.4613157	–2.5867963
N	0.6587534	1.1036417	–2.8483286
C	–0.2792745	0.8220643	–1.8103187
C	0.4286628	2.9531504	–1.4634734
C	–0.4162228	1.9568270	–0.9931470
C	–1.0045811	–0.3845368	–1.7325994
C	–1.4373633	–1.0789526	–2.8780277
N	–1.4413895	–0.5603538	–4.1639969
C	–2.6266739	–2.5264532	–4.1492562
C	–2.1421303	–2.3393765	–2.8847318
C	–2.2098426	–0.0133431	–7.0235876
N	–1.1790407	0.8169843	–6.6820383
C	–0.8687026	1.5731868	–7.7944848
C	–1.8550319	1.3109733	–8.8278684
C	–2.6773340	0.3311877	–8.3575461
C	0.3159946	2.3073302	–7.9477681
C	–2.6732975	–1.0928704	–6.2469518
C	–2.2258223	–1.3771887	–4.9338767
H	4.1954323	2.5379423	–5.3632287
H	3.1771846	2.2056764	–7.8574728
H	0.5163248	3.9727728	–1.1023842
H	–1.1293882	2.0305296	–0.1778846
H	–3.2159354	–3.3586251	–4.5196213
H	–2.2312484	–3.0037059	–2.0315613
H	–1.9096157	1.8255716	–9.7814124
H	–3.5226728	–0.1268752	–8.8605103
Co	–0.3798590	0.9105270	–4.8663894
C	3.0975055	3.9457937	–2.8092078
C	5.0218931	5.6583062	–1.6860122
C	3.5659155	3.7316945	–1.4935324
C	3.6123907	5.0296434	–3.5542780
C	4.5668533	5.8741577	–2.9921302
C	4.5177708	4.5856744	–0.9413142
H	3.2002068	2.8664633	–0.9367389
H	3.2228633	5.2146696	–4.5572431
H	4.9492403	6.7163147	–3.5710434
H	4.8821219	4.4047221	0.0711211
H	5.7691277	6.3233322	–1.2502495
C	0.7626184	2.7954508	–9.2671090
C	1.6647572	3.7862341	–11.7458387
C	1.3272276	4.0852387	–9.3648513
C	0.6883269	2.0029541	–10.4301377
C	1.1317543	2.4964805	–11.6567186
C	1.7655408	4.5741194	–10.5945722
H	1.4069673	4.6957016	–8.4629841
H	0.3101084	0.9830554	–10.3564482
H	1.0763678	1.8650349	–12.5447839
H	2.1868072	5.5787684	–10.6547212
H	2.0114302	4.1702341	–12.7063188
C	–3.6878447	–2.0012751	–6.8464727
C	–5.6138542	–3.7160398	–7.9847650
C	–4.9532941	–2.1565357	–6.2538465
C	–3.4053395	–2.7234290	–8.0190518
C	–4.3589723	–3.5725462	–8.5831778
C	–5.9074613	–3.0047974	–6.8175931
H	–5.1839372	–1.5947387	–5.3476121
H	–2.4220816	–2.6179749	–8.4796388
H	–4.1181366	–4.1297994	–9.4897513
H	–6.8868457	–3.1054474	–6.3473955
H	–6.3593555	–4.3793124	–8.4253636
C	–1.4107092	–0.8106460	–0.3785319
C	–2.1141239	–1.5708371	2.2390683
C	–0.4569969	–0.7765125	0.6606080
C	–2.7272912	–1.2100874	–0.0757036
C	–3.0732044	–1.5880827	1.2210779
C	–0.8081178	–1.1598388	1.9544717
H	0.5612597	–0.4552040	0.4308499
H	–3.4831316	–1.1918264	–0.8612114
H	–4.0998922	–1.8836653	1.4422323
H	–0.0562074	–1.1405842	2.7447322
H	–2.3872379	–1.8677675	3.2527092
C	1.7262749	0.1010057	–3.0367955
C	2.5664808	–0.0934052	–1.8771911
O	2.4270342	0.5253115	–0.8151879
O	3.5472197	–1.0333780	–2.0316420
C	1.8451603	–0.4842726	–4.3068781
O	2.8723936	–1.3204361	–4.5483994
O	1.0388446	–0.2653353	–5.2843672
C	4.3848681	–1.2118227	–0.8760230
H	4.8983316	–0.2763945	–0.6117812
H	5.1112218	–1.9797224	–1.1639490
H	3.7970259	–1.5452684	–0.0088636
C	2.9335331	–1.8715191	–5.8802815
H	3.8204148	–2.5136565	–5.8749625
H	3.0382296	–1.0743703	–6.6294326
H	2.0333130	–2.4589473	–6.1064099
C	–0.1259340	3.7586783	–5.2687519
C	–1.3255058	3.4127841	–4.6265350
O	–1.6573328	2.2092469	–4.3243232
O	–2.1890355	4.3865585	–4.2814435
C	0.3374843	5.0674720	–5.6620635
O	1.4499838	5.2826556	–6.1596274
O	–0.5562856	6.0796445	–5.4495824
C	–3.3873514	3.9501567	–3.6069621
H	–3.1422798	3.4409388	–2.6644540
H	–3.9712753	3.2686241	–4.2403177
H	–3.9482252	4.8703042	–3.4128960
C	–0.0805499	7.3816360	–5.8336977
H	0.8259887	7.6521911	–5.2737553
H	–0.8991435	8.0686838	–5.5929320
H	0.1477575	7.4182609	–6.9085165

[Co(TPP)] *trans*-*Bis*-Enolate Adduct (*t*-I^{E-E}):

107 atoms

C	3.2343855	3.5879818	–5.4534913
C	2.7846139	3.3698785	–6.7405206
C	1.4041675	3.1047530	–6.6846527
C	2.1393456	3.4725416	–4.5770003
N	0.9494413	3.1875601	–5.3278171
C	2.2261298	3.4732633	–3.1814153
C	1.4371664	2.6507154	–2.3575170
N	0.5788502	1.6441393	–2.7728407
C	0.1934229	0.9794297	–1.6211761
C	1.5603907	2.6326418	–0.9178922
C	0.8249012	1.5804764	–0.4677847
C	–0.7682389	–0.0424462	–1.5152936
C	–1.4367406	–0.5985886	–2.6083267
N	–0.9143406	–0.6912741	–3.9450630
C	–3.1588708	–1.3029841	–3.8919846
C	–2.7887245	–0.9945248	–2.5999090
C	–1.4407880	–0.1370175	–6.9363122
N	–0.6194803	0.8943316	–6.5131763
C	–0.3339981	1.6408759	–7.6475880
C	–1.0290494	1.0878811	–8.7884246
C	–1.6663018	–0.0350674	–8.3618886
C	0.6357051	2.6520686	–7.7649767
C	–2.1210896	–1.0672772	–6.1293754
C	–2.0478211	–1.0917471	–4.7324895
H	4.2594336	3.7273134	–5.1264151
H	3.3781605	3.3009218	–7.6461884
H	2.1383119	3.3392948	–0.3329328
H	0.7173753	1.2334022	0.5536173
H	–4.1512461	–1.5533138	–4.2521536
H	–3.4267549	–0.9519514	–1.7234664
H	–1.0195798	1.5067094	–9.7882777
H	–2.2449521	–0.7345774	–8.9542324
Co	–0.0110185	1.2647109	–4.6482364
C	3.3321541	4.2848685	–2.6198011
C	5.4411839	5.8815321	–1.6606264
C	4.2925540	3.7512950	–1.7403436
C	3.4623647	5.6255108	–3.0335695
C	4.5048939	6.4165480	–2.5506291
C	5.3360582	4.5446397	–1.2636412
H	4.2284202	2.7008606	–1.4546803
H	2.7376195	6.0303391	–3.7433194
H	4.5874572	7.4555370	–2.8727197
H	6.0783565	4.1138007	–0.5900364
H	6.2577776	6.5003602	–1.2859175
C	1.0531213	3.1820747	–9.0854977
C	1.9077328	4.2976989	–11.5245226
C	1.1857750	4.5778071	–9.2302509
C	1.3897431	2.3552721	–10.1734761
C	1.8095772	2.9098214	–11.3826771
C	1.6016134	5.1282580	–10.4423848
H	0.9681451	5.2197590	–8.3740899
H	1.3484971	1.2722960	–10.0539491
H	2.0756938	2.2549403	–12.2137364
H	1.6905566	6.2111164	–10.5404583
H	2.2357561	4.7288248	–12.4714406
C	–3.1381698	–1.9837012	–6.7061229
C	–5.0573450	–3.7969709	–7.6787188
C	–4.2116811	–1.5346603	–7.4962266
C	–3.0611439	–3.3518995	–6.3829708
C	–4.0075211	–4.2510810	–6.8748722
C	–5.1619558	–2.4350925	–7.9790245
H	–4.3102967	–0.4690031	–7.7058225
H	–2.2546964	–3.6945019	–5.7319023
H	–3.9273654	–5.3098504	–6.6245932
H	–5.9953776	–2.0701933	–8.5812752
H	–5.8001855	–4.4995052	–8.0591371
C	–1.2506127	–0.5003891	–0.1881878
C	–2.2031187	–1.4720409	2.2740564
C	–1.2929997	–1.8846114	0.0682033
C	–1.7207908	0.3860473	0.7974414
C	–2.1919878	–0.0970688	2.0185725
C	–1.7573546	–2.3632913	1.2934870
H	–0.9657780	–2.5749073	–0.7121111
H	–1.7362741	1.4562481	0.5881103
H	–2.5637140	0.6017486	2.7694401
H	–1.7738553	–3.4377362	1.4816295
H	–2.5695727	–1.8474900	3.2305548
C	0.2848430	–1.5547463	–4.0917678
C	0.0969366	–2.9275610	–3.6737333
O	–0.9642589	–3.3826929	–3.2345567
O	1.2113920	–3.7177202	–3.7942620
C	1.4531578	–0.9678515	–4.6101084
O	2.5534277	–1.7325066	–4.7737031
O	1.5548514	0.2609675	–4.9480312
C	1.0233247	–5.0762006	–3.3650008
H	0.7411862	–5.1221400	–2.3031051
H	1.9915163	–5.5641990	–3.5241532
H	0.2405483	–5.5756481	–3.9541062
C	3.7101841	–1.0504039	–5.2978392
H	4.0206440	–0.2304077	–4.6353478
H	3.5093582	–0.6406321	–6.2975302
H	4.4885538	–1.8191135	–5.3477730
C	–0.1924250	4.1033331	–5.1010293
C	–1.3906814	3.5479757	–4.6156290
O	–1.5610566	2.3073519	–4.3540684
O	–2.4435703	4.3653612	–4.4041642
C	0.0764665	5.4834362	–5.4399923
O	1.1651586	5.8932880	–5.8592954
O	–0.9834995	6.3346903	–5.2696695
C	–3.6334471	3.7312236	–3.8956543

H	–4.0095284	2.9738843	–4.5974149
H	–4.3580552	4.5449940	–3.7857773
H	–3.4427049	3.2523079	–2.9251741
C	–0.7077656	7.6998499	–5.6256103
H	0.1074840	8.1138134	–5.0150413
H	–1.6414128	8.2405880	–5.4349042
H	–0.4256883	7.7844276	–6.6851186

[Co(TPP)] Terminal Carbene Toluene Adduct ($I^{T–Tol}$):

107 atoms

C	3.3266459	3.8698131	–4.0924411
C	3.2108128	3.4026384	–5.3660640
C	2.0312212	2.5791136	–5.4080813
C	2.2589868	3.2805384	–3.3279834
N	1.4676305	2.4865870	–4.1392047
C	2.1043503	3.4370734	–1.9494150
C	1.2175653	2.6556343	–1.2109579
N	0.4171076	1.6441669	–1.7218788
C	–0.0358042	0.9459674	–0.6179371
C	1.1317579	2.6733427	0.2270411
C	0.3907606	1.5908193	0.5938307
C	–0.8115190	–0.2134319	–0.6476785
C	–1.4873701	–0.6032659	–1.8029402
N	–1.3899617	0.0519954	–3.0225502
C	–3.1090646	–1.4962185	–3.0830641
C	–2.5168493	–1.6050700	–1.8583819
C	–1.7156743	0.5862899	–5.9009012
N	–0.5133748	1.1056613	–5.4319250
C	0.1836784	1.4943722	–6.5615958
C	–0.6066998	1.2694812	–7.7413013
C	–1.7941938	0.7359755	–7.3304874
C	1.4572745	2.0714503	–6.5715681
C	–2.6192500	–0.1657755	–5.1527679
C	–2.3806841	–0.4958799	–3.8177619
H	4.1055585	4.5020729	–3.6832319
H	3.8694819	3.5908893	–6.2051462
H	1.5955054	3.4171704	0.8654928
H	0.1203157	1.2647027	1.5926099
H	–3.9591579	–2.0504534	–3.4657963
H	–2.7787414	–2.2736451	–1.0456630
H	–0.2905388	1.5132170	–8.7500709
H	–2.6413553	0.4333071	–7.9368528
Co	0.1185448	1.1820059	–3.5733735
C	3.0118005	4.3798904	–1.2414662
C	4.7716074	6.1507418	0.0550368
C	3.9479247	3.9032413	–0.3089311
C	2.9729119	5.7558682	–1.5172959
C	3.8448896	6.6351644	–0.8723753
C	4.8205972	4.7819440	0.3344001
H	3.9922516	2.8323446	–0.1072122
H	2.2500316	6.1304047	–2.2435635
H	3.7984298	7.7025446	–1.0935242
H	5.5471325	4.3945547	1.0503469
H	5.4543239	6.8375526	0.5573570
C	2.1662758	2.1737284	–7.8736111
C	3.5234896	2.2781342	–10.3342615
C	2.5141800	3.4082946	–8.4445824
C	2.4917697	0.9915619	–8.5609715
C	3.1679874	1.0449815	–9.7799056
C	3.1905972	3.4595059	–9.6653038
H	2.2396113	4.3301733	–7.9300770
H	2.2356394	0.0358004	–8.1026567
H	3.4293447	0.1182088	–10.2929476
H	3.4522117	4.4262013	–10.0984158
H	4.0553944	2.3191787	–11.2859626
C	–3.8222167	–0.7142138	–5.8416537
C	–6.0851638	–1.7176996	–7.1795850
C	–4.8639731	0.1440350	–6.2266022
C	–3.9291844	–2.0816026	–6.1393121
C	–5.0525985	–2.5805473	–6.8015932
C	–5.9872470	–0.3539112	–6.8905733
H	–4.7840338	1.2083941	–6.0004631
H	–3.1200382	–2.7515605	–5.8463658
H	–5.1184480	–3.6457358	–7.0285641
H	–6.7898762	0.3260635	–7.1799843
H	–6.9623356	–2.1067402	–7.6983769
C	–0.8995580	–1.0185062	0.5982215
C	–0.9461851	–2.5546937	2.9511054
C	0.2851849	–1.5798617	1.1076437
C	–2.1033604	–1.2239563	1.2899717
C	–2.1255310	–1.9879751	2.4590906
C	0.2591671	–2.3460079	2.2737780
H	1.2196071	–1.4021269	0.5707201
H	–3.0194153	–0.7643048	0.9160276
H	–3.0662395	–2.1338229	2.9923945
H	1.1839753	–2.7817607	2.6552270
H	–0.9656823	–3.1518674	3.8640030
C	1.2683094	–0.2852991	–3.6326527
C	1.2550814	–1.0092648	–4.9241921
O	2.1033959	–0.8504545	–5.7927325
O	0.1869130	–1.8300208	–5.0678855
C	2.1849068	–0.7431446	–2.6045192
O	2.4594717	–0.2379089	–1.5185094
O	2.7815235	–1.9265378	–3.0147975
C	0.0492132	–2.4218316	–6.3794474
H	0.9530377	–2.9826669	–6.6518313
H	–0.8144217	–3.0902228	–6.3082597
H	–0.1368779	–1.6368513	–7.1261974
C	3.8012924	–2.4203304	–2.1300391
H	4.1757588	–3.3363731	–2.5995306
H	3.3865740	–2.6372172	–1.1350731
H	4.6113524	–1.6839092	–2.0249977
H	4.3715303	–0.0294371	–6.5628300
C	5.2834514	0.5798818	–6.5784620
H	6.1223139	–0.0610098	–6.8941849
H	5.1584775	1.3542486	–7.3502326
C	5.5457111	1.1903210	–5.2262502
C	5.9970849	2.3602420	–2.7011188
C	6.4981104	2.2090433	–5.0654169
C	4.8288539	0.7664067	–4.0985047
C	5.0461172	1.3467852	–2.8462961
C	6.7241251	2.7895993	–3.8160211
H	7.0597475	2.5580303	–5.9358277
H	4.0660270	–0.0025020	–4.2269547
H	4.4438529	1.0232975	–1.9961064
H	7.4633683	3.5862998	–3.7121690
H	6.1554899	2.8306626	–1.7300985

[Co(TPP)] Alkyl (I^{A}):

93 atoms

C	2.8600271	4.0050374	–4.9476968
C	2.3225923	3.8258401	–6.1860910
C	1.2097237	2.9259042	–6.0325846
C	2.0622739	3.2349864	–4.0317187
N	1.0425013	2.5749651	–4.6999188
C	2.2552672	3.2510121	–2.6551724
C	1.3677925	2.6424933	–1.7743517
N	0.3393084	1.7846882	–2.1415874
C	–0.1801928	1.3284992	–0.9363887
C	1.4464189	2.7655111	–0.3437391
C	0.4719099	1.9674524	0.1756111
C	–1.0825213	0.2821589	–0.7859911
C	–1.6368326	–0.3928734	–1.8659125
N	–1.4456108	–0.0821201	–3.2025405
C	–2.8147005	–1.9522917	–2.9782202
C	–2.4943691	–1.5391522	–1.7222240
C	–1.7630012	–0.1469567	–6.1236205
N	–0.8697585	0.8472490	–5.7513884
C	–0.5283110	1.4739057	–6.9406214
C	–1.2834802	0.9307335	–8.0386142
C	–2.0403387	–0.0809233	–7.5347305
C	0.4651266	2.4336483	–7.1000269
C	–2.3375099	–1.0897233	–5.2743901
C	–2.1800225	–1.0379695	–3.8922268
H	3.7039107	4.6232381	–4.6603732
H	2.6448011	4.2525352	–7.1298448
H	2.1671205	3.3794200	0.1855066
H	0.2259017	1.7896832	1.2172139
H	–3.4324431	–2.7930385	–3.2741588
H	–2.7948557	–1.9669586	–0.7718122
H	–1.2278666	1.2881196	–9.0611247
H	–2.7411599	–0.7242979	–8.0555300
Co	–0.1221769	1.1717736	–3.9658951
C	3.4823365	3.9038860	–2.1213856
C	5.8498412	5.0537513	–1.1418005
C	4.7175160	3.2644869	–2.3163158
C	3.4464001	5.1270043	–1.4377015
C	4.6246267	5.6983075	–0.9501516
C	5.8937668	3.8358847	–1.8273395
H	4.7332583	2.3150935	–2.8548865
H	2.4888113	5.6304100	–1.2967640
H	4.5855184	6.6529896	–0.4235178
H	6.8473834	3.3283293	–1.9806446
H	6.7687140	5.5011247	–0.7604882
C	0.8382766	2.8525723	–8.4802318
C	1.6025981	3.5987965	–11.0760571
C	0.5615799	4.1412136	–8.9576112
C	1.5028050	1.9390966	–9.3147527
C	1.8835786	2.3126380	–10.6049859
C	0.9401640	4.5114596	–10.2504404
H	0.0454040	4.8499382	–8.3083862
H	1.7160430	0.9397117	–8.9304660
H	2.4030353	1.5971300	–11.2441079
H	0.7144280	5.5148224	–10.6143674
H	1.8987365	3.8892558	–12.0849465
C	–3.1631587	–2.1746385	–5.8758119
C	–4.6998223	–4.2239922	–7.0336883
C	–4.5508347	–2.2266738	–5.6728341
C	–2.5554024	–3.1597390	–6.6700389
C	–3.3186349	–4.1788597	–7.2428237
C	–5.3141675	–3.2442181	–6.2487498
H	–5.0272942	–1.4572685	–5.0636039
H	–1.4774777	–3.1171754	–6.8324094
H	–2.8318454	–4.9413695	–7.8524752
H	–6.3928546	–3.2687300	–6.0875457
H	–5.2962019	–5.0194689	–7.4825187
C	–1.3645032	–0.2186849	0.5906535
C	–1.8365237	–1.1943850	3.1772036
C	–0.6377137	–1.3169486	1.0755560
C	–2.3268420	0.3863383	1.4089106
C	–2.5614964	–0.1000147	2.6981172
C	–0.8750544	–1.8017063	2.3633720
H	0.1084072	–1.7773676	0.4251507
H	–2.8899960	1.2399716	1.0286611
H	–3.3144539	0.3759944	3.3280137
H	–0.3061408	–2.6560988	2.7332157
H	–2.0210248	–1.5740402	4.1831273
C	1.2018401	–0.3467051	–4.1817540
C	2.0957374	–0.0939355	–5.3619528
O	1.8138142	–0.4746731	–6.4896030
O	3.2396985	0.5809456	–5.0852302
C	1.7485667	–0.6478091	–2.8192007
O	1.2402169	–1.4751091	–2.0749279
O	2.8376622	0.0836438	–2.4707270
C	4.0784708	0.8374621	–6.2306629
H	3.5232805	1.3911065	–6.9992873
H	4.4474241	–0.1046573	–6.6593618
H	4.9058781	1.4451167	–5.8505829
C	3.2963272	–0.1267453	–1.1188115
H	3.6885075	–1.1458986	–0.9969113
H	2.4770067	0.0340555	–0.4060854
H	4.0850827	0.6169311	–0.9633610
H	0.5251767	–1.1601046	–4.4585099

[Co(TPP)] Alkyl Tolyl Radical Adduct ($I^{A–Tol•}$):

107 atoms

C	3.1774187	3.5727270	–4.9919605
C	2.7465968	3.2666847	–6.2467349
C	1.5724446	2.4490581	–6.0968049
C	2.2782847	2.9287910	–4.0709321
N	1.2966019	2.2275125	–4.7540453
C	2.3476804	3.0874463	–2.6895037
C	1.4492044	2.4738758	–1.8214329
N	0.5020822	1.5238159	–2.1878330
C	0.0206388	1.0271930	–0.9838699
C	1.4866372	2.6274453	–0.3906923
C	0.5977481	1.7339298	0.1274497
C	–0.8145976	–0.0752530	–0.8361942
C	–1.4175167	–0.7058038	–1.9169242
N	–1.3281392	–0.2960515	–3.2384451
C	–2.7491763	–2.1264747	–3.0394196
C	–2.2789960	–1.8503124	–1.7920682
C	–1.8302653	–0.1558035	–6.1290259
N	–0.7523283	0.6490768	–5.7817162
C	–0.3341554	1.2093672	–6.9780728
C	–1.2179643	0.8419355	–8.0511993
C	–2.1544357	0.0083463	–7.5227731
C	0.8075480	1.9843140	–7.1616317
C	–2.4744548	–1.0621214	–5.2886467
C	–2.1743527	–1.1516873	–3.9302577
H	4.0144368	4.1991530	–4.7035230
H	3.1683117	3.5755991	–7.1969588
H	2.1336304	3.3167340	0.1407416
H	0.3568123	1.5447054	1.1682157
H	–3.4182522	–2.9228207	–3.3451887
H	–2.4873311	–2.3654706	–0.8604967
H	–1.1292582	1.1979946	–9.0719320
H	–2.9969371	–0.4578703	–8.0211010
Co	0.0395405	0.9104541	–4.0077695
C	3.4544389	3.9072735	–2.1214192
C	5.5703560	5.4157873	–1.0470540
C	4.7744357	3.4332010	–2.1861807
C	3.2092213	5.1497865	–1.5183763
C	4.2602653	5.8982754	–0.9834653
C	5.8250295	4.1817597	–1.6524429
H	4.9633385	2.4728546	–2.6683548
H	2.1861961	5.5264185	–1.4754003
H	4.0551653	6.8646686	–0.5206127
H	6.8452953	3.7990881	–1.7072085
H	6.3905212	6.0010261	–0.6292050
C	1.2526735	2.2647717	–8.5540452
C	2.1257321	2.7255249	–11.1833973
C	1.2406624	3.5611614	–9.0895443
C	1.7034669	1.1986998	–9.3508516
C	2.1401983	1.4305206	–10.6565022
C	1.6729492	3.7895222	–10.3979628
H	0.8833105	4.3877989	–8.4736709
H	1.7109541	0.1950046	–8.9217341
H	2.4943112	0.5965025	–11.2643440
H	1.6517398	4.8009386	–10.8064763
H	2.4643047	2.9053346	–12.2047303
C	–3.5060346	–1.9679392	–5.8623131
C	–5.4439812	–3.7037049	–6.9384272
C	–4.8287117	–1.9464242	–5.3896579
C	–3.1731211	–2.8661872	–6.8895092
C	–4.1322380	–3.7290409	–7.4208938
C	–5.7898993	–2.8066605	–5.9237781
H	–5.0984113	–1.2427012	–4.6010253
H	–2.1465640	–2.8869342	–7.2533785
H	–3.8523436	–4.4275345	–8.2109359
H	–6.8139603	–2.7723498	–5.5492334

H	–6.1945064	–4.3777683	–7.3534725
C	–1.0137525	–0.6371265	0.5293927
C	–1.3338047	–1.7220455	3.0972264
C	0.0194222	–1.3843211	1.1162599
C	–2.2085315	–0.4431720	1.2360359
C	–2.3665592	–0.9811892	2.5159504
C	–0.1424271	–1.9245199	2.3935706
H	0.9336348	–1.5463168	0.5428610
H	–3.0112252	0.1350695	0.7759117
H	–3.2981219	–0.8198360	3.0604148
H	0.6630866	–2.5099730	2.8396691
H	–1.4582839	–2.1431569	4.0958873
C	1.3201299	–0.6570837	–4.1858922
C	2.1357110	–0.5575748	–5.4404046
O	1.7432411	–0.9787982	–6.5199867
O	3.3508392	0.0273951	–5.2871749
C	1.9622682	–0.8278724	–2.8456511
O	1.5189344	–1.5854991	–1.9901847
O	3.0595712	–0.0584537	–2.6322631
C	4.1366288	0.1082938	–6.4918223
H	3.6089553	0.6858279	–7.2623730
H	4.3519048	–0.8963253	–6.8831136
H	5.0598593	0.6188062	–6.2000411
C	3.6016418	–0.1510374	–1.2995305
H	3.9549081	–1.1706348	–1.0914673
H	2.8432341	0.1283918	–0.5560300
H	4.4330677	0.5605132	–1.2732400
H	0.6075170	–1.4726612	–4.3291540
C	2.9757915	–3.4405266	–4.4118042
H	3.3334755	–3.2926352	–3.3941694
H	3.6513825	–3.2048223	–5.2332163
C	1.6754021	–3.9117339	–4.6587799
C	–0.9753022	–4.7732715	–5.1586067
C	1.1929742	–4.0844493	–5.9914731
C	0.7710166	–4.1855283	–3.5869446
C	–0.5265274	–4.6009474	–3.8401245
C	–0.1031014	–4.5134931	–6.2278142
H	1.8542997	–3.8432296	–6.8241523
H	1.1038662	–4.0110804	–2.5644521
H	–1.2074849	–4.7767344	–3.0070599
H	–0.4510659	–4.6395365	–7.2544609
H	–2.0018269	–5.0838760	–5.3544426

[Co(TPP)] *Mono* Alkyl *Mono* Iodonium Ylide ($I^{A–IY}$):

120 atoms

C	3.1802392	4.7611260	–4.8907242
C	2.7217691	4.4113069	–6.1221763
C	1.7364019	3.3789563	–5.9227327
C	2.4686802	3.9530076	–3.9347711
N	1.5732595	3.1129042	–4.5721894
C	2.6432067	4.0674433	–2.5617721
C	1.9291274	3.3031829	–1.6480566
N	0.9892035	2.3343839	–1.9539280
C	0.6036828	1.8171244	–0.7296211
C	2.1189293	3.3985149	–0.2234369
C	1.3006699	2.4744014	0.3450699
C	–0.3208515	0.8023977	–0.5258278
C	–1.0063607	0.1916046	–1.5692266
N	–0.8859401	0.5021430	–2.9133314
C	–2.4906756	–1.1510416	–2.5978820
C	–2.0037319	–0.8267497	–1.3687468
C	–1.2918021	0.3410280	–5.8457799
N	–0.3441403	1.3116551	–5.5373782
C	0.0817104	1.7953722	–6.7721544
C	–0.6320749	1.1522437	–7.8389579
C	–1.4858835	0.2556178	–7.2644451
C	1.0485763	2.7755080	–6.9707806
C	–1.9875164	–0.4336027	–4.9262669
C	–1.7916000	–0.3313573	–3.5533880
H	3.9198621	5.5111602	–4.6324811
H	3.0088570	4.8111384	–7.0886561
H	2.7997109	4.0893392	0.2614572
H	1.1651978	2.2476419	1.3967735
H	–3.2512920	–1.8813027	–2.8524789
H	–2.2943932	–1.2223124	–0.4015203
H	–0.4811455	1.3594526	–8.8930089
H	–2.1815338	–0.4201227	–7.7503698
Co	0.4177252	1.7392416	–3.7400091
C	3.6162567	5.0689471	–2.0469921
C	5.4391056	6.9660012	–1.0824651
C	4.9954648	4.8356938	–2.1470104
C	3.1528438	6.2557717	–1.4589511
C	4.0642267	7.2002644	–0.9806099
C	5.9027057	5.7822424	–1.6647105
H	5.3393546	3.9055339	–2.6030832
H	2.0755932	6.4178880	–1.3863404
H	3.6989336	8.1231170	–0.5271845
H	6.9746378	5.5934186	–1.7412986
H	6.1489053	7.7044746	–0.7066522
C	1.3464360	3.2085813	–8.3666668
C	1.8965990	4.0385653	–10.9948674
C	0.4379163	4.0197199	–9.0630462
C	2.5344069	2.8185810	–9.0019479
C	2.8075404	3.2309949	–10.3081343
C	0.7104716	4.4325687	–10.3689469
H	–0.4832870	4.3276716	–8.5654768
H	3.2418515	2.1885849	–8.4610145
H	3.7339431	2.9176975	–10.7917129
H	–0.0025992	5.0672990	–10.8972820
H	2.1107401	4.3606068	–12.0148371
C	–2.9188511	–1.4773963	–5.4393921
C	–4.6306684	–3.4818250	–6.4012932
C	–4.3092077	–1.3105635	–5.3781444
C	–2.3903232	–2.6568470	–5.9871693
C	–3.2442799	–3.6533174	–6.4650748
C	–5.1616254	–2.3086656	–5.8573593
H	–4.7147210	–0.3922541	–4.9501302
H	–1.3053059	–2.7723637	–6.0264291
H	–2.8253408	–4.5684388	–6.8864775
H	–6.2426604	–2.1688726	–5.8079914
H	–5.2964514	–4.2610854	–6.7749294
C	–0.6608981	0.4141803	0.8714493
C	–1.3490324	–0.2948377	3.4972330
C	–0.2311795	–0.8063284	1.4107686
C	–1.4370377	1.2806225	1.6576708
C	–1.7788470	0.9243792	2.9641897
C	–0.5734395	–1.1588374	2.7186122
H	0.3759602	–1.4717942	0.7951728
H	–1.7621868	2.2285569	1.2243086
H	–2.3843864	1.6020028	3.5681406
H	–0.2303635	–2.1086225	3.1318295
H	–1.6160123	–0.5704578	4.5184931
C	1.8766878	0.3555163	–4.0542311
C	3.0452632	0.6597551	–3.1626115
O	3.9911771	1.3406625	–3.5337009
O	2.9671831	0.1269977	–1.9191497
C	1.2847624	–1.0218786	–4.1007298
O	0.9358807	–1.5498807	–5.1486344
O	1.1670633	–1.6378042	–2.8988442
C	4.0593024	0.4788423	–1.0448221
H	3.8057096	0.0373389	–0.0757602
H	4.1422546	1.5702038	–0.9562491
H	5.0074847	0.0735326	–1.4248899
C	0.5597169	–2.9445817	–2.9500062
H	–0.4377456	–2.8877654	–3.4058946
H	0.4816084	–3.2668757	–1.9066548
H	1.1828210	–3.6405273	–3.5289226
H	2.1708594	0.6141061	–5.0751860
C	–1.5741914	3.8649890	–3.3162452
I	–2.4391489	3.4819204	–5.1722102
C	–0.6894767	5.0228603	–3.2325697
O	–0.2089445	5.4635865	–2.1998414
O	–0.4409679	5.5932014	–4.4618121
C	–2.2579940	3.3193813	–2.1488161
O	–1.9448192	3.5373131	–0.9885868
O	–3.3241735	2.5112740	–2.4825844
C	0.4079830	6.7551291	–4.4188462
H	1.3520446	6.5300325	–3.9071243
H	–0.0966968	7.5819175	–3.8985167
H	0.5994206	7.0128979	–5.4653500
C	–4.0350794	1.9693871	–1.3544075
H	–4.5391620	2.7705284	–0.7948705
H	–3.3522236	1.4350532	–0.6821054
H	–4.7656397	1.2731573	–1.7787673
C	–4.0122069	4.9575002	–5.1798451
C	–6.0296910	6.8501283	–5.1889664
C	–4.1553039	5.7869104	–4.0734824
C	–4.8469525	5.0436225	–6.2928974
C	–5.8643811	6.0035929	–6.2886574
C	–5.1778282	6.7411319	–4.0864043
H	–3.4844356	5.6936037	–3.2176303
H	–4.7197366	4.3832729	–7.1524880
H	–6.5272598	6.0855924	–7.1510992
H	–5.3036701	7.3999810	–3.2262508
H	–6.8245501	7.5965288	–5.1917869

[Co(TPP)] *Bis*-Terminal Carbene Toluene Adduct ($I^{T–T–Tol}$):

122 atoms

C	3.0478944	3.6961393	–4.8239729
C	2.4557289	3.6705163	–6.0547684
C	1.2918517	2.8275383	–5.9468574
C	2.2255332	2.9038394	–3.9450200
N	1.1585471	2.3894713	–4.6489079
C	2.4366223	2.7816278	–2.5703555
C	1.4920146	2.2139790	–1.7144901
N	0.3474851	1.5551614	–2.0982021
C	–0.3463837	1.2612833	–0.9481553
C	1.5274650	2.3243541	–0.2768551
C	0.3681398	1.7819498	0.1925115
C	–1.4989896	0.4779393	–0.8641873
C	–2.0191997	–0.2180283	–1.9570174
N	–1.6108076	–0.1068870	–3.2686194
C	–3.1544236	–1.8088420	–3.0857389
C	–2.9986535	–1.2664266	–1.8418276
C	–1.6222516	–0.3075721	–6.2113838
N	–0.7529576	0.6845903	–5.8223052
C	–0.4277943	1.3989221	–6.9557362
C	–1.1469232	0.8611125	–8.0837981
C	–1.8573394	–0.2118056	–7.6308916
C	0.5147994	2.4253532	–7.0358813
C	–2.2959051	–1.2031082	–5.3734946
C	–2.3167042	–1.0538461	–3.9844804
H	3.9493906	4.2167177	–4.5178495
H	2.7838620	4.1519536	–6.9697925
H	2.3327336	2.7836876	0.2863276
H	0.0282920	1.7080382	1.2197272
H	–3.7849760	–2.6415161	–3.3775505
H	–3.4696432	–1.5675773	–0.9122460
H	–1.0977619	1.2570664	–9.0923192
H	–2.5138903	–0.8688759	–8.1912317
Co	–0.2062626	1.1312053	–3.9576654
C	3.7045525	3.3245845	–2.0082699
C	6.1295964	4.3193422	–1.0040283
C	4.8974631	2.6108836	–2.2026926
C	3.7379976	4.5384708	–1.3070818
C	4.9443676	5.0336337	–0.8066243
C	6.1027474	3.1079536	–1.7014564
H	4.8590999	1.6590554	–2.7362834
H	2.8094065	5.0922536	–1.1602176
H	4.9591708	5.9808770	–0.2653233
H	7.0240211	2.5430840	–1.8516493
H	7.0719809	4.7059503	–0.6134592
C	0.7826418	3.0621685	–8.3532297
C	1.3297374	4.2942528	–10.8166807
C	0.4423174	4.4070642	–8.5645578
C	1.4018189	2.3426088	–9.3872298
C	1.6738184	2.9547790	–10.6120627
C	0.7136561	5.0175078	–9.7911106
H	–0.0428231	4.9576052	–7.7570250
H	1.6772402	1.3004243	–9.2158002
H	2.1614717	2.3869394	–11.4058685
H	0.4394719	6.0617671	–9.9479935
H	1.5426210	4.7732689	–11.7733113
C	–3.0603088	–2.3119234	–6.0047903
C	–4.4558685	–4.4271030	–7.2335946
C	–4.4595078	–2.3945067	–5.9169785
C	–2.3722437	–3.3022984	–6.7260984
C	–3.0637061	–4.3516896	–7.3340268
C	–5.1517063	–3.4436674	–6.5247977
H	–5.0029870	–1.6201489	–5.3746509
H	–1.2865941	–3.2371675	–6.8031324
H	–2.5125897	–5.1141067	–7.8866086
H	–6.2393716	–3.4884803	–6.4515379
H	–4.9970586	–5.2458731	–7.7095056
C	–2.1713323	0.3014859	0.4521067
C	–3.4961569	–0.0393969	2.9031248
C	–1.5813325	–0.4515410	1.4786709
C	–3.4340679	0.8776921	0.6615306
C	–4.0905519	0.7087680	1.8826738
C	–2.2410841	–0.6201036	2.6979318
H	–0.6084549	–0.9133689	1.3044584
H	–3.8835037	1.4623640	–0.1428661
H	–5.0688526	1.1659819	2.0386010
H	–1.7762623	–1.2128443	3.4872462
H	–4.0106638	–0.1720255	3.8559481
C	1.0959909	–0.3115908	–4.0040215
C	–1.4830535	2.5603689	–3.9342298
C	–2.9195751	2.3121300	–3.7557850
O	–3.4694680	2.5338944	–2.6842186
O	–3.5205625	1.7708684	–4.8314996
C	–1.0563960	3.9567106	–4.1154980
O	–1.2314757	4.5423561	–5.1763722
O	–0.4121574	4.4676657	–3.0500095
C	2.4968436	–0.1627768	–4.4255169
O	3.4327299	–0.3208366	–3.6486920
O	2.6312745	0.2002775	–5.7154355
C	0.7611696	–1.5900141	–3.3497154
O	0.7871946	–1.7580793	–2.1447612
O	0.3897145	–2.5418346	–4.2476279
C	3.9906641	0.4331610	–6.1571634
H	4.4482630	1.2244075	–5.5498910
H	3.8971870	0.7514344	–7.1991851
H	4.5781742	–0.4913144	–6.0883109
C	–0.1186816	–3.7698426	–3.6681007
H	–0.9782471	–3.5480239	–3.0219076
H	0.6627792	–4.2711289	–3.0828411
H	–0.4272188	–4.3834658	–4.5198860
C	–4.8843543	1.3347509	–4.6181084
H	–5.2098267	0.9373512	–5.5843328
H	–5.5192495	2.1744488	–4.3063274
H	–4.9046021	0.5527417	–3.8458320
C	0.2029459	5.7615714	–3.2659713
H	–0.5408674	6.4982784	–3.5956145
H	0.9944265	5.6699978	–4.0223441
H	0.6261518	6.0421145	–2.2969508
H	1.0943105	–0.7846706	–7.9256715
C	1.1776260	–1.8378140	–7.6256735
H	0.6111967	–2.4291535	–8.3622559
H	0.6854178	–1.9317876	–6.6506279
C	2.6164302	–2.2713798	–7.5589625

C	5.3361068	–3.0144822	–7.4166939
C	3.4923043	–2.0121178	–8.6245130
C	3.1281100	–2.9150387	–6.4234589
C	4.4748082	–3.2811995	–6.3488881
C	4.8378483	–2.3788994	–8.5583824
H	3.1122455	–1.5042898	–9.5145404
H	2.4638089	–3.1019624	–5.5780235
H	4.8545649	–3.7632994	–5.4468953
H	5.5019425	–2.1619545	–9.3968447
H	6.3888424	–3.2940548	–7.3581325

[Co(TPP)] *Mono*-Alkyl *Mono*-Terminal Carbene (I^{A-T}):

108 atoms

C	2.6012052	3.6598792	–5.4937309
C	1.9166510	3.6929752	–6.6738461
C	0.7688529	2.8324721	–6.5231192
C	1.8398102	2.8375198	–4.5876078
N	0.7405532	2.3288234	–5.2460628
C	2.1070767	2.6882939	–3.2239480
C	1.1856008	2.1047191	–2.3460270
N	0.0617877	1.3983436	–2.7066654
C	–0.6363131	1.1383430	–1.5448414
C	1.1992874	2.2923888	–0.9173025
C	0.0489867	1.7397806	–0.4301984
C	–1.7539589	0.3103607	–1.4482944
C	–2.2007474	–0.4571135	–2.5293593
N	–1.8160975	–0.3218418	–3.8388521
C	–3.1310021	–2.1994011	–3.6244666
C	–3.0514410	–1.6111726	–2.3943010
C	–1.8958919	–0.4852182	–6.7676478
N	–1.1081006	0.5771599	–6.3840540
C	–0.9370328	1.3709174	–7.5001383
C	–1.6811687	0.8139345	–8.6017857
C	–2.2347397	–0.3546908	–8.1606905
C	–0.0804004	2.4737318	–7.5784062
C	–2.4079405	–1.4852847	–5.9314301
C	–2.3967273	–1.3623548	–4.5396035
H	3.5332108	4.1559201	–5.2457548
H	2.1781089	4.2157434	–7.5878348
H	1.9685560	2.8338174	–0.3766549
H	–0.3145280	1.7353909	0.5914365
H	–3.6573350	–3.1064225	–3.9010045
H	–3.4980204	–1.9358682	–1.4602243
H	–1.7621617	1.2630234	–9.5856342
H	–2.8619286	–1.0506505	–8.7079085
Co	–0.4847414	0.9670828	–4.5465491
C	3.3625945	3.2339807	–2.6438175
C	5.7401860	4.1974112	–1.4949683
C	4.2926058	2.3450201	–2.0789174
C	3.6348733	4.6108828	–2.6181532
C	4.8162798	5.0891369	–2.0475942
C	5.4745071	2.8249585	–1.5116795
H	4.0765330	1.2758328	–2.1048638
H	2.9034383	5.3044728	–3.0346842
H	5.0117340	6.1623895	–2.0269510
H	6.1925141	2.1235584	–1.0838224
H	6.6630087	4.5717860	–1.0495312
C	0.0143613	3.2501542	–8.8433007
C	0.2066854	4.7712409	–11.2043117
C	–0.3237964	4.6140512	–8.8466351
C	0.4584578	2.6633946	–10.0396438
C	0.5529317	3.4169938	–11.2111064
C	–0.2303774	5.3675123	–10.0180122
H	–0.6653907	5.0740541	–7.9181711
H	0.7403086	1.6095821	–10.0411071
H	0.9052498	2.9469286	–12.1305897
H	–0.5044581	6.4234261	–10.0046934
H	0.2798545	5.3600650	–12.1196444
C	–3.0470804	–2.6648133	–6.5732681
C	–4.1933313	–4.8955142	–7.8466899
C	–4.4205171	–2.9297267	–6.4502481
C	–2.2557724	–3.5293370	–7.3489384
C	–2.8256852	–4.6375088	–7.9781415
C	–4.9891448	–4.0375022	–7.0822526
H	–5.0433425	–2.2508179	–5.8670605
H	–1.1880144	–3.3238847	–7.4348117
H	–2.1974778	–5.3052829	–8.5698314
H	–6.0592794	–4.2261464	–6.9835353
H	–4.6383656	–5.7608563	–8.3399556
C	–2.4831608	0.1885081	–0.1599148
C	–3.9457716	–0.0087480	2.2269436
C	–1.9110724	–0.4028769	0.9765885
C	–3.7983926	0.6786487	–0.0934825
C	–4.5209721	0.5811445	1.0970747
C	–2.6391814	–0.5019894	2.1644284
H	–0.8936551	–0.7938103	0.9199746
H	–4.2222871	1.1499941	–0.9817622
H	–5.5377473	0.9742885	1.1435013
H	–2.1874827	–0.9694692	3.0408747
H	–4.5141326	–0.0843770	3.1552413
C	–2.0460416	2.5960953	–4.5072436
H	–1.8712268	2.9604706	–5.5204053
C	0.7549522	–0.3799097	–4.6495947
C	–3.3671578	1.9610502	–4.3627456
O	–4.0150785	1.7615473	–3.3480880
O	–3.8182221	1.5537091	–5.6016720
C	–1.6500863	3.5739629	–3.4785081
O	–1.9639871	3.6109952	–2.3013070
O	–0.7845708	4.5019914	–4.0297292
C	–5.0291714	0.7830273	–5.5732671
H	–4.9452100	–0.0387850	–4.8472605
H	–5.1489418	0.3895819	–6.5888935
H	–5.8898497	1.4087279	–5.2962271
C	–0.2143692	5.4159730	–3.0794801
H	0.4721934	6.0457962	–3.6568536
H	0.3314313	4.8682630	–2.2966559
H	–0.9911000	6.0291287	–2.6008352
C	1.1456394	–0.9488373	–5.9544522
O	0.7138359	–2.0497839	–6.2703862
O	1.8795815	–0.1372514	–6.7185761
C	1.3769156	–0.9484114	–3.4451899
O	2.5315265	–0.6091967	–3.2089252
O	0.5963960	–1.6970894	–2.6697402
C	2.0449195	–0.5647968	–8.0957536
H	2.6464282	0.2193674	–8.5640328
H	1.0571339	–0.6384053	–8.5715346
H	2.5551028	–1.5354857	–8.1437410
C	1.1262878	–1.9912783	–1.3497893
H	0.3490309	–2.5866069	–0.8626155
H	1.2924581	–1.0487414	–0.8103335
H	2.0665353	–2.5524661	–1.4241924

[Co(TPP)] *Mono*-Alkyl *Mono*-Terminal Carbene Tolyl Radical ($I^{A-T-Tol\cdot}$):

