Supporting Information for

Thermodynamic and Reactivity Studies of a Tin Corrole-Cobalt Porphyrin Heterobimetallic complex

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Contents:

1. General considerations.

C_6D_6 and toluene-d_8 were purchased from Cambridge Isotope Laboratory, Inc., degassed, dried by refluxing over freshly fused sodium, and stored over molecular sieves. Benzene and toluene were distilled from sodium benzophenone ketyl, degassed, refluxed over freshly fused sodium for at least 12 h and stored over molecular sieves. Na[(TPFC)Sn^{II}] (**4**)[1] and (TAP)Co^{II} (**3**)[2] were synthesized according to published procedures. All other solvents and reagents were used as received.

^{1}H, ^{13}C, ^{19}F and ^{119}Sn NMR spectra were recorded on a Bruker AVII^{+}-400 NMR spectrometer or a Bruker AVII^{+}-500 NMR spectrometer. ^{1}H-^{1}H ROESY spectra were recorded on a Bruker AVII^{+}-500 NMR spectrometer. ESI-MS results were obtained by a Bruker Apex IV FTMS. Stopped-flow experiments were conducted using a SX20 stopped-flow spectrometer purchased from the Applied Photophysics Ltd. GC–MS experiments were performed on an Agilent 7890A/5975C GC/MSD system with a DB–17MS (30 m, 0.25 mm, 0.25 μm) column. X-ray diffraction data were collected on a Rigaku MM007HF Saturn724+ diffractometer. Light irradiation experiments were performed using a 500 W xenon lamp (CHF-XM-500W, Beijing Trusttech Co., Ltd.) or a 500 W mercury lamp (CEL-M500, Beijing CeAuLight Science & Technology Co., Ltd.), and the reaction vessels were placed at a distance of 15 cm from the lamp, where the light intensity was 30 mW/cm^2. EPR spectra were recorded on a JEOL FA-200 spectrometer. The program easyspin[3] (version 5.0.12) was used to fit the experimental spectra.

2. Synthesis and characterization of 1.

Synthesis of (TAP)Co-Cl (5). The procedure was a modified version of that reported by Nakamoto *et al.*[4] 258.3 mg (0.3265 mmol) of (TAP)Co^{II} (**3**) was suspended in 250 mL of MeOH in a 500 mL round-bottom flask. 3 mL of concentrated HCl was added, and the mixture was vigorously stirred under air for 2 d until TLC indicated near-quantitative conversion of **3**. The solution was concentrated to about half the original volume, filtered, and evaporated to almost dryness. The residue was washed with H_2O and recrystallized with EtOH/H_2O to give (TAP)Co-Cl (**5**, 133.2 mg, 49 %) as a purple crystalline solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.65 (br s, 8H), 8.15 (br s, 8H), 7.25 (br s, 8H), 4.07 (br s, 12H). The characterization data matched those reported by Huet *et al.*[5] The complex is light sensitive and should be stored in the dark.

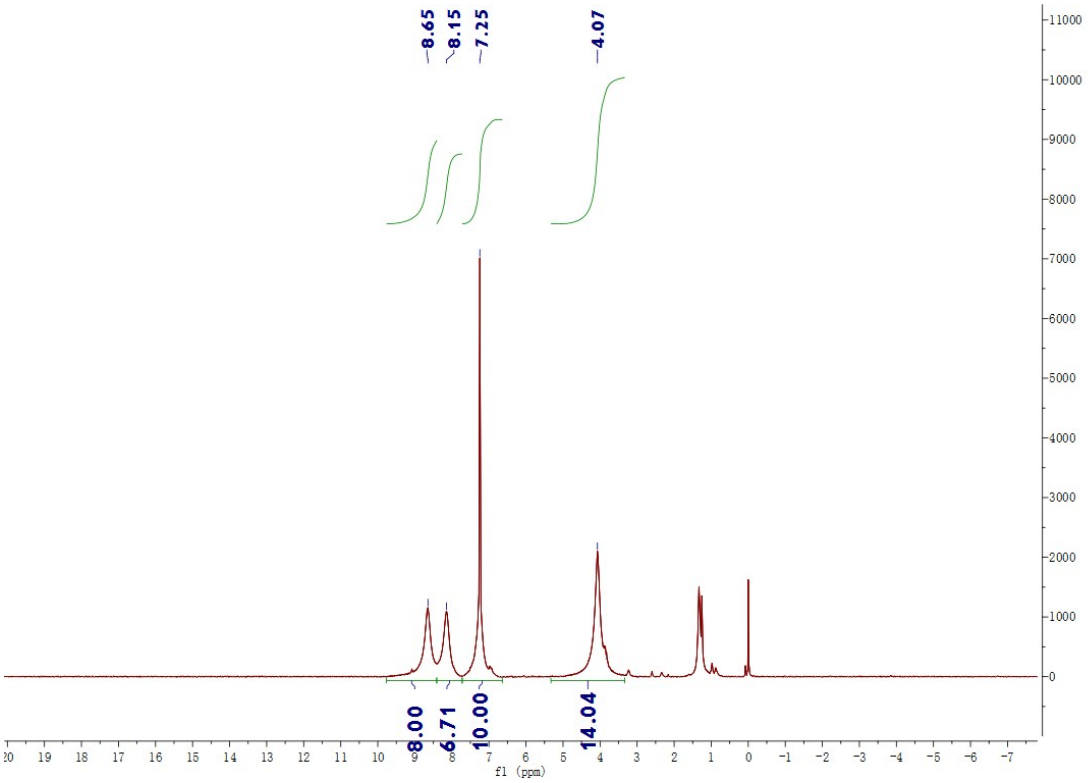


Figure S1. ^{1}H NMR spectrum of **5** in $CDCl_3$.

Synthesis of (TPFC)Sn-Co(TAP) (1). 31.6 mg (0.0382 mmol) of **5** was dissolved in a minimal amount of degassed benzene and added onto 0.0417 mmol (1.1 eq.) of freshly prepared Na[(TPFC)Sn^{II}] (**4**). The mixture was stirred overnight under N_2 in the dark, followed by column chromatography on basic alumina with PE:DCM = 1:2 as eluent. A fraction that appeared brownish-green on the column and brown in the solution was collected and evaporated to give (TPFC)Sn-Co(TAP) (**1**, 50.3 mg, 77 %) as a black solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 8.55 (d, J = 7.1 Hz, 4H), 8.51 (s, 8H), 8.33 (d, J = 4.1 Hz, 2H), 8.07 (d, J = 4.3 Hz, 2H), 7.93 (d, J = 2.4 Hz, 2H), 7.85 (d, J = 4.3 Hz, 2H), 7.58 (dd, J = 8.2, 2.5 Hz, 4H), 7.39 (dd, J = 8.2, 1.8 Hz, 4H), 7.09 (dd, J = 8.2, 2.5 Hz, 4H), 4.18 (s, 12H); ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 8.84 (d, J = 8.4 Hz, 4H), 8.77 (s, 8H), 8.18 (br s, 4H), 7.98 – 7.84 (m, 4H), 7.67 (d, J = 6.4 Hz, 4H), 7.39 (d, J = 8.3 Hz, 4H), 6.93 (d, J = 8.2 Hz, 4H), 3.58 (s, 12H); ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm): 159.3, 145.8, 143.8, 141.1, 139.2, 136.7, 135.2, 134.5, 133.8, 132.3, 125.8, 123.8, 122.4, 120.7, 116.3, 112.2, 112.1, 100.8, 55.6

(the peaks of C_6F_5 groups were not resolved due to excessive coupling by ^{19}F); ^{19}F NMR (377 MHz, $CDCl_3$) δ (ppm): -131.3 – -131.9 (m, 3F), -136.0 (d, J = 22.9 Hz, 1F), -136.4 (d, J = 19.4 Hz, 2F), -153.4 (t, J = 21.0 Hz, 2F), -153.9 (t, J = 21.1 Hz, 1F), -162.2 (qd, J = 23.2, 7.9 Hz, 4F), -162.3 – -162.5 (m, 1F), -162.5 – -162.8 (m, 1F); HR-ESI-MS m/z calcd for $C_{85}H_{44}CoF_{15}N_8O_4Sn$ $[M]^+$ 1705.16942, found 1705.17145; UV-Vis (toluene) λ_{max} (nm) (ε): 311(5.5×10^4), 413(2.6×10^5), 534(1.7×10^4), 624(1.3×10^4). Single crystals suitable for XRD studies were obtained by slow evaporation of DCM from a concentrated DCM/acetone solution.

1 is extremely sensitive towards light, and care must be taken to shield **1** from light during any operation. Once purified, **1** was immediately dissolved in benzene to make a stock solution and stored at -18 °C, at which temperature the complex was reasonably stable (< 1 % decomposition as observed by ^1H NMR) within a month. When used in EPR and laser flash photolysis experiments, **1** must be completely free of even trace amount of the paramagnetic decomposition product **3**, and were thus always purified immediately before use; low-temperature (-170 °C) EPR experiments showed no hint of the presence of **3**.

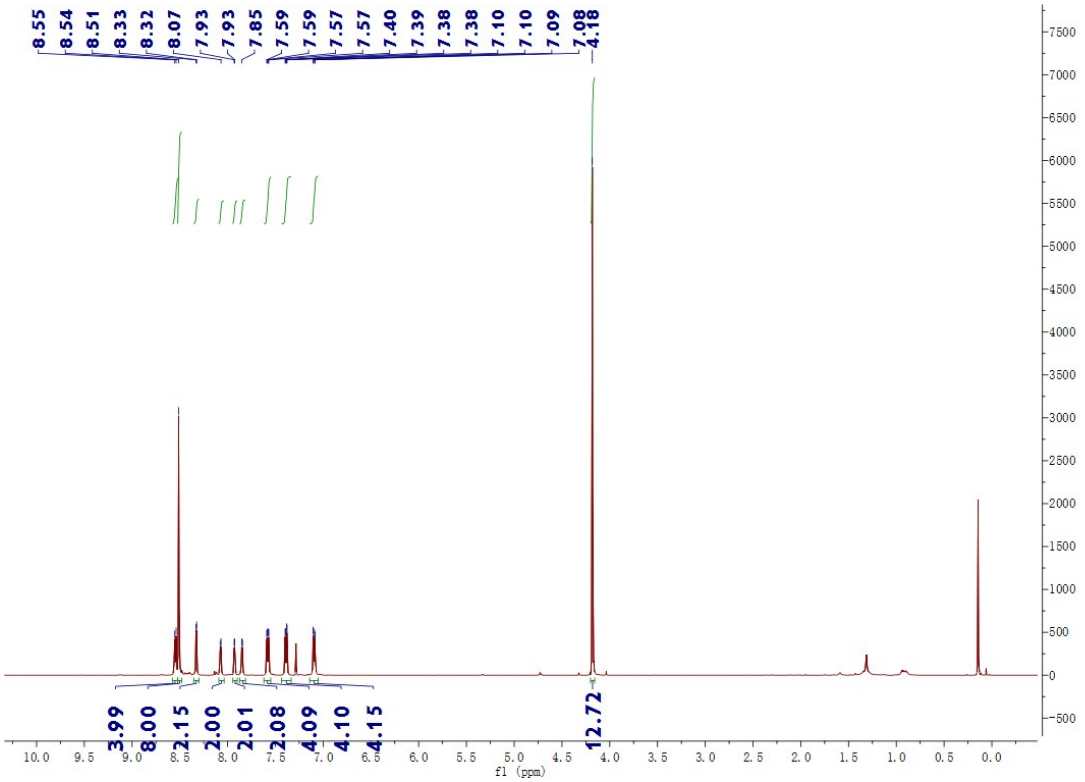


Figure S2. ^1H NMR spectrum of **1** in $CDCl_3$.

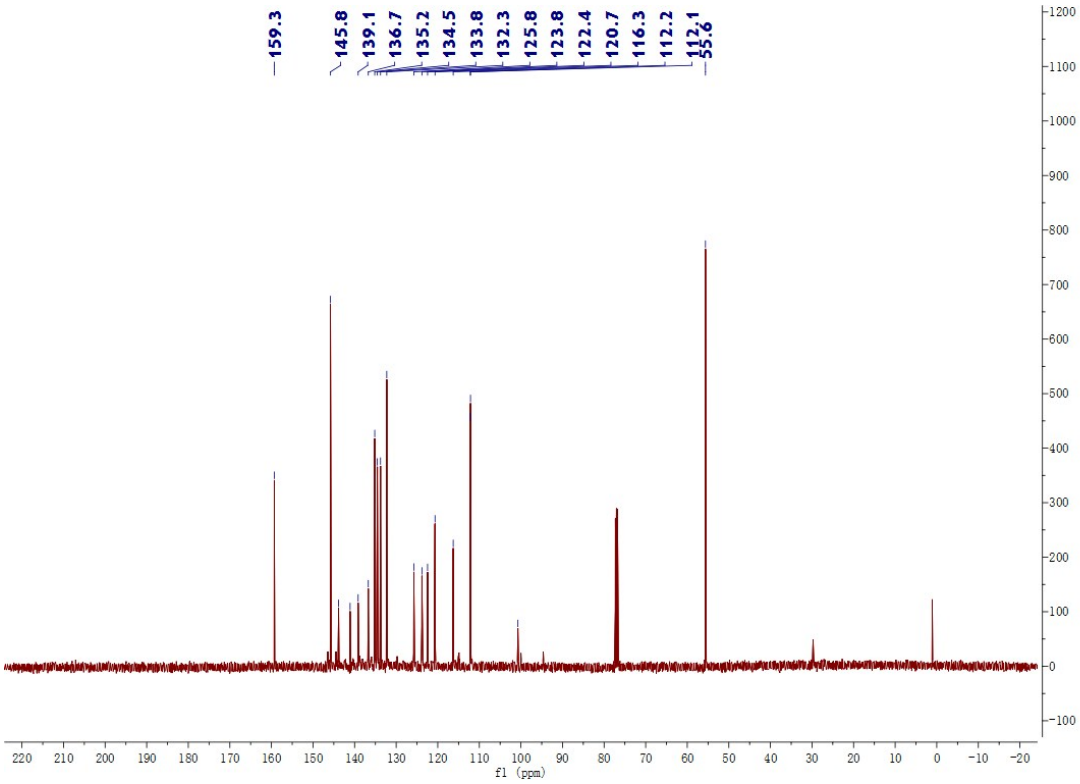


Figure S3. ^{13}C NMR spectrum of **1** in $CDCl_3$.

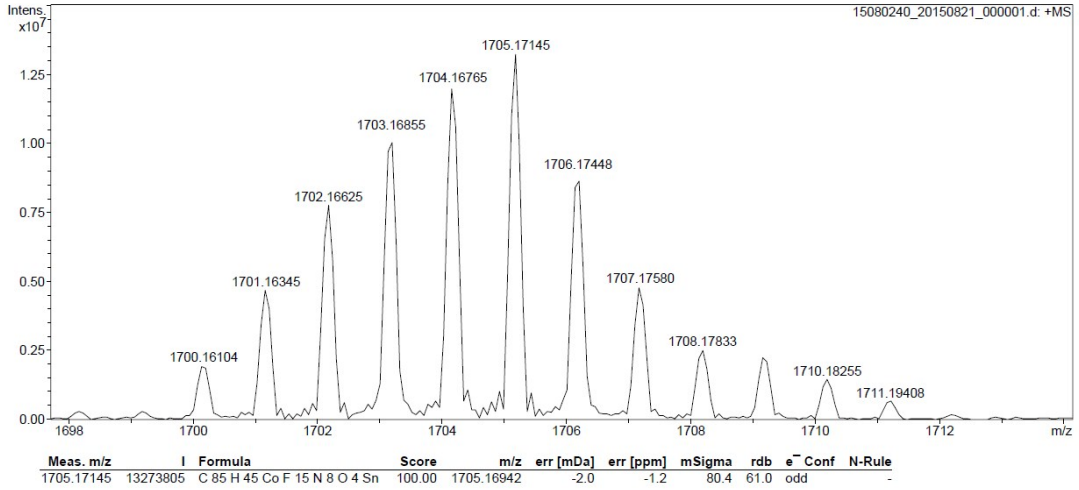


Figure S4. ESI-MS spectrum of **1**.

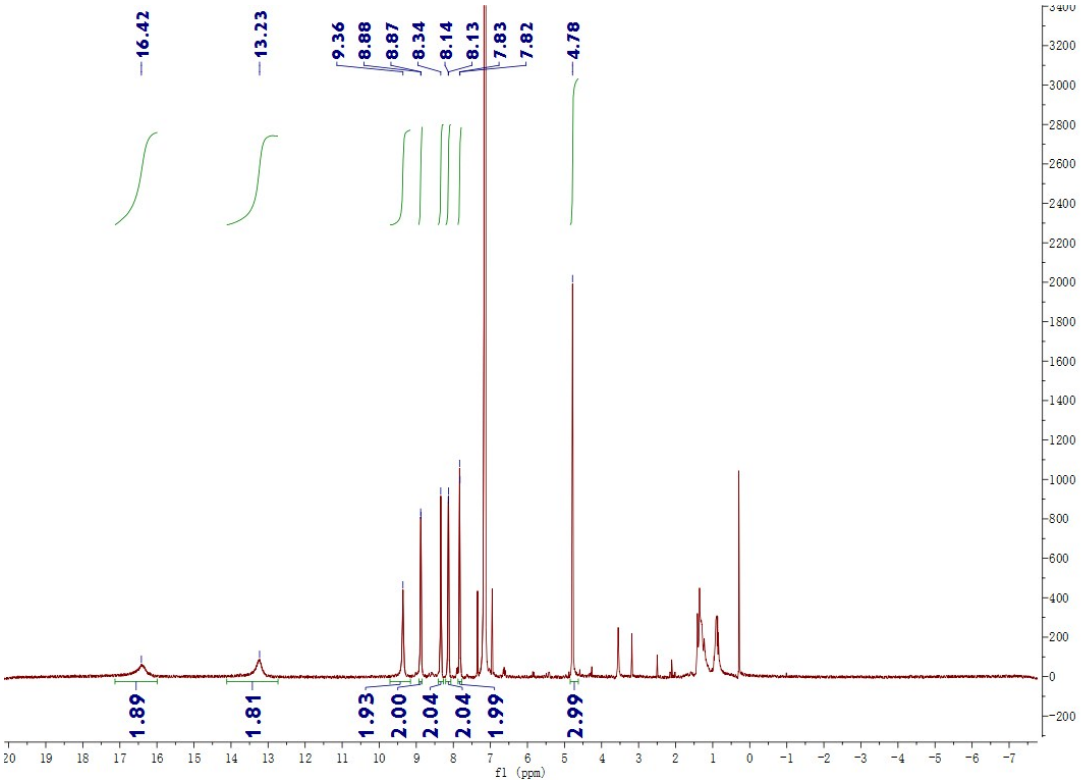
Table S1. Crystal data and structure refinement for **1**.

Identification code	mx4830a_sq
Empirical formula	C85 H44 Co F15 N8 O4 Sn
Formula weight	1703.90
Temperature	173.1500 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a = 17.250(5) Å α= 90°.

	b = 13.082(3) Å β= 96.735(4)°.
	c = 32.044(9) Å γ = 90°.
Volume	7181(3) $Å^3$
Z	4
Density (calculated)	1.576 Mg/m^3
Absorption coefficient	0.679 mm^{-1}
F(000)	3416
Crystal size	0.193 x 0.109 x 0.046 mm^3
Theta range for data collection	1.683 to 27.409°.
Index ranges	-22<=h<=22, -16<=k<=16, -32<=l<=41
Reflections collected	47149
Independent reflections	16271 [R(int) = 0.0653]
Completeness to theta = 26.000°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.61813
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16271 / 294 / 1104
Goodness-of-fit on F^2	1.173
Final R indices [I>2sigma(I)]	R1 = 0.0940, wR2 = 0.2020
R indices (all data)	R1 = 0.1103, wR2 = 0.2127
Extinction coefficient	n/a
Largest diff. peak and hole	1.558 and -0.996 $e.Å^{-3}$

3. ^{1}H NMR study of photolysis of 1.

(a)



(b)

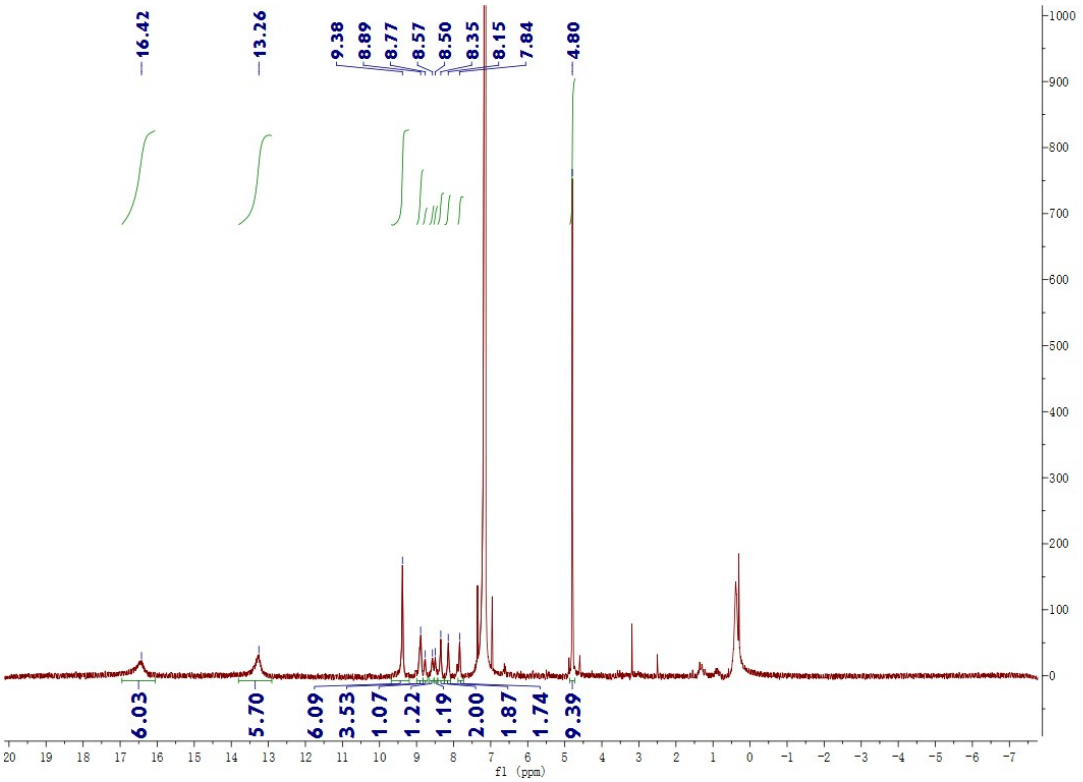


Figure S5. ^{1}H NMR spectra after visible light photolysis of **1**. Conditions: (a) 1 μmol of **1**, 1 atm of dry O_2, C_6D_6; (b) 1 μmol of **1**, 1 atm of air, C_6D_6. In both cases the reaction was complete within 1 h. The large discrepancy between the integration of **3** and (**6** + **7**) was due to partial precipitation of

3. Single crystals of **3** suitable for X-ray diffraction study were obtained from the precipitate (Figure S6).

3: ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 16.42 (br s, 8H), 13.23 (br s, 8H), 9.36 (br s, 8H), 4.78 (br s, 12H).

6: ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 8.88 (d, J = 3.7 Hz, 4H), 8.34 (br s, 4H), 8.13 (d, J = 3.8 Hz, 4H), 7.83 (d, J = 4.5 Hz, 4H).

7: ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 8.89 (br s, 2H), 8.77 (br s, 2H), 8.57 (br s, 2H), 8.50 (br s, 2H).

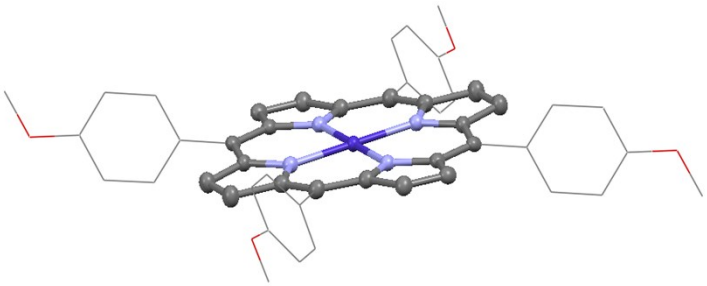


Figure S6. Solid state structure of **3**. Hydrogens and a crystallographic benzene molecule were omitted for clarity.

Table S2. Crystal data and structure refinement for **3**.

Identification code	mx4168	
Empirical formula	C54 H42 Co N4 O4	
Formula weight	869.84	
Temperature	173.1500 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 14.361(3) Å	α= 90°.
	b = 9.5170(19) Å	β= 99.257(3)°.
	c = 15.449(3) Å	γ = 90°.
Volume	2084.0(8) Å^3	
Z	2	
Density (calculated)	1.386 Mg/m^3	
Absorption coefficient	0.467 mm^{-1}	
F(000)	906	
Crystal size	0.28 x 0.2 x 0.05 mm^3	
Theta range for data collection	2.523 to 27.497°.	
Index ranges	-18<=h<=17, -12<=k<=11, -20<=l<=19	
Reflections collected	15827	
Independent reflections	4765 [R(int) = 0.0365]	

Completeness to theta = 26.000°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.7749
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4765 / 0 / 288
Goodness-of-fit on F^2	1.128
Final R indices [I>2sigma(I)]	R1 = 0.0459, wR2 = 0.1042
R indices (all data)	R1 = 0.0493, wR2 = 0.1062
Extinction coefficient	n/a
Largest diff. peak and hole	0.384 and -0.246 e.Å^{-3}

4. Independent synthesis and characterization of 6.

Synthesis of (TPFC)Sn-O-Sn(TPFC) (6). 0.0212 mmol of freshly prepared **4** was dissolved in a minimal amount of benzene under air, and 5 drops of water were added. A color change from dark green to bright violet was observed within 10 min. The solution was then evaporated to dryness under gentle heating, re-dissolved in dry benzene, filtered, and evaporated to give (TPFC)Sn-O-Sn(TPFC) (**6**, 18.9 mg, 97 %) as a dark-violet solid. ^{1}H NMR (400 MHz, C_6D_6): δ (ppm): 8.97 (d, J = 4.0 Hz, 4H), 8.37 (d, J = 3.6 Hz, 4H), 8.14 (d, J = 4.5 Hz, 4H), 7.84 (d, J = 4.6 Hz, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm): 142.5, 140.0, 138.3, 135.8, 127.2, 125.7, 124.0, 118.6 (C_6F_5 carbons were not resolved); ^{19}F NMR (471 MHz, C_6D_6) δ (ppm): -134.9 – -135.4 (m, 4F), -135.6 (d, J = 23.8 Hz, 2F), -138.4 (dd, J = 24.6, 7.4 Hz, 4F), -138.8 (dd, J = 24.4, 7.1 Hz, 2F), -152.4 (q, J = 21.2 Hz, 6F), -161.7 (t, J = 22.6 Hz, 4F), -162.6 (ddd, J = 29.3, 21.9, 8.1 Hz, 4F), -163.2 – -163.5 (m, 4F); ^{119}Sn NMR (186 MHz, C_6D_6) δ (ppm): -429 (s); HR-ESI-MS m/z calcd for $C_{74}H_{16}F_{30}N_8OSn_2$ $[M]^+$ 1841.900645, found 1841.903980; UV-Vis (toluene) λ_{max}: 406(sh), 425, 513(sh), 540(sh), 580, 599. Single crystals suitable for XRD analysis were obtained by slow evaporation of a concentrated petroleum ether solution. If the synthesis was carried out in the absence of water, an unknown impurity would be present.

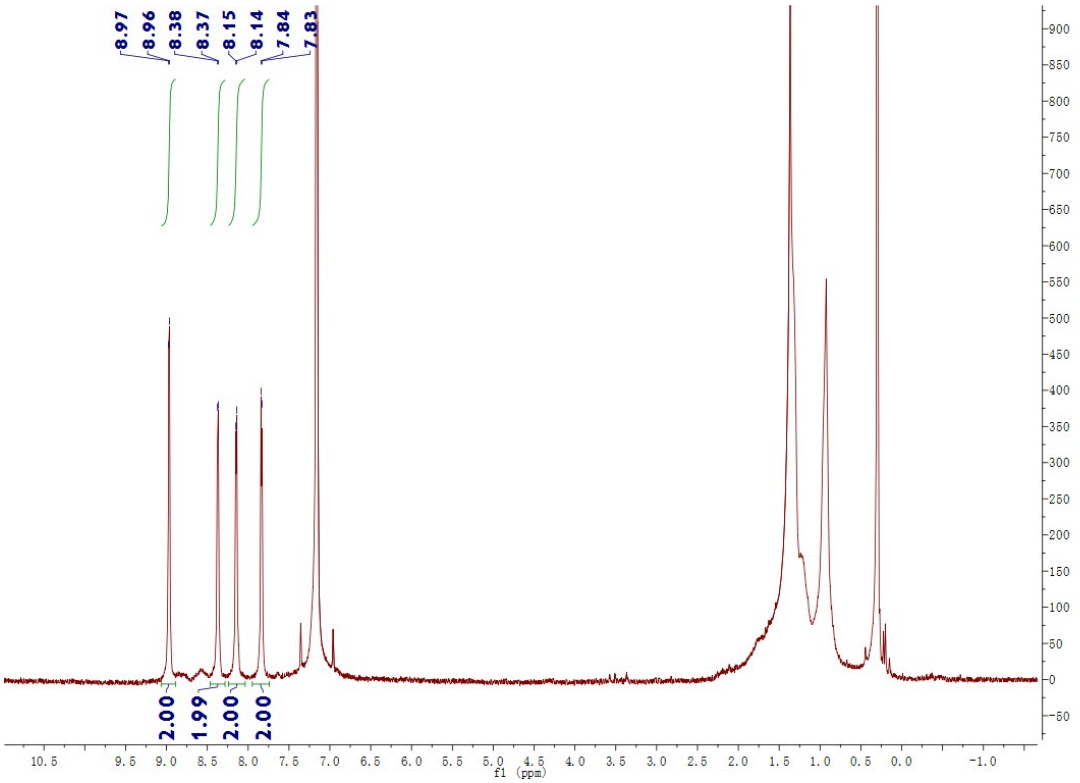


Figure S7. ^{1}H NMR spectrum of **6** in C_6D_6.

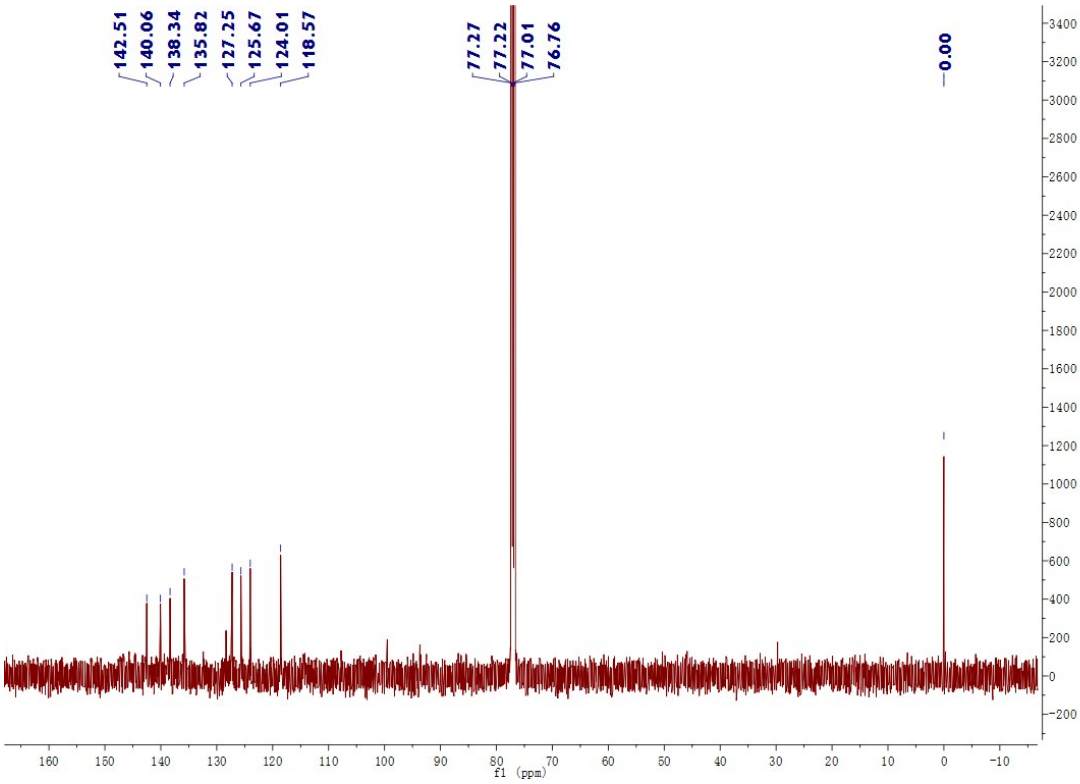


Figure S8. ^{13}C NMR spectrum of **6** in C_6D_6.

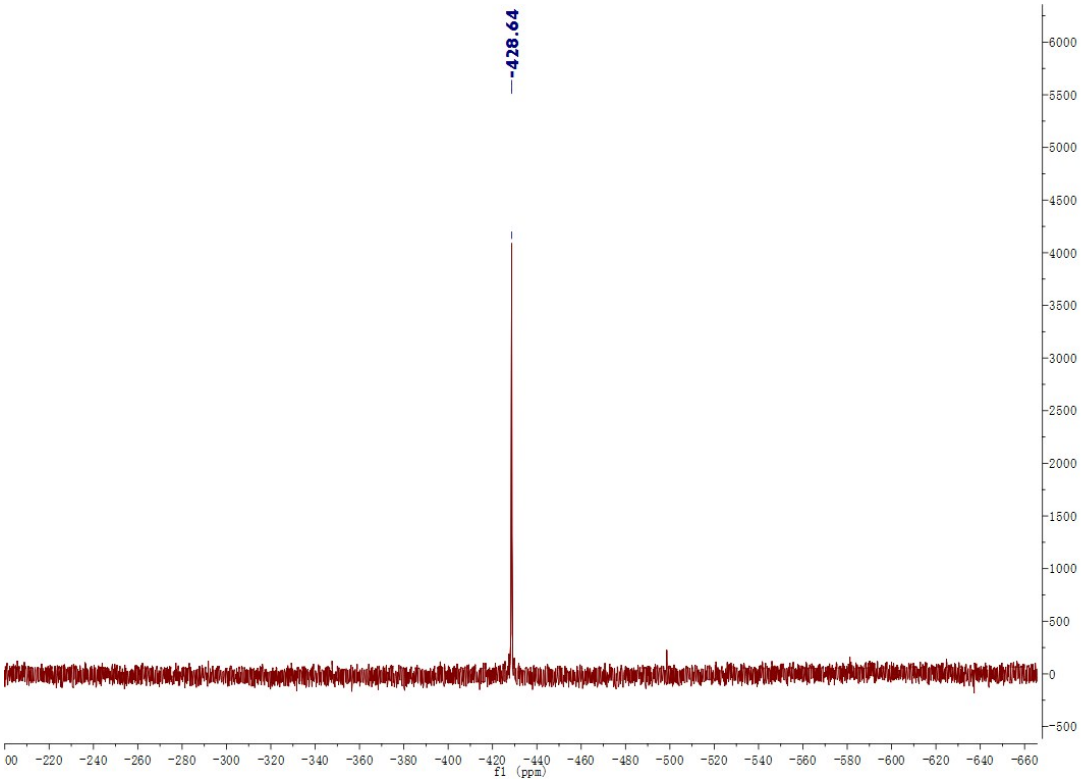


Figure S9. ^{119}Sn NMR spectrum of **6** in C_6D_6.

