Electronic Supplementary Material (ESI) for Chemical Science.

Supporting information

Reversible Reduction Drives Anion Ejection and C_{60} Binding within a $Fe^{II}_4L_6$ Cage

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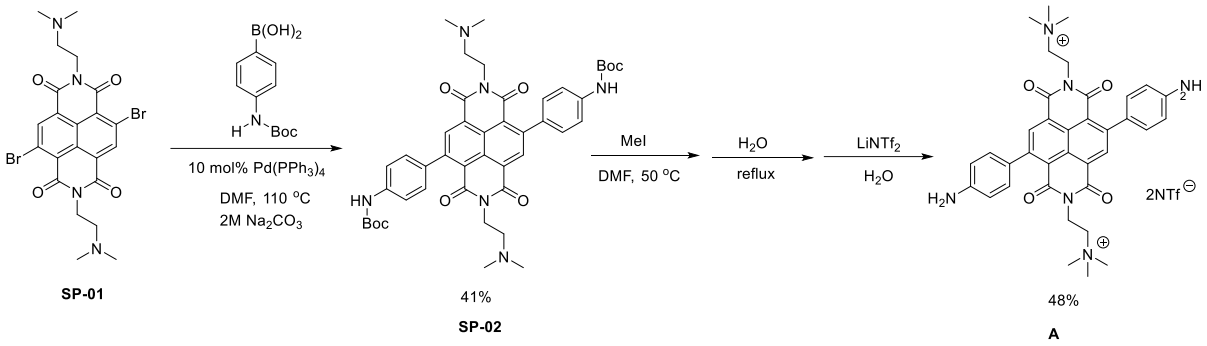
Contents

1. General Experimental Procedures

All the starting materials were purchased from commercial sources and used as received. Acetonitrile (99.9%, extra dry over molecular sieves) was bought from Acros and used as received. NMR solvents ($CDCl_3$, CD_3CN) were degassed (by 3 freeze-pump-thaw cycles) and dried over 3 Å molecular sieves. Air-sensitive compounds (For instance, reactions involving Cp_2Co) were handled under N_2 atmosphere using standard Schlenk and glovebox techniques. NMR spectra were recorded on a Bruker DRX-400, Bruker Avance 500 Cryo and Bruker 500 TCI-ATM Cryo. Chemical shifts (δ) for ^1H NMR spectra are reported in parts per million (ppm) and are reported relative to the solvent residual peak. DOSY experiments were performed on a Bruker DRX-400 spectrometer. ^1H and ^{13}C NMR spectra are referenced to the residual solvent peak for CD_3CN (^1H: 1.94 ppm for CHD_2CN, ^{13}C: 1.32 ppm for CD_3CN) and $CDCl_3$ (^1H: 7.26 ppm for $CHCl_3$, ^{13}C:77.16 ppm for $CDCl_3$). Low-resolution electrospray ionization mass spectra (ESI-MS) were obtained on a Micromass Quattro LC infused from a Harvard Syringe Pump at a rate of 10 μL per minute. High-resolution mass spectra were acquired using a Thermofisher LTQ Orbitrap XL.

2. Synthesis and characterization of subcomponent A



SP-01 was synthesized according to a literature procedure.[1]

SP-02: A mixture of Na_2CO_3 (318 mg) in H_2O (2 mL) and DMF (8 mL) was degassed by bubbling N_2 for 30 min. Then 4-(N-tert-butoxycarbonyl)aminophenylboronic acid (378 mg, 1.59 mmol, 2.94 equiv), **SP-01** (300 mg, 0.54 mmol, 1 equiv) and $Pd(PPh_3)_4$ (40 mg, 0.065 mmol, 0.12 equiv) were added to the mixture. The reaction mixture was then stirred at reflux in the dark under N_2 overnight. Then dichloromethane (100 mL) was added into the mixture for dilution, and the precipitate was removed by filtration, the organic layer was washed consecutively with water and brine before being dried over $MgSO_4$ and concentrated. The crude product was then purified by column chromatography flash silica gel, with DCM/Methanol (95 : 5) as eluent to afford the target product (**SP-02**, red solid, 170 mg, 41%).

^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 8.63 (s, 2H), 7.52 (d, J_{HH} = 8 Hz, 4H), 7.39 (d, J_{HH} = 8 Hz, 4H), 6.62 (s, 2H, N*H*), 4.24 (t, J_{HH} = 6.6 Hz, 4H), 2.57 (t, J_{HH} = 6.6 Hz, 4H), 2.28 (s, 18H) ppm.

A: SP-02 (170 mg, 0.22 mmol, 1.0 equiv) and MeI (0.1 mL, 1.6 mmol, 7.2 equiv) were mixed in dry DMF (4 mL) at room temperature in a schlenk tube. The mixture was then stirred at 50 °C in an oil bath overnight. Then all the volatile compounds were removed under high vacuum. 50 mL H_2O was added into the residue to obtain an orange solution. The solution was heated to reflux overnight resulting in a blue solution. An excess of $LiNTf_2$ (248 mg, 0.88 mmol, 4 equiv) was added into the solution, and a blue solid precipitated immediately. The blue solid was obtained as the target compound (**A**, 124 mg, 48% over three steps) after filtration and dried under high vacuum.

^{1}H NMR (500 MHz, CD_3CN, 298 K): δ = 8.53 (s, 2H, H^4), 7.29 (d, J_{HH} = 10 Hz, 4H, H^3), 6.76 (d, J_{HH} = 10 Hz, 4H, H^2), 4.49 (s, 4H, H^1), 4.44 (t, J_{HH} = 5 Hz, 4H, H^5), 3.53 (t, J_{HH} = 5 Hz, 4H, H^6), 3.15 (s, 18H, H^7) ppm.

^{13}C NMR (126 MHz, CD_3CN, 298 K): δ = 163.75, 163.74, 149.81, 148.49, 136.62, 131.29, 129.53, 128.29, 126.20, 125.58 (NTf_2^-, due to the C-F coupling), 123.03 (NTf_2^-), 122.19 (NTf_2^-), 119.64 (NTf_2^-, 114.94, 63.59, 59.29, 54.23 ppm.

HRMS (ESI) calcd. For 900.2278 $[C_{36}H_{40}N_6O_4]^{2+}$ $[C_2F_6NO_4S_2]^-$, Found 900.2163.