122 atoms

C	2.4662221	3.5768963	–5.6867847
C	1.7231731	3.6092854	–6.8310856
C	0.6025003	2.7215908	–6.6353020
C	1.7653084	2.7309339	–4.7538000
N	0.6482989	2.2032485	–5.3652046
C	2.0890409	2.5845596	–3.4020046
C	1.2070468	1.9920079	–2.4895716
N	0.0827180	1.2678498	–2.8093218
C	–0.5709295	1.0009574	–1.6231220
C	1.2649471	2.1894303	–1.0630630
C	0.1398804	1.6225953	–0.5352512
C	–1.6614838	0.1431609	–1.4845563
C	–2.1199963	–0.6447392	–2.5468220
N	–1.7814391	–0.5040715	–3.8683898
C	–3.0192374	–2.4274854	–3.6023172
C	–2.9243099	–1.8276015	–2.3785033
C	–1.9422046	–0.6888159	–6.7906745
N	–1.1897912	0.4082009	–6.4338942
C	–1.0874580	1.2071960	–7.5546540
C	–1.8359059	0.6118087	–8.6328298
C	–2.3261192	–0.5785361	–8.1737268
C	–0.2846315	2.3499016	–7.6554122
C	–2.3894639	–1.7031188	–5.9344016
C	–2.3434673	–1.5706947	–4.5440652
H	3.3997889	4.0885295	–5.4796169
H	1.9295394	4.1463378	–7.7507512
H	2.0430802	2.7461608	–0.5513289
H	–0.1891925	1.6191983	0.4980081
H	–3.5200679	–3.3551956	–3.8569687
H	–3.3293574	–2.1626195	–1.4292152
H	–1.9550574	1.0488761	–9.6172233
H	–2.9331793	–1.3054036	–8.7033167
Co	–0.5137704	0.8157184	–4.6231249
C	3.3597259	3.1435090	–2.8701587
C	5.7705118	4.1277424	–1.8121258
C	4.3181241	2.2624722	–2.3411613
C	3.6205038	4.5228088	–2.8544939
C	4.8185059	5.0113953	–2.3289553
C	5.5164143	2.7529830	–1.8191546
H	4.1107452	1.1913341	–2.3603430
H	2.8676558	5.2101345	–3.2425385
H	5.0052981	6.0863458	–2.3153416
H	6.2563197	2.0578404	–1.4192400
H	6.7063269	4.5102149	–1.4019690
C	–0.2886578	3.1639973	–8.8977029
C	–0.2921807	4.7756209	–11.2051370
C	–0.6262087	4.5260051	–8.8207078
C	0.0575448	2.6253854	–10.1479251
C	0.0511768	3.4236259	–11.2935798
C	–0.6271314	5.3237384	–9.9641870
H	–0.9125196	4.9443611	–7.8552697
H	0.3496267	1.5763368	–10.2133538
H	0.3273485	2.9906553	–12.2564135
H	–0.9116103	6.3733018	–9.8862421
H	–0.2980224	5.3991670	–12.1003240
C	–2.9994838	–2.9107710	–6.5512806
C	–4.0926639	–5.1928093	–7.7785465
C	–4.3583297	–3.2258578	–6.3907165
C	–2.1956198	–3.7509241	–7.3407049
C	–2.7394216	–4.8847901	–7.9469492
C	–4.9007980	–4.3592706	–6.9999821
H	–4.9906611	–2.5664318	–5.7952675
H	–1.1386618	–3.5061578	–7.4544268
H	–2.1016288	–5.5336636	–8.5493571
H	–5.9600761	–4.5876694	–6.8720343
H	–4.5170155	–6.0784847	–8.2536952
C	–2.3362694	–0.0016116	–0.1691342
C	–3.6959557	–0.2540186	2.2737679
C	–1.6969097	–0.5664046	0.9451159
C	–3.6672117	0.4331593	–0.0511993
C	–4.3384838	0.3086801	1.1665845
C	–2.3734598	–0.6927896	2.1604446
H	–0.6674266	–0.9156309	0.8490606
H	–4.1453220	0.8842375	–0.9220222
H	–5.3682536	0.6592437	1.2521332
H	–1.8688773	–1.1394344	3.0187502
H	–4.2242203	–0.3511000	3.2235204
C	–2.1209558	2.4158326	–4.5378999
H	–1.9969689	2.7454052	–5.5699458
C	0.7698081	–0.4966844	–4.7740424
C	–3.4052430	1.7447384	–4.3041531
O	–4.0058937	1.5696846	–3.2570559
O	–3.9023241	1.2671629	–5.5064554
C	–1.6927604	3.4302776	–3.5619904
O	–1.9373513	3.4918225	–2.3692435
O	–0.8880935	4.3658104	–4.1889388
C	–5.0870014	0.4634739	–5.3905652
H	–4.9308828	–0.3465842	–4.6635363
H	–5.2593577	0.0535162	–6.3921339
H	–5.9456539	1.0686587	–5.0664364
C	–0.2712326	5.3080673	–3.2979898
H	0.3711258	5.9303147	–3.9316010
H	0.3284572	4.7847190	–2.5381551
H	–1.0237680	5.9243256	–2.7854583
C	1.1397738	–1.0394171	–6.0956130
O	0.7779816	–2.1664497	–6.4093124
O	1.7848380	–0.1751786	–6.8870035
C	1.4441954	–1.0537653	–3.5923273
O	2.6101917	–0.7300371	–3.3925999
O	0.6857088	–1.7918567	–2.7794591
C	1.9206184	–0.5838651	–8.2715989
H	2.4416819	0.2441896	–8.7607035
H	0.9217626	–0.7282882	–8.7065099
H	2.4978397	–1.5144278	–8.3491118
C	1.2634790	–2.0831499	–1.4811544
H	0.5011782	–2.6692741	–0.9598465
H	1.4594497	–1.1399658	–0.9524670
H	2.1958698	–2.6525657	–1.5876988
C	–3.8886943	5.0927667	–6.0247611
H	–3.9024697	4.2547338	–5.3313400
H	–3.8778777	6.0980468	–5.6040199
C	–3.8901561	4.8910970	–7.4124605
C	–3.9498864	4.4921347	–10.2158105
C	–3.9186486	5.9963952	–8.3204808
C	–3.8771182	3.5747008	–7.9725013
C	–3.9112986	3.3923228	–9.3463086
C	–3.9523990	5.7947000	–9.6903181
H	–3.9225208	7.0097647	–7.9134611
H	–3.8355294	2.7145246	–7.3016357
H	–3.9033621	2.3802235	–9.7516862
H	–3.9741649	6.6515664	–10.3656631
H	–3.9635763	4.3378952	–11.2949870

[Co(TPP)] *Mono*-Bridged *Mono*-Terminal Carbene Toluene Adduct ($I^{B-T-Tol}$):

122 atoms

C	–1.5626695	1.6014138	–3.0360498
C	–1.7978189	1.8668535	–4.3576783
C	–0.9685548	1.0095584	–5.1493711
C	–0.5938947	0.5533947	–2.9580611
N	–0.1334162	0.3018419	–4.2582318
C	–0.4027668	–0.2490388	–1.8267442
C	–0.0205438	–1.6065182	–1.8212251
N	0.1916223	–2.4485178	–2.9051331
C	0.5893044	–3.6640523	–2.3834976
C	0.2348717	–2.3353375	–0.5982799
C	0.5871558	–3.6063920	–0.9432015
C	1.0895783	–4.7566845	–3.1044561
C	1.3573498	–4.7345230	–4.4784323
N	0.9848979	–3.7221137	–5.3322057
C	1.9365709	–5.4313478	–6.5477908
C	1.9756600	–5.7994048	–5.2333264
C	0.1869728	–2.2942553	–7.8248900
N	–0.1786729	–1.5341099	–6.7287545
C	–0.7548391	–0.3803876	–7.2259020
C	–0.7865062	–0.4433844	–8.6682691
C	–0.2025907	–1.6207351	–9.0376013
C	–1.1881301	0.7503918	–6.5028243
C	0.8620577	–3.5169436	–7.7842509
C	1.2685621	–4.1534924	–6.6076463
H	–2.1066302	1.9796695	–2.1778406
H	–2.5718389	2.5005360	–4.7751124
H	0.1949586	–1.9053222	0.3961662
H	0.8815910	–4.4213775	–0.2907332
H	2.2942877	–5.9838031	–7.4105864
H	2.3646314	–6.7183605	–4.8083272

H	–1.1643321	0.3449931	–9.3097047
H	–0.0260131	–1.9976421	–10.0393389
Co	–0.0360595	–2.1351096	–4.8492858
C	1.0782397	–0.4294413	–4.5762260
C	1.8023073	0.0639433	–5.8146226
C	2.1128379	–0.4281573	–3.4569208
O	2.2674507	0.4614628	–2.6387552
O	1.6551835	1.1487369	–6.3462105
O	2.6772929	–0.8740696	–6.2547595
O	2.8883776	–1.5309434	–3.5175788
C	3.3463615	–0.5390692	–7.4866262
H	3.8974360	0.4066471	–7.3953109
H	4.0305837	–1.3721847	–7.6771928
H	2.6092714	–0.4502436	–8.2979738
C	3.9010902	–1.6164313	–2.4932877
H	4.4526697	–2.5358446	–2.7120815
H	3.4269362	–1.6757653	–1.5038701
H	4.5666815	–0.7432787	–2.5238047
C	–1.7652094	–2.6929612	–4.8267918
C	–0.6822098	0.4231361	–0.5301788
C	–1.1747149	1.7763458	1.8840369
C	–1.6573563	–0.0456600	0.3649401
C	0.0404809	1.5834594	–0.2020415
C	–0.2019693	2.2510578	0.9992099
C	–1.9030882	0.6268082	1.5626811
H	–2.2275822	–0.9373994	0.1070379
H	0.8052155	1.9334638	–0.8963738
H	0.3739543	3.1437640	1.2470674
H	–2.6708068	0.2571192	2.2439798
H	–1.3665102	2.3011222	2.8208981
C	1.0720622	–4.2410463	–9.0711772
C	1.3928167	–5.6367639	–11.4846741
C	2.0997674	–3.8939037	–9.9575438
C	0.2046583	–5.2926300	–9.4039700
C	0.3636538	–5.9860233	–10.6047092
C	2.2599344	–4.5900177	–11.1589145
H	2.7715829	–3.0743351	–9.6981536
H	–0.5982106	–5.5538939	–8.7127030
H	–0.3211523	–6.7979098	–10.8542110
H	3.0650989	–4.3146001	–11.8415382
H	1.5183941	–6.1781704	–12.4232131
C	–2.0140724	1.7451308	–7.2370369
C	–3.5780594	3.6222488	–8.6131088
C	–1.5777507	3.0732421	–7.3641725
C	–3.2437258	1.3646729	–7.7998423
C	–4.0210958	2.3022110	–8.4815930
C	–2.3551372	4.0054349	–8.0537901
H	–0.6175702	3.3551141	–6.9300891
H	–3.5844035	0.3362084	–7.6695906
H	–4.9809501	2.0028735	–8.9051759
H	–2.0034020	5.0328323	–8.1582817
H	–4.1865173	4.3524030	–9.1487261
C	1.3142132	–6.0252431	–2.3582071
C	1.6447346	–8.4352040	–0.9560123
C	0.1956608	–6.7326420	–1.8874445
C	2.5979484	–6.5348941	–2.1161852
C	2.7619635	–7.7335083	–1.4178372
C	0.3619910	–7.9316626	–1.1921948
H	–0.7993955	–6.3292690	–2.0847486
H	3.4671314	–5.9802082	–2.4729115
H	3.7655243	–8.1177634	–1.2294596
H	–0.5139083	–8.4768889	–0.8376011
H	1.7738920	–9.3718055	–0.4119975
C	–2.3907546	–3.2566172	–3.6169236
O	–2.3988431	–4.4601315	–3.3845885
O	–2.9234652	–2.3257315	–2.7940122
C	–2.6426376	–2.6021711	–6.0143299
O	–3.4602140	–1.7048736	–6.1694232
O	–2.4120419	–3.5927477	–6.8993693
C	–3.4733183	–2.8493892	–1.5610987
H	–4.1935052	–3.6524076	–1.7640952
H	–3.9689762	–1.9990057	–1.0826357
H	–2.6625720	–3.2382995	–0.9288420
C	–3.2036296	–3.5596632	–8.1125852
H	–3.0248284	–4.5249701	–8.5955406
H	–2.8652016	–2.7285576	–8.7456729
H	–4.2677631	–3.4448173	–7.8747059
C	–1.3294883	–6.5416603	–5.7523227
H	–0.4816280	–7.0536387	–6.2234642
H	–1.4453157	–6.9233826	–4.7285842
H	–1.0764367	–5.4760315	–5.6543636
C	–2.5919476	–6.6968250	–6.5522893
C	–4.9593239	–6.8735733	–8.0835995
C	–2.5866251	–7.2842794	–7.8253207
C	–3.8118827	–6.2092919	–6.0538701
C	–4.9813142	–6.2958266	–6.8085949
C	–3.7566983	–7.3710181	–8.5886034
H	–1.6508236	–7.6838864	–8.2238477
H	–3.8220347	–5.7392920	–5.0687556
H	–5.9165659	–5.9042480	–6.4044278
H	–3.7268555	–7.8309745	–9.5779684
H	–5.8737039	–6.9380933	–8.6750087

[Co(TPP)] *Mono*-Alkyl *Mono*-Bridged Carbene ($I^{A–B}$):

108 atoms

C	2.9066763	3.7533557	–5.5379540
C	2.4901650	3.4905411	–6.8198267
C	1.5282560	2.4509952	–6.7878740
C	2.2378139	2.8824162	–4.6417516
N	1.4902227	1.9271291	–5.4387774
C	2.1062273	3.0856056	–3.2825839
C	1.2389165	2.3686207	–2.4349858
N	0.3013398	1.4342453	–2.8072426
C	–0.1399899	0.8522322	–1.6334427
C	1.3411490	2.4206302	–0.9958069
C	0.4968307	1.4742963	–0.5007207
C	–0.9897804	–0.2452199	–1.5553986
C	–1.5588803	–0.8559089	–2.6793195
N	–1.4450088	–0.4125296	–3.9807901
C	–2.9978393	–2.1187583	–3.8710049
C	–2.5012168	–1.9460694	–2.6134296
C	–2.0737208	0.0125840	–6.8676704
N	–0.9963385	0.7949928	–6.4893101
C	–0.5421810	1.3947746	–7.6417822
C	–1.3916913	1.0349954	–8.7525105
C	–2.3478370	0.1898679	–8.2704087
C	0.6185525	2.1807112	–7.7897992
C	–2.7179899	–0.9085818	–6.0465714
C	–2.3660726	–1.1332105	–4.7119793
H	3.5298322	4.5796972	–5.2135625
H	2.7212947	4.0646045	–7.7106649
H	2.0154504	3.0723889	–0.4516228
H	0.3269216	1.1966311	0.5336275
H	–3.7438362	–2.8299515	–4.2088871
H	–2.7650731	–2.4779028	–1.7057930
H	–1.2452956	1.3694603	–9.7737600
H	–3.1508671	–0.2976901	–8.8124792
Co	–0.3692316	1.0472063	–4.6154508
C	2.9289185	4.1649371	–2.6715589
C	4.4522516	6.2202669	–1.5307188
C	4.3272392	4.0641817	–2.6263771
C	2.2943294	5.2990114	–2.1390775
C	3.0580395	6.3223397	–1.5738680
C	5.0850626	5.0891896	–2.0557081
H	4.8049498	3.1708372	–3.0317261
H	1.2051781	5.3603033	–2.1860918
H	2.5613249	7.2045966	–1.1672459
H	6.1718887	5.0018320	–2.0155880
H	5.0454818	7.0206468	–1.0859331
C	0.8963184	2.7840865	–9.1227542
C	1.4528000	3.9247070	–11.6238902
C	0.0716836	3.7949704	–9.6391049
C	2.0028091	2.3492436	–9.8680183
C	2.2770290	2.9169633	–11.1140790
C	0.3502945	4.3630094	–10.8839081
H	–0.7833480	4.1326369	–9.0512445
H	2.6317004	1.5578894	–9.4574053
H	3.1353891	2.5686895	–11.6904834
H	–0.2921284	5.1533658	–11.2749080
H	1.6693081	4.3686772	–12.5965430
C	–3.8537858	–1.6921420	–6.6102981
C	–6.0174931	–3.1502723	–7.6470802
C	–5.1668767	–1.3884292	–6.2201956
C	–3.6356394	–2.7314891	–7.5257863
C	–4.7120424	–3.4581995	–8.0401357
C	–6.2425680	–2.1126039	–6.7375594
H	–5.3285334	–0.5713813	–5.5155504
H	–2.6140433	–2.9662462	–7.8285709
H	–4.5303208	–4.2682576	–8.7479847
H	–7.2598203	–1.8634854	–6.4321050
H	–6.8579698	–3.7171277	–8.0497370
C	–1.3963557	–0.7261126	–0.2068596
C	–2.2117738	–1.5844041	2.3351993
C	–0.9575494	–1.9579753	0.2983595
C	–2.2493507	0.0754444	0.5692842
C	–2.6538809	–0.3561106	1.8342284
C	–1.3623870	–2.3844500	1.5653815
H	–0.2942213	–2.5768584	–0.3080201
H	–2.5883008	1.0273599	0.1557512
H	–3.3197584	0.2698044	2.4301565
H	–1.0104427	–3.3413316	1.9536862
H	–2.5279692	–1.9180000	3.3245267
C	–2.0231202	2.5998742	–4.3435023
H	–2.5060981	2.4924632	–5.3146631
C	1.4352266	0.4799236	–5.1509448
C	1.5472127	–0.4438043	–6.3485916
O	2.2054307	–0.2301418	–7.3505133
O	0.8308187	–1.5697352	–6.1422408
C	2.3456627	–0.0097351	–4.0439084
O	3.3987717	0.5017467	–3.7119480
O	1.8309993	–1.1227418	–3.4739288
C	0.8230169	–2.4944021	–7.2501317
H	0.2374996	–3.3515758	–6.9033244
H	1.8435941	–2.7993366	–7.5178372
H	0.3457349	–2.0248254	–8.1219061
C	2.5666349	–1.6106582	–2.3312626
H	2.5176190	–0.8717308	–1.5186340
H	3.6173260	–1.8008258	–2.5881183
H	2.0616714	–2.5366891	–2.0390289
C	–2.8470657	2.1533759	–3.2187796
O	–2.6781627	2.3344853	–2.0219891
O	–3.9154222	1.4006199	–3.6891728
C	–4.7408723	0.8433931	–2.6528840
H	–4.1469140	0.2234774	–1.9669602
H	–5.4832058	0.2219710	–3.1669014
H	–5.2376979	1.6361660	–2.0751884
C	–1.2197111	3.8174097	–4.2083838
O	–0.8424052	4.3785638	–3.1901789
O	–0.8767746	4.2933198	–5.4697403
C	–0.1006586	5.5020835	–5.4589520
H	0.2033015	5.6654907	–6.4991325
H	0.7853927	5.3993653	–4.8180778
H	–0.7010407	6.3492007	–5.0950998

[Co(TPP)] *Mono*-Alkyl *Mono*-Bridged Carbene Tolyl Radical ($I^{A–B–Tol·}$):

122 atoms

C	2.6810828	3.6793534	–5.8359820
C	2.2808912	3.4063232	–7.1202497
C	1.3822525	2.3095893	–7.0996138
C	2.0632928	2.7597961	–4.9502514
N	1.3837929	1.7672267	–5.7585187
C	1.9034563	2.9531939	–3.5926571
C	1.0724431	2.1876761	–2.7512582
N	0.1902371	1.2022157	–3.1274208
C	–0.2265491	0.5978616	–1.9559879
C	1.1626000	2.2458184	–1.3114849
C	0.3705322	1.2530617	–0.8203412
C	–1.0261433	–0.5378124	–1.8839179
C	–1.5613095	–1.1738563	–3.0110592
N	–1.4566979	–0.7293759	–4.3134291
C	–2.9312026	–2.5025865	–4.2133307
C	–2.4550911	–2.3042002	–2.9515243
C	–2.0808595	–0.3331574	–7.2078625
N	–1.0523706	0.5058426	–6.8165774
C	–0.6408677	1.1602493	–7.9546162
C	–1.4683631	0.7712607	–9.0719278
C	–2.3621493	–0.1485841	–8.6092023
C	0.4677236	2.0196909	–8.0912302
C	–2.6856275	–1.2868768	–6.3924752
C	–2.3383105	–1.4911059	–5.0523061
H	3.2511598	4.5391582	–5.5012667
H	2.4719107	4.0068743	–8.0028860
H	1.7963077	2.9347103	–0.7641619
H	0.2116961	0.9668160	0.2133794
H	–3.6369170	–3.2518301	–4.5552016
H	–2.7020135	–2.8474135	–2.0458893
H	–1.3489503	1.1407604	–10.0843679
H	–3.1306464	–0.6755810	–9.1637271
Co	–0.4510991	0.7800906	–4.9367709
C	2.6489369	4.0842101	–2.9749963
C	4.0219559	6.2359384	–1.8234693
C	4.0483255	4.0607817	–2.8874601
C	1.9371612	5.1891428	–2.4813652
C	2.6262942	6.2610336	–1.9103959
C	4.7313666	5.1340229	–2.3109650
H	4.5860646	3.1899621	–3.2655723
H	0.8484782	5.1906397	–2.5641684
H	2.0702749	7.1209034	–1.5338510
H	5.8195965	5.1075060	–2.2377159
H	4.5567938	7.0740528	–1.3742734
C	0.6418223	2.7235225	–9.3915446
C	0.9581860	4.0871381	–11.8199421
C	–0.2897609	3.6973106	–9.7819410
C	1.7337159	2.4371919	–10.2232701
C	1.8881657	3.1166350	–11.4342958
C	–0.1305330	4.3764105	–10.9907735
H	–1.1345824	3.9119567	–9.1255593
H	2.4478792	1.6740998	–9.9103577
H	2.7358049	2.8848143	–12.0808331
H	–0.8560519	5.1370029	–11.2840160
H	1.0818277	4.6170843	–12.7653968
C	–3.7819085	–2.1155110	–6.9666949
C	–5.8787613	–3.6439393	–8.0435987
C	–5.1014944	–1.9228421	–6.5289299
C	–3.5247614	–3.0847012	–7.9476227
C	–4.5669211	–3.8457188	–8.4816644
C	–6.1435798	–2.6800263	–7.0662562
H	–5.2961312	–1.1650234	–5.7692302
H	–2.4987931	–3.2375043	–8.2856505
H	–4.3531453	–4.6002934	–9.2399727
H	–7.1658750	–2.5137341	–6.7238876
H	–6.6928034	–4.2367001	–8.4626762
C	–1.4190231	–1.0357873	–0.5375408
C	–2.2114860	–1.9284636	2.0005292
C	–0.9417090	–2.2544927	–0.0349647
C	–2.2984547	–0.2647353	0.2403358
C	–2.6916433	–0.7132089	1.5028992
C	–1.3350558	–2.6979043	1.2297997
H	–0.2572273	–2.8495040	–0.6417321

H	–2.6660877	0.6782544	–0.1692974
H	–3.3781098	–0.1107914	2.0996684
H	–0.9528778	–3.6440307	1.6158066
H	–2.5186683	–2.2754310	2.9880566
C	–2.1785799	2.2141386	–4.6755182
H	–2.6609502	2.0229185	–5.6318446
C	1.3936681	0.3202312	–5.4731250
C	1.5431068	–0.5910239	–6.6743797
O	2.1581274	–0.3296396	–7.6922497
O	0.9084677	–1.7643132	–6.4573121
C	2.3206060	–0.1247752	–4.3624649
O	3.3391288	0.4448329	–4.0166880
O	1.8661103	–1.2680831	–3.8007497
C	0.9291771	–2.6773892	–7.5742001
H	0.4045135	–3.5713487	–7.2228776
H	1.9592501	–2.9181818	–7.8700640
H	0.4036804	–2.2293286	–8.4297748
C	2.6220961	–1.7186589	–2.6564139
H	2.5340886	–0.9840892	–1.8434901
H	3.6815819	–1.8552146	–2.9102221
H	2.1643640	–2.6693213	–2.3661947
C	–2.9702620	1.7846972	–3.5239999
O	–2.8050452	2.0212227	–2.3373473
O	–4.0148436	0.9691449	–3.9546344
C	–4.7995235	0.4044895	–2.8911188
H	–4.1718097	–0.1932746	–2.2157558
H	–5.5386588	–0.2410856	–3.3795013
H	–5.3007491	1.1905432	–2.3084268
C	–1.4637141	3.4931565	–4.6250220
O	–1.1474553	4.1565964	–3.6483724
O	–1.1405589	3.8908642	–5.9139218
C	–0.4974926	5.1698910	–6.0049205
H	–0.2013637	5.2744038	–7.0546801
H	0.3843358	5.2185341	–5.3518093
H	–1.1951206	5.9727578	–5.7252131
H	–4.8580348	0.9604456	–8.0037946
C	–4.8618225	1.6684907	–7.1773212
H	–5.1407151	1.3042676	–6.1897287
C	–4.4630823	3.0035860	–7.3595261
C	–3.6318085	5.6944640	–7.6986720
C	–4.4929590	3.9352378	–6.2758097
C	–3.9967865	3.4823552	–8.6212800
C	–3.5971097	4.8015341	–8.7811800
C	–4.0826235	5.2473433	–6.4465158
H	–4.8278830	3.5861487	–5.2977220
H	–3.9469622	2.7863969	–9.4605853
H	–3.2506103	5.1465562	–9.7573132
H	–4.0996671	5.9325387	–5.5975889
H	–3.3075261	6.7274797	–7.8287672

[Co(TPP)] *Mono*-Enolate *Mono*-Terminal Carbene Toluene Adduct ($I^{E-T-Tol}$):

122 atoms

C	1.6168806	4.4941305	–4.6491410
C	1.0049211	4.4022190	–5.8885162
C	0.7984426	3.0489354	–6.1847295
C	1.7612043	3.2040060	–4.1272742
N	1.2749690	2.2443909	–5.0793052
C	2.1662493	2.8571004	–2.8290033
C	1.5024892	1.8579559	–2.0944308
N	0.2908845	1.2676308	–2.4442218
C	–0.1932766	0.6655186	–1.3095997
C	1.8188381	1.5052746	–0.7281851
C	0.7551113	0.8094211	–0.2321694
C	–1.4117959	–0.0220549	–1.1993186
C	–2.1249041	–0.4849070	–2.3116659
N	–1.7312866	–0.3189360	–3.6213705
C	–3.4718711	–1.8115804	–3.5470758
C	–3.2539480	–1.3811331	–2.2688456
C	–1.5540860	–0.5270426	–6.5795464
N	–0.8679202	0.5881307	–6.1518730
C	–0.3721890	1.2061790	–7.2834077
C	–0.7053086	0.4167986	–8.4461683
C	–1.4350399	–0.6509506	–8.0140136
C	0.2419459	2.4777370	–7.3288085
C	–2.3810230	–1.3235412	–5.7782372
C	–2.5232721	–1.1321996	–4.3968610
H	1.8504100	5.4037797	–4.1063158
H	0.6735083	5.2232351	–6.5128483
H	2.7423368	1.7634809	–0.2213583
H	0.6284470	0.3893511	0.7603575
H	–4.2033117	–2.5349293	–3.8908367
H	–3.7802636	–1.6712665	–1.3660069
H	–0.3971791	0.6540202	–9.4589050
H	–1.8656028	–1.4511397	–8.6065429
Co	–0.4809972	0.9991244	–4.2583925
C	3.1959451	3.7317101	–2.2286767
C	5.1932691	5.4415280	–1.2164298
C	4.3222925	4.0667152	–3.0099230
C	3.0796698	4.2912932	–0.9414726
C	4.0706250	5.1351076	–0.4407438
C	5.3115687	4.9087576	–2.5037158
H	4.4058655	3.6572261	–4.0190028
H	2.1911376	4.0842682	–0.3457643
H	3.9592455	5.5674120	0.5548043
H	6.1801681	5.1492056	–3.1182978
H	5.9672118	6.1015413	–0.8220007
C	0.2868535	3.2627860	–8.5774547
C	0.3945922	4.8548736	–10.8988267
C	–0.8130469	3.3336077	–9.4542119
C	1.4504440	3.9943348	–8.8955081
C	1.4976976	4.7853120	–10.0422574
C	–0.7585875	4.1209361	–10.6028017
H	–1.7258676	2.7923487	–9.2083021
H	2.3185577	3.9146161	–8.2379514
H	2.4061242	5.3431704	–10.2739761
H	–1.6270649	4.1771237	–11.2607952
H	0.4328114	5.4769110	–11.7943003
C	–3.1837467	–2.3932798	–6.4346819
C	–4.6871036	–4.4114227	–7.6938247
C	–4.5788866	–2.2817452	–6.5459823
C	–2.5528506	–3.5315284	–6.9613685
C	–3.2987265	–4.5321402	–7.5876524
C	–5.3250977	–3.2837174	–7.1697578
H	–5.0740419	–1.3996277	–6.1379098
H	–1.4695256	–3.6249333	–6.8721966
H	–2.7934380	–5.4119264	–7.9889363
H	–6.4081478	–3.1799626	–7.2513514
H	–5.2697100	–5.1935370	–8.1823681
C	–1.9237950	–0.2932609	0.1692221
C	–2.8765718	–0.7237768	2.7755493
C	–2.0273059	–1.5959497	0.6821448
C	–2.2991320	0.7934070	0.9773209
C	–2.7765088	0.5762105	2.2709153
C	–2.4991152	–1.8089494	1.9791043
H	–1.7192597	–2.4388048	0.0616230
H	–2.2338058	1.7994424	0.5606335
H	–3.0768749	1.4262082	2.8854945
H	–2.5662822	–2.8250394	2.3708035
H	–3.2473237	–0.8915372	3.7877966
C	2.2780988	1.2055343	–5.4392066
C	3.4436585	1.7132697	–6.1218032
O	3.6457020	2.9119195	–6.3585616
O	4.3393385	0.7551578	–6.5176544
C	2.0042681	–0.1186030	–5.0407880
O	2.9389935	–1.0623824	–5.3043724
O	0.9469072	–0.4875674	–4.4444843
C	5.4932983	1.2707424	–7.2013167
H	6.0993342	0.3908233	–7.4445467
H	6.0607000	1.9611727	–6.5604625
H	5.2063089	1.8044983	–8.1188763
C	2.5929262	–2.4005466	–4.9014571
H	3.4453245	–3.0155289	–5.2098368
H	1.6739702	–2.7389840	–5.4005471
H	2.4476435	–2.4629181	–3.8138517
C	–1.7849814	2.3470450	–4.0387599
C	–1.6865880	3.1373318	–2.7787557
O	–2.3109424	2.8766761	–1.7623199
O	–0.7847176	4.1454199	–2.8607766
C	–3.0802464	2.5256937	–4.6844420
O	–3.8303874	3.4741979	–4.4368366
O	–3.4035544	1.5716709	–5.6047241
C	–0.5151572	4.8279735	–1.6196668
H	–0.2207470	4.1031601	–0.8474385
H	–1.4017474	5.3789841	–1.2777362
H	0.3113065	5.5128122	–1.8373408
C	–4.7032181	1.7044384	–6.2019125
H	–5.4909256	1.6317868	–5.4380450
H	–4.8050516	2.6658741	–6.7222765
H	–4.7757884	0.8759728	–6.9156431
H	–3.8642716	4.7954315	–6.7085446
C	–2.9215428	4.7621591	–7.2696548
H	–3.1309048	4.8650253	–8.3422850
H	–2.4894828	3.7616285	–7.1048079
C	–1.9723568	5.8247820	–6.7855276
C	–0.1537249	7.7637877	–5.8463735
C	–1.8459802	6.0828790	–5.4111917
C	–1.1703390	6.5482833	–7.6804641
C	–0.2686048	7.5118239	–7.2170937
C	–0.9449457	7.0420518	–4.9467336
H	–2.4489767	5.5077614	–4.7065341
H	–1.2358177	6.3373702	–8.7499248
H	0.3512357	8.0592291	–7.9290783
H	–0.8550192	7.2194851	–3.8736335
H	0.5513802	8.5130236	–5.4830660

[Co(TPP)] *Mono*-Alkyl *Mono*-Enolate Adduct (I^{E-A}):

108 atoms

C	2.4248208	4.6889520	–5.4119031
C	1.9892206	4.4640279	–6.6819717
C	1.2252349	3.2385903	–6.6559016
C	1.9308855	3.6033944	–4.5971732
N	1.1847098	2.7466547	–5.3721630
C	2.2808464	3.3973460	–3.2608533
C	1.8287650	2.3054463	–2.5117202
N	0.8170011	1.4529207	–2.8913436
C	0.5597361	0.6428658	–1.7954881
C	2.2764215	1.9783364	–1.1785983
C	1.5138038	0.9323468	–0.7498632
C	–0.5979324	–0.1352998	–1.6187447
C	–1.4532984	–0.4218903	–2.6863241
N	–0.9779588	–0.5866360	–4.0411056
C	–3.2912738	–0.7514173	–3.9661105
C	–2.8482509	–0.5210808	–2.6692882
C	–1.2192977	–0.2827531	–7.0022026
N	–0.4490941	0.7954962	–6.5929106
C	0.0393906	1.3778965	–7.7403303
C	–0.3616981	0.6087476	–8.8944657
C	–1.1119054	–0.4331415	–8.4351334
C	0.7288130	2.5943487	–7.7912657
C	–2.1638944	–0.9512199	–6.2036274
C	–2.1802738	–0.7996695	–4.8142053
H	3.0471768	5.4979409	–5.0449359
H	2.1793820	5.0498354	–7.5747950
H	3.0751563	2.4892125	–0.6514394
H	1.5732863	0.4021389	0.1945496
H	–4.3182940	–0.8117865	–4.3109350
H	–3.4549398	–0.3627446	–1.7837646
H	–0.0933737	0.8447442	–9.9187553
H	–1.5690705	–1.2334669	–9.0070507
Co	0.1027238	1.2802190	–4.7415347
C	3.1089122	4.4324164	–2.5809194
C	4.5991306	6.4241823	–1.2840681
C	4.4623815	4.2222468	–2.2830527
C	2.5056946	5.6505382	–2.2281843
C	3.2505196	6.6400786	–1.5832035
C	5.2035163	5.2140267	–1.6356426
H	4.9310464	3.2789226	–2.5677834
H	1.4513953	5.7994503	–2.4692531
H	2.7743046	7.5834780	–1.3118402
H	6.2574572	5.0429763	–1.4115048
H	5.1792464	7.1986768	–0.7804414
C	0.8731457	3.2751613	–9.1085508
C	1.0751507	4.5988223	–11.5736687
C	0.0483371	4.3763949	–9.3899032
C	1.8003492	2.8458107	–10.0681234
C	1.8993103	3.5045747	–11.2963074
C	0.1518831	5.0334201	–10.6177894
H	–0.6668763	4.6996019	–8.6310289
H	2.4469889	1.9963846	–9.8425112
H	2.6267461	3.1658298	–12.0354886
H	–0.4930255	5.8877412	–10.8290428
H	1.1546032	5.1136292	–12.5321577
C	–3.2656907	–1.7356444	–6.7963591
C	–5.3827608	–3.2688261	–7.8388119
C	–4.0134136	–1.2731437	–7.8959267
C	–3.6092793	–2.9738656	–6.2153321
C	–4.6558619	–3.7327101	–6.7379941
C	–5.0611210	–2.0344316	–8.4123211
H	–3.7799234	–0.2989704	–8.3251744
H	–3.0371789	–3.3297288	–5.3554855
H	–4.9028485	–4.6940039	–6.2851762
H	–5.6383941	–1.6571457	–9.2577288
H	–6.2025904	–3.8631886	–8.2446622
C	–1.0406196	–0.5745529	–0.2801907
C	–1.9444627	–1.4724250	2.2289260
C	–1.5278175	–1.8883968	–0.1209208
C	–1.0323549	0.2845196	0.8352021
C	–1.4791825	–0.1620724	2.0781181
C	–1.9700662	–2.3308789	1.1253374
H	–1.5449605	–2.5531055	–0.9875854
H	–0.6952257	1.3134304	0.7107082
H	–1.4771676	0.5191080	2.9303324
H	–2.3332871	–3.3535931	1.2362093
H	–2.2930091	–1.8201662	3.2024126
C	0.0611666	–1.6359371	–4.2106590
C	–0.3677662	–2.9596957	–3.8302630
O	–1.4974632	–3.2222601	–3.3952957
O	0.5766337	–3.9378538	–3.9838698
C	1.3140094	–1.2302332	–4.7110897
O	2.2682010	–2.1737695	–4.8708601
O	1.6168744	–0.0339678	–5.0259721
C	0.1363541	–5.2519436	–3.6020133
H	0.9962317	–5.9061351	–3.7834224
H	–0.7243237	–5.5736515	–4.2058919
H	–0.1512495	–5.2820006	–2.5412250
C	3.5289461	–1.7017843	–5.3855709
H	3.9772240	–0.9577076	–4.7127218
H	3.4065608	–1.2526427	–6.3808669
H	4.1589784	–2.5956911	–5.4431230
C	–1.5653441	2.5299516	–4.3907146
H	–2.2874079	1.8011358	–4.0102847
C	–2.0024710	3.0847075	–5.6980875
O	–1.5634012	4.0540277	–6.2906395
O	–3.0161125	2.3055537	–6.2090999
C	–1.1898155	3.5102127	–3.3390074
O	–0.5913592	4.5631102	–3.4687284
O	–1.6044063	3.0446877	–2.1114193
C	–1.1349384	3.8178418	–0.9922191
H	–1.4145384	4.8751745	–1.0950246
H	–0.0399258	3.7436502	–0.9112256

H	–1.6136034	3.3782938	–0.1105465
C	–3.3956888	2.6330679	–7.5579226
H	–3.6712773	3.6927371	–7.6465173
H	–4.2549865	1.9927827	–7.7845626
H	–2.5659210	2.4204118	–8.2489127

[Co(TPP)] *Mono*-Alkyl *Mono*–Enolate Adduct Tolyl Radical ($I^{E–A–Tol}$):

122 atoms

C	2.4225695	4.5463859	–5.3606475
C	1.9592454	4.3320915	–6.6229790
C	1.1622371	3.1281344	–6.5817090
C	1.9115783	3.4767330	–4.5353635
N	1.1296150	2.6394064	–5.2963476
C	2.2705882	3.2674800	–3.2018734
C	1.7910161	2.1962330	–2.4396769
N	0.7450385	1.3784535	–2.8016229
C	0.4570741	0.6007587	–1.6904458
C	2.2328528	1.8708759	–1.1037847
C	1.4274688	0.8665411	–0.6535370
C	–0.7350424	–0.1191860	–1.4969207
C	–1.5996178	–0.3942119	–2.5595395
N	–1.1272328	–0.6044910	–3.9101170
C	–3.4443251	–0.7022190	–3.8343576
C	–2.9965441	–0.4483944	–2.5433711
C	–1.3694320	–0.3370129	–6.8783434
N	–0.5710986	0.7269114	–6.4846152
C	–0.0837489	1.2921554	–7.6410753
C	–0.5132298	0.5238851	–8.7856611
C	–1.2787832	–0.5002083	–8.3110766
C	0.6305352	2.4941292	–7.7069070
C	–2.3253673	–0.9731562	–6.0667409
C	–2.3349296	–0.7993466	–4.6795694
H	3.0734150	5.3382526	–5.0055152
H	2.1508546	4.9109456	–7.5201929
H	3.0549692	2.3566053	–0.5886766
H	1.4671050	0.3511089	0.3002343
H	–4.4715076	–0.7475234	–4.1787002
H	–3.5996709	–0.2406451	–1.6659825
H	–0.2509076	0.7470397	–9.8144910
H	–1.7569447	–1.2956230	–8.8728399
Co	0.0085700	1.2116413	–4.6422641
C	3.1259759	4.2873592	–2.5323785
C	4.6596742	6.2527787	–1.2456044
C	4.4767540	4.0521975	–2.2412736
C	2.5470873	5.5170691	–2.1777914
C	3.3136032	6.4934186	–1.5380835
C	5.2396362	5.0310890	–1.5988853
H	4.9262476	3.0995383	–2.5264021
H	1.4938704	5.6838484	–2.4128956
H	2.8563046	7.4458446	–1.2649628
H	6.2914122	4.8407052	–1.3795153
H	5.2567016	7.0169179	–0.7455784
C	0.7624310	3.1715780	–9.0274429
C	0.9365675	4.4907546	–11.4978120
C	–0.0448869	4.2903434	–9.2910671
C	1.6588661	2.7230812	–10.0074619
C	1.7438645	3.3795841	–11.2380928
C	0.0445620	4.9449197	–10.5214552
H	–0.7358375	4.6288006	–8.5163733
H	2.2928882	1.8604418	–9.7960127
H	2.4473630	3.0256431	–11.9933385
H	–0.5869806	5.8127011	–10.7185727
H	1.0049697	5.0035214	–12.4584022
C	–3.4513033	–1.7368232	–6.6416256
C	–5.6204028	–3.2263645	–7.6414155
C	–4.1940715	–1.2725380	–7.7439874
C	–3.8264636	–2.9543080	–6.0362842
C	–4.8988229	–3.6914307	–6.5374614
C	–5.2672798	–2.0122541	–8.2393880
H	–3.9358126	–0.3134626	–8.1929720
H	–3.2594268	–3.3107887	–5.1731808
H	–5.1704155	–4.6367395	–6.0651575
H	–5.8396234	–1.6335488	–9.0876831
H	–6.4603153	–3.8037509	–8.0306366
C	–1.1986802	–0.5047448	–0.1492124
C	–2.1492797	–1.2941857	2.3789958
C	–1.7460259	–1.7904310	0.0422306
C	–1.1528048	0.3819085	0.9434686
C	–1.6228322	–0.0112254	2.1960134
C	–2.2117676	–2.1792554	1.2978940
H	–1.7905010	–2.4761448	–0.8070564
H	–0.7687215	1.3905829	0.7927137
H	–1.5906609	0.6908821	3.0306536
H	–2.6220063	–3.1810629	1.4340725
H	–2.5158644	–1.6000853	3.3600328
C	–0.1227281	–1.6906048	–4.0556949
C	–0.5910728	–2.9895722	–3.6381978
O	–1.7280856	–3.2063885	–3.1967484
O	0.3242434	–3.9994007	–3.7616592
C	1.1385081	–1.3384917	–4.5762418
O	2.0593148	–2.3174113	–4.7200658
O	1.4774445	–0.1613837	–4.9238892
C	–0.1550981	–5.2881356	–3.3428331
H	0.6852466	–5.9726135	–3.5036326
H	–1.0244133	–5.6018248	–3.9387560
H	–0.4446968	–5.2790407	–2.2820875
C	3.3317339	–1.9003842	–5.2526980
H	3.8081993	–1.1548462	–4.6009853
H	3.2185602	–1.4723454	–6.2584572
H	3.9318479	–2.8158228	–5.2908996
C	–1.6140863	2.5194500	–4.2827104
H	–2.3595946	1.8268742	–3.8804129
C	–2.0500557	3.0681903	–5.5887858
O	–1.6150178	4.0341034	–6.1896492
O	–3.0767859	2.2948342	–6.0937754
C	–1.1883216	3.5025146	–3.2517274
O	–0.5656708	4.5374609	–3.4127819
O	–1.5808037	3.0592976	–2.0134602
C	–1.0773298	3.8306204	–0.9106141
H	–1.2654204	4.9012326	–1.0621185
H	0.0042825	3.6619744	–0.7939301
H	–1.6223564	3.4733949	–0.0305497
C	–3.4655437	2.6259759	–7.4384180
H	–3.7355463	3.6877520	–7.5243882
H	–4.3310765	1.9914824	–7.6584305
H	–2.6441192	2.4090891	–8.1376902
C	–5.3102325	2.0310716	–3.5005407
H	–5.1942429	1.9055430	–4.5759270
H	–5.7442988	1.2117288	–2.9282205
C	–4.8789207	3.2052671	–2.8621155
C	–3.9655339	5.5634775	–1.5800334
C	–4.9421471	3.3507025	–1.4427467
C	–4.3420621	4.2986695	–3.6082638
C	–3.8869760	5.4453769	–2.9759523
C	–4.4985145	4.5077805	–0.8221117
H	–5.3427196	2.5276749	–0.8471278
H	–4.2831730	4.2135166	–4.6936405
H	–3.4505197	6.2497576	–3.5686213
H	–4.5549545	4.5954110	0.2644211
H	–3.6066053	6.4669267	–1.0857327

[Co(TPP)] Diazo Adduct (I^{D}):

94 atoms

C	2.9975757	4.0845091	–5.0514005
C	2.5363293	3.8646090	–6.3108051
C	1.4319775	2.9460601	–6.1972480
C	2.1729866	3.3061910	–4.1625799
N	1.2157828	2.5991882	–4.8729169
C	2.3039512	3.3401699	–2.7788043
C	1.4657912	2.6226398	–1.9286764
N	0.5052421	1.7027498	–2.3259377
C	0.0365353	1.1452699	–1.1446525
C	1.5573627	2.6719504	–0.4921398
C	0.6662657	1.7634083	–0.0068052
C	–0.8753157	0.0977961	–1.0393107
C	–1.4992755	–0.4693931	–2.1475826
N	–1.3474379	–0.0576749	–3.4647168
C	–2.8108877	–1.8621899	–3.3343251
C	–2.3981952	–1.5912332	–2.0655326
C	–1.7468113	0.0876029	–6.3888382
N	–0.7720262	0.9916036	–5.9925571
C	–0.3912632	1.6387389	–7.1600687
C	–1.1749125	1.1739914	–8.2758329
C	–2.0137992	0.2131754	–7.7978940
C	0.6768675	2.5239890	–7.2858803
C	–2.3762957	–0.8484113	–5.5722152
C	–2.1712156	–0.9030677	–4.1965224
H	3.8104381	4.7275346	–4.7318311
H	2.8912239	4.2887405	–7.2437956
H	2.2311209	3.3175066	0.0611266
H	0.4482765	1.5192097	1.0274462
H	–3.4820676	–2.6444069	–3.6722782
H	–2.6608170	–2.1054813	–1.1473065
H	–1.0718988	1.5333717	–9.2941893
H	–2.7523343	–0.3683249	–8.3395838
Co	–0.0748629	1.2865582	–4.1684433
C	3.4294485	4.1181532	–2.1856518
C	5.5844865	5.5296915	–1.0660834
C	4.7377836	3.6192930	–2.2930783
C	3.2129398	5.3312010	–1.5164327
C	4.2847774	6.0328169	–0.9588357
C	5.8078409	4.3228125	–1.7355519
H	4.8964226	2.6773937	–2.8210296
H	2.1969967	5.7218519	–1.4390317
H	4.1045077	6.9778156	–0.4440401
H	6.8203830	3.9257276	–1.8241994
H	6.4212765	6.0786710	–0.6317068
C	1.0853836	2.9582442	–8.6525290
C	1.8834565	3.7150656	–11.2370606
C	0.3358317	3.8917901	–9.3822253
C	2.2421997	2.4083169	–9.2284777
C	2.6373918	2.7860377	–10.5136648
C	0.7325903	4.2677832	–10.6680356
H	–0.5602306	4.3223445	–8.9325109
H	2.8214711	1.6862492	–8.6500136
H	3.5374043	2.3518461	–10.9519962
H	0.1435758	4.9982977	–11.2247466
H	2.1932505	4.0098998	–12.2407052
C	–3.2838205	–1.8471631	–6.2065431
C	–4.9633373	–3.7488584	–7.4198019
C	–4.6745923	–1.7811755	–6.0364051
C	–2.7454598	–2.8790837	–6.9911627
C	–3.5781949	–3.8243446	–7.5932382
C	–5.5090618	–2.7252265	–6.6399499
H	–5.0963977	–0.9794819	–5.4283225
H	–1.6625744	–2.9344421	–7.1143927
H	–3.1445784	–4.6243666	–8.1953887
H	–6.5895416	–2.6587053	–6.5034149
H	–5.6153451	–4.4861007	–7.8904085
C	–1.1693072	–0.4594036	0.3121733
C	–1.7048555	–1.5218796	2.8609021
C	–0.1972790	–1.2085066	0.9932430
C	–2.4144468	–0.2518760	0.9243504
C	–2.6801559	–0.7783452	2.1905419
C	–0.4621228	–1.7369574	2.2581088
H	0.7675970	–1.3781045	0.5128238
H	–3.1726124	0.3298437	0.3980004
H	–3.6512150	–0.6040477	2.6564196
H	0.3018051	–2.3220468	2.7724514
H	–1.9128321	–1.9333844	3.8495288
C	1.9252404	–0.7489465	–4.5035807
C	2.0430447	–0.5885128	–5.9723063
O	2.7958368	0.1821044	–6.5276223
O	1.1934040	–1.4415898	–6.6086908
C	2.8792483	–0.1581008	–3.5354129
O	3.7410948	0.6471300	–3.8146861
O	2.6575189	–0.6609737	–2.2900614
C	1.2256159	–1.3586582	–8.0522689
H	0.3936575	–1.9807849	–8.3952742
H	2.1837224	–1.7382744	–8.4327687
H	1.0811053	–0.3226146	–8.3802147
C	3.5330927	–0.1392737	–1.2641764
H	3.5060682	0.9568023	–1.2581096
H	4.5627309	–0.4838440	–1.4316290
H	3.1380774	–0.5312268	–0.3222367
N	1.1485705	–1.7303480	–4.0616020
N	0.4678005	–2.5489162	–3.6791700