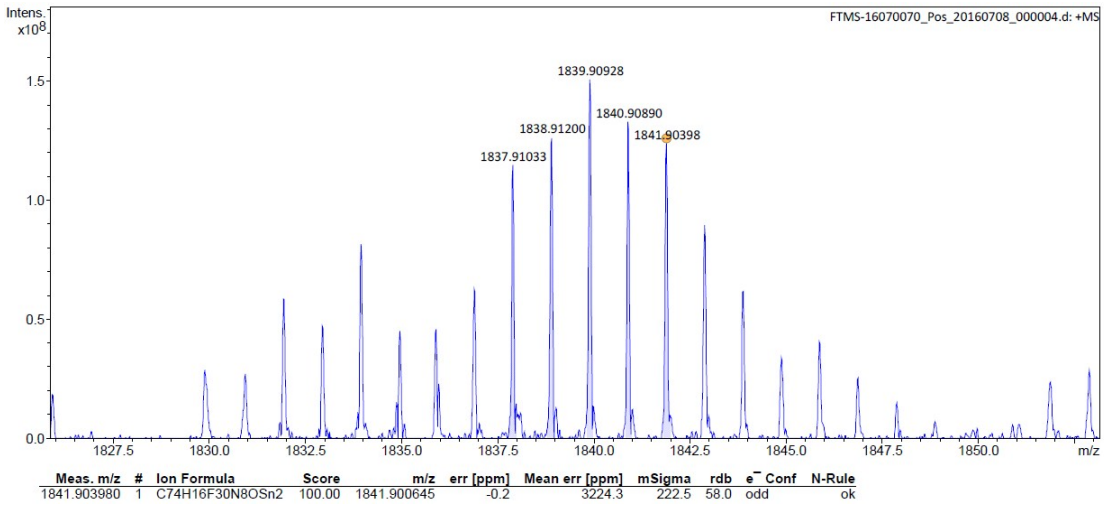


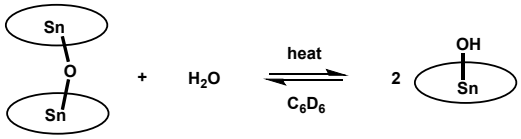
Figure S10. ESI-MS spectrum of **6**.

Table S3. Crystal data and structure refinement for **6**.

Identification code	mx5350_sq
Empirical formula	C74 H16 F30 N8 O Sn2
Formula weight	1840.33
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1

Unit cell dimensions	a = 12.8962(18) Å	α= 101.533(2)°.
	b = 15.333(2) Å	β= 90.070(2)°.
	c = 21.248(3) Å	γ = 106.286(2)°.
Volume	3944.1(10) $Å^3$	
Z	2	
Density (calculated)	1.550 Mg/m^3	
Absorption coefficient	0.751 mm^{-1}	
F(000)	1788	
Crystal size	0.27 x 0.15 x 0.13 mm^3	
Theta range for data collection	1.415 to 27.476°.	
Index ranges	-16<=h<=16, -19<=k<=19, -27<=l<=27	
Reflections collected	55543	
Independent reflections	17963 [R(int) = 0.0451]	
Completeness to theta = 26.000°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.886	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17963 / 427 / 1148	
Goodness-of-fit on F^2	1.089	
Final R indices [I>2sigma(I)]	R1 = 0.0557, wR2 = 0.1298	
R indices (all data)	R1 = 0.0606, wR2 = 0.1333	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.444 and -0.907 $e.Å^{-3}$	

5. Hydration of 6.



Variable-temperature (VT)-NMR study of the reaction of 6 with water. Approximately 1 mg of **6** was dissolved in 300 µL of C_6D_6 in a vacuum adapted NMR tube. 5 µL of mesitylene (0.0360 mmol) was added as an internal standard. Then, 1 µL of water was added, which was enough to ensure its saturation in benzene within the investigated temperature interval. VT-NMR spectra were recorded on a Bruker AVII$^+$-500 NMR spectrometer. The amount of **6** and **7** could be calculated from the integration of the peaks at 7.84 and 8.85 ppm, respectively (Figure S11), while the concentration of water was calculated based on the reported solubility of water in benzene at various temperatures.[6] The equilibrium constant of the reaction could be calculated through $K = \frac{[7]^2}{[6][H_2O]}$. The results were listed in Table S4. The reaction enthalpy ΔH and entropy ΔS were

derived from the temperature dependence of Δ*G* (Figure S12).

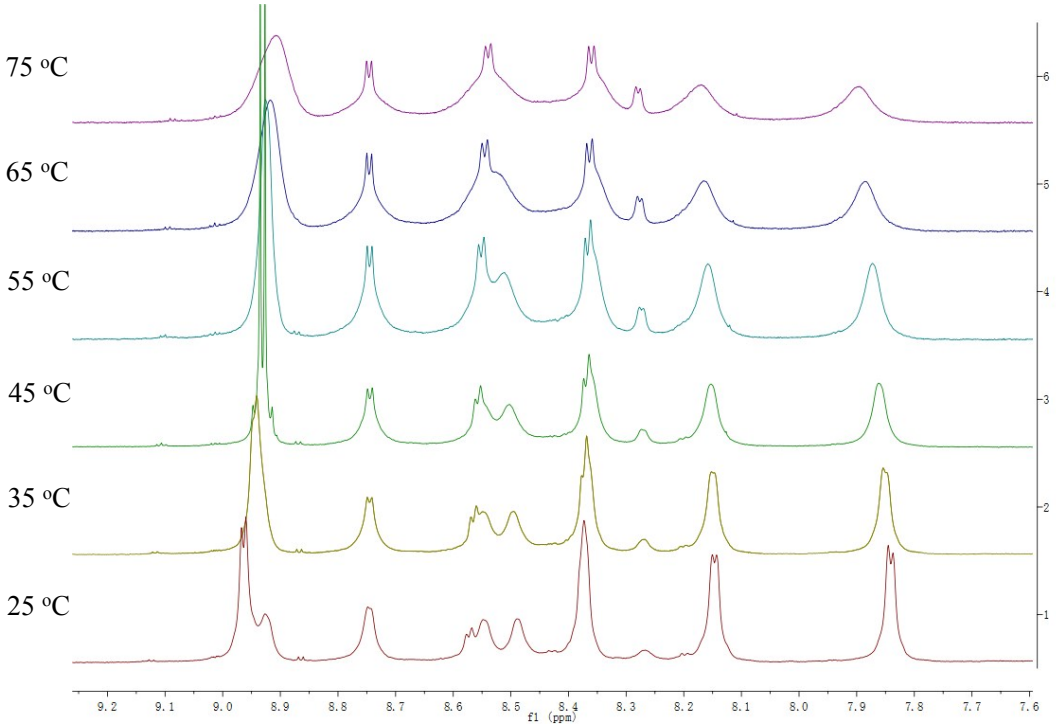


Figure S11. Variable-temperature (VT) ^{1}H NMR spectra of a C_6D_6 solution of **6** containing water, recorded in the range 25 ~ 75 °C.

Table S4. Equilibrium constants for hydration of **6** derived from the VT-NMR experiment.

Temperature(°C)	7(mmol/L)	6(mmol/L)	H_2O(mmol/L)	K
25	5.77	4.67	37.3	0.191
35	5.87	3.93	50.4	0.174
45	6.13	3.76	66.2	0.151
55	6.40	3.50	85.4	0.137
65	6.77	3.43	108.6	0.123
75	7.00	3.20	135.5	0.113

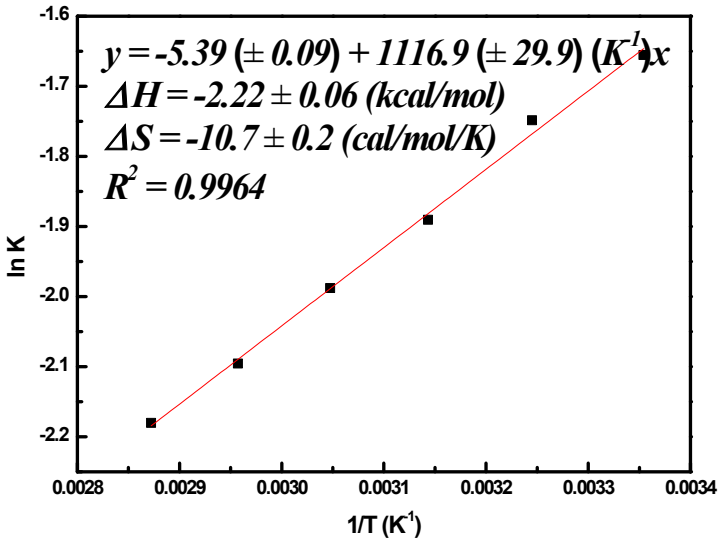


Figure S12. Temperature dependence of ΔG for hydration of **6**.

6. Laser flash photolysis of 1.

Instrument. The transient absorption profiles were recorded by a transient absorption detection system from Edinburgh Instruments, equipped with a monochromator and a pulsed xenon lamp. The excitation light was provided by a Continuum Surelite Laser, which delivered ca. 5 ns pulses at a repeating frequency of 10 Hz, with tunable wavelength. The monitoring light from xenon lamp was allowed to pass through the sample cell in a right-angle configuration with respect to the excitation light. The output was processed with Edinburgh Instruments L900 software.

Sample preparation. Since **2** is extremely air-sensitive, and the sample concentration must be kept below 1×10^{-5} mol/L due to the large extinction coefficient of **1** (2.6×10^{5} at 413 nm), due care was taken to avoid contact of the sample with oxygen. Thus, it was found mandatory to further deoxygenate the degassed toluene with molten sodium for 48 h under N_2, until fresh sodium surface was seen and persisted for 24 h. Freshly-prepared **1**, shown by ^{1}H NMR to be free (< 1 %) of **3** and **6**, was dissolved, under dark, in oxygen-free toluene in a glovebox whose oxygen level was consistently below 0.5 ppm, to make a 2.6×10^{-5} mol/L stock solution which was stored at -30 ^{o}C in the glovebox. A stock solution of **3** was similarly made, but was stored at room temperature to avoid precipitation. Appropriate amounts of stock solutions were added to a specially designed 1×1 cm UV absorption cell fitted with a Schlenk valve, and diluted to 2.5 mL with oxygen-free toluene. The cell was taken out of the glovebox under careful shielding against ambient light, and immediately inserted into the spectrometer. No sample was measured for over 30 minutes because of possible air leakage. The transient absorption spectra exhibited the same shape for at least three independent measurements, while samples that were deoxygenated less stringently gave strong negative peaks that coincided with those of **6**, whose lifetime was about 100-200 μs (details of the corresponding reaction are unknown).

Data processing. The spectra in Figure 5b and 5c were smoothed with window sizes of 5 and 20 points, respectively, to reduce overlapping of curves caused by noise. Since there are 876 and 9983 data points per curve, respectively, for Figure 5b and 5c, such smoothing procedure should

have negligible impact on spectral shapes and data fitting.

The data in Figure 5c were fitted according to $\Delta OD = \Delta OD_{res} + \Delta OD_0 e^{-k_{obs}t}$, where ΔOD_{res} is a constant that partly corrects for undetected side reactions (such as homo-coupling of **2**), and possibly baseline shifts. The fitted ΔOD_{res} was consistently below 15 % of ΔOD_0, indicating negligible side reaction.

The so-obtained k_{obs} were plotted against [**3**], as shown in Figure 5d. As noticed in the main text, the intercept was not zero. However, as illustrated above, the sample of **1** was free of **3** as shown by ^{1}H NMR, and oxygen leakage was absent as deduced from the lack of negative peak of **6** (see above), so it was concluded that the non-zero intercept was due to **3** from photolysis of **1**. One may argue that this would lead to second-order kinetics if no external [**3**] was added. However, the kinetic curve did not decay to a significant extent over 3 ms for [**3**] to change significantly, and the light output from the xenon lamp was unstable for periods longer than 3 ms, preventing following the reaction at longer timescales. Thus it was decided to fit all curves in Figure 5c according to first-order kinetics. This might lead to slight systematic error in the recombination rate, but since the dissociation barrier was determined at a much lower accuracy, this should have no impact on the estimated thermodynamics.

7. Spin trapping of 2.

2.6 μmol of freshly purified **1** and 20 μmol of PBN were dissolved in 500 μL of dry toluene in a glovebox, and transferred to a quartz tube equipped with a J. Young valve. The solution was kept in the dark until inserted into the EPR cavity, and then cooled to -50 °C. An initial spectrum was taken, before visible light (Xe lamp, with a 420-780 nm filter) was introduced into the cavity, and spectral changes were monitored continuously. After about 20 minutes, the sample was warmed to -20 °C to record the isotropic fast-motion spectrum, and then cooled to -150 °C to record the anisotropic spectrum. At the latter temperature, a weak signal centered at g = 2.25 was evident (Figure S13) whose g value indicated transition metal origin. Nevertheless anisotropic and hyperfine splittings were obscured, probably due to precipitation of **3** during cooling.

The reference sample of **3** was prepared by dissolving *ca.* 0.25 μmol of **3** in 400 μL of C_6D_6, and cooling to -170 °C. The use of benzene as solvent circumvented the low solubility of **3** at low temperature by rapidly forming a glass upon cooling. This allowed for resolution of ^{59}Co hyperfine lines of **3**, confirming the assignment of the signal as a Co(II) complex.

Direct EPR observation of **2** would have been a stronger evidence for its existence, and may allow a better investigation of its electronic structure. However, no signals of **2** or **3** were found during photolysis of **1**, even if the solution was gradually frozen upon irradiation and cooled to -170 °C (to trap any transient radicals in the forming glass) or heated to 110 °C (to increase the equilibrium concentration of the radicals). This is attributed to the fast recombination rate of the two complexes, and the low HOMO-LUMO gaps of the complexes, which decrease the signal strengths through rapid spin relaxation.

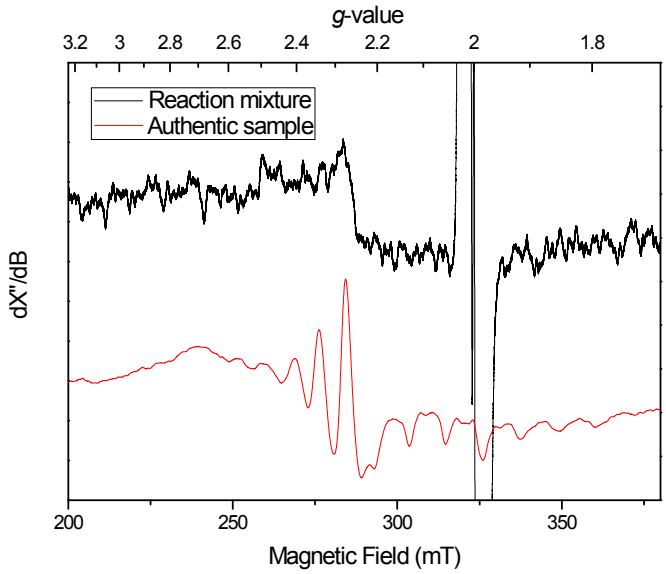


Figure S13. Anisotropic EPR spectrum of the reaction mixture of **1** and PBN, recorded at -150 °C. The reference spectrum of **3** is shown for comparison ($g_{\perp}$ = 2.49, $g_{//}$ = 2.02, $A_{\perp}$ = 300 MHz, $A_{//}$ = 320 MHz). The large signal centered at 323 mT was due to the PBN adduct of **2**.

8. Kinetic experiments and mechanistic discussions for the reaction of 1 with TEMPO

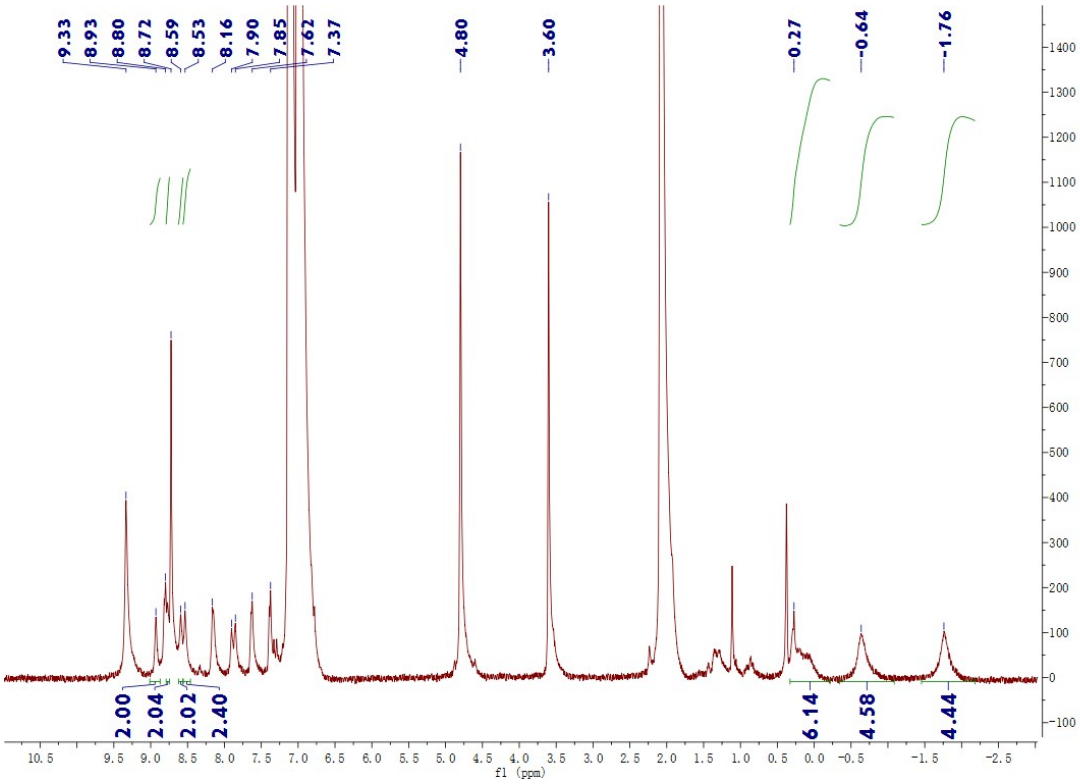


Figure S14. Typical ^{1}H NMR spectrum obtained during the kinetic experiments. Conditions: 1.6 mmol/L of **1**, 10 eq. of TEMPO, toluene-d_8 (containing 15 % v/v C_6D_6), 70.0 °C, under dark and N_2 atmosphere. Conversions were determined by relative integration of the methoxy signals of **1** (3.60 ppm) and **3** (4.80 ppm). The addition of C_6D_6 was a remedy to the difficulty in locking field due to

the presence of TEMPO.

8: ^{1}H NMR (400 MHz, toluene-d_8) δ (ppm): 8.93 (br s, 2H), 8.79 (br s, 2H), 8.59 (br s, 2H), 8.53 (br s, 2H), 0.35 – -0.10 (m, 6H), -0.64 (br s, 6H), -1.76 (br s, 6H); ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 8.92 (br s, 2H), 8.84 (br s, 2H), 8.59 (br s, 2H), 8.51 (br s, 2H), 0.26 (br s, 2H), 0.18 – -0.03 (m, 4H), -0.60 (br s, 6H), -1.68 (br s, 6H).

To eliminate the possibility of Sn-Co bond heterolysis, additional experiments were performed. Although independent treatment of **4** with TEMPO produced **8**, which is the product of the reaction of **1** with TEMPO, quantitative conversion was observed only after 2 h at room temperature. This ruled out heterolytic dissociation of **1** to $[(TPFC)Sn^{II}]^-$ and $[(TAP)Co^{III}]^+$ as a productive pathway, since otherwise the reaction of $[(TPFC)Sn^{II}]^-$ with TEMPO would be the rate-limiting step of the reaction based on its slow rate, which contradicts with the observed zeroth order dependence on TEMPO. Furthermore, no organocobalt nor organotin complexes were detected by NMR when **1** was heated at 110 ^{o}C in the presence of methyl acrylate, which is known as an efficient and irreversible trap for both Co(I)[7] and corrole Sn(II)[1] species. Neither were the use of benzoic acid or cyclohexene oxide effective in trapping the two highly nucleophilic species. This provided additional evidence against the involvement of $[(TPFC)Sn^{II}]^-$ and $[(TAP)Co^{III}]^+$, and further excluded heterolytic dissociation of **1** to $[(TPFC)Sn^{IV}]^+$ and $[(TAP)Co^{I}]^-$. Besides, homolysis of Sn-Co bond is a known pattern of reactivity with many examples,[8] and to our best knowledge, heterolysis of Sn-Co bond is rare and only occurs in strong polar solvents under the action of strong nucleophiles.[8d] Consequently, the measured activation enthalpy for the reaction of **1** with TEMPO represents the barrier for the homolysis of **1**, which justifies the estimation of Sn-Co BDE from the data.

Although **8** could not be isolated as a pure form from the reaction mixture of **1** and TEMPO, the reaction of **4** with TEMPO provided a route for its independent synthesis. A solution of 0.0053 mmol of freshly prepared **4** in dry benzene was treated with 8.3 mg (0.053 mmol) of TEMPO under N_2. After 2 h, the solution was evaporated under gentle heating, followed by washing with dry *n*-hexane to give (TPFC)Sn-TEMPO (**8**, 4.8 mg, 85 %) as a dark-purple solid. ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 8.95 (d, J = 3.9 Hz, 2H), 8.78 (d, J = 3.2 Hz, 2H), 8.60 (d, J = 3.6 Hz, 2H), 8.53 (d, J = 3.4 Hz, 2H), 0.27 (m, 2H), 0.20 (br s, 4H), -0.60 (br s, 6H), -1.67 (br s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm): 143.0, 141.0, 138.9, 136.7, 127.9, 127.7, 125.7, 124.3, 118.3, 38.1, 38.0, 31.1, 15.6 (C_6F_5 carbons were not resolved); HR-ESI-MS m/z calcd for $C_{46}H_{27}F_{15}N_5OSn$ $[M+H]^+$ 1070.10021, found 1070.09591. The ^{1}H NMR signals matched those observed in the reaction mixture of **1** and TEMPO.

Previously, we have reported a complex that was in direct analogy with **8**, namely (TPFC)Ge-TEMPO.[9] The complex possessed a weak Ge-O bond (calculated BDFE = 20.6 kcal/mol) and readily underwent photolysis under visible light irradiation. The resulting (TPFC)Ge and TEMPO radicals could activate the N-H bonds of amines in a cooperative manner, through a proton coupled electron transfer (PCET) mechanism.[9b] However, no reaction was observed during irradiation of a mixture of **8** with various amines with a Hg lamp. This hinted on a stronger Sn-O bond in **8**. In fact, from the absence of backward reaction from **8** and **3**, one is able to deduce that the BDFE of the Sn-O bond in **8** should be at least 2 kcal/mol larger than that of the Sn-Co bond of **1**, i.e. at least 23 kcal/mol.

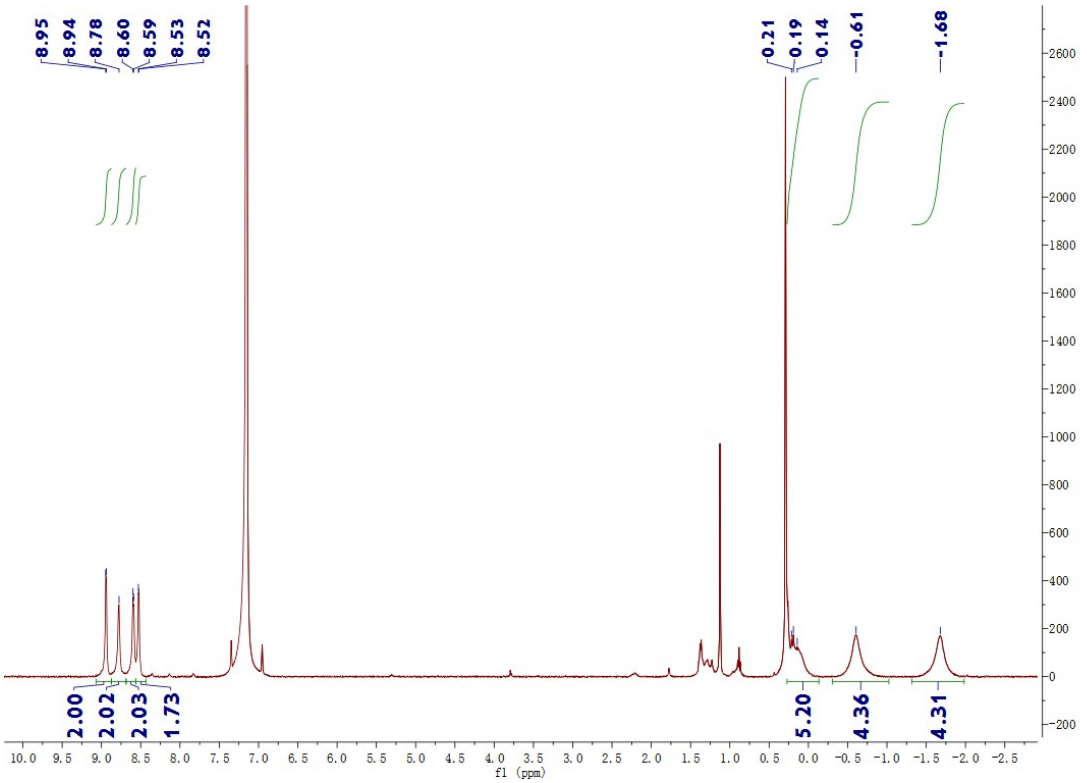


Figure S15. ^{1}H NMR spectrum of **8** in C_6D_6.

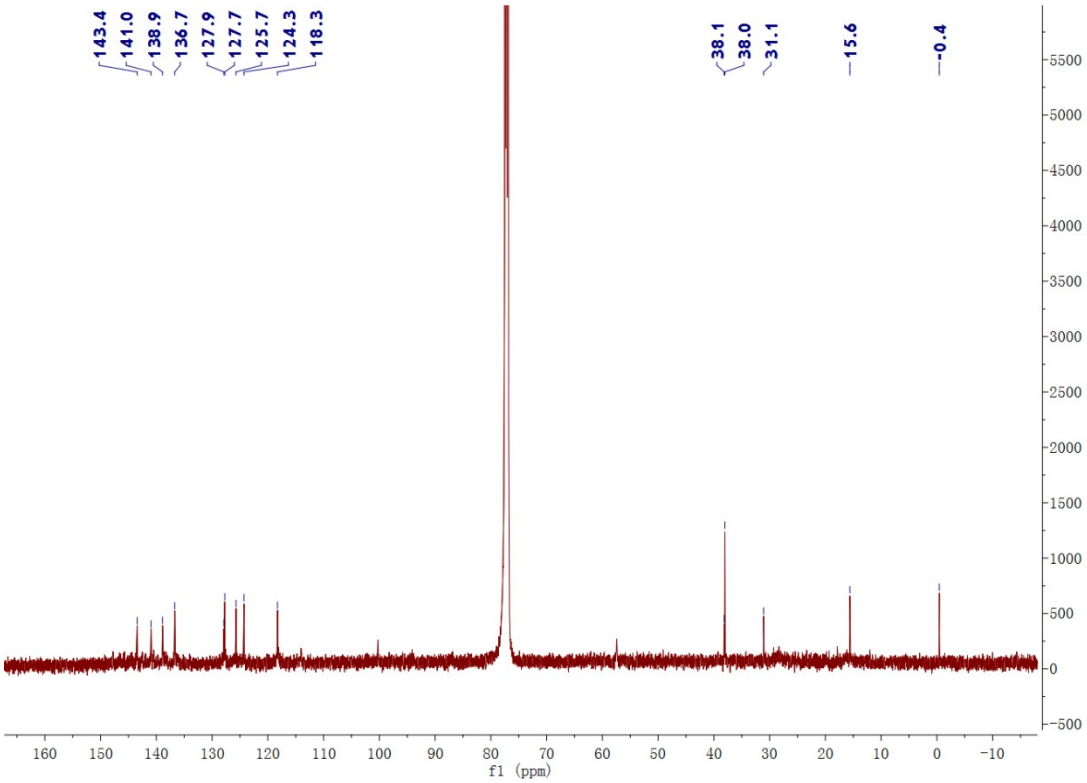


Figure S16. ^{13}C NMR spectrum of **8** in $CDCl_3$.

Configuration transformation energy barrier calculation for 8. The *o*-CH_3 peaks in the TEMPO ligand of **8** were significantly broadened and thus integrated to a number much smaller than the expected number of 6H. A VT-NMR experiment revealed that this was due to slow exchange of the TEMPO ring between two equivalent boat configurations (Figure S17), similar to the situation of (TPFC)Ge-TEMPO.[9] The DNMR package implanted in Bruker TopSpin 3.1 program was used to calculate the rate constants at different temperatures. The energy barrier was calculated using the Arrhenius equation. An activation energy (E_a) of 17.1 kcal/mol was obtained, which is comparable to that of (TPFC)Ge-TEMPO (15.0 kcal/mol).[9]

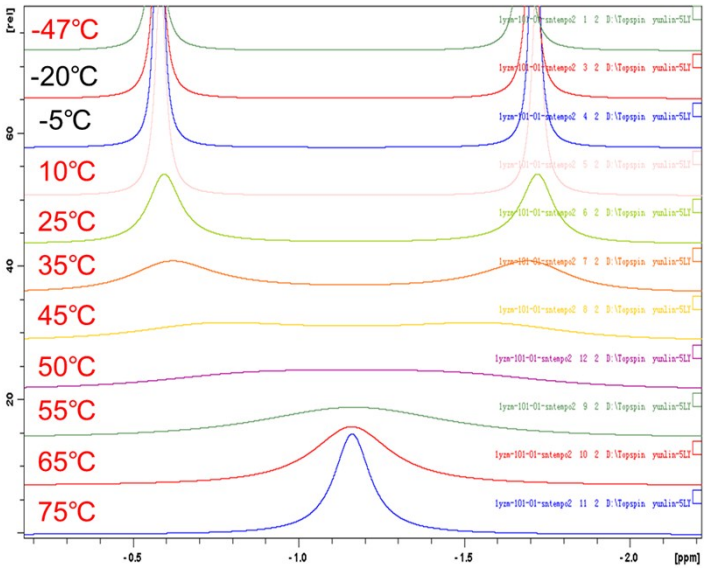


Figure S17. Resonances of the four methyl groups of **8** at different temperatures in toluene-d_8.

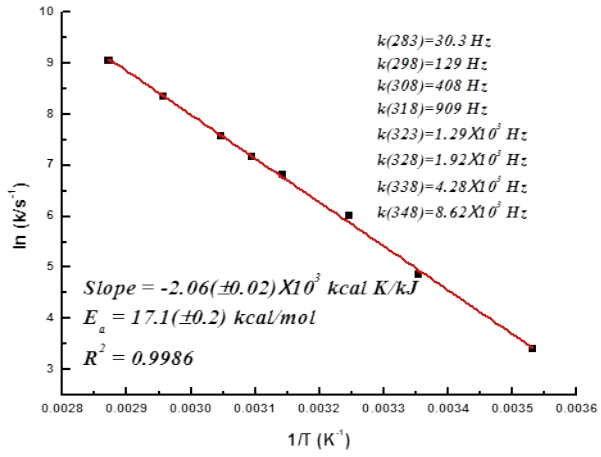


Figure S18. Measurement of apparent topomerization energy barrier using ^{1}H NMR.

9. Product analysis for the reaction of 1 with *p*-fluorophenylacetylene.

1.0 μmol of **1** was added to a vacuum adapted NMR tube, followed by addition of 25 μL of *p*-fluorophenylacetylene and 0.4 mL of C_6D_6. The solution was degassed by three freeze-pump-thaw cycles and irradiated with a Xe lamp at room temperature for 2 days. The reaction mixture was then chromatographed on silica gel with PE:DCM = 2:1 as eluent. Four fractions were collected and characterized. This, together with the relative integral intensity changes of the ^{1}H NMR signals

during the reaction, allowed unambiguous assignment of the products. Detailed assignment of ^{1}H NMR signals of **9-11** was aided by the ^{1}H NMR data of isolated **9'-11'** (*vide infra*).

3: ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 16.33 (br s, 8H), 13.21 (br s, 8H), 9.36 (br s, 8H), 4.80 (br s, 12H).

9: ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 8.63 (s, 8H), 8.45 (m, 2H), 8.27 (d, J = 4.2 Hz, 2H), 8.19 (d, J = 4.1 Hz, 2H), 7.94 (d, J = 3.9 Hz, 2H), 5.27 (m, 2H), 3.63 (s, 12H), 0.72 (m, 2H), -6.02 (s, 1H); HR-ESI-MS m/z calcd for $C_{93}H_{50}CoF_{16}N_8O_4Sn$ $[M]^+$ 1825.20524, found 1825.21182.

10: ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 8.75 (s, 8H), 8.51 (d, J = 4.1 Hz, 2H), 8.42 (d, J = 2.3 Hz, 2H), 8.16 (d, J = 4.2 Hz, 2H), 8.03 (d, J = 4.0 Hz, 2H), 6.07 (t, J = 8.6 Hz, 2H), 5.46 (t, J = 8.6 Hz, 2H), 3.55 (s, 12H), 3.12 – 3.04 (m, 2H), 1.98 – 1.90 (m, 2H), -1.50 (s, 1H), -2.90 (s, 1H); HR-ESI-MS m/z calcd for $C_{101}H_{55}CoF_{17}N_8O_4Sn$ $[M]^+$ 1945.24281, found 1945.24484.

11: ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 8.85 (s, 8H), 8.62 (d, J = 5.6 Hz, 2H), 8.54 (m, 2H), 8.29 (d, J = 4.1 Hz, 2H), 8.18 – 8.17 (m, 2H), 5.83 (m, 2H), 5.77 (m, 2H), 5.27 (m, 2H), 4.15 (m, 2H), 3.52 (s, 12H), 3.16 – 3.10 (m, 2H), 2.42 (m, 2H), 2.17 (s, 1H), 0.09 (s, 1H), -1.88 (s, 1H); HR-ESI-MS m/z calcd for $C_{109}H_{60}CoF_{18}N_8O_4Sn$ $[M]^+$ 2065.28036, found 2065.27943.

12: ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 9.09 (s, 8H), 8.03 (br s, 16H), 5.73 (t, J = 8.8 Hz, 2H), 3.53 (s, 12H), 3.20 (dd, J = 8.6, 5.7 Hz, 2H), 0.05 (d, J = 2.2 Hz, 1H), -1.51 (d, J = 2.3 Hz, 1H).

13: ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 9.08 (s, 8H), 8.03 (s, 16H), 6.50 (t, J = 8.6 Hz, 2H), 5.71 – 5.65 (m, 2H), 5.57 – 5.50 (m, 2H), 3.52 (s, 12H), 3.16 – 3.07 (m, 2H), -1.17 (s, 1H).

14: HR-ESI-MS m/z calcd for $C_{61}H_{23}F_{18}N_4Sn$ $[M+H]^+$ 1273.06655, found 1273.06321.

15: ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 7.46 (s, 3H), 7.23 (dd, J = 8.8, 5.3 Hz, 6H), 6.92 (t, J = 8.7 Hz, 6H); ^{19}F NMR (471 MHz, C_6D_6) δ (ppm): -114.9 (tt, J = 8.5, 5.7 Hz, 3F); GC-MS (EI) m/z (I): 360.1 (100, calcd for $C_{24}H_{15}F_3$ $[M]^+$ 360.1).