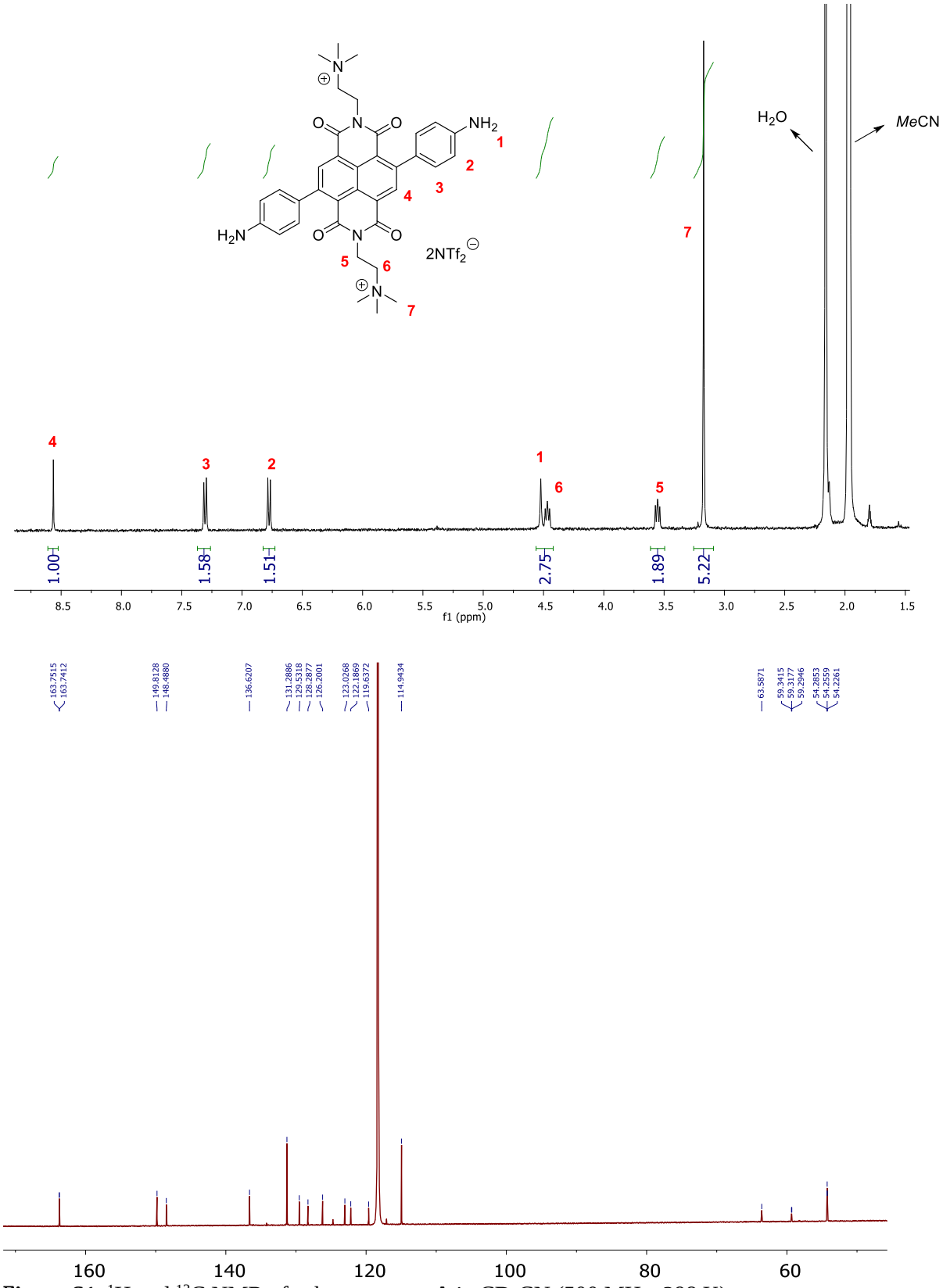
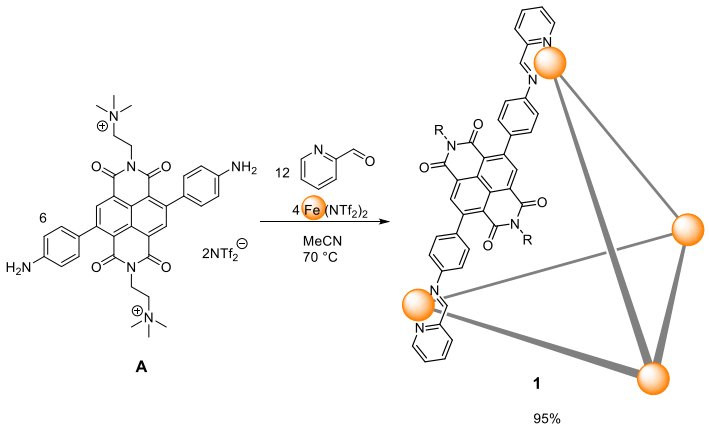


Figure S1. ^{1}H and ^{13}C NMR of subcomponent **A** in CD_3CN (500 MHz, 298 K).

3. Synthesis and characterization of cage 1.



Subcomponent **A** (50 mg, 0.042 mmol, 1 equiv), $Fe(NTf_2)_2$ (20 mg, 0.028 mmol, 0.69 equiv) and 2-formylpyridine (8.0 µL, 0.084 mmol, 2 equiv) were mixed in MeCN (3 mL) at room temperature. The solution was then stirred at 70 ºC in an oil bath overnight. The crude product was purified by filtration through Celite and precipitation with diethyl ether. The resulting dark purple crystalline solid was collected by centrifugation, washed with excess diethyl ether and dried under vacuum (71 mg, 95%).

^{1}H NMR (500 MHz, CD_3CN, 298 K): δ = 8.90 (s, 1H, H^5), 8.65 (d, J_{HH} = 10 Hz, 1H, H^4), 8.46 (t, J_{HH} = 10 Hz, 1H, H^3), 8.19 (s, 1H, H^8), 7.83 (t, J_{HH} = 5 Hz, 1H, H^2), 7.45 (m, 2H, $H^{1,7}$), 7.01 (br s, 1H, H^7), 6.07 (br s, 1H, H^6), 5.82 (br s, 1H, H^6), 4.51 (m,1H, H^9) 4.31 (m, 1H, H^9), 3.54 (m, 2H, H^{10}), 3.16 (s, 9H, H^{11}) ppm.

^{13}C NMR (126 MHz, CD_3CN, 298 K): δ = 175.07, 163.30, 163.20, 158.97, 150.86, 146.07, 141.51, 140.48, 135.73, 131.88, 130.58, 130.45, 129.91, 127.93, 126.27, 124.13, 123.52, 121.58, 63.47, 53.99, 35.09 ppm.

m/z (high resolution FT-ICR ESI-MS) calcd. For 1047.1176 $[\mathbf{1}(NTf_2)_{12}]^{8+}$, 1489.7954 $[\mathbf{1}(NTf_2)_{14}]^{6+}$, 1843.5365 $[\mathbf{1}(NTf_2)_{15}]^{5+}$, Found 1047.1142 $[\mathbf{1}(NTf_2)_{12}]^{8+}$, 1489.7901 $[\mathbf{1}(NTf_2)_{14}]^{6+}$, 1843.5306 $[\mathbf{1}(NTf_2)_{15}]^{5+}$.