[Co(TPP)] *Mono*-Diazo *Mono*-Terminal Carbene Adduct ($I^{D–T}$):

109 atoms

C	2.4358609	3.5480822	–5.1941683
C	1.8715726	3.5321064	–6.4375414
C	0.7412727	2.6449758	–6.3730336
C	1.6255036	2.7062705	–4.3561897
N	0.5851267	2.1558753	–5.0867102
C	1.8117719	2.5598106	–2.9847880
C	0.8728961	1.9261284	–2.1768573
N	–0.2490227	1.2463117	–2.6273152
C	–0.9220444	0.8560765	–1.4846123
C	0.9009922	1.9499321	–0.7386074
C	–0.2297795	1.3233672	–0.3112880
C	–0.2216716	0.0002036	–1.4307177
C	–2.4778930	–0.6773718	–2.5595430
N	–2.0090040	–0.4983782	–3.8522604
C	–3.5571246	–2.2237612	–3.7964247
C	–3.4704373	–1.7210979	–2.5328497
C	–2.0014918	–0.5885463	–6.7953185
N	–1.2607072	0.4801104	–6.3151053
C	–0.9115413	1.2101681	–7.4399656
C	–1.4889326	0.6245065	–8.6205860
C	–2.1246425	–0.5132136	–8.2276242
C	–0.0154171	2.2703470	–7.4779695
C	–2.6166034	–1.5558042	–6.0061158
C	–2.6638287	–1.4486086	–4.6165125
H	3.3042541	4.1019229	–4.8533648
H	2.1861354	4.0617380	–7.3308251
H	1.6825288	2.4086439	–0.1427883
H	–0.5612954	1.1554989	0.7075197
H	–4.1996694	–3.0164091	–4.1650258
H	–4.0301320	–2.0218997	–1.6542390
H	–1.3759400	1.0244679	–9.6226206
H	–2.6457638	–1.2390231	–8.8421136
Co	–0.6224101	0.7312089	–4.4755483
C	3.0324675	3.1551608	–2.3752552
C	5.3683453	4.2568538	–1.2763486
C	4.2774505	2.5479336	–2.6004304
C	2.9684449	4.3217285	–1.5991866
C	4.1316079	4.8688416	–1.0525206
C	5.4387735	3.0955094	–2.0513834
H	4.3165062	1.6399524	–3.2046792
H	2.0000880	4.7972407	–1.4363459
H	4.0718615	5.7788228	–0.4536305
H	6.4009340	2.6118067	–2.2263322
H	6.2757691	4.6848225	–0.8480899
C	0.2422056	2.9536326	–8.7775608
C	0.7393585	4.2624920	–11.2077758
C	–0.4858051	4.0993084	–9.1255825
C	1.2175385	2.4635851	–9.6576260
C	1.4651187	3.1168307	–10.8671494
C	–0.2381811	4.7513325	–10.3365757

H	–1.2527787	4.4667820	–8.4415327
H	1.7694566	1.5634483	–9.3815790
H	2.2252159	2.7287465	–11.5468182
H	–0.8114118	5.6412240	–10.6009326
H	0.9330626	4.7715137	–12.1529281
C	–3.3349775	–2.6900714	–6.6513424
C	–4.6847575	–4.8564372	–7.8274897
C	–4.5311133	–2.4861992	–7.3566427
C	–2.8258667	–3.9927213	–6.5377122
C	–3.4957834	–5.0685304	–7.1242422
C	–5.2013854	–3.5625954	–7.9413880
H	–4.9342285	–1.4754774	–7.4361767
H	–1.8952185	–4.1515192	–5.9913103
H	–3.0846641	–6.0750060	–7.0346005
H	–6.1324957	–3.3906078	–8.4833750
H	–5.2079308	–5.6970873	–8.2851914
C	–2.6573118	–0.2551480	–0.1081259
C	–3.8449240	–0.6981304	2.4043541
C	–2.6096392	–1.5237612	0.4931426
C	–3.3027212	0.7925754	0.5710097
C	–3.8937082	0.5688386	1.8164765
C	–3.1987114	–1.7441411	1.7393473
H	–2.1003371	–2.3379486	–0.0238730
H	–3.3422886	1.7754569	0.1013581
H	–4.3963218	1.3906764	2.3287230
H	–3.1463598	–2.7340502	2.1950332
H	–4.3050247	–0.8697470	3.3784428
C	–2.9348193	2.9739991	–4.3320106
C	0.7368277	–0.5440760	–4.6113421
C	–3.7017317	2.4448006	–3.1874571
O	–3.5450702	2.7863102	–2.0337674
O	–4.6300921	1.5439121	–3.6120048
C	–1.8927253	4.0153696	–4.2037436
O	–1.3716344	4.3490814	–3.1625267
O	–1.6134037	4.5561418	–5.4243617
C	–5.4939477	1.0269049	–2.5740323
H	–4.9023853	0.6111769	–1.7498701
H	–6.0817770	0.2405454	–3.0561090
H	–6.1437691	1.8254909	–2.1902298
C	–0.5980987	5.5862053	–5.4048998
H	–0.9991396	6.4995598	–4.9445719
H	–0.3392803	5.7581654	–6.4541542
H	0.2827192	5.2477538	–4.8474725
C	1.6908404	–0.3713987	–5.7446279
O	1.4486874	–0.5723893	–6.9214226
O	2.8927169	0.0963362	–5.3016178
C	1.0371066	–1.6435821	–3.7195908
O	1.8606214	–2.5175002	–4.0087726
O	0.3493584	–1.6457175	–2.5423204
C	3.8603956	0.3540478	–6.3422501
H	4.7415884	0.7524371	–5.8285472
H	3.4659192	1.0943912	–7.0517099
H	4.1070826	–0.5723912	–6.8779649
C	0.6610863	–2.7336717	–1.6581285
H	1.7421141	–2.7908927	–1.4699376
H	0.3251274	–3.6907230	–2.0830220
H	0.1222095	–2.5129454	–0.7302417
N	–3.3489526	2.6465925	–5.5439063
N	–3.6923958	2.3424899	–6.5794301

[Co(TPP)] *Mono*-Diazo *Mono*-Enolate (I^{D-E}):

109 atoms

C	2.0081058	5.0938081	–5.3355036
C	1.6634859	4.8301192	–6.6288593
C	1.0854620	3.5072277	–6.6493558
C	1.6746465	3.9184581	–4.5654587
N	1.0441334	2.9906417	–5.3707442
C	2.0774028	3.6829577	–3.2454984
C	1.7689180	2.4995507	–2.5645271
N	0.8352236	1.5717338	–2.9742938
C	0.6984183	0.6820459	–1.9116545
C	2.3187734	2.1233218	–1.2821500
C	1.6755305	0.9853811	–0.8919987
C	–0.4201272	–0.1460067	–1.7273837
C	–1.3221241	–0.3583249	–2.7769118
N	–0.8926024	–0.4444409	–4.1525081
C	–3.2086922	–0.5837358	–4.0004145
C	–2.7160091	–0.4388730	–2.7101375
C	–1.1835364	–0.0962633	–7.0644557
N	–0.4085875	0.9698156	–6.6237880
C	0.1205317	1.5432088	–7.7633394
C	–0.2473098	0.7680048	–8.9281670
C	–1.0379847	–0.2525410	–8.4934208
C	0.7496554	2.7921607	–7.8071522
C	–2.1459091	–0.7497435	–6.2777606
C	–2.1282374	–0.6093897	–4.8864647
H	2.4689579	5.9904656	–4.9353268
H	1.7946149	5.4647137	–7.4981335
H	3.1067354	2.6615371	–0.7653752
H	1.8301370	0.4028069	0.0100030
H	–4.2480255	–0.6198797	–4.3103187
H	–3.2865275	–0.3390416	–1.7921921
H	0.0512491	0.9964664	–9.9456822
H	–1.4993904	–1.0404905	–9.0791945
Co	0.1699493	1.3443822	–4.7961365
C	2.8796022	4.7168388	–2.5382151
C	4.3786128	6.6716492	–1.1778944
C	4.1569812	5.0831243	–2.9925656
C	2.3661646	5.3442837	–1.3914007
C	3.1079338	6.3159637	–0.7176045
C	4.9011970	6.0513722	–2.3162647
H	4.5641790	4.5927083	–3.8775123
H	1.3702786	5.0700794	–1.0409978
H	2.6903730	6.8004107	0.1660604
H	5.8952624	6.3188598	–2.6770824
H	4.9598846	7.4297249	–0.6513782
C	1.0615342	3.3931415	–9.1350074
C	1.6470744	4.5101045	–11.6489417
C	0.3773524	4.5350992	–9.5838394
C	2.0465060	2.8237274	–9.9579471
C	2.3358766	3.3770884	–11.2066363
C	0.6702676	5.0872142	–10.8330766
H	–0.3826184	4.9887603	–8.9450468
H	2.5875285	1.9440471	–9.6059662
H	3.1067555	2.9253045	–11.8327853
H	0.1281993	5.9722293	–11.1698733
H	1.8736649	4.9431527	–12.6241909
C	–3.2531440	–1.5263524	–6.8693133
C	–5.3792902	–3.0501852	–7.9166958
C	–3.9776661	–1.0779288	–7.9907832
C	–3.6234511	–2.7506258	–6.2735854
C	–4.6745785	–3.5026778	–6.7970333
C	–5.0286550	–1.8329171	–8.5094220
H	–3.7237083	–0.1192136	–8.4434680
H	–3.0639444	–3.1041301	–5.4045998
H	–4.9407174	–4.4523531	–6.3304586
H	–5.5852692	–1.4638819	–9.3722142
H	–6.2017038	–3.6401502	–8.3237676
C	–0.7998053	–0.6796726	–0.4040604
C	–1.6017494	–1.7549601	2.0716726
C	–1.2769979	–2.0040547	–0.3165993
C	–0.7545913	0.1006280	0.7676117
C	–1.1498375	–0.4337089	1.9934570
C	–1.6681000	–2.5342160	0.9124815
H	–1.3312003	–2.6055035	–1.2268378
H	–0.4292838	1.1394991	0.7046185
H	–1.1177794	0.1873249	2.8899533
H	–2.0241854	–3.5640559	0.9656111
H	–1.9091963	–2.1718557	3.0317691
C	0.1082680	–1.5237817	–4.3958543
C	–0.3520222	–2.8510961	–4.0784732
O	–1.4721954	–3.1100706	–3.6130844
O	0.5492677	–3.8519491	–4.3330126
C	1.3786034	–1.1282597	–4.8752580
O	2.3001220	–2.1009945	–5.0807552
O	1.7113097	0.0677264	–5.1196986
C	0.0769202	–5.1694040	–4.0106679
H	–0.1683143	–5.2551451	–2.9420229
H	0.9039722	–5.8409796	–4.2670259
H	–0.8191596	–5.4255065	–4.5944989
C	3.5739437	–1.6429103	–5.5699989
H	4.0459902	–0.9495445	–4.8597516
H	3.4674089	–1.1367883	–6.5398225
H	4.1769219	–2.5512441	–5.6765683
C	–1.6022904	4.7097654	–4.8383526
C	–1.6463544	3.6900457	–3.7820036
O	–1.8586944	2.5042619	–3.9824930
O	–1.4065339	4.2411220	–2.5618655
C	–1.9614927	4.5587667	–6.2648535
O	–1.8183457	5.4492092	–7.0904664
O	–2.4777849	3.3440900	–6.5108940
C	–2.8418675	3.0886656	–7.8852954
H	–1.9799388	3.2329062	–8.5472085
H	–3.6610682	3.7514740	–8.1943548
H	–3.1536498	2.0405061	–7.8979031
C	–1.3795399	3.3404824	–1.4266825
H	–0.3399996	3.2432976	–1.0881826
H	–1.7673858	2.3543681	–1.7056047
H	–1.9959628	3.8012072	–0.6462596
N	–1.1450404	5.9077720	–4.5140700
N	–0.7467098	6.9290381	–4.2358823

[Co(TPP)] *Mono*-Enolate *Mono*-Terminal Carbene (I^{E-T}) (Q):

107 atoms

C	1.9988234	4.2512414	–5.4153100
C	1.3996065	3.9727593	–6.6364515
C	1.2612180	2.5783622	–6.7502632
C	2.2088755	3.0317529	–4.7501892
N	1.7780867	1.9689388	–5.5748665
C	2.5758219	2.8566930	–3.4006157
C	1.9252275	1.9477079	–2.5391843
N	0.7136283	1.3145496	–2.7674339
C	0.3040148	0.7923292	–1.5687192
C	2.3230222	1.7242636	–1.1678435
C	1.3156173	1.0315263	–0.5628310
C	–0.9076220	0.1056373	–1.3058232
C	–1.7471524	–0.4138218	–2.3010263
N	–1.4433822	–0.3923361	–3.6404265
C	–3.4272277	–1.5161402	–3.3380717
C	–3.0096427	–1.0951194	–2.1060288
C	–1.5274861	–0.7201515	–6.5875404
N	–0.6221357	0.2833731	–6.3201746
C	–0.0979789	0.6811157	–7.5447474
C	–0.6055551	–0.1842780	–8.5828707
C	–1.4863482	–1.0431707	–7.9969563
C	0.6455831	1.8512869	–7.7828688
C	–2.4465425	–1.2895606	–5.6826395
C	–2.4274689	–1.0806620	–4.2923756
H	2.1595151	5.2233739	–4.9626090
H	1.0059749	4.6821517	–7.3569342
H	3.2627748	2.0503225	–0.7351293
H	1.2678975	0.6797748	0.4622171
H	–4.3388101	–2.0517252	–3.5832524
H	–3.5146097	–1.2250844	–1.1544285
H	–0.3054515	–0.1394218	–9.6243707
H	–2.0547850	–1.8390401	–8.4663987
Co	–0.1115791	0.8647676	–4.5210169
C	3.5395108	3.8403053	–2.8781263
C	5.3981654	5.7497197	–1.9839063
C	4.6962862	4.1239936	–3.6343047
C	3.3128199	4.5551693	–1.6855265
C	4.2376442	5.4996994	–1.2434385
C	5.6210448	5.0641307	–3.1826389
H	4.8563668	3.5908160	–4.5739025
H	2.3833786	4.3918561	–1.1406211
H	4.0443328	6.0575129	–0.3260085
H	6.5192362	5.2636170	–3.7686086
H	6.1204197	6.4888189	–1.6340403
C	0.7200395	2.4363629	–9.1347043
C	0.9181107	3.5986757	–11.6857081
C	–0.4188912	2.5610676	–9.9538188
C	1.9573414	2.9228370	–9.6050809
C	2.0522320	3.4927514	–10.8741062
C	–0.3175470	3.1374754	–11.2191525
H	–1.3856488	2.2330308	–9.5707658
H	2.8372864	2.8317532	–8.9642316
H	3.0173908	3.8531320	–11.2329710
H	–1.2093296	3.2413415	–11.8389446
H	0.9944324	4.0478553	–12.6770580
C	–3.5609078	–2.0962348	–6.2455044
C	–5.7151086	–3.5711475	–7.2906998
C	–4.4640075	–1.5028644	–7.1455407
C	–3.7542240	–3.4372749	–5.8761216
C	–4.8215939	–4.1702639	–6.3980771
C	–5.5340772	–2.2352335	–7.6613621
H	–4.3182852	–0.4569105	–7.4209116
H	–3.0525685	–3.9024108	–5.1823154
H	–4.9532779	–5.2143309	–6.1103803
H	–6.2318667	–1.7594322	–8.3519004
H	–6.5500314	–4.1440108	–7.6964236
C	–1.2843743	–0.0952843	0.1167402
C	–1.9951237	–0.4518058	2.8176401
C	–1.4901042	–1.3836403	0.6405758
C	–1.4367858	1.0114677	0.9710389
C	–1.7927777	0.8343895	2.3084552
C	–1.8403505	–1.5600742	1.9798874
H	–1.3551502	–2.2477946	–0.0110847
H	–1.2829058	2.0134104	0.5683579
H	–1.9162421	1.7045802	2.9546571
H	–1.9849094	–2.5674917	2.3728680
H	–2.2699436	–0.5902051	3.8641454
C	2.7072192	0.8476628	–5.7288735
C	3.9251585	1.1873727	–6.4315555
O	4.1675153	2.3151101	–6.8769245
O	4.8071078	0.1526689	–6.5814226
C	2.3316654	–0.3778298	–5.1579272
O	3.1780456	–1.4248726	–5.2539029
O	1.2399289	–0.5593534	–4.5277790
C	6.0093393	0.4965066	–7.2917473
H	5.7819067	0.8439350	–8.3097079
H	6.5976326	–0.4270811	–7.3248346
H	6.5657624	1.2879080	–6.7693668
C	2.7258439	–2.6476309	–4.6382238
H	3.5233738	–3.3715827	–4.8357415
H	1.7794547	–2.9861972	–5.0821202
H	2.5851693	–2.5161181	–3.5564705
C	–1.2520446	2.3882681	–4.5221541
C	–1.0384025	3.7135064	–3.9783305
O	–0.1235818	4.1094736	–3.2587812
O	–2.0514224	4.5739879	–4.3801388
C	–2.6174468	2.1053647	–5.0401709
O	–2.9321611	2.0343569	–6.2177724
O	–3.4973012	1.8845803	–4.0246759
C	–1.9347223	5.9130606	–3.8754006
H	–1.9618872	5.9236151	–2.7759248
H	–2.7923794	6.4575494	–4.2858353
H	–0.9924981	6.3757230	–4.2039481
C	–4.8347433	1.5349611	–4.4423435
H	–5.2812977	2.3479291	–5.0310488
H	–4.8183551	0.6172688	–5.0469067

H	–5.3937956	1.3690818	–3.5161705

[Co(TPP)] *Mono*-Enolate *Mono*-Gamma Radical (I^{E-G}) (Q):

123 atoms

C	0.4088609	4.4800727	–5.4245392
C	0.0235046	4.1248522	–6.7077160
C	–0.2991690	2.7522782	–6.7031360
C	0.3536273	3.3303004	–4.6106525
N	–0.0298212	2.2162807	–5.4135305
C	0.5334231	3.2622794	–3.2252600
C	–0.0811573	2.3077260	–2.3862211
N	–1.1833839	1.5188696	–2.6734235
C	–1.5241642	0.8716532	–1.5014579
C	0.2949525	2.1205684	–1.0028427
C	–0.5926210	1.2421563	–0.4568002
C	–2.6468251	0.0475268	–1.2958179
C	–3.5226263	–0.3860297	–2.3056815
N	–3.3803999	–0.0933845	–3.6349600
C	–5.1837507	–1.4948126	–3.3721264
C	–4.6572269	–1.2654974	–2.1295638
C	–3.6006018	–0.1392975	–6.6063674
N	–2.6141797	0.7653854	–6.2992996
C	–1.9562562	1.0549454	–7.4871326
C	–2.5402767	0.2707086	–8.5559173
C	–3.5668156	–0.4459749	–8.0185701
C	–0.9720088	2.0463079	–7.7164897
C	–4.4920821	–0.7735456	–5.7121760
C	–4.3591589	–0.7760539	–4.3167144
H	0.6208204	5.4774805	–5.0548374
H	–0.1461355	4.7893073	–7.5486004
H	1.1435494	2.5982494	–0.5249304
H	–0.6240801	0.8793303	0.5646668
H	–6.0468709	–2.1018452	–3.6245729
H	–4.9987874	–1.6672729	–1.1809966
H	–2.1831945	0.2568544	–9.5799650
H	–4.2181317	–1.1574843	–8.5151359
Co	–2.0854312	1.1985338	–4.4136605
C	1.3369237	4.3466166	–2.6220557
C	2.8582854	6.4390683	–1.5352817
C	2.6123784	4.6419540	–3.1396188
C	0.8228521	5.1274780	–1.5709853
C	1.5812987	6.1665336	–1.0326313
C	3.3692043	5.6779236	–2.5917316
H	2.9950442	4.0456883	–3.9709361
H	–0.1931895	4.9345210	–1.2253147
H	1.1691275	6.7768447	–0.2276058
H	4.3618935	5.8919457	–2.9903948
H	3.4503241	7.2513210	–1.1107750
C	–0.7017170	2.5201446	–9.0917914
C	–0.1068399	3.4836690	–11.6666303
C	–1.7345339	2.8396325	–9.9937876
C	0.6351423	2.7151836	–9.4939940
C	0.9272767	3.1857155	–10.7736016
C	–1.4376428	3.3159786	–11.2701865
H	–2.7716596	2.7363798	–9.6731999
H	1.4367705	2.4903133	–8.7875292
H	1.9669293	3.3202410	–11.0751566
H	–2.2483852	3.5712273	–11.9540271
H	0.1228456	3.8557154	–12.6661076
C	–5.6578062	–1.4793739	–6.3090043
C	–7.8971091	–2.7375058	–7.4467822
C	–6.6243283	–0.7257550	–6.9977092
C	–5.8244691	–2.8687655	–6.2008649
C	–6.9365912	–3.4938405	–6.7685856
C	–7.7380597	–1.3530136	–7.5588900
H	–6.4904142	0.3552696	–7.0647790
H	–5.0669665	–3.4562828	–5.6800572
H	–7.0498961	–4.5758771	–6.6868574
H	–8.4859513	–0.7571888	–8.0843082
H	–8.7658509	–3.2269721	–7.8892118
C	–2.9517979	–0.3911998	0.0961248
C	–3.5724741	–1.1989443	2.7185229
C	–2.1297483	–1.3033715	0.7755214
C	–4.0946664	0.1033248	0.7452734
C	–4.4021399	–0.2963884	2.0471505
C	–2.4369531	–1.7027434	2.0779686
H	–1.2481574	–1.7008661	0.2706519
H	–4.7398679	0.8027615	0.2115527
H	–5.2909962	0.1007907	2.5396482
H	–1.7899731	–2.4153016	2.5916968
H	–3.8117412	–1.5114381	3.7357798
C	0.8889542	1.0651680	–5.3955019
C	2.2342738	1.3635852	–5.8358192
O	2.6137769	2.4812553	–6.2024154
O	3.0912422	0.2935455	–5.8138178
C	0.3621594	–0.1670424	–4.9837844
O	1.1737738	–1.2491041	–4.9637533
O	–0.8483190	–0.3394440	–4.6416091
C	4.4281409	0.5986581	–6.2434386
H	4.9766329	–0.3470107	–6.1691605
H	4.8888557	1.3608055	–5.5984283
H	4.4389292	0.9679589	–7.2791455
C	0.5546818	–2.4766542	–4.5333069
H	1.3579330	–3.2206140	–4.5627692
H	–0.2620180	–2.7664952	–5.2090990
H	0.1544083	–2.3823007	–3.5141585
C	–3.4668255	2.9406041	–4.3170463
C	–4.8309182	2.3505929	–4.5540213
O	–5.3196089	2.2463748	–5.6752435
O	–5.5056654	1.9513744	–3.4471848
C	–6.8307956	1.4436780	–3.7015425
H	–6.8048746	0.6081175	–4.4126671
H	–7.4748112	2.2366729	–4.1076948
H	–7.1980738	1.1031029	–2.7282745
C	–3.0969442	3.8627788	–5.4930928
H	–3.1799286	3.2879998	–6.4234111
H	–2.0698899	4.2024025	–5.3713645
C	–4.0535421	5.0020165	–5.4961113
C	–3.0991183	3.5702350	–3.0081118
O	–2.2637519	4.4629148	–2.9055940
O	–3.7217709	3.0524530	–1.9174026
C	–3.2835795	3.6113717	–0.6632991
H	–3.4915196	4.6893568	–0.6234530
H	–3.8507141	3.0773415	0.1060110
H	–2.2076292	3.4452986	–0.5186854
H	–5.0826609	4.7530765	–5.7664751
C	–3.7796200	6.3471231	–5.1614560
C	–3.3119179	9.0798252	–4.5705156
C	–4.8273701	7.3155428	–5.2350629
C	–2.4885456	6.8075858	–4.7663054
C	–2.2681430	8.1467800	–4.4795620
C	–4.5944505	8.6517943	–4.9493340
H	–5.8254244	6.9845376	–5.5301509
H	–1.6839004	6.0859297	–4.6511255
H	–1.2739474	8.4737495	–4.1705701
H	–5.4111257	9.3723591	–5.0165296
H	–3.1303094	10.1308166	–4.3421861

[Co(TPP)] Enolate (I^{E})(Q):

92 atoms

C	1.9827381	4.1400441	–5.2362757
C	1.5409645	3.8603443	–6.5243294
C	1.4119561	2.4700101	–6.6519545
C	2.1325654	2.9263703	–4.5504310
N	1.7913237	1.8490079	–5.4233518
C	2.4442216	2.7728304	–3.1795219
C	1.7627143	1.8586313	–2.3520596
N	0.5811261	1.2162721	–2.6930831
C	0.1142597	0.6182369	–1.5416361
C	2.0714361	1.5991321	–0.9650835
C	1.0466067	0.8503801	–0.4598162
C	–1.1022976	–0.0895519	–1.3937110
C	–1.9529709	–0.4671823	–2.4448618
N	–1.6864487	–0.2593348	–3.7752001
C	–3.6024960	–1.5250532	–3.5802040
C	–3.1704591	–1.2478948	–2.3150453
C	–1.6707919	–0.5209478	–6.7635739
N	–0.6985722	0.4000834	–6.4346926
C	–0.0388941	0.7147852	–7.6138776
C	–0.5742889	–0.0799545	–8.6945787
C	–1.5923729	–0.8283282	–8.1753478
C	0.8735854	1.7780526	–7.7615309
C	–2.6385695	–1.0725448	–5.8903245
C	–2.6533741	–0.9157375	–4.4950046
H	2.1119879	5.1159552	–4.7791989
H	1.2500806	4.5703291	–7.2920283
H	2.9648623	1.9360087	–0.4495659
H	0.9325158	0.4800268	0.5538897
H	–4.4678426	–2.1099725	–3.8760457
H	–3.6137693	–1.5617687	–1.3751311
H	–0.2082474	–0.0743896	–9.7160751
H	–2.2317370	–1.5320205	–8.6985274
Co	–0.0591126	0.5840551	–4.5149229
C	3.4062562	3.7453044	–2.6260185
C	5.2785624	5.6138178	–1.6582698
C	4.5762266	4.0385450	–3.3594209
C	3.1809576	4.4287092	–1.4137461
C	4.1106279	5.3505244	–0.9346781
C	5.5033655	4.9595183	–2.8737088
H	4.7454326	3.5289852	–4.3104845
H	2.2535598	4.2545528	–0.8675858
H	3.9155043	5.8788811	–0.0001564
H	6.4082625	5.1659653	–3.4471933
H	6.0045025	6.3356235	–1.2810295
C	1.1894184	2.3445593	–9.0870854
C	1.8709304	3.4673407	–11.5786409
C	0.2071889	2.5503332	–10.0770159
C	2.5167952	2.7395055	–9.3601502
C	2.8509839	3.2891321	–10.5970268
C	0.5471450	3.1030123	–11.3109057
H	–0.8317445	2.3035123	–9.8569621
H	3.2780268	2.6032899	–8.5889631
H	3.8839398	3.5783004	–10.7962504
H	–0.2274212	3.2659320	–12.0619249
H	2.1343184	3.8997343	–12.5450658
C	–3.7102529	–1.9246072	–6.4891141
C	–5.7387835	–3.5335580	–7.5893672
C	–5.0180925	–1.4342245	–6.6204340
C	–3.4329115	–3.2336031	–6.9125889
C	–4.4390835	–4.0316295	–7.4613041
C	–6.0259202	–2.2332374	–7.1657301
H	–5.2382119	–0.4178622	–6.2903218
H	–2.4189452	–3.6214876	–6.8035472
H	–4.2081690	–5.0481332	–7.7835830
H	–7.0377177	–1.8366629	–7.2630031
H	–6.5252700	–4.1573778	–8.0161976
C	–1.4994148	–0.5078691	–0.0151120
C	–2.2701158	–1.3067268	2.5694720
C	–0.8750329	–1.5974227	0.6113348
C	–2.5175214	0.1732900	0.6685015
C	–2.9012636	–0.2237145	1.9517580
C	–1.2556738	–1.9927054	1.8956037
H	–0.0889029	–2.1347194	0.0786889
H	–3.0068184	1.0193111	0.1834684
H	–3.6934345	0.3173583	2.4714666
H	–0.7625277	–2.8433167	2.3685414
H	–2.5687933	–1.6163972	3.5718704
C	2.7844293	0.7606139	–5.5273766
C	4.0616589	1.1868757	–6.0594993
O	4.3131240	2.3507453	–6.3979466
O	5.0030396	0.2005437	–6.1708291
C	2.4115548	–0.5319835	–5.1164931
O	3.3299559	–1.5194063	–5.2146169
O	1.2640883	–0.8449491	–4.6546543
C	6.2640729	0.6420345	–6.7014816
H	6.8944606	–0.2537829	–6.7250839
H	6.7163817	1.4129208	–6.0611025
H	6.1462054	1.0551000	–7.7136428
C	2.8929926	–2.8217120	–4.7810518
H	3.7602597	–3.4726441	–4.9353057
H	2.0391004	–3.1723095	–5.3772413
H	2.6049941	–2.8107040	–3.7206933

[Co(TPP)] *Mono*-Enolate *Mono*-Iodonium Ylide (I^{E-IY}) (Q):

119 atoms

C	2.5176294	4.7878448	–5.4076331
C	1.9942392	4.6368341	–6.6579438
C	1.2618643	3.3839477	–6.6621648
C	2.1021692	3.6322308	–4.6311252
N	1.3503995	2.8038404	–5.4227381
C	2.3869871	3.3891417	–3.2766367
C	1.8948609	2.2927952	–2.5278196
N	0.8886200	1.4197182	–2.9036845
C	0.6691234	0.5767891	–1.8178397
C	2.3630893	1.9446850	–1.2083172
C	1.6109527	0.8854150	–0.7743860
C	–0.4495696	–0.2740623	–1.6889428
C	–1.2688455	–0.6186810	–2.7837274
N	–0.7845012	–0.8303702	–4.1097433
C	–3.0905391	–0.9022801	–4.0951979
C	–2.6726253	–0.6687684	–2.7939697
C	–1.1283805	–0.2620053	–7.1243359
N	–0.4130031	0.8345307	–6.6622784
C	–0.0356373	1.5566708	–7.7729581
C	–0.4700699	0.8695890	–8.9681878
C	–1.1095022	–0.2707634	–8.5683930
C	0.6176182	2.8135401	–7.7684925
C	–1.9561343	–1.0706015	–6.3209508
C	–1.9525728	–0.9934864	–4.9102819
H	3.1175584	5.6113191	–5.0351781
H	2.0825780	5.3104761	–7.5035867
H	3.1799054	2.4352903	–0.6886697
H	1.7010087	0.3446842	0.1624840
H	–4.1065779	–0.8876567	–4.4735313
H	–3.2960771	–0.4468857	–1.9339899
H	–0.3019362	1.2122912	–9.9836194
H	–1.5388213	–1.0449848	–9.1955353
Co	0.4922024	1.1114860	–4.8825511
C	3.2183132	4.3870388	–2.5520240
C	4.7402674	6.3163439	–1.1785089
C	4.5395166	4.6646964	–2.9390746
C	2.6730481	5.0891317	–1.4629358
C	3.4264017	6.0472103	–0.7833072
C	5.2945617	5.6207881	–2.2569202
H	4.9719665	4.1158212	–3.7767334
H	1.6419005	4.8844526	–1.1714205
H	2.9845367	6.5897370	0.0538946
H	6.3219519	5.8193926	–2.5656252
H	5.3304543	7.0642141	–0.6472810
C	0.5521319	3.6395718	–9.0085972
C	0.3535273	5.2571536	–11.2939932
C	–0.2796294	4.7728761	–9.0037338
C	1.2907495	3.3330498	–10.1604900
C	1.1898864	4.1371342	–11.2985262
C	–0.3757944	5.5738049	–10.1438434
H	–0.8338503	5.0139874	–8.0935962
H	1.9536609	2.4662210	–10.1551482
H	1.7728212	3.8924543	–12.1878715
H	–1.0239218	6.4515582	–10.1308437
H	0.2765788	5.8852918	–12.1827397

C	–3.0287636	–1.9010366	–6.9029997
C	–5.0834032	–3.5428245	–7.9103936
C	–3.8637974	–1.4512773	–7.9448616
C	–3.2653541	–3.1788854	–6.3527016
C	–4.2784476	–3.9917992	–6.8590056
C	–4.8779739	–2.2665160	–8.4446828
H	–3.7358490	–0.4412291	–8.3337881
H	–2.6417619	–3.5206710	–5.5239239
H	–4.4403375	–4.9815374	–6.4296385
H	–5.5237078	–1.8974613	–9.2429004
H	–5.8779986	–4.1787359	–8.3034417
C	–0.9516624	–0.6687240	–0.3590284
C	–2.0192927	–1.4498910	2.1273596
C	–1.4587794	–1.9716817	–0.1719238
C	–1.0073858	0.2386607	0.7185661
C	–1.5348291	–0.1497070	1.9496016
C	–1.9815885	–2.3558059	1.0622363
H	–1.4317367	–2.6714413	–1.0102452
H	–0.6508462	1.2597066	0.5742899
H	–1.5788596	0.5677130	2.7705568
H	–2.3603940	–3.3702672	1.1944774
H	–2.4310491	–1.7530301	3.0910059
C	0.2605851	–1.8604330	–4.2604139
C	–0.1627588	–3.1826358	–3.8468811
O	–1.2903074	–3.4384897	–3.4062163
O	0.7848526	–4.1618090	–3.9752084
C	1.5148400	–1.4764485	–4.7665801
O	2.4624914	–2.4303644	–4.9079151
O	1.8290185	–0.2867879	–5.1066720
C	0.3478805	–5.4668108	–3.5603718
H	0.0595309	–5.4705817	–2.4993278
H	1.2093296	–6.1234976	–3.7250312
H	–0.5122008	–5.8056845	–4.1556993
C	3.7289332	–1.9795745	–5.4261688
H	4.1825973	–1.2275630	–4.7658084
H	3.6156968	–1.5483117	–6.4304234
H	4.3509284	–2.8802802	–5.4645071
C	–1.7373889	3.8265742	–4.3902539
C	–2.5155577	3.0424502	–5.3381888
O	–3.2204687	2.0764475	–5.0437430
O	–2.3949359	3.4956742	–6.6187469
C	–1.0213574	5.0608789	–4.6191516
O	–0.9734037	5.6636994	–5.6847456
O	–0.3794995	5.5311696	–3.4865400
C	0.2882410	6.7937785	–3.6607524
H	0.9331582	6.7725666	–4.5481609
H	0.8891803	6.9347280	–2.7558830
H	–0.4444140	7.6067021	–3.7707279
C	–3.1605132	2.7571266	–7.5894517
H	–2.8477145	3.1559050	–8.5604831
H	–4.2381648	2.9087081	–7.4327493
H	–2.9374596	1.6849017	–7.5259213
I	–1.7326570	2.9903270	–2.5113502
C	–3.6324146	3.6736081	–1.7391537
C	–6.0784218	4.5021140	–0.7621395
C	–4.0687004	3.1671135	–0.5166640
C	–4.3791838	4.5692642	–2.4923216
C	–5.6165563	4.9850880	–1.9902598
C	–5.3078766	3.5954219	–0.0283430
H	–3.4714934	2.4476271	0.0482639
H	–4.0034615	4.9244884	–3.4548757
H	–6.2208255	5.6867771	–2.5669890
H	–5.6705460	3.2112285	0.9261310
H	–7.0452552	4.8288420	–0.3778878

[Co(TPP)] *Mono* Iodonium Ylide Carbonyl Adduct ($I^{IY(C=O)}$):

104 atoms

C	2.9783807	4.4639058	–3.5003447
C	2.4572291	4.6130530	–4.7521134
C	1.1949326	3.9127340	–4.7696985
C	2.0036837	3.7359267	–2.7250410
N	0.9303137	3.3776572	–3.5230997
C	2.0703352	3.5383866	–1.3454613
C	0.9695397	3.0851774	–0.6094734
N	–0.1885583	2.5521919	–1.1386620
C	–1.0351385	2.3436736	–0.0613089
C	0.8403102	3.2419549	0.8182458
C	–0.4162587	2.8234132	1.1522684
C	–2.2439031	1.6425823	–0.1157771
C	–2.6899557	1.0177243	–1.2872759
N	–2.0910753	1.1210260	–2.5296792
C	–3.6476932	–0.5951540	–2.5465545
C	–3.6888242	–0.0228633	–1.3049538
C	–1.7287576	0.9219051	–5.4265792
N	–0.9623968	1.9428463	–4.9004791
C	–0.5443767	2.6982818	–5.9835226
C	–1.1245372	2.1787927	–7.1993866
C	–1.8071291	1.0460704	–6.8609594
C	0.4492293	3.6799234	–5.9318699
C	–2.4468013	–0.0222246	–4.6865316
C	–2.6850414	0.1501007	–3.3193993
H	3.9263855	4.8303225	–3.1207904
H	2.8973067	5.1148850	–5.6076792
H	1.6030953	3.6648327	1.4642416
H	–0.8841105	2.8234964	2.1309593
H	–4.2315850	–1.4307857	–2.9172056
H	–4.3022944	–0.3086585	–0.4567429
H	–1.0012730	2.6162517	–8.1842587
H	–2.3650965	0.3761628	–7.5071529
Co	–0.5307981	2.1895093	–3.0212718
C	3.3075369	3.8960643	–0.5984779
C	5.6314139	4.5034681	0.8658431
C	4.0768563	2.8729313	–0.0212821
C	3.7171647	5.2277097	–0.4308125
C	4.8714226	5.5290263	0.2959528
C	5.2307577	3.1738671	0.7047063
H	3.7618640	1.8372999	–0.1562648
H	3.1149483	6.0264721	–0.8660922
H	5.1743842	6.5694494	0.4233761
H	5.8216202	2.3666397	1.1408329
H	6.5323299	4.7401945	1.4335823
C	0.8394477	4.4074064	–7.1712628
C	1.6110854	5.8181367	–9.4820377
C	0.6449450	5.7949762	–7.2617354
C	1.4360612	3.7392881	–8.2528258
C	1.8175211	4.4381357	–9.3996365
C	1.0251577	6.4947240	–8.4087442
H	0.1894897	6.3200966	–6.4209371
H	1.6089891	2.6645486	–8.1810415
H	2.2848003	3.9041720	–10.2284393
H	0.8609420	7.5718436	–8.4647552
H	1.9092468	6.3644556	–10.3778756
C	–2.9908333	–1.2087026	–5.3984597
C	–3.9212086	–3.4986421	–6.7366643
C	–4.3669621	–1.4201523	–5.5752587
C	–2.0838785	–2.1507627	–5.9132707
C	–2.5487930	–3.2902676	–6.5718143
C	–4.8288191	–2.5579836	–6.2408225
H	–5.0726748	–0.6782749	–5.1984091
H	–1.0136964	–1.9919120	–5.7748612
H	–1.8327703	–4.0191068	–6.9546519
H	–5.9009716	–2.7073979	–6.3773454
H	–4.2835753	–4.3890359	–7.2525046
C	–3.0118279	1.4067067	1.1374183
C	–4.4931235	0.9058352	3.4785910
C	–2.4713934	0.6301232	2.1761112
C	–4.3086969	1.9224087	1.2877655
C	–5.0428510	1.6758023	2.4499319
C	–3.2046398	0.3821321	3.3377076
H	–1.4680914	0.2154809	2.0612419
H	–4.7355362	2.5209792	0.4818563
H	–6.0472908	2.0889670	2.5529653
H	–2.7714229	–0.2279840	4.1316825
H	–5.0672627	0.7121463	4.3855435
C	0.2742942	–1.9408544	–3.0105745
C	0.7387900	–0.7033085	–3.5804949
O	0.8096169	0.3650948	–2.9411352
O	1.1174650	–0.8120623	–4.8785710
C	0.3785542	–3.3307984	–3.4242311
O	0.1594255	–4.3069309	–2.7076176
O	0.7510429	–3.4633602	–4.7350115
I	–0.5223021	–1.7014020	–1.1312675
C	0.8340850	–4.8274583	–5.1916681
H	–0.1421224	–5.3254364	–5.1073959
H	1.5710116	–5.3959368	–4.6075015
H	1.1440170	–4.7586839	–6.2401745
C	1.7432743	0.3367595	–5.4929019
H	1.7944058	1.1789587	–4.7945802
H	1.1367931	0.6105573	–6.3648158
H	2.7487433	0.0313702	–5.8113277
C	1.2393600	–1.4684616	0.0692711
C	3.5339141	–1.1017902	1.5539886
C	2.1724981	–2.5031562	0.1134006
C	1.4176422	–0.2564524	0.7301691
C	2.5792501	–0.0835896	1.4897232
C	3.3343994	–2.3038242	0.8653330
H	2.0021542	–3.4319076	–0.4322057
H	0.6896496	0.5489291	0.6467230
H	2.7361063	0.8634507	2.0075952
H	4.0826512	–3.0959752	0.9149511
H	4.4424781	–0.9580979	2.1400521

[Co(TPP)] *Mono* Iodonium Ylide Methoxy Adduct ($I^{IY(C-OMe)}$):

104 atoms

C	1.6801926	5.3008626	–4.2229055
C	1.5820179	4.9341440	–5.5316779
C	0.7551042	3.7539821	–5.5764030
C	0.9698799	4.3081507	–3.4541234
N	0.4123968	3.3579214	–4.2924994
C	0.9881876	4.2590003	–2.0580954
C	0.5770462	3.1289424	–1.3479249
N	0.0209328	1.9894118	–1.9061168
C	–0.0218982	1.0606839	–0.8762678
C	0.8314674	2.9253330	0.0571551
C	0.5121873	1.6297043	0.3347162
C	–0.5593508	–0.2213695	–0.9671600
C	–1.3004118	–0.6352694	–2.0751367
N	–1.4541521	0.0712354	–3.2562801
C	–2.7921306	–1.8238302	–3.2758381
C	–2.1135776	–1.8214166	–2.0886782
C	–2.0914485	0.5975779	–6.0861084
N	–1.1132778	1.4657213	–5.6214419
C	–0.6835921	2.1609914	–6.7342487
C	–1.4275814	1.7560146	–7.9004133
C	–2.3176008	0.8073682	–7.4943083
C	0.2805568	3.1705231	–6.7500363
C	–2.7084896	–0.4018517	–5.3368785
C	–2.3600448	–0.6580444	–4.0082374
H	2.2160119	6.1433276	–3.7982412
H	2.0154029	5.4203460	–6.3989485
H	1.2310756	3.6757259	0.7307099
H	0.6003992	1.1035393	1.2790865
H	–3.5142290	–2.5487769	–3.6372017
H	–2.1720548	–2.5378201	–1.2759787
H	–1.2950937	2.1767869	–8.8916909
H	–3.0584592	0.2821255	–8.0874198
Co	–0.4858194	1.6919130	–3.7823989
C	1.5774416	5.4157809	–1.3250299
C	2.6877769	7.6284465	0.0141688
C	2.8229165	5.3141327	–0.6850253
C	0.9005456	6.6448533	–1.2909350
C	1.4500982	7.7424324	–0.6247648
C	3.3737646	6.4110775	–0.0194632
H	3.3604179	4.3653572	–0.7214054
H	–0.0638373	6.7311321	–1.7938097
H	0.9082769	8.6890154	–0.6033205
H	4.3448173	6.3159058	0.4687945
H	3.1175166	8.4858277	0.5337459
C	0.7598579	3.6545512	–8.0734989
C	1.6631452	4.4973894	–10.5986073
C	0.4727408	4.9475776	–8.5383337
C	1.4994878	2.7833802	–8.8917726
C	1.9496244	3.2065327	–10.1441496
C	0.9212860	5.3662786	–9.7930665
H	–0.1176524	5.6184222	–7.9123102
H	1.7168657	1.7795969	–8.5224580
H	2.5313062	2.5249458	–10.7672820
H	0.6840016	6.3715326	–10.1451458
H	2.0143117	4.8250022	–11.5783132
C	–3.6761797	–1.3202800	–6.0002186
C	–5.4795799	–3.1024663	–7.2180647
C	–5.0300627	–1.3277394	–5.6321499
C	–3.2356122	–2.2189683	–6.9861512
C	–4.1317156	–3.1036617	–7.5896578
C	–5.9262147	–2.2113450	–6.2381887
H	–5.3743518	–0.6317059	–4.8658715
H	–2.1801516	–2.2162855	–7.2638011
H	–3.7750019	–3.7993420	–8.3511040
H	–6.9773413	–2.2010886	–5.9464247
H	–6.1798221	–3.7925508	–7.6909140
C	–0.3879959	–1.1832994	0.1571001
C	–0.0486726	–3.0576944	2.2211043
C	0.4662065	–2.2844776	–0.0178211
C	–1.0720258	–1.0337435	1.3726084
C	–0.9027732	–1.9656033	2.3994109
C	0.6346437	–3.2136179	1.0112659
H	0.9994687	–2.3881127	–0.9644256
H	–1.7448450	–0.1848606	1.5032611
H	–1.4441300	–1.8413299	3.3384784
H	1.3075029	–4.0609639	0.8684192
H	0.0835486	–3.7851739	3.0232842
O	1.6565033	0.5024876	–4.1255163
C	1.4969831	–0.8633324	–4.0202207
C	2.6587831	1.0623475	–3.2380112
H	3.6416054	0.6416478	–3.4883623
H	2.4149890	0.8500288	–2.1910217
H	2.6337046	2.1382366	–3.4306306
O	1.8833423	–1.4896488	–3.0377179
C	0.8249470	–1.4171969	–5.1799261
C	0.8904052	–0.9305972	–6.5397323
O	1.5502080	0.0315817	–6.9111095
O	0.1699559	–1.7070070	–7.4277403
C	0.3036470	–1.3101786	–8.8062106
H	–0.3275511	–2.0054704	–9.3705180
H	1.3499610	–1.3902197	–9.1330266
H	–0.0439115	–0.2786394	–8.9456018
I	–0.0657849	–3.2223018	–4.7891099
C	1.5469800	–4.5880393	–5.2961989
C	3.6283811	–6.2835562	–5.9351978
C	2.8041646	–4.0411869	–5.5129134
C	1.2891653	–5.9530342	–5.3863470
C	2.3514330	–6.8048564	–5.7099469
C	3.8532983	–4.9072697	–5.8377673
H	2.9595635	–2.9633613	–5.4298404
H	0.2906215	–6.3592061	–5.2161246
H	2.1731531	–7.8781614	–5.7888127
H	4.8500275	–4.4990003	–6.0101782
H	4.4511737	–6.9528807	–6.1883819

[Co(TPP)] *Mono* Iodonium Ylide Iodine Adduct ($I^{Y(IPh)}$):