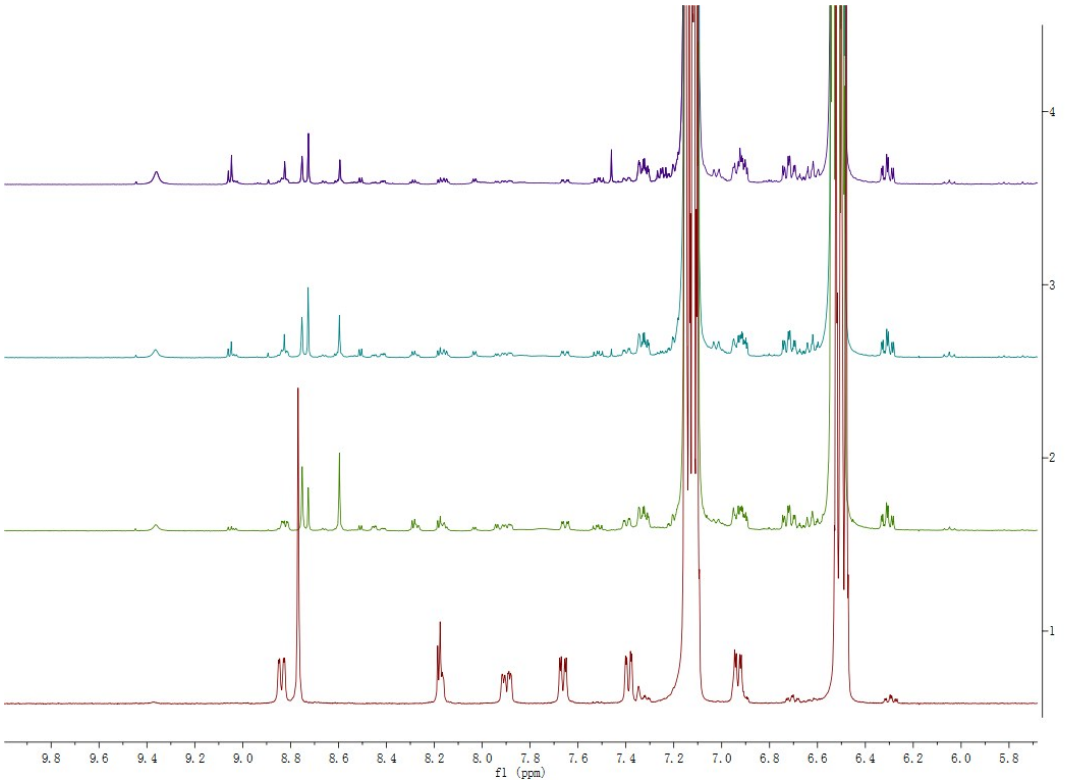
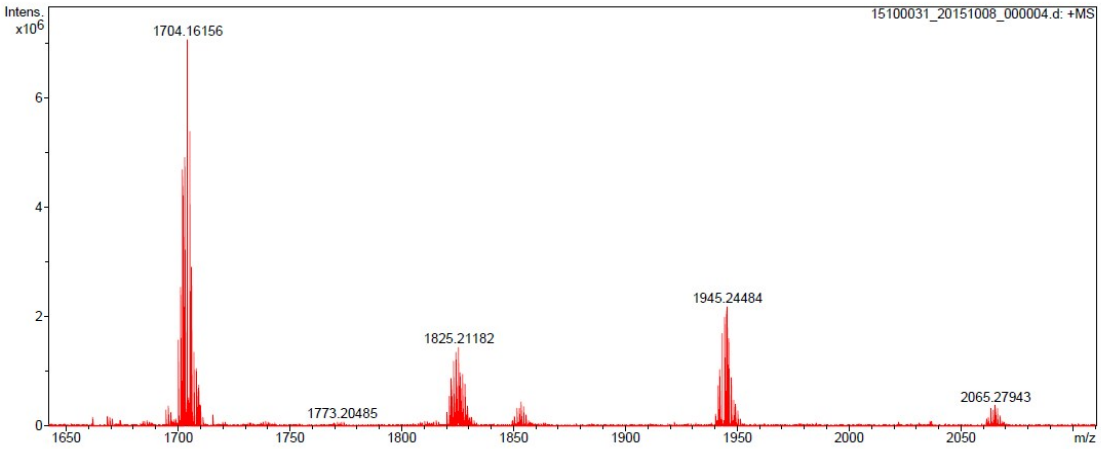


Figure S19. ^{1}H NMR spectrum of the reaction mixture of **1** with *p*-fluorophenylacetylene. From bottom to top: before irradiation, and after being irradiated for 4 h, 18.5 h, and 47 h. The complexes

9 (8.59 ppm), **10** (8.73 ppm) and **11** (8.82 ppm) appeared in a sequential manner. When a sufficient concentration of **10** was accumulated, the signals of **12** (9.06 ppm), **13** (9.05 ppm) and **15** (7.46 ppm) increased rapidly.



Meas. m/z	I	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1704.16156	7065584	C 85 H 44 Co F 15 N 8 O 4 Sn	100.00	1704.16158	0.0	0.0	25.2	61.5	even	-
1825.21182	1445666	C 93 H 50 Co F 16 N 8 O 4 Sn	100.00	1825.20524	-6.6	-3.6	107.2	66.0	odd	-
1945.24484	2196404	C 101 H 55 Co F 17 N 8 O 4 Sn	100.00	1945.24281	-2.0	-1.0	65.3	71.0	odd	-
2065.27943	395150	C 109 H 60 Co F 18 N 8 O 4 Sn	100.00	2065.28036	0.9	0.5	62.4	76.0	odd	-

Figure S20. ESI-MS spectrum of the reaction mixture of **1** with *p*-fluorophenylacetylene, showing the presence of **1** (m/z 1704.16156, $[M+H]^+$), **9** (m/z 1825.21182, $[M]^+$), **10** (m/z 1945.24484, $[M]^+$) and **11** (m/z 2065.27943, $[M]^+$).

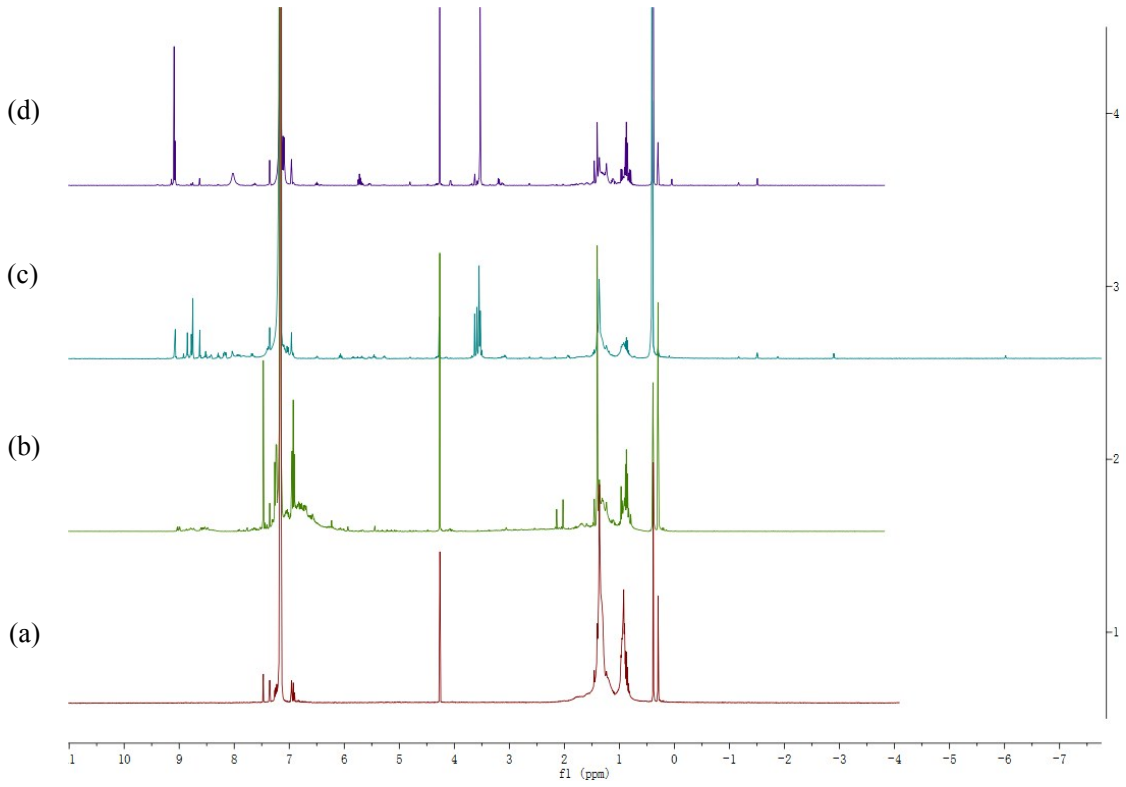


Figure S21. ^{1}H NMR spectra of the isolated fractions. (a) **15**; (b) a mixture of **14**, **15** and other unidentified organotin corrole complexes; (c) a mixture of **1**, **9**, **10**, **11**, **12** and **13**; (d) a mixture of **12** and **13.**

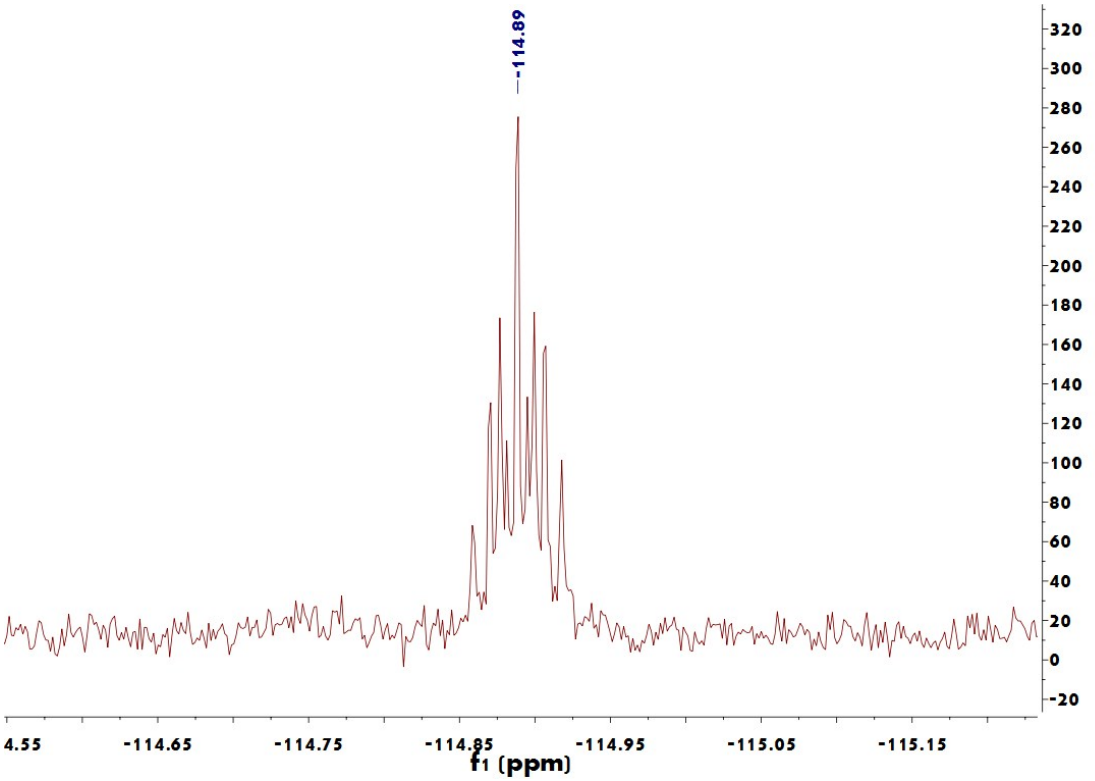
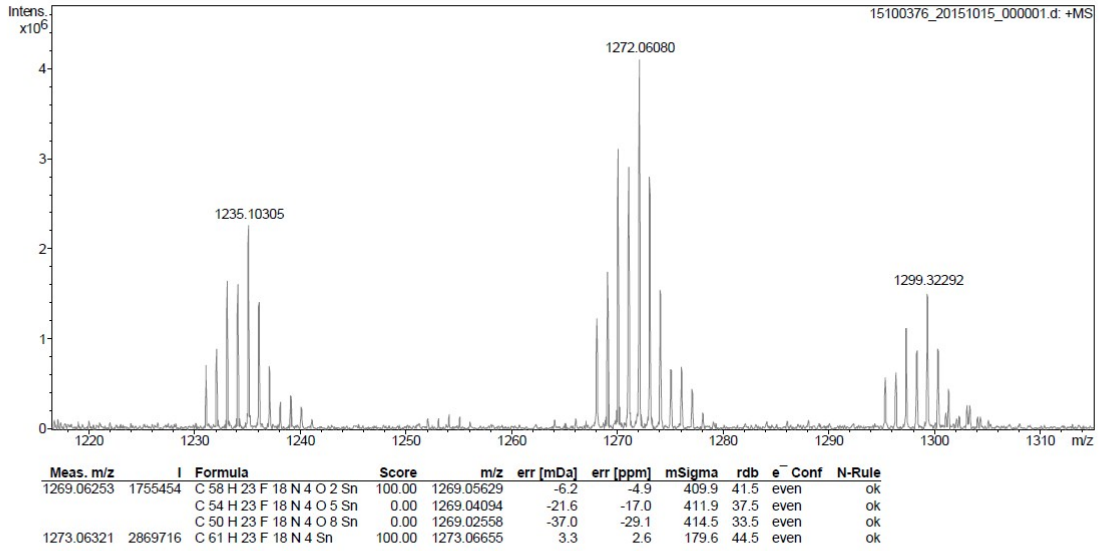


Figure S22. ^{19}F NMR spectrum of **15** in C_6D_6.



Meas. m/z	I	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1269.06253	1755454	C 58 H 23 F 18 N 4 O 2 Sn	100.00	1269.05629	-6.2	-4.9	409.9	41.5	even	ok
		C 54 H 23 F 18 N 4 O 5 Sn	0.00	1269.04094	-21.6	-17.0	411.9	37.5	even	ok
		C 50 H 23 F 18 N 4 O 8 Sn	0.00	1269.02558	-37.0	-29.1	414.5	33.5	even	ok
1273.06321	2869716	C 61 H 23 F 18 N 4 Sn	100.00	1273.06655	3.3	2.6	179.6	44.5	even	ok

Figure S23. ESI-MS spectrum of the organotin corrole fraction, showing the presence of **14** (m/z = 1273.06321, $[M+H]^+$).

10. Independent synthesis of 12 and 13.

The synthetic procedure for **12** was adopted from Wayland *et al.*[10] A $CHCl_3$ (1.72 mL) solution containing 20 μmol of **3**, 30 μL of *p*-fluorophenylacetylene and 3.4 mg (21 μmol) of azobisisobutyronitrile (AIBN) was degassed by three freeze-pump-thaw cycles, and heated at 60 °C for 24 h under N_2, at which point complete consumption of **3** was observed by TLC. The solution was further heated at 70 °C for 45 h to destroy excess AIBN. The mixture was then evaporated to

dryness and chromatographed on silica gel using PE:$CHCl_3$ = 1:1 as eluent, giving 11.8 mg (65 %) of **12** as an orange-red solid. ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 9.10 (s, 8H), 8.02 (br s, 8H), 7.10 (d, J = 8.5 Hz, 8H), 5.73 (t, J = 8.7 Hz, 2H), 3.52 (s, 12H), 3.20 (dd, J = 8.1, 5.8 Hz, 2H), 0.06 (d, J = 1.7 Hz, 1H), -1.50 (d, J = 1.7 Hz, 1H); HR-ESI-MS m/z calcd for $C_{56}H_{42}CoFN_4O_4^+$ $[M+H]^+$ 912.25166, found 912.24968. Single crystals suitable for XRD studies were obtained by recrystallization in benzene. **12** is light sensitive, and all manipulations should be conducted in the dark.

Approximately 2.6 μmol of **12** was placed in a vacuum adapted NMR tube and dissolved in 0.4 mL of C_6D_6. 25 μL of *p*-fluorophenylacetylene was then added. The solution was degassed by three freeze-pump-thaw cycles and irradiated with a Hg lamp equipped with a 420-780 nm band pass filter. After 3 h, a conversion of 63 % was achieved, giving **13** (NMR yield 32 %) and **3** (NMR yield 31 %) as products. Although **13** was not isolable, *in situ* NMR and ESI-MS characterization data were consistent with its structure. ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 9.05 (s, 8H), 8.02 (br s, 8H), 5.71 – 5.64 (m, 2H), 5.56 – 5.49 (m, 2H), 3.52 (s, 12H), 3.14 – 3.06 (m, 2H), -1.20 (s, 1H) (the $=CH_2$ group could not be unambiguously assigned due to the complexity of the mixture); HR-ESI-MS m/z calcd for $C_{64}H_{47}CoF_2N_4O_4^+$ $[M+H]^+$ 1032.28919, found 1032.28906.

Since Wayland's synthesis of porphyrin cobalt alkenyl complexes is known to proceed through initial formation of (por)Co-H from (por)Co^{II} and 2-cyano-2-propyl radical, followed by formal alkyne insertion into the Co-H bond,[10] the above syntheses are also experimental proofs of the catalytic chain transfer reaction shown in Figure 10.

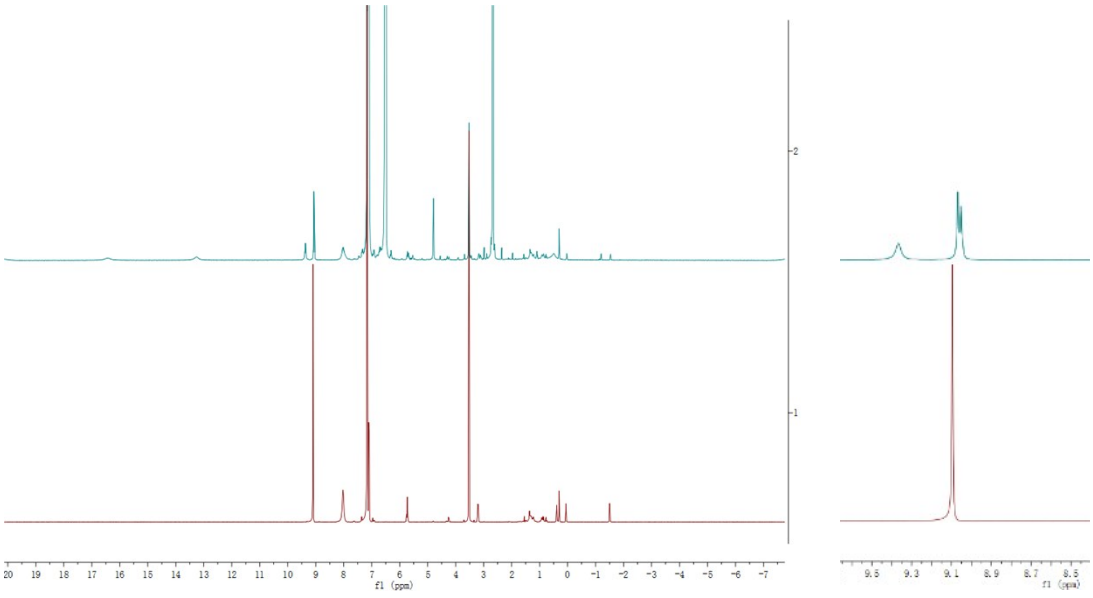
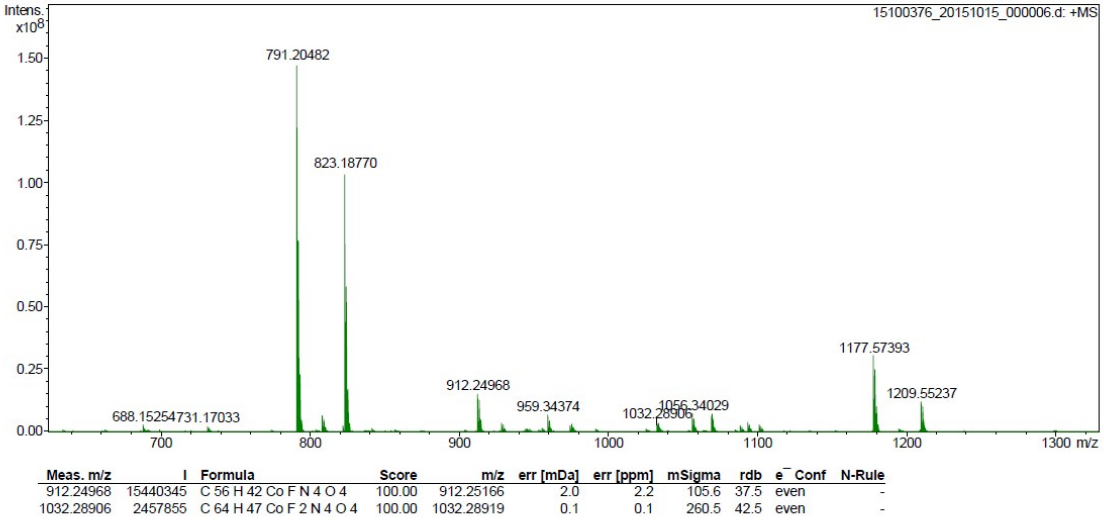


Figure S24. ^{1}H NMR spectrum of **12** (bottom) and a mixture of **12**, **13** and **3** (top) in C_6D_6. The region around 9.1 ppm (characteristic of porphyrin pyrrole proton resonances) was magnified to show the emergence of (apart from the signal of **3** at 9.36 ppm) a new porphyrin cobalt species, i.e. **13**.



Meas. m/z	I	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
912.24968	15440345	C 56 H 42 Co F N 4 O 4	100.00	912.25166	2.0	2.2	105.6	37.5	even	-
1032.28906	2457855	C 64 H 47 Co F 2 N 4 O 4	100.00	1032.28919	0.1	0.1	260.5	42.5	even	-

Figure S25. ESI-MS spectrum of a mixture of **12** and **13**.

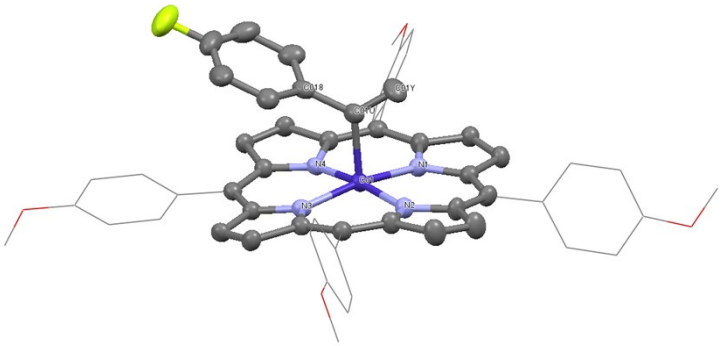


Figure S26. Solid state structure of **12**. Hydrogen atoms and a crystallographic benzene molecule were omitted for clarity. Selected bond lengths (Å) and angles (°): Co1-N1 1.963(4), Co1-N2 1.975(4), Co1-N3 1.962(4), Co1-N4 1.960(4), Co1-C01U 1.969(5), C01U-C01Y 1.326(8), C01U-C018 1.480(8), C01Y-C01U-Co1 119.1(4), C018-C01U-Co1 117.0(4), C01Y-C01U-C018 123.8(5).

Table S5. Crystal data and structure refinement for **12**.

Identification code	a	
Empirical formula	C62 H48 Co F N4 O4	
Formula weight	990.97	
Temperature	173.1500 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P c a 21	
Unit cell dimensions	a = 21.495(2) Å	α= 90°.
	b = 13.598(3) Å	β= 90°.
	c = 16.434(4) Å	γ = 90°.
Volume	4803.3(15) Å^3	

Z	4
Density (calculated)	1.370 Mg/m^3
Absorption coefficient	0.417 mm^{-1}
F(000)	2064
Crystal size	0.23 x 0.16 x 0.04 mm^3
Theta range for data collection	1.772 to 27.465°.
Index ranges	-27<=h<=26, -17<=k<=16, -21<=l<=21
Reflections collected	38144
Independent reflections	10871 [R(int) = 0.0641]
Completeness to theta = 26.000°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.8165
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10871 / 1 / 653
Goodness-of-fit on F^2	1.093
Final R indices [I>2sigma(I)]	R1 = 0.0581, wR2 = 0.1610
R indices (all data)	R1 = 0.0626, wR2 = 0.1663
Absolute structure parameter	0.019(9)
Extinction coefficient	n/a
Largest diff. peak and hole	0.377 and -0.538 $e.Å^{-3}$

11. Synthesis and characterization of 9', 10' and 11'

4.0 μmol of **1** and 40 μL of *p*-methoxyphenylacetylene were dissolved in 460 μL of benzene in a 10 mL round-bottom Schlenk flask. After three freeze-pump-thaw cycles, the flask was irradiated with a Hg lamp equipped with a 420-780 nm band pass filter for 24 h. The flask was placed at a distance of 5 cm from the lamp, and a mirror was placed at the opposite side of the flask to make a total light intensity of *ca.* 60 mW/cm^2. Product mixtures from two parallel batches were combined (i.e. the total amount of starting complex, **1**, was 8.0 μmol) and subjected to silica column chromatography with PE:DCM = 1:1 as eluent, giving recovered **1** (7.0 mg, 51 %), **9'** (*ca.* 1 mg, ~ 10 %), **10'** (5.5 mg, 35 %) and **11'** (trace). No MeO analogs of **12**, **13**, **14** or **15** were isolated. Note: the column should be pre-saturated with Et_3N before chromatographing. Otherwise, depending on the specific batch of silica used, acid-catalyzed Sn-C bond hydrolysis might occur.

9': ^1H NMR (400 MHz, C_6D_6) δ (ppm): 8.64 (s, 8H), 8.46 (d, J = 2.9 Hz, 2H), 8.29 (d, J = 3.9 Hz, 2H), 8.23 (d, J = 4.0 Hz, 2H), 7.95 (d, J = 3.7 Hz, 2H), 7.76 (br s, 4H), 7.35 (br s, 8H), 6.95 (br s, 4H), 5.06 (d, J = 8.5 Hz, 2H), 3.62 (s, 12H), 3.39 (s, 3H), 0.73 (d, J = 8.4 Hz, 2H), -5.96 (s, 1H); HR-ESI-MS m/z calcd for $C_{94}H_{53}CoF_{15}N_8O_5Sn^+$ $[M]^+$ 1837.22523, found 1837.22550; UV-Vis (toluene) λ_{max} (nm): 419, 536, 582, 616. Single crystals suitable for XRD studies were obtained by slow evaporation of MeOH from a MeOH/H_2O solution.

10': ^1H NMR (400 MHz, C_6D_6) δ (ppm): 8.76 (s, 8H), 8.47 (d, J = 4.1 Hz, 2H), 8.42 (d, J = 2.4 Hz, 2H), 8.14 (d, J = 4.3 Hz, 2H), 8.06 (d, J = 3.9 Hz, 2H), 7.86 (br s, 4H), 7.35 (br s, 4H), 6.95 (br s,

4H), 5.89 (d, J = 8.4 Hz, 2H), 5.26 (d, J = 8.5 Hz, 2H), 3.55 (s, 12H), 3.47 (s, 3H), 3.45 (s, 3H), 3.15 (d, J = 8.3 Hz, 2H), 2.02 (d, J = 8.6 Hz, 2H), -1.34 (s, 1H), -2.88 (s, 1H); HR-ESI-MS m/z calcd for $C_{103}H_{61}CoF_{15}N_8O_6Sn^+$ $[M]^+$ 1969.28279, found 1969.28354; UV-Vis (toluene) λ_{max} (nm): 425, 536, 582, 612.

11': ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 8.86 (s, 8H), 8.60 (d, J = 4.2 Hz, 2H), 8.52 (m, 2H), 8.29 (m, 2H), 8.17 (m, 2H), 7.00 (d, J = 8.5 Hz, 8H), 5.82 (d, J = 8.1 Hz, 2H), 5.60 (d, J = 7.8 Hz, 2H), 5.10 (d, J = 8.4 Hz, 2H), 4.34 (d, J = 8.6 Hz, 2H), 3.51 (s, 12H), 3.31 (s, 3H), 3.21 (s, 3H), 3.00 (s, 3H), 2.54 (d, J = 8.2 Hz, 2H), 2.25 (s, 1H), 0.29 (s, 1H), -1.88 (s, 1H); HR-ESI-MS m/z calcd for $C_{112}H_{69}CoF_{15}N_8O_7Sn^+$ $[M]^+$ 2101.339811, found 2101.349346; UV-Vis (toluene) λ_{max} (nm): 412(sh), 432, 538, 580, 610.

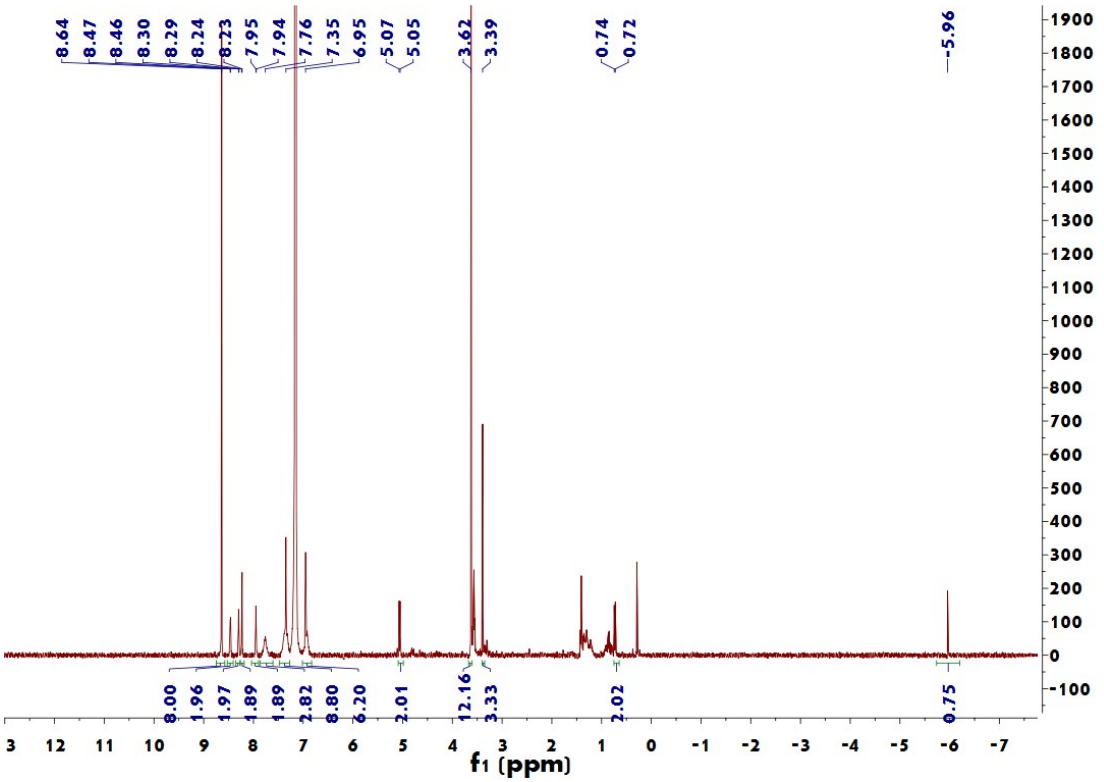


Figure S27. ^{1}H NMR spectrum of **9'** in C_6D_6.

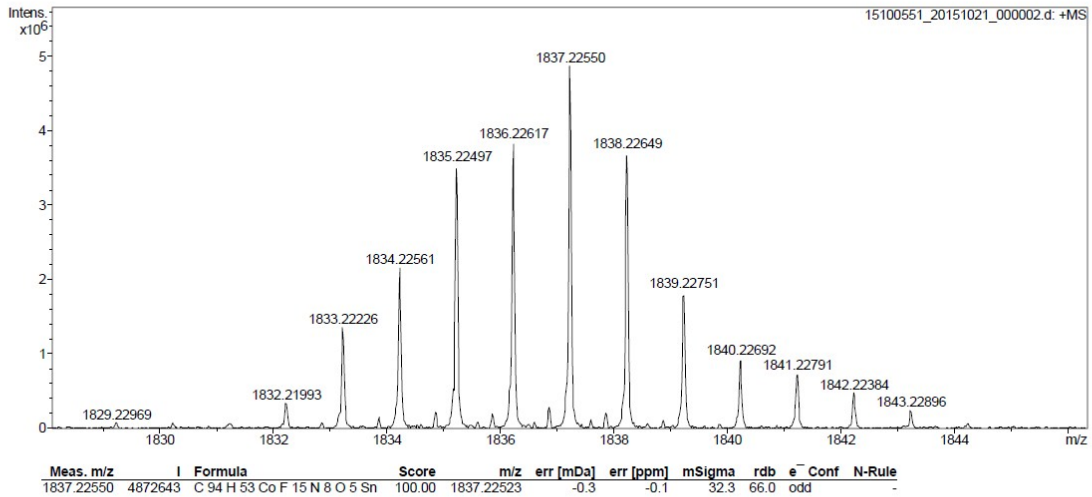


Figure S28. ESI-MS spectrum of **9'**.

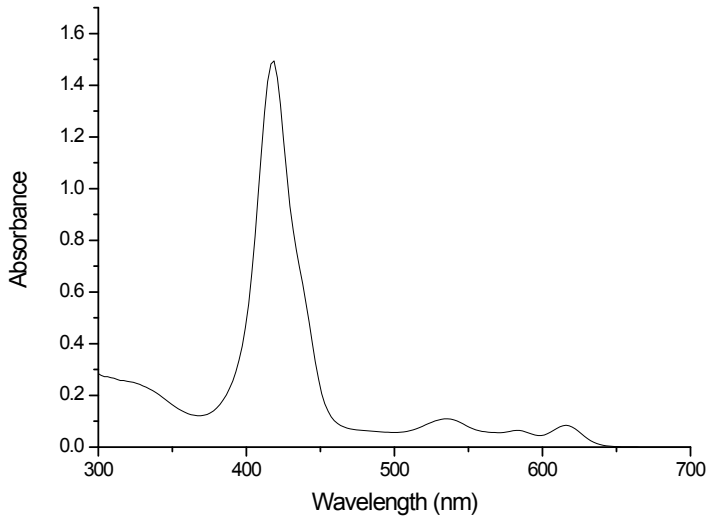


Figure S29. UV-Vis spectrum of **9'** in toluene. The spectrum was recorded by a stopped-flow spectrometer, and data from the first 0.5 s after sample injection were averaged. **9'** decomposed under the light used by the spectrometer within 100 s.

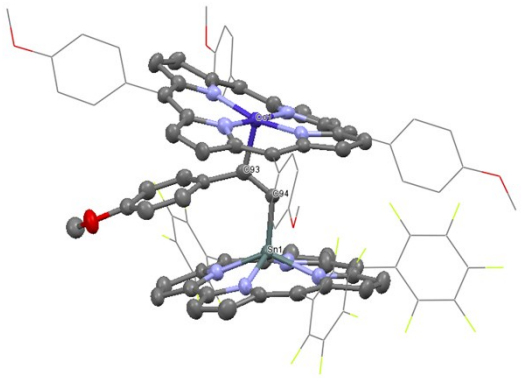


Figure S30. Solid state structure of **9'**. Hydrogen atoms were omitted for clarity. Selected bond lengths (Å) and angles (°): Sn1-C94 2.070(6), Co1-C93 1.966(7), C93-C94 1.331(9), C94-C93-Co1 118.5(5), C93-C94-Sn1 126.1(5).

Table S6. Crystal data and structure refinement for **9'**.

Identification code	a_sq	
Empirical formula	C94 H52 Co F15 N8 O5 Sn	
Formula weight	1836.05	
Temperature	173.1500 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 15.523(4) Å	α= 93.436(10)°.
	b = 16.499(2) Å	β= 111.524(10)°.
	c = 20.024(2) Å	γ = 102.953(11)°.
Volume	4591.7(14) $Å^3$	
Z	2	
Density (calculated)	1.328 Mg/m^3	
Absorption coefficient	0.537 mm^{-1}	
F(000)	1848	
Crystal size	0.2 x 0.05 x 0.03 mm^3	
Theta range for data collection	1.449 to 27.482°.	
Index ranges	-19<=h<=20, -21<=k<=21, -25<=l<=25	
Reflections collected	45658	
Independent reflections	20689 [R(int) = 0.0970]	
Completeness to theta = 26.000°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.73395	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20689 / 0 / 1122	
Goodness-of-fit on F^2	1.173	
Final R indices [I>2sigma(I)]	R1 = 0.1133, wR2 = 0.2258	
R indices (all data)	R1 = 0.1385, wR2 = 0.2423	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.836 and -0.869 $e.Å^{-3}$	

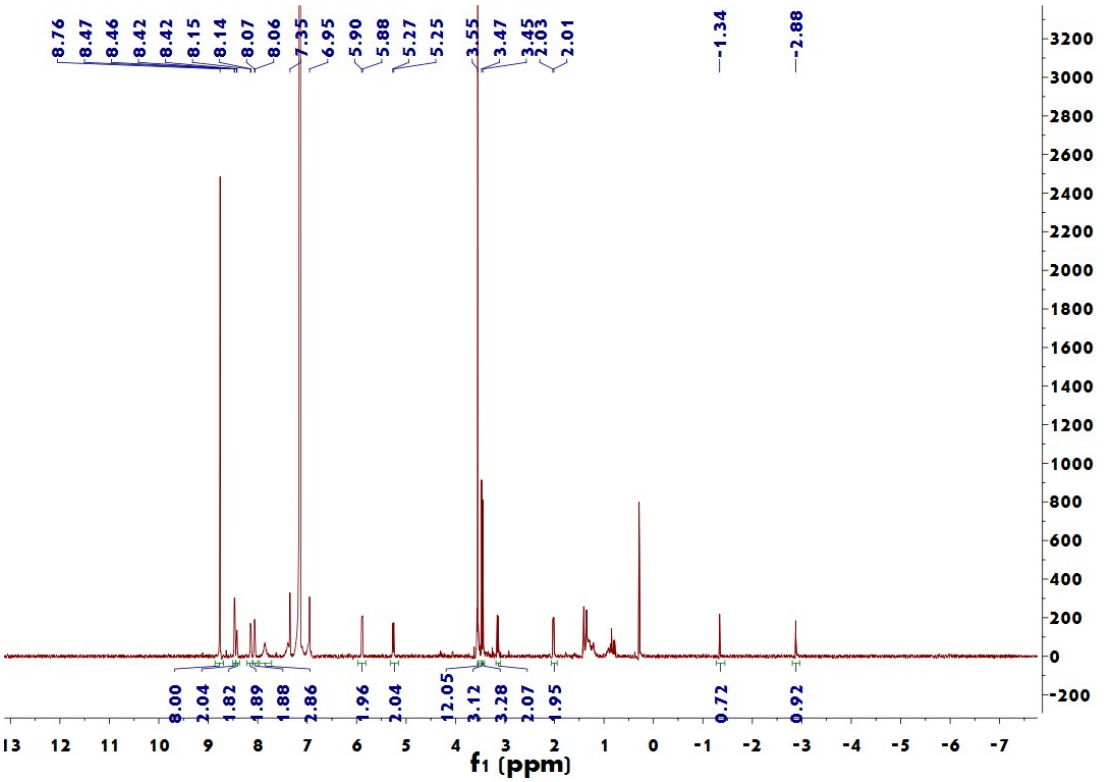


Figure S31. ^{1}H NMR spectrum of **10'** in C_6D_6.