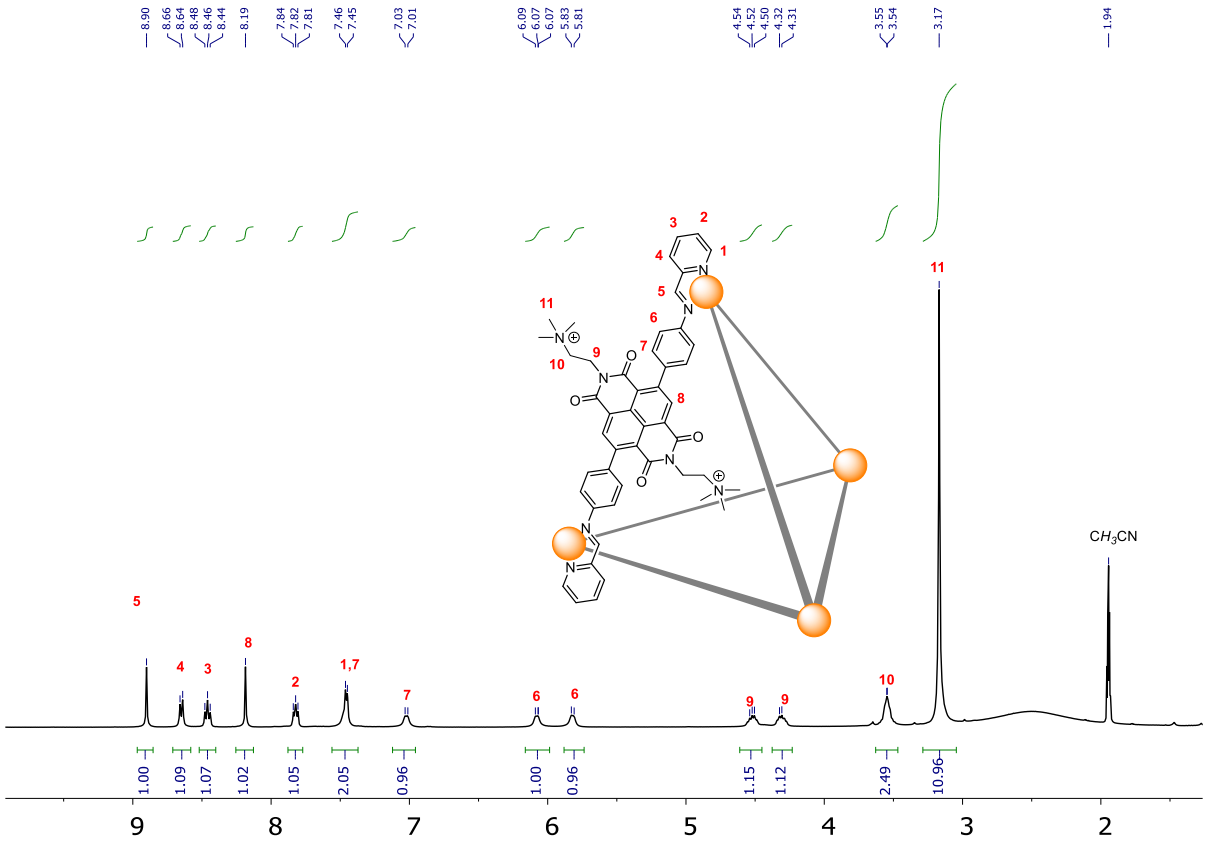


Figure S2. ^{1}H NMR (500 MHz, 298 K, CD_3CN) of **1** with assignments.

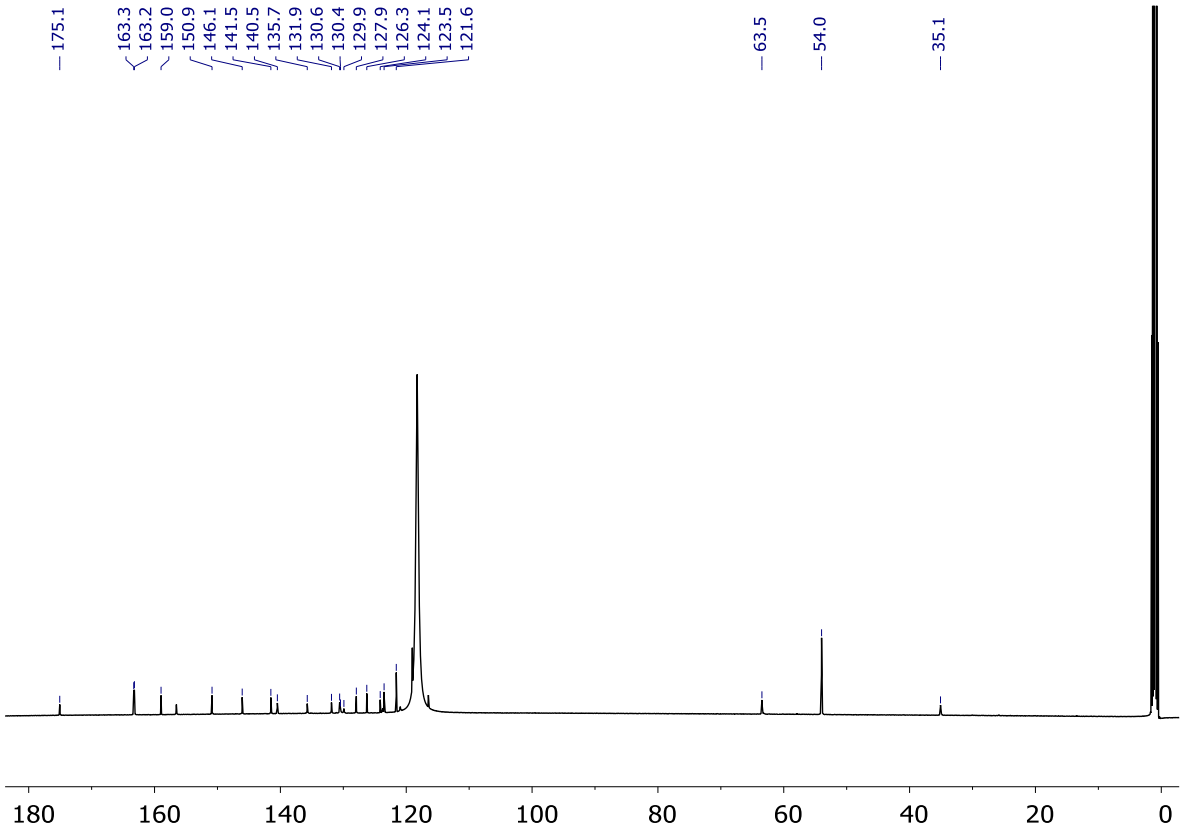


Figure S3. ^{13}C NMR (126 MHz, 298 K, CD_3CN) of **1**.

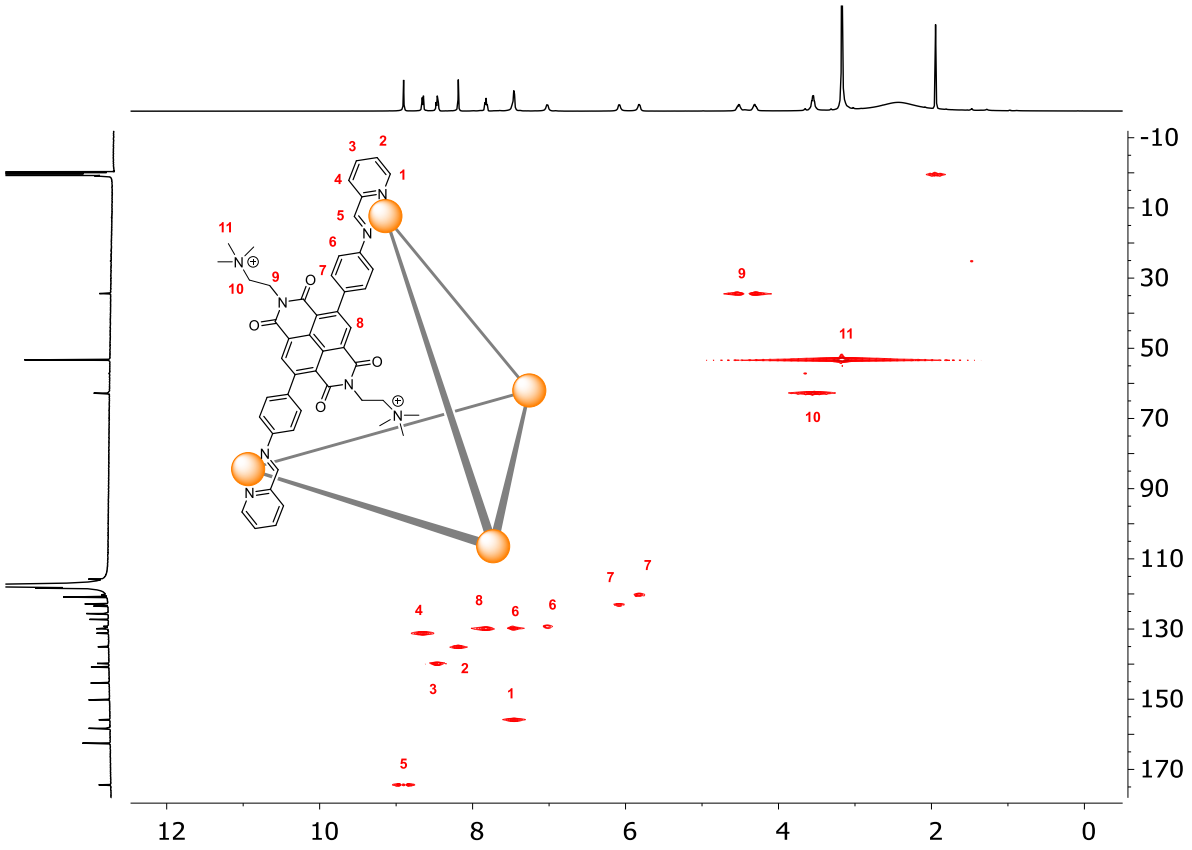


Figure S4. HSQC NMR of **1** (500 MHz, 298 K, CD_3CN).