104 atoms

C	1.6175899	4.0666716	–4.5489637
C	1.0120685	3.9448954	–5.7634677
C	–0.1663778	3.1370618	–5.5700588
C	0.7725470	3.3986257	–3.5925648
N	–0.3080437	2.8104165	–4.2343259
C	0.9691414	3.4262836	–2.2117885
C	0.0099182	2.9436317	–1.3160694
N	–1.0936082	2.1766535	–1.6497890
C	–1.7724229	1.9648310	–0.4573851
C	–0.0061533	3.2572379	0.0885245
C	–1.1321628	2.6908434	0.6107271
C	–2.8197742	1.0590281	–0.2804656
C	–3.2639457	0.2227345	–1.3106590
N	–2.8919900	0.3044838	–2.6435692
C	–4.2203801	–1.5643122	–2.3028313
C	–4.0990908	–0.9310161	–1.0990763
C	–2.9421960	–0.0967497	–5.5506632
N	–2.1542257	0.9928293	–5.2281330
C	–1.8637974	1.6081561	–6.4334216
C	–2.5504186	0.9407624	–7.5117238
C	–3.1880204	–0.1339088	–6.9713311
C	–0.9394440	2.6357649	–6.6178687
C	–3.5057481	–1.0018056	–4.6471944
C	–3.5083152	–0.7703870	–3.2697051
H	2.5495747	4.5668783	–4.3105497
H	1.3463337	4.3312316	–6.7203861
H	0.7359295	3.8695179	0.5904368
H	–1.4953906	2.7412642	1.6315186
H	–4.7526963	–2.4829403	–2.5240475
H	–4.5111357	–1.2273840	–0.1400243
H	–2.5303727	1.2567698	–8.5489609
H	–3.8057141	–0.8717582	–7.4721133
Co	–1.5644661	1.5245153	–3.4454992
C	2.2105973	4.0248791	–1.6502181
C	4.5736261	5.0857673	–0.5588007
C	3.1255409	3.1932926	–0.9850573
C	2.4899746	5.3960383	–1.7547082
C	3.6641728	5.9226480	–1.2119082
C	4.3004751	3.7195726	–0.4465550
H	2.9071691	2.1272556	–0.9118940
H	1.7742667	6.0476500	–2.2581098
H	3.8672937	6.9913691	–1.2957646
H	5.0081068	3.0596066	0.0576817
H	5.4922969	5.4975643	–0.1387235
C	–0.6236054	3.0850798	–8.0012280
C	0.0492983	3.9199426	–10.5997603
C	–0.8771218	4.4016669	–8.4142295
C	–0.0232235	2.1914891	–8.9045189
C	0.3105994	2.6073430	–10.1944808
C	–0.5450683	4.8157321	–9.7064677
H	–1.3386183	5.0983500	–7.7127108
H	0.1940020	1.1775906	–8.5650444
H	0.7832868	1.9057047	–10.8837251
H	–0.7533093	5.8407787	–10.0168835
H	0.3101422	4.2444186	–11.6081606
C	–4.1528509	–2.2237738	–5.1942832
C	–5.3087493	–4.5604785	–6.2549844
C	–5.5261807	–2.4751116	–5.0413643
C	–3.3710705	–3.1538570	–5.8986904
C	–3.9428902	–4.3144071	–6.4208950
C	–6.0993084	–3.6349108	–5.5669411
H	–6.1451475	–1.7447965	–4.5182780
H	–2.3047032	–2.9611548	–6.0197219
H	–3.3165678	–5.0302091	–6.9557090
H	–7.1691214	–3.8121183	–5.4460134
H	–5.7575241	–5.4664053	–6.6649615
C	–3.4296967	0.8924785	1.0685717
C	–4.6204154	0.5578858	3.5975337
C	–2.6866762	0.3901645	2.1493419
C	–4.7807324	1.2168512	1.2730135
C	–5.3711007	1.0532201	2.5276794
C	–3.2767001	0.2249803	3.4039541
H	–1.6406697	0.1220039	1.9937494
H	–5.3638772	1.6027508	0.4355418
H	–6.4201174	1.3169502	2.6706171
H	–2.6863236	–0.1711528	4.2316242
H	–5.0813085	0.4294527	4.5778817
C	2.1921438	0.0966069	–3.9431141
I	0.3988647	–0.3315270	–3.0307079
C	2.0401978	0.4472856	–5.3448225
O	1.0227852	0.2384649	–6.0132944
O	3.1511337	1.0326608	–5.8637668
C	3.3966350	0.0830700	–3.1436964
O	4.5269970	0.2943995	–3.5547328
O	3.1502939	–0.2121885	–1.8063238
C	3.0601850	1.3671237	–7.2609063
H	4.0476132	1.7597535	–7.5258819
H	2.2852610	2.1271443	–7.4281285
H	2.8208383	0.4803300	–7.8649478
C	4.3375559	–0.3052303	–0.9985689
H	4.9744557	–1.1364013	–1.3327953
H	3.9824148	–0.4817043	0.0228298
H	4.9210572	0.6247377	–1.0509533
C	–0.1051161	–2.3243762	–3.7248030
C	–0.7262999	–4.8790523	–4.5452833
C	0.5480414	–2.8334291	–4.8401136
C	–1.0701364	–3.0320275	–3.0127955
C	–1.3797530	–4.3269591	–3.4400318
C	0.2282686	–4.1350815	–5.2448321
H	1.2773094	–2.2303042	–5.3808471
H	–1.5870532	–2.5962125	–2.1562866
H	–2.1408304	–4.8978321	–2.9072015
H	0.7258872	–4.5596334	–6.1179737
H	–0.9761327	–5.8885459	–4.8729907

[Co(TPP)] *Mono* Diazo Carbonyl Adduct ($I^{D(C=O)}$):

94 atoms

C	2.6031125	4.9119898	–4.5278654
C	1.9159725	4.8627782	–5.7041733
C	0.7827239	3.9964598	–5.4921194
C	1.8595593	4.1256046	–3.5751534
N	0.7693367	3.5321236	–4.1891507
C	2.1284076	4.0791680	–2.2061557
C	1.2661133	3.4499749	–1.3042179
N	0.2147195	2.6182680	–1.6342640
C	–0.3425675	2.2325736	–0.4269467
C	1.3251078	3.6443361	0.1242017
C	0.3061123	2.9210191	0.6640131
C	–1.2824719	1.2149301	–0.2619905
C	–1.7648677	0.4654451	–1.3399021
N	–1.5370506	0.7348704	–2.6773629
C	–2.6624829	–1.2822646	–2.4520142
C	–2.4727113	–0.7817738	–1.1967343
C	–1.8711007	0.6768144	–5.5915914
N	–1.0982766	1.7610662	–5.2143422
C	–0.9894650	2.5491528	–6.3524246
C	–1.7774838	1.9905979	–7.4215762
C	–2.2879936	0.8104344	–6.9638323
C	–0.1072279	3.6212029	–6.5029955
C	–2.2600599	–0.3791571	–4.7612354
C	–2.1259223	–0.3133283	–3.3729215
H	3.5240947	5.4425169	–4.3118733
H	2.1621407	5.3392188	–6.6474302
H	2.0401163	4.2834195	0.6316507
H	0.0199338	2.8435552	1.7071491
H	–3.1327741	–2.2176332	–2.7350765
H	–2.7604388	–1.2266821	–0.2500834
H	–1.9084411	2.4422679	–8.3989668
H	–2.9274520	0.1066691	–7.4864000
Co	–0.3672147	2.1268309	–3.4301641
C	3.3283336	4.7716302	–1.6619093
C	5.6063233	6.0361281	–0.5963609
C	4.3343138	4.0218089	–1.0299086
C	3.4769321	6.1656876	–1.7432611
C	4.6073614	6.7928423	–1.2154166
C	5.4652472	4.6486330	–0.5037124
H	4.2180683	2.9393960	–0.9600577
H	2.6899835	6.7559216	–2.2147981
H	4.7043814	7.8776186	–1.2811422
H	6.2402427	4.0504953	–0.0219876
H	6.4894371	6.5264828	–0.1842899
C	–0.0271694	4.3320746	–7.8091583
C	0.1488310	5.7106308	–10.2584656
C	–0.3597873	5.6940326	–7.8909740
C	0.4033773	3.6745234	–8.9731166
C	0.4898323	4.3569232	–10.1880083
C	–0.2748954	6.3773961	–9.1055832
H	–0.6885596	6.2117041	–6.9887686
H	0.6790338	2.6206349	–8.9137586
H	0.8316711	3.8315559	–11.0810998
H	–0.5434604	7.4338082	–9.1518318
H	0.2162141	6.2443177	–11.2074572
C	–2.8706961	–1.5766593	–5.3981973
C	–3.9648886	–3.8501330	–6.6475211
C	–4.1982570	–1.9604123	–5.1492541
C	–2.1045958	–2.3438016	–6.2925941
C	–2.6451030	–3.4725639	–6.9098130
C	–4.7402711	–3.0888084	–5.7680858
H	–4.8070542	–1.3567026	–4.4748637
H	–1.0727078	–2.0471048	–6.4867933
H	–2.0314432	–4.0626233	–7.5920760
H	–5.7754994	–3.3699466	–5.5686892
H	–4.3890861	–4.7322358	–7.1290843
C	–1.6755436	0.8010496	1.1119021
C	–2.4184897	–0.0448471	3.6927901
C	–0.7128768	0.3059736	2.0090906
C	–3.0154433	0.8619985	1.5276254
C	–3.3840253	0.4437728	2.8079888
C	–1.0817527	–0.1127564	3.2887720
H	0.3242249	0.2400469	1.6773175
H	–3.7666976	1.2442292	0.8350432
H	–4.4286618	0.5038474	3.1170554
H	–0.3227604	–0.4989721	3.9711379
H	–2.7066369	–0.3712323	4.6930626
C	1.1651948	–0.4777399	–3.9942659
O	1.4570439	0.6435279	–3.6043814
O	1.1132699	–0.8594843	–5.2958507
C	1.3959171	0.1558558	–6.2943528
H	2.3136926	–0.1413887	–6.8170993
H	1.5162184	1.1374828	–5.8238735
H	0.5437051	0.1708532	–6.9846111
C	0.8086951	–1.5852738	–3.1036129
C	0.8515741	–1.5197960	–1.6274731
O	1.2609367	–0.5817987	–0.9779442
O	0.3723382	–2.6829890	–1.1015226
C	0.2754831	–2.7036353	0.3390022
H	1.2459420	–2.4720918	0.7976330
H	–0.0427358	–3.7193872	0.5934661
H	–0.4673983	–1.9691508	0.6770097
N	0.3242144	–2.6855855	–3.6509569
N	–0.1089857	–3.6252119	–4.1129644

[Co(TPP)] *Mono* Diazo Methoxy Adduct ($I^{D(C–OMe)}$):

94 atoms

C	2.5783690	3.7892099	–4.4925602
C	2.0430680	3.6558762	–5.7383499
C	0.7796615	2.9796776	–5.5839893
C	1.6341665	3.2186400	–3.5669949
N	0.5606272	2.6656346	–4.2504402
C	1.7401803	3.3144369	–2.1799473
C	0.7788575	2.7781053	–1.3205843
N	–0.2464178	1.9222861	–1.6918239
C	–0.8500424	1.5405203	–0.5014064
C	0.7531241	3.0055250	0.1013745
C	–0.2667972	2.2548958	0.6060027
C	–1.7773164	0.5054112	–0.3657621
C	–2.2674238	–0.2012062	–1.4673849
N	–2.0595541	0.1359181	–2.7940610
C	–3.4117625	–1.7460077	–2.6451805
C	–3.0891356	–1.3832188	–1.3720401
C	–2.5640645	0.3320936	–5.6812165
N	–1.5315128	1.1825005	–5.3162894
C	–1.2194154	1.8894347	–6.4696122
C	–2.1392453	1.5535114	–7.5261394
C	–2.9568451	0.5743468	–7.0446718
C	–0.0914041	2.6946119	–6.6380332
C	–3.0836811	–0.6845844	–4.8823557
C	–2.8023372	–0.7795496	–3.5224342
H	3.5267426	4.2346709	–4.2129703
H	2.4661787	3.9652139	–6.6878089
H	1.4276510	3.6689762	0.6323792
H	–0.5970804	2.1771462	1.6362910
H	–4.0303479	–2.5740060	–2.9757150
H	–3.3774078	–1.8621587	–0.4423286
H	–2.1383396	2.0020958	–8.5135744
H	–3.7581118	0.0529899	–7.5582319
Co	–0.7931205	1.4432145	–3.5148997
C	2.8970812	4.0400645	–1.5865816
C	5.0813884	5.3970914	–0.4440580
C	3.8328058	3.3528562	–0.7965734
C	3.0716876	5.4178082	–1.7948599
C	4.1550191	6.0914934	–1.2274644
C	4.9174631	4.0253459	–0.2308879
H	3.7056832	2.2809006	–0.6395797
H	2.3436312	5.9575522	–2.4022833
H	4.2729713	7.1633947	–1.3937367
H	5.6401176	3.4749645	0.3735917
H	5.9284235	5.9231300	–0.0014985
C	0.2353711	3.2057102	–7.9968365
C	0.8900014	4.1595728	–10.5631795
C	0.3165919	4.5850032	–8.2490775
C	0.4872036	2.3110840	–9.0515618
C	0.8131734	2.7845339	–10.3233141
C	0.6396270	5.0583079	–9.5222044
H	0.1194690	5.2841590	–7.4350930
H	0.4327929	1.2391765	–8.8558505
H	1.0161522	2.0766090	–11.1285045
H	0.6924225	6.1331185	–9.7025997
H	1.1454054	4.5295814	–11.5571028
C	–3.9698572	–1.7074337	–5.5089288
C	–5.5987243	–3.6580095	–6.7067915
C	–5.3140389	–1.4312192	–5.7980042
C	–3.4489340	–2.9730903	–5.8214826
C	–4.2611880	–3.9419005	–6.4161552
C	–6.1234574	–2.4002446	–6.3960300
H	–5.7204278	–0.4499113	–5.5478010
H	–2.4006830	–3.1763585	–5.5984969
H	–3.8460776	–4.9224889	–6.6548903
H	–7.1681822	–2.1737404	–6.6145533
H	–6.2316755	–4.4154020	–7.1714716
C	–2.2198083	0.0967295	0.9962570
C	–3.0699260	–0.6991507	3.5599432
C	–1.3052189	–0.4276248	1.9246350
C	–3.5680540	0.2132100	1.3727086
C	–3.9896018	–0.1800266	2.6442642
C	–1.7259786	–0.8224852	3.1958109
H	–0.2576982	–0.5281969	1.6364055

H	–4.2835472	0.6188177	0.6559854
H	–5.0398056	–0.0773030	2.9217866
H	–1.0027909	–1.2334970	3.9019197
H	–3.3993602	–1.0077200	4.5530197
O	0.9619370	–0.4938523	–3.4424474
C	1.9632106	–0.1663768	–4.3011242
C	1.3786103	–0.6599155	–2.0613061
H	2.0850896	–1.4973386	–1.9944005
H	0.4555097	–0.8740613	–1.5163746
H	1.8436458	0.2588194	–1.6876848
O	3.0739111	0.2009403	–3.9666315
C	1.5185754	–0.3041781	–5.7018385
C	0.4220523	–1.1440482	–6.2161899
O	–0.2074830	–1.9510334	–5.5625279
O	0.2403404	–0.9259667	–7.5515360
C	–0.7403928	–1.7861703	–8.1775569
H	–0.3978991	–2.8299142	–8.1560816
H	–0.8232197	–1.4253214	–9.2073400
H	–1.7057874	–1.7053170	–7.6647995
N	2.2835562	0.3188650	–6.5805166
N	2.9426336	0.8652447	–7.3207597

[Co(TPP)] ***Mono*** **Diazo Nitrogen Adduct ($I^{D(C=N=N)}$):**

94 atoms

C	2.1978785	3.9860626	–4.8633973
C	1.7244768	3.7629795	–6.1224366
C	0.4811804	3.0495432	–5.9823969
C	1.2439383	3.4154866	–3.9474827
N	0.2167339	2.8019903	–4.6457722
C	1.3230214	3.5278391	–2.5566060
C	0.4161758	2.8897116	–1.7076819
N	–0.5163331	1.9367255	–2.0892869
C	–1.0420230	1.4503072	–0.9018526
C	0.3831256	3.0795805	–0.2801717
C	–0.5177104	2.1889987	0.2181224
C	–1.8993463	0.3548015	–0.7781762
C	–2.4957187	–0.2501169	–1.8879647
N	–2.4306502	0.2212464	–3.1891702
C	–3.8205644	–1.6314549	–3.0788776
C	–3.3318953	–1.4210280	–1.8234401
C	–2.9831504	0.5241559	–6.0768875
N	–1.8770721	1.2807536	–5.7271472
C	–1.5066861	1.9419402	–6.8861028
C	–2.4489295	1.6688813	–7.9425717
C	–3.3634659	0.7926788	–7.4413935
C	–0.3545788	2.7142164	–7.0499769
C	–3.6101976	–0.4233676	–5.2648918
C	–3.2775921	–0.5954098	–3.9192188
H	3.1105605	4.4936362	–4.5708427
H	2.1701178	4.0508598	–7.0685765
H	0.9723393	3.8103424	0.2624033
H	–0.8146757	2.0439141	1.2507825
H	–4.4879059	–2.4168830	–3.4171874
H	–3.5188392	–2.0002287	–0.9258179
H	–2.4099134	2.1061634	–8.9344800
H	–4.2273231	0.3646841	–7.9385924
Co	–1.0753640	1.4699760	–3.9337721
C	2.4090067	4.3427587	–1.9491480
C	4.4775877	5.8716534	–0.7996015
C	3.3086508	3.7635115	–1.0356725
C	2.5582684	5.7037184	–2.2669261
C	3.5828176	6.4614161	–1.6972235
C	4.3358059	4.5207816	–0.4701057
H	3.2079722	2.7079611	–0.7786797
H	1.8535304	6.1660475	–2.9593659
H	3.6778093	7.5184712	–1.9499901
H	5.0297328	4.0483692	0.2264478
H	5.2792289	6.4636109	–0.3558640
C	–0.0055877	3.1997802	–8.4134645
C	0.6562522	4.1156517	–10.9918403
C	0.0344133	4.5749558	–8.6971906
C	0.2905874	2.2909279	–9.4427444
C	0.6207110	2.7448793	–10.7209085
C	0.3609537	5.0293548	–9.9761594
H	–0.2010961	5.2854938	–7.9036299
H	0.2649668	1.2218812	–9.2271576
H	0.8553357	2.0254134	–11.5067690
H	0.3794668	6.1007099	–10.1813409
H	0.9126039	4.4705428	–11.9909407
C	–4.6712691	–1.2848731	–5.8552900
C	–6.6771923	–2.9160462	–6.9691800
C	–5.9907515	–1.2255920	–5.3772311
C	–4.3731457	–2.1746659	–6.9005089
C	–5.3672986	–2.9849618	–7.4518197
C	–6.9860426	–2.0330089	–5.9307099
H	–6.2295697	–0.5325232	–4.5694341
H	–3.3491460	–2.2284359	–7.2724098
H	–5.1168006	–3.6758312	–8.2580922
H	–8.0074349	–1.9683016	–5.5529522
H	–7.4545179	–3.5478889	–7.4009204
C	–2.1751694	–0.1780644	0.5827972
C	–2.6827754	–1.2007636	3.1586916
C	–1.1190743	–0.6099678	1.4059466
C	–3.4879683	–0.2567660	1.0788119
C	–3.7395498	–0.7630788	2.3550435
C	–1.3720212	–1.1208323	2.6800783
H	–0.0938256	–0.5565884	1.0368132
H	–4.3113931	0.0946491	0.4556680
H	–4.7646141	–0.8088149	2.7257961
H	–0.5391490	–1.4620405	3.2963357
H	–2.8799502	–1.5982868	4.1551934
N	0.2708574	–0.0114376	–4.1121285
N	1.0199496	–0.3201164	–3.2980243
C	1.8112515	–0.5519802	–2.2759830
C	3.0895158	0.1880669	–2.2272596
O	3.8526721	0.2212785	–1.2835018
O	3.2862004	0.8295132	–3.4141396
C	1.3499105	–1.5305955	–1.2696929
O	1.8778992	–1.7462564	–0.1977816
O	0.2351083	–2.1644663	–1.7329729
C	4.5198759	1.5713434	–3.5306519
H	4.5510203	2.3887122	–2.7994824
H	4.5109613	1.9730713	–4.5483445
H	5.3810204	0.9076951	–3.3749827
C	–0.3124992	–3.1842663	–0.8692058
H	0.4401003	–3.9585113	–0.6671190
H	–1.1616233	–3.5955701	–1.4236262
H	–0.6521917	–2.7476736	0.0784088

TS1 (I^{IY}-I^{T}):

92 atoms

C	3.1923367	3.5645790	–4.8072929
C	2.6612346	3.5387199	–6.0614667
C	1.4525167	2.7578614	–5.9901787
C	2.2929768	2.8274605	–3.9567863
N	1.2394418	2.3158733	–4.6975705
C	2.4523813	2.6925428	–2.5771199
C	1.4895208	2.0817233	–1.7724088
N	0.3854710	1.3810235	–2.2171189
C	–0.3071772	1.0299920	–1.0669224
C	1.4800656	2.1883555	–0.3351398
C	0.3531602	1.5609184	0.0997974
C	–1.4412035	0.2210749	–1.0100618
C	–2.0197265	–0.3457816	–2.1500743
N	–1.6274177	–0.1100730	–3.4594785
C	–3.2623390	–1.7593615	–3.3907809
C	–3.0437153	–1.3593382	–2.1054147
C	–1.7546951	–0.0420209	–6.3899999
N	–0.7896361	0.8382190	–5.9329294
C	–0.4073943	1.5686484	–7.0460988
C	–1.2007477	1.1922029	–8.1901184
C	–2.0118699	0.1720623	–7.7916358
C	0.6538202	2.4711535	–7.0985467
C	–2.4471739	–0.9748457	–5.6194447
C	–2.4092194	–0.9593967	–4.2279920
H	4.1091302	4.0406480	–4.4771861
H	3.0534099	3.9902358	–6.9664972
H	2.2251438	2.7169613	0.2497383
H	–0.0127023	1.4637011	1.1161953
H	–3.9492725	–2.5168672	–3.7526892
H	–3.5069897	–1.7298743	–1.1972969
H	–1.1342411	1.6542602	–9.1691720
H	–2.7498962	–0.3728190	–8.3712247
Co	–0.0586878	0.9450492	–4.1013839
C	3.6721848	3.2333492	–1.9178314
C	5.9902396	4.1917697	–0.6464065
C	4.5629288	2.3436633	–1.2920548
C	3.9535430	4.6082704	–1.8892316
C	5.1048953	5.0839757	–1.2582686
C	5.7148232	2.8213569	–0.6641080
H	4.3377463	1.2761989	–1.3198248
H	3.2543542	5.3031728	–2.3565603
H	5.3070750	6.1559429	–1.2377801
H	6.4010848	2.1193231	–0.1878970
H	6.8894154	4.5643998	–0.1537274
C	0.9864189	3.1219073	–8.3968323
C	1.6280645	4.3631327	–10.8406057
C	0.8355558	4.5086721	–8.5568326
C	1.4673114	2.3678855	–9.4789286
C	1.7858924	2.9823311	–10.6912946
C	1.1521209	5.1244121	–9.7694380
H	0.4631990	5.0996629	–7.7188779
H	1.5940047	1.2919855	–9.3550903
H	2.1637762	2.3818301	–11.5201625
H	1.0224604	6.2021466	–9.8790008
H	1.8759835	4.8440862	–11.7877692
C	–3.2874898	–1.9846316	–6.3217478
C	–4.8213689	–3.9012133	–7.6857313
C	–4.6866314	–1.8883402	–6.3464287
C	–2.6622256	–3.0516307	–6.9861357
C	–3.4272636	–4.0042895	–7.6626158
C	–5.4495622	–2.8412340	–7.0256321
H	–5.1707921	–1.0552734	–5.8344388
H	–1.5745460	–3.1279097	–6.9419397
H	–2.9322573	–4.8337241	–8.1704129
H	–6.5369751	–2.7528161	–7.0427317
H	–5.4174289	–4.6453258	–8.2160416
C	–2.0093959	–0.1385625	0.3193494
C	–3.0925703	–0.8523095	2.8148357
C	–1.2849971	–0.9504976	1.2068796
C	–3.2850077	0.3076902	0.6977204
C	–3.8221337	–0.0449407	1.9376728
C	–1.8226358	–1.3051708	2.4454483
H	–0.2965465	–1.3052253	0.9101023
H	–3.8515918	0.9367099	0.0094944
H	–4.8125202	0.3148351	2.2205556
H	–1.2502406	–1.9418622	3.1216975
H	–3.5128357	–1.1288707	3.7827371
C	1.2080097	–0.6254119	–4.2509161
I	0.5796661	–2.3491727	–2.4009555
C	0.9948123	–1.4524915	–5.4850409
O	0.3735621	–2.5071177	–5.5472519
O	1.5158875	–0.8542003	–6.5874495
C	2.6317256	–0.3395147	–3.8585884
O	3.1106205	–0.4647302	–2.7389898
O	3.3499317	0.1468926	–4.9035210
C	1.2229947	–1.5205369	–7.8335791
H	0.1443050	–1.4926667	–8.0376953
H	1.5669403	–2.5634428	–7.8090071
H	1.7673347	–0.9522919	–8.5949481
C	4.7116934	0.5149678	–4.5946621
H	5.2757127	–0.3621744	–4.2484434
H	4.7399801	1.2915531	–3.8201348
H	5.1205469	0.9008729	–5.5335545
C	2.1446857	–3.6806854	–2.8707829
C	4.2169044	–5.4017574	–3.5347140
C	1.9260253	–4.6633468	–3.8406105
C	3.3804538	–3.5321182	–2.2346749
C	4.4168574	–4.4053897	–2.5749079
C	2.9760124	–5.5256758	–4.1665738
H	0.9657536	–4.7302455	–4.3484177
H	3.5350020	–2.7323074	–1.5132491
H	5.3867801	–4.2988085	–2.0870819
H	2.8191996	–6.2954557	–4.9234709
H	5.0310364	–6.0795148	–3.7945934

TS2 (I^{T}-I^{G}):

108 atoms

C	4.0968143	0.1153663	–2.7751209
C	3.7597099	–0.2469926	–4.0439512
C	2.7471918	–1.2621553	–3.9351153
C	3.2997062	–0.6882953	–1.8857251
N	2.4426224	–1.5144459	–2.6058392
C	3.4336554	–0.6560912	–0.4991692
C	2.6140214	–1.4003046	0.3450763
N	1.5500540	–2.1950643	–0.0587674
C	1.0321747	–2.7113909	1.1197093
C	2.7855794	–1.4640755	1.7727892
C	1.8105158	–2.2854340	2.2517093
C	–0.1316369	–3.4614186	1.2279714
C	–0.9068698	–3.7974791	0.1238008
N	–0.5528081	–3.6123023	–1.2061895
C	–2.5609784	–4.7744029	–1.0464065
C	–2.1662049	–4.4827882	0.2249571
C	–0.5252108	–4.0019799	–4.1285888
N	0.4888440	–3.1358245	–3.7421178
C	1.1212329	–2.7813937	–4.9235611
C	0.5193180	–3.4508037	–6.0444327
C	–0.5042286	–4.2030593	–5.5537830
C	2.1848821	–1.8946474	–5.0376675
C	–1.5079953	–4.5244730	–3.2945376
C	–1.5455018	–4.2636697	–1.9279453
H	4.8144274	0.8620853	–2.4534641
H	4.1396559	0.1430747	–4.9821244
H	3.5621063	–0.9453849	2.3243112
H	1.6123228	–2.5743849	3.2783361
H	–3.4484961	–5.3073538	–1.3696417
H	–2.6645941	–4.7161120	1.1599590
H	0.8414820	–3.3376974	–7.0738737
H	–1.2070514	–4.8232555	–6.0995671
Co	1.1129833	–2.7933743	–1.9042774
C	4.5449790	0.1408821	0.0902981
C	6.6659645	1.6100943	1.2017934
C	5.8755106	–0.2511420	–0.1305404
C	4.2900074	1.2757071	0.8746036
C	5.3446291	2.0073227	1.4251355
C	6.9283758	0.4785857	0.4238162
H	6.0770396	–1.1369722	–0.7357260
H	3.2569027	1.5820876	1.0452689
H	5.1332748	2.8920963	2.0274084
H	7.9567001	0.1587942	0.2497959
H	7.4892947	2.1809161	1.6333968
C	2.8200624	–1.6828978	–6.3669154
C	4.0885729	–1.3219137	–8.8433277
C	2.1942012	–0.9462264	–7.3820094
C	4.0869406	–2.2424987	–6.6018794
C	4.7146625	–2.0623066	–7.8354802
C	2.8273165	–0.7648446	–8.6143841
H	1.2113281	–0.5104606	–7.1959533
H	4.5541914	–2.8307889	–5.8108738
H	5.6959105	–2.5061203	–8.0109661

H	2.3354521	–0.1834838	–9.3957018
H	4.5818658	–1.1799890	–9.8059998
C	–2.5283668	–5.4382992	–3.8812681
C	–4.4194947	–7.2056685	–4.9760125
C	–3.8651934	–5.0434115	–4.0350751
C	–2.1479723	–6.7269889	–4.2878585
C	–3.0876186	–7.6050029	–4.8314319
C	–4.8051173	–5.9225684	–4.5781849
H	–4.1614503	–4.0393171	–3.7280454
H	–1.1046883	–7.0260811	–4.1752245
H	–2.7790221	–8.6046108	–5.1410867
H	–5.8411989	–5.6016870	–4.6958086
H	–5.1541401	–7.8912161	–5.4004298
C	–0.5570642	–3.9528079	2.5695505
C	–1.3499000	–4.9285567	5.0775242
C	–0.3203662	–5.2924262	2.9143018
C	–1.1888386	–3.1063558	3.4909801
C	–1.5857247	–3.5931851	4.7391331
C	–0.7146274	–5.7752246	4.1639683
H	0.1907759	–5.9333103	2.1940060
H	–1.3697938	–2.0649862	3.2202759
H	–2.0812718	–2.9278935	5.4477509
H	–0.5209543	–6.8163054	4.4268465
H	–1.6586760	–5.3079349	6.0526572
C	2.1722178	–4.4207587	–1.8775558
C	2.9398954	–4.8747862	–3.0512286
O	3.3945183	–4.1832195	–3.9518412
O	3.2204501	–6.2185957	–2.9776656
C	1.5152548	–5.4874697	–1.0563944
O	1.6539750	–5.6547748	0.1463034
O	0.6813621	–6.2608831	–1.8085586
C	4.0732628	–6.7088975	–4.0318571
H	3.5878973	–6.5830493	–5.0099305
H	5.0330749	–6.1748799	–4.0388743
H	4.2238310	–7.7711839	–3.8107334
C	–0.0481241	–7.2648248	–1.0711509
H	–0.7403150	–7.7106187	–1.7930732
H	–0.6082360	–6.8053632	–0.2465025
H	0.6404675	–8.0214665	–0.6702126
C	4.0954972	–4.0153331	–0.6651226
H	3.5369165	–4.3217394	0.2159147
H	4.0141999	–2.9742887	–0.9527934
C	5.1617419	–4.7569333	–1.1158332
H	5.3137881	–5.7590945	–0.7055687
C	6.0815852	–4.3456569	–2.1570001
C	7.8954613	–3.6116617	–4.2048192
C	5.9320798	–3.1308322	–2.8700637
C	7.1679148	–5.1800855	–2.5093555
C	8.0598308	–4.8197730	–3.5172576
C	6.8245597	–2.7710698	–3.8717732
H	5.0821094	–2.4836440	–2.6650098
H	7.2991055	–6.1262665	–1.9794472
H	8.8882874	–5.4834472	–3.7702542
H	6.6726204	–1.8323658	–4.4074490
H	8.5925678	–3.3295119	–4.9949732

TS3 (I^{G}-P):

108 atoms

C	4.0324543	0.3058706	–2.8279273
C	3.7150057	–0.0977790	–4.0882119
C	2.7029513	–1.1134611	–3.9589548
C	3.2257997	–0.4753709	–1.9242843
N	2.3904200	–1.3332361	–2.6279152
C	3.3219599	–0.3830641	–0.5378087
C	2.5314869	–1.1440105	0.3206636
N	1.5353956	–2.0308311	–0.0641547
C	1.0745385	–2.5791468	1.1251178
C	2.7072608	–1.1632205	1.7500738
C	1.8153217	–2.0649748	2.2465909
C	0.0074190	–3.4609525	1.2513335
C	–0.7413621	–3.8887966	0.1598087
N	–0.4349855	–3.6669481	–1.1744406
C	–2.3370076	–4.9930953	–0.9782943
C	–1.9327851	–4.6859276	0.2858945
C	–0.4891080	–3.9631987	–4.1096241
N	0.5013824	–3.0697411	–3.7334911
C	1.0764688	–2.6549328	–4.9267538
C	0.4428712	–3.2990234	–6.0481432
C	–0.5284976	–4.1070360	–5.5422920
C	2.1300972	–1.7552663	–5.0524244
C	–1.3933220	–4.5903334	–3.2562560
C	–1.3942957	–4.3814752	–1.8795321
H	4.7373401	1.0714798	–2.5218840
H	4.1053814	0.2661080	–5.0327253
H	3.4356080	–0.5684462	2.2908899
H	1.6543735	–2.3583716	3.2785005
H	–3.1836117	–5.5980433	–1.2841394
H	–2.3840559	–4.9731027	1.2298206
H	0.7123889	–3.1380392	–7.0864926
H	–1.2320590	–4.7315688	–6.0821663
Co	1.0909794	–2.6328424	–1.8985896
C	4.3503868	0.5203278	0.0519285
C	6.3024624	2.2048402	1.1770434
C	5.7154407	0.2186551	–0.0764525
C	3.9769341	1.6768860	0.7532173
C	4.9459818	2.5140446	1.3107855
C	6.6848401	1.0537470	0.4821146
H	6.0092906	–0.6830036	–0.6164644
H	2.9170731	1.9144431	0.8554325
H	4.6401960	3.4127624	1.8486247
H	7.7414356	0.8019506	0.3787665
H	7.0591840	2.8582269	1.6135219
C	2.7147554	–1.5136338	–6.4018721
C	3.8638347	–1.1059166	–8.9325842
C	2.0388013	–0.7660823	–7.3769290
C	3.9752468	–2.0541733	–6.7053993
C	4.5436023	–1.8517220	–7.9648423
C	2.6107648	–0.5624960	–8.6351894
H	1.0620679	–0.3419597	–7.1387767
H	4.4881843	–2.6377326	–5.9390830
H	5.5211498	–2.2803631	–8.1922160
H	2.0777995	0.0258883	–9.3837393
H	4.3097938	–0.9468201	–9.9155195
C	–2.3558077	–5.5666923	–3.8394490
C	–4.1258291	–7.4592108	–4.9347452
C	–3.7334266	–5.3073355	–3.8921976
C	–1.8753397	–6.7840285	–4.3501544
C	–2.7535981	–7.7238109	–4.8930838
C	–4.6124261	–6.2478786	–4.4350150
H	–4.1098549	–4.3584710	–3.5069520
H	–0.8015185	–6.9766735	–4.3186385
H	–2.3655650	–8.6664585	–5.2825776
H	–5.6810989	–6.0307279	–4.4729731
H	–4.8131446	–8.1928500	–5.3584735
C	–0.3362148	–3.9997451	2.5976417
C	–0.9660343	–5.0750142	5.1130601
C	0.0035850	–5.3263834	2.9065985
C	–0.9910602	–3.2175817	3.5594188
C	–1.3060668	–3.7534268	4.8108261
C	–0.3092894	–5.8585970	4.1591425
H	0.5290724	–5.9173939	2.1543489
H	–1.2554332	–2.1872058	3.3164916
H	–1.8209320	–3.1378360	5.5501172
H	–0.0352522	–6.8886662	4.3929037
H	–1.2113276	–5.4927919	6.0906626
C	2.7204842	–4.4502300	–1.8387184
C	3.1141050	–4.5242700	–3.2739302
O	3.9692094	–3.7942473	–3.7671738
O	2.4771341	–5.4748203	–4.0015185
C	1.9062545	–5.4803551	–1.1287629
O	1.9715508	–5.6488183	0.0867020
O	1.0881075	–6.2136621	–1.9185975
C	2.9133097	–5.5731505	–5.3730268
H	2.8144642	–4.6101510	–5.8883670
H	3.9618649	–5.9003995	–5.4182998
H	2.2526491	–6.3164251	–5.8306577
C	0.2960863	–7.1932325	–1.2153034
H	–0.4013896	–7.5893529	–1.9603000
H	–0.2574437	–6.7291918	–0.3903064
H	0.9397616	–7.9913755	–0.8186919
C	3.7963210	–3.8245063	–0.9406716
H	3.3938665	–3.6537625	0.0600333
H	4.1773873	–2.8966876	–1.3700474
C	4.7215660	–4.9680255	–0.9975396
H	4.4163139	–5.8434066	–0.4194025
C	5.9113914	–5.0759470	–1.7668241
C	8.3090381	–5.3671390	–3.2234922
C	6.4683959	–3.9796567	–2.4805453
C	6.5986666	–6.3213965	–1.8099982
C	7.7784143	–6.4627305	–2.5254211
C	7.6502430	–4.1311597	–3.1945405
H	5.9496395	–3.0237701	–2.4830441
H	6.1788931	–7.1713707	–1.2681947
H	8.2911904	–7.4252054	–2.5487506
H	8.0631353	–3.2818944	–3.7404518
H	9.2349120	–5.4789712	–3.7896642

TS4 (I^{IY-T}-I^{T-T}):

119 atoms

C	2.6308371	3.6477998	–5.2666107
C	2.1167653	3.6851866	–6.5310772
C	0.9737522	2.8048212	–6.5447990
C	1.7638706	2.8014915	–4.4834289
N	0.7554707	2.3092730	–5.2801274
C	1.8719239	2.6397450	–3.0992056
C	0.8504788	2.0828230	–2.3267262
N	–0.3069965	1.5186252	–2.8139045
C	–1.0770461	1.1921954	–1.7257265
C	0.8140947	2.0905884	–0.8846878
C	–0.3946318	1.5795723	–0.5148530
C	–2.2589166	0.4401562	–1.7409327
C	–2.6790519	–0.2542820	–2.8802055
N	–2.0864216	–0.1750006	–4.1243412
C	–3.7149056	–1.8021678	–4.1561219
C	–3.7359352	–1.2359838	–2.9139587
C	–1.6537289	–0.5151185	–7.0476666
N	–1.0265272	0.6259612	–6.5881254
C	–0.5469852	1.2896778	–7.7000472
C	–0.9080848	0.5604714	–8.8891894
C	–1.5432380	–0.5796576	–8.4828817
C	0.2938152	2.4052335	–7.6953149
C	–2.4184173	–1.3801042	–6.2609108
C	–2.6891700	–1.1270862	–4.9113161
H	3.4971529	4.1714397	–4.8759859
H	2.4873975	4.2320501	–7.3916319
H	1.6128321	2.4535202	–0.2469587
H	–0.7837217	1.4298748	0.4867014
H	–4.3491839	–2.5906671	–4.5475822
H	–4.3963755	–1.4671876	–2.0854091
H	–0.6502092	0.8667641	–9.8977328
H	–1.9217317	–1.3897679	–9.0968040
Co	–0.6965606	1.1007637	–4.7099014
C	3.0892633	3.1729856	–2.4288807
C	5.4144425	4.1742141	–1.2071516
C	4.3282868	2.5449471	–2.6315507
C	3.0297891	4.3127884	–1.6115751
C	4.1853084	4.8088152	–1.0040520
C	5.4831298	3.0414336	–2.0232907
H	4.3715686	1.6576972	–3.2653975
H	2.0695006	4.8106559	–1.4697326
H	4.1265268	5.6987163	–0.3752843
H	6.4386393	2.5395924	–2.1839909
H	6.3165164	4.5626252	–0.7320533
C	0.5667448	3.0915321	–8.9870027
C	1.0345892	4.4001196	–11.4290227
C	–0.4128266	3.9266380	–9.5463033
C	1.7804588	2.9119120	–9.6683990
C	2.0123381	3.5635246	–10.8818173
C	–0.1793675	4.5788021	–10.7594856
H	–1.3570356	4.0604640	–9.0151140
H	2.5303821	2.2455608	–9.2397446
H	2.9574415	3.4118350	–11.4056575
H	–0.9477666	5.2278575	–11.1827951
H	1.2167823	4.9075640	–12.3774972
C	–3.0053024	–2.6045558	–6.8672059
C	–4.0818007	–4.9614918	–7.9516917
C	–4.0060188	–2.5432063	–7.8493274
C	–2.5518178	–3.8602069	–6.4288026
C	–3.0870989	–5.0301100	–6.9713099
C	–4.5411049	–3.7153450	–8.3885651
H	–4.3682347	–1.5673901	–8.1775929
H	–1.7675733	–3.8956414	–5.6703632
H	–2.7215487	–6.0000006	–6.6300599
H	–5.3228949	–3.6556320	–9.1476181
H	–4.4992341	–5.8768992	–8.3740153
C	–3.0332359	0.3361949	–0.4756581
C	–4.4972277	0.2188959	1.9262557
C	–3.2188476	–0.8861666	0.1910150
C	–3.5820005	1.5032909	0.0862790
C	–4.3101121	1.4421553	1.2760594
C	–3.9463895	–0.9447164	1.3812686
H	–2.7737434	–1.7910405	–0.2241016
H	–3.4374572	2.4512242	–0.4340657
H	–4.7345926	2.3556456	1.6957114
H	–4.0749546	–1.9014400	1.8900828
H	–5.0644991	0.1725684	2.8570354
C	–2.0181713	2.6676418	–4.6730870
C	0.6105546	–0.3453734	–4.6249147
C	–3.2056788	2.6773340	–3.7608808
O	–3.2530241	3.3471802	–2.7388233
O	–4.1954074	1.8410212	–4.1416520
C	–1.3727654	4.0080330	–4.7571849
O	–0.7821857	4.4624169	–3.7929480
O	–1.4437300	4.6321321	–5.9576654
C	–5.3538787	1.8356090	–3.2802168
H	–5.0798063	1.4978151	–2.2723630
H	–6.0489805	1.1322154	–3.7473911
H	–5.7925195	2.8417635	–3.2295891
C	–0.6542737	5.8437232	–6.0541414
H	–1.0484455	6.6147914	–5.3787186
H	–0.7396838	6.1551161	–7.0999974
H	0.3918852	5.6310286	–5.7995034
C	1.8106523	–0.4310029	–5.4609335
O	1.9655991	–0.0018248	–6.5958157
O	2.8214306	–1.0819573	–4.7836448
C	0.3167909	–1.5370676	–3.8090510
O	0.0408490	–2.6243497	–4.3043538
O	0.3226935	–1.3086206	–2.4749315
C	4.0422851	–1.2319984	–5.5320354
H	4.7377685	–1.7464436	–4.8599892
H	4.4405098	–0.2499780	–5.8265258
H	3.8707243	–1.8267007	–6.4404908
C	–0.1496253	–2.4036243	–1.6638241
H	0.5168404	–3.2726136	–1.7514607
H	–1.1628862	–2.6933312	–1.9778661
H	–0.1567720	–2.0185131	–0.6387723
I	–3.4916915	2.4873510	–7.1355794
C	–5.1511746	3.5413235	–6.3588808
C	–7.3009702	4.8532487	–5.1772588
C	–4.9365236	4.7620583	–5.7133732
C	–6.4233337	2.9671289	–6.4243274
C	–7.4998735	3.6367725	–5.8357293

C	–6.0207257	5.4106862	–5.1158370
H	–3.9356060	5.1896669	–5.6617898
H	–6.5721615	2.0044906	–6.9128331
H	–8.4958078	3.1939732	–5.8832487
H	–5.8562707	6.3551469	–4.5956121
H	–8.1421844	5.3643070	–4.7078272

TS5 (I^{T-T}-I^{B-T}):

107 atoms

C	3.9337559	1.4947545	0.0255250
C	4.2405973	0.1991764	–0.2623020
C	2.9994792	–0.5356477	–0.2519223
C	2.5026244	1.5608559	0.1877736
N	1.9481200	0.3150332	0.0181619
C	1.8093125	2.7376320	0.5015123
C	0.4288148	2.8032946	0.6023823
N	–0.4516741	1.7318731	0.3899021
C	–1.7116225	2.3069867	0.2041435
C	–0.3239349	4.0169386	0.7168240
C	–1.6312747	3.7155646	0.4540567
C	–2.8234647	1.6543403	–0.3107948
C	–2.8938055	0.2674608	–0.4626475
N	–1.8844484	–0.6159402	–0.1671744
C	–3.8678611	–1.7631596	–0.4263599
C	–4.1258518	–0.4483914	–0.6816879
C	–0.3963636	–3.1309895	0.1784277
N	0.4699550	–2.0726168	–0.0097467
C	1.7228389	–2.6264582	–0.1533652
C	1.6457349	–4.0612712	–0.0339308
C	0.3431018	–4.3684569	0.2207904
C	2.9154107	–1.9222811	–0.3471243
C	–1.7918148	–3.0510426	0.1750532
C	–2.4644393	–1.8582901	–0.1028829
H	4.6056409	2.3392788	0.1310801
H	5.2170116	–0.2401681	–0.4353990
H	0.1136785	4.9897193	0.9135083
H	–2.4742322	4.3956542	0.3916837
H	–4.5522322	–2.6038523	–0.4626005
H	–5.0700394	0.0172640	–0.9437070
H	2.4902648	–4.7361928	–0.1188314
H	–0.0910343	–5.3461608	0.3966506
Co	0.0123602	–0.1779348	0.0177972
C	2.5821879	3.9977718	0.6655943
C	4.0129770	6.3880622	0.9631234
C	2.7259232	4.5787971	1.9336383
C	3.1589981	4.6185333	–0.4529863
C	3.8709520	5.8104563	–0.3024763
C	3.4409855	5.7700222	2.0792375
H	2.2796078	4.0773842	2.7934881
H	3.0378774	4.1538995	–1.4335418
H	4.3132922	6.2910324	–1.1763878
H	3.5551677	6.2149694	3.0688993
H	4.5700330	7.3188718	1.0793382
C	4.1712108	–2.6828718	–0.6045172
C	6.5590441	–4.0786643	–1.1001962
C	4.7687599	–2.6420456	–1.8733802
C	4.7860238	–3.4267700	0.4142038
C	5.9723042	–4.1208139	0.1678313
C	5.9547790	–3.3373272	–2.1192342
H	4.2945294	–2.0585442	–2.6637291
H	4.3267460	–3.4515751	1.4035507
H	6.4426649	–4.6911588	0.9701743
H	6.4067892	–3.3001109	–3.1113486
H	7.4860127	–4.6203774	–1.2926442
C	–2.6098359	–4.2767543	0.3793309
C	–4.2152459	–6.5539109	0.7795089
C	–2.5573072	–5.3567221	–0.5169902
C	–3.4861436	–4.3523480	1.4748335
C	–4.2795141	–5.4831271	1.6753522
C	–3.3537126	–6.4858424	–0.3189671
H	–1.8918128	–5.2997885	–1.3790319
H	–3.5371511	–3.5114874	2.1676906
H	–4.9495118	–5.5280849	2.5350625
H	–3.3063830	–7.3120275	–1.0297541
H	–4.8371163	–7.4365352	0.9342545
C	–4.0205777	2.4650544	–0.6636492
C	–6.2674361	3.9883965	–1.3634682
C	–4.8782321	2.9556650	0.3311749
C	–4.2959706	2.7392324	–2.0111963
C	–5.4158615	3.4987467	–2.3581709
C	–5.9969546	3.7150783	–0.0192182
H	–4.6604010	2.7253707	1.3750481
H	–3.6189474	2.3554987	–2.7761533
H	–5.6224364	3.7099781	–3.4083977
H	–6.6626939	4.0898609	0.7597403
H	–7.1421753	4.5807500	–1.6354883
C	–0.1612707	0.1746601	1.8929386
C	0.0497563	0.1299494	–1.9456188
C	–0.3555362	–0.7602175	–3.0168039
O	–0.3056239	–0.4631585	–4.2144111
O	–0.8042571	–1.9825122	–2.5941177
C	0.4561197	1.4732364	–2.4193398
O	1.6096159	1.8305739	–2.5961532
O	–0.6128366	2.3003088	–2.5842118
C	1.0924449	0.4571354	2.6617432
O	1.4303884	1.5363140	3.1180509
O	1.8266984	–0.6760715	2.7710750
C	–1.3785659	0.2129099	2.7115174
O	–2.5207155	0.5069762	2.3974244
O	–1.0568123	–0.2510496	3.9720191
C	3.1162569	–0.5046376	3.4012066
H	3.7447237	0.1505440	2.7816849
H	3.5466012	–1.5093764	3.4574267
H	3.0085192	–0.0680311	4.4030491
C	–2.1867264	–0.4537435	4.8412698
H	–2.9058757	–1.1519572	4.3894195
H	–2.6979585	0.4989294	5.0378744
H	–1.7732449	–0.8696577	5.7658193
C	–1.2561345	–2.8534860	–3.6418706
H	–1.6442285	–3.7420352	–3.1318862
H	–0.4286388	–3.1235470	–4.3135827
H	–2.0488002	–2.3759735	–4.2351620
C	–0.2860323	3.6621346	–2.9383486
H	0.2043437	3.6985877	–3.9202389
H	0.3774433	4.1029450	–2.1811857
H	–1.2437062	4.1927323	–2.9585321