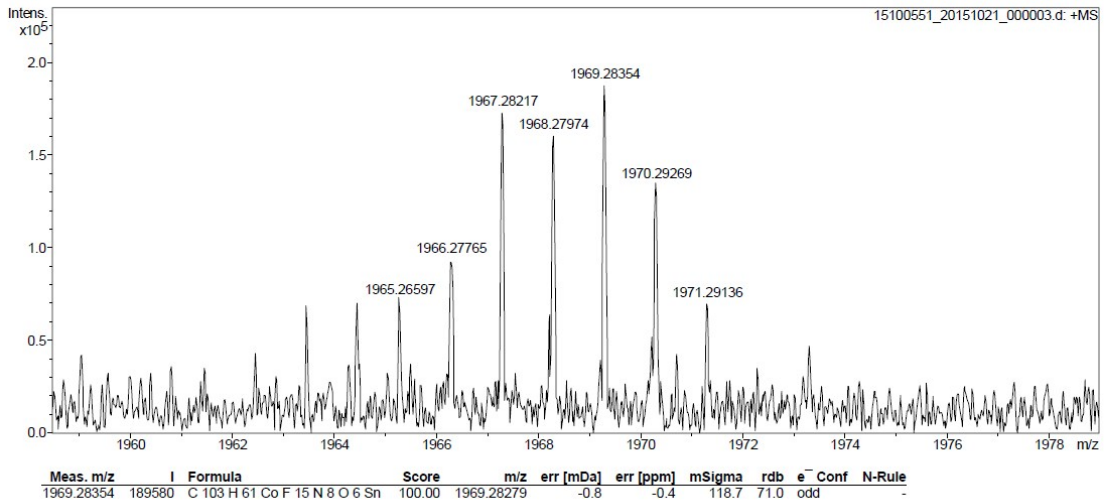


Figure S32. ESI-MS spectrum of **10'**.

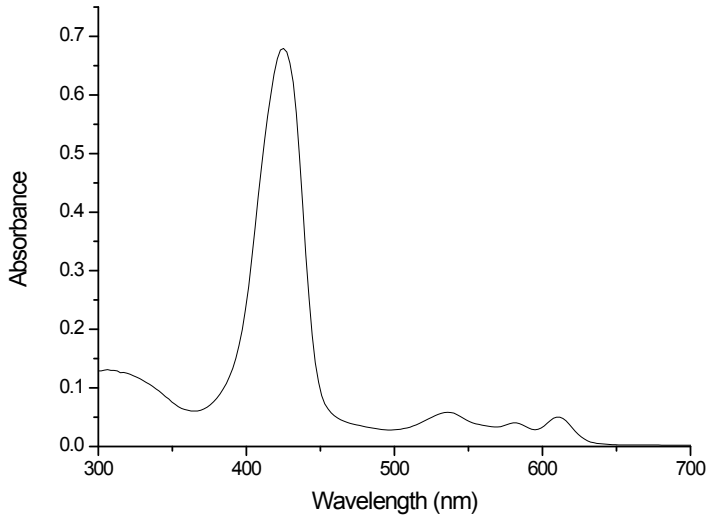


Figure S33. UV-Vis spectrum of **10'** in toluene. The spectrum was recorded by a stopped-flow spectrometer, and data from the first 0.02 s after sample injection were averaged. **10'** decomposed under the light used by the spectrometer within 500 s.

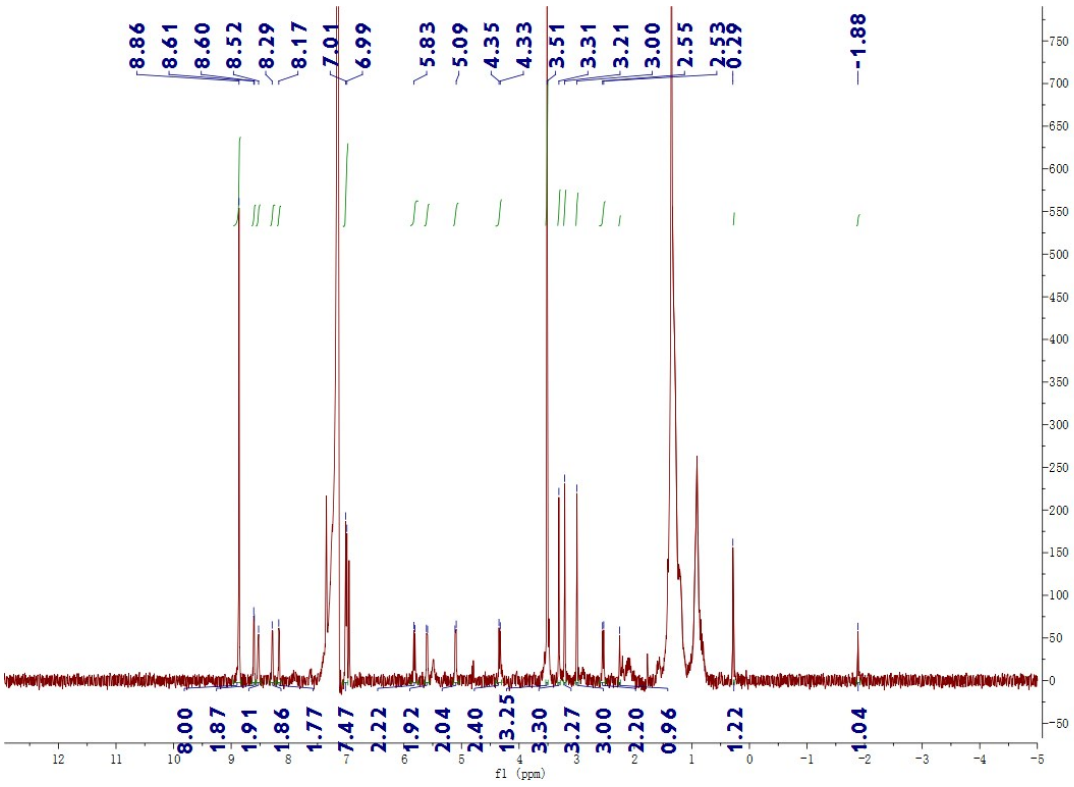


Figure S34. ^{1}H NMR spectrum of **11'** in C_6D_6.

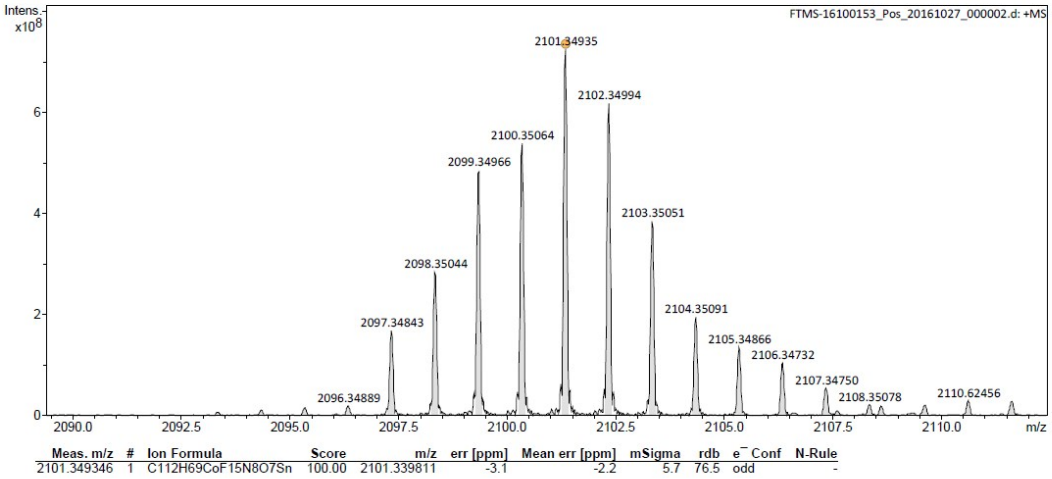


Figure S35. ESI-MS spectrum of **11'**.

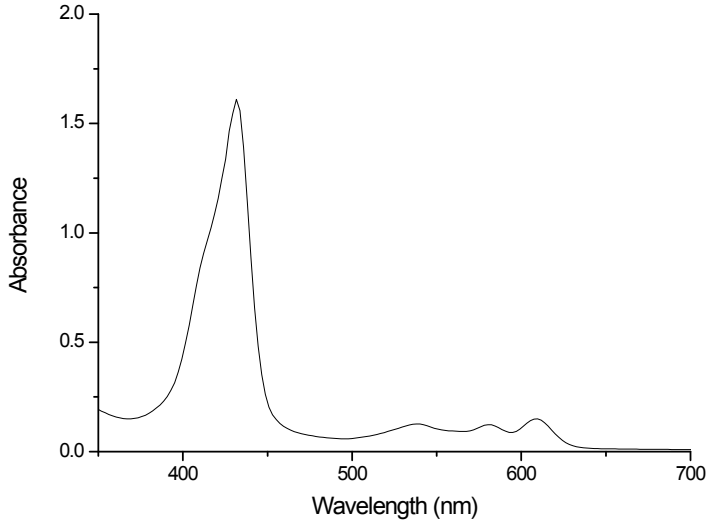


Figure S36. UV-Vis spectrum of **11'** in toluene. The spectrum was recorded by a stopped-flow spectrometer, and data from the first 0.01 s after sample injection were averaged. **11'** decomposed under the light used by the spectrometer within 200 s.

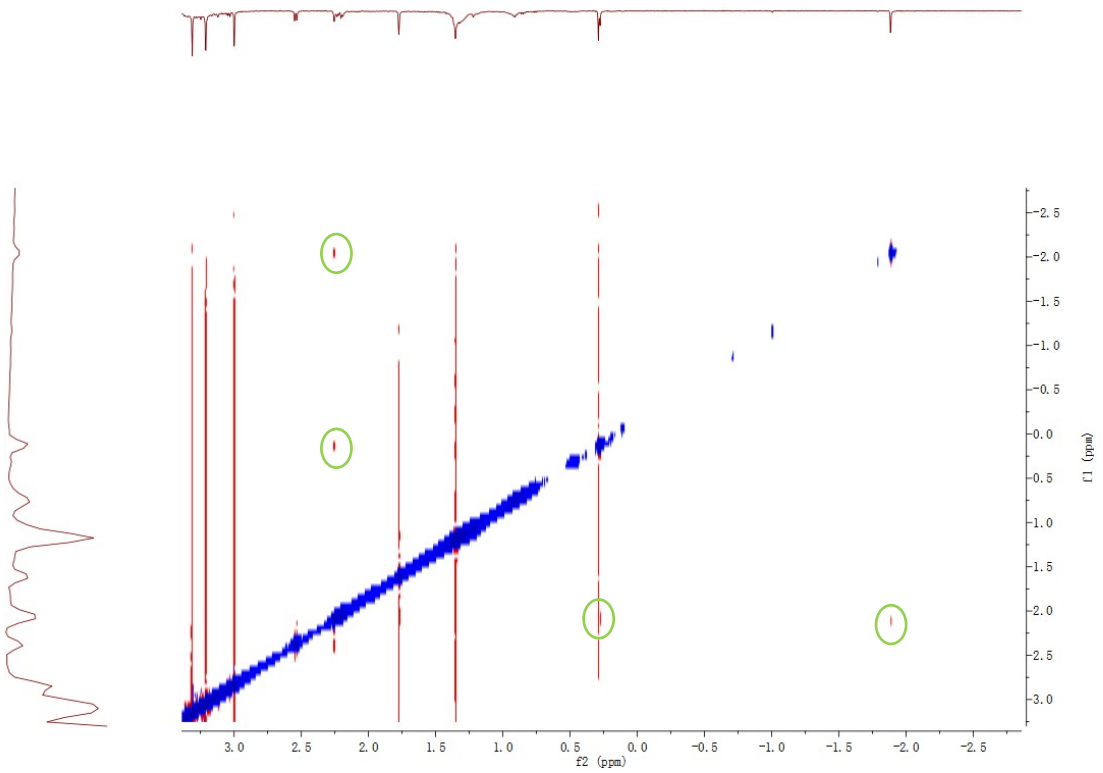


Figure S37. ^{1}H-^{1}H ROESY spectrum of **11'** in C_6D_6. The high field region was magnified to show the cross peaks (circled) due to H_a-H_b and H_b-H_c (see below).

The ROESY spectrum unambiguously showed that the oligoalkyne methine protons in **11'** are *cis* to each other. This leaves only two possible stereochemical configurations of **11'**, i.e. (A) and (B) in Figure S38. Configuration (B) can be safely ruled out since the (TAP)Co group is too bulky to allow for such a conformation. Nevertheless, in either case, Co-C bond homolysis of **11'** should yield **11-rad-trans**, rather than **11-rad-cis**.

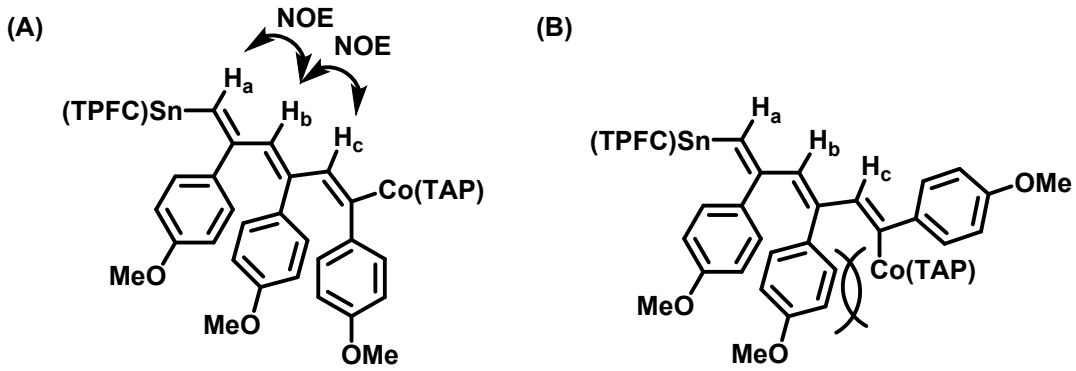


Figure S38. Possible configurations of **11'**.

12. ^{1}H NMR monitoring of the photolysis of 9', 10' and 11'.

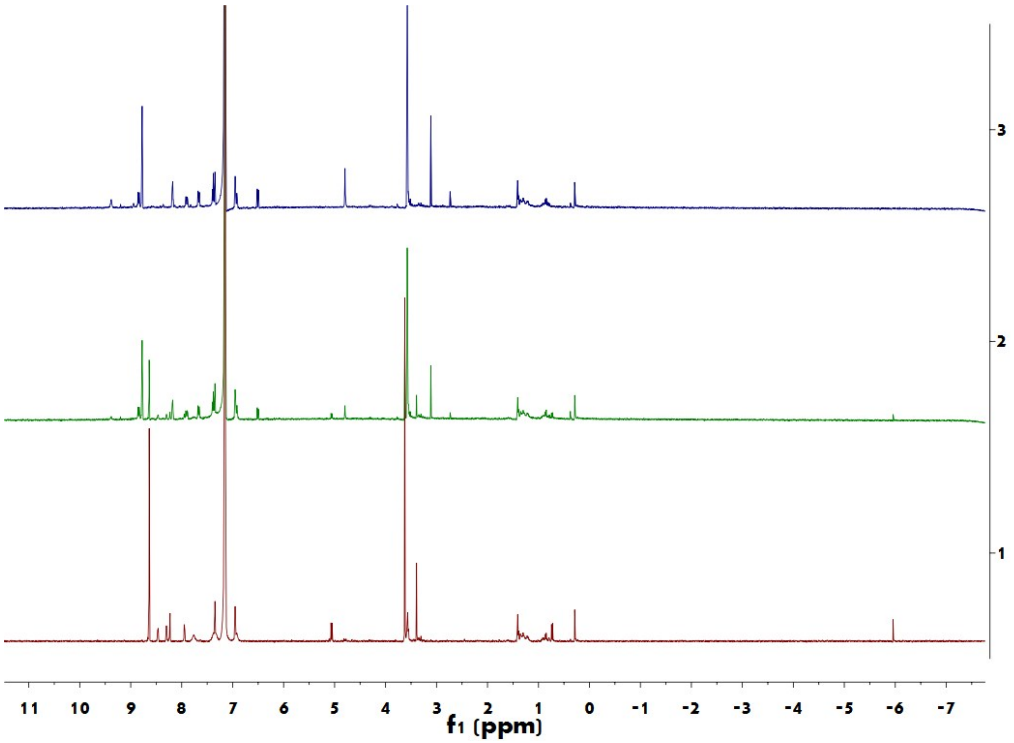


Figure S39. ^{1}H NMR spectra of **9'** in C_6D_6 during photolysis. From bottom to top: before irradiation, irradiated for 15 min and 2 h under N_2. The signals at 9.38 and 8.78 ppm were characteristic of **3** and **1**, respectively. The formation of *p*-methoxyphenylacetylene (6.92, 6.51, 3.11, 2.73 ppm) was additionally confirmed by GC-MS analysis.

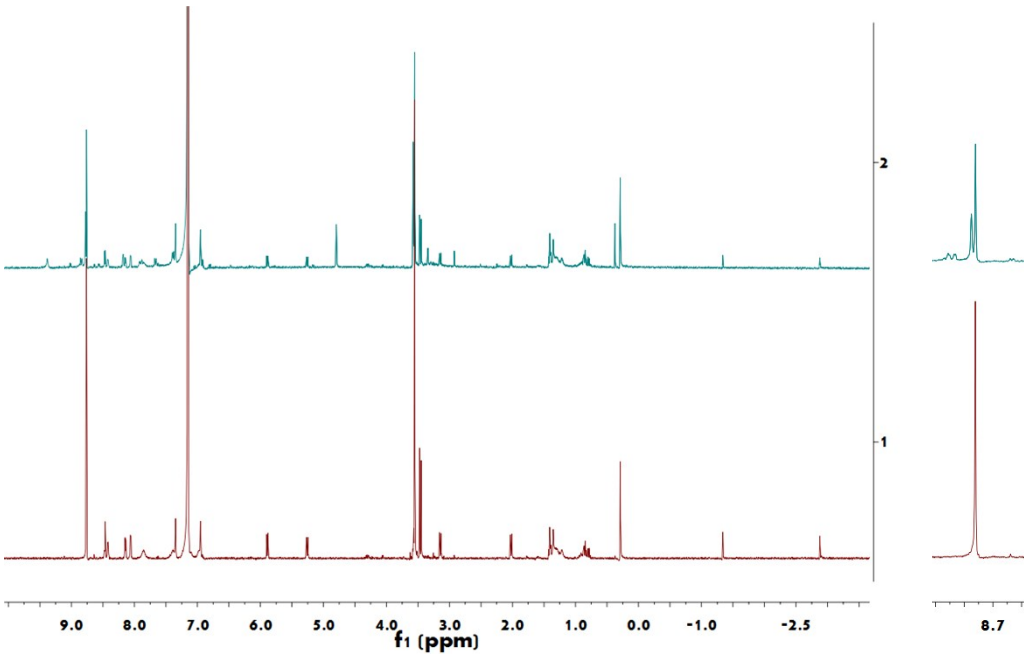


Figure S40. ^{1}H NMR spectra of **10'** in C_6D_6 during photolysis. From bottom to top: before irradiation, and irradiated for 2.5 h under N_2. The signals at 9.38 and 8.78 ppm were characteristic of **3** and **1**, respectively.

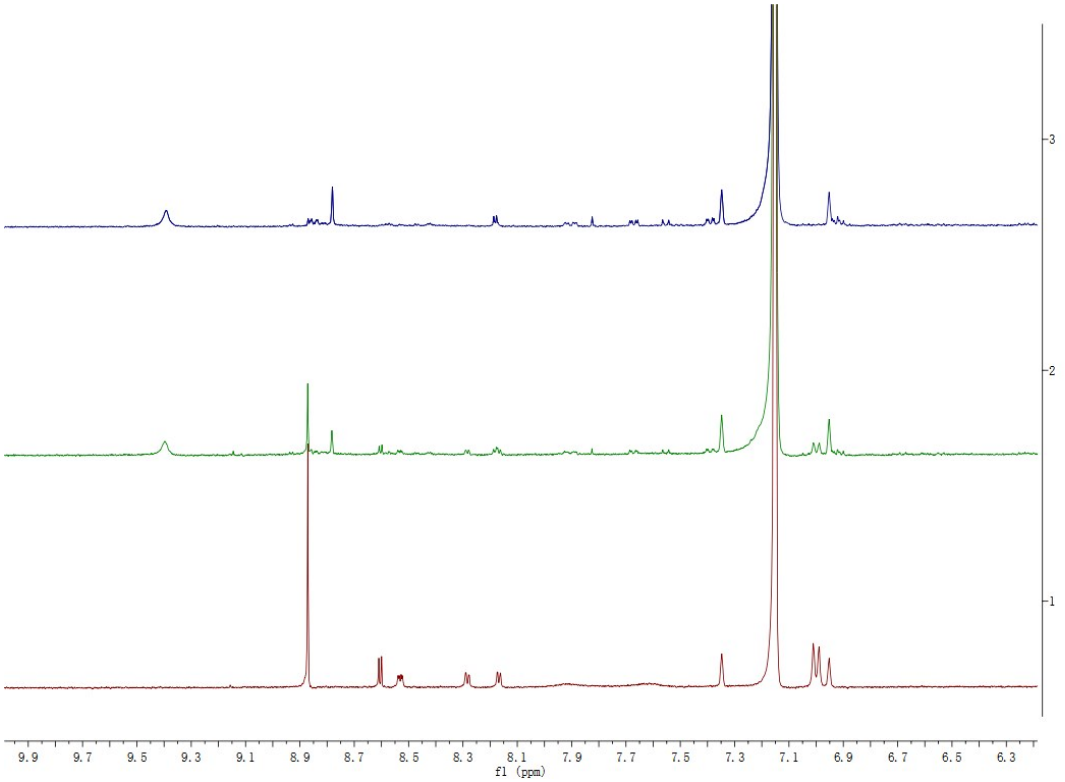


Figure S41. ^{1}H NMR spectra of **11'** in C_6D_6 during photolysis. A Hg lamp with a 420-780 nm band-pass filter was used. From bottom to top: before irradiation, irradiated for 45 min and 3 h under N_2. The signals at 9.37 and 8.77 ppm were characteristic of **3** and **1**, respectively, while the singlet at 7.82 ppm was attributed to **15'**. Integration of the peak at 7.82 ppm against the total integration of porphyrin pyrrole signals gave a yield of 8 %. Using a Xe lamp, or conducting the experiment without a light filter, led to similar or lower yields of **15'**.

13. Catalytic synthesis and isolation of 15'.

1 (1.0 μmol) was added to a J. Young Valve NMR tube, and *p*-methoxyphenylacetylene (25 μL) was added. The mixture was degassed by three freeze-pump-thaw cycles. Degassed C_6D_6 (0.4 mL) was then added in a glove box, and the NMR tube was subjected to photolysis by a Hg lamp (without using a light filter). After 92 h, the majority of **1** had decomposed to **3**, mononuclear (TAP)Co-R complexes, and mononuclear (TPFC)Sn-R species. Integration of the peak at 7.82 ppm against the total integration of porphyrin pyrrole signals yielded a TON of 4.3 for **15'**. ^{1}H NMR (400 MHz, C_6D_6) δ (ppm): 7.82 (s, 3H), 7.56 (d, J = 8.8 Hz, 6H), 6.91 (d, J = 8.8 Hz, 6H) (the methoxy peak could not be unambiguously assigned).

The mixture was subsequently chromatographed on silica gel with PE:DCM = 1:1 as eluent to yield pure **15'**. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.66 (s, 3H), 7.63 (d, J = 8.8 Hz, 6H), 7.01 (d, J = 8.8 Hz, 6H), 3.87 (s, 9H); HR-ESI-MS m/z calcd for $C_{27}H_{25}O_3$ $[M+H]^+$ 397.179821, found 397.180360. The characterization data were consistent with literature results.[11] Note that complete bleaching of active catalyst was crucial for the successful isolation of **15'**, since the polarity of **15'** was similar to that of **1**.

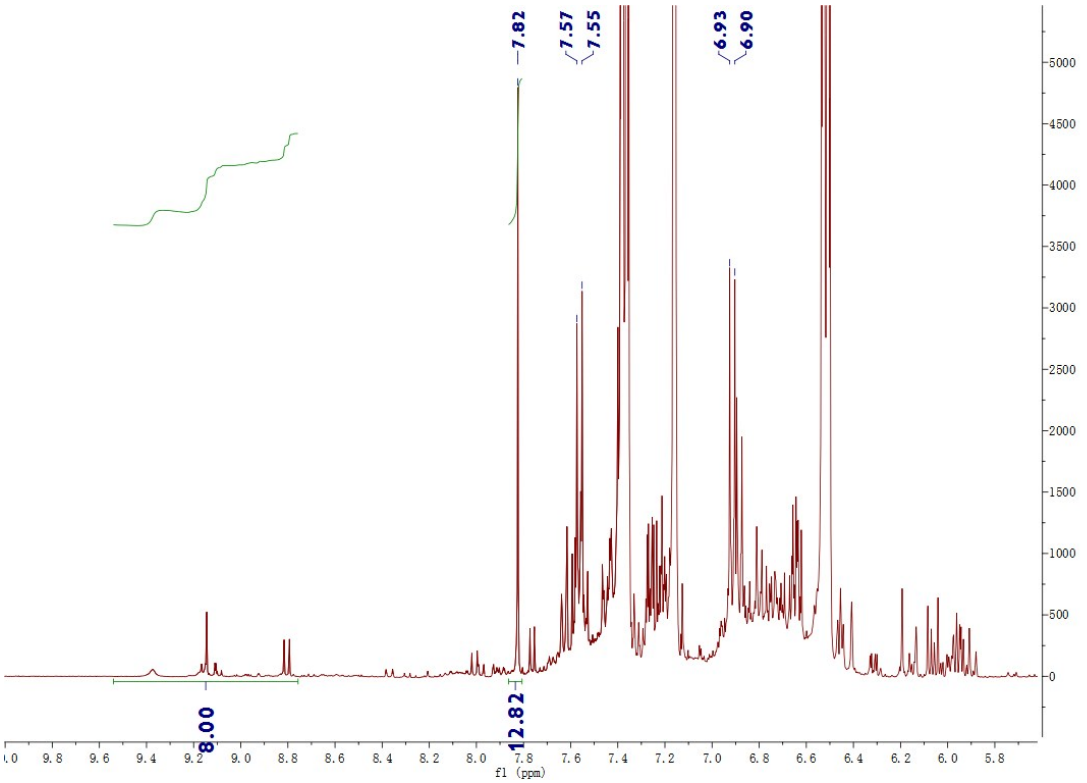


Figure S42. ^{1}H NMR spectrum of the reaction mixture of **1** with *p*-methoxyphenylacetylene after irradiation with a Hg lamp for 92 h. Labeled peaks are due to **15'**.

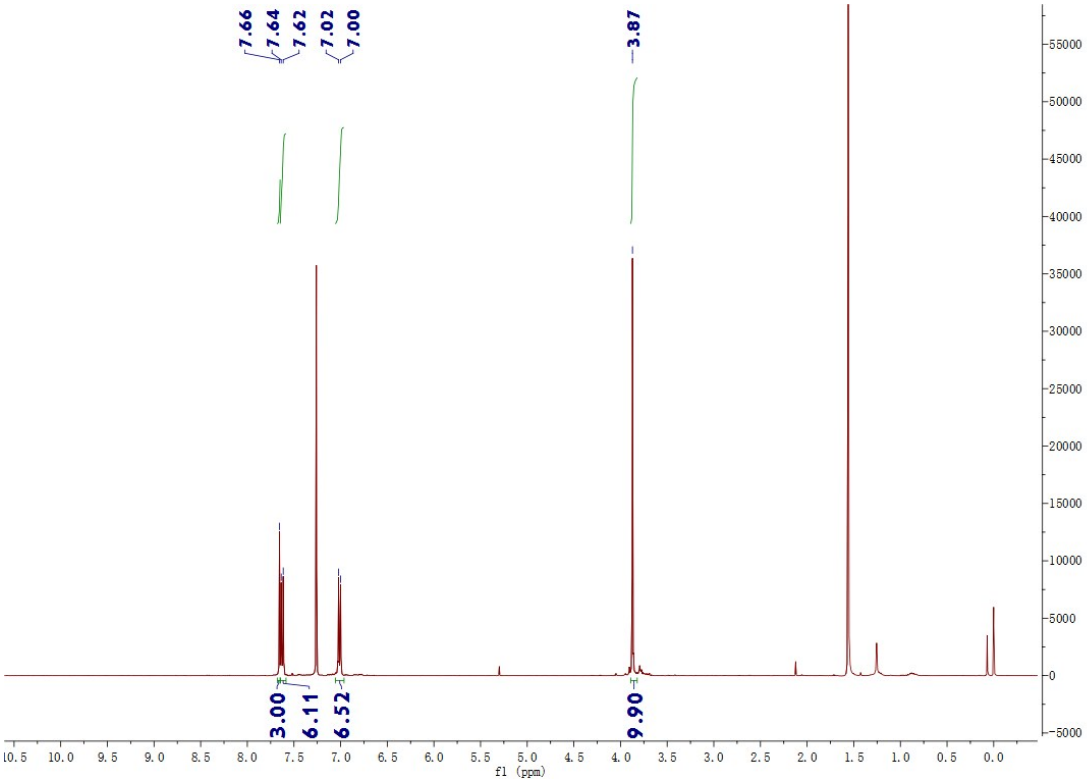


Figure S43. ^{1}H NMR spectrum of **15'** in $CDCl_3$.

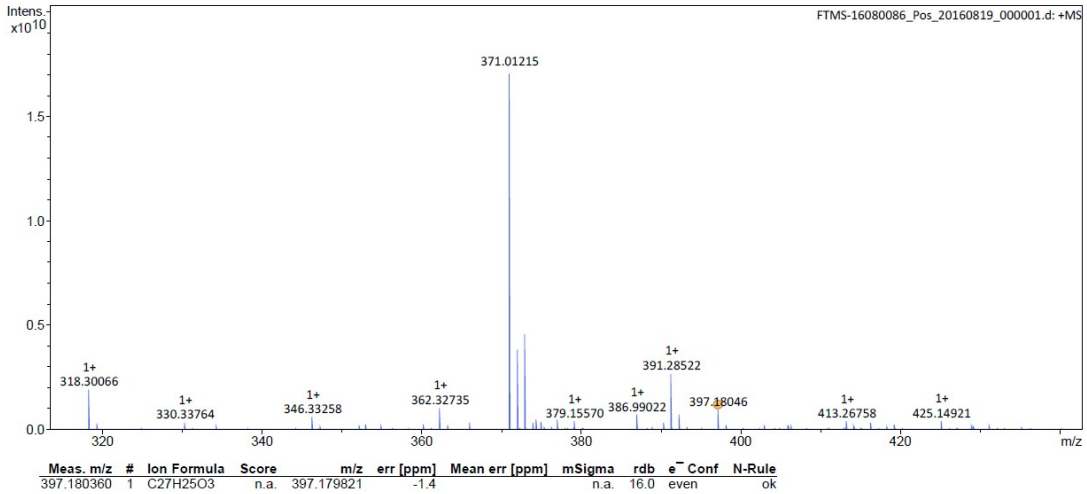


Figure S44. ESI-MS spectrum of **15'**.

14. Computational studies.

All calculations were performed with the ORCA software package,[12] version 3.0.3, except for TDDFT calculations which were performed with ORCA 4.0.0.

For geometry optimizations, the BP86[13] functional was employed with def2-TZVP(-f)[14] basis set on Sn, and def2-SV(P)[15] on all other atoms. The resolution-of-the-identity (RI) approximation[16] was used with the Coulomb fitting set def2-TZVP/J[17] for Sn and def2-SVP/J[17] for all other atoms. Numerical harmonic frequencies were calculated for converged structures to verify the nature of the stationary points. For transition states, we further confirmed the direct connection with the presumed reactants and products by relaxed surface scans. Gibbs free energy corrections based on the standard state of ideal gas (298 K, 1 atm) were corrected to the standard state of solution (298 K, 1 mol/L) by adding 1.89 kcal/mol.[18] For calculations involving **1**, the above level of theory greatly underestimated the Sn-Co bond length (Table S8) due to excessive basis set superposition error (BSSE); thus we re-optimized all relevant structures using the def2-TZVP(-f) basis set on all atoms, while still using the Gibbs free energy corrections computed at the lower level. This resulted in a change of the Sn-Co bond dissociation enthalpy (BDE) of only 1.8 kcal/mol. It was thus deemed that re-optimization using a larger basis set for non-metal atoms was unnecessary for mononuclear (TPFC)Sn-R species, where the BSSE would be significantly smaller, and energies rather than geometries are the major concern.

Single point energies were computed using the B3LYP[19] functional combined with the def2-TZVPP[14] basis set on all atoms. The RIJCOSX approximation[20] was used together with the def2-TZVPP/J[17] Coulomb fitting set. The SMD solvation model[18] was employed at this stage, with benzene as solvent.

For both geometry optimizations and single point calculations, the unrestricted Kohn-Sham (UKS) formalism was used throughout for open-shell species, and restricted Kohn-Sham (RKS) was used otherwise; relativistic effects were explicitly described at the zeroth order regular approximation (ZORA)[21] level, and dispersion effects were accounted for by means of Grimme's DFT-D3 correction with Becke-Johnson (BJ) damping.[22]

NBO calculations were carried out using NBO 5.0[23] on the B3LYP/def2-TZVPP wavefunctions. The (TPFC)Ge^{III} complex, whose computational results have already been published in our previous

paper,[9] was recalculated with ZORA turned on to maximize comparability with the Sn analog. Spin populations were calculated using natural population analysis (NPA) to minimize basis set dependence.

TDDFT calculations were performed at the B3LYP/def2-TZVP(-f) (Sn)/def2-SV(P) (other atoms) level at optimized geometries, employing both ZORA and SMD.

All isosurface plots (molecular orbitals, spin densities, density difference maps etc.) and NBO second-order perturbative interaction energy estimates were generated by the BMV program, version 0.1.1.[24]

Table S7. Benchmark studies on geometry optimization of (TPFC)Sn-CH_2CH_2COOMe.

	Sn-C (Å)	Sn-C-C (°)	N-Sn-C-C (°) [a]	Sn-N (Å, mean)
Standard level of theory [b]	2.156	109.43	10.26	2.080
TPSS instead of BP86	2.159	110.08	5.29	2.079
B3LYP instead of BP86	2.152	109.85	14.67	2.071
def2-TZVP(-f) also on C, N	2.152	109.92	6.90	2.074
Use SMD solvation	2.154	110.18	7.72	2.081
def2-SD [c] instead of ZORA	2.176	111.36	2.28	2.120
Experiment	**2.123**	**111.50**	**7.74**	**2.090**

[a] The nitrogen atom is the one that gives the smallest dihedral angle among all 4 possible choices. [b] BP86/def2-TZVP(-f)(Sn)/def2-SV(P)(other atoms), with ZORA and DFT-D3 correction. [c] def2-SD is the pseudopotential inherent in the def2-TZVP(-f) and def2-SV(P) basis sets, which was automatically turned off if ZORA was turned on.