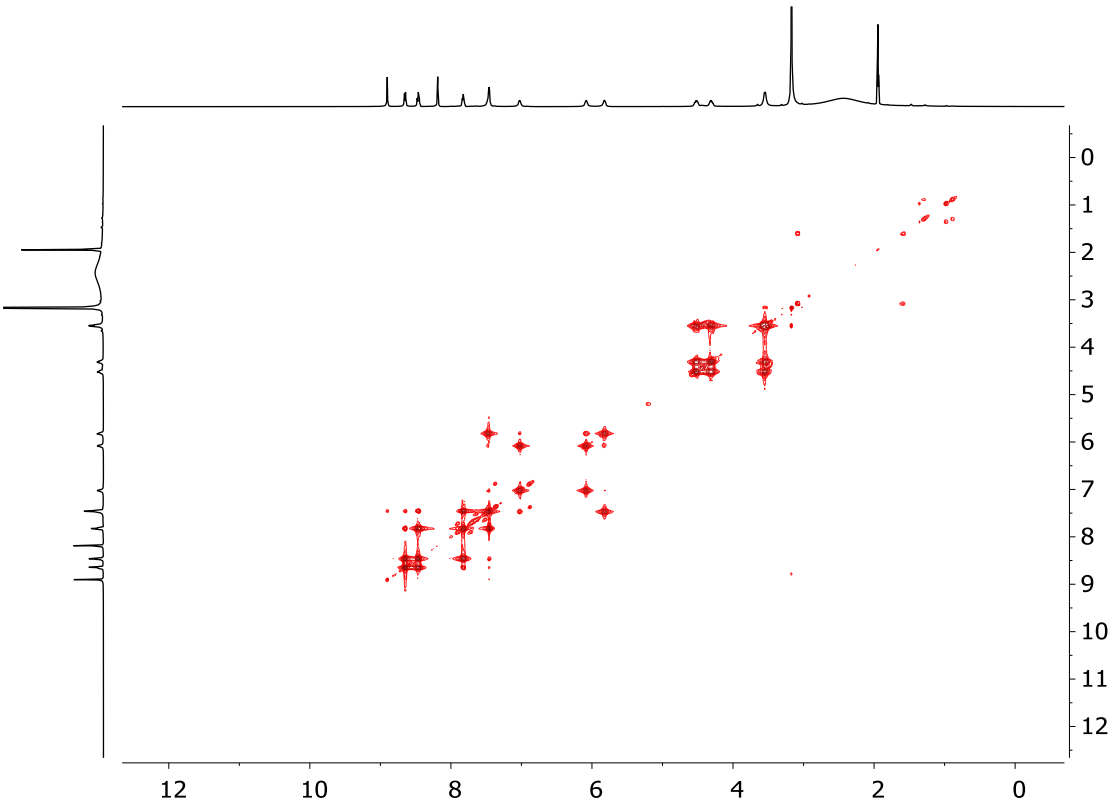


Figure S5. ^{1}H COSY NMR of cage **1** (500 MHz, 298 K, CD_3CN)

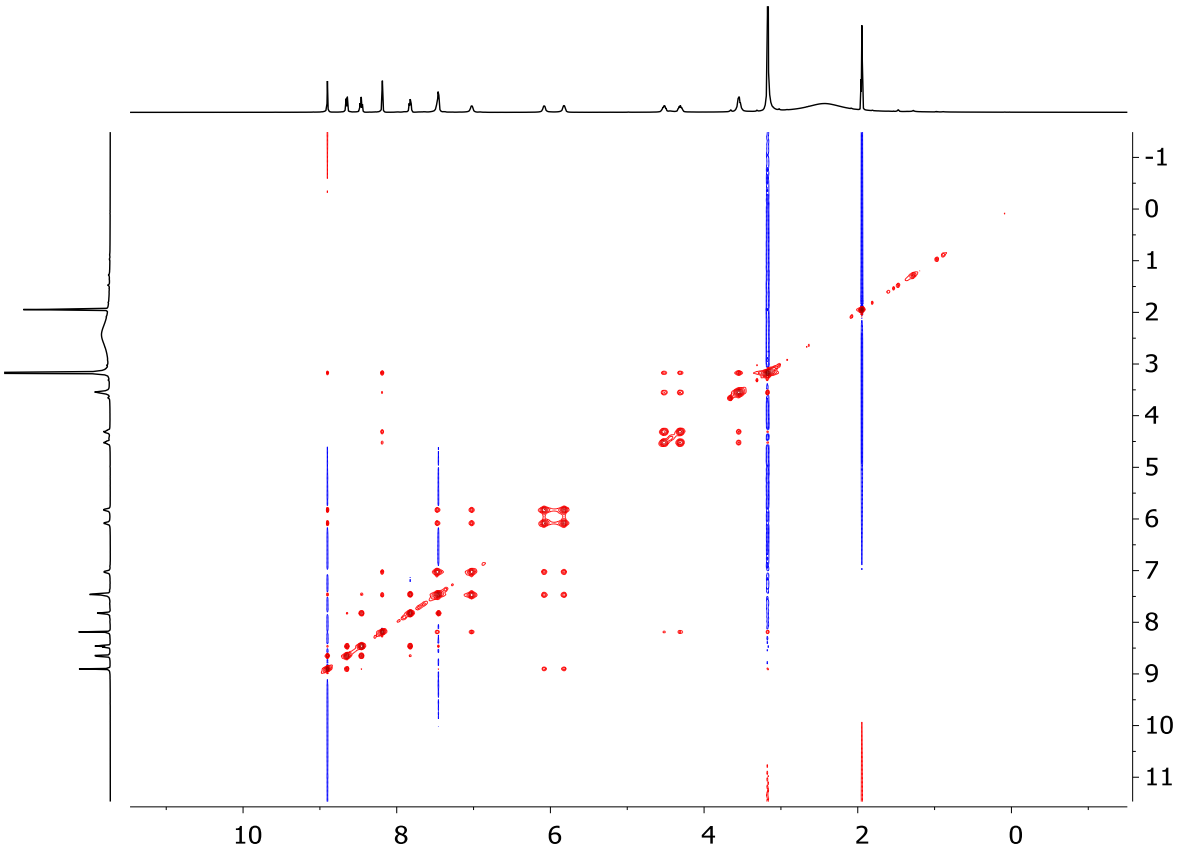


Figure S6. HMBC NMR of **1** (500 MHz, 298 K, CD_3CN).