TS6 (I^{B-T}-I^{E-T}):

107 atoms

C	3.9999887	1.3943230	–1.0867684
C	3.9540570	0.1067002	–1.5920871
C	2.8727056	–0.5797743	–1.0215991
C	2.8601281	1.6125119	–0.2916951
N	2.2016376	0.3210983	–0.0674275
C	2.2813691	2.8640380	–0.0751373
C	0.8901986	3.0676374	–0.1354969
N	–0.0637636	2.0814422	–0.2411122
C	–1.2685343	2.7132733	–0.4490388
C	0.2557132	4.3620047	–0.2459749
C	–1.0672274	4.1423352	–0.5008629
C	–2.5264336	2.1084440	–0.3830219
C	–2.7007279	0.8361090	0.1922467
N	–1.6708464	–0.0205649	0.4997969
C	–3.6406995	–0.8684599	1.3335163
C	–3.9429602	0.2923316	0.6737061
C	–0.3456370	–2.6236124	0.8127175
N	0.4250297	–1.7326503	0.1082207
C	1.4173781	–2.4604935	–0.5050978
C	1.2636357	–3.8580575	–0.1901688
C	0.2006465	–3.9545216	0.6644042
C	2.4971043	–1.8994945	–1.2123576
C	–1.5778807	–2.3185442	1.4026661
C	–2.2311069	–1.1024757	1.1501701
H	4.6873400	2.1832514	–1.3781423
H	4.6100316	–0.3211843	–2.3431145
H	0.7595359	5.3147631	–0.1278241
H	–1.8594671	4.8724887	–0.6296161
H	–4.3201241	–1.5283114	1.8617861
H	–4.9161777	0.7566077	0.5564416
H	1.9244757	–4.6434112	–0.5423902
H	–0.2041103	–4.8447378	1.1346159
Co	0.1522629	0.1641927	–0.1106627
C	3.2272037	4.0078902	–0.0125395
C	5.1091419	6.0923832	0.1612840
C	4.1922140	4.0189912	1.0099350
C	3.2314558	5.0481381	–0.9575864
C	4.1646443	6.0825431	–0.8694138
C	5.1215090	5.0559811	1.0993669
H	4.1936928	3.2070953	1.7387951
H	2.5101639	5.0306044	–1.7747569
H	4.1602414	6.8790824	–1.6149872
H	5.8565935	5.0552417	1.9054145
H	5.8369523	6.9020851	0.2290878
C	3.2942876	–2.7752161	–2.1031542
C	4.7532139	–4.4547560	–3.8044260
C	2.6729242	–3.3594628	–3.2199777
C	4.6484660	–3.0395897	–1.8401329
C	5.3712924	–3.8797978	–2.6890544
C	3.4052723	–4.1919993	–4.0682756
H	1.6264538	–3.1265225	–3.4290174
H	5.1044328	–2.6010548	–0.9512933
H	6.4199358	–4.0923571	–2.4748135
H	2.9223267	–4.6306804	–4.9427321
H	5.3222715	–5.1080388	–4.4677981
C	–2.2386202	–3.3821467	2.2052132
C	–3.3959481	–5.4302818	3.7472016
C	–3.4151039	–4.0188798	1.7790235
C	–1.6423394	–3.7952792	3.4086600
C	–2.2192837	–4.8092023	4.1752347
C	–3.9900114	–5.0345559	2.5454713
H	–3.8680020	–3.7227544	0.8318616
H	–0.7218044	–3.3086302	3.7347064
H	–1.7481525	–5.1139505	5.1109208
H	–4.9005130	–5.5248246	2.1976840
H	–3.8457361	–6.2239889	4.3452200
C	–3.6920411	2.8854723	–0.8750370
C	–5.8373596	4.3673577	–1.9156488
C	–4.7085503	3.3534781	–0.0275792
C	–3.7533196	3.1776536	–2.2491482
C	–4.8244205	3.9105491	–2.7638059
C	–5.7745486	4.0912192	–0.5463712
H	–4.6440181	3.1582612	1.0438628
H	–2.9591109	2.8079673	–2.9015626
H	–4.8673367	4.1233181	–3.8330310
H	–6.5540626	4.4593328	0.1224628
H	–6.6722008	4.9421769	–2.3193036
C	2.3611568	–0.0989249	1.3583641
C	3.1948020	–1.2689925	1.6396232
O	4.2630500	–1.5550751	1.1024856
O	2.6174929	–2.0892034	2.5699001
C	1.8243686	0.7263578	2.3995658
O	2.3425290	0.3980034	3.6377639
O	1.0414086	1.6748464	2.2766764
C	3.4122665	–3.2298658	2.9368123
H	2.8435181	–3.7428854	3.7199397
H	4.3978311	–2.9211084	3.3129584
H	3.5535839	–3.8921211	2.0702236
C	1.7404158	1.1055675	4.7325384
H	2.2010935	0.6885779	5.6353953
H	0.6512081	0.9528196	4.7523913
H	1.9376708	2.1852380	4.6660985
C	–0.1897883	–0.0502917	–1.9377667
C	0.0763807	1.0594339	–2.8684779
O	–0.7670742	1.5581280	–3.6026170
O	1.3541011	1.5209550	–2.7922978
C	–0.7852153	–1.2421219	–2.5336567
O	–0.4365867	–1.6737729	–3.6334791
O	–1.7128472	–1.8721564	–1.7621710
C	1.6186326	2.7286294	–3.5301100
H	0.9513641	3.5333654	–3.1889693
H	1.4712468	2.5700211	–4.6067746
H	2.6637389	2.9758329	–3.3130241
C	–2.1308580	–3.1630264	–2.2417075
H	–2.6032193	–3.0841879	–3.2303841
H	–1.2691978	–3.8429194	–2.3050256
H	–2.8458205	–3.5292347	–1.4969268

TS7 (I^{E-T}-I^{E-G}):

123 atoms

C	1.2719468	4.1255311	–4.6535489
C	0.8396753	4.0045712	–5.9602084
C	0.2620206	2.7300410	–6.1232475
C	0.9808511	2.9283570	–3.9753990
N	0.3854449	1.9907592	–4.8923450
C	1.1522902	2.6641963	–2.6186174
C	0.3198218	1.7838977	–1.8967320
N	–0.9164117	1.2977511	–2.2876079
C	–1.4666571	0.7058995	–1.1692962
C	0.5684691	1.4208027	–0.5191676
C	–0.5442828	0.7822135	–0.0614988
C	–2.7468687	0.1494607	–1.0836738
C	–3.5632972	–0.0868670	–2.1924599
N	–3.2317890	0.1669879	–3.5005387
C	–5.2541841	–0.9258535	–3.4272576
C	–4.8370409	–0.7623336	–2.1400424
C	–3.2053297	0.1080657	–6.4706318
N	–2.1312562	0.8503591	–6.0222586
C	–1.4573692	1.2803317	–7.1486397
C	–2.0847244	0.7253699	–8.3265050
C	–3.1713392	0.0176710	–7.9113426
C	–0.4471309	2.2635838	–7.2233616
C	–4.2477817	–0.3867746	–5.6756581
C	–4.2414244	–0.3433758	–4.2765260
H	1.6818573	5.0101526	–4.1775413
H	0.8299159	4.7793533	–6.7195459
H	1.4871323	1.6318806	0.0173668
H	–0.7294679	0.3788555	0.9283060
H	–6.1510670	–1.4196108	–3.7847543
H	–5.3208650	–1.0923412	–1.2269665
H	–1.7256522	0.8688083	–9.3400040
H	–3.8925936	–0.5180726	–8.5183911
Co	–1.7051576	1.1898572	–4.1249460
C	2.2081899	3.4407442	–1.9300505
C	4.2525513	4.9346261	–0.7032467
C	3.4898758	3.5144815	–2.5114721
C	1.9655731	4.1410857	–0.7339719
C	2.9798247	4.8802530	–0.1257265
C	4.5021822	4.2526479	–1.8982326
H	3.6752847	2.9833779	–3.4479590
H	0.9672894	4.1134644	–0.2962999
H	2.7739017	5.4257947	0.7964350
H	5.4923203	4.2927736	–2.3545427
H	5.0452638	5.5125367	–0.2258727
C	–0.2147638	2.9756306	–8.5026899
C	0.2573074	4.4210952	–10.8668518
C	–1.2814150	3.5641968	–9.2063628
C	1.0941775	3.1329714	–8.9933454
C	1.3252000	3.8459212	–10.1705703
C	–1.0460746	4.2822354	–10.3785389
H	–2.2912297	3.4730568	–8.8054306
H	1.9222615	2.6913132	–8.4353696
H	2.3437933	3.9533052	–10.5462072

H	–1.8815158	4.7422811	–10.9087280
H	0.4407828	4.9817114	–11.7845407
C	–5.4639235	–0.9331118	–6.3394961
C	–7.7956145	–1.9011647	–7.5721452
C	–6.6768024	–0.2329825	–6.2175510
C	–5.4355495	–2.1269857	–7.0757846
C	–6.5948293	–2.6072727	–7.6890834
C	–7.8334994	–0.7150412	–6.8331775
H	–6.6936081	0.6904858	–5.6347914
H	–4.4991244	–2.6812617	–7.1558632
H	–6.5612705	–3.5401475	–8.2539681
H	–8.7677230	–0.1599295	–6.7354490
H	–8.7004046	–2.2773526	–8.0517081
C	–3.2975161	–0.1683550	0.2647757
C	–4.3777924	–0.7001710	2.7988390
C	–2.8884465	–1.2990824	0.9853415
C	–4.2570986	0.6933566	0.8197832
C	–4.7925467	0.4260336	2.0816690
C	–3.4257958	–1.5626264	2.2478466
H	–2.1504053	–1.9726294	0.5467702
H	–4.5692009	1.5668453	0.2443804
H	–5.5369422	1.1014546	2.5063174
H	–3.1040850	–2.4473054	2.7995408
H	–4.7980837	–0.9077392	3.7839994
C	1.1468724	0.7188261	–5.0287499
C	2.5030653	0.8697473	–5.5069616
O	3.0386673	1.9549502	–5.7611077
O	3.1852012	–0.3085394	–5.6706454
C	0.4901415	–0.4683560	–4.6587205
O	1.1688824	–1.6343581	–4.7581146
O	–0.7041782	–0.5297108	–4.2283312
C	4.5365525	–0.1493584	–6.1316731
H	4.9358213	–1.1671223	–6.2065365
H	5.1319655	0.4444044	–5.4228630
H	4.5673793	0.3477040	–7.1121357
C	0.4394043	–2.8114054	–4.3617549
H	1.1404484	–3.6389838	–4.5150349
H	–0.4585604	–2.9485735	–4.9801840
H	0.1372835	–2.7542036	–3.3066193
C	–2.8168938	2.8077834	–3.9959534
C	–4.0332176	2.8268660	–4.8725368
O	–5.1792494	2.6100978	–4.5112832
O	–3.7317854	3.0947399	–6.1754729
C	–4.8597808	3.0644278	–7.0720343
H	–4.4507849	3.2942591	–8.0601984
H	–5.6030799	3.8208628	–6.7864201
H	–5.3224580	2.0689046	–7.0747840
C	–1.9450367	4.8620834	–4.7340168
H	–1.6246379	4.4295507	–5.6765681
H	–1.2627509	4.7767577	–3.8964228
C	–2.9948890	5.7388830	–4.7047844
C	–3.0841173	3.1742362	–2.5686556
O	–4.0387716	2.8090207	–1.9026472
O	–2.0847930	3.9383569	–2.0260684
C	–2.1953550	4.1480758	–0.6056607
H	–3.1556807	4.6152103	–0.3479838
H	–2.1062186	3.1911388	–0.0712877
H	–1.3631106	4.8106924	–0.3448454
H	–3.3080700	6.1514725	–3.7405890
C	–3.8018373	6.0932305	–5.8602331
C	–5.4252823	6.7145987	–8.0903103
C	–5.1197616	6.5700301	–5.6918703
C	–3.3102748	5.9636844	–7.1801118
C	–4.1100899	6.2680491	–8.2754840
C	–5.9235544	6.8668648	–6.7919483
H	–5.5188250	6.6757387	–4.6810073
H	–2.2871414	5.6229404	–7.3414157
H	–3.7046380	6.1612783	–9.2834787
H	–6.9457146	7.2159054	–6.6371786
H	–6.0523983	6.9511892	–8.9509467

TS8 (I^{E-G}-P):

123 atoms

C	1.1628596	4.1396031	–4.7453354
C	0.6849538	4.0137631	–6.0350965
C	0.1234465	2.7334464	–6.1825790
C	0.9002865	2.9470832	–4.0518367
N	0.2676661	1.9878340	–4.9416885
C	1.1069621	2.7095313	–2.6982540
C	0.2860035	1.8491145	–1.9457171
N	–0.9449852	1.3353355	–2.3299171
C	–1.4890529	0.7825057	–1.1841926
C	0.5311046	1.5546642	–0.5534224
C	–0.5766072	0.9243020	–0.0754931
C	–2.7589846	0.2109429	–1.0780717
C	–3.5728144	–0.0479776	–2.1827136
N	–3.2366861	0.1887156	–3.4946688
C	–5.2560790	–0.9324473	–3.3882129
C	–4.8422323	–0.7313567	–2.1083811
C	–3.2217211	0.0119391	–6.4501712
N	–2.1787171	0.8143881	–6.0243792
C	–1.5304753	1.2223530	–7.1787913
C	–2.1359265	0.6031090	–8.3330314
C	–3.1891452	–0.1344591	–7.8854041
C	–0.5593170	2.2371403	–7.2821224
C	–4.2454238	–0.4846952	–5.6399706
C	–4.2421189	–0.3702304	–4.2485816
H	1.5943771	5.0234427	–4.2871771
H	0.6567599	4.7809190	–6.8018312
H	1.4391616	1.8107120	–0.0186740
H	–0.7662125	0.5743635	0.9332749
H	–6.1529271	–1.4332374	–3.7354780
H	–5.3283544	–1.0332517	–1.1873994
H	–1.7898829	0.7309618	–9.3530990
H	–3.8935649	–0.7202850	–8.4656598
Co	–1.6529631	1.1024358	–4.1514429
C	2.1666886	3.5144162	–2.0468313
C	4.2115123	5.0654839	–0.8961772
C	3.4471539	3.5589562	–2.6317339
C	1.9226136	4.2758222	–0.8894014
C	2.9378029	5.0434982	–0.3187205
C	4.4608509	4.3248498	–2.0556668
H	3.6297067	2.9878384	–3.5445239
H	0.9223021	4.2746193	–0.4547964
H	2.7316057	5.6365371	0.5735215
H	5.4508307	4.3420274	–2.5137015
H	5.0048772	5.6650055	–0.4475919
C	–0.3271052	2.9210934	–8.5753606
C	0.1500073	4.3078316	–10.9748113
C	–1.3971579	3.4341015	–9.3310231
C	0.9877621	3.1214075	–9.0352574
C	1.2210132	3.8061607	–10.2285073
C	–1.1598558	4.1225180	–10.5205621
H	–2.4148098	3.3015525	–8.9621586
H	1.8176333	2.7351790	–8.4395316
H	2.2444960	3.9473604	–10.5786464
H	–1.9992348	4.5211202	–11.0927012
H	0.3352361	4.8450247	–11.9059737
C	–5.4353473	–1.1037858	–6.2881303
C	–7.7102648	–2.2099048	–7.5057605
C	–6.6585431	–0.4129347	–6.2651372
C	–5.3650891	–2.3541118	–6.9194350
C	–6.4970413	–2.9037936	–7.5256574
C	–7.7876438	–0.9655966	–6.8730301
H	–6.7010020	0.5562859	–5.7643450
H	–4.4175068	–2.8950052	–6.9256446
H	–6.4322277	–3.8797195	–8.0090914
H	–8.7324947	–0.4202991	–6.8522396
H	–8.5941279	–2.6402969	–7.9786716
C	–3.2934465	–0.1135836	0.2745886
C	–4.3403729	–0.6781493	2.8184430
C	–2.7794171	–1.1743696	1.0348914
C	–4.3452781	0.6579364	0.7960809
C	–4.8621561	0.3754752	2.0622479
C	–3.2995448	–1.4541163	2.3005502
H	–1.9738105	–1.7836089	0.6222052
H	–4.7449776	1.4724714	0.1894929
H	–5.6777314	0.9820235	2.4591559
H	–2.8952985	–2.2853400	2.8802462
H	–4.7471197	–0.8980431	3.8065337
C	1.0995817	0.7523796	–5.1160987
C	2.4214767	0.9589592	–5.6646375
O	2.8971824	2.0585448	–5.9703014
O	3.1492514	–0.1915411	–5.8384134
C	0.5226309	–0.4682924	–4.7147681
O	1.2578025	–1.5975496	–4.8340623
O	–0.6493382	–0.5868285	–4.2407385
C	4.4627292	0.0171884	–6.3807576
H	4.9052659	–0.9827325	–6.4520506
H	5.0686534	0.6580834	–5.7239124
H	4.4143127	0.4862261	–7.3742663
C	0.6018895	–2.8088463	–4.4118341
H	1.3383788	–3.6003254	–4.5873650
H	–0.3079067	–2.9927985	–4.9999702
H	0.3325958	–2.7635941	–3.3474068
C	–3.2377106	3.2932793	–3.9465070
C	–4.2952744	2.8847885	–4.8927999
O	–5.3571388	2.3446582	–4.6284178
O	–3.9395355	3.1881637	–6.1881707
C	–4.9537834	2.9279612	–7.1710732
H	–4.5897807	3.3920139	–8.0944299
H	–5.9117560	3.3753025	–6.8730891
H	–5.0873559	1.8476193	–7.3156001
C	–2.1430834	4.2369572	–4.4092214
H	–1.7681363	3.9568736	–5.3913580
H	–1.3206515	4.2706398	–3.6926974
C	–2.9934097	5.4420030	–4.4254202
C	–3.5400052	3.2551173	–2.5007324
O	–4.4543533	2.6736534	–1.9413535
O	–2.6057945	3.9882720	–1.7916403
C	–2.7745744	3.9559447	–0.3646655
H	–3.7823734	4.2881416	–0.0784332
H	–2.6109752	2.9404481	0.0213167
H	–2.0152543	4.6370192	0.0347843
H	–3.3033239	5.8291700	–3.4527533
C	–3.4949361	6.0849894	–5.5940989
C	–4.4655096	7.4444391	–7.8744649
C	–4.4948032	7.0880641	–5.4817913
C	–2.9939593	5.7924389	–6.8927708
C	–3.4705356	6.4652651	–8.0084824
C	–4.9719693	7.7531669	–6.6040458
H	–4.8940385	7.3241683	–4.4934202
H	–2.2283106	5.0279176	–7.0156519
H	–3.0625233	6.2261665	–8.9920294
H	–5.7452122	8.5150034	–6.4963282
H	–4.8423149	7.9668783	–8.7546890

TS9 (I^{E-IY}-I^{E-T}):

119 atoms

C	2.5970672	4.9634610	–5.2181394
C	2.1161085	4.7834176	–6.4833732
C	1.2207889	3.6364760	–6.4298077
C	2.0011588	3.9242226	–4.3964213
N	1.1343116	3.1872531	–5.1457963
C	2.3851540	3.5990925	–3.0869698
C	1.9601786	2.4554121	–2.3825561
N	0.9073529	1.6079740	–2.7167861
C	0.8443156	0.6375205	–1.7060734
C	2.5562952	2.0129948	–1.1507035
C	1.8910122	0.8855545	–0.7525827
C	–0.1895544	–0.3032234	–1.5105161
C	–1.1530714	–0.5983190	–2.4873018
N	–0.8868229	–0.5500948	–3.8812158
C	–3.1239586	–0.9783737	–3.5293868
C	–2.5209874	–0.8729507	–2.2890350
C	–1.5267136	0.2156286	–6.7077382
N	–0.7448376	1.2810936	–6.2855701
C	–0.2702159	1.8980084	–7.4280343
C	–0.7378385	1.1793045	–8.5944268
C	–1.5092516	0.1483636	–8.1510259
C	0.5749908	3.0252370	–7.5189613
C	–2.3128530	–0.6434914	–5.9046348
C	–2.1425744	–0.7589725	–4.5178999
H	3.3129705	5.7031038	–4.8733890
H	2.3504766	5.3615175	–7.3713877
H	3.3930711	2.4961076	–0.6575967
H	2.0988116	0.2634539	0.1114117
H	–4.1828029	–1.0967326	–3.7311745
H	–3.0063685	–0.8820522	–1.3192263
H	–0.4724047	1.4159549	–9.6190037
H	–1.9869463	–0.6278322	–8.7392861
Co	–0.0273622	1.6273592	–4.4707725
C	3.3764537	4.5015691	–2.4303111
C	5.2172079	6.2509130	–1.2234676
C	4.7298236	4.1479177	–2.3212311
C	2.9573016	5.7459092	–1.9354195
C	3.8720791	6.6146547	–1.3350681
C	5.6441177	5.0155504	–1.7194322
H	5.0594996	3.1867415	–2.7189233
H	1.9062335	6.0228537	–2.0330323
H	3.5328314	7.5786325	–0.9522921
H	6.6943362	4.7287444	–1.6445617
H	5.9317577	6.9293933	–0.7551062
C	0.8633430	3.5672229	–8.8758345
C	1.4273051	4.5941171	–11.4394293
C	–0.1627878	4.0811914	–9.6862584
C	2.1766639	3.5705762	–9.3772826
C	2.4565316	4.0789906	–10.6464201
C	0.1159730	4.5918548	–10.9552607
H	–1.1864087	4.0704440	–9.3099917
H	2.9766947	3.1583820	–8.7610360
H	3.4815063	4.0647583	–11.0202275
H	–0.6934899	4.9916885	–11.5678828
H	1.6456450	4.9911133	–12.4316636
C	–3.4221666	–1.4198645	–6.4941003
C	–5.5531149	–2.9435681	–7.5321657
C	–4.3076615	–0.8696713	–7.4419233
C	–3.6287316	–2.7504694	–6.0723814
C	–4.6839004	–3.5014947	–6.5894447
C	–5.3610727	–1.6241627	–7.9554979
H	–4.1701866	0.1648510	–7.7563335
H	–2.9393192	–3.1847572	–5.3446711
H	–4.8234115	–4.5321328	–6.2599264
H	–6.0429081	–1.1778811	–8.6811854
H	–6.3780911	–3.5329303	–7.9350103
C	–0.3842110	–0.9566676	–0.1987575
C	–0.8070547	–2.2772066	2.2509181
C	–0.6512573	–2.3409456	–0.1655491
C	–0.3572915	–0.2439087	1.0150262
C	–0.5651052	–0.8996071	2.2282808
C	–0.8544090	–2.9929015	1.0504105
H	–0.6907641	–2.8919082	–1.1081204
H	–0.1947924	0.8344492	0.9952478
H	–0.5504382	–0.3318706	3.1599398
H	–1.0467868	–4.0667797	1.0606573
H	–0.9659247	–2.7890564	3.2012632
C	0.2198671	–1.3993350	–4.3567133
C	–0.0009706	–2.8140445	–4.1658698
O	–1.0141575	–3.2949921	–3.6417491
O	1.0129320	–3.6195942	–4.6164786
C	1.3323835	–0.7621043	–4.9288930
O	2.3599587	–1.5253729	–5.3682768

O	1.4522695	0.4966048	–5.0660715
C	0.7810347	–5.0244149	–4.4281467
H	0.6603166	–5.2692670	–3.3628419
H	1.6699659	–5.5193822	–4.8352797
H	–0.1204822	–5.3544421	–4.9645960
C	3.4548316	–0.8018526	–5.9618793
H	3.9122699	–0.1111168	–5.2396252
H	3.1211311	–0.2275491	–6.8375396
H	4.1716499	–1.5746243	–6.2601741
C	–1.5171576	2.8316079	–3.8985992
C	–2.9386228	2.3047366	–3.9128049
O	–3.5911036	1.9681628	–2.9351215
O	–3.4307686	2.2416024	–5.1709148
C	–1.3417502	4.2173302	–4.4981780
O	–0.8411822	5.1850175	–3.9451976
O	–1.7939175	4.2587611	–5.7712842
C	–1.5958601	5.5239314	–6.4398637
H	–0.5250643	5.7583413	–6.5035330
H	–2.1151171	6.3295505	–5.9037555
H	–2.0183321	5.3854487	–7.4398304
C	–4.8040219	1.8065835	–5.2629584
H	–5.4422252	2.3860911	–4.5828401
H	–4.8850773	0.7401720	–5.0180775
H	–5.0877298	1.9747028	–6.3062082
I	–1.1806765	3.2569991	–1.5972986
C	–2.7766185	4.5996443	–1.2208308
C	–4.8515900	6.3657052	–0.7130750
C	–2.5784521	5.9629257	–1.4559755
C	–3.9920455	4.0982633	–0.7483139
C	–5.0306056	4.9970024	–0.4913203
C	–3.6312009	6.8450792	–1.1977180
H	–1.6333683	6.3197048	–1.8613043
H	–4.1305160	3.0274591	–0.6130087
H	–5.9854682	4.6203194	–0.1222857
H	–3.4929165	7.9115252	–1.3809388
H	–5.6681314	7.0606159	–0.5127924

TS10 (I^{B}-I^{E}):

92 atoms

C	3.5490091	3.5715759	–4.6467290
C	3.0041516	3.5004091	–5.9001045
C	1.7964341	2.7427163	–5.8185980
C	2.6601546	2.9069885	–3.7470346
N	1.6569704	2.2272870	–4.4979324
C	2.6201095	3.0860806	–2.3806268
C	1.5842296	2.6015595	–1.5679562
N	0.5812646	1.7361271	–1.9602889
C	–0.0780488	1.3912253	–0.7882036
C	1.4859684	2.8849407	–0.1634618
C	0.4446856	2.1464560	0.3202528
C	–1.0210121	0.3689294	–0.6740897
C	–1.4832024	–0.3410573	–1.7835135
N	–1.2155239	–0.0198717	–3.1048370
C	–2.6493388	–1.8403720	–2.9974824
C	–2.3554079	–1.4853632	–1.7149041
C	–1.6633159	0.2360822	–5.9993469
N	–0.6923624	1.1251888	–5.5594187
C	–0.3127348	1.8401009	–6.6871702
C	–1.1295880	1.4681934	–7.8101541
C	–1.9466992	0.4570751	–7.3917070
C	0.8487637	2.6161782	–6.8174863
C	–2.1974009	–0.8014967	–5.2314204
C	–1.9692194	–0.9058007	–3.8591782
H	4.4360479	4.1134855	–4.3356421
H	3.3659463	3.9693746	–6.8089035
H	2.1400655	3.5624291	0.3755204
H	0.0681661	2.0984572	1.3362269
H	–3.3034015	–2.6349377	–3.3403615
H	–2.7041768	–1.9420571	–0.7948132
H	–1.0389530	1.8901610	–8.8054051
H	–2.6594059	–0.1110887	–7.9794122
Co	0.1153366	1.2063910	–3.7749671
C	3.7489786	3.8085224	–1.7257359
C	5.8983210	5.1040291	–0.4713891
C	4.7060148	3.0663531	–1.0164890
C	3.8765250	5.2022010	–1.8008925
C	4.9468142	5.8473575	–1.1752047
C	5.7756085	3.7131355	–0.3942571
H	4.5959220	1.9820209	–0.9730418
H	3.1288979	5.7768478	–2.3499909
H	5.0357216	6.9331426	–1.2358609
H	6.5177445	3.1282251	0.1515287
H	6.7340930	5.6078404	0.0165069
C	1.1383551	3.2327674	–8.1432908
C	1.6844795	4.3599067	–10.6546428
C	0.3964858	4.3294055	–8.6045311
C	2.1546726	2.7007514	–8.9522094
C	2.4247080	3.2636819	–10.2012113
C	0.6693839	4.8911564	–9.8541123
H	–0.3956232	4.7386646	–7.9754368
H	2.7133507	1.8374970	–8.5878501
H	3.2129543	2.8403426	–10.8257743
H	0.0895153	5.7476125	–10.2015402
H	1.8970513	4.7984780	–11.6307239
C	–3.0499219	–1.8307953	–5.8870814
C	–4.6193505	–3.8145470	–7.1218386
C	–4.3026812	–1.5128621	–6.4344498
C	–2.6008843	–3.1600249	–5.9569249
C	–3.3779483	–4.1440750	–6.5703916
C	–5.0802817	–2.4970600	–7.0487210
H	–4.6669855	–0.4867663	–6.3662577
H	–1.6353455	–3.4122720	–5.5157610
H	–3.0115641	–5.1706785	–6.6193945
H	–6.0539870	–2.2346946	–7.4652714
H	–5.2274292	–4.5824365	–7.6019470
C	–1.5342399	0.0039138	0.6746989
C	–2.5150407	–0.6828600	3.2210169
C	–0.6726136	–0.5077704	1.6587638
C	–2.8948781	0.1636748	0.9846596
C	–3.3812149	–0.1747799	2.2487423
C	–1.1598518	–0.8497135	2.9216489
H	0.3835969	–0.6394001	1.4199770
H	–3.5674851	0.5629279	0.2241127
H	–4.4393751	–0.0368286	2.4760393
H	–0.4788565	–1.2516736	3.6733531
H	–2.8949807	–0.9481913	4.2086035
C	1.7448796	0.3923399	–4.3560695
C	1.7727051	–0.2401617	–5.7222125
O	2.4310866	0.1488715	–6.6710158
O	0.9639002	–1.3261665	–5.7694582
C	2.7988388	–0.1037743	–3.4618881
O	3.1726036	0.3332134	–2.3820960
O	3.3485821	–1.2470724	–4.0102030
C	0.9026923	–1.9675256	–7.0633695
H	1.8974268	–2.3179556	–7.3702914
H	0.2116321	–2.8068623	–6.9402448
H	0.5157715	–1.2626891	–7.8119500
C	4.3306307	–1.8953338	–3.1835552
H	4.6363137	–2.7878927	–3.7398494
H	3.8999583	–2.1740172	–2.2111028
H	5.1918113	–1.2343672	–3.0109728

TS11 (I^{T}-I^{B}):

92 atoms

C	3.5490091	3.5715759	–4.6467290
C	3.0041516	3.5004091	–5.9001045
C	1.7964341	2.7427163	–5.8185980
C	2.6601546	2.9069885	–3.7470346
N	1.6569704	2.2272870	–4.4979324
C	2.6201095	3.0860806	–2.3806268
C	1.5842296	2.6015595	–1.5679562
N	0.5812646	1.7361271	–1.9602889
C	–0.0780488	1.3912253	–0.7882036
C	1.4859684	2.8849407	–0.1634618
C	0.4446856	2.1464560	0.3202528
C	–1.0210121	0.3689294	–0.6740897
C	–1.4832024	–0.3410573	–1.7835135
N	–1.2155239	–0.0198717	–3.1048370
C	–2.6493388	–1.8403720	–2.9974824
C	–2.3554079	–1.4853632	–1.7149041
C	–1.6633159	0.2360822	–5.9993469
N	–0.6923624	1.1251888	–5.5594187
C	–0.3127348	1.8401009	–6.6871702
C	–1.1295880	1.4681934	–7.8101541
C	–1.9466992	0.4570751	–7.3917070
C	0.8487637	2.6161782	–6.8174863
C	–2.1974009	–0.8014967	–5.2314204
C	–1.9692194	–0.9058007	–3.8591782
H	4.4360479	4.1134855	–4.3356421
H	3.3659463	3.9693746	–6.8089035
H	2.1400655	3.5624291	0.3755204
H	0.0681661	2.0984572	1.3362269
H	–3.3034015	–2.6349377	–3.3403615
H	–2.7041768	–1.9420571	–0.7948132
H	–1.0389530	1.8901610	–8.8054051
H	–2.6594059	–0.1110887	–7.9794122
Co	0.1153366	1.2063910	–3.7749671
C	3.7489786	3.8085224	–1.7257359
C	5.8983210	5.1040291	–0.4713891
C	4.7060148	3.0663531	–1.0164890
C	3.8765250	5.2022010	–1.8008925
C	4.9468142	5.8473575	–1.1752047
C	5.7756085	3.7131355	–0.3942571
H	4.5959220	1.9820209	–0.9730418
H	3.1288979	5.7768478	–2.3499909
H	5.0357216	6.9331426	–1.2358609
H	6.5177445	3.1282251	0.1515287
H	6.7340930	5.6078404	0.0165069
C	1.1383551	3.2327674	–8.1432908
C	1.6844795	4.3599067	–10.6546428
C	0.3964858	4.3294055	–8.6045311
C	2.1546726	2.7007514	–8.9522094
C	2.4247080	3.2636819	–10.2012113
C	0.6693839	4.8911564	–9.8541123
H	–0.3956232	4.7386646	–7.9754368
H	2.7133507	1.8374970	–8.5878501
H	3.2129543	2.8403426	–10.8257743
H	0.0895153	5.7476125	–10.2015402
H	1.8970513	4.7984780	–11.6307239
C	–3.0499219	–1.8307953	–5.8870814
C	–4.6193505	–3.8145470	–7.1218386
C	–4.3026812	–1.5128621	–6.4344498
C	–2.6008843	–3.1600249	–5.9569249
C	–3.3779483	–4.1440750	–6.5703916
C	–5.0802817	–2.4970600	–7.0487210
H	–4.6669855	–0.4867663	–6.3662577
H	–1.6353455	–3.4122720	–5.5157610
H	–3.0115641	–5.1706785	–6.6193945
H	–6.0539870	–2.2346946	–7.4652714
H	–5.2274292	–4.5824365	–7.6019470
C	–1.5342399	0.0039138	0.6746989
C	–2.5150407	–0.6828600	3.2210169
C	–0.6726136	–0.5077704	1.6587638
C	–2.8948781	0.1636748	0.9846596
C	–3.3812149	–0.1747799	2.2487423
C	–1.1598518	–0.8497135	2.9216489
H	0.3835969	–0.6394001	1.4199770
H	–3.5674851	0.5629279	0.2241127
H	–4.4393751	–0.0368286	2.4760393
H	–0.4788565	–1.2516736	3.6733531
H	–2.8949807	–0.9481913	4.2086035
C	1.7448796	0.3923399	–4.3560695
C	1.7727051	–0.2401617	–5.7222125
O	2.4310866	0.1488715	–6.6710158
O	0.9639002	–1.3261665	–5.7694582
C	2.7988388	–0.1037743	–3.4618881
O	3.1726036	0.3332134	–2.3820960
O	3.3485821	–1.2470724	–4.0102030
C	0.9026923	–1.9675256	–7.0633695
H	1.8974268	–2.3179556	–7.3702914
H	0.2116321	–2.8068623	–6.9402448
H	0.5157715	–1.2626891	–7.8119500
C	4.3306307	–1.8953338	–3.1835552
H	4.6363137	–2.7878927	–3.7398494
H	3.8999583	–2.1740172	–2.2111028
H	5.1918113	–1.2343672	–3.0109728

TS12 (I^{E-T}-I^{E-G}) (Q):

123 atoms

C	0.7297171	4.2736190	–5.2907236
C	0.1724008	4.0747876	–6.5430328
C	–0.1809024	2.7166748	–6.6590199
C	0.7167124	3.0425724	–4.6076415
N	0.1971804	2.0391144	–5.4644427
C	0.9522375	2.8626218	–3.2335896
C	0.1855148	2.0276479	–2.3913682
N	–1.0176714	1.4078349	–2.6905709
C	–1.5676088	1.0043745	–1.4977419
C	0.4235008	1.9268021	–0.9680756
C	–0.6753971	1.3379641	–0.4124344
C	–2.8201816	0.3737956	–1.3229271
C	–3.5658491	–0.2060328	–2.3538232
N	–3.2178510	–0.1596715	–3.6803441
C	–5.1084375	–1.4459175	–3.4444978
C	–4.7619469	–1.0041801	–2.1969201
C	–3.2565608	–0.3719486	–6.6442414
N	–2.3261961	0.5966232	–6.3255905
C	–1.7677645	1.0208504	–7.5227248
C	–2.3259651	0.2493672	–8.6104261
C	–3.2404235	–0.6043911	–8.0719139
C	–0.8866249	2.1071572	–7.7067010
C	–4.1472861	–1.0229034	–5.7696358
C	–4.1338135	–0.9012891	–4.3698759
H	1.0017279	5.2187899	–4.8338580
H	–0.0728694	4.8306258	–7.2817894
H	1.3184948	2.2739545	–0.4632464
H	–0.8593425	1.1259228	0.6351820
H	–5.9526999	–2.0706491	–3.7187943
H	–5.2566783	–1.2112321	–1.2531724
H	–2.0239829	0.3390734	–9.6484810
H	–3.8431854	–1.3470418	–8.5840628
Co	–1.8364902	1.0746631	–4.4930496
C	1.9113504	3.8223213	–2.6432225
C	3.7427814	5.6932081	–1.6256600
C	3.1951784	3.9448456	–3.2077793
C	1.5453706	4.6767268	–1.5865728
C	2.4568117	5.6037634	–1.0821367
C	4.1072468	4.8659886	–2.6928668
H	3.4625045	3.3083313	–4.0533391
H	0.5248417	4.6326157	–1.2057393
H	2.1579140	6.2713136	–0.2725568
H	5.1043909	4.9418908	–3.1286874
H	4.4546696	6.4180946	–1.2279836
C	–0.7394071	2.7270722	–9.0395094
C	–0.4036967	3.9563338	–11.5449651
C	–1.8558537	3.0404825	–9.8380562
C	0.5490365	3.0541456	–9.5088628
C	0.7114669	3.6587842	–10.7550312
C	–1.6872444	3.6502655	–11.0804836
H	–2.8564186	2.8246478	–9.4614329
H	1.4131186	2.8174501	–8.8838610
H	1.7143647	3.8965290	–11.1127247

H	–2.5614047	3.9006402	–11.6832543
H	–0.2741515	4.4328324	–12.5178506
C	–5.2601500	–1.8038086	–6.3753449
C	–7.4200359	–3.2105788	–7.4912246
C	–6.2424944	–1.1270841	–7.1185625
C	–5.3748382	–3.1902792	–6.1937837
C	–6.4468997	–3.8900503	–6.7525995
C	–7.3162188	–1.8276109	–7.6705970
H	–6.1533832	–0.0457195	–7.2364326
H	–4.6123883	–3.7160090	–5.6168275
H	–6.5206274	–4.9696872	–6.6133466
H	–8.0773618	–1.2909002	–8.2391211
H	–8.2581324	–3.7577210	–7.9253422
C	–3.4275458	0.3630655	0.0375963
C	–4.6629650	0.4273444	2.5583776
C	–2.9631155	–0.4571441	1.0754107
C	–4.5250813	1.2092218	0.2702245
C	–5.1366580	1.2414199	1.5247337
C	–3.5776805	–0.4234232	2.3299630
H	–2.1237920	–1.1293632	0.8900208
H	–4.8775521	1.8387734	–0.5492131
H	–5.9852817	1.9057138	1.6962752
H	–3.2113104	–1.0691087	3.1296044
H	–5.1412768	0.4523792	3.5385621
C	1.0319738	0.8410832	–5.6217336
C	2.2936104	1.0727131	–6.2926084
O	2.6476094	2.1698185	–6.7366703
O	3.0861548	–0.0373309	–6.4126537
C	0.5216554	–0.3594383	–5.1094260
O	1.2584183	–1.4852892	–5.2221298
O	–0.6010248	–0.4502002	–4.5172674
C	4.3247147	0.1918542	–7.1059706
H	4.8318830	–0.7792910	–7.1171460
H	4.9390047	0.9403468	–6.5850380
H	4.1449474	0.5427829	–8.1324271
C	0.6549148	–2.6781045	–4.6824637
H	1.3772973	–3.4748997	–4.8889956
H	–0.3048952	–2.8914455	–5.1733905
H	0.4874300	–2.5819317	–3.6007536
C	–3.0068886	2.6591753	–4.3278790
C	–4.4117972	2.2566388	–4.6274325
O	–4.8327222	2.0107442	–5.7513472
O	–5.2249372	2.1636070	–3.5343607
C	–6.5762444	1.7537244	–3.8282742
H	–6.5839783	0.7918307	–4.3584455
H	–7.0832647	2.5084155	–4.4459885
H	–7.0663481	1.6564074	–2.8536240
C	–3.0490764	4.3916572	–5.9573454
H	–3.0401446	3.6192528	–6.7227790
H	–2.0847267	4.7321988	–5.5901202
C	–4.2053817	5.0764624	–5.6942619
C	–2.6375151	3.5674123	–3.2192102
O	–1.6550042	4.3032753	–3.2366764
O	–3.4605175	3.5207073	–2.1313962
C	–3.0387189	4.3509194	–1.0298421
H	–2.9879732	5.4044194	–1.3372398
H	–3.7961604	4.2065388	–0.2520159
H	–2.0534982	4.0248469	–0.6652515
H	–5.1243733	4.7050009	–6.1570205
C	–4.3774705	6.1735108	–4.7589238
C	–4.8292101	8.2594265	–2.8978854
C	–5.6822352	6.6448260	–4.4842362
C	–3.3010857	6.7905435	–4.0787145
C	–3.5278275	7.8119869	–3.1616453
C	–5.9061989	7.6703145	–3.5687577
H	–6.5274015	6.1830927	–5.0000419
H	–2.2841267	6.4434077	–4.2534467
H	–2.6807548	8.2673595	–2.6452525
H	–6.9244986	8.0112791	–3.3740616
H	–5.0004519	9.0620581	–2.1791114

TS13 (I^{E-G}-P) (Q):

123 atoms

C	0.4132230	4.4591040	–5.4753665
C	0.0302236	4.0950729	–6.7569224
C	–0.2872864	2.7217280	–6.7473815
C	0.3662551	3.3144030	–4.6542946
N	–0.0209280	2.1935240	–5.4501284
C	0.5638936	3.2579505	–3.2701252
C	–0.0489396	2.3164964	–2.4164749
N	–1.1483964	1.5257812	–2.7058881
C	–1.5183363	0.9078095	–1.5257094
C	0.3032407	2.1568573	–1.0242352
C	–0.6019278	1.2973999	–0.4738091
C	–2.6521688	0.0964813	–1.3251501
C	–3.5177508	–0.3561465	–2.3400532
N	–3.3747797	–0.0771397	–3.6683641
C	–5.1672312	–1.4923039	–3.3995039
C	–4.6460388	–1.2481246	–2.1587575
C	–3.5963172	–0.1431316	–6.6485754
N	–2.6047084	0.7608646	–6.3540058
C	–1.9434441	1.0289870	–7.5422074
C	–2.5312816	0.2380392	–8.6027357
C	–3.5655385	–0.4650188	–8.0569241
C	–0.9474735	2.0111098	–7.7667131
C	–4.4847077	–0.7696781	–5.7437401
C	–4.3468736	–0.7688005	–4.3478882
H	0.6289605	5.4584340	–5.1124223
H	–0.1348073	4.7528180	–7.6042748
H	1.1454183	2.6401927	–0.5401593
H	–0.6544549	0.9629525	0.5566362
H	–6.0225328	–2.1114099	–3.6495558
H	–4.9840618	–1.6484747	–1.2081715
H	–2.1742383	0.2073934	–9.6267050
H	–4.2226025	–1.1758807	–8.5473331
Co	–2.0324778	1.1739080	–4.4534605
C	1.3668097	4.3546048	–2.6865981
C	2.8797729	6.4776709	–1.6449722
C	2.6387187	4.6481371	–3.2136327
C	0.8521636	5.1527312	–1.6487242
C	1.6064231	6.2062936	–1.1323945
C	3.3910923	5.6995735	–2.6888579
H	3.0211476	4.0397884	–4.0363812
H	–0.1616093	4.9604023	–1.2957412
H	1.1935334	6.8286788	–0.3367712
H	4.3807540	5.9125081	–3.0959636
H	3.4683959	7.3015765	–1.2381692
C	–0.6464820	2.4680974	–9.1413776
C	0.0141808	3.3855773	–11.7189111
C	–1.6554707	2.7699533	–10.0762585
C	0.7002437	2.6584058	–9.5136354
C	1.0249207	3.1069687	–10.7933208
C	–1.3261428	3.2222466	–11.3537185
H	–2.7008301	2.6713620	–9.7817055
H	1.4841448	2.4467766	–8.7833149
H	2.0721027	3.2380136	–11.0698406
H	–2.1193492	3.4619957	–12.0635412
H	0.2692324	3.7385701	–12.7192876
C	–5.6566787	–1.4737049	–6.3323796
C	–7.9090890	–2.7249016	–7.4531589
C	–6.6323124	–0.7156687	–7.0031614
C	–5.8207367	–2.8641177	–6.2339633
C	–6.9393954	–3.4857153	–6.7931084
C	–7.7525477	–1.3393350	–7.5557808
H	–6.5007324	0.3661812	–7.0622401
H	–5.0565143	–3.4549231	–5.7266927
H	–7.0508429	–4.5685971	–6.7187398
H	–8.5075460	–0.7397968	–8.0669212
H	–8.7829730	–3.2116151	–7.8887724
C	–2.9944833	–0.2970059	0.0715962
C	–3.6933105	–1.0060574	2.7041184
C	–2.1890119	–1.1757899	0.8124640
C	–4.1614705	0.2128216	0.6650306
C	–4.5076893	–0.1376651	1.9713326
C	–2.5348151	–1.5258469	2.1196481
H	–1.2900226	–1.5875540	0.3513681
H	–4.7934015	0.8856250	0.0829812
H	–5.4148818	0.2711843	2.4192088
H	–1.8999767	–2.2129880	2.6812926
H	–3.9624979	–1.2800369	3.7251528
C	0.9034956	1.0439952	–5.4237465
C	2.2511051	1.3505974	–5.8550363
O	2.6226370	2.4680313	–6.2301075
O	3.1186663	0.2904319	–5.8139264
C	0.3843058	–0.1958337	–5.0202484
O	1.2099631	–1.2671619	–4.9938988
O	–0.8299268	–0.3846922	–4.6966883
C	4.4548536	0.6037070	–6.2396970
H	5.0125746	–0.3352729	–6.1499981
H	4.9038154	1.3789537	–5.6018942
H	4.4678978	0.9597950	–7.2800919
C	0.6015768	–2.5046362	–4.5766960
H	1.4152011	–3.2376789	–4.5987058
H	–0.2023284	–2.8024039	–5.2643760
H	0.1867416	–2.4201911	–3.5624859
C	–3.5402144	3.0059395	–4.3273521
C	–4.8792877	2.3761687	–4.5506785
O	–5.3750080	2.2571817	–5.6687821
O	–5.5259925	1.9538649	–3.4361333
C	–6.8387338	1.4076971	–3.6738241
H	–6.8013056	0.5874422	–4.4018206
H	–7.5161887	2.1877047	–4.0504214
H	–7.1743009	1.0361388	–2.7004289
C	–3.1226070	3.8553791	–5.5360535
H	–3.2459558	3.2687847	–6.4523659
H	–2.0865923	4.1737920	–5.4313508
C	–4.0819243	4.9799959	–5.4487794
C	–3.1136060	3.6024316	–3.0307523
O	–2.2333060	4.4542055	–2.9407975
O	–3.7448684	3.1132263	–1.9318249
C	–3.2700787	3.6578573	–0.6845536
H	–3.4502962	4.7409241	–0.6405059
H	–3.8376022	3.1372571	0.0936514
H	–2.1965736	3.4648766	–0.5581632
H	–5.1150623	4.7346887	–5.7064309
C	–3.8236915	6.2947271	–4.9920804
C	–3.3980316	8.9540832	–4.1322413
C	–4.9057353	7.2169915	–4.8748701
C	–2.5188421	6.7589104	–4.6589866
C	–2.3183319	8.0658607	–4.2376105
C	–4.6939420	8.5213250	–4.4555510
H	–5.9133951	6.8768840	–5.1229860
H	–1.6820256	6.0673001	–4.7086042
H	–1.3125492	8.3996286	–3.9783064
H	–5.5355186	9.2105998	–4.3720100
H	–3.2327446	9.9788687	–3.7965457