(TPFC)Sn-CH_2CH_2COOMe was selected as a benchmark molecule due to the availability of its single crystal structure,[1] and the relatively large size of the axial ligand resembling, e.g. **9-rad**, in terms of the strength of non-covalent interactions. As can be seen from the table above, the quality of key bond lengths and angles are relatively insensitive to the functional used, but the N-Sn-C-C dihedral angle worsens upon using the hybrid functional B3LYP. Furthermore, enlarging the basis sets on all N atoms and the C atom directly bonded to Sn, or including solvation effects, give negligible impact on the geometry. Nevertheless, ZORA improves the bond lengths noticeably compared to the pseudopotential approach. These results led to the choice of the level of theory as mentioned before.

Table S8. Benchmark studies on geometry optimization of **1**.

	Sn-Co (Å)
Standard level of theory	2.378
def2-TZVP(-f) on all atoms	2.423
B3LYP instead of BP86	2.396
Experiment	**2.456**

In contrast with (TPFC)Sn-CH_2CH_2COOMe, basis set effects are more pronounced for **1**: upon enlarging the basis set of non-metal atoms to def2-TZVP(-f), the Sn-Co bond lengthens by 0.05 Å, and is brought into much better agreement to the XRD result than at the lower level of theory. Substituting BP86 by B3LYP also changes the result in the correct direction, but the improvement

is minuscule, and such a procedure incurs significant difficulty in geometrical convergence. Thus it was decided to use the BP86 functional also for this system, while using the def2-TZVP(-f) basis set for all atoms. The structures of **2** and **3** are similarly re-optimized at the BP86/def2-TZVP(-f) level, and the single point energies at the optimized geometries are used to calculate the Sn-Co bond dissociation energetics.

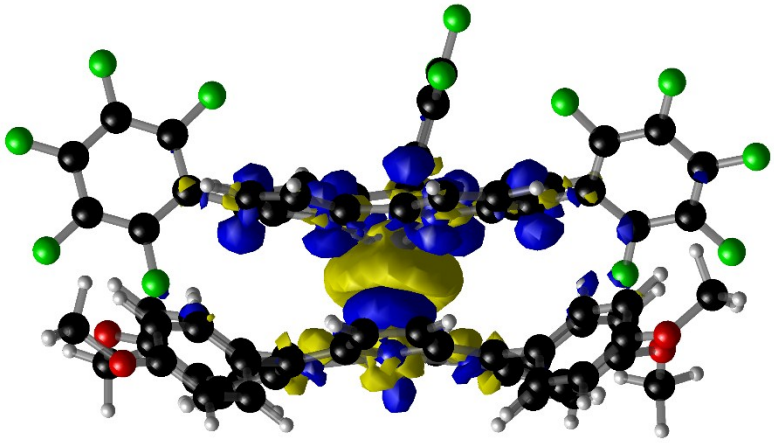


Figure S45. Plot of density change upon Sn-Co bonding, $\Delta\rho = \rho$(**1**, fully optimized geometry) − ρ(**2**, frozen fragment from fully optimized **1**) − ρ(**3**, frozen fragment from fully optimized **1**), with blue indicating density accumulation ($\Delta\rho > 0$) and yellow indicating density depletion ($\Delta\rho < 0$) (isovalue = 0.001).

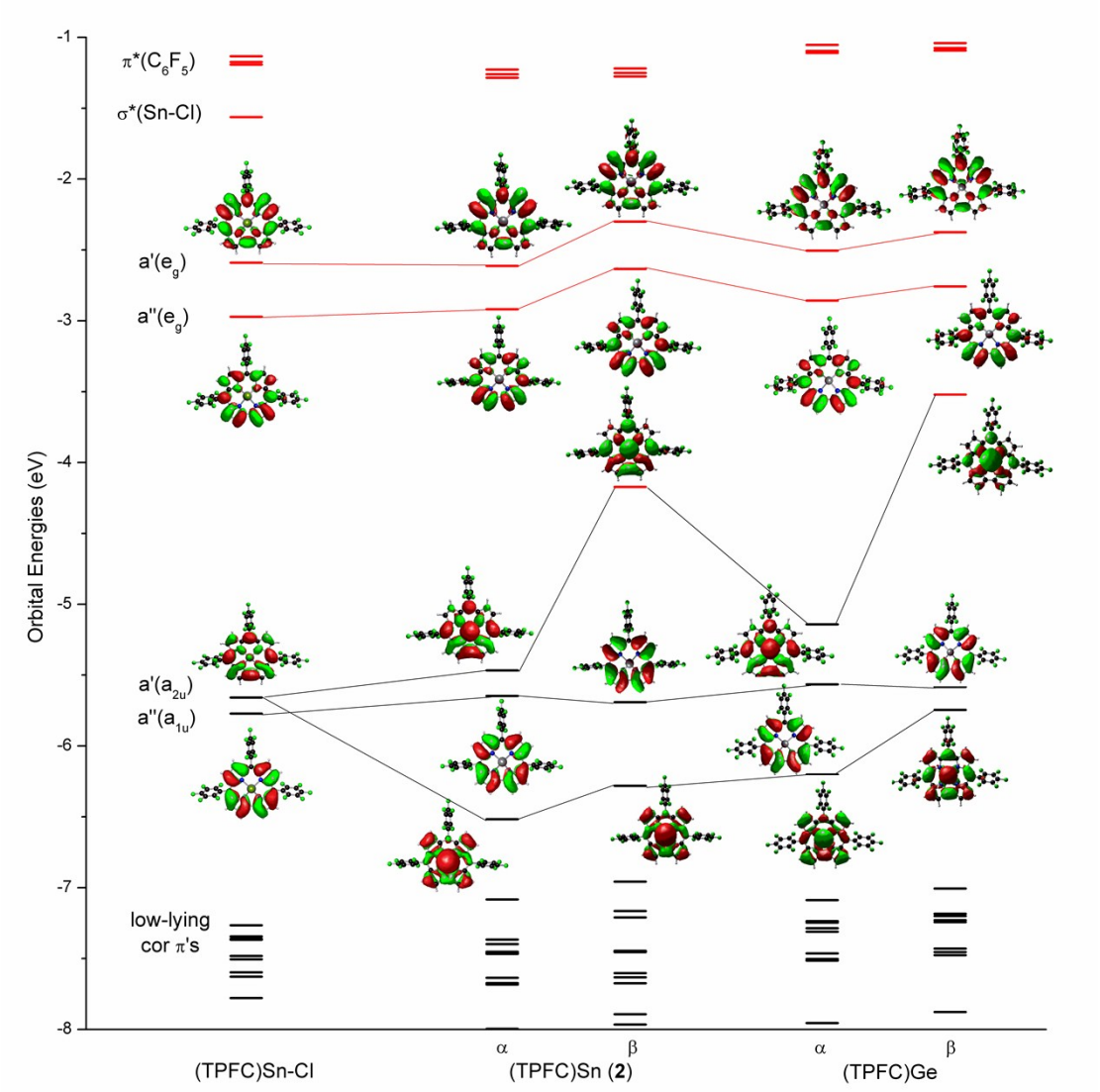


Figure S46. Orbital energy level plots of (TPFC)Sn-Cl (a model complex containing an unperturbed corrole ligand), (TPFC)Sn (**2**), and (TPFC)Ge.

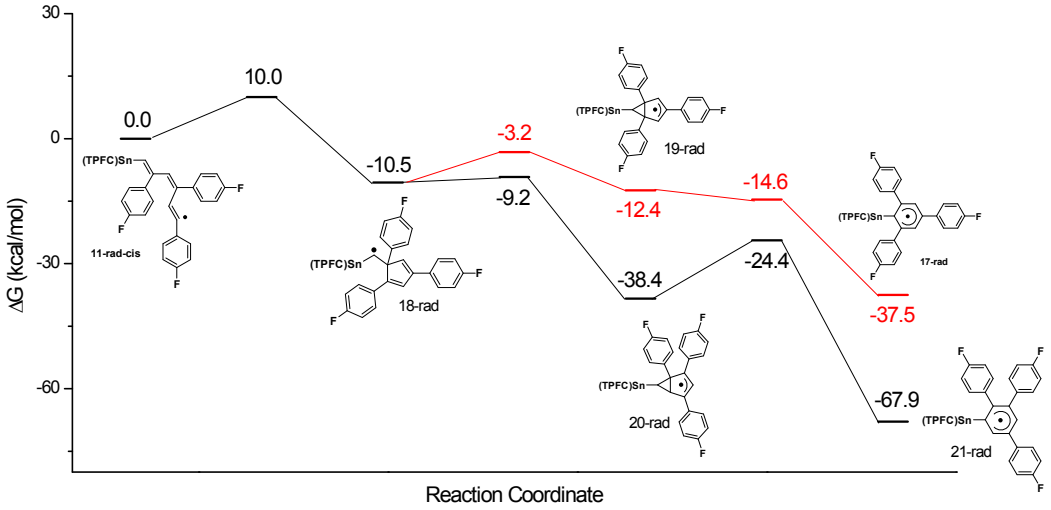


Figure S47. Fate of **11-rad-cis** after 5-exo-trig cyclization. The cyclized radical **18-rad** rapidly undergoes an intramolecular addition to yield **20-rad**. The highly strained bridge C-C bond is then ruptured to give the ring expanded product **21-rad**, which is expected to yield 1,2,4-triarylbenzene upon product release. Radical **17-rad**, on the other hand, could be generated through **19-rad** and would lead to the experimentally observed 1,3,5-product, but the corresponding intramolecular radical addition step requires a much higher activation energy than that of the 1,2,4-product, and should thus be non-operative.

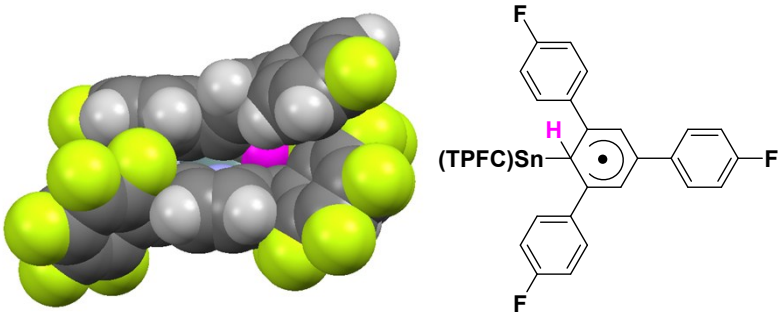


Figure S48. Space filling diagram of **17-rad**, with the HAT-active hydrogen highlighted in magenta. Although an explicit calculation of HAT barrier was not attempted, it is obvious from the figure that the hydrogen could not undergo HAT with the large rigid planar molecule **3** (see Figure S6) with a reasonable barrier, due to extreme steric demands.

List of DFT-optimized structures.

Unless otherwise specified, all structures correspond to singlet (for even-electron species) or doublet (for odd-electron species) electronic states.

(TPFC)Sn-Co(TAP), **1**

E = -13166.305447975 a.u.

Sn	9.03287879043548	3.75855870397056	19.30028483190361
Co	9.11452736627684	5.31159411616235	17.44237167594155
F	5.43199728421076	3.46416565047765	23.69483622673856
F	3.19046941485433	4.10233251749902	25.06904054871697
F	1.33830555854982	5.79355083613110	23.97220636124142
F	1.75716450774669	6.84807132984642	21.47665494626445
F	4.00664419879058	6.24381112623506	20.10778854787238
F	11.86388404459087	7.17525895405437	23.10148557195396
F	13.17475522404224	7.51006668855335	25.41795553032764
F	13.62889043059497	5.38021386720291	27.08118783473486
F	13.83872004094185	1.83060801443035	17.32414193343056
F	15.64552484133346	0.00090825874383	16.52003117493894
F	15.26021417494411	-2.65706962515777	17.06663422697548
F	13.06215190931101	-3.44719308183049	18.49858747395701
F	11.27162781505457	-1.62791036654577	19.36073981480456
O	11.70311963139443	-1.53272488368968	12.04211496987141
O	0.42312399025247	4.00489992626057	15.08794634200233
O	6.20294172213736	11.41350597337531	23.49590808824155
O	17.82365472735522	6.54468591943953	19.69426000590240
N	10.81280056157735	4.64809295502130	16.78182954696692
N	8.17126313460833	4.06953572976579	16.25067230968927
N	7.44390936848901	6.21945882959315	17.81354874989857
N	10.04290171718378	6.52976296480052	18.65441495113692
N	7.03045336380494	3.02810810958789	19.45682364747995
N	9.04934670500572	1.73906122616564	18.60197686435347
N	10.86661909782614	3.09929466477715	20.18804387164639
N	8.55924864125954	4.52345270435065	21.23948702033887
C	12.08472170322507	5.11926380627572	17.10184871148739
C	13.05868937412143	4.58540839640961	16.19158319886980
H	14.11004479399059	4.85001911309438	16.19180328806350
C	12.40503497401721	3.71142014239020	15.37426409005331
H	12.81292333128542	3.11294825960077	14.56770532348585
C	11.02560089059858	3.70770194369387	15.77488409645071
C	10.06685833051982	2.83176407463166	15.26987801031085
C	8.71570330255099	2.98850606913793	15.56185338281221
C	7.67502733378945	2.11405751392443	15.09259412584004
H	7.84606108989607	1.17625975289466	14.57753304180589
C	6.48683036111817	2.68598706886533	15.43842630308469

H	5.48413379493761	2.31328190236574	15.26369639892105
C	6.79302409427934	3.91162231032180	16.12404605914330
C	5.84654333726549	4.85955000737104	16.49927375459044
C	6.20859935436732	6.00455168340568	17.20471170207394
C	5.31140204873456	7.08635020086165	17.50071085379061
H	4.31265031911138	7.18568085186408	17.09103291946296
C	5.95275874076550	7.90961725205408	18.37787048481209
H	5.58943545590297	8.82518819291728	18.82963355537230
C	7.25051768613125	7.34162140410742	18.61567736690185
C	8.14430268616888	7.80682364136759	19.57885055029099
C	9.46050425034453	7.35554900653161	19.61731237846816
C	10.44235998416263	7.76808952420848	20.57847233531463
H	10.22977751138332	8.35491016928414	21.46337687886262
C	11.64128769068815	7.25677045308900	20.17489997881789
H	12.60617658080094	7.34856091105438	20.65723875616343
C	11.40109027997790	6.51236506991960	18.97270846008328
C	12.39366162935599	5.91742516881025	18.20050042111981
C	10.50806366295484	1.70230870801476	14.41748691287662
C	11.45348573119435	0.79320556553303	14.90435996644787
H	11.84044979210039	0.93512107193832	15.90896013050682
C	11.88216787495134	-0.30055026624388	14.15389577201772
H	12.61055679300705	-0.98781905831060	14.58169000047948
C	11.36040345148308	-0.49747183145873	12.86801791991232
C	10.41955029590793	0.41125960361961	12.35582728165828
H	10.03537514701336	0.25290039005105	11.34833428933344
C	10.00135389721034	1.49173945247175	13.12215295734878
H	9.28005248292591	2.19778199835042	12.70907919196579
C	12.65983559663875	-2.47123637228630	12.54064380680454
H	12.79641978815239	-3.20830519369376	11.74232814292457
H	12.28939132095229	-2.97510583884427	13.44826092179502
H	13.62295454653701	-1.98372433357702	12.76090779203097
C	4.42269179458870	4.64814788781643	16.14640526960851
C	4.01604286049302	4.45958791763272	14.81238220526431
H	4.76224606053622	4.49440161171335	14.01803329330064
C	2.68177767208404	4.25010239831943	14.49087570218394
H	2.36532266017902	4.11433969385770	13.45640878801803
C	1.70904853084741	4.22170427860449	15.50314255393899
C	2.09366521927810	4.41411928360067	16.83697298877764
H	1.36222422532343	4.39739882926617	17.64248013189096
C	3.43889050393751	4.62579314125176	17.14252112876912
H	3.73718047880812	4.76122582493181	18.18053896691534
C	-0.59170938066808	3.98754028901154	16.09313693039499
H	-1.53321833605395	3.81487958376165	15.56127269926757
H	-0.64324065744590	4.94985547285342	16.62790636923556

H	-0.42480129992184	3.17423570669685	16.81804060521360
C	7.66439692529767	8.78781329319009	20.57831196574473
C	6.51215979798132	8.51086648620857	21.33928999946179
H	5.98863426788850	7.57067639020237	21.17697799138132
C	6.04978554779560	9.39855545573917	22.29896749548381
H	5.16335542738178	9.17715363475550	22.89386436171510
C	6.73019154644936	10.60544333147366	22.52580642407738
C	7.87006796577893	10.90919009906584	21.76892717224928
H	8.40535782339586	11.84580405952907	21.91029196822330
C	8.32263679377942	10.00252322549479	20.80809136243300
H	9.20027669518456	10.25428795746062	20.21183658807737
C	6.88023690655509	12.64428020977044	23.75844642958277
H	6.88693932330075	13.29567605404851	22.86935153662617
H	7.91574646474258	12.46814024187128	24.09188629733684
H	6.31503265850088	13.12793969298408	24.56209663613397
C	13.81506455561933	6.11785716641139	18.56865754988334
C	14.64383922142498	5.01366941178690	18.84081120479979
H	14.22405563227577	4.01061065287080	18.77997995078524
C	15.96916692585679	5.18514565079863	19.21322547679842
H	16.60619903767172	4.33037051107263	19.44024725653258
C	16.50987128229341	6.47678940786831	19.31605701423048
C	15.70399059612474	7.58924187967127	19.03735792124307
H	16.10288885084395	8.60023476849185	19.09513619372310
C	14.36969143911124	7.39959953497372	18.67131450839635
H	13.74809923203145	8.26769740328911	18.44983040890628
C	18.40016311065416	7.84645149946871	19.81826252087829
H	18.39359997940880	8.38082743740788	18.85445937481220
H	19.43440108363683	7.68310646523610	20.13884987337857
H	17.87053679520426	8.44885898501921	20.57401398113141
C	6.71074682619198	1.91354749415956	18.72314534674678
C	5.30153892888611	1.71231184365182	18.83909015165990
H	4.73031477361546	0.91159947533338	18.38009234368505
C	4.81398180194993	2.70006923346285	19.68940284578044
H	3.78962497735932	2.80800501086560	20.03368968460652
C	5.92706755679906	3.51732638877114	20.09563829431192
C	6.05405935865884	4.48538762651947	21.11878664429868
C	7.28715999340916	4.93131050683028	21.64963373553530
C	7.45873683060070	5.71018252807769	22.84556984713070
H	6.65599859880453	6.17462120277026	23.40808989122435
C	8.79315849466112	5.70342905358362	23.17596223241909
H	9.24786781628890	6.15700405452035	24.05034195293107
C	9.49140868854755	4.94661812008428	22.17608927098948
C	10.84743630309945	4.55510828948308	22.20102115417217
C	11.48587217140485	3.70329185874020	21.27230186549983

C	12.81840918797371	3.17788620355031	21.36098977571672
H	13.55207581716884	3.45440825760354	22.11140513062056
C	12.96861120938785	2.23809039021773	20.36747946972760
H	13.83951765389613	1.61389831083162	20.19274943119954
C	11.73562380095792	2.15848914642062	19.63356433200956
C	11.39399438170676	1.15648000419370	18.69142810886467
C	10.07891839078404	0.92247075520762	18.22002141340019
C	9.48966099240230	-0.17658933817505	17.49879954898861
H	10.02734588379479	-1.00514316534112	17.05011380188071
C	8.11103992825648	-0.00808801551907	17.52146349159577
H	7.36932121838560	-0.67610336143897	17.09528844733629
C	7.84282208605857	1.20332518607575	18.22707692448626
C	4.81678892554054	4.85387205255859	21.86101023036625
C	4.56030287243245	4.32181784182063	23.13419897658853
C	3.40501199736637	4.63215123585671	23.85181299366913
C	2.45513746462836	5.48879351463446	23.29200499127499
C	2.66903503711734	6.02120417736740	22.02074720853851
C	3.83594032265687	5.69650480217986	21.32782089665912
C	11.59902902638033	4.82931935901744	23.46335643299533
C	12.06166720109483	6.08612361250020	23.86968758268958
C	12.74131092556534	6.28290972933204	25.07393793917878
C	12.97523665859221	5.20196308597368	25.92194733911154
C	12.44307337343923	0.17231344568385	18.31773019091433
C	13.61077348240972	0.53875645303267	17.63092488194031
C	14.55767545125896	-0.39344388423997	17.20645688196338
C	14.36292847965437	-1.74723767775693	17.48104028211332
C	13.23533572665698	-2.14750358817804	18.19902657433168
C	12.30674720167450	-1.19352860415337	18.61755741919999
F	11.38007727049088	2.53399314377971	24.06936216543133
F	12.72160400150814	2.89056165779182	26.38336838126591
C	11.83694569301715	3.76770545411891	24.35449933603858
C	12.51744042619880	3.93428840748418	25.56004048222167

(TPFC)Sn, **2** (BP86/def2-TZVP(-f) geometry, used in calculation of Sn-Co BDFE, and various structural and electronic properties of **2**)

E = -9394.67343510208 a.u.

C	-1.76262192033212	1.27418740534449	1.26548273368558
C	-0.89413946071849	1.34175884596784	2.34392528043372
C	0.43829294219637	1.28017366099766	1.81126218722391
N	0.35885550062641	1.16538024405449	0.46059909901763
C	-0.95737750601691	1.19362398143380	0.07109206059058
C	0.55912612904258	2.13205500233255	-4.33280414529534
C	-0.63124002271620	1.84707160240457	-3.70271107468049
C	-0.33372631687964	1.54220449106427	-2.32753058135027

N	1.03317006483459	1.64359062654781	-2.14529669616981
C	1.60197764369257	2.01272943899033	-3.34947970677191
C	-1.28436907344192	1.31248654058099	-1.29004564926487
C	5.89235965468545	2.69689371196557	-1.36860068252303
C	5.32764753024619	2.76787846158596	-2.62242388383341
C	3.97020617527695	2.30627483743336	-2.50563898078886
N	3.73372443496565	1.96031154207656	-1.19012044197121
C	4.88862593402506	2.19383655910212	-0.46751849097926
C	2.97921594845017	2.29331969970489	-3.51727022562099
C	2.44244396968798	1.74467994719634	3.53090855468547
C	3.78259231275355	1.94711199865566	3.23846047392596
C	3.93813965435094	1.79056671644383	1.81257408165132
N	2.71111507957595	1.45204668823279	1.29656315904175
C	1.78518613820002	1.44384720682509	2.28984219370490
C	5.00490260431516	2.09003224624492	0.94985529535653
Sn	2.17412697317584	0.45934433618672	-0.62533899637276
C	-2.72209397725225	1.30334889285245	-1.67027644053086
C	3.42488281928714	2.68797382169853	-4.88230304767200
C	6.32140216397134	2.42976460171843	1.55289378600744
C	-3.28872769508100	0.20321123312855	-2.32421760506155
C	-4.63648296348184	0.17084899438460	-2.68339079150611
C	-5.45211556510091	1.26479005730852	-2.38560161595330
C	-4.91554618083096	2.37848258397843	-1.73647023190051
C	-3.56369839344201	2.38606189364968	-1.38954639535392
C	4.18323490596967	1.82029651476130	-5.67652153648958
C	4.61856888172176	2.17835857219063	-6.95329117836931
C	4.29431761834489	3.43838040838631	-7.46055517217144
C	3.54086857031221	4.32727748162576	-6.69096929521211
C	3.11790752969817	3.94438961508160	-5.41740729322929
C	7.39389273121012	1.53258920387379	1.49572008012671
C	8.63608146256400	1.82961628750453	2.05739429980733
C	8.82351430905032	3.05704597494849	2.69694969993417
C	7.77355455199982	3.97463116780489	2.76710205313284
C	6.54104622354512	3.65294742372392	2.19668618558015
F	5.55470020578180	4.56734129457283	2.26078170439043
F	7.95968331474764	5.15881876374682	3.37471084030806
F	10.01184712736264	3.35392839285562	3.24345565395671
F	9.64664858101868	0.94644935785298	1.99557271027223
F	7.23500252000047	0.33675918239739	0.89636799505632
F	-3.07002781850628	3.48447990721832	-0.78692158393350
F	-5.70032973957877	3.43300024530757	-1.45757624144979
F	-6.75040938701084	1.24521116424032	-2.72242947239420
F	-5.15668735592747	-0.90217394527560	-3.30261764472901
F	-2.52760715429907	-0.87045853750784	-2.61169226294889

F	2.41266069601107	4.83110101791754	-4.69009544348079
F	3.23875872427186	5.54289100581636	-7.17704930570802
F	4.70705146429791	3.79545793402308	-8.68579897242638
F	5.33876450432153	1.32261025662613	-7.69780792689916
F	4.49832248337916	0.59401478907866	-5.21810413456974
H	-2.84683967698983	1.33328466547512	1.30108268915510
H	-1.16323595173441	1.45922465643425	3.38929803547543
H	0.69420875211413	2.43272090017015	-5.36687478249236
H	-1.62529029276105	1.88058391731106	-4.13848175658681
H	6.89490532042301	3.00159348006340	-1.08479984183246
H	5.79235580714200	3.14185315066770	-3.52928035613767
H	1.96788215783458	1.83431549085201	4.50351048214624
H	4.56409133561952	2.23147439016315	3.93706954999444

(TPFC)Sn, **2** (BP86/def2-TZVP(-f)(Sn)/def2-SV(P) geometry, used in calculations regarding the alkyne trimerization process, i.e. in Figure 10)

E = -9394.66220518423 a.u.

C	-1.79353587827887	1.35992902239650	1.29535079665446
C	-0.92313270300180	1.44011436243919	2.38459110292767
C	0.41262928368300	1.38187010774860	1.85589628179084
N	0.33263768071208	1.24802697246767	0.49648690333036
C	-0.98323099543541	1.27873309072404	0.10076214711544
C	0.54713847479602	2.11221695144437	-4.33024951579180
C	-0.65180987216292	1.85387210268046	-3.68902559793107
C	-0.35714664327242	1.56848556017646	-2.30348682814606
N	1.01976391046610	1.64796663665995	-2.13233351868428
C	1.59471772001038	2.00106238814105	-3.34365545351831
C	-1.32201191034898	1.36213938901058	-1.27116104507848
C	5.88658668909822	2.70517568853352	-1.35615694853169
C	5.31918873368093	2.76519538059193	-2.61766153637825
C	3.95937960519694	2.29625575072408	-2.49957313326210
N	3.72921914529650	1.94840969525404	-1.17894008557535
C	4.88169727008654	2.20437445076652	-0.44678912265520
C	2.97671279376334	2.27492047671805	-3.52653806673548
C	2.42860428335719	1.82808967144643	3.57023141945577
C	3.78026620026675	2.00817862407070	3.26743611092754
C	3.92617046724797	1.85172846581584	1.83752685661176
N	2.69171870174207	1.52057732283690	1.33040483609569
C	1.75894282096736	1.53756969299779	2.33175849836308
C	5.01361962666352	2.11852428832159	0.97260402889542
Sn	2.11109071543414	0.67657503492125	-0.54531931913936
C	-2.75396078242583	1.32233708072250	-1.66610596908725
C	3.43159173004176	2.65064668796438	-4.89273094776418
C	6.34468260507609	2.42358720334874	1.55810245894467

C	-3.23444159517843	0.27667765836183	-2.47862279874985
C	-4.58079877104288	0.21771366169319	-2.86949068023340
C	-5.46962283250892	1.22060543579625	-2.44504665248343
C	-5.01042982501565	2.27483535880128	-1.63721890996882
C	-3.65965814113983	2.31940095340713	-1.25660088064765
C	4.32671285961331	1.82513179454481	-5.59948396104275
C	4.77522349177609	2.17238193916931	-6.88362571762279
C	4.32703468248886	3.36644441784614	-7.47441892686669
C	3.43810678830758	4.20717964117303	-6.78307119780111
C	2.99913293459594	3.84470811384702	-5.50010682179386
C	7.43925165971922	1.57439961352183	1.30280997453866
C	8.70742334564202	1.83913484157208	1.84219352291568
C	8.89225693510448	2.97322038136192	2.65167516425238
C	7.81502398222214	3.83690407010577	2.91370916430216
C	6.55280287842736	3.55773126264021	2.36589061748706
F	5.55228367121636	4.40364166498381	2.60983008322371
F	8.00002651338390	4.91525849596601	3.67300603737598
F	10.08961585855646	3.23078120810152	3.16857489293282
F	9.73151281723142	1.02331412908739	1.59949107166018
F	7.27872904887036	0.49165293280112	0.54378051311184
F	-3.24388245153122	3.34057327183457	-0.50762807896648
F	-5.85529275871735	3.22654231890297	-1.24469434819981
F	-6.74723433656285	1.17153145469768	-2.80947466098922
F	-5.02211430691822	-0.77956886532686	-3.63378632252480
F	-2.40724775775695	-0.68602654433615	-2.88355884211879
F	2.17134388704186	4.66356656635820	-4.85301610212391
F	3.02444850440027	5.34108392159382	-7.34576875028277
F	4.74638294634302	3.70281111108119	-8.69028107193991
F	5.61528494554675	1.38010687874916	-7.54662385688022
F	4.75697670303509	0.68820506375088	-5.05538097096807
H	-2.88553705226273	1.40736381773689	1.32767581032638
H	-1.19552603201949	1.56124924195595	3.43677818676234
H	0.68652816338119	2.38598826543397	-5.37857429998410
H	-1.65374325430559	1.89702182930544	-4.12420980953651
H	6.89053560648579	3.02647281884015	-1.06779404120367
H	5.78019608729945	3.14369667360685	-3.53332911272963
H	1.95585933081035	1.92400197787600	4.55172720051528
H	4.57660280080018	2.27360252423458	3.96754122341990

(TPFC)Ge

E = -5245.679411351014 a.u.

Ge	0.77343091014110	16.66337561251040	-0.44816125647797
F	3.94627110923084	12.37434733277182	-0.39245041908030
F	5.49686978099782	10.36928303759891	0.59255442273934

F	6.00783753466950	10.22945232117132	3.27201834909360
F	4.97289837082117	12.10163551099352	4.97092011132409
F	3.43885791912797	14.12189509128569	3.99588246497733
F	-3.25530544833148	13.90892633630991	1.28479092264839
F	-5.49179021517080	13.26339193139577	2.69544367369350
F	-6.36948721400360	14.91127952450979	4.68916638266777
F	-5.00851378827890	17.20464111241990	5.28017357544844
F	-2.76565554845923	17.85226528963100	3.88196342815484
F	-1.21715205724846	22.03479572863277	0.30130711480594
F	-2.22192603595221	24.32587876747946	-0.75822065957545
F	-2.38215799565833	24.62322352769150	-3.46857169031774
F	-1.54237518774969	22.62051534742563	-5.12525322669168
F	-0.55804925716782	20.31279341150437	-4.07748854947639
N	1.59360206254284	18.35694136826876	-1.12436876281008
N	2.73434165579488	16.35966515293526	-0.21290375384236
N	0.60830690537106	15.59119695631969	1.25056631848923
N	-0.69372743042476	17.87717283077367	0.21077579299407
C	1.03394807089580	19.52119643783480	-1.59944200054226
C	2.06675947917421	20.25021206686914	-2.29045330811132
H	1.94583014109304	21.23058322761225	-2.75858786754588
C	3.24182611071156	19.49725584680206	-2.20682165624371
H	4.22538899071843	19.76179849870757	-2.60374132326052
C	2.92314698299995	18.31304274312965	-1.46472238461628
C	3.58120932708604	17.16102136959402	-0.93845481428014
C	4.89922513009115	16.60115453416746	-0.87912674673473
H	5.79641887305919	17.01816337633778	-1.34392550709691
C	4.81483559210489	15.45113068184851	-0.08830882987161
H	5.63565011853393	14.78855127951795	0.20034315843625
C	3.44358759022558	15.31302348108192	0.33202493008301
C	2.82389305321037	14.41124129604151	1.22449827983965
C	3.63858639031259	13.29935189444520	1.77426362964583
C	4.18996552520054	12.32718124892246	0.91615121063011
C	4.98956119746089	11.28656291794263	1.41422430634926
C	5.25012991242585	11.21114398654676	2.79317134351308
C	4.71374221229790	12.17285350641365	3.66658139464075
C	3.91683224464510	13.20748182189193	3.15257997315842
C	1.47704516336741	14.56652536605117	1.64372052967044
C	0.78006567494391	13.72675515429237	2.58457028250701
H	1.20232498110837	12.84250562579670	3.06755448861419
C	-0.48785390615816	14.24873339123544	2.76175162081442
H	-1.27076471534704	13.87800818398809	3.42772505407408
C	-0.59909994173788	15.40765102931819	1.91512122600727
C	-1.72607911879109	16.25088144309449	1.77694109320561
C	-2.95051732355093	15.89880458469855	2.54411872971822

C	-3.66528419207869	14.71997679120173	2.25942103563521
C	-4.82109472502470	14.37895385223357	2.97866749578354
C	-5.27521172418733	15.22721814762053	4.00291994694065
C	-4.57591849101474	16.40843333877254	4.30399858723287
C	-3.42184910094297	16.73422535578189	3.57481194112114
C	-1.76266398982299	17.41184466239134	0.96961831441597
C	-2.87784999369319	18.30453644992581	0.79273502558960
H	-3.85643858224398	18.19166245716848	1.26499359549566
C	-2.47516338230332	19.30355641167063	-0.07421096180838
H	-3.07103466440565	20.14647870852011	-0.43216388009603
C	-1.10640396270972	19.04521940910848	-0.44219496731712
C	-0.30492340342268	19.85056604752027	-1.29343743797379
C	-0.86913451259196	21.10146313007342	-1.85759706763129
C	-1.30473482154782	22.15039254120102	-1.02306833316036
C	-1.81828871868413	23.34144082565953	-1.55915335136561
C	-1.89679296917552	23.49793686828288	-2.95359276120799
C	-1.46201983073738	22.46755756543548	-3.80473954333248
C	-0.95212676174675	21.28204625162085	-3.25290868969037

(TAP)Co, **3**

E = -3771.56531832104 a.u.