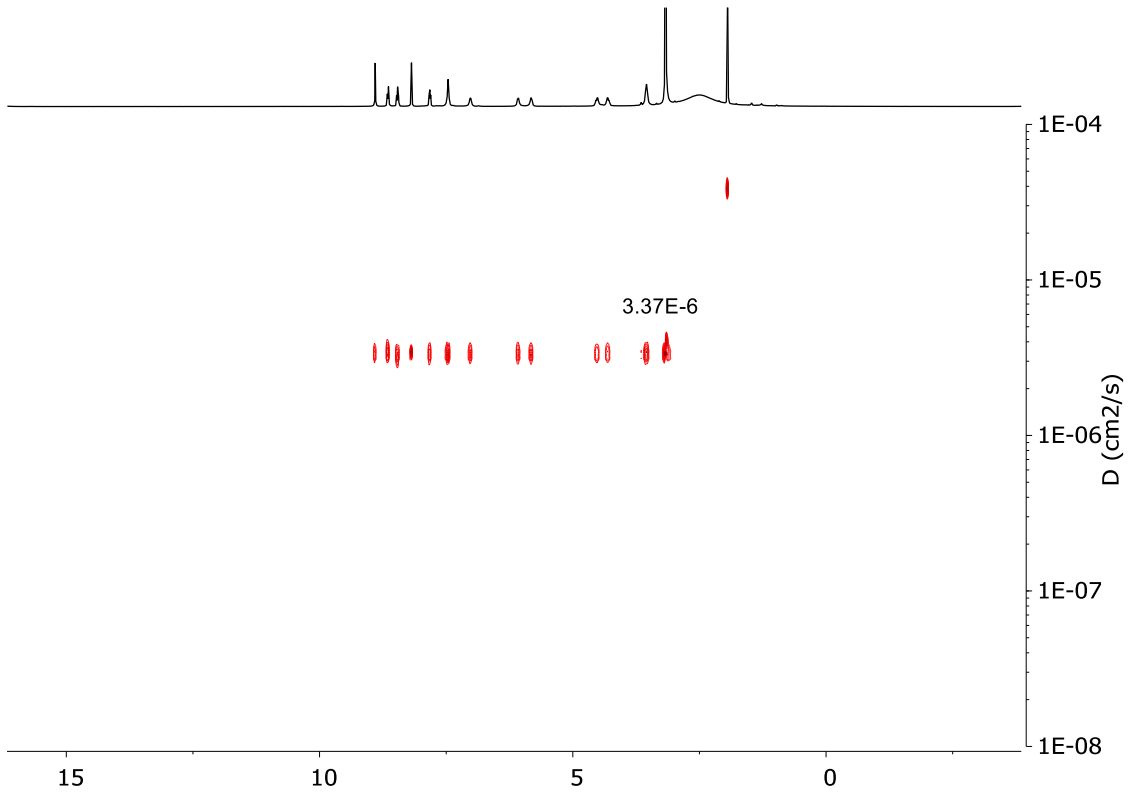


Figure S7. ^1H DOSY NMR of cage **1** (400 MHz, 298 K, CD_3CN). Vertical axis corresponds to diffusion coefficient D (in cm^2s^{-1}).