TS14 (I^{E-IY}-I^{E-T}) (Q):

119 atoms

C	2.9799120	4.6796796	–5.5132042
C	2.4687522	4.5495813	–6.7757580
C	1.4606031	3.5123989	–6.7158132
C	2.2855870	3.7235447	–4.6705421
N	1.3539122	3.0586752	–5.4242684
C	2.5379293	3.4943603	–3.3014175
C	1.9068370	2.5161489	–2.5019129
N	0.8151100	1.7540645	–2.8532416
C	0.5368849	0.9266167	–1.7773056
C	2.3496994	2.1391626	–1.1739659
C	1.5106496	1.1543492	–0.7327981
C	–0.6197063	0.1246741	–1.6682972
C	–1.4428240	–0.1842594	–2.7743808
N	–0.9501763	–0.3787623	–4.1017108
C	–3.2461587	–0.5582314	–4.0964055
C	–2.8440493	–0.2913248	–2.7954048
C	–1.2503440	0.1112831	–7.1369504
N	–0.5044165	1.1838828	–6.6962513
C	–0.0382012	1.8297966	–7.8087202
C	–0.4844625	1.1375653	–9.0038361
C	–1.1968698	0.0515368	–8.5869074
C	0.7820556	2.9803934	–7.8237190
C	–2.0870974	–0.6862530	–6.3247521
C	–2.1047784	–0.5934686	–4.9114125
H	3.7569074	5.3615782	–5.1830518
H	2.7606467	5.0878795	–7.6720021
H	3.2139396	2.5518496	–0.6627312
H	1.5680305	0.6007534	0.1991768
H	–4.2642667	–0.6053018	–4.4664336
H	–3.4899711	–0.1001337	–1.9461833
H	–0.2538780	1.4290070	–10.0233483
H	–1.6266876	–0.7325118	–9.2013224
Co	0.0652132	1.6858063	–4.7547867
C	3.5643822	4.3463228	–2.6368885
C	5.4686612	5.9838681	–1.3613801
C	4.9168457	4.2986367	–3.0125031
C	3.1836752	5.2231060	–1.6067153
C	4.1262929	6.0367489	–0.9751052
C	5.8607953	5.1105304	–2.3801905
H	5.2220889	3.6097402	–3.8013782
H	2.1345991	5.2584966	–1.3077564
H	3.8113157	6.7155333	–0.1808867
H	6.9086085	5.0555956	–2.6797018
H	6.2068352	6.6178036	–0.8680986
C	0.9647504	3.6963794	–9.1203504
C	1.2744369	5.1222072	–11.5205474
C	0.3036605	4.9207645	–9.3094923
C	1.7865544	3.1976948	–10.1414542
C	1.9392735	3.9064538	–11.3358843
C	0.4579750	5.6275367	–10.5042493
H	–0.3313880	5.3000506	–8.5068432
H	2.3113650	2.2533677	–9.9883252
H	2.5845854	3.5106848	–12.1218354
H	–0.0636997	6.5760509	–10.6424512
H	1.3947632	5.6753676	–12.4532685
C	–3.1120058	–1.5820784	–6.9013037
C	–5.0587960	–3.3682058	–7.8919554
C	–3.9118644	–1.2382863	–8.0101737
C	–3.3243357	–2.8361201	–6.2864365
C	–4.2841945	–3.7175803	–6.7816808
C	–4.8714928	–2.1228457	–8.5002973
H	–3.7954221	–0.2581782	–8.4704307
H	–2.7194095	–3.1087828	–5.4187033
H	–4.4250594	–4.6854864	–6.2982745
H	–5.4870588	–1.8326261	–9.3532266
H	–5.8108691	–4.0584209	–8.2771798
C	–1.1259751	–0.2969918	–0.3486815
C	–2.2228949	–1.1095208	2.1187142
C	–1.6976353	–1.5791376	–0.2014008
C	–1.1181286	0.5673128	0.7659647
C	–1.6608700	0.1644777	1.9860463
C	–2.2378577	–1.9768877	1.0209488
H	–1.6998929	–2.2541444	–1.0605585
H	–0.7090688	1.5724554	0.6560969
H	–1.6579141	0.8528626	2.8326963
H	–2.6684651	–2.9746170	1.1192629
H	–2.6473177	–1.4240660	3.0733411
C	0.1321536	–1.3669481	–4.2539641
C	–0.2294847	–2.6969267	–3.8355448
O	–1.3433715	–3.0059736	–3.3844271
O	0.7616692	–3.6354556	–3.9673341
C	1.3581471	–0.9022418	–4.7736608
O	2.3657494	–1.8023180	–4.9102134

O	1.5689035	0.2913571	–5.1257747
C	0.3870953	–4.9551013	–3.5436377
H	0.1047075	–4.9679117	–2.4806633
H	1.2766303	–5.5735153	–3.7094075
H	–0.4598267	–5.3379412	–4.1318972
C	3.5906248	–1.2662101	–5.4413549
H	3.9911806	–0.4739083	–4.7929363
H	3.4397861	–0.8530203	–6.4488025
H	4.2796266	–2.1174510	–5.4758565
C	–1.6740075	3.1641163	–4.4089808
C	–2.9788707	2.7073102	–4.9497918
O	–3.9331821	2.3148801	–4.2864134
O	–2.9742428	2.7160924	–6.3029508
C	–1.1314509	4.4579713	–4.8919658
O	–1.2518061	4.8778055	–6.0309179
O	–0.3997130	5.1017360	–3.9307782
C	0.2257928	6.3363844	–4.3408267
H	0.7166095	6.2131855	–5.3129143
H	0.9682687	6.5563371	–3.5663954
H	–0.5233617	7.1385970	–4.4006439
C	–4.1731478	2.1994225	–6.9133099
H	–3.9675553	2.2119741	–7.9885249
H	–5.0379573	2.8336512	–6.6735799
H	–4.3713542	1.1762119	–6.5686678
I	–1.9185228	3.3891673	–2.1267229
C	–3.9216832	3.1486856	–1.4496810
C	–6.4939596	2.8119254	–0.4924312
C	–4.1582660	2.1588480	–0.4955942
C	–4.9332888	3.9718110	–1.9423654
C	–6.2292788	3.7909619	–1.4560613
C	–5.4616935	2.0034940	–0.0114088
H	–3.3543435	1.5191268	–0.1295002
H	–4.7225700	4.7211440	–2.7033763
H	–7.0353315	4.4193304	–1.8372246
H	–5.6614075	1.2364309	0.7379203
H	–7.5098976	2.6775514	–0.1192219

TS15 (I^{B-T}-*c*-I^{B-B}):

107 atoms

C	–1.2996625	1.6023853	–2.7978233
C	–1.4513576	2.0162157	–4.1009079
C	–0.7803867	1.0821934	–4.9400747
C	–0.5102561	0.4150594	–2.7910582
N	–0.0764782	0.1986668	–4.1098049
C	–0.4617465	–0.4929934	–1.7199112
C	–0.1595802	–1.8669188	–1.7828738
N	0.0569335	–2.6502571	–2.9150936
C	0.5234809	–3.8739739	–2.4571676
C	0.1147998	–2.6521637	–0.6007249
C	0.5407380	–3.8782355	–1.0126672
C	1.0341358	–4.9263139	–3.2392410
C	1.1854200	–4.8861828	–4.6311422
N	0.7908518	–3.8354997	–5.4187579
C	1.5675231	–5.5469398	–6.7579911
C	1.6847287	–5.9651524	–5.4649038
C	–0.1239210	–2.2637553	–7.7903262
N	–0.5599785	–1.5840014	–6.6203414
C	–0.9471803	–0.2713736	–7.0608157
C	–0.9462687	–0.2675530	–8.4887715
C	–0.4263200	–1.4589530	–8.9246608
C	–1.0783402	0.8987259	–6.3049735
C	0.5783119	–3.4718694	–7.8380427
C	0.9911396	–4.2146981	–6.7181407
H	–1.7924377	2.0030008	–1.9189390
H	–2.0891723	2.8108675	–4.4713938
H	0.0591156	–2.2774219	0.4152827
H	0.8810602	–4.7047602	–0.3984667
H	1.8181602	–6.0937261	–7.6613798
H	2.0452470	–6.9226585	–5.1036458
H	–1.2015901	0.5945029	–9.0949385
H	–0.2086627	–1.7409992	–9.9491564
Co	–0.1326274	–2.1999750	–4.7772564
C	1.0552613	–0.6220124	–4.5237716
C	1.7698689	–0.0872808	–5.7591283
C	2.1101968	–0.8105642	–3.4475146
O	2.2490854	–0.1176545	–2.4550331
O	1.8087758	1.0806552	–6.1049976
O	2.4019080	–1.0831107	–6.4173119
O	2.9025290	–1.8701309	–3.7360496
C	3.1053401	–0.6728123	–7.6084487
H	3.8500504	0.1012836	–7.3797631
H	3.5869333	–1.5810690	–7.9832953
H	2.3917192	–0.2849522	–8.3484489
C	3.8715875	–2.1921369	–2.7177252
H	4.4489421	–3.0277086	–3.1259966
H	3.3551048	–2.4951342	–1.7956404
H	4.5231129	–1.3343215	–2.5028717
C	–1.7951033	–2.5706662	–5.5994436
C	–0.7776655	0.0872123	–0.3875891
C	–1.3528668	1.2339257	2.1106926
C	–1.8518853	–0.3870217	0.3828074
C	0.0050041	1.1436969	0.1077316
C	–0.2794086	1.7093039	1.3514258
C	–2.1389882	0.1853677	1.6228300
H	–2.4634847	–1.2026076	–0.0056632
H	0.8464361	1.4945893	–0.4909863
H	0.3422274	2.5213717	1.7312954
H	–2.9824407	–0.1842665	2.2077449
H	–1.5769174	1.6793460	3.0809818
C	0.8732407	–4.0370223	–9.1846283
C	1.4230036	–5.1256629	–11.7154603
C	2.1969163	–4.1666796	–9.6322830
C	–0.1748088	–4.4634518	–10.0170358
C	0.1017026	–5.0059990	–11.2735013
C	2.4707705	–4.7046259	–10.8914690
H	3.0104562	–3.8425659	–8.9813386
H	–1.1997734	–4.3724813	–9.6548921
H	–0.7194401	–5.3418624	–11.9087105
H	3.5040411	–4.7925181	–11.2307644
H	1.6360442	–5.5475089	–12.6986756
C	–1.6400190	2.0931035	–6.9907900
C	–2.7057433	4.3743444	–8.2296127
C	–0.8951229	3.2819569	–7.0477511
C	–2.9242802	2.0591216	–7.5575526
C	–3.4544786	3.1944205	–8.1721780
C	–1.4257584	4.4144508	–7.6679718
H	0.1047979	3.2935455	–6.6119349
H	–3.5019029	1.1350311	–7.5017114
H	–4.4566814	3.1603994	–8.6018596
H	–0.8361592	5.3310786	–7.7164973
H	–3.1200739	5.2613335	–8.7108792
C	1.4750928	–6.1607549	–2.5300189
C	2.3024580	–8.4963973	–1.1983129
C	0.5389575	–6.9864598	–1.8874912
C	2.8311606	–6.5211648	–2.4949318
C	3.2424671	–7.6800121	–1.8333029
C	0.9494172	–8.1463917	–1.2277929
H	–0.5158387	–6.7093371	–1.9141803
H	3.5613121	–5.8794457	–2.9902064
H	4.3008929	–7.9435977	–1.8098064
H	0.2092708	–8.7810782	–0.7383175
H	2.6231473	–9.4020121	–0.6817710
C	–3.0598438	–1.9493890	–5.1928457
O	–4.0964637	–2.6059141	–5.1223895
O	–2.9820356	–0.6480116	–4.8163153
C	–2.0909939	–3.8382038	–6.3750918
O	–2.3871721	–3.9094611	–7.5536165
O	–1.9923153	–4.9091818	–5.5585485
C	–4.2276915	–0.0588644	–4.3936855
H	–5.0099962	–0.2162009	–5.1483575
H	–4.0103254	1.0061294	–4.2681373
H	–4.5552560	–0.4995609	–3.4423987
C	–2.2725242	–6.1780303	–6.1905405
H	–2.1748829	–6.9240454	–5.3960352
H	–1.5407352	–6.3658775	–6.9882560
H	–3.2858348	–6.1836889	–6.6138735

TS16 (I^{B-T}-*t*-I^{B-B}):

107 atoms

C	–1.2566133	1.8237605	–3.1062981
C	–1.4517969	2.1134045	–4.4296100
C	–0.7265947	1.1645889	–5.2168133
C	–0.4173623	0.6713566	–3.0186049
N	0.0072631	0.3466748	–4.3229013
C	–0.2963174	–0.1309348	–1.8833151
C	–0.0083116	–1.5119754	–1.8666542
N	0.1391593	–2.3676701	–2.9457398
C	0.4061604	–3.6196616	–2.4086244
C	0.1705625	–2.2470467	–0.6344666
C	0.4142679	–3.5449674	–0.9674259
C	0.6576655	–4.8075915	–3.1160794
C	0.6578727	–4.9248936	–4.5073502
N	0.2423301	–3.9359632	–5.3989337
C	1.2237829	–5.6523012	–6.5732182
C	1.2325461	–6.0056456	–5.2488696
C	0.1132071	–2.2411020	–7.8697389
N	–0.1825853	–1.4396717	–6.7757817
C	–0.6117369	–0.2297904	–7.2896926
C	–0.6092177	–0.2835457	–8.7307260
C	–0.1457524	–1.5164084	–9.0888330
C	–0.9404065	0.9414525	–6.5750766
C	0.5378204	–3.5814698	–7.8360372
C	0.6215750	–4.3559891	–6.6782370
H	–1.7543157	2.2693434	–2.2519642
H	–2.1406030	2.8376094	–4.8500268
H	0.1406637	–1.8100278	0.3574427
H	0.5881518	–4.3828549	–0.3015030
H	1.6467526	–6.2030223	–7.4066470
H	1.6580048	–6.8976937	–4.8011265
H	–0.8842914	0.5398693	–9.3805887
H	–0.0113283	–1.9118115	–10.0896093
Co	–0.0448996	–1.9720943	–4.8715180
C	1.2142041	–0.4270276	–4.6260233
C	1.9686372	0.0358955	–5.8554590
C	2.2291469	–0.4686125	–3.4940698
O	2.4158371	0.4077113	–2.6679095
O	1.9115855	1.1408937	–6.3635139
O	2.7621036	–0.9603014	–6.3244194
O	2.9532992	–1.6091045	–3.5460005
C	3.4756827	–0.6366683	–7.5342263
H	4.1057414	0.2530304	–7.3988150
H	4.0890231	–1.5173921	–7.7512552
H	2.7614732	–0.4492651	–8.3494622
C	3.9509851	–1.7371451	–2.5116536
H	4.4646425	–2.6803825	–2.7228919
H	3.4656514	–1.7712634	–1.5261630
H	4.6557381	–0.8947579	–2.5366745
C	–1.5064878	–3.1435648	–5.0619907
C	–0.5573995	0.5563409	–0.5898901
C	–1.0218817	1.9175947	1.8227660
C	–1.6172824	0.1762414	0.2494016
C	0.2632708	1.6315886	–0.2104055
C	0.0339365	2.3036296	0.9915079
C	–1.8486038	0.8537786	1.4475571
H	–2.2630194	–0.6488711	–0.0543693
H	1.0885454	1.9124977	–0.8660197
H	0.6843029	3.1302562	1.2814789
H	–2.6808159	0.5557938	2.0871233
H	–1.2023816	2.4457359	2.7601544
C	0.9007677	–4.2350587	–9.1220811
C	1.5794123	–5.4823514	–11.5522591
C	1.9467665	–3.7359526	–9.9157207
C	0.2048018	–5.3733662	–9.5620898
C	0.5394583	–5.9905376	–10.7684635
C	2.2837344	–4.3545154	–11.1205593
H	2.4965710	–2.8584384	–9.5728430
H	–0.6012554	–5.7677474	–8.9419096
H	–0.0156439	–6.8697222	–11.0991004
H	3.1035842	–3.9583954	–11.7216608
H	1.8422427	–5.9651254	–12.4944284
C	–1.6299890	2.0257143	–7.3230217
C	–2.9471276	4.0770432	–8.7153078
C	–1.0573959	3.3046713	–7.4113293
C	–2.8704783	1.7851417	–7.9376002
C	–3.5251712	2.8064710	–8.6274607
C	–1.7121766	4.3229171	–8.1070899
H	–0.0888706	3.4791630	–6.9406096
H	–3.3175982	0.7934009	–7.8515192
H	–4.4935039	2.6120896	–9.0913069
H	–1.2547038	5.3109049	–8.1785821
H	–3.4594982	4.8744766	–9.2557189
C	0.9625672	–6.0457763	–2.3451340
C	1.5058886	–8.4085781	–0.9259039
C	0.0710206	–7.1296331	–2.4014569
C	2.1310085	–6.1614281	–1.5761129
C	2.4016091	–7.3362670	–0.8716367
C	0.3412078	–8.3014742	–1.6917199
H	–0.8368448	–7.0282435	–2.9971773
H	2.8276972	–5.3224676	–1.5408916
H	3.3166176	–7.4168204	–0.2827756
H	–0.3633855	–9.1335586	–1.7351129
H	1.7165657	–9.3257873	–0.3739626
C	–2.1612847	–3.9490947	–3.9692776
O	–2.2046338	–5.1665585	–3.9164085
O	–2.7312704	–3.1299807	–3.0591646
C	–2.4194537	–3.0615124	–6.2388356
O	–3.2785803	–2.1952790	–6.2788921
O	–2.2495599	–4.0040364	–7.1908721
C	–3.3737061	–3.8073633	–1.9542462
H	–4.1301959	–4.5166421	–2.3153295
H	–3.8348073	–3.0135751	–1.3590422
H	–2.6191258	–4.3460068	–1.3646001
C	–3.0267222	–3.7856364	–8.3944610
H	–2.7659132	–4.6124830	–9.0619003
H	–2.7437012	–2.8251220	–8.8472777
H	–4.1005111	–3.7860171	–8.1683543

TS17 (*c*-I^{B-B}-*c*-I^{B-E}):

107 atoms

C	–0.7730518	1.9441026	–3.3342079
C	–0.7197210	2.2241521	–4.6670285
C	–0.4346029	0.9732021	–5.3450946
C	–0.5360965	0.5201057	–3.1908446
N	–0.3243049	–0.0440494	–4.4241634
C	–0.5560729	–0.1929959	–1.9828488
C	–0.2686507	–1.5521287	–1.8529252
N	0.3331744	–2.4092475	–2.8741151
C	0.1865600	–3.7924467	–2.3116754
C	–0.5349044	–2.3303796	–0.7157083
C	–0.2289199	–3.6494696	–0.9710867
C	0.2549843	–5.0290405	–2.9651319
C	0.1186675	–5.2994175	–4.3495024
N	–0.4445608	–4.4668240	–5.3086428
C	0.7160772	–6.0984118	–6.3773348
C	0.7479043	–6.3806819	–5.0319907
C	0.2277863	–2.6049508	–7.7458263
N	0.0873484	–1.6569325	–6.7255208
C	–0.0608974	–0.4321980	–7.3542928
C	0.0444362	–0.5935714	–8.7838029
C	0.2260285	–1.9221096	–9.0214950
C	–0.3033099	0.8038024	–6.7253781
C	0.2595916	–4.0147628	–7.6746773

C	0.0592108	–4.8406853	–6.5527954
H	–0.9524654	2.6315964	–2.5140815
H	–0.8530633	3.1836947	–5.1556608
H	–0.9970972	–1.9397344	0.1843318
H	–0.4249051	–4.4911087	–0.3145244
H	1.2173803	–6.6337796	–7.1756635
H	1.2756559	–7.1864825	–4.5348048
H	–0.0238365	0.2104822	–9.5083031
H	0.2964025	–2.4151252	–9.9844869
Co	0.0675778	–1.9138463	–4.8163391
C	1.7175291	–1.9717644	–3.2241666
C	–1.3000216	–3.3315704	–5.0355378
C	0.5947878	–4.7546726	–8.9219066
C	1.2043112	–6.2095939	–11.2458089
C	–0.3139598	–5.6975475	–9.4301105
C	1.8152428	–4.5543889	–9.5876878
C	2.1186834	–5.2796756	–10.7404876
C	–0.0126356	–6.4149800	–10.5889993
H	–1.2622269	–5.8407561	–8.9107327
H	2.5253361	–3.8324297	–9.1825248
H	3.0744069	–5.1235663	–11.2429696
H	–0.7318227	–7.1349277	–10.9822735
H	1.4412442	–6.7740455	–12.1487903
C	0.4480833	–6.2215915	–2.0990554
C	0.8054661	–8.4924107	–0.4777006
C	–0.4111563	–7.3285977	–2.2174710
C	1.4919131	–6.2720678	–1.1581616
C	1.6690282	–7.3987596	–0.3554024
C	–0.2349309	–8.4534855	–1.4112239
H	–1.2202472	–7.2886764	–2.9478829
H	2.1663139	–5.4188033	–1.0711826
H	2.4895698	–7.4273612	0.3629330
H	–0.9144264	–9.3015318	–1.5085279
H	0.9448862	–9.3730609	0.1506974
C	–0.9758383	0.5293424	–0.7491326
C	–1.7752542	1.9019810	1.5676922
C	–2.2643944	1.0801601	–0.6564001
C	–0.0930252	0.6661313	0.3350280
C	–0.4923815	1.3524802	1.4835519
C	–2.6614304	1.7613420	0.4956396
H	–2.9533820	0.9569240	–1.4930032
H	0.9048384	0.2325621	0.2557222
H	0.2042180	1.4607456	2.3164159
H	–3.6679115	2.1777924	0.5585907
H	–2.0850774	2.4359143	2.4673052
C	–0.4632121	2.0090501	–7.5899579
C	–0.7792267	4.2928331	–9.2011437
C	0.5158751	3.0138064	–7.6035016
C	–1.6034172	2.1645842	–8.3933623
C	–1.7610713	3.2979319	–9.1933012
C	0.3594186	4.1475852	–8.4041343
H	1.4032373	2.8957548	–6.9800984
H	–2.3677114	1.3861752	–8.3821358
H	–2.6553433	3.4066943	–9.8087015
H	1.1313774	4.9184222	–8.4072574
H	–0.9017083	5.1785285	–9.8259639
C	2.3963784	–1.0377524	–2.3095219
O	2.3208267	–1.0229364	–1.0853056
O	3.1427325	–0.1323136	–3.0038703
C	2.4871187	–2.7336280	–4.1695647
O	2.0219769	–3.4296300	–5.0854098
O	3.8373859	–2.6391016	–3.9776135
C	4.6313095	–3.1949203	–5.0431380
H	4.3788151	–2.7231454	–6.0034472
H	4.4696569	–4.2783013	–5.1285178
H	5.6706385	–2.9807770	–4.7717418
C	–2.2281687	–3.5152790	–3.8280678
O	–2.6154749	–4.8149139	–3.6801439
O	–2.6572027	–2.6131897	–3.1400299
H	–4.3864513	–4.4936090	–2.5957186
C	–3.4476763	–5.0590968	–2.5253694
H	–3.6400805	–6.1367593	–2.5265610
H	–2.9157979	–4.7616883	–1.6108113
C	–2.2645230	–3.0198781	–6.1808196
O	–2.5258122	–3.7488494	–7.1196057
O	–2.8228457	–1.8009543	–5.9978830
C	–3.6707732	–1.3577537	–7.0755022
H	–4.0468442	–0.3793683	–6.7602016
H	–4.4987853	–2.0596800	–7.2444587
H	–3.0807444	–1.2679830	–7.9994083
C	3.9607852	0.7251506	–2.1850605
H	4.5187800	1.3531392	–2.8877974
H	4.6486487	0.1323430	–1.5653305
H	3.3348478	1.3446414	–1.5273558

TS18 (*t*-I$^{B–B}$-*t*-I$^{B–E}$):

107 atoms

C	–1.3283479	1.3803301	–3.3766514
C	–1.4796316	1.5604676	–4.7390478
C	–0.6454855	0.6510649	–5.4126651
C	–0.4545562	0.2974396	–3.1679812
N	0.0407129	–0.1654308	–4.4354225
C	–0.3438167	–0.4179752	–1.9696811
C	–0.2777773	–1.8168653	–1.9149934
N	–0.3771312	–2.7008785	–2.9851683
C	–0.4285578	–3.9697947	–2.4156416
C	–0.2498865	–2.5427458	–0.6685585
C	–0.3834475	–3.8584491	–0.9706112
C	–0.4118280	–5.2321183	–3.0441908
C	–0.3048733	–5.4765101	–4.4197463
N	–0.5603637	–4.5473264	–5.4372519
C	0.6372772	–6.2739521	–6.3197467
C	0.3674460	–6.5850446	–5.0073828
C	0.4584781	–2.7774637	–7.7607391
N	0.0731883	–1.8826416	–6.7717820
C	0.0185800	–0.6373053	–7.3876499
C	0.4429936	–0.7457134	–8.7594041
C	0.7238701	–2.0582618	–8.9884647
C	–0.4835199	0.5306642	–6.7981730
C	0.5084728	–4.1810539	–7.6849869
C	0.1287551	–4.9701195	–6.5919218
H	–1.8855742	1.8679360	–2.5826457
H	–2.1664279	2.2347432	–5.2392910
H	–0.1388007	–2.0929138	0.3113661
H	–0.4338141	–4.6920355	–0.2800123
H	1.2467127	–6.8379698	–7.0171695
H	0.7181013	–7.4451050	–4.4477042
H	0.5283400	0.0882375	–9.4476539
H	1.0505886	–2.5152046	–9.9158046
Co	–0.2421713	–2.2065647	–4.8741980
C	1.5068360	–0.2729648	–4.6413551
C	–1.5707705	–3.5018287	–5.3395582
C	–2.3108335	–3.2316443	–6.6515163
O	–2.3975226	–3.9988939	–7.5902720
O	–2.9190373	–2.0268288	–6.5947836
C	–2.7107802	–3.7509043	–4.3354468
O	–3.2587249	–2.8881918	–3.6881814
O	–3.1240692	–5.0478899	–4.3707555
C	–3.6618501	–1.6706941	–7.7794362
H	–3.0061756	–1.7082989	–8.6604202
H	–4.0170616	–0.6514203	–7.6008098
H	–4.5046256	–2.3589990	–7.9321793
C	–4.2088672	–5.3521356	–3.4646489
H	–3.8812027	–5.2082106	–2.4256611
H	–4.4590138	–6.4015690	–3.6504258
H	–5.0723248	–4.7040312	–3.6633212
C	1.0581436	–4.9289123	–8.8489035
C	2.0749556	–6.3853164	–11.0245376
C	0.2501770	–5.8601474	–9.5212522
C	2.3824907	–4.7390891	–9.2757079
C	2.8873881	–5.4638981	–10.3565067
C	0.7555776	–6.5804750	–10.6049380
H	–0.7796271	–5.9961791	–9.1880482
H	3.0113685	–4.0218627	–8.7461343
H	3.9201678	–5.3134395	–10.6743199
H	0.1157360	–7.2939729	–11.1263370
H	2.4700646	–6.9506743	–11.8697387
C	–0.3201788	–6.4604322	–2.2016728
C	–0.1467932	–8.8344599	–0.7031167
C	–1.3110874	–7.4491136	–2.3104289
C	0.7732939	–6.6889823	–1.3496351
C	0.8575939	–7.8664996	–0.6051518
C	–1.2301088	–8.6240201	–1.5606658
H	–2.1423653	–7.2850387	–2.9965442
H	1.5617118	–5.9377746	–1.2875021
H	1.7159009	–8.0328140	0.0473585
H	–2.0133341	–9.3783917	–1.6486206
H	–0.0801877	–9.7536407	–0.1195705
C	–0.5112174	0.3842764	–0.7322580
C	–0.8186680	1.9971979	1.5511974
C	–1.5377693	0.1252179	0.1932702
C	0.3435015	1.4781591	–0.5076234
C	0.1957129	2.2726240	0.6296849
C	–1.6884134	0.9256127	1.3260500
H	–2.2298756	–0.6955273	0.0018663
H	1.1303278	1.6889422	–1.2332626
H	0.8751728	3.1094830	0.7967194
H	–2.4956211	0.7190869	2.0303337
H	–0.9370602	2.6208929	2.4383520
C	–0.8999675	1.6686279	–7.6491772
C	–1.7189352	3.8421347	–9.2418481
C	–0.4843217	2.9788496	–7.3414090
C	–1.7314368	1.4692584	–8.7676831
C	–2.1375489	2.5455228	–9.5561183
C	–0.8914873	4.0519718	–8.1342792
H	0.1871788	3.1227396	–6.4944438
H	–2.0671417	0.4600971	–9.0058022
H	–2.7896162	2.3727696	–10.4137289
H	–0.5504319	5.0594495	–7.8908279
H	–2.0353553	4.6843914	–9.8589418
C	2.1630859	0.9336973	–5.0336737
O	1.6222518	2.0434201	–5.1632490
O	3.5263259	0.7912547	–5.1984994
C	2.2594881	–1.4871099	–4.2905699
O	2.2686835	–2.0910203	–3.2184848
O	3.0511194	–1.8954481	–5.3390439
C	4.2109972	2.0074159	–5.5287747
H	3.8341354	2.4339557	–6.4700679
H	5.2652010	1.7261541	–5.6346721
H	4.0952045	2.7609565	–4.7355351
C	3.9481725	–2.9749448	–5.0268726
H	4.5808744	–2.7279601	–4.1622964
H	4.5606109	–3.1159400	–5.9245016
H	3.3844541	–3.8920096	–4.7991086

TS19 (*c*-I$^{B–E}$-*c*-I$^{E–E}$):

107 atoms

C	3.2922752	3.0700968	–5.4531475
C	2.8766945	2.7467685	–6.7243378
C	1.4579570	2.6028233	–6.7210450
C	2.1461266	3.1373617	–4.6145951
N	1.0070538	2.8707446	–5.4177853
C	2.0667082	3.2750602	–3.2228342
C	1.0901135	2.5482640	–2.5078685
N	0.6508433	1.2067338	–2.9154674
C	–0.2411632	0.7961405	–1.8634108
C	0.4736767	2.8732862	–1.2991370
C	–0.3368569	1.8133781	–0.9072616
C	–0.9523788	–0.4245330	–1.8563260
C	–1.4700390	–1.0126816	–3.0210377
N	–1.5400162	–0.3938754	–4.2582469
C	–2.8472221	–2.2925824	–4.2878272
C	–2.2388313	–2.2433763	–3.0699788
C	–2.2664169	0.2755310	–7.0569908
N	–1.1762674	0.9913690	–6.6273598
C	–0.6154984	1.5996000	–7.7364718
C	–1.4871801	1.3767494	–8.8674454
C	–2.5185594	0.5829232	–8.4446127
C	0.6535562	2.2171513	–7.8096860
C	–2.8657463	–0.7580796	–6.3071692
C	–2.4292958	–1.1146970	–5.0228114
H	4.3102807	3.1302743	–5.0817718
H	3.5005884	2.5252363	–7.5835893
H	0.5853918	3.8341651	–0.8062199
H	–0.9963909	1.7735917	–0.0463344
H	–3.5031404	–3.0647615	–4.6767626
H	–2.3006772	–2.9673794	–2.2645160
H	–1.3323365	1.7971742	–9.8554797
H	–3.3585407	0.2150600	–9.0239300
Co	–0.5251313	1.1038795	–4.8590806
C	3.0445601	4.0992038	–2.5040151
C	4.9393546	5.6707211	–1.1406758
C	3.5313082	3.6996790	–1.2403904
C	3.5285595	5.2965878	–3.0716745
C	4.4679109	6.0722774	–2.3954425
C	4.4676511	4.4836607	–0.5690571
H	3.1928723	2.7508876	–0.8186809
H	3.1394787	5.6196598	–4.0382993
H	4.8252054	7.0013107	–2.8423424
H	4.8447188	4.1578380	0.4016509
H	5.6735299	6.2801291	–0.6115580
C	1.2498506	2.4211795	–9.1524500
C	2.4269751	2.8192737	–11.6747450
C	1.7481863	3.6861398	–9.5161567
C	1.3568477	1.3583648	–10.0683477
C	1.9430206	1.5563947	–11.3187092
C	2.3266915	3.8814119	–10.7705995
H	1.6426415	4.5084682	–8.8084802
H	0.9921044	0.3720021	–9.7794101
H	2.0307570	0.7203369	–12.0142390
H	2.6959368	4.8704421	–11.0463028
H	2.8832583	2.9739531	–12.6536634
C	–3.9575651	–1.5581732	–6.9235906
C	–6.0330657	–3.0879092	–8.0553819
C	–5.2301046	–1.5931383	–6.3280852
C	–3.7407699	–2.3068563	–8.0929677
C	–4.7695938	–3.0655679	–8.6534690
C	–6.2597440	–2.3497879	–6.8903573
H	–5.4043664	–1.0131859	–5.4206372
H	–2.7506323	–2.2995775	–8.5506185
H	–4.5812622	–3.6480459	–9.5566860
H	–7.2436137	–2.3594257	–6.4186525
H	–6.8369348	–3.6804407	–8.4943160
C	–1.2726001	–0.9706735	–0.5186049
C	–1.8175582	–1.9578090	2.0623738
C	–0.2472271	–1.0690786	0.4446812
C	–2.5794156	–1.3498061	–0.1545221
C	–2.8471599	–1.8412961	1.1229385
C	–0.5202222	–1.5642763	1.7196232
H	0.7621583	–0.7504354	0.1759575
H	–3.3897673	–1.2269938	–0.8737513
H	–3.8671745	–2.1206889	1.3915960
H	0.2867095	–1.6445234	2.4496620
H	–2.0288137	–2.3434245	3.0608865
C	1.7680891	0.2673553	–3.1765750
C	2.6118711	–0.0033787	–2.0399485
O	2.4568367	0.4993080	–0.9173193
O	3.6245187	–0.8953546	–2.2757506
C	1.9238607	–0.1853884	–4.5050221
O	3.0347906	–0.9008573	–4.8056401
O	1.0992883	0.0447733	–5.4384940
C	4.4650557	–1.1513667	–1.1392187

H	4.9441211	–0.2279187	–0.7826593
H	5.2204300	–1.8610165	–1.4951090
H	3.8904656	–1.5882657	–0.3094398
C	3.1481612	–1.2932825	–6.1865020
H	4.0981825	–1.8352449	–6.2476104
H	3.1632089	–0.4127133	–6.8450143
H	2.3144948	–1.9441267	–6.4850611
C	–0.3144281	3.4286645	–5.2532743
C	–1.1195599	3.4880121	–4.0136969
O	–1.7656525	2.5363448	–3.5546586
O	–1.2164243	4.7313593	–3.4886850
C	–0.6938946	4.4336343	–6.2516058
O	0.0350192	4.9929956	–7.0646463
O	–2.0446691	4.6672735	–6.2010137
C	–2.2257423	4.8853474	–2.4657821
H	–2.0035777	4.2334394	–1.6102807
H	–3.2144904	4.6256054	–2.8685312
H	–2.1874109	5.9397571	–2.1742380
C	–2.5076951	5.7146307	–7.0722135
H	–2.0359210	6.6741845	–6.8156360
H	–3.5907093	5.7655401	–6.9172976
H	–2.2784914	5.4764842	–8.1200278

TS20 (t-I^{B-E}-t-I^{E-E}):

107 atoms

C	2.0605874	4.3668407	–5.4662540
C	1.6635054	3.9579698	–6.7222409
C	1.3072242	2.5949511	–6.6560686
C	1.9774097	3.2665098	–4.5899558
N	1.5294221	2.1114407	–5.3233075
C	2.1703933	3.2877900	–3.2086336
C	1.4763366	2.4306299	–2.3267908
N	0.3689577	1.6657546	–2.6457073
C	–0.0054673	1.0082010	–1.4790297
C	1.7887349	2.2810489	–0.9289643
C	0.8779996	1.4102890	–0.4078669
C	–1.0384551	0.0672030	–1.2794084
C	–2.0019646	–0.3599797	–2.2050035
N	–2.3330573	0.2825643	–3.4060138
C	–3.2965384	–1.8000494	–3.3943254
C	–2.6694316	–1.6260338	–2.1882639
C	–2.1232409	–0.0817191	–6.4959099
N	–1.0183652	0.7128703	–6.2097578
C	–0.3802083	0.9472208	–7.4235679
C	–1.0753992	0.2563179	–8.4766544
C	–2.1667580	–0.3401954	–7.9143364
C	0.6550862	1.8794172	–7.6636004
C	–3.0554793	–0.6778528	–5.6092537
C	–3.0223439	–0.6548266	–4.2140842
H	2.3044451	5.3750616	–5.1478567
H	1.5243187	4.5766246	–7.6028410
H	2.6131313	2.7689179	–0.4205981
H	0.7931548	1.0796560	0.6211308
H	–3.7550174	–2.7090070	–3.7699259
H	–2.5588269	–2.3566587	–1.3945092
H	–0.7702555	0.2343900	–9.5168133
H	–2.9361679	–0.9124796	–8.4199428
Co	–0.3166089	1.3031347	–4.4375827
C	3.0943144	4.3179041	–2.6868121
C	4.8891099	6.2803476	–1.7681837
C	4.3536476	4.4809676	–3.2985919
C	2.7449641	5.1642208	–1.6176075
C	3.6361632	6.1357959	–1.1628658
C	5.2424497	5.4526183	–2.8384895
H	4.6213206	3.8293253	–4.1335046
H	1.7587492	5.0662680	–1.1622793
H	3.3476793	6.7915487	–0.3398630
H	6.2178821	5.5608456	–3.3152621
H	5.5852047	7.0401104	–1.4095755
C	0.9959841	2.2980284	–9.0446505
C	1.7512375	3.1598908	–11.6166347
C	0.0243723	2.6845991	–9.9866065
C	2.3557263	2.3763130	–9.4064654
C	2.7271251	2.7972810	–10.6834152
C	0.3993257	3.1095695	–11.2610400
H	–1.0286734	2.6722629	–9.7028052
H	3.1130261	2.1084561	–8.6666424
H	3.7840387	2.8435374	–10.9501194
H	–0.3659500	3.4161648	–11.9759144
H	2.0423631	3.4913970	–12.6144264
C	–4.0755953	–1.6127476	–6.1712963
C	–6.0455898	–3.3813739	–7.1206517
C	–5.4381524	–1.3348610	–5.9788061
C	–3.7127665	–2.7992789	–6.8303465
C	–4.6906747	–3.6768151	–7.3010290
C	–6.4166159	–2.2085139	–6.4575315
H	–5.7200678	–0.4221137	–5.4518576
H	–2.6547676	–3.0322501	–6.9580207
H	–4.3938300	–4.5988526	–7.8031939
H	–7.4715925	–1.9736434	–6.3088884
H	–6.8092506	–4.0672251	–7.4900732
C	–1.0927479	–0.6381943	0.0318779
C	–1.2602071	–2.0030427	2.4807821
C	–0.0235856	–1.4317437	0.4799297
C	–2.2524748	–0.5431578	0.8196474
C	–2.3293638	–1.2170758	2.0396989
C	–0.1078164	–2.1114998	1.6961073
H	0.8706725	–1.5156177	–0.1395843
H	–3.0707328	0.0824518	0.4619082
H	–3.2288899	–1.1258028	2.6506069
H	0.7256077	–2.7319183	2.0292925
H	–1.3250456	–2.5323262	3.4327017
C	2.3823473	0.9055732	–5.2135611
C	3.7429533	1.0967460	–5.6706950
O	4.1715828	2.1570418	–6.1374654
O	4.5475249	–0.0042623	–5.5468106
C	1.7976167	–0.2679829	–4.7037429
O	2.5499057	–1.3827200	–4.6051139
O	0.5771080	–0.3668693	–4.3189647
C	5.8971661	0.1950777	–6.0006096
H	5.9220925	0.4651912	–7.0661777
H	6.3998075	–0.7647268	–5.8374056
H	6.3944821	0.9911371	–5.4279584
C	1.8909404	–2.5318593	–4.0354612
H	1.0414624	–2.8492447	–4.6560366
H	1.5277071	–2.3165410	–3.0206947
H	2.6601890	–3.3108897	–4.0113538
C	–2.4993559	1.7040112	–3.4046673
C	–2.3337969	2.5348914	–4.6243235
O	–1.2952125	3.1935792	–4.8465004
O	–3.3831122	2.5538370	–5.4552792
C	–2.9908839	2.3649536	–2.2282327
O	–3.3165212	1.8704727	–1.1471065
O	–3.0929895	3.7270342	–2.4630298
C	–3.1807135	3.2775645	–6.6983881
H	–4.0884194	3.1048268	–7.2839381
H	–2.2955237	2.8821243	–7.2140090
H	–3.0396700	4.3465351	–6.4942965
C	–3.6177325	4.4854495	–1.3628871
H	–3.5979423	5.5301191	–1.6929939
H	–2.9977276	4.3543100	–0.4644553
H	–4.6469797	4.1787688	–1.1254212

TS21 (I^{E-T}-c-I^{B-E}):

107 atoms

C	2.1256640	4.3201555	–5.1725565
C	1.6500009	4.0972583	–6.4643931
C	1.3122256	2.7522759	–6.5812059
C	2.1001166	3.1133499	–4.4747739
N	1.6272434	2.0641635	–5.3414532
C	2.4152153	2.9185686	–3.1156926
C	1.7061076	2.0188582	–2.3031206
N	0.5353532	1.3555099	–2.6299801
C	0.0809017	0.7799157	–1.4641254
C	2.0264056	1.7788579	–0.9085077
C	1.0140015	1.0379305	–0.3856365
C	–1.0813354	0.0162470	–1.3164092
C	–1.8589284	–0.4415844	–2.3996961
N	–1.5417980	–0.2987921	–3.7288227
C	–3.4375632	–1.5865947	–3.5436908
C	–3.0619889	–1.2229175	–2.2774254
C	–1.7363775	–0.3744627	–6.7166184
N	–0.8743813	0.6761575	–6.3473353
C	–0.2176471	1.0816360	–7.5394085
C	–0.6952403	0.2715590	–8.6213538
C	–1.6151970	–0.6056796	–8.1253397
C	0.6887838	2.1314474	–7.6747488
C	–2.5405666	–1.1074259	–5.8508691
C	–2.4852370	–1.0036293	–4.4477038
H	2.4094571	5.2701286	–4.7313646
H	1.4707374	4.8331473	–7.2412759
H	2.9246463	2.1280363	–0.4107602
H	0.9150172	0.6575104	0.6256526
H	–4.3008430	–2.1702965	–3.8454184
H	–3.5452037	–1.4781438	–1.3405497
H	–0.3235975	0.3437516	–9.6379020
H	–2.1411894	–1.3903246	–8.6588207
Co	–0.2111925	0.9117704	–4.4745872
C	3.4370707	3.8297169	–2.5579931
C	5.4203592	5.5822598	–1.5892506
C	4.6432220	4.0155996	–3.2663434
C	3.2345719	4.5616480	–1.3713949
C	4.2188581	5.4254936	–0.8909403
C	5.6246627	4.8787205	–2.7810091
H	4.7944827	3.4740846	–4.2027400
H	2.2854198	4.4666249	–0.8428582
H	4.0412496	5.9906335	0.0254894
H	6.5560793	5.0013324	–3.3358954
H	6.1891171	6.2581130	–1.2117282
C	0.9412614	2.7257724	–9.0042192
C	1.4554957	3.8942134	–11.5036614
C	–0.1203564	3.0635867	–9.8633799
C	2.2636242	3.0045420	–9.4005699
C	2.5151333	3.5783670	–10.6467030
C	0.1381967	3.6427759	–11.1053415
H	–1.1441415	2.9014216	–9.5248630
H	3.0824996	2.7675241	–8.7175311
H	3.5433914	3.7799196	–10.9507612
H	–0.6921829	3.9136729	–11.7591865
H	1.6550367	4.3464942	–12.4763889
C	–3.5608765	–2.0078492	–6.4478519
C	–5.5170869	–3.6759385	–7.5788719
C	–4.5615256	–1.4705188	–7.2755804
C	–3.5546664	–3.3881396	–6.1899147
C	–4.5251114	–4.2172515	–6.7554046
C	–5.5337898	–2.3013998	–7.8348631
H	–4.5719096	–0.3937817	–7.4502104
H	–2.7768202	–3.8048003	–5.5483142
H	–4.5042181	–5.2898145	–6.5562783
H	–6.3115898	–1.8722743	–8.4684080
H	–6.2762060	–4.3243541	–8.0189052
C	–1.5017178	–0.3570853	0.0609976
C	–2.2770454	–1.0449979	2.6802524
C	–1.5718985	–1.7034051	0.4587153
C	–1.8250590	0.6381297	0.9992226
C	–2.2105673	0.2973877	2.2970925
C	–1.9547619	–2.0442525	1.7568025
H	–1.3096651	–2.4812483	–0.2598004
H	–1.7744138	1.6847293	0.6955689
H	–2.4635265	1.0833855	3.0103917
H	–1.9939826	–3.0942182	2.0509631
H	–2.5766561	–1.3118414	3.6946777
C	2.5970089	0.9434928	–5.5112524
C	3.8593519	1.3092095	–6.1118221
O	4.1705322	2.4596599	–6.4441150
O	4.7231720	0.2627681	–6.3081993
C	2.2020690	–0.3253407	–5.0474230
O	3.0788532	–1.3485523	–5.1544521
O	1.0700683	–0.5843746	–4.5252555
C	5.9776112	0.6353105	–6.9011518
H	6.5463795	–0.2981284	–6.9786630
H	6.5153953	1.3608621	–6.2737613
H	5.8314409	1.0783735	–7.8970877
C	2.6119782	–2.6199274	–4.6635550
H	3.4459733	–3.3086641	–4.8364277
H	1.7190774	–2.9525268	–5.2111290
H	2.3721613	–2.5672687	–3.5924479
C	–1.5586692	2.0263230	–5.1429466
C	–1.3836094	3.4276092	–5.6544382
O	–1.6684711	3.8205680	–6.7716143
O	–0.9698281	4.2268194	–4.6364097
C	–3.0476548	1.8013051	–5.0358444
O	–3.8028552	1.6034415	–5.9705025
O	–3.4462376	1.9322017	–3.7476217
C	–0.9713149	5.6399493	–4.9377176
H	–1.9917692	5.9787773	–5.1647594
H	–0.3247505	5.8512375	–5.7987605
H	–0.5886980	6.1283849	–4.0363114
C	–4.8659775	1.7492278	–3.5356375
H	–5.4414321	2.4955261	–4.1002228
H	–5.1620637	0.7410160	–3.8543163
H	–5.0132888	1.8703581	–2.4582726