Co	5.93751108661153	4.75920416221145	7.62394743596073
O	-2.40948399258688	3.05513665938029	4.36686574753685
O	2.46147845878875	5.25094896540478	16.04096737310515
N	5.19917205975572	4.36373339470647	5.83719630348409
N	4.13649911267303	4.58248884699122	8.40682532437021
C	3.87174086367251	4.12262135016114	5.50026294459514
C	2.79791714544921	4.07443227812079	6.38232887172034
C	2.94704733921311	4.29323646470667	7.74744150053133
C	1.84799588493035	4.24107180672894	8.67587108616898
H	0.82229778346774	4.02161535238810	8.40134017910607
C	2.35636841364389	4.51818035525631	9.90832476638219
H	1.83273951940270	4.58317296906324	10.85572405280704
C	3.77316070652630	4.71582487894411	9.74253125406155
C	4.62838088008548	5.00357704766666	10.80061873512851
C	5.99361876881291	5.19742266453852	10.62157510260380
C	6.90238029291721	5.44232828418491	11.71107578905072
H	6.61189474756917	5.49358436917377	12.75437331658125
C	8.14632933981729	5.56355376636657	11.17042513256002
H	9.08959520337246	5.73374013216698	11.67738406819588
C	1.43978746806618	3.78198817744517	5.84600398682556
C	1.11201366779044	2.50603338557455	5.37688559980791
H	1.86530835959188	1.71744806790556	5.41053558991993
C	-0.16000071633874	2.21682707014080	4.87478498645296

H	-0.37856790276721	1.21020478235665	4.52349425722632
C	-1.13311736392407	3.22370973255399	4.83661927838433
C	-0.81834956217034	4.50983132630171	5.30178715973218
H	-1.58444783676244	5.28451267865007	5.25900224317866
C	0.45075019012201	4.77948110657534	5.79869579082047
H	0.68929857847994	5.78275120531612	6.15432155208698
C	-2.75933479779275	1.75495864981560	3.89005388116796
H	-2.12356681175421	1.45370508418814	3.04183770649433
H	-3.79995087440977	1.83103701235694	3.55782252423363
H	-2.68225305489382	1.00033932475054	4.69019669930460
C	4.06388996553788	5.09701285492738	12.17551133020144
C	3.60344491995770	3.95094220238483	12.84583979215617
H	3.66743563810852	2.98223102693325	12.34834760027573
C	3.07750417422899	4.03187021601282	14.12922006357610
H	2.72594104271388	3.14255219196543	14.65218888287939
C	2.99619927431305	5.27329048529336	14.77944870477163
C	3.45058332450527	6.42673318899788	14.12709553260677
H	3.39467287199031	7.40289431562371	14.60559999296970
C	3.97832039892204	6.32635518741112	12.83628286042666
H	4.32735671370520	7.22714512524632	12.32999939125136
C	2.36195553028487	6.49945868197426	16.72778154783673
H	1.71112833147743	7.20482429363376	16.18546235369541
H	3.35372380696162	6.95669291792507	16.87488958044095
H	1.91850526167304	6.26734691276566	17.70186898099598
O	14.28762509491305	6.44476448671814	10.88253966754370
O	9.41263424219674	4.28247945146912	-0.79426397598128
N	6.67593481709042	5.15442682308321	9.41071934956697
N	7.73864905937263	4.93503919196116	6.84119955632858
C	8.00371846109257	5.39309968631442	9.74803425261852
C	9.07792673116520	5.43880178950995	8.86631545648770
C	8.92857222383131	5.22133954079756	7.50101662919747
C	10.02765696469307	5.27341762551782	6.57262843354558
H	11.05371031840690	5.49076611700731	6.84751006085783
C	9.51871632019039	4.99973028643502	5.33964294859230
H	10.04215221614680	4.93584311967450	4.39206301238993
C	8.10167029704390	4.80369231795972	5.50521093976710
C	7.24608385218339	4.51831559338479	4.44676989142454
C	5.88103795443170	4.32326942028132	4.62598562377465
C	4.97220040897726	4.07810987986790	3.53661026403962
H	5.26227238765321	4.02874667027817	2.49310907370386
C	3.72880728031592	3.95340970457223	4.07775512891791
H	2.78564650567420	3.78181839310995	3.57106767180223
C	10.43665438477925	5.72785936611148	9.40297214205824
C	10.76758702723178	7.00289512678072	9.87237055360593

H	10.01628200086837	7.79337895191931	9.83881768873135
C	12.04028434227246	7.28879746022819	10.37463514349302
H	12.26136613051318	8.29479793249419	10.72614275602655
C	13.01087855503954	6.27948065663479	10.41264871824343
C	12.69293690405011	4.99426233941337	9.94713653372055
H	13.45710597017591	4.21766797850913	9.98974119324571
C	11.42320255294185	4.72790641558331	9.45007009340906
H	11.18220491783979	3.72534736079311	9.09409592692708
C	14.64076454676010	7.74405566049815	11.35935975384701
H	14.00569034395193	8.04696642624481	12.20751271364721
H	15.68115544733539	7.66532672585169	11.69167980449201
H	14.56567087557848	8.49883760991201	10.55917361707020
C	7.81026920558435	4.42781577819563	3.07156675407774
C	8.27091047492926	5.57534245966953	2.40386011614048
H	8.20715465002306	6.54291112364290	2.90360123322465
C	8.79681991090140	5.49727879935526	1.12028852340073
H	9.14855154254587	6.38773740693083	0.59937586604995
C	8.87790064165711	4.25734581524969	0.46720110395697
C	8.42331517502975	3.10248607521829	1.11690711325426
H	8.47902442566531	2.12741865193900	0.63615516697783
C	7.89562627415888	3.19997985429357	2.40795996029798
H	7.54650237297354	2.29807243544003	2.91218533319621
C	9.51177969011679	3.03554427223485	-1.48398457715727
H	10.16229830267977	2.32868263442996	-0.94324251411180
H	8.51986115097431	2.57901611004100	-1.63225686338448
H	9.95541088727197	3.26976745860584	-2.45748319125517

[(TPFC)Sn]$^-$

E = -9394.79563317872 a.u.

Sn	-0.06409446176725	0.00327538702918	0.25091340964339
N	-1.59267565660422	1.25640525140674	1.35334740037280
N	-1.58192165476223	-1.29002770193663	1.31981558207312
N	1.16742021100649	-1.42679248236437	1.51731566917323
N	1.14590145168359	1.46298678519018	1.50899093702916
F	-1.68753120685347	-7.85358123901911	0.21994345222710
F	-1.48274307216325	7.26761516007287	4.45014186132099
F	-1.39933814122406	-5.19999741235862	-0.23993939483197
F	-1.24768499954679	4.59011440400856	4.12161780774885
F	-0.93951768368252	-8.92332942426431	2.62861603168391
F	-0.89448836572375	8.96642682339722	2.38248400438748
F	8.79115159985196	-0.01919136484490	2.25529777411562
F	7.63735906478405	-0.69433095385736	-0.13633221574790
F	7.21884820746954	0.68675327645699	4.38444996032462
F	4.94048779864615	-0.64564320060994	-0.40766118680960

F	4.52009383275518	0.70116688699784	4.13911622159747
F	0.31944887346185	-4.64156883609218	4.16843265871671
F	0.10268246053634	5.27617475072474	-0.39252951522442
F	0.07575429376191	-7.30185266330779	4.59046555784908
F	-0.09121122791411	7.95615660278175	-0.03440228460673
C	-3.71773329540177	1.72548106494465	2.00085107027836
C	-3.67374042610198	-1.78381162803703	2.05310450841620
C	-3.00026934807855	2.91780667623689	1.98030773459687
C	-2.92954920934628	-2.96003314327973	2.04563213308140
C	-2.80858911825678	0.68900784045504	1.61597774939132
C	-2.79906795650914	-0.73954945501558	1.61398305388412
C	-1.64625395665794	2.59423917050180	1.60700107625511
C	-1.59784066716367	-2.61922507599574	1.61191581325479
C	-1.19057603946805	-7.04958586396711	1.18492663961185
C	-1.09631969735943	6.76450277879162	3.25785611451307
C	-1.04065726652366	-5.67964340695275	0.96706460206810
C	-0.98072427907620	5.38641722199526	3.06810347585931
C	-0.80297801479406	-7.59944548065043	2.40673889733389
C	-0.79110010328075	7.63239866974393	2.20974228012054
C	-0.57512632068998	4.83025748997289	1.84724768467290
C	-0.50892215623912	-4.81758206633982	1.93784490162038
C	-0.45594677232448	3.36322640505003	1.64908860065349
C	-0.39046337572600	-3.36114137965100	1.68805659732178
C	-0.37692972622392	7.11473439205815	0.98262977281297
C	-0.27635597667143	-6.77266780733914	3.39883352262451
C	-0.27815552232556	5.73269400745914	0.81686449985740
C	-0.14411543412402	-5.40434054227041	3.15913742134991
C	7.44830782083095	-0.00095371034169	2.12528342146905
C	6.85705052994629	-0.35014205484176	0.91123509757047
C	6.64477079163470	0.36569299908561	3.20473910183109
C	5.46709349478094	-0.32399659575717	0.79007230655857
C	5.25669324048970	0.37578222597936	3.05833994313313
C	4.62745681955870	0.03844907498337	1.85224361133043
C	3.14855187470437	0.03959141664775	1.70300908126130
C	3.14415530938263	-2.50602612365046	1.92140556469247
C	3.09291585573236	2.59290540371535	1.91752687391457
C	2.51821997448871	-1.22864399293980	1.67941235333779
C	2.49786432762073	1.29761343100080	1.69158594756773
C	2.14982566047426	-3.45704688348499	1.91079436373956
C	2.07563129794637	3.51975272315590	1.89045428992145
C	0.89896180466544	-2.77855988332488	1.67420928188931
C	0.84556843442314	2.80973072091301	1.63673230511921
H	-4.75794439922268	1.59587889455104	2.28800239761990
H	-4.70534586654650	-1.66670504341777	2.37428603438703

H	-3.36607280885672	3.89904611137351	2.27152390301308
H	-3.25903535310268	-3.94054182188604	2.38054881669068
H	4.19943483823302	-2.66648560219263	2.12674745699016
H	4.14237527347187	2.78327163484502	2.12568336708411
H	2.26686344126286	-4.52203343589979	2.09265755902855
H	2.16113997670892	4.58805559436451	2.07295904122916

[(TAP)Co]$^{+}$ (triplet ground state, with S = 1 Co(III) center and essentially redox innocent ligand)
E = -3771.36658301839 a.u.

Co	5.83775745759269	4.76673741716932	7.65303676967595
O	-1.53556655462774	0.43899275461614	4.79192624089009
O	2.30652009528011	7.89908430193809	15.34568385752981
N	5.14014338341431	4.30109988504641	5.91611915584666
N	4.06552171062210	4.59626126044226	8.42350863139910
C	3.93271094209615	3.68872758930806	5.64029921828237
C	2.93222827481058	3.39643580194220	6.58237366840629
C	2.98132106134547	3.92481796133941	7.88186108736745
C	1.85979136162278	3.99791067356982	8.77903288386487
H	0.90104638756760	3.51882555774809	8.62346888491714
C	2.23083789686903	4.80413058818498	9.81735957168995
H	1.62066555327589	5.13067960447931	10.65062576195189
C	3.62215168363246	5.11688552560936	9.63059591528787
C	4.44753327561292	5.70450237795198	10.60075814608000
C	5.84974981335194	5.64115947100649	10.49901194324792
C	6.72623466912968	5.72962758680493	11.63610734843278
H	6.41356191232859	5.99414480048177	12.63985713642503
C	7.96310076476459	5.32056810625894	11.21952539125718
H	8.85490148152732	5.19138882757738	11.82099337996962
C	1.76130668102300	2.62644591052215	6.12198658836906
C	1.95298338479310	1.34066745535856	5.58851986323917
H	2.96181627718936	0.92760379106423	5.54737622147674
C	0.88208704293149	0.56861979383342	5.14544785127513
H	1.06679890629262	-0.43403779502072	4.76654965251860
C	-0.41968832668816	1.09359918392436	5.20017985671267
C	-0.62300381196944	2.39477303726041	5.69791654904433
H	-1.63462291039094	2.80059555705751	5.69970720500675
C	0.44878281529845	3.14140553408823	6.15780952366706
H	0.27990037891687	4.16013848283232	6.50521088218219
C	-1.38024706369647	-0.89312052532040	4.27833826593788
H	-0.74745776491729	-0.89864641243624	3.37781656913635
H	-2.38979810468094	-1.22568795700222	4.02000315594029
H	-0.95339621209150	-1.56194748532080	5.04122384373412
C	3.87757483776599	6.27968387916554	11.83334802783125
C	3.04385789323631	5.54133495824286	12.69958494047609

H	2.82771827321427	4.49686327873353	12.47606114819530
C	2.54757002392567	6.10344692923389	13.86360796839989
H	1.92568392262571	5.52663761736935	14.54829925863173
C	2.85595491251559	7.43680404266540	14.19450918995157
C	3.69504182970609	8.18408979135622	13.35103949393499
H	3.94977068581579	9.21546978491300	13.58438199025796
C	4.20586996146346	7.59738043063043	12.19590562409690
H	4.85466361554312	8.18160242171102	11.54200321114201
C	2.59266312755405	9.25362804042847	15.72694006456153
H	2.23351367410869	9.96130098352540	14.96466560025040
H	3.67099489463057	9.39701325355201	15.89342646115036
H	2.05100397449534	9.41378808519566	16.66343811661981
O	14.16900042459817	3.89818004713575	10.91287822934576
O	8.89778537113630	6.74238231928997	-0.56393354245858
N	6.55727301186390	5.23162211139679	9.38694932377163
N	7.59239579229762	4.93906366545940	6.89054691636166
C	7.86942817278566	5.06893485077868	9.80752520357738
C	8.95534657891208	4.81596051693984	8.95311557163532
C	8.80191354312406	4.85553572435947	7.55592898920613
C	9.88506311433310	5.03851816871531	6.62846689360027
H	10.93662972806307	5.03175149879944	6.89266310140076
C	9.32728079511344	5.26751953083937	5.40093133503054
H	9.83568261123537	5.44103409686168	4.45933944730978
C	7.90127158985566	5.18349648009405	5.56474367908120
C	6.98397741585059	5.13660512698181	4.49913200116549
C	5.68592910038942	4.63723071371390	4.68460867447131
C	4.77238806432839	4.28122034206637	3.63276576940301
H	4.91404442302756	4.49959336939983	2.58112869163031
C	3.71555845587916	3.64249492217784	4.21865699751529
H	2.82858171038780	3.24057095327599	3.74206876575470
C	10.31041305897019	4.62199107334317	9.49598682902558
C	10.91166965530161	5.54464200439239	10.36850688314229
H	10.37833065086791	6.45723813578151	10.63337400207282
C	12.20029407417665	5.34865282302702	10.85703352409765
H	12.64414005274102	6.09820441766785	11.50952177205685
C	12.91740835894533	4.19847278835810	10.48669905319292
C	12.33285929512064	3.26983717124162	9.60447196293902
H	12.90053679037790	2.38113693269272	9.32974337878239
C	11.05912572456398	3.48845640706762	9.11056386584267
H	10.61102139716499	2.75960693382972	8.43428381447448
C	14.80347946785919	4.80950913554243	11.82384311618115
H	14.22621669832068	4.89866305240525	12.75654183095026
H	15.78386475495746	4.37389451864420	12.03713522455627
H	14.93056259808280	5.80188935292466	11.36510921186990

C	7.46168060184023	5.50961743272188	3.15640937322326
C	8.03254040538349	6.78433361552296	2.94930324840109
H	8.08629564638214	7.48425578827613	3.78390370590649
C	8.49099184755744	7.16946196901074	1.70146186170080
H	8.90781275230618	8.16216340410378	1.53398063439030
C	8.41934504837216	6.27538941319765	0.61607287852424
C	7.88268873419653	4.99120453479083	0.80975905347046
H	7.84663945558708	4.27137126891220	-0.00565960866403
C	7.40582806875792	4.62553986289302	2.06586681995877
H	7.02451018478637	3.61524850605906	2.21442986749802
C	8.83957461417498	5.86928707253728	-1.70256848340470
H	9.44512828876939	4.96524857674892	-1.53738886396764
H	7.80023294121110	5.58855423854235	-1.93039219993517
H	9.25680289218315	6.44508290979077	-2.53388941891816

[(TPFC)Sn]$^{+}$

E = -9394.46208943867 a.u.

C	-1.76058128002239	1.29040991687557	1.24974869302859
C	-0.88835873998522	1.30717527738541	2.32016215356117
C	0.34499776932937	1.87784896414759	1.84349709538378
N	0.20269361770597	2.21669158909078	0.54664819744097
C	-1.05985920574468	1.84269458429753	0.11237730131046
C	0.56800828729614	2.21448938056301	-4.34746875544311
C	-0.63105547639822	1.98283978289856	-3.71205595845063
C	-0.39452351650429	2.06558354371103	-2.29710198523575
N	0.93264244324196	2.36118124145992	-2.08639098051675
C	1.54807331970602	2.46080492503519	-3.32910123817051
C	-1.35316221565257	1.80113825632041	-1.25058903135726
C	5.87446292101896	2.95875297989124	-1.36618813098988
C	5.32411845408474	2.98730324018567	-2.62787420082695
C	3.91205852509476	2.78336419853865	-2.47976890498668
N	3.61953003072436	2.65211748390960	-1.12477548701989
C	4.80521985250457	2.74241372450341	-0.43175522711893
C	2.93795418835925	2.67671616402913	-3.50200042954953
C	2.45337061719055	1.67550757463965	3.50707748572988
C	3.78341872173384	1.91213829168560	3.22152196612126
C	3.85323177180618	2.40741027590990	1.86537230659064
N	2.55428435945459	2.48562365496332	1.38674363204492
C	1.70520310114624	2.02885153560455	2.32754830492178
C	4.93394289796850	2.56763793306406	0.99727625102883
Sn	1.71583436350386	3.53391542656987	-0.36923065500077
C	-2.72076555674750	1.40079109885065	-1.64518271631542
C	3.42231578066315	2.78302564185135	-4.90008739051371
C	6.29537379634206	2.49132452688874	1.56365584319535

C	-2.96912561909853	0.23034854866483	-2.38011353474606
C	-4.26079401789169	-0.15358861469208	-2.73490885848837
C	-5.34419688954570	0.65015631110985	-2.36053007587333
C	-5.12946825139493	1.82267946778686	-1.62820741178466
C	-3.82955468374594	2.17766115429460	-1.27008008408584
C	4.29060709803898	1.82783073230012	-5.44993263263406
C	4.74820954650279	1.92363969158968	-6.76352827143550
C	4.34459031648647	3.00437792209893	-7.55530189808733
C	3.48143143818274	3.97408835543583	-7.03322053572809
C	3.02617859574537	3.84939727177227	-5.72155079818725
C	7.21409487500835	1.51349750806862	1.14409736930170
C	8.49418831068968	1.42607375077938	1.68656821079011
C	8.88703164145451	2.33855596621710	2.67251905974190
C	7.99619520524723	3.32387255376942	3.11253893379562
C	6.71508968566330	3.38336929265644	2.56581075963798
F	5.89129765966616	4.35947743002392	2.98595122268066
F	8.37992790325846	4.20168800938663	4.04443940554580
F	10.10977067058217	2.26583677570250	3.19510006545756
F	9.33921627330770	0.47130692721693	1.28539112807402
F	6.84555883340935	0.59543205819204	0.23355026360385
F	-3.64691509415599	3.32260816039296	-0.58908548964948
F	-6.16521831558459	2.59440427075866	-1.28408166849750
F	-6.58239926544736	0.29516317223778	-2.70008582461022
F	-4.47309934003428	-1.28618223478601	-3.41236682525105
F	-1.94747537852578	-0.57831208838476	-2.71475697141180
F	2.21931076603017	4.80819215221270	-5.23051306149072
F	3.10962598608810	5.01363115077571	-7.78731953674415
F	4.78360015655305	3.11078462510874	-8.80896842082888
F	5.56057215224615	0.99078270345619	-7.27050723701018
F	4.66620500782172	0.76365540646743	-4.71836151421339
H	-2.76718745657652	0.88465182667196	1.23751747270076
H	-1.07062404252930	0.91794229466181	3.31690932342841
H	0.75603163903826	2.18743503113801	-5.41582186568729
H	-1.58084086729643	1.74893888454577	-4.18143012170239
H	6.92403082105141	3.06590783684645	-1.11267881102163
H	5.85240495398180	3.12156574406236	-3.56576771223907
H	2.04657311582797	1.25682981347236	4.42219550595314
H	4.63202274212495	1.71445292511762	3.86877430183489

$[(TAP)Co]^-$

E = -3771.62568312428 a.u.

Co	5.88314562936200	4.77072386645152	7.63540773563058
O	-2.10393967598397	1.74630658505981	4.47159724130976
O	2.33275230075768	6.56177498476503	15.83228484456343

N	5.17026933549966	4.35378196560948	5.87579018813948
N	4.09968501056768	4.61929083821898	8.39831845368668
C	3.89681648991299	3.88059530461682	5.56046078307266
C	2.84583171268487	3.73134787647600	6.45904550578828
C	2.93987129147692	4.14790344091376	7.78193734671594
C	1.81544994539715	4.21500042132201	8.67877981093195
H	0.80878497733820	3.89051984218321	8.43748352717408
C	2.26687426551735	4.77204616133898	9.83965161535599
H	1.70180007230305	5.00433174619747	10.73623166265813
C	3.68326319520183	4.97902732933988	9.68151496002632
C	4.52423025560376	5.37090374636669	10.71734775100536
C	5.90929495662367	5.37478784196525	10.58272892242884
C	6.81055249281575	5.50330614229140	11.69846336621021
H	6.50194524490706	5.65949064222278	12.72703131663108
C	8.07390667720471	5.33663049857472	11.20982507130678
H	9.01130789168326	5.33716732554696	11.75617457376739
C	1.55466545284701	3.19288627385622	5.95172221437455
C	1.43483190216696	1.84597269515240	5.59458405489505
H	2.30193879273089	1.19416500873095	5.70985576818582
C	0.23770554371808	1.31920435483499	5.09591167767929
H	0.18890735468497	0.26426111343090	4.83136658271349
C	-0.87459194331148	2.15557203094887	4.95008315952461
C	-0.77483280013797	3.50904398695489	5.29970764707323
H	-1.64768581542513	4.15029633250691	5.16966382990433
C	0.42506894458566	4.01452528871163	5.78994712073039
H	0.50256115490826	5.07022234258344	6.05195159838240
C	-2.22317554784594	0.37418329577394	4.11418316677005
H	-1.52654633620787	0.10478547233505	3.30207124125975
H	-3.25492529956701	0.24221379204395	3.76759628490117
H	-2.03881899358648	-0.28725757434364	4.97770884626767
C	3.94441179763611	5.70425419106442	12.04594265127644
C	3.30245480958950	4.73240830908364	12.83428922162762
H	3.22710825870862	3.71345864289371	12.45324546099258
C	2.77592361659426	5.04356400510529	14.08325350308735
H	2.28502606514998	4.28527999199977	14.69442057690080
C	2.88371636803205	6.34811296426129	14.58418176805043
C	3.52425439877941	7.33115683742925	13.82181350022136
H	3.62090123035473	8.35302705547356	14.18560391687956
C	4.04381741950080	6.99933022386582	12.56559032228092
H	4.54167792380457	7.76606143295610	11.97077619602357
C	2.44095408487857	7.87973021903875	16.35866461400978
H	1.92528715795073	8.61546071511472	15.71834873099177
H	3.49495197710866	8.18379154441273	16.47691008568473
H	1.95781526741561	7.85094462077947	17.34212894520071

O	14.34695089151242	5.13866022959225	10.95883243292092
O	9.18894547158151	5.54755965209689	-0.81004149797360
N	6.60895667958777	5.14275214636480	9.39965649048962
N	7.65468966339350	4.96456401680852	6.86705533847737
C	7.95079500100944	5.15455842747534	9.78661528704662
C	9.03465273511054	5.08770523102326	8.91886515141276
C	8.87410086690415	5.05768643563140	7.53752143357606
C	9.96289505272301	5.21405544871826	6.60876034983342
H	11.00615203040242	5.31603652916624	6.88924881873380
C	9.41781574055621	5.23238579400984	5.35766467680648
H	9.92681500017419	5.32357865070678	4.40364256055918
C	7.99701490085450	5.05968165738449	5.51780075960469
C	7.12352080514610	4.87886517680233	4.45027993997872
C	5.80042223604908	4.49387123742274	4.63785812648999
C	4.90998529716665	4.13585124629867	3.56423888662051
H	5.15524296088567	4.19889587632174	2.50921970353302
C	3.74185671439238	3.72422618913635	4.13720393678776
H	2.83250015451260	3.39062408790185	3.64764044947776
C	10.41520793610859	5.13057309552061	9.47094048970708
C	10.91762839098838	6.27603047293310	10.09824371073637
H	10.27466615012614	7.15295599947268	10.18386496941431
C	12.21893085467046	6.32458918569847	10.61049912350891
H	12.57062092091432	7.23856822403355	11.08679562349081
C	13.04892317123546	5.20404496495982	10.49139192359907
C	12.56749026061675	4.04893428231575	9.86059018520053
H	13.22536184935926	3.18286925787072	9.77664659032928
C	11.26950498360158	4.01907791808916	9.36107539620379
H	10.89694373867705	3.11887079683702	8.87127127992992
C	14.85091666085300	6.30250616713718	11.60480664378916
H	14.25550716730200	6.56192202835837	12.49651752133938
H	15.87472077464828	6.05705798407950	11.90984048402348
H	14.86986073597517	7.16939487859139	10.92213855887803
C	7.65383286576529	5.02013458739469	3.06792898791707
C	8.05969030163883	6.27386733246593	2.57714364562226
H	7.97046085773139	7.14473490630842	3.22790588120099
C	8.56762528100766	6.42042749687391	1.29049656627574
H	8.87701743950255	7.39562838816491	0.91276404547463
C	8.68004543910807	5.30455014697839	0.45027804900695
C	8.28465374022714	4.04584320152682	0.91665324405710
H	8.36877023743436	3.15971661853992	0.28890625354801
C	7.78224225612940	3.91765316991232	2.21628404735618
H	7.48551255873222	2.93368682433717	2.58111167366029
C	9.29019047849405	4.42855517067202	-1.68295329084363
H	9.97057960244000	3.65847160448217	-1.27995473376381

H	8.30382182736421	3.97149289608325	-1.87220051722336
H	9.69781451441661	4.81679257839119	-2.62358505767356

p-fluorophenylacetylene

E = -407.957985823894 a.u.

C	-1.53998163966896	-0.58920207735867	-0.03167475264441
C	-0.14438914490176	-0.27866056185929	-0.03088239251822
C	0.42474494536927	0.50912861753357	-1.06492214538724
C	-2.73625872774652	-0.85927709679409	-0.03238272452479
H	-3.78761669798619	-1.10028251283348	-0.03280393310607
C	2.60792831911337	0.32625853824719	-0.03141200277273
C	2.07068870947919	-0.45453758312209	1.00444529852042
C	1.79219504405173	0.81015337660549	-1.06657796447111
C	0.70295615792321	-0.75399811053324	1.00358713714776
F	3.91307238096468	0.61133884158526	-0.03237290032527
H	2.24065974846456	1.41718384582882	-1.86350365303415
H	2.73275225903301	-0.81899559318078	1.79994727842110
H	-0.21999295183192	0.88284713195946	-1.86989813287912
H	0.27424159773634	-1.36295681607814	1.80945088757387

TS(2 + *p*-fluorophenylacetylene → **9-rad)**

E = -9802.60975225004 a.u.

C	4.24780565827348	-0.77374295517784	-1.22099906710024
C	-1.18651278245140	-0.54312442210835	-7.89418193173411
C	4.07759412007759	-0.06934462439097	0.91834776896271
C	3.42064552563186	0.52321407359641	2.02941757291232
C	-0.67519443471282	0.65072437341740	-7.33705554262955
C	5.47995834508772	-0.18418089187301	0.60265381394127
C	2.02681941101037	0.79807212988251	2.06028575899374
C	3.59038548824721	-1.03929795354059	-2.46798752853828
C	5.58369119511219	-0.62105319564299	-0.72338495284257
C	-1.19644285208980	-1.74055368222962	-7.14694773442088
C	4.25761702467075	0.97929357537210	3.16687075358269
C	1.31626374674496	1.52962386883991	3.08282864744046
C	-0.12812707472527	1.01332336418107	1.39728969740922
C	-0.18162385775085	0.63745126850564	-6.02133256132036
C	5.01648353289146	0.06827747255365	3.92452778859773
C	0.31166575771286	-3.16014250499423	1.19220684726580
C	-4.80434201236784	2.73131779979427	2.31779054726567
C	1.95948427026085	-1.01666092555843	5.28073338478171
C	-0.70100059393437	-1.73319880955081	-5.83203162921933
C	-1.25945018200749	1.03802643922125	0.54261783022652
C	3.95385091909877	-1.10232483995505	-3.85446946070828
C	1.67962884883713	-0.90280666232690	-3.65715626938108

C	4.35157813327098	2.34680344801412	3.49788897464610
C	0.36080392203497	-2.58303089439101	2.28274184702884
C	-0.00045904505761	1.66045895378397	2.68086262077825
C	-1.27695493631417	0.65549005513758	-0.82265672863335
C	5.82037863215979	0.49343145616263	4.99357984709275
C	5.15277771761007	2.79125025930454	4.56164380065771
C	0.51950679670748	-1.84329688962041	3.48208136525305
C	-3.97089113071522	3.53822965968179	1.52961099921309
C	-2.28954817057084	0.97059470887440	-1.79799734707213
C	-0.54463550257888	-0.08638811547420	-2.83283257212122
C	-2.49644058567744	1.63090081737890	1.12549222939909
C	5.89023988898759	1.85991624194206	5.31096907807014
C	-4.49561669729928	1.37506623427269	2.51117633215465
C	0.85312554196777	-0.35644702869655	5.84310585365522
C	-0.58311396184251	-1.16237295732354	4.06644632068664
C	-2.82728861924013	2.98108881549287	0.93569904085269
C	-0.19335994469108	-0.55047448259773	-5.25668746538122
C	0.31944079082347	-0.55724350438380	-3.85653422480792
C	-3.34959987517351	0.83751664889466	1.90798807474294
C	2.77002108035191	-1.03056632726585	-4.59470969698299
C	-1.83861050153257	0.51968886901194	-3.02936007110926
C	1.79208823956593	-1.76235318556738	4.11004704731499
C	-0.41762884988525	-0.43389732297829	5.25118333813214
F	6.51380363554837	-0.39106283338374	5.71149252133262
F	6.65522192170337	2.27104662519726	6.31808272327715
F	5.22508475619334	4.08818803585963	4.85518473679901
F	-1.65522950826808	-0.54078182459281	-9.14013042343118
F	-0.65902876909069	1.77637391235410	-8.06164614877537
F	4.97697957033633	-1.23702592418075	3.64934605003008
F	-0.72038433264940	-2.86733167184885	-5.12612592391519
F	3.68675031374660	3.25820489707111	2.78827036023281
F	0.30830026562620	1.76839977873579	-5.50155532474948
F	-5.29548049265569	0.61391443434094	3.24534352376564
F	-5.88685577444212	3.25609072079446	2.88095602616845
F	-4.26835732502568	4.82509018333266	1.35609382420127
F	1.02246877624088	0.36763564676321	6.95531618028661
F	-3.07308648161244	-0.45915144755859	2.09330011688591
F	-2.03994005649103	3.76252384029703	0.19847818178363
F	-1.67576733082325	-2.86573056984203	-7.69104270251398
H	6.30420962313768	0.08097276764480	1.27100390867928
H	-1.25787439742563	0.10411997734971	5.70666625667476
H	2.67632107762738	-1.01842830221664	-5.68506909621106
H	4.97295659293023	-1.15185189484126	-4.24905437826346
H	-3.21760035825061	1.50581729726648	-1.58528841516069

H	2.93893130527256	-0.93272923487602	5.77140374887024
H	2.63973607681523	-2.29139166116847	3.66459307990080
H	1.76238445532788	1.91059778213661	4.00334403334463
H	-0.80679063510827	2.17117383537584	3.21230188477709
H	-2.33919016792485	0.61231265056965	-3.99720196969151
H	6.50378572905670	-0.77434285757535	-1.29359062265875
H	-1.55492045066661	-1.18065744737368	3.55846110676108
H	0.17592278994972	-3.77646086364413	0.31661532299401
N	-0.25631577645754	-0.02216150008519	-1.47057345430485
N	2.21398696205723	-0.98540891759209	-2.39717029292871
N	1.10611721935157	0.48108127690192	1.06480748315217
N	3.38182996081933	-0.47285100859134	-0.19600056556235
Sn	1.35808020863245	-0.93200806028905	-0.47164378880609

(TPFC)Sn-CH=C(C_6H_4F)·, **9-rad**

E = -9802.62760450113 a.u.

C	4.42611569784882	-0.72138617807937	-1.48734518318959
C	-1.29194829304217	-0.75165172994664	-7.92377108792127
C	4.33247925231058	-0.11777706565290	0.69510931617164
C	3.70466086954409	0.39826586147741	1.86659747762546
C	-1.29210334680925	0.47678399779731	-7.24109538297176
C	5.72058531831095	-0.20183034864447	0.31882966758332
C	2.32852800774472	0.73753311453135	1.94382037807247
C	3.70675746406571	-0.91900497723364	-2.71660898385142
C	5.77565773893219	-0.56557147151798	-1.03634622397153
C	-0.77101075367375	-1.90141266291839	-7.30587549039897
C	4.54815474307598	0.59320382622199	3.07185191159076
C	1.64026038646753	1.34247550073627	3.06035426578726
C	0.14792437383033	1.02774584416600	1.35934653399933
C	-0.76978599408720	0.54787343631016	-5.94009456275115
C	5.14152905636361	-0.52073708441307	3.69730011667239
C	0.98701519827044	-2.61790724990131	0.28864662087518
C	-4.69895525464964	2.11584501172855	2.58010897233448
C	1.42475622519280	-1.33718045025626	5.02613298441326
C	-0.25617371816771	-1.81351411633604	-6.00321808087982
C	-1.04023777221783	0.99345108983917	0.58148644398009
C	3.98375230844615	-1.01031197394904	-4.11712789532711
C	1.71673491467715	-0.81117157370240	-3.79900808177124
C	4.77383397537429	1.86604259221045	3.63020109946233
C	0.70459750006722	-2.50675904322375	1.55871819362243
C	0.31527344943972	1.51948339458048	2.70632745273765
C	-1.13372693594554	0.59834559110775	-0.78300059480146
C	5.92613668685293	-0.38176684294210	4.85178884923633
C	5.55833516415871	2.02565074325943	4.78368517801094

C	0.52088733735696	-1.97427369540013	2.82954752293272
C	-3.69549111395871	3.07746479602841	2.37312577882250
C	-2.27292867898694	0.72284559944253	-1.65753801099382
C	-0.50054106662114	-0.09956162516142	-2.85636677631785
C	-2.30428622431208	1.39999450703157	1.25209721897471
C	6.13448620837066	0.89844369941825	5.39401383419140
C	-4.51716682509652	0.79798882665775	2.12550595904503
C	0.14862875443915	-0.88596591215686	5.41259492289431
C	-0.76965236986948	-1.50879711050582	3.25780328970240
C	-2.51158163592351	2.71430221027212	1.71066798077126
C	-0.25096716126534	-0.59357758396588	-5.29747981175735
C	0.32800001033638	-0.52274633537158	-3.93189381002529
C	-3.32796133146126	0.45682119264490	1.46456492980108
C	2.75367091201809	-0.94985981388397	-4.78923138266842
C	-1.88791203895457	0.29248722191382	-2.91879964864438
C	1.61588449158272	-1.87645320242262	3.75527734203941
C	-0.94577011748253	-0.97346417644087	4.53239365690636
F	6.47019136926221	-1.44730532959660	5.43703467856437
F	6.87800989525121	1.04260150509275	6.48667840289253
F	5.76587434677693	3.23591404519086	5.29951210143891
F	-1.78325388106604	-0.82602358223352	-9.15705114611415
F	-1.77880628499310	1.56537051736804	-7.83509883438137
F	4.94307547688943	-1.74890802064640	3.20656967411569
F	0.22326328652703	-2.91765360523307	-5.43123885139068
F	4.24819270171650	2.95028836350781	3.06209926875613
F	-0.75735687719464	1.73004834221653	-5.32513090177731
F	-5.46935014722208	-0.11146673022946	2.32654677456854
F	-5.82253483786301	2.45236151795644	3.20681869481177
F	-3.87667276922413	4.32557629040644	2.80089096471856
F	-0.02328109775984	-0.35915226630846	6.63084247949575
F	-3.17065265908019	-0.80632323418980	1.05137503497723
F	-1.57799625022588	3.64569053175560	1.51834956027047
F	-0.77544816564636	-3.06351221697924	-7.95683351514690
H	6.56778775462422	0.04398793396436	0.96556516255913
H	-1.92607750356545	-0.60284784300386	4.85812678125960
H	2.60009608052961	-0.94446823968388	-5.87256040619881
H	4.97586012021879	-1.07293906357840	-4.57277688375162
H	-3.24592920862811	1.12713203712922	-1.36702735844417
H	2.26117029227472	-1.24441804023804	5.73080804151240
H	2.61291293827702	-2.20306578791968	3.44109343801859
H	2.09969309407826	1.60528991332674	4.01500880543024
H	-0.47317487201817	1.95165518145489	3.32517030483174
H	-2.50598986322442	0.26939133697647	-3.81945065281384
H	6.67521957511470	-0.67982392644105	-1.64744871232266

H	-1.60938349801906	-1.55671527306969	2.55612254017848
H	0.95076254119783	-3.55156899327315	-0.29675162296215
N	-0.08963530347083	0.08503867952623	-1.53348733092294
N	2.33375401868686	-0.85053659296787	-2.57334835751139
N	1.38304345230438	0.56632721388854	0.93126797016815
N	3.60549166944551	-0.48263884915356	-0.40469071996464
Sn	1.58172310347338	-0.75235838836435	-0.65183827487972

TS(9-rad + *p*-fluorophenylacetylene → **10-rad(cis)**)

E = -10210.5554162893 a.u.