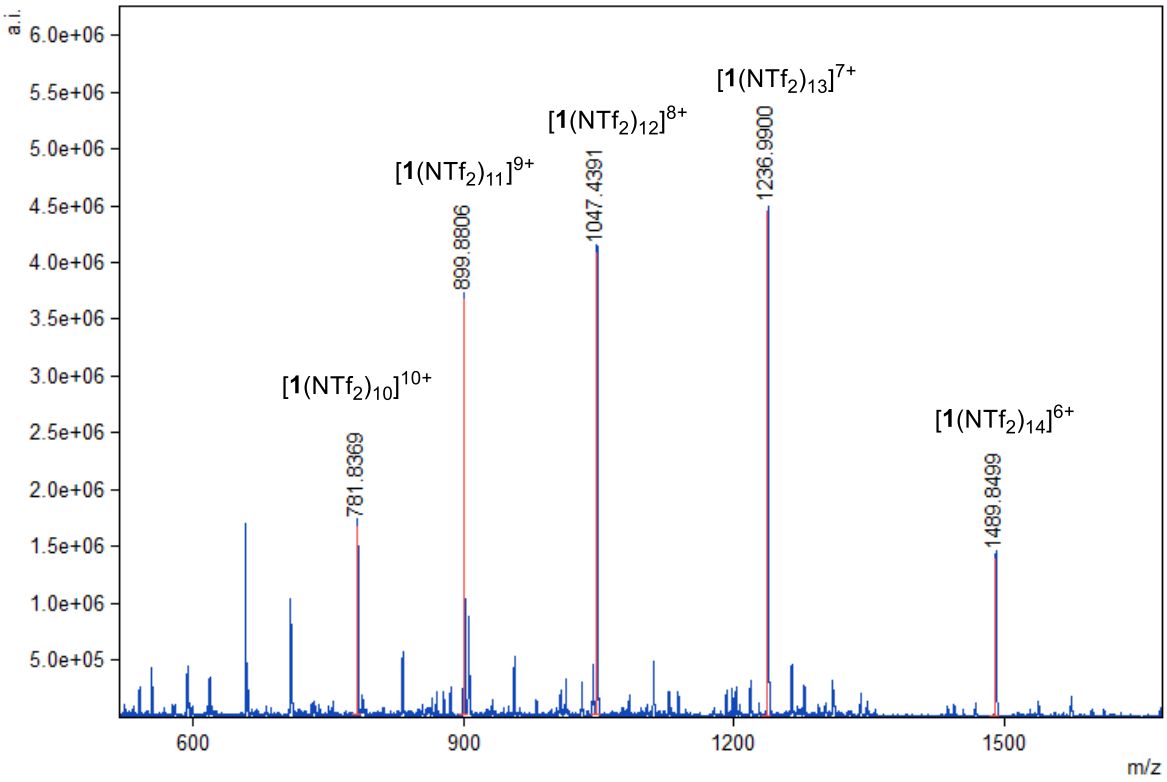


Figure S8. Low-resolution ESI-mass spectrum of **1**·20NTf_2

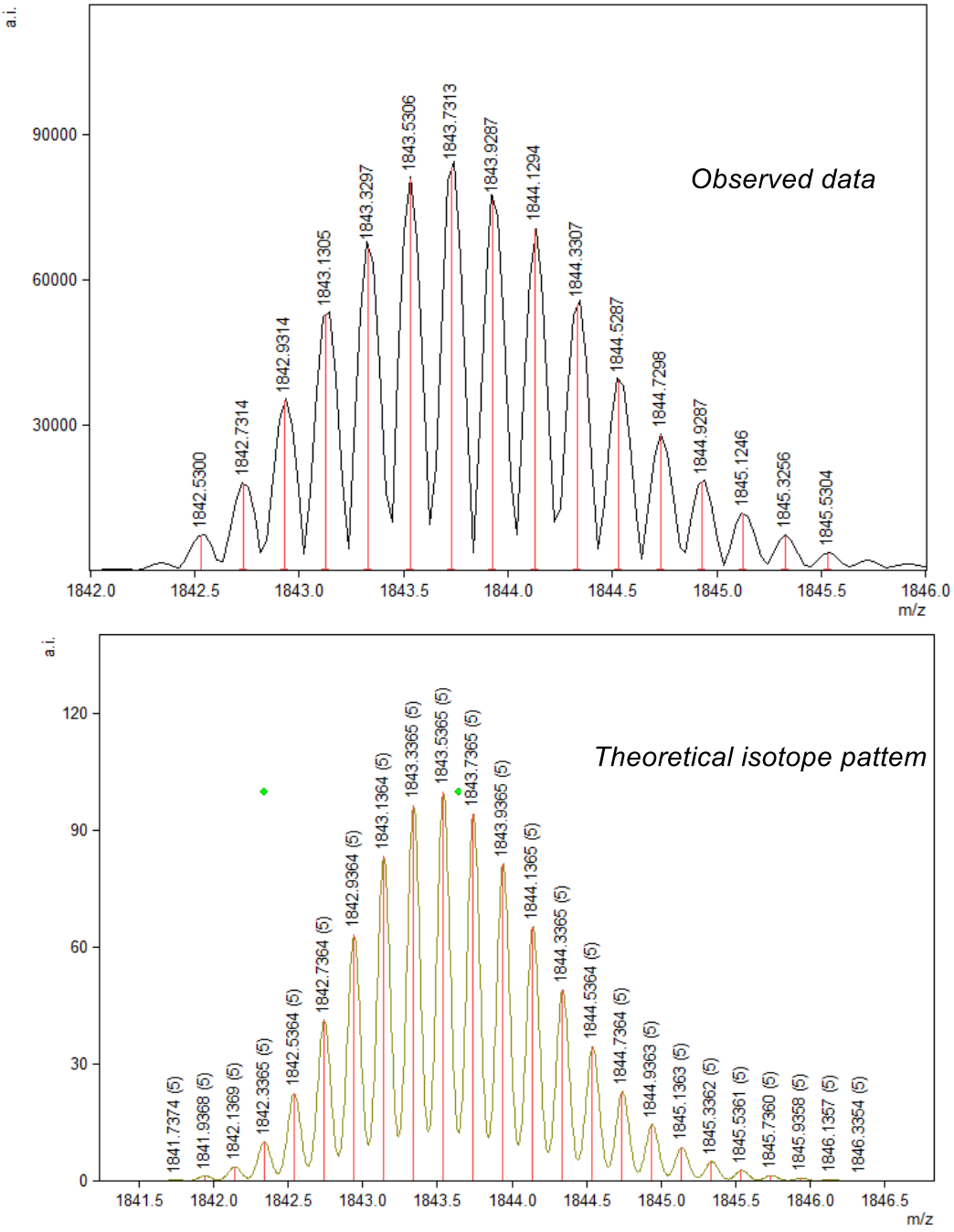


Figure S9. High-resolution ESI-mass spectrum of **1**·20NTf_2 showing the 5+ corresponding to the loss of 5 NTf_2^- anions.

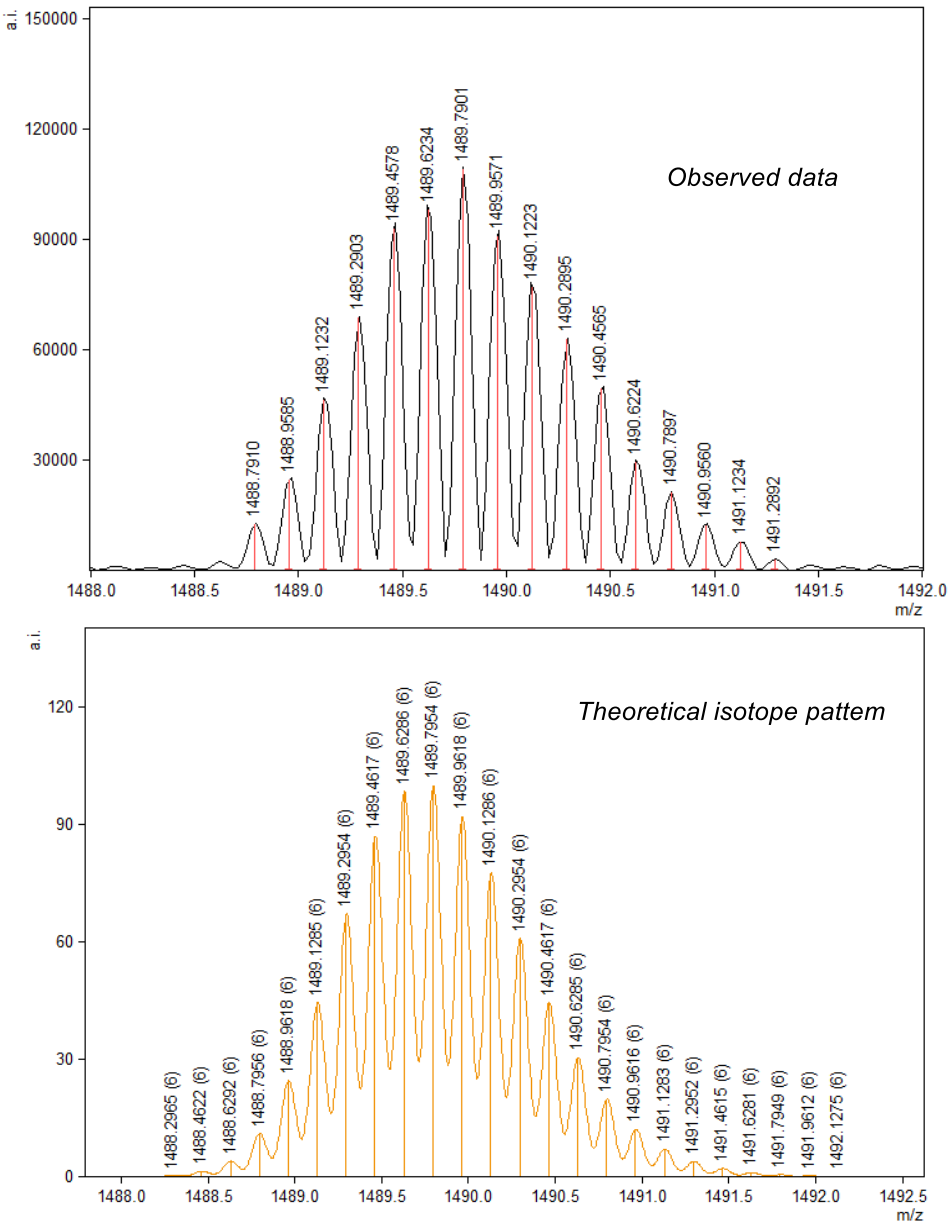


Figure S10. High-resolution ESI-mass spectrum of **1**·20NTf_2 showing the 6+ corresponding to the loss of 6 NTf_2^- anions.