TS22 (I^{E-T}-t-I^{B-E}):

107 atoms

C	1.8933525	4.2782307	–5.3740596
C	1.3663446	3.9941399	–6.6226639
C	1.2144821	2.6007704	–6.7303674
C	2.0699769	3.0668485	–4.6833721
N	1.6536658	1.9866415	–5.5168710
C	2.4509324	2.9049672	–3.3410254
C	1.8341383	1.9642871	–2.4932915
N	0.6378985	1.3082405	–2.7616034
C	0.1882306	0.8028628	–1.5631177
C	2.1898390	1.7500110	–1.1101438
C	1.1669626	1.0549266	–0.5310680
C	–1.0792632	0.2256676	–1.3336677
C	–2.0175644	–0.0707916	–2.3218651
N	–1.8689413	0.1829716	–3.6920080
C	–3.6016148	–1.2976529	–3.3811170
C	–3.1534238	–0.9298002	–2.1413441
C	–1.7297879	–0.5331502	–6.6253248
N	–0.7702724	0.4150427	–6.3530734
C	–0.1942025	0.7634718	–7.5689268
C	–0.7526807	–0.0624902	–8.6106266
C	–1.7054680	–0.8539912	–8.0329032
C	0.6268887	1.8880790	–7.7856661
C	–2.6980914	–1.0109178	–5.7123209
C	–2.7668877	–0.6616866	–4.3632669
H	2.0554586	5.2565316	–4.9339302
H	1.0197608	4.7002658	–7.3695636
H	3.1084222	2.0934810	–0.6464615
H	1.0710358	0.7513120	0.5058326
H	–4.3825633	–2.0142545	–3.6124442
H	–3.5023724	–1.2862020	–1.1778153
H	–0.4478172	–0.0371027	–9.6513987
H	–2.3542811	–1.5726840	–8.5215889
Co	–0.1708804	0.9173604	–4.5297909
C	3.4138349	3.8990365	–2.8242849
C	5.2724927	5.8269524	–1.9539909
C	4.5485525	4.2076097	–3.6038909
C	3.2181667	4.5911248	–1.6130698

C	4.1404337	5.5441477	–1.1824167
C	5.4696215	5.1589173	–3.1665825
H	4.6934821	3.6856337	–4.5525598
H	2.3218992	4.3933338	–1.0249553
H	3.9687457	6.0787618	–0.2468845
H	6.3477303	5.3782678	–3.7756748
H	5.9933058	6.5721585	–1.6145037
C	0.8020425	2.4602770	–9.1352150
C	1.2152471	3.6018174	–11.6735444
C	–0.2729120	2.6327106	–10.0281360
C	2.0865410	2.8904158	–9.5282950
C	2.2879044	3.4507554	–10.7892842
C	–0.0665071	3.1968008	–11.2861057
H	–1.2770847	2.3481770	–9.7129397
H	2.9187662	2.7692752	–8.8310116
H	3.2890071	3.7687252	–11.0841418
H	–0.9115196	3.3358941	–11.9620723
H	1.3745940	4.0426110	–12.6586992
C	–3.7428982	–1.9404352	–6.2247603
C	–5.7402827	–3.6727101	–7.1897169
C	–5.0927058	–1.5515764	–6.2191079
C	–3.4100149	–3.2143817	–6.7123211
C	–4.4008733	–4.0728850	–7.1922950
C	–6.0837236	–2.4099349	–6.6986612
H	–5.3541733	–0.5679070	–5.8261255
H	–2.3651691	–3.5278992	–6.7044590
H	–4.1263676	–5.0617173	–7.5626158
H	–7.1269604	–2.0905785	–6.6909195
H	–6.5136958	–4.3442293	–7.5647454
C	–1.4616137	–0.0958248	0.0708398
C	–2.2325225	–0.6673398	2.7096442
C	–0.8501551	–1.1412705	0.7786428
C	–2.4670046	0.6588648	0.6956039
C	–2.8477754	0.3740177	2.0086511
C	–1.2336759	–1.4250625	2.0912804
H	–0.0768978	–1.7344477	0.2880693
H	–2.9332150	1.4714039	0.1365393
H	–3.6264186	0.9700385	2.4870544
H	–0.7557037	–2.2444891	2.6301422
H	–2.5319114	–0.8897684	3.7348212
C	2.6013133	0.8615777	–5.6506659
C	3.8520303	1.2331207	–6.2682645
O	4.1208646	2.3819021	–6.6459244
O	4.7499658	0.2098769	–6.4187123
C	2.1973070	–0.3997317	–5.1677230
O	3.0713287	–1.4267458	–5.2799111
O	1.0700012	–0.6458634	–4.6302047
C	5.9892636	0.5957166	–7.0352927
H	6.5859162	–0.3222960	–7.0794037
H	6.5079367	1.3616774	–6.4408177
H	5.8232717	0.9938868	–8.0467619
C	2.6088362	–2.6920828	–4.7726939
H	3.4380066	–3.3853213	–4.9506418
H	1.7075152	–3.0270951	–5.3049736
H	2.3836564	–2.6306114	–3.6987542
C	–1.6000166	2.0403302	–4.2451242
C	–1.6626886	2.9319514	–3.0327634
O	–2.4179944	2.7960640	–2.0874846
O	–0.7455206	3.9181452	–3.1393974
C	–2.4014914	2.5333233	–5.3964356
O	–2.0736256	3.5700221	–5.9526107
O	–3.4487937	1.7723546	–5.7692963
C	–0.6319669	4.7745229	–1.9809387
H	–0.3471072	4.1752636	–1.1044170
H	–1.5809548	5.2879608	–1.7765474
H	0.1560222	5.4914943	–2.2316126
C	–4.0013062	2.1037568	–7.0660119
H	–4.4284636	3.1146329	–7.0624885
H	–3.2135416	2.0382954	–7.8291334
H	–4.7726267	1.3502153	–7.2524403

TS23 (I^{T}-I^{A}):

107 atoms

C	3.0705450	3.9124981	–4.9283483
C	2.8318738	3.5183814	–6.2104658
C	1.7812973	2.5378964	–6.1579202
C	2.2023264	3.1392107	–4.0808599
N	1.4104404	2.2924625	–4.8413041
C	2.1624912	3.2645809	–2.6929145
C	1.3898033	2.4345848	–1.8856484
N	0.6172708	1.3686076	–2.3317208
C	0.2722700	0.6741336	–1.1834355
C	1.4505528	2.4437759	–0.4469407
C	0.7763870	1.3404809	–0.0138653
C	–0.4821318	–0.4959774	–1.1362012
C	–1.1735513	–0.9671034	–2.2445661
N	–1.0996753	–0.4363096	–3.5253660
C	–2.7361167	–2.0821301	–3.4116332
C	–2.1646062	–2.0077072	–2.1804870
C	–1.5253099	–0.1700865	–6.4318320
N	–0.4364028	0.5883762	–6.0222949
C	0.0737004	1.1334459	–7.1875589
C	–0.7247165	0.7545770	–8.3223859
C	–1.7311486	–0.0308110	–7.8511591
C	1.1769877	1.9791374	–7.2820659
C	–2.3057640	–0.9871682	–5.6155654
C	–2.0588874	–1.1257726	–4.2503919
H	3.7658711	4.6675420	–4.5783684
H	3.3017026	3.8753586	–7.1203436
H	1.9757386	3.1859094	0.1445624
H	0.6162659	0.9991640	1.0036968
H	–3.5129827	–2.7582375	–3.7459314
H	–2.3852955	–2.6000612	–1.3007728
H	–0.5488279	1.0876646	–9.3395530
H	–2.5523919	–0.4725985	–8.4044220
Co	0.2710967	0.8205412	–4.1952004
C	3.0557549	4.2608127	–2.0364018
C	4.7566791	6.1077915	–0.7690978
C	4.4466080	4.0678501	–2.0358414
C	2.5288345	5.3923527	–1.3961605
C	3.3737471	6.3094623	–0.7665072
C	5.2912259	4.9845577	–1.4070504
H	4.8559498	3.1911746	–2.5403041
H	1.4488314	5.5471057	–1.3965293
H	2.9498047	7.1867449	–0.2756170
H	6.3697043	4.8190935	–1.4119459
H	5.4159043	6.8240464	–0.2768485
C	1.7083336	2.2895035	–8.6373938
C	2.7216071	2.8078956	–11.2071453
C	1.6458329	3.5823035	–9.1800722
C	2.2763274	1.2553059	–9.4013965
C	2.7827719	1.5161267	–10.6761309
C	2.1487064	3.8393430	–10.4573343
H	1.1885287	4.3827091	–8.5964181
H	2.3183390	0.2532718	–8.9711555
H	3.2272932	0.7062466	–11.2567470
H	2.0864780	4.8471330	–10.8707785
H	3.1148953	3.0099486	–12.2044893
C	–3.4116057	–1.7807838	–6.2197680
C	–5.5043590	–3.3168605	–7.3126978
C	–4.7399279	–1.5779499	–5.8107294
C	–3.1513262	–2.7599261	–7.1926475
C	–4.1872923	–3.5235977	–7.7324672
C	–5.7775231	–2.3385115	–6.3526926
H	–4.9512643	–0.8150808	–5.0600759
H	–2.1240695	–2.9188655	–7.5220099
H	–3.9635713	–4.2858686	–8.4802601
H	–6.8035940	–2.1637265	–6.0256594
H	–6.3144635	–3.9139419	–7.7335978
C	–0.5753702	–1.2375572	0.1527350
C	–0.6990889	–2.6768282	2.5602137
C	0.5211839	–2.0041556	0.5774182
C	–1.7302406	–1.1944110	0.9468571
C	–1.7914492	–1.9100668	2.1449758
C	0.4560150	–2.7211963	1.7740845
H	1.4111632	–2.0359885	–0.0524676
H	–2.5799424	–0.5943633	0.6176879
H	–2.6941516	–1.8668409	2.7562880
H	1.3109421	–3.3203230	2.0915934
H	–0.7481055	–3.2374358	3.4948916
C	1.7312794	–0.4939812	–4.3145797
C	2.5652527	–0.3796946	–5.5611690
O	2.2303106	–0.8260212	–6.6486176
O	3.7549181	0.2526568	–5.3719464
C	2.4557315	–0.6710724	–3.0089054
O	2.2515405	–1.6127601	–2.2534832
O	3.3428376	0.3109129	–2.7148122
C	4.5666331	0.4012748	–6.5561981
H	4.0551360	1.0324197	–7.2949557
H	4.7812639	–0.5774781	–7.0069295
H	5.4871896	0.8859135	–6.2151946
C	3.9716180	0.1931591	–1.4192872
H	4.6311516	–0.6851864	–1.3904340
H	3.2139082	0.1081313	–0.6302323
H	4.5454126	1.1167199	–1.2920388
H	1.1587177	–1.7798289	–4.5007114
C	1.2162007	–3.0673007	–4.7813345
H	2.2369731	–3.2631235	–4.4381311
H	1.1403982	–3.0217664	–5.8719382
C	0.1834943	–3.8446948	–4.0990723
C	–1.7720081	–5.4429097	–2.8258885
C	–0.9370195	–4.3299336	–4.8055787
C	0.2801065	–4.1537929	–2.7236989
C	–0.6839152	–4.9416846	–2.0996223
C	–1.8955049	–5.1274428	–4.1830079
H	–1.0400106	–4.0875679	–5.8637437
H	1.1155996	–3.7462904	–2.1553066
H	–0.5909801	–5.1597714	–1.0341186
H	–2.7466873	–5.4946321	–4.7593056
H	–2.5224770	–6.0641205	–2.3348016

TS24 (I^{T-T}-I^{A-T}):

122 atoms

C	3.0388249	3.6802569	–5.1074150
C	2.3790454	3.7108643	–6.3015991
C	1.2315673	2.8479197	–6.1712115
C	2.2650580	2.8479714	–4.2192240
N	1.1812390	2.3282391	–4.9002159
C	2.5322868	2.6645683	–2.8606918
C	1.6192081	2.0394089	–2.0040395
N	0.4771304	1.3776154	–2.3792175
C	–0.2172963	1.1019961	–1.2214363
C	1.6600424	2.1647971	–0.5671109
C	0.5034371	1.6263046	–0.0876618
C	–1.3894746	0.3503294	–1.1339786
C	–1.9188880	–0.3419234	–2.2252697
N	–1.4854195	–0.2475280	–3.5311888
C	–3.0955567	–1.8886706	–3.3737087
C	–2.9380870	–1.3550682	–2.1248499
C	–1.6517729	–0.3044515	–6.4737016
N	–0.8006369	0.6984384	–6.0613032
C	–0.5352417	1.4716488	–7.1715823
C	–1.2472911	0.9456863	–8.3093979
C	–1.8938794	–0.1810984	–7.8893953
C	0.3781969	2.5268676	–7.2309143
C	–2.2486143	–1.2610724	–5.6489971
C	–2.2127053	–1.1651860	–4.2550056
H	3.9624929	4.1814165	–4.8395998
H	2.6507450	4.2415599	–7.2079943
H	2.4594545	2.6467582	–0.0143919
H	0.1640504	1.5677856	0.9407152
H	–3.7739841	–2.6742644	–3.6899495
H	–3.4438853	–1.6285852	–1.2048120
H	–1.2300744	1.3768148	–9.3044795
H	–2.5020037	–0.8600608	–8.4769955
Co	–0.1445632	1.0265729	–4.2248979
C	3.7906223	3.1997576	–2.2751111
C	6.1801766	4.1482893	–1.1347858
C	4.7296435	2.3022480	–1.7379752
C	4.0617403	4.5766414	–2.2260926
C	5.2481799	5.0478287	–1.6606672
C	5.9164102	2.7761430	–1.1748520
H	4.5172998	1.2335837	–1.7847857
H	3.3273803	5.2775083	–2.6247887
H	5.4411318	6.1210910	–1.6228672
H	6.6393721	2.0679871	–0.7669463
H	7.1065331	4.5165627	–0.6916252
C	0.4845735	3.3394703	–8.4734783
C	0.6816073	4.9449457	–10.7701445
C	0.0585256	4.6776371	–8.4438604
C	1.0141570	2.8175886	–9.6632106
C	1.1115984	3.6153624	–10.8055150
C	0.1557963	5.4731129	–9.5872398
H	–0.3552919	5.0738255	–7.5147192
H	1.3575594	1.7819515	–9.6828988
H	1.5302738	3.1996221	–11.7233289
H	–0.1845392	6.5091999	–9.5547897
H	0.7577907	5.5681031	–11.6623003
C	–3.0369703	–2.3690758	–6.2536336
C	–4.5005147	–4.5104732	–7.3467570
C	–4.2481795	–2.1387153	–6.9246353
C	–2.5733595	–3.6888108	–6.1345795
C	–3.2975387	–4.7519064	–6.6774368
C	–4.9737072	–3.2007047	–7.4683002
H	–4.6188771	–1.1165144	–7.0119564
H	–1.6324789	–3.8657680	–5.6124971
H	–2.9200928	–5.7710455	–6.5808805
H	–5.9158652	–3.0053566	–7.9825720
H	–5.0684132	–5.3396789	–7.7705555
C	–2.0847170	0.2198054	0.1750556
C	–3.4550361	–0.0172761	2.6120177
C	–1.5398576	–0.5366894	1.2232572
C	–3.3241858	0.8542475	0.3549300
C	–4.0031243	0.7362074	1.5696855
C	–2.2227998	–0.6538010	2.4360600
H	–0.5828396	–1.0381755	1.0723231
H	–3.7334612	1.4480922	–0.4645354
H	–4.9618848	1.2393955	1.7037706
H	–1.7935413	–1.2482435	3.2440554
H	–3.9870239	–0.1087175	3.5601268
C	1.2641724	–0.5282116	–4.2944526
C	–1.4103032	2.4600706	–4.0217101
C	–2.8448463	2.2510868	–3.7829096
O	–3.4063840	2.6472196	–2.7659874
O	–3.4703617	1.5508512	–4.7575174
C	–0.9648805	3.8645285	–4.0251548
O	–1.1884103	4.6097477	–4.9718915
O	–0.2612906	4.2260478	–2.9321070
C	2.7207314	–0.2092157	–4.2615330
O	3.4476275	–0.3525538	–3.2904673
O	3.1547708	0.2926703	–5.4453305
C	0.9143977	–1.6693494	–3.4059840
O	1.0313739	–1.6138982	–2.1966335
O	0.4146580	–2.7619346	–4.0553073
C	4.5594675	0.6216153	–5.4798668
H	4.8010758	1.3434171	–4.6885667
H	4.7255854	1.0623043	–6.4672045
H	5.1658957	–0.2855463	–5.3522675
C	–0.0399963	–3.8126198	–3.1690605
H	–0.9106694	–3.4672394	–2.5960815
H	0.7595467	–4.1119508	–2.4791850
H	–0.3182157	–4.6461310	–3.8225716

C	–4.8357133	1.1823763	–4.4629085
H	–5.1796655	0.6263296	–5.3406980
H	–5.4551397	2.0739598	–4.2978515
H	–4.8665556	0.5430981	–3.5701634
C	0.3318665	5.5420638	–2.9909999
H	–0.4404558	6.3146889	–3.1020315
H	1.0284055	5.5987359	–3.8397668
H	0.8652033	5.6570153	–2.0420481
H	0.3736725	–2.3466955	–6.5194269
C	1.1714429	–1.6273868	–6.7202694
H	1.1182501	–0.9861605	–5.6364610
H	0.8751274	–0.8410839	–7.4209146
C	2.5087713	–2.1795902	–6.9318907
C	5.1167887	–3.1790495	–7.2836441
C	3.4120545	–1.5466142	–7.8089329
C	2.9419735	–3.3228833	–6.2302134
C	4.2335229	–3.8143147	–6.4021348
C	4.6996785	–2.0451990	–7.9897879
H	3.0908140	–0.6472682	–8.3370577
H	2.2546012	–3.8009160	–5.5312075
H	4.5585515	–4.6947815	–5.8461737
H	5.3855133	–1.5455275	–8.6753797
H	6.1278705	–3.5658724	–7.4176866

TS25 (I^{B-T}-I^{A-B}):

122 atoms

C	–1.6514390	1.3699066	–2.9772832
C	–1.9494581	1.6124412	–4.2935010
C	–1.1508805	0.7529876	–5.1068212
C	–0.6819555	0.3258320	–2.9259592
N	–0.2882655	0.0448743	–4.2412353
C	–0.4164298	–0.4540890	–1.7907083
C	–0.0373258	–1.8128615	–1.8041261
N	0.1089105	–2.6580781	–2.9002872
C	0.5862454	–3.8555299	–2.3991372
C	0.3327037	–2.5220813	–0.5984169
C	0.6967705	–3.7813237	–0.9611298
C	1.0828541	–4.9433944	–3.1333738
C	1.2645570	–4.9525767	–4.5254613
N	0.8655398	–3.9489077	–5.3733705
C	1.7137763	–5.6990658	–6.6104381
C	1.7981576	–6.0559244	–5.2931046
C	0.0550075	–2.4787018	–7.8334245
N	–0.3499885	–1.7528063	–6.7268407
C	–0.9157878	–0.5871978	–7.2088987
C	–0.8852395	–0.5946790	–8.6526928
C	–0.2705660	–1.7499666	–9.0371559
C	–1.3708648	0.5203303	–6.4651042
C	0.7274360	–3.7077390	–7.8198010
C	1.1135958	–4.3843709	–6.6521913
H	–2.1477728	1.7715284	–2.1007171
H	–2.7390032	2.2430557	–4.6859609
H	0.3630323	–2.0845842	0.3928736
H	1.0664092	–4.5777705	–0.3246021
H	2.0010847	–6.2857585	–7.4769624
H	2.1643034	–6.9898646	–4.8802244
H	–1.2337181	0.2189024	–9.2794501
H	–0.0315131	–2.0741869	–10.0441055
Co	–0.1761867	–2.3374770	–4.8480694
C	0.9255271	–0.6668183	–4.6052964
C	1.6232378	–0.1195794	–5.8427363
C	2.0046050	–0.6522419	–3.5217040
O	2.2052781	0.2645321	–2.7450753
O	1.4678207	0.9886754	–6.3194594
O	2.4941433	–1.0345318	–6.3321265
O	2.7654839	–1.7633070	–3.5837269
C	3.1539676	–0.6432648	–7.5536514
H	3.7042696	0.2981482	–7.4219696
H	3.8373718	–1.4657694	–7.7871651
H	2.4112441	–0.5213571	–8.3547180
C	3.8169700	–1.8339961	–2.5975592
H	4.3439012	–2.7696628	–2.8080673
H	3.3808798	–1.8551812	–1.5893500
H	4.4945410	–0.9736776	–2.6826139
C	–2.0018101	–3.0617691	–4.8208641
C	–0.5809294	0.2521613	–0.4935994
C	–0.8495651	1.6930156	1.9109483
C	–1.4141762	–0.2189602	0.5357553
C	0.1168224	1.4587490	–0.2969801
C	–0.0153482	2.1701479	0.8957851
C	–1.5478693	0.4957545	1.7266116
H	–1.9659528	–1.1474310	0.3933474
H	0.7812770	1.8088829	–1.0875874
H	0.5413232	3.0979646	1.0353229
H	–2.2065432	0.1198106	2.5109176
H	–0.9552537	2.2507026	2.8425385
C	1.0135206	–4.3605648	–9.1267356
C	1.5267676	–5.6286476	–11.5854156
C	2.3317763	–4.5697443	–9.5613388
C	–0.0438961	–4.7933118	–9.9431226
C	0.2102583	–5.4243485	–11.1616681
C	2.5866432	–5.1978878	–10.7822349
H	3.1561905	–4.2316619	–8.9318440
H	–1.0670882	–4.6407834	–9.5996789
H	–0.6229272	–5.7612083	–11.7805565
H	3.6165643	–5.3478386	–11.1093152
H	1.7262950	–6.1207449	–12.5381859
C	–2.1895726	1.5298087	–7.1850930
C	–3.7310028	3.4348941	–8.5491817
C	–1.7537044	2.8615156	–7.2748324
C	–3.4078299	1.1604405	–7.7789288
C	–4.1740302	2.1116647	–8.4544594
C	–2.5196628	3.8075527	–7.9582023
H	–0.8009617	3.1340773	–6.8188352
H	–3.7513637	0.1306859	–7.6693634
H	–5.1260041	1.8209757	–8.9014768
H	–2.1676681	4.8374629	–8.0338401
H	–4.3305398	4.1757686	–9.0802710
C	1.4511396	–6.1705312	–2.3737147
C	2.0980323	–8.4990181	–0.9357642
C	0.4497400	–6.9081062	–1.7209591
C	2.7807791	–6.6127529	–2.2921447
C	3.1022001	–7.7685942	–1.5777915
C	0.7712964	–8.0650630	–1.0089884
H	–0.5830177	–6.5611504	–1.7803909
H	3.5624603	–6.0361789	–2.7889999
H	4.1410493	–8.0963763	–1.5170136
H	–0.0180660	–8.6309252	–0.5121729
H	2.3493120	–9.4022680	–0.3782596
C	–2.6645648	–2.9439644	–3.4833829
O	–2.8418336	–3.8566525	–2.6901391
O	–3.0239648	–1.6591238	–3.2279082
C	–2.8713140	–2.6754325	–5.9735987
O	–3.6423437	–1.7282613	–6.0015414
O	–2.6798418	–3.5054386	–7.0324297
C	–3.7006319	–1.4492153	–1.9740517
H	–4.7426609	–1.7915239	–2.0451168
H	–3.6605036	–0.3702073	–1.7966092
H	–3.1975830	–1.9968169	–1.1679302
C	–3.4732472	–3.2268078	–8.2017859
H	–3.3453707	–4.1019691	–8.8473185
H	–3.1066944	–2.3179152	–8.6977645
H	–4.5305315	–3.1021637	–7.9337621
C	–1.9977418	–5.7273550	–4.9331299
H	–0.9398690	–5.9707922	–4.8082810
H	–2.5781082	–5.7703566	–4.0100046
H	–1.8182831	–4.3641287	–4.9755109
C	–2.6273947	–6.1855378	–6.1535937
C	–3.8619322	–7.0002217	–8.5567105
C	–1.8555461	–6.5249374	–7.2874040
C	–4.0351999	–6.2567096	–6.2597289
C	–4.6433108	–6.6587127	–7.4448068
C	–2.4654156	–6.9313060	–8.4703098
H	–0.7685708	–6.4531553	–7.2257078
H	–4.6434840	–5.9795215	–5.3965788
H	–5.7314154	–6.7079575	–7.5076908
H	–1.8490968	–7.1913074	–9.3323017
H	–4.3394395	–7.3185687	–9.4844172

TS26 (I^{E-T}-I^{E-A}):

122 atoms

C	1.4399209	4.2884858	–5.1567695
C	0.8065194	4.0853355	–6.3771276
C	0.6054044	2.7130619	–6.5508384
C	1.6531134	3.0458893	–4.5570514
N	1.1211927	2.0072956	–5.4041329
C	2.2348770	2.7713785	–3.3124924
C	1.7507347	1.7333282	–2.4990745
N	0.5195692	1.1064301	–2.6540989
C	0.2650826	0.4615433	–1.4686776
C	2.3188030	1.3606799	–1.2232065
C	1.3885659	0.6042901	–0.5733836
C	–0.9127748	–0.2230412	–1.1480925
C	–1.8586215	–0.5967291	–2.1061044
N	–1.7579539	–0.3659405	–3.4594569
C	–3.5079767	–1.8066318	–3.0578023
C	–2.9881052	–1.4555941	–1.8466905
C	–2.1749297	–0.5559782	–6.4007611
N	–1.2796538	0.4559162	–6.1360161
C	–0.8214406	0.9015324	–7.3673329
C	–1.4177939	0.1092805	–8.4187674
C	–2.2722666	–0.7701141	–7.8273883
C	–0.0494801	2.0546355	–7.5979856
C	–2.9191219	–1.2645429	–5.4481372
C	–2.7357975	–1.1192166	–4.0680520
H	1.6622590	5.2382367	–4.6829784
H	0.4410371	4.8464586	–7.0576555
H	3.3062815	1.6497647	–0.8800013
H	1.4522823	0.1529334	0.4113513
H	–4.3361246	–2.4762854	–3.2619649
H	–3.3065361	–1.7754577	–0.8604723
H	–1.1939418	0.2163278	–9.4745689
H	–2.9052242	–1.5111534	–8.3030264
Co	–0.5554629	0.8808240	–4.3239311
C	3.2894636	3.6988707	–2.8570153
C	5.3212416	5.4924181	–2.0895070
C	4.2848031	4.0953819	–3.7755796
C	3.3248624	4.2315906	–1.5535709
C	4.3316691	5.1183335	–1.1747977
C	5.2912432	4.9798990	–3.3900046
H	4.2599069	3.6894740	–4.7892296
H	2.5405539	3.9644838	–0.8467885
H	4.3365091	5.5305306	–0.1646696
H	6.0594586	5.2672457	–4.1092723
H	6.1082194	6.1863322	–1.7907466
C	0.0204747	2.6917511	–8.9272695
C	0.2298422	3.9646276	–11.4306022
C	–1.1105142	2.8470737	–9.7526587
C	1.2588474	3.1982831	–9.3756959
C	1.3585648	3.8249152	–10.6172567
C	–1.0052708	3.4764439	–10.9917391
H	–2.0791755	2.4955131	–9.3993476
H	2.1386881	3.0797264	–8.7394489
H	2.3254048	4.2018773	–10.9538017
H	–1.8940797	3.5996762	–11.6122409
H	0.3098901	4.4572978	–12.4006500
C	–3.9411655	–2.2444087	–5.9193189
C	–5.8574099	–4.1070742	–6.8020509
C	–5.3118343	–2.0035486	–5.7324165
C	–3.5448039	–3.4362683	–6.5472046
C	–4.4951765	–4.3595198	–6.9868730
C	–6.2622131	–2.9276187	–6.1717967
H	–5.6324377	–1.0838890	–5.2416728
H	–2.4805926	–3.6342944	–6.6824335
H	–4.1695908	–5.2822543	–7.4693452
H	–7.3230332	–2.7209437	–6.0238133
H	–6.6001925	–4.8282627	–7.1453725
C	–1.1499817	–0.5581538	0.2818209
C	–1.5851927	–1.1114088	2.9985467
C	–1.0872583	–1.8769099	0.7556929
C	–1.4350363	0.4823972	1.1807010
C	–1.6543358	0.2044638	2.5310413
C	–1.3013447	–2.1511993	2.1084694
H	–0.8591709	–2.6832346	0.0570665
H	–1.5093184	1.4992089	0.7917769
H	–1.8855569	1.0181805	3.2200773
H	–1.2424200	–3.1793441	2.4686419
H	–1.7539832	–1.3269658	4.0545278
C	2.0823527	0.9211538	–5.7298631
C	3.2565493	1.3613103	–6.4414650
O	3.4702623	2.5382379	–6.7650054
O	4.1496259	0.3709816	–6.7484775
C	1.7502582	–0.3806065	–5.3097399
O	2.6184348	–1.3793533	–5.5889045
O	0.6878259	–0.6866850	–4.6821074
C	5.3164117	0.8235162	–7.4556226
H	5.9182004	–0.0769386	–7.6210557
H	5.8803424	1.5579001	–6.8626575
H	5.0449477	1.2851332	–8.4159231
C	2.2242222	–2.6875729	–5.1323337
H	3.0379841	–3.3500699	–5.4460145
H	1.2761183	–2.9984073	–5.5929090
H	2.1111089	–2.7080872	–4.0395085
C	–1.7408374	2.4702637	–3.9305670
C	–1.5766226	2.8930481	–2.5060634
O	–2.2258669	2.4379694	–1.5724978
O	–0.5968947	3.8182196	–2.3278194
C	–1.9534997	3.5848515	–4.8877463
O	–1.8596304	4.7791759	–4.6343012
O	–2.4132025	3.1324263	–6.0894719
C	–0.3419688	4.1731906	–0.9565362
H	0.0839857	3.3143472	–0.4151604
H	–1.2643818	4.4931554	–0.4536187
H	0.3795891	4.9955398	–0.9996999
C	–2.8246952	4.1592226	–7.0084945
H	–3.4811992	4.8836995	–6.5110562
H	–1.9503930	4.6791393	–7.4242707
H	–3.3720802	3.6370359	–7.7979643
C	–4.3614626	1.7366656	–3.8152740
H	–3.0253141	1.9677855	–3.9449004
H	–4.3402476	0.6459505	–3.7885602
H	–4.5120239	2.1863434	–2.8305746
C	–5.0584711	2.3452449	–4.9348493
C	–6.3925399	3.5488079	–7.1231438
C	–5.6124228	3.6419867	–4.8307882
C	–5.1644376	1.6843681	–6.1822185
C	–5.8277104	2.2723689	–7.2536763
C	–6.2722541	4.2316092	–5.9068404
H	–5.5182058	4.1812101	–3.8863279
H	–4.6897686	0.7111134	–6.3077330
H	–5.8996593	1.7376032	–8.2025856
H	–6.6972059	5.2310392	–5.7984941
H	–6.9132147	4.0094658	–7.9636622

TS27 (I^{A-IV}-I^{A-T})

120 atoms

C	2.8396399	4.9419925	–4.9185916
C	2.5757895	4.3794097	–6.1305493
C	1.6631685	3.2850324	–5.8974543
C	2.1144547	4.1784119	–3.9327182
N	1.3907845	3.1810069	–4.5530897
C	2.1614858	4.4275386	–2.5607440

C	1.5699686	3.5835091	–1.6203949
N	0.8049301	2.4730300	–1.8988026
C	0.5851635	1.8416043	–0.6954850
C	1.8133486	3.6668214	–0.2018536
C	1.2346557	2.5702696	0.3649818
C	–0.1591976	0.6782083	–0.5067851
C	–0.9581303	0.1198304	–1.5020389
N	–1.0304373	0.5300944	–2.8164066
C	–2.5673478	–1.1522006	–2.4434691
C	–1.9067793	–0.9401357	–1.2676494
C	–1.4744053	0.3367251	–5.7364538
N	–0.4636330	1.2515013	–5.4752000
C	0.0993242	1.5654581	–6.6990158
C	–0.5681241	0.8323840	–7.7424188
C	–1.5613718	0.1042793	–7.1543813
C	1.1034195	2.5112117	–6.9189432
C	–2.2531780	–0.3222464	–4.7847497
C	–1.9878762	–0.2585556	–3.4165804
H	3.4766758	5.7911419	–4.6962770
H	2.9495733	4.6752127	–7.1049489
H	2.3950656	4.4470367	0.2772326
H	1.2400576	2.2687817	1.4068041
H	–3.3474795	–1.8749547	–2.6589726
H	–2.0456979	–1.4401102	–0.3146465
H	–0.3064922	0.8784720	–8.7937826
H	–2.2733432	–0.5635757	–7.6267138
Co	0.1021385	1.9245375	–3.6942592
C	2.9175362	5.6102422	–2.0662734
C	4.3153545	7.8512649	–1.1171031
C	4.3188178	5.6501222	–2.1288631
C	2.2217564	6.6985075	–1.5163695
C	2.9197043	7.8138489	–1.0466173
C	5.0130040	6.7662090	–1.6568391
H	4.8524417	4.7920259	–2.5403932
H	1.1325454	6.6536131	–1.4673802
H	2.3705756	8.6567768	–0.6238988
H	6.1029180	6.7853962	–1.7040714
H	4.8592008	8.7220074	–0.7477782
C	1.5657199	2.7504558	–8.3150731
C	2.4497911	3.2178637	–10.9438162
C	0.7144475	3.3444477	–9.2603973
C	2.8671823	2.3967128	–8.7036641
C	3.3055450	2.6282126	–10.0091965
C	1.1524890	3.5760367	–10.5657737
H	–0.2957049	3.6247086	–8.9568882
H	3.5305116	1.9351348	–7.9708960
H	4.3178427	2.3420067	–10.2981378
H	0.4806687	4.0413371	–11.2887864
H	2.7925432	3.3976859	–11.9636971
C	–3.3200354	–1.2521325	–5.2472924
C	–5.3322109	–3.0256269	–6.0745583
C	–4.6714919	–0.9053404	–5.1101757
C	–2.9836211	–2.4972392	–5.8009006
C	–3.9859368	–3.3784169	–6.2124214
C	–5.6735040	–1.7872883	–5.5230305
H	–4.9250019	0.0661387	–4.6817674
H	–1.9282646	–2.7596132	–5.8971468
H	–3.7150613	–4.3459357	–6.6380198
H	–6.7225210	–1.5062632	–5.4168248
H	–6.1140828	–3.7151916	–6.3961332
C	–0.0746727	–0.0298822	0.7994573
C	0.1540050	–1.4385980	3.2144804
C	0.6911189	–1.2053700	0.8641594
C	–0.7253273	0.4327863	1.9511511
C	–0.6106419	–0.2698586	3.1538584
C	0.8044515	–1.9047973	2.0674518
H	1.1981602	–1.5441726	–0.0417854
H	–1.3230348	1.3437417	1.8926423
H	–1.1228916	0.0949665	4.0455758
H	1.4054206	–2.8146371	2.1110127
H	0.2425739	–1.9855612	4.1543303
C	1.8827860	0.3102465	–3.9350294
C	2.8988903	0.7042481	–2.9496626
O	3.7598192	1.5494583	–3.1742899
O	2.8052635	0.0695910	–1.7419709
C	1.2341787	–1.0038559	–4.0377754
O	0.8417724	–1.4765795	–5.1019271
O	1.0694659	–1.6712641	–2.8543982
C	3.7713949	0.4951298	–0.7641924
H	3.4854464	–0.0132230	0.1637801
H	3.7344746	1.5838172	–0.6277542
H	4.7878325	0.2064794	–1.0685899
C	0.4122375	–2.9444118	–2.9761500
H	–0.5671797	–2.8340548	–3.4611551
H	0.2838586	–3.3037252	–1.9490344
H	1.0236695	–3.6465774	–3.5610747
H	2.1546123	0.6736067	–4.9248454
C	–1.3204706	3.3009425	–3.5108650
I	–2.8336798	3.2506726	–5.8017586
C	–0.9317968	4.7560032	–3.5390020
O	–0.8480822	5.4310585	–2.5266852
O	–0.6291977	5.2224092	–4.7694936
C	–2.3202437	2.9757734	–2.4381157
O	–2.0694436	3.1865029	–1.2663272
O	–3.4641878	2.3830837	–2.8622128
C	–0.1953755	6.6007012	–4.8003580
H	0.6822117	6.7374113	–4.1555030
H	–1.0092398	7.2607630	–4.4703877
H	0.0647128	6.7913986	–5.8455176
C	–4.3104748	1.8964234	–1.7917738
H	–4.6566292	2.7280044	–1.1633512
H	–3.7580910	1.1746794	–1.1774108
H	–5.1516911	1.4078752	–2.2930544
C	–3.5900089	5.1907060	–5.4324374
C	–4.4514878	7.7725201	–4.8717836
C	–4.3010338	5.4318108	–4.2544939
C	–3.3006136	6.2179686	–6.3341347
C	–3.7443894	7.5119386	–6.0488291
C	–4.7251188	6.7344198	–3.9774724
H	–4.5050727	4.6195612	–3.5577692
H	–2.7226870	6.0171410	–7.2354672
H	–3.5224774	8.3198916	–6.7473148
H	–5.2686587	6.9338701	–3.0532656
H	–4.7847669	8.7865365	–4.6489385

TS28 (I^{A-T}-I^{A-B}):

108 atoms

C	2.7568369	3.3647946	–5.3465644
C	2.1737239	3.3211188	–6.5867809
C	1.0069846	2.5033332	–6.5023724
C	1.9239601	2.6328245	–4.4503369
N	0.9148988	1.9763210	–5.1934427
C	1.9759031	2.6897779	–3.0679577
C	0.9624216	2.1562695	–2.2513050
N	–0.1019354	1.3896095	–2.6634980
C	–0.8276848	1.1011786	–1.5243116
C	0.8825852	2.3904290	–0.8291155
C	–0.2447197	1.7673826	–0.3861635
C	–1.8692373	0.1825361	–1.4523534
C	–2.2649125	–0.5917386	–2.5515507
N	–1.8884735	–0.3924383	–3.8568038
C	–3.1994247	–2.2896840	–3.7046112
C	–3.0924835	–1.7672897	–2.4487613
C	–2.0449386	–0.4319317	–6.7908151
N	–1.2115842	0.5760575	–6.3620633
C	–0.9263920	1.3429638	–7.4674456
C	–1.6798609	0.8661479	–8.5990063
C	–2.3394372	–0.2602496	–8.1889470
C	0.0920303	2.3085525	–7.5269793
C	–2.5630388	–1.4476552	–5.9834011
C	–2.4944827	–1.3964736	–4.5906854
H	3.6541791	3.8970905	–5.0500182
H	2.5044903	3.8167729	–7.4936997
H	1.5897126	2.9887869	–0.2646856
H	–0.6531884	1.7468691	0.6179378
H	–3.7281532	–3.1828556	–4.0187465
H	–3.5089563	–2.1461369	–1.5215098
H	–1.6762782	1.3203362	–9.5839745
H	–2.9919056	–0.9070123	–8.7661032
Co	–0.6364340	0.9340093	–4.5128655
C	3.1509505	3.3303731	–2.4095554
C	5.3823576	4.4649611	–1.1277747
C	4.0574529	2.5212155	–1.7051665
C	3.3803949	4.7128461	–2.4678706
C	4.4882806	5.2765732	–1.8304971
C	5.1645152	3.0853515	–1.0694384
H	3.8929529	1.4436525	–1.6879942
H	2.6800717	5.3475236	–3.0098965
H	4.6486067	6.3546681	–1.8786384
H	5.8638894	2.4432729	–0.5317902
H	6.2465522	4.9056467	–0.6288039
C	0.2543228	3.1283594	–8.7598740
C	0.5583981	4.7366660	–11.0443146
C	–0.0199200	4.5045603	–8.7040845
C	0.6871827	2.5697028	–9.9717058
C	0.8381442	3.3686764	–11.1072694
C	0.1294782	5.3024532	–9.8399785
H	–0.3542873	4.9345499	–7.7582045
H	0.9096680	1.5028849	–10.0151725
H	1.1803068	2.9225309	–12.0423366
H	–0.0932318	6.3690538	–9.7850202
H	0.6758893	5.3603743	–11.9314777
C	–3.2517086	–2.5835374	–6.6515550
C	–4.5009691	–4.7281744	–7.9672843
C	–4.6354663	–2.7832318	–6.5308358
C	–2.5001229	–3.4695411	–7.4406356
C	–3.1216826	–4.5368987	–8.0913002
C	–5.2562349	–3.8484343	–7.1864701
H	–5.2210219	–2.0893241	–5.9266723
H	–1.4222838	–3.3172765	–7.5178917
H	–2.5258723	–5.2246644	–8.6932304
H	–6.3340080	–3.9884900	–7.0911377
H	–4.9865126	–5.5610757	–8.4777149
C	–2.5777251	–0.0342330	–0.1633522
C	–3.9795802	–0.4418062	2.2327820
C	–1.9415660	–0.6233517	0.9396695
C	–3.9250362	0.3484389	–0.0583040
C	–4.6175947	0.1475524	1.1370427
C	–2.6400034	–0.8278951	2.1315778
H	–0.8976855	–0.9285301	0.8516903
H	–4.3992708	0.8239336	–0.9178034
H	–5.6602996	0.4592312	1.2145679
H	–2.1380904	–1.2933142	2.9812198
H	–4.5245865	–0.5992911	3.1646670
C	–2.0273078	2.6200926	–4.5467968
H	–2.0262178	2.8097241	–5.6209671
C	0.9454110	–0.0047206	–4.8388949
C	–3.3083945	2.0694268	–4.0803487
O	–3.7555212	2.0276886	–2.9446785
O	–3.9895084	1.5187871	–5.1505512
C	–1.4472061	3.7437264	–3.7949169
O	–1.5618227	4.0243508	–2.6164292
O	–0.6551908	4.5025318	–4.6527218
C	–5.1825282	0.8043272	–4.7929589
H	–4.9493928	–0.0238736	–4.1065416
H	–5.5833885	0.4166675	–5.7365209
H	–5.9136924	1.4674988	–4.3090759
C	0.0230305	5.5968271	–4.0205088
H	0.7976650	5.9150109	–4.7286478
H	0.4704092	5.2774482	–3.0690059
H	–0.6724628	6.4245628	–3.8153931
C	1.1417122	–0.8371349	–6.0445454
O	0.8378441	–2.0208199	–5.9818527
O	1.6442061	–0.2291381	–7.1303913
C	1.9041396	–0.3566570	–3.7308102
O	3.0567153	0.0248009	–3.6391190
O	1.2959711	–1.1819682	–2.8555679
C	1.6181334	–1.0207668	–8.3430283
H	2.1492175	–0.4199833	–9.0877630
H	0.5755519	–1.1853075	–8.6494733
H	2.1194670	–1.9849048	–8.1908267
C	2.0862262	–1.5404157	–1.6986719
H	1.4914385	–2.2870306	–1.1642531
H	2.2398061	–0.6490960	–1.0737757
H	3.0588304	–1.9523340	–1.9981916

TS29 (I^{A-B}-I^{E-A}):

108 atoms

C	2.5651084	3.7079669	–5.3799471
C	1.7186710	3.7956367	–6.4700394
C	0.8454451	2.6988390	–6.4704569
C	2.1614925	2.6286156	–4.5744491
N	1.1630100	1.8444815	–5.3139286
C	2.4206801	2.5260737	–3.2091595
C	1.4581168	2.0725245	–2.2889590
N	0.2248529	1.5472150	–2.6031857
C	–0.4392214	1.3753537	–1.4098627
C	1.5755545	2.2144264	–0.8538945
C	0.3799824	1.8415908	–0.3161409
C	–1.6183532	0.6551634	–1.2273792
C	–2.1184312	–0.2051493	–2.2171478
N	–1.6770838	–0.2340395	–3.5173783
C	–3.1852509	–1.9472535	–3.1691537
C	–3.0884322	–1.2449629	–1.9998862
C	–1.8263586	–0.6074781	–6.4311594
N	–1.0873337	0.5057995	–6.1031449
C	–0.9059962	1.2061124	–7.2743333
C	–1.5522583	0.5231519	–8.3668404
C	–2.0914955	–0.6194840	–7.8517689
C	–0.1137395	2.3625631	–7.4130973
C	–2.3750611	–1.5097412	–5.5143782
C	–2.3567301	–1.2691262	–4.1344666
H	3.3156884	4.4325918	–5.0786198
H	1.6852029	4.5945998	–7.2030841
H	2.4665668	2.5436890	–0.3313786
H	0.0905328	1.8033791	0.7287767
H	–3.7927063	–2.8219169	–3.3744541
H	–3.6035712	–1.4289030	–1.0633489
H	–1.5435824	0.8627539	–9.3971954
H	–2.6396187	–1.3980354	–8.3719472
Co	–0.4662823	1.0466046	–4.3429857
C	3.7043471	3.1220079	–2.7542117
C	6.1900102	4.2137825	–2.0117550
C	4.9018330	2.6004010	–3.2751351
C	3.7717453	4.2107768	–1.8684028
C	5.0050640	4.7505571	–1.4998142
C	6.1342687	3.1380263	–2.9025740
H	4.8505692	1.7606441	–3.9699667
H	2.8493868	4.6455185	–1.4837464
H	5.0397759	5.6006045	–0.8167704
H	7.0538840	2.7140750	–3.3082953
H	7.1528383	4.6365303	–1.7216943
C	–0.2588428	3.1802328	–8.6413417
C	–0.5815267	4.7155513	–10.9696028
C	–1.5149908	3.7169220	–8.9723767
C	0.8331048	3.4105749	–9.4956861
C	0.6681818	4.1738690	–10.6526620
C	–1.6734025	4.4836281	–10.1275001
H	–2.3616744	3.5312506	–8.3092357
H	1.7928449	2.9533492	–9.2524939
H	1.5187305	4.3377041	–11.3161810
H	–2.6507494	4.9040369	–10.3688994