C	9.99987406555400	6.85628342696979	2.05852736307324
C	11.22759004313033	6.53681503280436	2.66189147084442
C	11.57427536819076	5.21178258971008	2.24348419657787
N	10.56995580269400	4.77834626755368	1.40957670459393
C	9.60105941642056	5.72831047221742	1.25257545280469
C	7.67766733317679	2.96291584724235	-2.14289429467853
C	7.35558939339770	4.12978665708366	-1.46716106959570
C	8.42887097981365	4.42641049929711	-0.54520268304417
N	9.39465506258273	3.43084193143919	-0.71066475410719
C	8.95279954618790	2.50726790118897	-1.64376154950235
C	8.50307570721303	5.51833713198395	0.36958366487874
C	12.77004467301203	-0.33095804356229	-0.98709314552718
C	11.67502432371136	-0.26104265260084	-1.83590825834580
C	10.85504903714449	0.84480762095366	-1.40480226258817
N	11.47574883678287	1.41671657288211	-0.30721472276682
C	12.65050256802958	0.72768206715142	-0.01221019810360
C	9.64376920676881	1.31152729380043	-1.98966357667578
C	13.88685896506800	4.12302453977739	3.06548490400330
C	14.42879265531949	2.88256229557356	2.69892117704274
C	13.49890146495863	2.24190491458717	1.80307032974843
N	12.40948666339486	3.07220239659898	1.71316915254490
C	12.61638037592110	4.24015265666326	2.42014090598885
C	13.59079104948559	1.06668287970957	1.00233712024408
Sn	10.50868776624227	2.76718119347642	0.95062460906306
C	7.33005683604063	6.41811021139578	0.49014571172406
C	9.02169840389688	0.43376960385873	-3.01522491863813
C	14.74419625324640	0.15519793590565	1.21250185302368
C	6.81148727867285	7.13128649661566	-0.60958659099309
C	5.63429077367412	7.88827040260324	-0.50225737023218
C	4.95101164388226	7.94471130038511	0.72534578844209
C	5.46092441463947	7.26350177976339	1.84292990708837
C	6.64380969756097	6.52219581220193	1.71829876249296
C	8.57445410382000	-0.85476871649526	-2.66212829676776
C	7.98864819268946	-1.70831603098325	-3.60919468696738

C	7.84135892200635	-1.26966584620517	-4.93686052160241
C	8.27565005694919	0.01420149920612	-5.30977824799924
C	8.86145544753006	0.85422166714120	-4.34913347045362
C	16.07254385656509	0.59469812896494	1.04411730103837
C	17.16190693243027	-0.25640337557010	1.28882532692956
C	16.93290734611666	-1.57941655358008	1.70195454303742
C	15.61751689810550	-2.04631789376144	1.86325892069049
C	14.54324766673966	-1.18127472279895	1.61124670595696
F	13.30212474506134	-1.65435372380261	1.78424626565990
F	15.40084305639091	-3.29923788131565	2.25826233770380
F	18.40944830005705	0.17904098312750	1.12348695841460
F	16.32280687322267	1.83681822154427	0.62952538004493
F	7.09076960056951	5.88888746839008	2.80599454814137
F	4.81314525928846	7.30628384972980	3.00576207093292
F	3.82988727862900	8.65146620019108	0.82921880235530
F	5.16026599427392	8.55428164942685	-1.55402020516941
F	7.44207546809361	7.10456381104247	-1.78372463330193
F	9.27699050086639	2.06309316533966	-4.72437370702440
F	8.13530653555741	0.42036097684892	-6.57077360840730
F	7.28747331014519	-2.07121161546861	-5.84212461810012
F	7.56602974794300	-2.92276978896066	-3.26102354166861
F	8.68951882494670	-1.27826086845302	-1.40217786779355
F	17.95963404254169	-2.39030675581137	1.93760673595128
C	9.31726710644784	3.77328572232243	3.85501168371592
C	10.27043926650453	3.13141555945014	4.33731394127462
C	8.00953955711933	2.47228726329372	2.50298370280818
C	11.29289991998808	2.21908236522599	4.72764539798958
C	8.79579095681954	1.74063858900094	1.73866153783689
C	11.54590919642716	1.05121781686855	3.96156045437953
C	12.12002370340783	2.48401309592402	5.85057861080678
C	13.16620215164154	1.61819372705302	6.18903288780884
C	13.39518935858678	0.47375078478237	5.40809056297239
F	14.40556398394757	-0.34503818997967	5.71944378352671
C	12.58316248639572	0.17893158736569	4.30421411218623
C	6.69473950805676	2.90711455963893	2.80809790338587
C	6.23363391828339	3.14900717749971	4.13528974837253
C	5.85070606319946	3.29223048693584	1.71972558923434
C	5.00176656728009	3.76778711026579	4.36051327342364
C	4.62428631614393	3.91972809301456	1.94923485062560
C	4.21146184767555	4.17051637315530	3.26896969035475
H	9.46150395004067	7.80563666283946	2.13480254002600
H	11.82122508477113	7.18277274125950	3.31480071275430
H	7.08397686339525	2.46687845535366	-2.91483502187578
H	6.45458548499082	4.73211022790622	-1.60452904061363

H	13.61134752891769	-1.02648061673161	-1.05434869186785
H	11.47610832271507	-0.88759718439888	-2.70942576285658
H	14.35604431102509	4.87841861875078	3.70166619932034
H	15.40338972653010	2.49006941061021	2.99630765373707
H	8.74870288297929	4.67264155084607	3.65135972967647
H	8.47322335889838	0.85060025486124	1.16761386751137
H	10.91691761634697	0.83379567731121	3.08989928233155
H	11.93869840135290	3.38746801188214	6.44563618626702
H	13.81755848315923	1.81939640941224	7.04892873675492
H	12.78018007488905	-0.71425893034955	3.70347699633560
H	6.87365197963545	2.86833015681088	4.98036561078742
H	6.19899047551204	3.11875331007582	0.69400818823231
H	4.64407822737900	3.96895627013671	5.37836279731675
H	3.97993107000591	4.23039676389583	1.11699799210742
F	3.04895753317603	4.79182362473491	3.48852838237168

TS(9-rad + *p*-fluorophenylacetylene → **10-rad**)

E = -10210.5737105828 a.u.

C	-3.53352553546666	1.72188528310542	2.27140669615832
C	-2.99074291279081	1.83735072070650	3.56035339912884
C	-1.58431171288086	1.60441247158923	3.44666923934293
N	-1.31645643926170	1.31751604251920	2.12468830313502
C	-2.45073924092100	1.43421723260340	1.36406257314552
C	0.29383594266897	1.75491626655157	-2.53191281910163
C	-1.05167002416111	1.61085544227118	-2.23544419964125
C	-1.18593391518112	1.49945159307418	-0.80255607565176
N	0.10367189124511	1.55206212709525	-0.26715270861057
C	1.02407755586966	1.72838954602290	-1.28747014489840
C	-2.39639751878599	1.43634193960247	-0.05917309927728
C	4.68292387579288	2.25758319470292	1.76597720707459
C	4.46679903911201	2.30374546387781	0.39920671612946
C	3.08823414194841	1.96069365621244	0.15855540178547
N	2.49658671747364	1.72606769777466	1.39124614898051
C	3.43295910353385	1.92873660308592	2.40847266671212
C	2.42091670017508	1.91440353315472	-1.09553501901245
C	-0.06285080459709	2.15370908873225	5.57599985989840
C	1.33697944773895	2.19657327988758	5.63993877838914
C	1.84723960106746	1.80937047563602	4.34820459340654
N	0.76500947834728	1.48124583892524	3.57654590440272
C	-0.40995055418038	1.71829985059576	4.25918717238372
C	3.15780844530710	1.92829039782958	3.80398123955280
Sn	0.63448697408690	0.83950237880345	1.61483242087975
C	-3.69122932540272	1.47160908968614	-0.78439120895696
C	3.24358763570443	2.18729670087581	-2.30638043095329

C	4.26470598902494	2.13178330418997	4.77024987841552
C	-4.06298550236769	2.57187851660291	-1.58243400807413
C	-5.30270085985809	2.60729830581295	-2.24007378322997
C	-6.19642959306252	1.53202635832975	-2.09632186636611
C	-5.85068495618954	0.42871038864189	-1.29692813637510
C	-4.60592909649154	0.40801577795090	-0.64888569051092
C	4.25412785113845	1.30472437439120	-2.72929526327033
C	5.04005460634698	1.57479021393778	-3.86017726806400
C	4.81519172158865	2.75222614583007	-4.59321870904886
C	3.81289053630174	3.65116620451727	-4.19083181519324
C	3.04082663188468	3.36476675580777	-3.05417341103115
C	5.08437339224851	3.27844288886803	4.75470298038430
C	6.13553873193082	3.44069685769294	5.67131404088213
C	6.37470967418369	2.45153288628817	6.63993082585147
C	5.55541664858384	1.31145421154119	6.69284545385764
C	4.50693265805273	1.16946813097193	5.77286462898236
F	3.74377912890902	0.07559028579989	5.86132684373170
F	5.78230630877973	0.36935924966856	7.60804253624748
F	6.89825987087819	4.53210877229315	5.63803182693228
F	4.86457534151383	4.25506349230354	3.87405862935172
F	-4.29049243668288	-0.65239207057619	0.09554276646522
F	-6.70155946356814	-0.58806809735706	-1.16690179597015
F	-7.37235353953719	1.55955409809271	-2.71640998531558
F	-5.64247225085649	3.65512898881467	-2.98956565665612
F	-3.24492674457209	3.61540514914905	-1.71161313866972
F	2.10992956774696	4.24087196227100	-2.68071125630218
F	3.60830931110103	4.76975712211775	-4.88424608220021
F	5.55204702637614	3.01701321034958	-5.66809547305485
F	5.98973275865266	0.72363497491334	-4.24584805047532
F	4.48612113383022	0.16980658817940	-2.06073415325641
F	7.36934953682507	2.59763545288021	7.50991223082759
C	1.88608130874702	-3.75604126374366	2.90330407299409
C	1.08076928897287	-3.34105232057799	3.75359831163351
C	2.14583497255008	-1.73794629868065	1.70297626222292
C	0.16493540787624	-2.51749710429896	4.45608141067345
C	0.94549901434862	-1.26880963336612	1.41662133360426
C	-1.13738390244079	-2.29017583621457	3.92845787769447
C	0.54382583848542	-1.83642273071969	5.64499128636174
C	-0.34487894967251	-0.96396159176887	6.27843648067644
C	-1.61732253370144	-0.75117000620704	5.72639047327171
F	-2.44702644424206	0.12482810586965	6.31163818527554
C	-2.02287184158187	-1.40891559463362	4.55657495290233
C	3.50513367183322	-1.38598717345296	1.90569108479432
C	4.08673421549523	-1.33731254947200	3.20670448252906

C	4.33288124593965	-1.09476121873893	0.78182614667961
C	5.42637221199944	-0.98219190168818	3.37493417575715
C	5.67276223157157	-0.74475198906324	0.95393048552051
C	6.21314664861174	-0.68445896660875	2.24908021251689
H	-4.57486718225366	1.88853429309797	1.98205697754773
H	-3.52512437767120	2.07851824366955	4.48229856209748
H	0.73819308148884	1.88404692982989	-3.52214278520104
H	-1.88163309810938	1.59805630487116	-2.94629713528690
H	5.62410193295850	2.45466895902675	2.28216600559259
H	5.19306456096522	2.56671038901425	-0.37362262722377
H	-0.76954206388517	2.41679644034628	6.36676490256771
H	1.94407203723156	2.53676187859350	6.48380980368537
H	2.56389185488976	-4.41546328184002	2.37942035495647
H	0.06895071528053	-1.91095684233781	1.24924929580277
H	-1.44291731180999	-2.81111735262426	3.01343429421779
H	1.54822040912733	-1.98648204591499	6.05791060394878
H	-0.05515928642132	-0.42209800357231	7.18569339616355
H	-3.01563646888838	-1.20429156661609	4.13922601678062
H	3.46216762554972	-1.55821980471514	4.07621260057866
H	3.89293103772237	-1.10888574459237	-0.21990765139397
H	5.87606332682544	-0.92540054641234	4.37399339613396
H	6.29810984296284	-0.48341197366374	0.09200204753878
F	7.49033943009065	-0.31690961799080	2.41576499311800

(TPFC)Sn-CH=C(C_6H_4F)-CH=C(C_6H_4F)·, **10-rad**

E = -10210.62922541 a.u.

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C	-2.82847668268550	1.66787333489848	3.56438885085656
C	-1.41341712292719	1.49714634760265	3.43343428525200
N	-1.14196673848956	1.26877515608723	2.10202342680843
C	-2.28713075204682	1.34683612462846	1.35571552015909
C	0.40755664489809	1.82099824790179	-2.55777419226337
C	-0.92866631622062	1.61835482582608	-2.25179115822719
C	-1.04563456332393	1.47273800554615	-0.82052312846316
N	0.24661108221391	1.55981391007047	-0.29578605805873
C	1.14794552463256	1.79919077252140	-1.32002185243816
C	-2.24653573733616	1.36083855669842	-0.06768881789125
C	4.78169112360397	2.50143909747859	1.72471919132093
C	4.55090385413251	2.56833752863859	0.35997868032459
C	3.19558226292880	2.14544963206896	0.12124134831768
N	2.62927088159049	1.84699049770593	1.35187110388511
C	3.56258778627269	2.07699030441902	2.36865011248446
C	2.53248524086598	2.05295820104208	-1.13120427612604
C	0.10153910412177	2.01534767001358	5.57835739864689

C	1.49891020759507	2.11448263958027	5.63452342934526
C	2.01181299661815	1.81025682219514	4.32048267484712
N	0.93804796548295	1.47715653157485	3.54312274587266
C	-0.23930400942893	1.62738705022705	4.24407304504368
C	3.30856576383968	2.00810945875173	3.76648172197887
Sn	0.82725050828367	0.84730851124707	1.57303513145459
C	-3.54786769341489	1.35268419333499	-0.78260362470115
C	3.35196685929482	2.31472311725206	-2.34597196010498
C	4.42426718567848	2.20099652652561	4.72502264445143
C	-3.96936293595896	2.44709299061171	-1.56373782186926
C	-5.21299903301898	2.43992177266788	-2.21483892545087
C	-6.06110675499792	1.32705789376818	-2.08048850717711
C	-5.66605351875242	0.22889786992026	-1.29692151850949
C	-4.41785168070991	0.25108677370862	-0.65542624149009
C	4.32553468068800	1.39272569691566	-2.76949117942029
C	5.11249435340315	1.62766199758215	-3.90711899663737
C	4.91857624855985	2.80744158821070	-4.64682769813424
C	3.94864532093180	3.74218800559320	-4.24534863038392
C	3.17506269822082	3.48974087687676	-3.10081532261694
C	5.20299319886871	3.37475342144291	4.76324652892741
C	6.26733584927831	3.51789950909859	5.66773948829978
C	6.56051838477105	2.47984361850850	6.56812135297605
C	5.78100157332124	1.31083993338466	6.56779186939765
C	4.71808510985619	1.18788634408287	5.66159102867738
F	3.98468532204910	0.07304427291164	5.70332623319663
F	6.05737003985951	0.32536243046591	7.42175606640968
F	6.99315813377869	4.63468922815509	5.68562039273839
F	4.93109611570129	4.39323886959458	3.94672369574130
F	-4.05575597148322	-0.80471611208076	0.07439861665607
F	-6.47382134355825	-0.82375409172870	-1.17638217116780
F	-7.24029736014290	1.31359974024288	-2.69480573979466
F	-5.59877479510130	3.48215885712151	-2.94979880847399
F	-3.19529056548426	3.52502405067834	-1.68350445843276
F	2.26781676043134	4.39037322200829	-2.72976032497520
F	3.77454465188093	4.85964569256072	-4.94882209316224
F	5.65460847743656	3.04018935351328	-5.72956285514033
F	6.02858684450900	0.74285799691145	-4.29673021469353
F	4.51367248765756	0.25450797523180	-2.09106870007403
F	7.56821724615136	2.60715517829954	7.42596667890149
C	1.57377192583674	-3.32619279262789	2.77803659718203
C	0.64160186966647	-3.35784773670750	3.72790213924986
C	1.85191688839630	-2.01616300115302	2.11030477827922
C	-0.25083053707114	-2.54605087632791	4.45583777259503
C	0.82867493893328	-1.26584647161620	1.61577822503972

C	-1.60160999253664	-2.33687178042865	4.03413505327316
C	0.20225663717723	-1.86420904747525	5.62962204318435
C	-0.63819383151182	-0.98905625217256	6.31586278853564
C	-1.94552150477243	-0.77523938577117	5.84794964966641
F	-2.72595367412581	0.12102738171469	6.47089766365391
C	-2.43618247182241	-1.45242165762318	4.71895615918757
C	3.25760830013894	-1.54818196231578	2.10412973343841
C	4.06264357235692	-1.65078288398425	3.26025908358061
C	3.81439350963201	-0.98032259563704	0.93381316302692
C	5.36965532261727	-1.14534221877717	3.27294225098041
C	5.13134430030481	-0.50798724896502	0.92758115981435
C	5.88952139427863	-0.56962601940062	2.10536218487131
H	-4.42559509790572	1.68899196062591	1.99927226577645
H	-3.36348427039640	1.85218944743326	4.49877116556183
H	0.83747937041143	1.99503050320062	-3.54749446456050
H	-1.76500884138413	1.59360955860970	-2.95470737965296
H	5.71576619649554	2.73905852383789	2.23662682092009
H	5.25235650507427	2.89144678981245	-0.41318203144910
H	-0.60970923750142	2.22244692162000	6.38191885462816
H	2.09934660953825	2.44041696415103	6.48861277308588
H	2.20894502909426	-4.19464270040923	2.53544056017945
H	-0.18029753561827	-1.70467348375235	1.59241827673230
H	-1.96912668818917	-2.85670945243403	3.14121483110480
H	1.23624428973965	-2.00728591262196	5.96385324291147
H	-0.28508622347806	-0.44173507821173	7.19722838351651
H	-3.45646044453135	-1.25122977914790	4.37289626905437
H	3.63938418483330	-2.09236017352998	4.17004266182251
H	3.21412015760761	-0.92248588317105	0.01687684604516
H	5.98671620602537	-1.18123368330867	4.17890788168531
H	5.56551723054215	-0.07539248173544	0.02205180851302
F	7.12818927875470	-0.06178318326600	2.11477896354003

TS(10-rad + *p*-fluorophenylacetylene → **11-rad-cis**)

E = -10618.5751120999 a.u.

C	11.09473198680102	3.68096633282521	-2.94117126520817
C	11.91081543769403	3.69014337062894	-1.79888605001408
C	11.46048999121111	2.62911497701243	-0.95118063144657
N	10.37701235807228	2.04334892608069	-1.56885356582395
C	10.15319701940576	2.59798956825483	-2.79803012451045
C	7.40875086936098	-1.16334932979933	-3.89595565441192
C	7.76932396882475	0.04535363249370	-4.46655988545394
C	8.66967980310032	0.72085627689339	-3.56200147260259
N	8.84392788251723	-0.11843380107682	-2.46043060377146
C	8.08647231155540	-1.26788900890051	-2.62503118012488

C	9.26078672419417	2.00172786279342	-3.73643253238365
C	9.67444502738659	-3.20098292621854	1.47626412685452
C	8.81260081145445	-3.54561792336997	0.44462632265314
C	8.76043665477013	-2.43402139420768	-0.47324659917020
N	9.59568908797704	-1.44761669286847	0.02126865318353
C	10.18196345584049	-1.87467747085923	1.21315596729392
C	8.01948274533165	-2.33434123690375	-1.68434169163462
C	12.96240853842366	1.97614609652891	1.17408343060920
C	12.82027998316339	0.85817105843181	2.01079027185994
C	11.66520299925767	0.12025671672668	1.56679725099645
N	11.12818449084672	0.82218904044044	0.52172593885906
C	11.88979813214173	1.93458312734644	0.22953529661441
C	11.14713773281576	-1.14710458912528	1.96366154510501
Sn	9.39264648673940	0.53482217328126	-0.55606668791730
C	8.93532807637807	2.78457993898002	-4.95232811058621
C	7.03740652042713	-3.41608931310442	-1.96776023806968
C	11.67666970744500	-1.71978125699147	3.22557164177777
C	9.22254801291244	2.31150948687587	-6.24813467435092
C	8.90746192365770	3.06923074605571	-7.38726417800923
C	8.30085046844856	4.32820875629324	-7.23927286034881
C	8.01230419469038	4.82526280678405	-5.95664055844588
C	8.33708832237219	4.05541926660977	-4.83053040138478
C	5.88604903843847	-3.53755576920421	-1.16846140849110
C	4.89803261582640	-4.49073605539083	-1.44669355311110
C	5.06208588856923	-5.36150818629159	-2.53653753912814
C	6.21357743609430	-5.27212835937863	-3.33804180883261
C	7.18771516407330	-4.30091643057295	-3.05110413091078
C	12.40825277158397	-2.92271188159026	3.25459541338159
C	12.92402779253108	-3.43132430853151	4.45717551705468
C	12.71449737543214	-2.72810989618630	5.65587544400518
C	11.99127943373048	-1.52249880197719	5.65028061604579
C	11.48059958065885	-1.03147746326348	4.43992012013626
F	10.77941451059251	0.10718232911609	4.46072801947148
F	11.78923666904194	-0.86516933971576	6.79096008433461
F	13.61893273983019	-4.56761875434028	4.46917998836087
F	12.64065315322535	-3.59439493335342	2.12753698430084
F	8.04225582623128	4.54807428294996	-3.62169535206706
F	7.43232870768125	6.01703928601062	-5.82106652013299
F	7.99847671867730	5.05047175730908	-8.31440279057234
F	9.18871793262760	2.60967941368581	-8.60512514161676
F	9.81849014577270	1.13158826540949	-6.41551961422843
F	8.26614569099672	-4.22917349845681	-3.82896750969009
F	6.37104208468229	-6.10715922804021	-4.36329162084852
F	4.12952603964673	-6.26818619698619	-2.80996967946014

F	3.78581441117087	-4.54735640985460	-0.70690661506991
F	5.69248142282093	-2.69678076846083	-0.14717305557017
F	13.20103801631050	-3.20394554621820	6.79810090212208
C	6.04161402645470	3.11846070822729	0.70036966213583
C	5.12405937617551	2.93249146469826	-0.25176944622961
C	7.37139855407757	2.46557256037390	0.68785943004111
C	3.77810575891475	2.94871540678599	-0.67026379771917
C	7.52567686807148	1.22003968085979	0.15563355040875
C	3.30075888720168	3.82264608850901	-1.69482098824453
C	2.90349556353803	1.91155708546035	-0.21720779657949
C	1.63088857943475	1.74629169417997	-0.76811035893239
C	1.20370677659281	2.61103224332296	-1.78805126036578
F	0.00397533321364	2.42566108148265	-2.35216312574023
C	2.02413634513017	3.66128081293508	-2.23638519897496
C	8.53634564381052	3.15547442491274	1.30026536454597
C	9.28579575648662	2.49628410586623	2.30346565102993
C	8.95081299857756	4.43528978705971	0.87118051509740
C	10.42772335020635	3.08902678024498	2.85601011746674
C	10.11527631663732	5.01888575963128	1.38984333509486
C	10.84670664601840	4.33649852439962	2.37505432949410
F	11.97040432975956	4.88217021461359	2.85645701450895
C	6.21177573570579	2.31658083259143	-2.31708557964669
C	5.43691129810088	1.47770988333838	-2.80482309451660
C	4.35864026261654	0.56915142217677	-2.94693933883293
C	4.34597612694643	-0.62820236881049	-2.17830883944267
C	2.12511713885444	0.01552564186516	-3.78419926890027
C	3.23576926781454	0.86521366099405	-3.76443859378794
C	3.23735282008520	-1.47962882030655	-2.19836394979777
C	2.12889520540429	-1.14672341821088	-2.99488763312878
H	11.19372828054209	4.32151875848317	-3.82265533486894
H	12.75902179107032	4.35212524819844	-1.60401771901374
H	6.73148836797623	-1.91094129044810	-4.31534033227444
H	7.42276925377781	0.44247863533983	-5.42230036982470
H	9.95142897318697	-3.82338123100371	2.33078022713258
H	8.28714506315496	-4.49499753246752	0.31198215897009
H	13.74554314312435	2.73776659171733	1.22362334857337
H	13.49122305905141	0.55885851543497	2.82158844977038
H	5.81708633580284	3.78000223228159	1.56162310046742
H	6.64022406632521	0.68407555528633	-0.21458019265180
H	3.96358043208161	4.60934349098796	-2.07542396845244
H	3.26041629984647	1.21607649824119	0.55272625527659
H	0.96959534041299	0.93483857389491	-0.43974294170485
H	1.65497861681830	4.32490307379820	-3.02938866548268
H	8.96656001796746	1.50746049230362	2.65530631367167

H	8.38006274464382	4.95494131919104	0.08979534277050
H	11.01425658650366	2.57166238627738	3.62235925550446
H	10.47425092259422	5.99188738343753	1.03371103165704
H	7.07297105370573	2.96297725844203	-2.23044529907694
H	5.20285885858224	-0.86298627779484	-1.53847856520655
H	1.23816844141381	0.25103354283847	-4.38554293551725
H	3.23286658658171	1.78912050816241	-4.35391714980174
H	3.21084691337378	-2.39400836041061	-1.59428713148898
F	1.06028574416875	-1.95067459397206	-3.00239693703378

(TPFC)Sn-CH=C(C_6H_4F)-CH=C(C_6H_4F)-CH=C(C_6H_4F)·, **11-rad-cis**

E = -10618.6401717068 a.u.

C	10.35028404402577	3.56322482031454	-2.89799778101122
C	11.19793651913985	3.71823746245663	-1.78929506643573
C	10.97820540806211	2.59482908138687	-0.93048659953797
N	10.00637585666511	1.81802744288703	-1.51751675926607
C	9.63291190930840	2.32314326894278	-2.72885409628795
C	7.75862592251843	-1.93968461380487	-3.79376189270224
C	7.85933066051301	-0.69320111502161	-4.38774080403555
C	8.54063891753017	0.18878387599451	-3.46925175074134
N	8.85932287809754	-0.57323610740873	-2.34174875338505
C	8.36533721830271	-1.85720141718415	-2.48813644532808
C	8.82258052518171	1.57604476245147	-3.63493680025397
C	10.12352940567011	-3.34232794357518	1.72617807511351
C	9.32344324586115	-3.85772233742602	0.71631337305447
C	9.14744866115495	-2.82451692866330	-0.27481283168677
N	9.84131198369878	-1.70637105667415	0.16223910360764
C	10.45521408902089	-1.97874491924416	1.38739042463100
C	8.42010402016544	-2.87889349656716	-1.49698921985731
C	12.56102866642144	2.27397830155799	1.21243774961946
C	12.59702149074793	1.18209757073365	2.09399157394651
C	11.58672969983313	0.24469619068655	1.67328860277367
N	10.95584452119568	0.80346989843978	0.59510680220461
C	11.52276357449663	2.01612542811441	0.26366129187354
C	11.27720608734188	-1.07446437193775	2.11612723245161
Sn	9.27376128147207	0.19958684786080	-0.45196002698982
C	8.18483839811530	2.31991234826648	-4.74838130100417
C	7.54403998074990	-4.05010166236395	-1.76347317081992
C	11.86638424303797	-1.50000554274932	3.40893783320812
C	8.32745007230678	1.97257031253048	-6.10615915748918
C	7.64369517686973	2.66580619589777	-7.11750612451509
C	6.81239175594776	3.74771834225478	-6.78597350429914
C	6.66455933978452	4.12343827665583	-5.43983633645098
C	7.34976211312824	3.41782216438840	-4.44102143213781

C	6.15262321176574	-3.84759791748300	-1.86610903865747
C	5.28072449462254	-4.88920601415942	-2.20894652988212
C	5.79848463580708	-6.17854210345924	-2.42360423097391
C	7.17960254477086	-6.41144857449100	-2.30109461372276
C	8.04007200198897	-5.34801244231457	-1.97963475899128
C	12.75447000240464	-2.58901599333118	3.50573244165347
C	13.32561383899434	-2.95523372169928	4.73475560252582
C	13.01486723503272	-2.22116802786369	5.89215053282269
C	12.13493009657205	-1.12741383751377	5.81904539406951
C	11.57054191888465	-0.77764971354658	4.58365947957795
F	10.72246722621283	0.25501483981551	4.54221327595434
F	11.83830351959603	-0.44020002394124	6.92099600972964
F	14.16748734331181	-3.98428930523224	4.81031168894180
F	13.08416123687493	-3.28504331837737	2.41802671543976
F	7.15491500117769	3.78806579085561	-3.17361466621859
F	5.84842265334025	5.12739882792654	-5.11292715369745
F	6.15743450801270	4.40354079668444	-7.73926646345462
F	7.76853637623127	2.29609351528934	-8.39218640947716
F	9.12323224945972	0.96547006619137	-6.46584110694938
F	9.34897463696358	-5.58638182259303	-1.89941767038301
F	7.66362436838018	-7.63548478774115	-2.50425681095802
F	4.98192478345485	-7.17897062166134	-2.74055091319171
F	3.97210227634512	-4.66306487796142	-2.33383585681150
F	5.63209544652180	-2.63419325244379	-1.64388266451935
F	13.55341449328707	-2.56210386173660	7.05878374998653
C	5.71019387473679	2.55648878745322	-0.01255983592581
C	5.05815525541068	2.30967069920534	-1.20282948169068
C	6.97814991079710	1.94023679017930	0.37415710908479
C	3.80527731206528	3.03054147017530	-1.53175021286251
C	7.28901561654296	0.62376419219039	0.13567771506434
C	3.62305995791938	3.62704660005828	-2.80279614654137
C	2.77244631458001	3.15909779151385	-0.57559707348843
C	1.58898050978540	3.84944408850411	-0.87559022482769
C	1.43515516666819	4.42962569432299	-2.14388128168289
F	0.30936848524652	5.08912275872809	-2.43620236151107
C	2.45043675358820	4.32979758163779	-3.10819384920492
C	8.00988943765840	2.81189903805528	0.99263545829708
C	8.74031779289936	2.34486899509115	2.11256576564511
C	8.31110153063783	4.08714220647731	0.46496796880849
C	9.76298713968429	3.11514355623516	2.67836845314912
C	9.34957873858604	4.85351534832245	1.00900428660539
C	10.07126621558057	4.35703892829685	2.10647258197675
F	11.08376710271902	5.07642908113897	2.60519639981975
C	5.62125887775420	1.40793473766364	-2.21588947223626

C	4.99647415134702	0.90296255843875	-3.27015611339715
C	4.85613710147869	0.18393118691193	-4.44893063220765
C	4.53251198226717	-1.21677516815946	-4.45278921278425
C	5.06031898880883	0.09454080472989	-6.90476282349995
C	5.08619760452694	0.82037121392911	-5.71561178575076
C	4.49217717719676	-1.93185847887067	-5.64868326094293
C	4.76447378347731	-1.28255865294916	-6.86977468449154
H	10.29442390133091	4.21360364384558	-3.77618270333969
H	11.91645160755768	4.52549819255666	-1.62146755699106
H	7.32132611721644	-2.83811149403561	-4.23487375859273
H	7.50334852713643	-0.42379590869667	-5.38176997854341
H	10.46584100121128	-3.86906678100047	2.62022711453695
H	8.92114827755226	-4.87128077131240	0.65326727213339
H	13.20459178085048	3.15746601458120	1.23629728316029
H	13.29694616479492	1.03087760042721	2.92103699257811
H	5.33370484617166	3.37483790768270	0.62046248029963
H	6.51955853897350	-0.08392368406977	-0.20540601155638
H	4.43373368856019	3.59236712952946	-3.53925357473815
H	2.88949454163294	2.68461014603090	0.40754497872081
H	0.77632015709961	3.93719576670969	-0.14310616896610
H	2.31451084308939	4.81202559741387	-4.08431447458325
H	8.49328425747289	1.36587435038372	2.54253817629281
H	7.76819811050990	4.44372449014556	-0.42017007074192
H	10.34352343083333	2.74403742813736	3.53021456350557
H	9.62819338757856	5.82331497453945	0.57954638398918
H	6.68163155879238	1.13210528542865	-2.05449251637129
H	4.37589027659110	-1.73100991770483	-3.49903812445533
H	5.28055246463671	0.57545672936764	-7.86683101216462
H	5.32888564685816	1.88687458273825	-5.72499538913946
H	4.26392091607866	-3.00536654529273	-5.65493898507554
F	4.74264940912919	-1.98269324509864	-8.00772641642475

TS(10-rad + *p*-fluorophenylacetylene → **11-rad-trans**)

E = -10618.5752844969 a.u.

C	10.59347870792337	3.54177147768495	-3.15803459820177
C	11.50642342284169	3.62847204946317	-2.09489342943776
C	11.20219635061169	2.56187549581459	-1.19199769222653
N	10.11998816204081	1.88538618437272	-1.70894409732608
C	9.73978075245742	2.40563334055431	-2.91249552138237
C	7.21122910940108	-1.57980712587115	-3.69964202154579
C	7.40921195458533	-0.36030531469988	-4.32257039715177
C	8.31239768387659	0.42455376963578	-3.50976150163134
N	8.65961802638439	-0.37361097444721	-2.41730215317707
C	7.98349145867639	-1.57991164573687	-2.48112929671804

C	8.78113503973560	1.75139412889439	-3.74492617440907
C	9.88614328687995	-3.21124867161449	1.61928651921360
C	8.98805257196938	-3.65555663438552	0.65919480101117
C	8.84794621507340	-2.61172619688133	-0.32645826148526
N	9.66608036247966	-1.56221868300201	0.05941177538601
C	10.31928160573889	-1.88428142416416	1.24986717553495
C	8.02799551241473	-2.59919381892719	-1.48863850277494
C	12.84598121856016	2.11460416268480	0.88055490426533
C	12.80898191116796	1.04203091669952	1.78535333657719
C	11.68083383035573	0.21495751562524	1.43975667523309
N	11.05125410886826	0.82626607686834	0.38997220373885
C	11.73412412466441	1.95789161148432	-0.00457009973611
C	11.26385993614640	-1.05941685559062	1.92165568081946
Sn	9.28213003205969	0.37953312975828	-0.57472245869537
C	8.20231622811545	2.54581982831426	-4.85366997869165
C	7.04021624831736	-3.69927573585701	-1.65958771960063
C	11.87593774750907	-1.53059744726981	3.18777486981093
C	8.14702030265730	2.08948725274206	-6.18738348882059
C	7.48744863803999	2.81730984200593	-7.19195527582907
C	6.90276303601288	4.05552667603658	-6.88105233530083
C	6.98961843588742	4.56034163510432	-5.57469264435608
C	7.62655234158951	3.80783965459042	-4.58021314582698
C	5.66998074011001	-3.40585980954600	-1.52838644417630
C	4.68765944062210	-4.38020721537948	-1.75004616721370
C	5.07927403020941	-5.68800336352268	-2.08547663918626
C	6.44330051765120	-6.00911518138198	-2.19969391074903
C	7.41233276546397	-5.01344774232256	-1.98967549166020
C	12.67296401555117	-2.69012435797866	3.24861305652419
C	13.26514185868772	-3.10333390731170	4.45259765174027
C	13.06782869296328	-2.34607969305316	5.61998697279710
C	12.28013061554257	-1.18218711301630	5.58204194590922
C	11.69367108143195	-0.78621248676871	4.37102322715277
F	10.93264144210109	0.31330411740882	4.36238804169546
F	12.08995342060007	-0.47397921291043	6.69395413180577
F	14.02124940987536	-4.19928380185832	4.49392930626678
F	12.89493685742979	-3.41009629685354	2.14979299558888
F	7.63260429769514	4.30805227553560	-3.33851528865759
F	6.44093950880908	5.74297004845467	-5.28609855128670
F	6.26277061489159	4.75303050979509	-7.81917843057749
F	7.43452335642661	2.35177271623366	-8.43727276236297
F	8.73706376939820	0.94582678168801	-6.53550762938641
F	8.69953575081955	-5.33143641491858	-2.12039024415738
F	6.80565378941080	-7.25109525080086	-2.51730780138621
F	4.15790226316136	-6.62502962742146	-2.29141424249087

F	3.39290223011816	-4.07414810770156	-1.64551873712923
F	5.28266712551475	-2.17395144833984	-1.18703242165469
F	13.62618228662191	-2.73155952777373	6.76337438294196
C	5.80212944355009	2.88536994158786	0.45775201252017
C	4.88918511911046	2.57396976794006	-0.46654190718616
C	7.13206164568534	2.22014460979139	0.52014162356240
C	4.70373851093322	1.78688228555829	-1.62879975207248
C	7.35529298865541	0.94671325670277	0.09391818868111
C	3.96581466304473	0.56780950718024	-1.63336234431206
C	5.21380070031557	2.26866106908625	-2.87112241199271
C	5.01273110613771	1.56159082397737	-4.05369811067575
C	4.28883101840025	0.36198437752440	-4.02234961719976
F	4.11519566881209	-0.32330429184425	-5.16203291129055
C	3.77076504619895	-0.14512145163624	-2.82082263360553
C	8.28120042181969	3.01325200392794	1.03842406697280
C	9.06419550823971	2.49747752755173	2.09791768132816
C	8.66127929029239	4.23283090846731	0.43742326755811
C	10.20545711709764	3.17468109744364	2.54560423589001
C	9.81945792945074	4.89978678513650	0.85840417306268
C	10.58238019975494	4.36332604311138	1.90754009581472
F	11.70440593157595	4.98740283122338	2.28842185343428
C	3.23746393554231	4.47782555520219	-0.80615867823461
C	2.97240898371092	4.40182499997911	-2.01193703540372
C	2.83871503197766	4.05233921153960	-3.38292856223112
C	3.62356042289270	4.69230814975546	-4.38088295913697
C	1.96755474721012	2.52839078573350	-5.09072442037709
C	1.99106191284978	2.97850742889435	-3.76777601606526
C	3.59627073615995	4.24503328768894	-5.70535844164707
C	2.77740120087991	3.15775281575966	-6.05020935378514
H	10.57091421724809	4.17083860906269	-4.05300926780530
H	12.32024033054379	4.35085839736600	-1.98647364891365
H	6.59595308993992	-2.40654219855187	-4.06311701344350
H	6.97575183180210	-0.05552496725252	-5.27404137507364
H	10.22864400246549	-3.76227469681039	2.49871721197161
H	8.48933246965000	-4.62725426830101	0.62608108569284
H	13.58560152858865	2.91933794795961	0.84728907099680
H	13.53388746159358	0.82626433425047	2.57591314306049
H	5.62890451757114	3.70856043460981	1.17187852933149
H	6.52567269150950	0.31001308207156	-0.24728632761257
H	3.56790266621433	0.17657698565369	-0.68913316140191
H	5.78098197405509	3.20220966933291	-2.87453536560963
H	5.40038454027938	1.93408808099550	-5.00813044053587
H	3.24152755332433	-1.10550823385468	-2.82255760590351
H	8.77542548515293	1.54804804081663	2.56689759622074

H	8.08010628172224	4.62271187140132	-0.40859737828286
H	10.82638203541185	2.76193522340084	3.34806881256642
H	10.15636647131190	5.82127571978090	0.36873553731564
H	3.27022985338780	4.78263561914355	0.22947460997692
H	4.29223814487244	5.51215059670005	-4.09805454364782
H	1.34670947895944	1.67518186820211	-5.39159193464700
H	1.39105855488065	2.47153172799088	-3.00308010911696
H	4.21671144270296	4.71340292714010	-6.47777707118245
F	2.77599822236503	2.71004357146595	-7.30949764517775

(TPFC)Sn-CH=C(C_6H_4F)-CH=C(C_6H_4F)-CH=C(C_6H_4F)·, **11-rad-trans**

E = -10618.642746076 a.u.