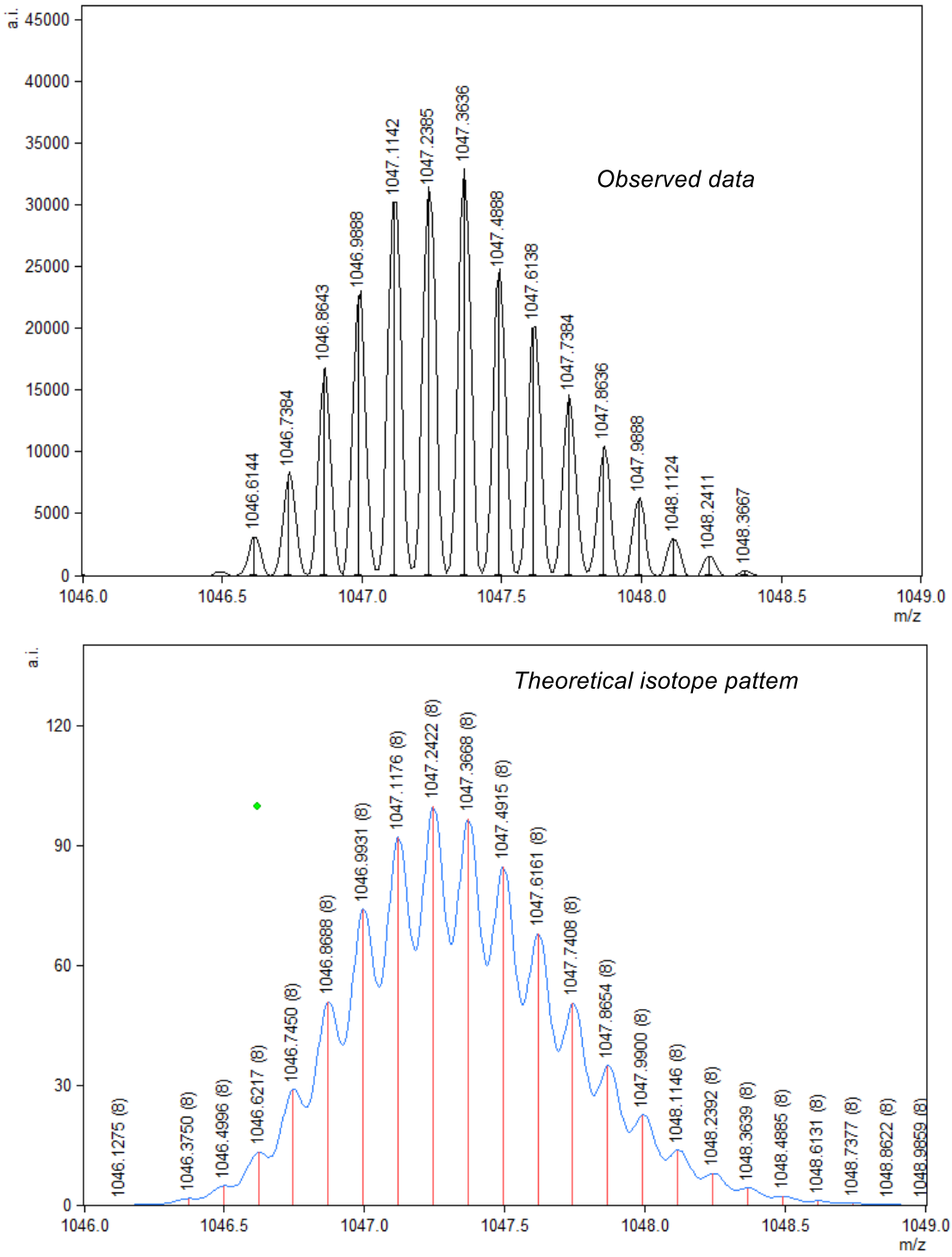


Figure S11. High-resolution ESI-mass spectrum of **1**·20NTf_2 showing the 8+ corresponding to the loss of 6 and 8 NTf_2^- anions.

4. Encapsulation of C_{60} within 1

Cage **1** (20 mg, 0.0019 mmol, 1 equiv) and C_{60} (5.4 mg, 0.0076 mmol, 4 equiv) were mixed in CD_3CN (0.5 mL). Cp_2Co (3.56 mg, 0.019 mmol, 10 equiv) was added into the mixture at room temperature. The reaction was kept at room temperature overnight. Then $AgNTf_2$ (11.1 mg, 0.029 mmol, 15 equiv) was added to the mixture, resulting in formation of $C_{60} \subset$ **1** which was characterized by NMR spectroscopy.

Figure S12-S17 are the data recorded 1 day after the addition of $AgNTf_2$.

Figure S18-S24 are the data recorded 10 days after the addition of $AgNTf_2$.

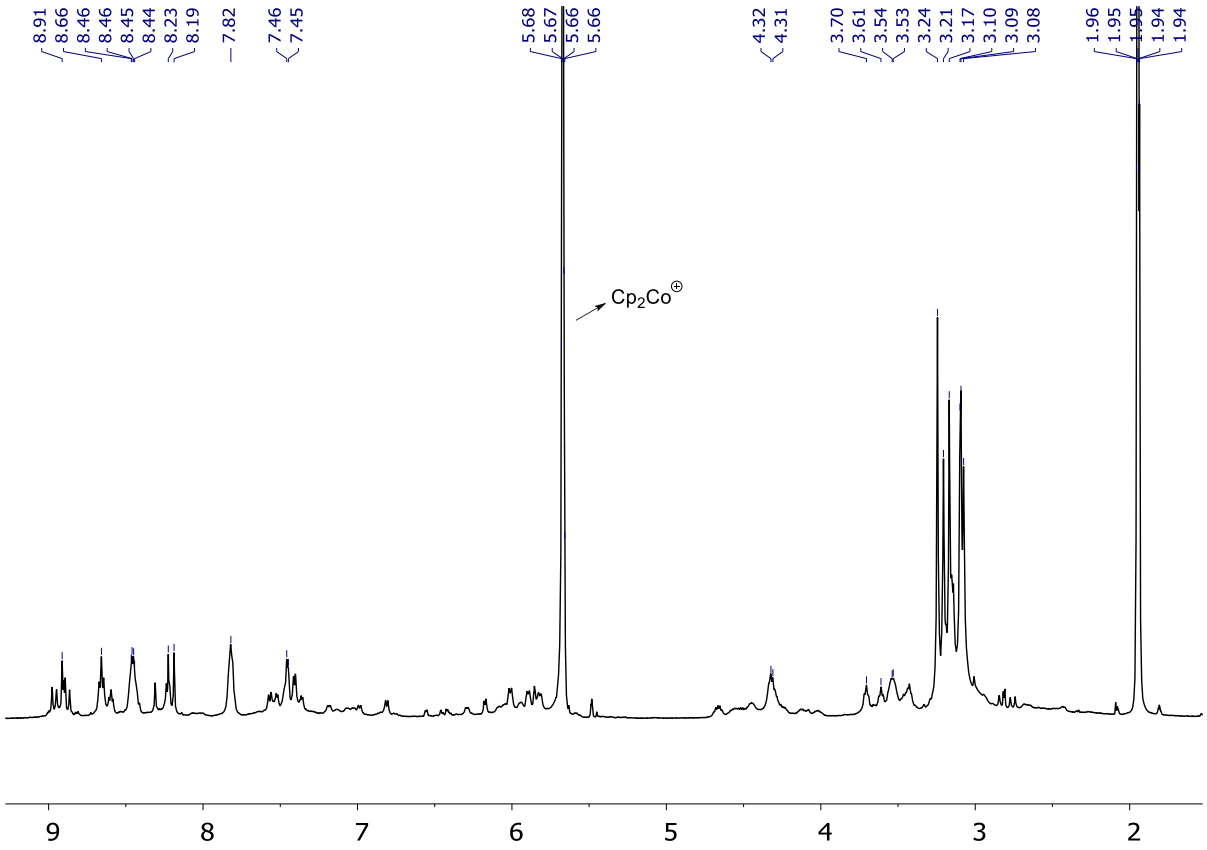


Figure S12.^{1}H NMR (500 MHz, 298 K, CD_3CN) of $C_{60}\subset$**1**. The sample was measured 1 day after the addition of $AgNTf_2$.