H	–0.7058946	5.3131852	–11.8738365
C	–3.0854066	–2.7020956	–6.0529135
C	–4.3783708	–4.9557062	–7.1298782
C	–4.4786413	–2.8414070	–5.9529015
C	–2.3495393	–3.7026245	–6.7087691
C	–2.9914593	–4.8225911	–7.2404528
C	–5.1201082	–3.9607024	–6.4869817
H	–5.0580035	–2.0573220	–5.4643684
H	–1.2676160	–3.5913211	–6.7941930
H	–2.4054110	–5.5947590	–7.7410326
H	–6.2043432	–4.0518115	–6.4067495
H	–4.8801634	–5.8300105	–7.5465978
C	–2.3211464	0.7836229	0.0741413
C	–3.6701068	1.1513694	2.5029081
C	–2.3663279	–0.2507569	1.0204739
C	–2.9512879	2.0081449	0.3521344
C	–3.6255901	2.1846247	1.5619798
C	–3.0371429	–0.0654856	2.2314789
H	–1.8559928	–1.1920421	0.8097215
H	–2.9149141	2.7954713	–0.4030224
H	–4.1207291	3.1346769	1.7688460
H	–3.0595907	–0.8708437	2.9673103
H	–4.1951857	1.2941319	3.4486918
C	–1.7427049	2.6566018	–4.3932481
H	–1.5825731	2.9932716	–5.4221922
C	1.7276146	0.5216187	–5.7206112
C	2.0186269	0.3007292	–7.1392113
O	2.5194387	1.1039670	–7.9236359
O	1.6155864	–0.9421501	–7.5436954
C	2.1415805	–0.4225742	–4.7220402
O	1.8380600	–0.4436413	–3.5252711
O	3.0275401	–1.3488522	–5.2367278
C	1.9422772	–1.2635628	–8.9069806
H	1.6051541	–2.2954038	–9.0532593
H	3.0241249	–1.1808285	–9.0835286
H	1.4171343	–0.5870516	–9.5969096
C	3.3468986	–2.4221555	–4.3366325
H	2.4361670	–2.9372868	–3.9973959
H	3.8861779	–2.0518561	–3.4531933
H	3.9811051	–3.1053054	–4.9129093
C	–3.1281078	2.1432424	–4.1938996
O	–3.7487914	2.0488751	–3.1516689
O	–3.6456459	1.7308166	–5.3990579
C	–4.9063992	1.0441177	–5.3012568
H	–4.8401396	0.2329639	–4.5617275
H	–5.0975420	0.6419831	–6.3019749
H	–5.7080799	1.7319191	–4.9973810
C	–1.2928120	3.6959097	–3.4245186
O	–1.7372049	3.9552536	–2.3228804
O	–0.2279521	4.3787038	–3.9651678
C	0.3781330	5.3373115	–3.0819712
H	1.3075047	5.6431579	–3.5744363
H	0.5878331	4.8773719	–2.1063548
H	–0.2828288	6.2020205	–2.9305111

TS30 (I^{D}-I^{T}):

94 atoms

C	2.8266555	4.2712685	–5.0257210
C	2.3807692	4.0349894	–6.2884844
C	1.3804552	3.0047094	–6.1919423
C	2.0984160	3.3875338	–4.1539072
N	1.1943350	2.6215046	–4.8728147
C	2.2930059	3.3515317	–2.7779537
C	1.5424170	2.5375984	–1.9361872
N	0.5756670	1.6277051	–2.3388914
C	0.1466842	1.0254947	–1.1659408
C	1.7049861	2.5094290	–0.5057816
C	0.8369493	1.5751047	–0.0284200
C	–0.8421080	0.0528600	–1.0573498
C	–1.5581824	–0.4184124	–2.1529520
N	–1.3475267	–0.0557185	–3.4774539
C	–3.0280025	–1.6600077	–3.3181214
C	–2.6055301	–1.3997062	–2.0512650
C	–1.6474837	–0.0113403	–6.4180559
N	–0.6937190	0.9121010	–6.0180788
C	–0.2879677	1.5319064	–7.1909240
C	–1.0058472	1.0034527	–8.3217671
C	–1.8484288	0.0469433	–7.8422593
C	0.7065388	2.4982400	–7.2970952
C	–2.3684183	–0.8590398	–5.5834621
C	–2.2433481	–0.8356199	–4.1982382
H	3.5726914	4.9848181	–4.6930777
H	2.6827787	4.5129261	–7.2141503
H	2.3952458	3.1365884	0.0482471
H	0.6574042	1.2833642	1.0008976
H	–3.7912009	–2.3579819	–3.6447805
H	–2.9494749	–1.8400555	–1.1216373
H	–0.8727817	1.3358497	–9.3458046
H	–2.5606892	–0.5618748	–8.3889754
Co	0.0813599	1.1320060	–4.1999727
C	3.3936563	4.1674920	–2.1902600
C	5.5032085	5.6555397	–1.0887941
C	4.7217702	3.7445202	–2.3575492
C	3.1322054	5.3408163	–1.4689686
C	4.1825512	6.0817503	–0.9212903
C	5.7696883	4.4863174	–1.8077283
H	4.9107902	2.8292586	–2.9207930
H	2.0992926	5.6693820	–1.3431022
H	3.9685483	6.9961870	–0.3658813
H	6.7988113	4.1489312	–1.9410471
H	6.3229964	6.2347836	–0.6613817
C	1.1196822	2.9512789	–8.6561585
C	1.9341825	3.7521579	–11.2197295
C	0.3380402	3.8454621	–9.4007257
C	2.3149248	2.4606813	–9.2049831
C	2.7178099	2.8602492	–10.4811618
C	0.7440706	4.2444563	–10.6768029
H	–0.5893375	4.2272013	–8.9709641
H	2.9126026	1.7641158	–8.6147831
H	3.6472643	2.4722092	–10.9007170
H	0.1307831	4.9443946	–11.2463610
H	2.2508547	4.0644070	–12.2159418
C	–3.3080333	–1.8350380	–6.2068574
C	–5.0459359	–3.6919290	–7.4008847
C	–4.6951073	–1.6318722	–6.1766765
C	–2.8009592	–2.9785031	–6.8420558
C	–3.6644120	–3.9018433	–7.4349715
C	–5.5590652	–2.5550964	–6.7704178
H	–5.0904623	–0.7414743	–5.6857656
H	–1.7214670	–3.1359463	–6.8583533
H	–3.2575907	–4.7896077	–7.9213129
H	–6.6361080	–2.3835689	–6.7435464
H	–5.7209968	–4.4125864	–7.8642389
C	–1.1344052	–0.5144068	0.2908178
C	–1.6550011	–1.5976740	2.8308434
C	–0.2425736	–1.4284146	0.8715876
C	–2.2897341	–0.1490423	0.9966002
C	–2.5484807	–0.6875671	2.2593450
C	–0.5012381	–1.9672867	2.1336113
H	0.6525117	–1.7150517	0.3174177
H	–2.9829316	0.5634927	0.5470998
H	–3.4491263	–0.3922995	2.7996812
H	0.1978291	–2.6811242	2.5717941
H	–1.8575989	–2.0182191	3.8167971
C	1.5119761	–0.2337699	–4.4293069
C	1.8751920	–0.4125693	–5.8856709
O	2.6430708	0.3053543	–6.4967101
O	1.1861501	–1.4329838	–6.4617630
C	2.7031076	0.0518621	–3.5433575
O	3.5986692	0.8257878	–3.8217818
O	2.6257307	–0.6063398	–2.3568743
C	1.4199276	–1.5865804	–7.8796096
H	0.7350887	–2.3777761	–8.1998176
H	2.4633811	–1.8730966	–8.0687313
H	1.1953627	–0.6507758	–8.4065715
C	3.6912080	–0.2970921	–1.4308517
H	3.7296625	0.7829595	–1.2409007
H	4.6577102	–0.6337302	–1.8299477
H	3.4397415	–0.8367332	–0.5127394
N	1.0991399	–1.9293880	–3.9433117
N	0.1857218	–2.4338296	–3.5181236

TS31 (I^{D-T}-I^{T-T}):

109 atoms

C	2.3731748	3.6594075	–5.2130261
C	1.7630308	3.7128848	–6.4351313
C	0.6531017	2.7948928	–6.3912457
C	1.5950726	2.7691317	–4.3922181
N	0.5471538	2.2527479	–5.1290996
C	1.8399847	2.5168472	–3.0432027
C	0.9413328	1.8323324	–2.2246270
N	–0.2362174	1.2399830	–2.6284027
C	–0.8618093	0.7968374	–1.4879029
C	1.0601434	1.7512915	–0.7908494
C	–0.0670278	1.1357233	–0.3332870
C	–2.0280773	0.0231611	–1.4339852
C	–2.5752276	–0.5658017	–2.5781044
N	–2.1126992	–0.3842772	–3.8688245
C	–3.6553969	–2.0961865	–3.8394908
C	–3.5941336	–1.5872339	–2.5739475
C	–1.9135890	–0.5844060	–6.8239483
N	–1.2947287	0.5644246	–6.3607097
C	–0.9140977	1.2744104	–7.4811097
C	–1.3399482	0.5784777	–8.6680057
C	–1.9072971	–0.5940075	–8.2637001
C	–0.1004419	2.4066682	–7.5011238
C	–2.5582873	–1.5224808	–6.0209399
C	–2.7310473	–1.3372100	–4.6434556
H	3.2591864	4.1899556	–4.8808806
H	2.0525292	4.2930946	–7.3046782
H	1.8936826	2.1454180	–0.2191259
H	–0.3372161	0.9035669	0.6910955
H	–4.2869036	–2.8938205	–4.2168345
H	–4.1680180	–1.8896989	–1.7050334
H	–1.1658120	0.9295121	–9.6797765
H	–2.3058225	–1.3947951	–8.8771896
Co	–0.8023060	0.9389566	–4.5001644
C	3.0970628	3.0336151	–2.4340121
C	5.4859746	3.9618018	–1.2883930
C	4.1397496	2.1402291	–2.1450935
C	3.2588461	4.3948214	–2.1379333
C	4.4484566	4.8558518	–1.5687957
C	5.3284432	2.6027855	–1.5760501
H	4.0024949	1.0823673	–2.3751034
H	2.4387190	5.0823449	–2.3498586
H	4.5626668	5.9159989	–1.3373451
H	6.1341776	1.9001737	–1.3574684
H	6.4140385	4.3229932	–0.8429395
C	0.0559185	3.1394639	–8.7864467
C	0.2913092	4.5387601	–11.2115122
C	–1.0031485	3.9307255	–9.2580762
C	1.2298378	3.0464415	–9.5495318
C	1.3462929	3.7432187	–10.7542495
C	–0.8851794	4.6288411	–10.4621042
H	–1.9186369	3.9909258	–8.6670834
H	2.0397750	2.4080688	–9.1940986
H	2.2611722	3.6577061	–11.3426014
H	–1.7143505	5.2432981	–10.8163302
H	0.3835079	5.0816994	–12.1531991
C	–3.1131754	–2.7615187	–6.6298842
C	–4.1157146	–5.1441056	–7.7240807
C	–4.2317092	–2.7379631	–7.4761288
C	–2.5002772	–3.9904731	–6.3350094
C	–2.9995263	–5.1739065	–6.8825244
C	–4.7307871	–3.9240765	–8.0196032
H	–4.7115340	–1.7831296	–7.6967089
H	–1.6185695	–3.9969813	–5.6907877
H	–2.5102863	–6.1224065	–6.6557421
H	–5.6048466	–3.8955108	–8.6721042
H	–4.5051650	–6.0698760	–8.1502104
C	–2.6360443	–0.2288870	–0.0998185
C	–3.7764953	–0.6379611	2.4422769
C	–2.7295736	–1.5205652	0.4448830
C	–3.1116796	0.8584997	0.6557293
C	–3.6799264	0.6526431	1.9142278
C	–3.2960921	–1.7237513	1.7045546
H	–2.3407679	–2.3662940	–0.1229028
H	–3.0368857	1.8606775	0.2322568
H	–4.0497913	1.5062850	2.4843737
H	–3.3536288	–2.7330364	2.1150573
H	–4.2184077	–0.7970271	3.4268831
C	–2.1842882	2.5359133	–4.2193912
C	0.5420174	–0.4446781	–4.6179404
C	–3.1668922	2.4590711	–3.0853744
O	–2.9383019	2.9053725	–1.9759057
O	–4.2961897	1.7874094	–3.4136053
C	–1.5681854	3.8917719	–4.3562264
O	–0.8862356	4.3664908	–3.4685907
O	–1.7816010	4.4789402	–5.5584017
C	–5.2375734	1.6099872	–2.3307968
H	–4.7934311	0.9902760	–1.5413516
H	–6.0960137	1.1015975	–2.7797061
H	–5.5304317	2.5811291	–1.9098917
C	–1.0612792	5.7188891	–5.7603189
H	–1.4461180	6.4977695	–5.0886870
H	–1.2358560	5.9826488	–6.8081012
H	0.0096762	5.5669854	–5.5756085
C	1.6944923	–0.2350010	–5.5229223
O	1.6550378	–0.1371175	–6.7358760
O	2.8489569	–0.1232569	–4.7994016
C	0.4417173	–1.7678585	–4.0063137
O	0.5540245	–2.8053009	–4.6568668
O	0.1920906	–1.7516976	–2.6731277
C	4.0125368	0.2500224	–5.5725774
H	4.8318721	0.3233854	–4.8501742
H	3.8411012	1.2215817	–6.0574046
H	4.2310298	–0.5064484	–6.3379182
C	–0.0878653	–3.0357742	–2.0823298
H	0.7087601	–3.7574208	–2.3064048
H	–1.0452574	–3.4213409	–2.4623395
H	–0.1501074	–2.8484328	–1.0053208
N	–3.4272546	2.4990267	–5.6851109
N	–3.6169640	1.8994851	–6.6055998

TS32 (I^{D-E}-I^{E-T}):

109 atoms

C	2.8596638	4.8651429	–5.4189166
C	2.2932952	4.8250996	–6.6614870
C	1.4611833	3.6481854	–6.7071333
C	2.3529806	3.7314469	–4.6845114
N	1.4847053	3.0250219	–5.4814750
C	2.6815103	3.4136222	–3.3577575
C	2.0413871	2.4030005	–2.6285464
N	0.9249591	1.7057690	–3.0325744
C	0.5401817	0.9272446	–1.9566410
C	2.4203826	1.9907855	–1.2961886
C	1.4898198	1.0862941	–0.8814119
C	–0.6757711	0.2233941	–1.8262100
C	–1.4568397	–0.1233246	–2.9240525
N	–0.8940998	–0.2750196	–4.2421442
C	–3.1844101	–0.6079040	–4.3057167
C	–2.8435952	–0.3296541	–2.9923904

C	–1.0262075	0.1424483	–7.2121222
N	–0.3601770	1.2696270	–6.7345729
C	0.0946142	1.9444707	–7.8421492
C	–0.2335174	1.2125752	–9.0412559
C	–0.8860390	0.0811574	–8.6495201
C	0.8122530	3.1502635	–7.8422017
C	–1.9149423	–0.6656576	–6.4777768
C	–2.0207501	–0.5609379	–5.0845864
H	3.5411798	5.6078815	–5.0186946
H	2.4199431	5.5269947	–7.4784313
H	3.2950981	2.3465763	–0.7626364
H	1.4453567	0.5494218	0.0602480
H	–4.1806355	–0.7503540	–4.7109594
H	–3.5180149	–0.2113943	–2.1518047
H	0.0464803	1.5160933	–10.0446421
H	–1.2430686	–0.7327986	–9.2709417
Co	0.2280428	1.6659438	–4.8647346
C	3.7366820	4.2143448	–2.6834473
C	5.7225608	5.7427954	–1.4064270
C	5.0495073	4.2418099	–3.1828690
C	3.4323629	4.9669113	–1.5363089
C	4.4180225	5.7264420	–0.9044797
C	6.0355725	4.9978648	–2.5470646
H	5.2908717	3.6556504	–4.0706488
H	2.4099564	4.9588688	–1.1565239
H	4.1642275	6.3131662	–0.0205252
H	7.0527946	5.0016751	–2.9412460
H	6.4927665	6.3355604	–0.9112013
C	0.8928654	3.9020949	–9.1199316
C	0.9670247	5.3195553	–11.5431786
C	–0.2914542	4.4010100	–9.6886820
C	2.1131895	4.1212556	–9.7786691
C	2.1488316	4.8233793	–10.9849493
C	–0.2515458	5.1085918	–10.8909419
H	–1.2301734	4.2484267	–9.1541993
H	3.0312592	3.7227318	–9.3444089
H	3.1016335	4.9787361	–11.4932450
H	–1.1752498	5.5030301	–11.3169351
H	0.9964616	5.8704351	–12.4843593
C	–2.8882122	–1.5669579	–7.1318988
C	–4.7545170	–3.3523526	–8.2612100
C	–3.6363002	–1.2040297	–8.2689335
C	–3.1087760	–2.8383647	–6.5601786
C	–4.0296243	–3.7205412	–7.1238533
C	–4.5575997	–2.0891105	–8.8277249
H	–3.5090839	–0.2116295	–8.6997461
H	–2.5438628	–3.1224914	–5.6696044
H	–4.1788177	–4.7028986	–6.6735709
H	–5.1345801	–1.7860939	–9.7027184
H	–5.4754333	–4.0430646	–8.7007929
C	–1.2175962	–0.0777227	–0.4865444
C	–2.3151900	–0.6580094	2.0315148
C	–1.7334699	–1.3593819	–0.2128454
C	–1.2695216	0.9126904	0.5129417
C	–1.8161735	0.6210531	1.7625447
C	–2.2739348	–1.6449907	1.0410321
H	–1.6911206	–2.1215809	–0.9942427
H	–0.9128273	1.9159638	0.2768155
H	–1.8639076	1.3984278	2.5265547
H	–2.6600525	–2.6440956	1.2483368
H	–2.7400851	–0.8837159	3.0107404
C	0.1903833	–1.2865721	–4.3358437
C	–0.1742139	–2.6092858	–3.8864894
O	–1.3007104	–2.9215449	–3.4802720
O	0.8423325	–3.5262017	–3.9301701
C	1.4160916	–0.8566322	–4.8687217
O	2.4079183	–1.7605752	–5.0214974
O	1.6592292	0.3399160	–5.2305470
C	0.4740218	–4.8406394	–3.4804805
H	0.1393097	–4.8230517	–2.4332915
H	1.3834762	–5.4433103	–3.5809766
H	–0.3338205	–5.2602016	–4.0972814
C	3.6480754	–1.2404105	–5.5404831
H	4.0543634	–0.4595268	–4.8827870
H	3.5113368	–0.8223460	–6.5474012
H	4.3209795	–2.1038414	–5.5720175
C	–1.2312359	3.1060935	–4.4534104
C	–1.8574624	3.0385044	–3.0883702
O	–1.2739708	3.3233973	–2.0550732
O	–3.1743133	2.6953157	–3.1128175
C	–2.0750063	3.2067422	–5.6938241
O	–1.9071081	4.0061482	–6.5990803
O	–3.0316244	2.2432898	–5.7311969
C	–3.7692038	2.1839457	–6.9678093
H	–3.0815793	2.0424114	–7.8139917
H	–4.3461970	3.1055250	–7.1234415
H	–4.4332991	1.3197933	–6.8643776
C	–3.8002721	2.6711455	–1.8124730
H	–3.8111819	3.6772218	–1.3711953
H	–3.2641475	1.9951887	–1.1322570
H	–4.8205466	2.3159677	–1.9911831
N	–0.4109031	4.5333483	–4.2724360
N	–0.4431705	5.4853309	–4.9102383

Co(Acacen)(Cl)(CHCO$_2$Et):

101 atoms

N	0.7542188	–0.5864958	2.0668621
N	1.4731615	–2.7940951	1.1286696
O	–0.9470017	–1.8386706	3.8437346
O	–0.1564012	–4.1383209	2.8927182
O	0.8188027	–7.5123172	0.5500309
C	0.0092907	0.4402656	2.3640034
H	0.3125783	1.4067109	1.9442406
C	–1.1675172	0.4369738	3.1559980
C	–1.5294812	–0.7113776	3.9397832
C	–1.9611753	1.6813539	3.1488101
C	1.6406477	–4.0063450	0.6706888
H	2.3334661	–4.1160951	–0.1686888
C	1.0080794	–5.1884874	1.1023373
C	0.1594690	–5.1944357	2.2643390
C	1.3211688	–6.4085329	0.3286176
C	2.0068573	–0.4286766	1.2963568
H	1.9051370	0.4677863	0.6649936
C	2.1166259	–1.6657626	0.3922393
H	3.1766925	–1.9232649	0.2517420
C	–2.6376268	–0.6665662	4.9508395
H	–3.5871842	–0.4545762	4.4389747
H	–2.4944774	0.1581299	5.6601549
H	–2.6880126	–1.6326565	5.4646388
C	–0.4023435	–6.4606308	2.8371577
H	0.3996695	–7.1872714	3.0219361
H	–1.0717986	–6.9346819	2.1066487
H	–0.9425838	–6.2238878	3.7600499
Co	0.2999869	–2.3423533	2.4698755
C	3.1878192	–0.2067000	2.2372102
C	5.2650689	0.2871376	4.0671098
C	4.1098935	–1.2114130	2.5552540
C	3.3260938	1.0519888	2.8392055
C	4.3549695	1.2996428	3.7484798
C	5.1405481	–0.9659177	3.4655478
H	4.0174948	–2.2074525	2.1227599
H	2.6200198	1.8493382	2.5958655
H	4.4483699	2.2853680	4.2061963
H	5.8399231	–1.7656790	3.7117300
H	6.0680182	0.4764564	4.7805906
C	1.5030983	–1.5032331	–0.9918786
C	0.3587301	–1.3691632	–3.5535389
C	0.3570465	–0.7304462	–1.2170191
C	2.0754289	–2.1988939	–2.0667960
C	1.5037313	–2.1395290	–3.3389317
C	–0.2067173	–0.6593580	–2.4908823
H	–0.1272053	–0.2109708	–0.3931043
H	2.9718265	–2.8051180	–1.9157658
H	1.9565672	–2.6986134	–4.1583906
H	–1.1064670	–0.0627371	–2.6449500
H	–0.0927167	–1.3222179	–4.5455734
C	2.3294515	–6.2544215	–0.7920814
C	4.2317843	–5.9264877	–2.8314584
C	1.9053867	–5.8558339	–2.0729432
C	3.6903350	–6.4818513	–0.5102052
C	4.6206861	–6.3127555	–1.5413661
C	2.8716114	–5.7035926	–3.0756204
H	5.6801955	–6.4821207	–1.3303892
H	2.5503034	–5.3932709	–4.0735349
C	4.1223678	–6.8647518	0.8836554
H	5.2120242	–6.9831712	0.9435967
H	3.6548560	–7.8122918	1.1902135
H	3.8177417	–6.1054075	1.6224860
C	0.4540790	–5.5454747	–2.3378266
H	0.2770119	–5.3504727	–3.4029999
H	0.1327451	–4.6502394	–1.7808017
H	–0.1954826	–6.3741538	–2.0214495
C	5.2533263	–5.7825649	–3.9316268
H	5.4878069	–6.7617884	–4.3782159
H	6.1968666	–5.3647680	–3.5526995
H	4.8895272	–5.1321041	–4.7386854
O	–2.9096443	1.9076838	3.9053622
C	–1.5657501	2.7209160	2.1210341
C	–0.7930762	4.6529176	0.2305132
C	–0.8352551	3.8489789	2.5399769
C	–1.9261483	2.5487148	0.7690441
C	–1.5308134	3.5261416	–0.1526316
C	–0.4551915	4.7958555	1.5822383
H	–1.8071045	3.4015607	–1.2031639
H	0.1221407	5.6683943	1.9001491
C	–2.7308877	1.3519120	0.3267228
H	–2.2352358	0.3957796	0.5604194
H	–2.9185341	1.3803860	–0.7543825
H	–3.7041548	1.3260285	0.8398795
C	–0.4547844	4.0149544	3.9906380
H	0.1132259	3.1452319	4.3588104
H	–1.3514551	4.0934630	4.6217834
H	0.1595351	4.9117300	4.1421069
C	–0.4041634	5.7034097	–0.7790423
H	–0.2676310	5.2702344	–1.7796850
H	0.5275333	6.2116771	–0.4938606
H	–1.1863254	6.4752985	–0.8601449
Cl	–1.5082363	–2.2826966	0.9680154
C	1.6163108	–2.3740642	3.8588232
H	1.5416486	–1.5683858	4.5928857
C	2.6016525	–3.3973875	4.0848643
O	2.9084941	–4.3349035	3.3436584
O	3.2453889	–3.1870224	5.2904543
C	4.2905384	–4.1316613	5.5795517
H	5.0663321	–4.1062449	4.7998111
H	3.8913350	–5.1545173	5.6366564
H	4.7058424	–3.8250702	6.5455933

Co(Acacen)(MeIm)(CHCO$_2$Et):

112 atoms

N	0.0866677	–0.4669927	1.5155115
N	1.0237557	–2.7298269	0.8546151
O	–1.6191616	–1.6677639	3.3619872
O	–0.5155182	–3.9975368	2.7764042
O	1.1624709	–7.5310502	1.1568351
C	–0.4970595	0.6038762	1.9729002
H	–0.1686321	1.5620591	1.5547323
C	–1.5064110	0.6864685	2.9728131
C	–2.0237859	–0.4854588	3.6140847
C	–1.9170724	2.0422419	3.3666917
C	1.3928068	–3.9582270	0.6265548
H	2.1203653	–4.1069430	–0.1767824
C	0.9417307	–5.1404599	1.2679766
C	0.0348234	–5.0730572	2.3774558
C	1.4587752	–6.4033201	0.7394343
C	1.2622915	–0.3176480	0.6096226
H	1.0179545	0.4471368	–0.1440543
C	1.4635711	–1.6679699	–0.0935450
H	2.5371464	–1.8072201	–0.2945242
C	–3.0953030	–0.4072198	4.6674664
H	–4.0168865	0.0181322	4.2492373
H	–2.7983189	0.2797863	5.4714773
H	–3.2742715	–1.4135726	5.0618213
C	–0.3428563	–6.2964267	3.1639271
H	0.5601643	–6.8037450	3.5282271
H	–0.8492192	–7.0281516	2.5203607
H	–0.9879381	–5.9962313	3.9971701
Co	–0.2344556	–2.2040753	2.1306297
C	2.4781023	0.1723411	1.3833457
C	4.6060244	1.1449345	2.9435137
C	3.3906783	–0.7131548	1.9736398
C	2.6601298	1.5506595	1.5642357
C	3.7146225	2.0351867	2.3401871
C	4.4436487	–0.2294044	2.7521678
H	3.2750870	–1.7891445	1.8478819
H	1.9659750	2.2618802	1.1113572
H	3.8315555	3.1110387	2.4742392
H	5.1321294	–0.9348616	3.2187979
H	5.4263550	1.5208165	3.5564264
C	0.7273210	–1.8108414	–1.4218597
C	–0.6717821	–2.2726164	–3.8237436
C	–0.4600254	–1.1226540	–1.7014429
C	1.2168998	–2.7160468	–2.3765657
C	0.5205449	–2.9536161	–3.5625624
C	–1.1546215	–1.3507097	–2.8908445
H	–0.8739971	–0.4301689	–0.9698070
H	2.1464602	–3.2596367	–2.1946463
H	0.9180127	–3.6700630	–4.2827654
H	–2.0832517	–0.8105093	–3.0810122
H	–1.2125992	–2.4484383	–4.7550540
C	2.4118371	–6.3025202	–0.4403378
C	4.1908076	–6.0820713	–2.6094283
C	1.9099069	–6.2968587	–1.7525149
C	3.7956148	–6.1987123	–0.1957806
C	4.6617214	–6.0897297	–1.2886612
C	2.8119339	–6.1879868	–2.8198299
H	5.7362464	–6.0032191	–1.1051001
H	2.4245773	–6.1833257	–3.8428375
C	4.3101411	–6.1771903	1.2215372
H	5.4007120	–6.0552345	1.2477560
H	4.0531001	–7.1129765	1.7397962
H	3.8537740	–5.3612329	1.8050496
C	0.4235593	–6.3333922	–2.0142633
H	0.2064336	–6.7255379	–3.0171465
H	0.0050028	–5.3139224	–1.9669525
H	–0.1019937	–6.9546761	–1.2769141
C	5.1520531	–5.9938331	–3.7684432
H	5.6083268	–6.9749279	–3.9756933
H	5.9727674	–5.2931146	–3.5576177
H	4.6478634	–5.6641478	–4.6872775
O	–2.9237018	2.3082888	4.0348629
C	–1.0125916	3.1842622	2.9392520
C	0.6262596	5.3403395	2.1644914
C	0.2569781	3.3418583	3.5305317
C	–1.4728641	4.0990709	1.9710411
C	–0.6379328	5.1538830	1.5889785
C	1.0481971	4.4294983	3.1378634
H	–0.9847519	5.8536200	0.8236174
H	2.0274984	4.5615563	3.6053623
C	–2.8361048	3.9306118	1.3469907
H	–2.9660741	2.9172346	0.9356893
H	–2.9944865	4.6533687	0.5361400
H	–3.6250369	4.0646904	2.1003419

C	0.7886116	2.3550218	4.5412134
H	1.2112505	1.4691976	4.0403766
H	0.0040911	2.0022768	5.2239245
H	1.5935028	2.8018967	5.1391509
C	1.4898902	6.5113892	1.7683756
H	1.3927514	6.7393666	0.6974739
H	2.5503025	6.3217677	1.9839516
H	1.1986907	7.4183052	2.3218119
C	1.0030172	–1.9042520	3.5144747
H	0.8232461	–1.0075928	4.1188610
C	2.0976546	–2.7307530	3.9395669
O	2.5657870	–3.7298437	3.3840175
O	2.6585916	–2.2361580	5.1116913
C	3.7959171	–2.9752119	5.5815712
H	4.6018076	–2.9760286	4.8319780
H	3.5278784	–4.0198971	5.7969849
H	4.1235355	–2.4662724	6.4949413
N	–1.7618503	–2.5250531	0.7545970
C	–2.8556848	–1.7265413	0.5013567
H	–3.0403395	–0.8244927	1.0731981
C	–3.5777785	–2.2702588	–0.5355445
H	–4.4884940	–1.9550026	–1.0304423
N	–2.9097037	–3.4249391	–0.9034853
C	–1.8198978	–3.5383135	–0.1018198
H	–1.1013276	–4.3476965	–0.1712337
C	–3.2411180	–4.3028026	–2.0158888
H	–2.9954599	–3.8129551	–2.9679090
H	–4.3079107	–4.5572257	–1.9903203
H	–2.6516386	–5.2223996	–1.9298960

Co(Salen)(I)(CHCO$_2$Et):

55 atoms

H	–0.5776761	3.3935107	3.0589890
C	0.1081455	2.5521795	2.9655936
C	1.9122937	0.3676789	2.7474374
C	–0.3471347	1.3238349	2.5202958
C	1.4730096	2.7062018	3.2979165
C	2.3551929	1.6510189	3.1858033
C	0.5203883	0.2141707	2.4044613
H	–1.3987577	1.1942714	2.2548098
H	1.8355182	3.6731593	3.6506819
H	3.4091798	1.7515109	3.4427247
O	2.7898343	–0.5810559	2.6713937
C	0.0027820	–1.0181931	1.9036516
H	–1.0440041	–1.0111214	1.5823034
N	0.6639322	–2.1326002	1.8037031
C	0.0832633	–3.3448486	1.2117704
C	0.2953312	–5.8576893	1.3578182
C	–1.8490292	–4.7758085	0.5250523
C	–1.2355045	–5.9642128	1.2729152
C	–1.4397286	–3.4337994	1.1529984
C	0.6768839	–4.5247849	1.9962841
H	0.7493327	–5.9138015	0.3555146
H	–1.5162406	–4.7958188	–0.5263466
H	–1.6517509	–6.0066992	2.2937557
H	–1.8523320	–3.3420109	2.1721280
H	0.2668613	–4.4628350	3.0256357
H	0.5052764	–3.4174790	0.1946235
H	0.6820842	–6.6975997	1.9535903
H	–2.9459859	–4.8577463	0.5118098
H	–1.5127927	–6.9079141	0.7802404
H	–1.8548438	–2.6109921	0.5521106
N	2.1062861	–4.2377208	2.1579044
C	3.0044468	–5.1748251	2.1806227
H	2.6843494	–6.1980743	1.9617697
C	4.3846500	–4.9942013	2.4965029
C	7.0828295	–4.7687513	3.2622375
C	4.8916185	–3.7308474	2.9721012
C	5.2578933	–6.1032778	2.4145176
C	6.5882555	–6.0019616	2.7798281
C	6.2618287	–3.6642733	3.3631527
H	4.8597182	–7.0551165	2.0562615
H	7.2478379	–6.8659805	2.7053740
H	6.6269915	–2.7067782	3.7330096
H	8.1296639	–4.6881012	3.5597800
O	4.1768652	–2.6557861	3.0815922
Co	2.4295269	–2.4122238	2.3958426
I	1.3796140	–2.6182189	4.9911802
C	3.1976142	–2.2388695	0.6567085
H	3.8678606	–1.3771961	0.5955437
C	3.1231171	–3.0931213	–0.4991671
O	2.3769921	–4.0603670	–0.7014270
O	4.0426129	–2.6932642	–1.4519862
C	4.0503274	–3.4880819	–2.6515989
H	4.8260605	–3.0496890	–3.2885783
H	3.0722555	–3.4509610	–3.1529113
H	4.2852556	–4.5378383	–2.4239258

Co(Salen)(MeIm)(CHCO$_2$Et):

66 atoms

H	–0.8697328	3.3885054	2.4102520
C	–0.1697759	2.5548687	2.4585391
C	1.6851327	0.3788674	2.5914739
C	–0.5292426	1.3028936	1.9971356
C	1.1280525	2.7352157	2.9854149
C	2.0271656	1.6875022	3.0482196
C	0.3609293	0.2002120	2.0494738
H	–1.5252170	1.1428712	1.5750007
H	1.4306505	3.7203094	3.3471763
H	3.0324294	1.8233938	3.4482022
O	2.5794092	–0.5558035	2.6901175
C	–0.0878739	–1.0537017	1.5275298
H	–1.0841810	–1.0521262	1.0686600
N	0.5706624	–2.1732875	1.5519326
C	0.0716018	–3.4056266	0.9264035
C	0.2736267	–5.9088354	1.1524119
C	–1.7584103	–4.8652175	0.0384167
C	–1.2330204	–6.0338634	0.8792778
C	–1.4328239	–3.5091570	0.6838275
C	0.5705158	–4.5613228	1.8096356
H	0.8483948	–5.9708148	0.2144868
H	–1.2973691	–4.9024736	–0.9625556
H	–1.7751111	–6.0625453	1.8409402
H	–1.9755457	–3.4019603	1.6403189
H	0.0250663	–4.5020731	2.7713498
H	0.6098298	–3.5049907	–0.0307561
H	0.5953994	–6.7376624	1.8005733
H	–2.8451366	–4.9570976	–0.1090391
H	–1.4404371	–6.9895435	0.3748897
H	–1.7764691	–2.6991217	0.0236672
N	1.9742601	–4.2653814	2.1287286
C	2.8795331	–5.1887853	2.2159790
H	2.5949742	–6.2190460	1.9767066
C	4.2434100	–4.9851102	2.6049925
C	6.9035419	–4.7411287	3.4677273
C	4.7020508	–3.7253714	3.1240201
C	5.1376396	–6.0802823	2.5356868
C	6.4532091	–5.9733268	2.9513034
C	6.0561632	–3.6497491	3.5552063
H	4.7656164	–7.0283896	2.1387102
H	7.1292066	–6.8250868	2.8814751
H	6.4024701	–2.6907802	3.9421239
H	7.9395341	–4.6405038	3.7980884
O	3.9505042	–2.6667850	3.2539903
Co	2.2652694	–2.4213889	2.3538471
C	3.1938818	–2.2558832	0.7383344
H	3.8838842	–1.4063388	0.7499917
C	3.2468670	–3.0943193	–0.4269646
O	2.5489987	–4.0773607	–0.7206604
O	4.2518508	–2.6664149	–1.2868423
C	4.3947026	–3.4544035	–2.4778834
H	5.2180701	–2.9965309	–3.0375615
H	3.4704860	–3.4414699	–3.0748621
H	4.6321655	–4.5001450	–2.2328705
N	1.3451973	–2.4241701	4.2563081
C	2.0795482	–2.2329187	5.3438010
N	1.2857002	–2.0884319	6.4386130
C	–0.0283368	–2.1904734	6.0163745
C	0.0275246	–2.3955325	4.6579448
H	3.1627912	–2.1768926	5.3435264
H	–0.8598148	–2.1010242	6.7055055
H	–0.7840095	–2.4959990	3.9471395
C	1.7360788	–1.8485646	7.8014257
H	2.8309373	–1.8173446	7.8116973
H	1.3964052	–2.6546177	8.4654027
H	1.3491690	–0.8884637	8.1680184

Cu(Box)(CHCO$_2$Et):

61 atoms

C	0.2927077	–0.3540371	0.8488345
C	–0.0204416	–1.5980859	1.7305051
H	0.6034424	–2.4403981	1.4091219
H	–1.0759082	–1.8704960	1.6152680
H	0.1812968	–1.3901976	2.7894506
C	–0.0521785	–0.6493868	–0.6356643
H	0.5287644	–1.5105625	–0.9827818
H	0.1807271	0.2130725	–1.2740881
H	–1.1194960	–0.8777006	–0.7272248
C	1.7733475	–0.0769416	0.9863364
C	–0.5756943	0.7971049	1.3056479
N	2.3625838	0.8209310	1.7052145
N	–0.2280596	1.9590959	1.7552867
O	2.5674498	–0.9311267	0.3284850
O	–1.8909670	0.5722645	1.1860285
C	3.9457632	–0.4467565	0.5243039
H	4.2568162	0.0212503	–0.4190346
H	4.5688231	–1.3228838	0.7261331
C	3.8297990	0.5496014	1.6955222
H	4.3465297	1.4954269	1.4799733
C	–1.4527281	2.8041691	1.8599089
H	–1.4484626	3.2928535	2.8437770
C	–2.5669197	1.7428862	1.7666634
H	–2.9607254	1.4364736	2.7448366
H	–3.3941772	2.0017287	1.0990457
Cu	1.5512654	2.4684271	2.3694072
C	4.3442793	0.0123706	3.0653176
C	4.0695444	1.0476909	4.1685630
H	4.5360294	0.7254538	5.1098872
H	2.9921961	1.1636518	4.3548313
H	4.4811633	2.0314505	3.8993169
C	3.6626617	–1.3155509	3.4332239
H	4.0343319	–1.6708296	4.4038000
H	3.8605226	–2.1100431	2.6994634
H	2.5735738	–1.1927687	3.5234314
C	5.8669616	–0.1828493	2.9417065
H	6.2772588	–0.5347139	3.8981043
H	6.3692392	0.7621182	2.6875307
H	6.1363391	–0.9297870	2.1809485
C	–1.4983869	3.9105621	0.7622437
C	–0.2642341	4.8206844	0.8824762
H	0.6583097	4.2970005	0.5934118
H	–0.1277226	5.1953192	1.9070743
H	–0.3720053	5.6874807	0.2159203
C	–1.5329668	3.2927377	–0.6454736
H	–0.6400998	2.6781747	–0.8323903
H	–1.5476131	4.0883442	–1.4025738
H	–2.4225689	2.6691190	–0.8122864
C	–2.7635474	4.7534630	1.0070136
H	–2.8275637	5.5580792	0.2618381
H	–2.7457727	5.2199445	2.0032024
H	–3.6867013	4.1619831	0.9236954
C	2.4431737	3.8404935	3.1470414
H	2.5994614	3.9462796	4.2339705
C	3.3459925	4.7191708	2.4097988
O	4.4475415	4.2333794	2.1522446
O	2.9070073	5.9225757	2.0561255
C	3.8506147	6.7475514	1.3006397
H	4.1130684	6.2492538	0.3594841
H	4.7556939	6.9218512	1.8945865
H	3.3186604	7.6836464	1.1138756

Ru(PyBox)(CHCO$_2$Et):

57 atoms

H	–2.8052269	0.0130931	–0.0070356
C	–2.1524827	–0.0285415	0.8645481
N	–0.5100707	–0.1320695	3.0723535
C	–1.9594142	–1.2466512	1.5277766
C	–1.5091969	1.1353008	1.3046450
C	–0.6796569	1.0420784	2.4269528
C	–1.1156518	–1.2614287	2.6435951
H	–2.4406800	–2.1644239	1.1947458
H	–1.6395958	2.0901272	0.7985736
C	–0.6957161	–2.3663904	3.4854256
C	0.0917625	2.0669645	3.1065972
N	0.1148544	–2.1220418	4.4800142
N	0.8402541	1.7279971	4.1230751
O	–1.0358785	–3.6473841	3.2722235
O	0.0208876	3.3742737	2.8027074
C	0.4822438	–3.3897235	5.1331558
H	1.5774483	–3.4767144	5.0661884
C	–0.2325296	–4.4321370	4.2314289
H	0.4646514	–5.0404105	3.6425832
H	–0.9265587	–5.0825678	4.7769706
C	1.3353087	2.9564876	4.7728623
H	0.7443007	3.0605281	5.6996491
C	0.9402232	4.0428869	3.7414034
H	0.4010796	4.8902609	4.1774860
H	1.7960584	4.4046017	3.1548763
Ru	0.7923218	–0.2272885	4.7024165
Cl	2.5521945	–0.8411062	3.1707953
Cl	–0.9479457	0.4005428	6.2246855
C	1.9404988	–0.3882628	6.1751338
H	1.5948438	–0.1391758	7.1938589
C	3.2703232	–1.0329917	6.1340900
O	3.4024849	–2.2389520	6.2925363
O	4.2843741	–0.1709357	5.9129017
C	5.5662625	–0.7908517	5.6458192
H	5.4916532	–1.3939173	4.7311677
H	5.8761991	–1.4265669	6.4856991
H	6.2657386	0.0392238	5.5065719
C	2.8243515	2.8948977	5.1459136
H	2.9122052	2.0565958	5.8566901
C	3.7328839	2.5790978	3.9564648
H	4.7696423	2.4691744	4.3033493
H	3.7242544	3.3837310	3.2041631
H	3.4409953	1.6363255	3.4734718
C	3.2324167	4.1859970	5.8663362
H	4.2675245	4.1121400	6.2269876
H	2.5860538	4.3923876	6.7326477
H	3.1843052	5.0556019	5.1909833
C	0.0853417	–3.4022225	6.6210756
H	0.6037101	–2.5344956	7.0605293
C	0.6301102	–4.6687851	7.2893037
H	1.7196258	–4.7447160	7.1630284
H	0.1675155	–5.5784770	6.8727636
H	0.4113807	–4.6581546	8.3661130
C	–1.4180410	–3.2163812	6.8358004
H	–1.7636534	–2.2707497	6.3962975
H	–1.6433640	–3.1822640	7.9107419
H	–2.0016208	–4.0475369	6.4078612

Co(TPP)(CH_2CO_2Et):

90 atoms

Co	12.4975227	22.1790354	0.4870069
O	9.1519484	22.2302551	1.6331142
O	10.5858700	21.4403010	3.2204518
N	11.9063537	23.8075623	1.4319058
N	13.6016566	21.7066608	2.0491772
N	13.3711283	20.7729733	-0.5638240
N	11.4672072	22.7322218	-1.0965479
C	12.3393939	24.2953165	2.6613073
C	13.1457852	23.6089056	3.5658241
C	13.6635834	22.3455812	3.2777261
C	14.3834733	21.5423678	4.2323674
H	14.5530874	21.8165206	5.2679494
C	14.7949692	20.4207539	3.5791472
H	15.3834203	19.5938655	3.9623963
C	14.3276432	20.5351061	2.2227448
C	14.6843338	19.6509324	1.2090265
C	14.2754210	19.8203767	-0.1116863
C	14.6968349	18.9677496	-1.1917833
H	15.4147906	18.1601996	-1.0962736
C	14.0263388	19.3764267	-2.3043510
H	14.0863407	18.9773970	-3.3111257
C	13.1692972	20.4612513	-1.9027477
C	12.2090555	21.0331325	-2.7349052
C	11.3781273	22.0685765	-2.3123777
C	10.2827674	22.5823842	-3.0941074
H	9.9987440	22.2166864	-4.0750162
C	9.6983960	23.5666749	-2.3571390
H	8.8384824	24.1778996	-2.6087424
C	10.4459857	23.6711465	-1.1321172
C	10.2050565	24.6358028	-0.1610526
C	10.9720627	24.7335420	0.9962930
C	10.8814021	25.8389210	1.9116522
H	10.2468877	26.7069471	1.7676408
C	11.7476069	25.5810287	2.9301917
H	11.9718876	26.1981487	3.7930776
C	11.0647564	20.9029040	0.9895266
H	10.5515534	20.6432311	0.0590511
H	11.5850224	20.0520612	1.4418105
C	10.1541316	21.5967861	1.9319219
C	9.8506355	22.1665646	4.2306292
H	10.0128006	23.2453234	4.0651204
H	8.7740335	21.9732917	4.1105472
C	10.3757035	21.6998261	5.5738471
H	9.8923973	22.2582264	6.3881753
H	11.4608488	21.8557598	5.6412265
H	10.1719026	20.6299645	5.7178772
C	13.4599215	24.2303148	4.8832241
C	14.7923248	24.5113942	5.2315045
H	15.5850489	24.2769821	4.5196210
C	15.1027400	25.0865169	6.4649069
H	16.1426359	25.3032580	6.7137587
C	14.0861435	25.3888763	7.3753925
H	14.3282414	25.8351099	8.3409019
C	12.7570411	25.1176410	7.0398954
H	11.9559944	25.3461534	7.7446413
C	12.4476913	24.5469460	5.8043132
H	11.4102759	24.3376589	5.5460378
C	9.0977756	25.6107147	-0.3574303
C	9.1698020	26.6054829	-1.3442548
H	10.0541787	26.6587448	-1.9812556
C	8.1278118	27.5218935	-1.5020027
H	8.1986504	28.2962791	-2.2674766
C	7.0011468	27.4499331	-0.6776602
H	6.1871440	28.1658035	-0.8013570
C	6.9209466	26.4577052	0.3043933
H	6.0399492	26.3933364	0.9448941
C	7.9636413	25.5430569	0.4669795
H	7.9125479	24.7558763	1.2209870
C	12.0158939	20.4761867	-4.1040075
C	12.3001252	21.2469750	-5.2420455
H	12.6805217	22.2614108	-5.1136565
C	12.0998528	20.7250445	-6.5219387
H	12.3294167	21.3347065	-7.3971130
C	11.6092642	19.4261241	-6.6822578
H	11.4497816	19.0196182	-7.6819508
C	11.3216698	18.6508248	-5.5553119
H	10.9318152	17.6384258	-5.6713390
C	11.5245868	19.1719146	-4.2762982
H	11.2962335	18.5722338	-3.3939924
C	15.5793240	18.5044228	1.5432171
C	15.0814959	17.3827549	2.2221027
H	14.0267404	17.3558023	2.4997023
C	15.9235471	16.3145702	2.5404452
H	15.5223337	15.4474256	3.0670555
C	17.2737462	16.3538321	2.1820029
H	17.9311771	15.5193769	2.4295871
C	17.7783761	17.4678649	1.5053892
H	18.8322243	17.5081274	1.2258160
C	16.9369041	18.5366701	1.1899563
H	17.3272733	19.4103320	0.6657471

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