C	3.35859009890719	8.62121821486308	2.80995492108583
C	1.97536324877606	8.73457752317640	2.60846776932168
C	1.43660723920158	7.40948612213792	2.63010200476737
N	2.48599232783043	6.53987382241382	2.83222448094107
C	3.66024959822402	7.22387265101467	2.99392993041390
C	5.56692125232164	3.31432477994558	4.95567557518766
C	5.98460674348552	4.57234585430612	4.54965180176539
C	4.86157051008655	5.23838792207022	3.93577430860300
N	3.77656781482334	4.37057042659242	4.01990956627670
C	4.17069906248427	3.18279224077552	4.61279169395773
C	4.84229141550782	6.56098504202516	3.42114799815764
C	-0.29549955939886	1.42587701865639	4.58171010241965
C	0.97182570518562	1.01033042951975	4.95599088466154
C	1.90156139491409	2.05320138007641	4.59439606336415
N	1.17426675486897	3.07528047813883	4.00925699754795
C	-0.17937567146659	2.73574624716206	3.98512171887832
C	3.30883280633336	2.06575822302154	4.81262055134325
C	-1.22339677646972	7.13943677208669	2.61959737152148
C	-1.96670103056978	5.97320608242165	2.85931680824497
C	-1.03598492003640	4.88576055006225	3.02066905916236
N	0.21737062162125	5.39956891757434	2.80169517260650
C	0.15596788457813	6.76647284010844	2.61908526380927
C	-1.23320427949953	3.56293188517498	3.51085924177106
Sn	2.08765536489213	4.50721450917745	2.80582448141849
C	6.13962452250689	7.27791063063029	3.30393343911922
C	3.93562367394072	0.77047652466699	5.18307310402811
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17-rad

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C	10.22761254187834	4.78642127166480	0.18501976503361
F	11.23840821703539	5.63124290570010	-0.05035269332958
C	4.43551674799868	0.82979256919565	0.78387070379135

C	5.15234540559050	0.90531902197705	-0.40002444240569
C	4.58408556107211	0.92481251195598	-1.74631462671765
C	5.12282984995881	1.81648671151112	-2.71536980629146
C	2.98337758921321	0.15566435273448	-3.43646064602299
C	3.49232262030027	0.11193690371008	-2.13254977457605
C	4.60090052878061	1.88887511816290	-4.00868677008501
C	3.55183223259343	1.03097966436154	-4.37219436085077
H	11.51413037550526	3.87621809816026	-3.85712897294940
H	12.52952796142418	3.01324319219484	-1.49531504636644
H	5.78520130941280	-0.46894335106383	-6.44291131245349
H	7.20526842367522	1.78359275169940	-6.80505883475030
H	6.81001934739242	-4.28170132038264	0.09532140071704
H	5.71477874276400	-4.25414162320373	-2.37591320350224
H	12.10605800877130	1.02557983230265	1.31512647850918
H	10.73921494130957	-0.99584500151594	2.47503014050672
H	6.54946960211206	2.53250504497177	2.89486161832207
H	6.87863204498280	0.04588318292084	0.30953722405007
H	3.47196306858398	-0.95447475913238	2.54740411979423
H	5.06209534358422	2.62711912549036	4.41550689740652
H	3.89810678395873	2.02403928191744	6.53831323432061
H	2.28129149262445	-1.52336476674945	4.67852998012854
H	9.11180806409054	2.60465068995005	2.56714450687029
H	7.44057154838250	3.55308236117754	-1.32714495215352
H	10.97103636345147	4.24934339611431	2.14316706746192
H	9.29467366603571	5.15711675341492	-1.73800912165029
H	3.34932807418088	0.65768847207319	0.76249521280355
H	5.93107083102660	2.50382964715341	-2.43266565568409
H	2.16579759979192	-0.50607951187825	-3.74762039215879
H	3.07337155335967	-0.60086365902520	-1.41239821991200
H	5.01147723213869	2.58451133835295	-4.74863297742010
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N	9.48576232734620	2.13118435313107	-2.01388615799585
C	9.78061716025621	2.86756373441556	-3.13459463574071
C	7.02254642125310	-0.10094961471024	-5.66373676398028
C	7.80806359419411	1.01639912720141	-5.88882769794438
C	8.37062986492736	1.43834936053355	-4.62782805168331
N	7.92758864197515	0.53102491137179	-3.66152186405824
C	7.14825126938648	-0.43855160941450	-4.26820137164378

C	9.27005121849922	2.52046758870999	-4.41818454042175
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C	7.22044420357506	-3.50804939871091	-1.94759296601535
C	7.26258614566271	-2.14396507489117	-2.41437862459960
N	7.99960832172013	-1.40346742856725	-1.50969508086695
C	8.43911229781955	-2.23478287561811	-0.48136113470326
C	6.75577204313243	-1.65454548332475	-3.64838479258451
C	11.07799499624286	1.28691355565364	1.29364781915633
C	10.73903871886693	-0.00260397511820	1.72460302737922
C	9.78412208610257	-0.54656659103939	0.78865963261133
N	9.51707838207402	0.44656965974346	-0.12179313944684
C	10.31893949202847	1.54616244560590	0.10859057463486
C	9.24527261749589	-1.85861344775440	0.62728124695268
Sn	7.99922882349349	0.70330035129889	-1.55817564215382
C	9.88609862959629	3.19398781938285	-5.59792094937933
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C	11.29276192101728	3.14121587867867	-5.75218351737082
C	11.94781766846419	3.76841798257412	-6.82289361593154
C	11.19885851533515	4.45093382896042	-7.79445821426082
C	9.80016264718624	4.48581482368433	-7.69106514895227
C	9.16330405302393	3.85511469092923	-6.61090771105774
C	4.49383028248636	-2.68314927092028	-3.83405542138557
C	3.55057500566109	-3.52298105197688	-4.44432879996806
C	3.91150407114262	-4.23762315843619	-5.60006941538842
C	5.20445192733222	-4.11172982755265	-6.13611065246323
C	6.13544426503553	-3.26713311993126	-5.50969821319122
C	10.84296598698554	-3.14885082127580	2.10800218901353
C	11.09705374657387	-4.00944375567651	3.18728720335901
C	10.02793589336833	-4.63570557430943	3.84934000394842
C	8.71381190670889	-4.41858106453472	3.40687244568516
C	8.48137767462822	-3.56708537036566	2.31803231661606
F	7.22187581587103	-3.43250610839543	1.90549816053350
F	7.69477731469827	-5.02157135828137	4.01625986944768
F	12.34833261446552	-4.24441914771585	3.58059052691134
F	11.89161319285307	-2.60749392210644	1.48529727890197
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F	9.08015190752501	5.11240771400250	-8.62077188980998
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F	12.04354718676419	2.45675905614044	-4.88977033453878
F	7.36207463165992	-3.17259342290444	-6.02343383407247
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F	2.32198998170524	-3.64643388021843	-3.94446942641396
F	4.13930734731747	-2.00409521136356	-2.74045476040620
F	10.26328959266023	-5.44597556282227	4.87691625489403
C	3.63403558191956	0.90514662648387	0.58499480561261
C	2.89730071875574	1.76817744954557	-0.26304148881270
C	4.90082720483077	0.40323472516462	0.26775974355807
C	1.53236865660193	2.21273825599558	0.06243757151693
C	5.48904286124946	0.72232592257407	-1.03740985987706
C	0.64533313645593	2.63358486915989	-0.96311146373733
C	1.04683188067032	2.23392512738390	1.39578098769427
C	-0.25572854879849	2.65216587338661	1.69289545091224
C	-1.10573033120616	3.06089054299935	0.65315890245809
F	-2.35021222374943	3.46070650065917	0.93280607162939
C	-0.65946640616398	3.05283123870503	-0.67776934085324
C	5.58488590612291	-0.35524513702116	1.34170911760910
C	4.89523503092055	-1.32515827391534	2.11210275706969
C	6.85034860062870	0.07546421731480	1.79809210198666
C	5.43910951943789	-1.82647025898803	3.29992318248609
C	7.40662814069031	-0.42060263093193	2.98545676849977
C	6.69565641923521	-1.37068345397278	3.72714259006309
F	7.23592161884548	-1.87976780438747	4.84379013286309
C	3.58851771196452	2.27087595295318	-1.39949298899041
C	4.85457485033626	1.82364352285567	-1.76518460567204
C	5.59499799473742	2.68559402291141	-2.72299352463242
C	6.59709852436036	3.51894752064274	-2.16626892759635
C	5.70643969016240	3.99753303214344	-4.77969690378503
C	5.16899129936376	2.93086565999691	-4.04344617398285
C	7.14725109926494	4.57745719073560	-2.89710861723748
C	6.68515701128779	4.81568002969457	-4.19846554023352
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H	11.84762682578619	4.13772128635541	-0.80680598579846
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H	7.98869745653788	1.49562974725877	-6.85194616582923
H	8.20142193258981	-4.46311940310433	-0.20473617295998
H	6.74622120457081	-4.33834828998374	-2.47724304649022
H	11.81492997797972	1.95552944725256	1.74809552929940
H	11.16693026237367	-0.52384745658818	2.58337449178169
H	3.20538862486448	0.60597004663362	1.54952707343280
H	5.69841682270798	-0.17648236567657	-1.64974695839385
H	0.97520320159818	2.60092641645282	-2.00940197662707
H	1.70844752934622	1.94821725244468	2.22312196544614
H	-0.62324983455345	2.67754012395691	2.72679763083369
H	-1.34500308482825	3.36611189220587	-1.47511118099336
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H	8.38762277712000	-0.07804365218499	3.33415243856120
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H	6.89453045187078	3.37248388646118	-1.11934421036203
H	5.38262271076234	4.19960617127089	-5.80658930788241
H	4.39079858858260	2.29594266718100	-4.48591811385205
H	7.91657716214221	5.22974705829285	-2.46640309521232
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C	12.00167281265125	2.76863273375383	-0.05054747830762
N	11.08448824995084	2.37541457302295	-0.99341492388290
C	11.13779834189033	3.18307445281766	-2.09694135867319
C	8.39573874986864	-0.01715338494038	-4.35439569149644
C	8.96915322155583	1.21365808051512	-4.62142921417756
C	9.64759566533172	1.65838007617257	-3.42514709767687
N	9.48756843965721	0.66075524496569	-2.46656517179303
C	8.70842277303711	-0.35905796889378	-2.98531570153717
C	10.39394920349384	2.85859640102703	-3.26433437186503
C	8.95074099082946	-2.91946998057935	1.07650599744354
C	8.39332120223475	-3.04625979831245	-0.18760414520673
C	8.71717541545181	-1.85154865942337	-0.92999936523344
N	9.50904466795437	-1.05749786916338	-0.11944683094199
C	9.65014698660315	-1.65555295391549	1.13250384992060
C	8.31233790504126	-1.51380213233303	-2.25347319657452
C	12.66054015487838	1.80989870300834	2.38603309138072
C	12.11414099532809	0.69217628395290	3.03645710710694
C	11.14855937229864	0.09820062031287	2.14266794421452
N	11.12860788545772	0.86784727670255	1.01111364014889
C	12.01497695935040	1.91391897466300	1.10746032046074
C	10.34663087014659	-1.07777734205236	2.23908461499240
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C	10.40669663638791	3.82021528756864	-4.39787823032157
C	7.31115040439212	-2.40784479748438	-2.89342709053065
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C	10.39619675239907	5.64766840931545	-6.55862014770208
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C	9.73161766749395	5.04971966477398	-4.30850093369578

C	6.01693390405601	-2.52635612718627	-2.35150065815005
C	5.03058564297356	-3.31891357708196	-2.95467524344222
C	5.33924698587398	-4.02160452006366	-4.13257223998959
C	6.62466239105513	-3.92592818411865	-4.69189548497361
C	7.59664303332707	-3.12532763640665	-4.07008501615495
C	10.30430229420374	-2.93293752700922	3.99750183132036
C	9.90177700576986	-3.39920695323643	5.25953166456599
C	9.27438065804306	-2.52130883368181	6.15901323412475
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C	9.46403481571293	-0.73437082378741	4.53121044911611
F	9.21080345693331	0.53402735413596	4.20274815851790
F	8.46490898187631	-0.34873675469878	6.64917577660489
F	10.11687404709783	-4.66640268185223	5.61100482871404
F	10.90977689687942	-3.79019556683805	3.17137495580405
F	9.05102083573357	5.36772804345824	-3.19394280478271
F	9.05859933546998	7.11920861326237	-5.26543841557789
F	10.39210346347846	6.50448770261368	-7.57495515312560
F	11.72494817771694	4.13356962559848	-7.80228917117546
F	11.73189940288623	2.37113619485508	-5.72877051225539
F	8.80959970073975	-3.05827394355898	-4.61671483247444
F	6.91347418013021	-4.59931878454482	-5.80371210090822
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F	3.81054593795733	-3.40662655838327	-2.42787329482175
F	5.68438805922192	-1.84855010370582	-1.24054194341137
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C	7.61143418532234	2.79115273863741	1.52656796485359
C	8.09297498542659	3.64873692338656	0.51139275327178
C	6.76942754809824	1.70108013118982	1.22111945095457
C	9.15468165495300	4.64195462974543	0.80643406617904
C	6.32737280964409	1.52729390726789	-0.10945623975494
C	9.33939888187522	5.78873240073349	-0.00089340687090
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F	12.24613093420388	7.32642468931493	1.55912977444909
C	10.37190614235890	6.69990762055382	0.25244280474753
C	6.48896444164192	0.68648839639350	2.26665205338598
C	6.24598583467132	1.05075638119552	3.61029831992466
C	6.59262152292481	-0.68737038353402	1.95120912172523
C	6.13046913661427	0.08054274109279	4.61406551977907
C	6.48414828200828	-1.66581874101293	2.94834535942677
C	6.27002490830882	-1.27291723331719	4.27600491771563
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C	6.31688447272524	2.17771937659705	-2.55426787530758
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C	6.14478816777029	2.95532847814097	-4.88099880664354
C	6.54502241743122	3.15422865359031	-3.55378386771587
C	5.26184079057655	0.77116185570913	-4.27475594096012
C	5.50129163185545	1.76161822068101	-5.23708870077353
H	12.44645552864310	4.98129459673831	-2.52319038366009
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H	8.92761355214624	1.76373484458873	-5.56433255782300
H	8.92506024621696	-3.66662290520593	1.87117616991529
H	7.83579242547143	-3.90243783910073	-0.57735406001410
H	13.44916846571205	2.46634482430755	2.76550545142166
H	12.39890266361878	0.30168033043132	4.01767540651224
H	7.97072604981067	2.90652358665682	2.55533264007428
H	5.64909699314463	0.69443629520959	-0.32384599711642
H	8.66001450351442	5.98155204201363	-0.83877672684317
H	9.97992950170233	3.53463674607100	2.49571951739268
H	11.79456604562535	5.17089794080705	2.96794478248168
H	10.51436823183571	7.58685948664806	-0.37718103358245
H	6.14426241317817	2.11172638646185	3.87477795821686
H	6.79484958502734	-0.99960126294749	0.91947182684242
H	5.95717678818221	0.35609117906449	5.66067902893571
H	6.59931416628404	-2.72983791129225	2.71032189595938
H	8.09761001530773	4.03281002659938	-1.61573340838023
H	5.51170589333851	0.17483833023139	-2.23309508760853
H	6.32822930998970	3.71897748101985	-5.64738606335736
H	7.04852731899739	4.09314546929532	-3.30472601937863
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15

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C	0.20423984905852	-0.19558964172132	1.43357782033625
C	0.47390575585082	1.05044450709120	0.82901389551010
C	-0.61430230539915	0.32825048728798	-2.76078982099383
C	-0.58063732396799	-2.58548168308455	1.34416996788958
C	1.00658716200972	2.18192066581409	1.62925373593884
C	1.95801753352617	3.07618624581085	1.08512316007086

C	2.46314116709014	4.14782788953440	1.83443561135873
C	2.01634194444022	4.33894389756755	3.15058671983459
C	-1.75694166234459	-0.25431957433976	-3.35746795023211
C	-2.03338369104673	-0.08538532150229	-4.72151048464964
C	-1.15904853909766	0.67545235895435	-5.51218532344836
C	0.28024106553966	-3.08268265413475	2.35058369359969
C	0.04146351201081	-4.31678103250143	2.97052585347057
C	-1.07309322052869	-5.07662289931197	2.58575391524167
C	-0.01699023055079	1.26563706898868	-4.95020027781535
C	0.24678168985142	1.09041710378653	-3.58454861362258
C	-1.94459886695638	-4.61250329032802	1.58898828601109
C	-1.69447766039954	-3.37646181521409	0.97722471060982
C	1.07322843358020	3.46964695059781	3.71893659269883
C	0.57661180799414	2.40145345208704	2.95909607382222
H	0.35039200428576	2.18583926971074	-1.01796216297750
H	-0.94036051433898	-1.93460288545697	-1.28055071660260
H	0.41235666158460	-0.32796971847948	2.50319277861508
H	2.33116472329642	2.91331450311887	0.06544577814924
H	3.20974046009373	4.83536332798939	1.41624769738960
F	2.49318778583467	5.36009448642155	3.87055578470738
H	-2.45924477729586	-0.82462979922019	-2.73520867091991
H	-2.92682759209456	-0.52574418967376	-5.18189097413163
F	-1.41645137294499	0.83972730085558	-6.81413741275616
H	1.17179409729096	-2.50699791507680	2.63349119770193
H	0.71629029794641	-4.70661787696913	3.74343374416736
F	-1.30686850370862	-6.25440576299384	3.17465393715095
H	0.65839316534126	1.84517510615118	-5.59250919590521
H	1.15587217865070	1.52992338876929	-3.15373903880764
H	-2.81552007659182	-5.22055353327588	1.31264716652717
H	-2.39592876740374	-3.00520944815374	0.21828906079233
H	0.72920409034344	3.64853095350028	4.74517252197265
H	-0.18451854316058	1.74191537720121	3.39743027990344

TS(11-rad-cis → 18-rad)

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C	9.81150360562778	2.92169430244057	-3.66495475576329
C	7.65955908527685	-1.19355255130057	-4.78488104912689
C	7.90624236163872	0.03218736804259	-5.38454229217845
C	8.59218906275232	0.86748942356281	-4.42583163114539
N	8.76378207114456	0.10840827163064	-3.27021423252533

C	8.20084994542509	-1.14433522275698	-3.44595061625912
C	9.06470703312342	2.19043765766325	-4.63149890017671
C	9.55591371996506	-2.61399570349602	0.91810531726922
C	8.91670025344838	-3.14400385501956	-0.19052751175079
C	8.79021007134087	-2.08811556937887	-1.16805807184566
N	9.38231354136506	-0.95775079105952	-0.63691858998962
C	9.83486169119826	-1.22066033831890	0.65099664266494
C	8.18333571799327	-2.16379154893052	-2.45223666442943
C	11.90704450837537	3.05010310002988	0.78238916834257
C	11.77069441793540	1.99254500047775	1.69787421929805
C	10.90490106574170	1.00270662609836	1.10805752493696
N	10.50573919262311	1.51202301243099	-0.10208549670253
C	11.10830905365954	2.72879272910401	-0.35612801400863
C	10.49728290923290	-0.30676237093638	1.51620073562083
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C	8.72207139603421	2.85741896521926	-5.91425678807825
C	7.40962801396661	-3.39916429444109	-2.74618964794481
C	10.63491551130013	-0.68077437742258	2.94471269867059
C	9.68762339688080	3.12588639328710	-6.89941697413706
C	9.33975532192169	3.76844302902934	-8.09894066572572
C	8.00591968577009	4.15336357380628	-8.31754349588759
C	7.02601720266952	3.89949116219866	-7.34162341525041
C	7.39282244107883	3.25644017961900	-6.14978561177136
C	6.25101422911409	-3.69324007736729	-2.00077619756231
C	5.49262374845802	-4.84552754817035	-2.25607304877791
C	5.89538114479227	-5.72626403860837	-3.27509703248048
C	7.04849348795247	-5.45303208133237	-4.03034559699031
C	7.79531808935549	-4.29545352545788	-3.75951954004750
C	11.85012697213596	-0.59667358834800	3.65092198280368
C	11.90631349394801	-0.78506448020615	5.04087148028859
C	10.73021241697370	-1.07118888142930	5.75468020113333
C	9.51010885582381	-1.19021605847269	5.07027030077427
C	9.47674213467682	-1.01771669087088	3.68058208004048
F	8.30458035872685	-1.16235949433599	3.06558358212194
F	8.39079201110294	-1.46127400741293	5.74003706560307
F	13.06886040930702	-0.69940778986789	5.68675613629353
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F	5.84668386069937	-2.86321696302922	-1.03517781547053
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C	4.75666170605076	0.47420984683868	0.08186750635336
C	3.67656380369937	1.30888554877250	0.01891985341901
C	6.13262258027877	1.04814589670368	0.18171890659245
C	2.27761897393882	0.84446007424107	-0.08924692369014
C	6.88118276734649	1.02685743880760	-0.99374231729426
C	1.29307582313808	1.61643354998559	-0.75106195556689
C	1.88309326712782	-0.40143198837425	0.45693397483084
C	0.56836887238912	-0.86770913553171	0.33605835112738
C	-0.38308156339082	-0.08033595518036	-0.33220812665795
F	-1.64109357383490	-0.51799209041268	-0.44497210936164
C	-0.02784642550187	1.16240301203372	-0.87604812009613
C	6.69828003268651	1.24150335011310	1.54654909099011
C	6.00079160726152	0.78056210780906	2.68998124222958
C	7.92283218088516	1.91372825281006	1.75371178135791
C	6.52158305409389	0.94673822254545	3.97830889796532
C	8.46423204558297	2.07611273725148	3.03623064970333
C	7.76393366353262	1.57823883349156	4.14073608008045
F	8.28887646238716	1.69839042731522	5.36956133390344
C	4.01257481473215	2.74954169443065	0.00515215892804
C	5.29168431125301	3.12096484115888	0.02443213788221
C	6.35914051669855	4.03107900846645	-0.06487686625049
C	6.92429390448208	4.64464015776950	1.09329991015762
C	8.20016122164044	4.95058303936397	-1.40180463929481
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C	8.10878296325671	5.38342015982994	1.00503801410478
C	8.74366801669503	5.52391519244209	-0.23948399405301
H	10.79059705206809	4.68922325063229	-4.67772355955218
H	11.99420779803318	5.06676785603206	-2.27646840679637
H	7.17341332320186	-2.05970993122201	-5.24001629236595
H	7.65930882327521	0.32667756698270	-6.40774425106520
H	9.84633026940183	-3.14513605856010	1.82838107113374
H	8.59748330191389	-4.17904820328011	-0.33831877713744
H	12.52675527598808	3.94321523313143	0.90167484513068
H	12.29550845985069	1.90052049995599	2.65022932234749
H	4.66268783918329	-0.61559733970599	-0.02191190836127
H	6.32229705768121	0.84455210631849	-1.92577639353887
H	1.56608834635697	2.57853588190446	-1.20279732800781
H	2.61827738467484	-1.00739018662672	1.00228845852044
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H	-0.78856950896964	1.75815372447211	-1.39612757677589

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18-rad

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N	10.07787938719613	2.35108006439460	-1.76510644221891
C	10.03798967055680	2.91768217181702	-3.00882909032864
C	7.59006445757170	-0.91906220178178	-4.50643837013882
C	7.96975127839698	0.31769426634842	-4.99988953049762
C	8.75358236646330	0.98469907747886	-3.98405870878997
N	8.89548263917534	0.08956745063544	-2.92212571821195
C	8.14643145456184	-1.04938655950149	-3.17761929175564
C	9.26001375869350	2.31051224737824	-4.05100777574369
C	9.09646133680003	-2.88366895034057	1.15781092884190
C	8.44329563687093	-3.27156050441416	-0.00438806485202
C	8.46120649796442	-2.15095242763236	-0.91141868349427
N	9.11518855048360	-1.11302245711813	-0.27578960931579
C	9.51372307598663	-1.51117890452657	0.99913619509144
C	7.91887009292196	-2.08707239878271	-2.22954410038545
C	11.84345824466085	2.58532225048684	1.54432489672545
C	11.63273772781186	1.45194408962620	2.34106004401618
C	10.69382776770113	0.60125637632362	1.65542273350363
N	10.32723015315177	1.26044721975278	0.50744019129489
C	11.02822551275635	2.44130446916274	0.37863194008652
C	10.24353854471029	-0.71979117296688	1.92528959569030
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C	8.73399405292712	3.21837119227203	-5.10386229499267
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C	9.06106575836638	5.03132659125482	-6.72251115727349
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C	6.82603380323951	4.54141324611435	-5.90205064342628

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C	4.70537153434686	-4.09690901792864	-2.03892040963753
C	4.85223395293841	-4.99595470165406	-3.10983111328426
C	6.01502876580042	-4.96455444092615	-3.89982116886018
C	7.02606584282973	-4.03034886544842	-3.61700801098599
C	11.87437963939088	-1.60180449339172	3.63833503851824
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C	11.10852427885597	-2.44553137510380	5.78285338605423
C	9.78004187437761	-2.16852511848489	5.41665152674056
C	9.51640372335119	-1.60878669513916	4.15795361955951
F	8.24660441923476	-1.33443570792284	3.83640337348017
F	8.78837404949962	-2.43158139896794	6.26559257737785
F	13.41497180667232	-2.43077526352730	5.24634111834904
F	12.88471971234879	-1.35478345664658	2.80547627864635
F	6.50914950662095	2.81822399378663	-4.34532609899158
F	5.52516813020243	4.82440671740217	-5.86075202717763
F	7.19716761349035	6.30775590585631	-7.43426939021141
F	9.87292241381981	5.75311768967864	-7.49408681004670
F	10.88652860513603	3.76102746919679	-5.95402415015748
F	8.11972201666493	-4.02241911842454	-4.37869353979959
F	6.15184673693463	-5.82487972530748	-4.90705095375202
F	3.89245841102365	-5.87682516236320	-3.37401971875243
F	3.59664024993420	-4.11884523197819	-1.29500515933704
F	5.55611101373553	-2.31377509954572	-0.76156809232983
F	11.37115057398826	-2.97637007602422	6.97316925543415
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C	3.81008349615954	1.43720152377669	-0.14797769417493
C	6.09168347311017	2.09824619190572	-0.02907499544357
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C	6.88486501058200	1.34596604715019	-1.06537569178036
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C	1.46434931950316	-1.54690928246909	-0.25450745180471
C	0.21627318459510	-0.91182499177926	-0.15548161110668
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C	7.00306592146699	2.51756076666766	1.12702997955132
C	7.40712871411329	1.54054048443812	2.06550508729110
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C	8.32031932662362	1.84157239260509	3.08437245759087
C	8.48854283767298	4.11533189734860	2.23938849619654
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C	3.95301703049628	2.74282377079413	-0.78857063805627
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C	5.80277790117763	4.29366527432590	-1.53715186371961
C	4.94861172676221	5.31719191014216	-2.02510783116255
C	7.65924640175543	5.37257448610602	-2.73644297253004
C	7.17077980982859	4.35836115225572	-1.90479546142646
C	5.42061418206918	6.32061786441255	-2.87941931115306
C	6.77728377748060	6.33721680216025	-3.23707110091576
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H	6.99876941410834	-1.67746988469584	-5.02505176707009
H	7.74167319189245	0.73240051340401	-5.98524056456407
H	9.30119723377387	-3.50268152648116	2.03536149666530
H	8.03194583572521	-4.25792115510968	-0.23403141070627
H	12.52452467276085	3.41509974904041	1.75188272904530
H	12.11632576713510	1.23021882946315	3.29504212800340
H	5.28023464849102	0.13405956777650	0.86106571497928
H	6.36158644214176	1.06283064331007	-1.99238146425309
H	1.23081426239039	2.34366986583703	0.04358313581340
H	3.60108599636268	-1.26960437376122	-0.35523247884004
H	1.51470941555271	-2.63731683452187	-0.36494491389142
H	-0.86039109483210	0.95566651361222	0.02406615532293
H	7.01425827430153	0.51833577437347	2.01680502737733
H	7.23871628470971	4.60315637444317	0.55167506307631
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H	8.92781711150667	5.11768452961471	2.31561621262920
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TS(18-rad → 19-rad)

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N	10.10200714168408	2.42762619810062	-1.77215364271903
C	10.06875407339400	3.05278737834147	-2.99169008359200
C	7.47909542204728	-0.61864032675009	-4.64582869625576
C	7.92309129999021	0.61329451782933	-5.09694253777777
C	8.66515280145637	1.24312634738341	-4.02806041888502
N	8.69866535764602	0.33740178784136	-2.96926534740910

C	7.95581773888581	-0.78670322480418	-3.29246487193574
C	9.26567140194287	2.53158213498619	-4.05592962216688
C	8.82133969858302	-2.85536700238117	0.95334115541176
C	8.12756275513362	-3.15281117298668	-0.21067787369017
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19-rad

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C	9.65393562445494	4.71400077801874	0.93729197455510
C	7.73796028554050	1.07225468391747	-0.03148997034001
C	10.02983529312700	5.75252496226693	0.05437784843677
C	10.34257672333775	4.61217455984856	2.16991127502050
C	11.36176937440274	5.50915785974225	2.51343726180523
C	11.71090609234164	6.52855065555000	1.61479241645081
F	12.69844544681208	7.37738495226580	1.92721580026276
C	11.04472806016518	6.65839075248689	0.38838135464056
C	5.63839903085483	1.69461698729009	1.34841780029320
C	4.90385439269837	2.73326947155579	1.97628680265788
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C	3.59144184879559	2.53212681147045	2.41558599888835
C	3.68705077120723	0.23076683866270	1.60970447664139
C	2.98576418438865	1.27873235221673	2.22532414392248
F	1.72944747909163	1.08311618540924	2.63782711976851
C	8.19609872519884	3.44010043375915	-0.75065094237730
C	7.36355064103635	2.26500474742758	-0.89775016082009
C	6.50096987369951	2.05540668359410	-2.07747746690706
C	5.79162626221256	0.84914118807756	-2.29458759604842
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C	6.43106197889844	3.04031010641107	-3.09544913382174
C	5.07863050777930	0.61609801355765	-3.47731652353749
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H	12.63136555721812	4.77159798183971	-2.40165566349225
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H	13.25040023150508	-0.11068736505504	3.79627200755352
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H	3.02054344702581	3.33567177066979	2.89767127282182
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TS(18-rad → 20-rad)

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C	7.65899944209308	0.32747516654233	-4.91370212485846
C	8.48907459312287	0.97376629978401	-3.92283060674631
N	8.65049454587520	0.06888723992199	-2.87200541972323
C	7.90024778527965	-1.06977444047132	-3.12002025977787
C	9.03921932238563	2.28204195928357	-4.00812041932729
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C	8.29963068873361	-2.20537879453142	-0.88620642568931
N	8.95680082049148	-1.16383325133571	-0.25493074712719
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C	7.73484626307241	-2.14132088522387	-2.19385028954422
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C	11.67937683467900	1.30330384610807	2.26482491134550
C	10.68259057677412	0.49163302581057	1.61524541700154
N	10.31428069303474	1.15512172014833	0.47256741630340
C	11.05767669848367	2.30594168081792	0.31275499950491
C	10.16373248766196	-0.79744875418883	1.91314619169326
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C	6.82173429694843	-3.24933938462875	-2.57684406172439
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F	11.08163660100840	-2.92630865615789	7.05370049770120
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C	6.83223028494724	1.47800486298827	-0.89548400695331
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F	-0.35372870740955	-1.99992114207751	-0.58573724434677
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C	7.15437736659849	2.78871786311497	1.23242150992567
C	7.61512276305888	1.81144382369511	2.14347586973963
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C	4.04338742371382	2.89946791221139	-0.69726155034863
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C	5.87048570231845	4.49405345959028	-1.42627626415117
C	5.02362972483739	5.49800291624824	-1.96263533414173
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C	5.50863063375387	6.46118471194486	-2.85519539632817
C	6.86736721247115	6.45071675667005	-3.20549647562493
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H	7.39498116217268	0.75688297354342	-5.88365206779830
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H	12.18668604511542	1.06347416708830	3.20233441722499
H	5.43769138716524	0.40644595483500	1.07641865482019
H	6.29294820523361	1.34765035029979	-1.84550958152137
H	1.25668205868793	2.20475322748990	-0.08918020351984
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H	2.18067120810865	-2.69691154084273	-0.57875590608004
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20-rad

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C	9.08604468955274	1.26152341386753	-4.72425874247045
C	9.68079377157456	1.81229910849322	-3.52914397638209
N	9.39940522972268	0.92322140182444	-2.49138561788135

C	8.67718911318925	-0.15487225319458	-2.97960221037312
C	10.46361369738013	2.98899636094594	-3.43635605872367
C	9.09072205483104	-2.62528621525224	1.10637584415777
C	8.43357903333099	-2.75554166148907	-0.10871253484502
C	8.70295293039081	-1.56624794590500	-0.88070470825006
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C	12.35250874002877	0.98765492106731	2.83526947914852
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N	11.04958685775417	1.29791967921078	1.01889849039929
C	11.96002004320057	2.33124386965171	1.03564224579637
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H	9.10747997885105	-3.35116747251118	1.92374530166726
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H	11.49013261662645	7.52496861178742	-0.34304100007876

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H	4.80363177697620	-0.19011626321392	-4.33423146317930
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TS(20-rad → 21-rad)

E = -10618.6795656085 a.u.

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21-rad

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