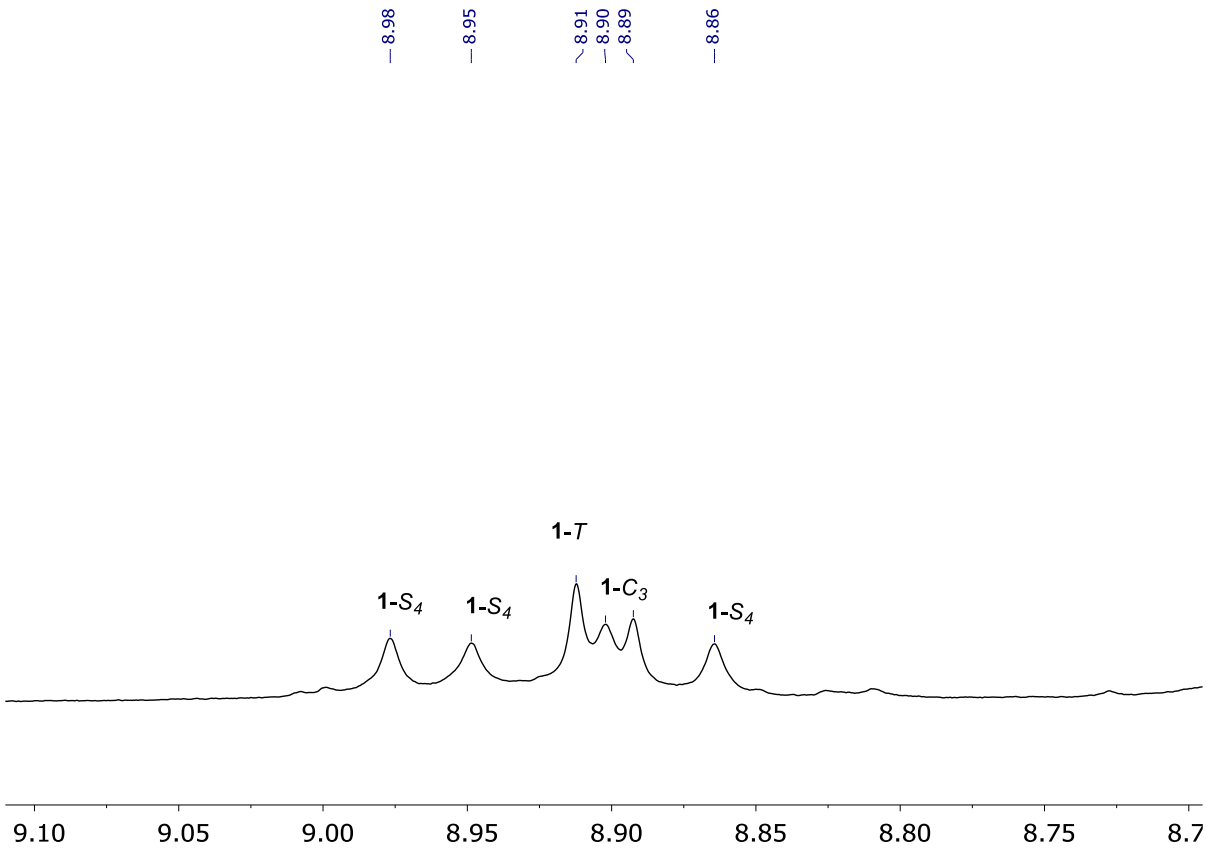


Figure S13. Expansion of the imine region of the ^{1}H NMR (500 MHz, 298 K, CD3CN) of C_{60}⊂**1**. The signals are consistent with the presence of **1**-*S*$_4$, **1**-*C*$_3$ and **1**-*T* diastereomers in the mixture

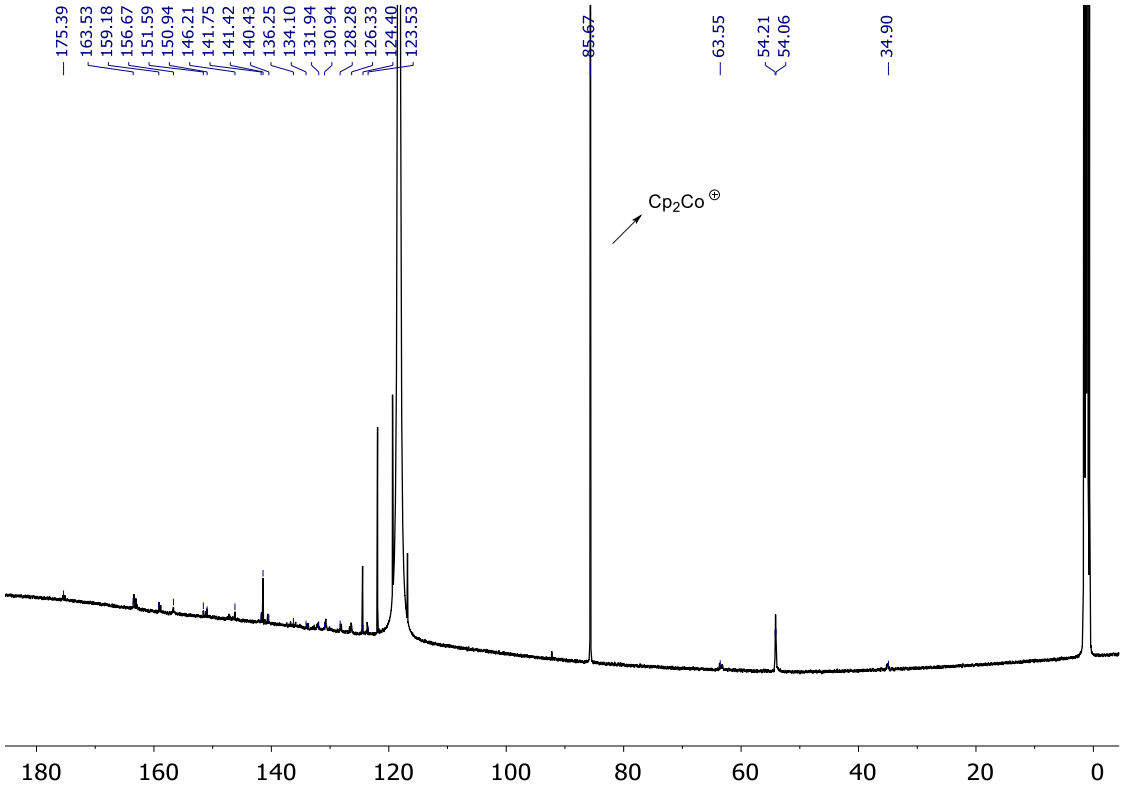


Figure S14. ^{13}C NMR (126 MHz, 298 K, CD_3CN) of C_{60}⊂**1**. The sample was measured 1 day after the addition of $AgNTf_2$.

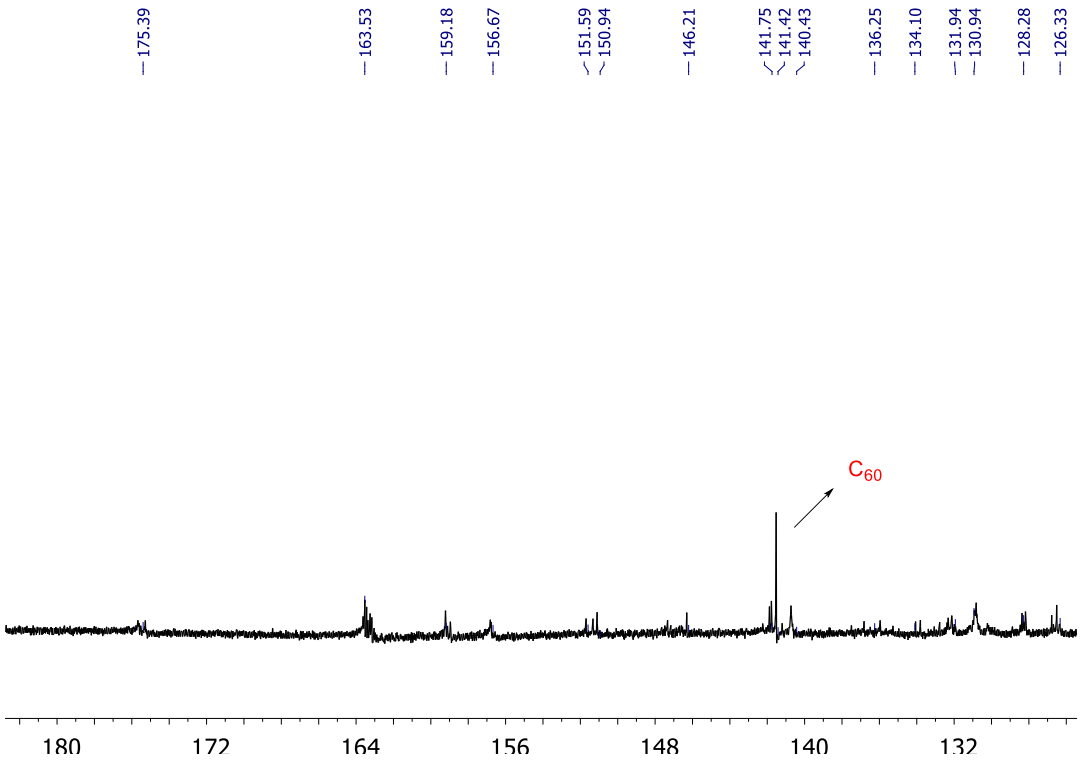


Figure S15. Aromatic region of the ^{13}C NMR (126 MHz, 298 K, CD_3CN) of C_{60}⊂**1**. The sample was measured 1 day after the addition of $AgNTf_2$.

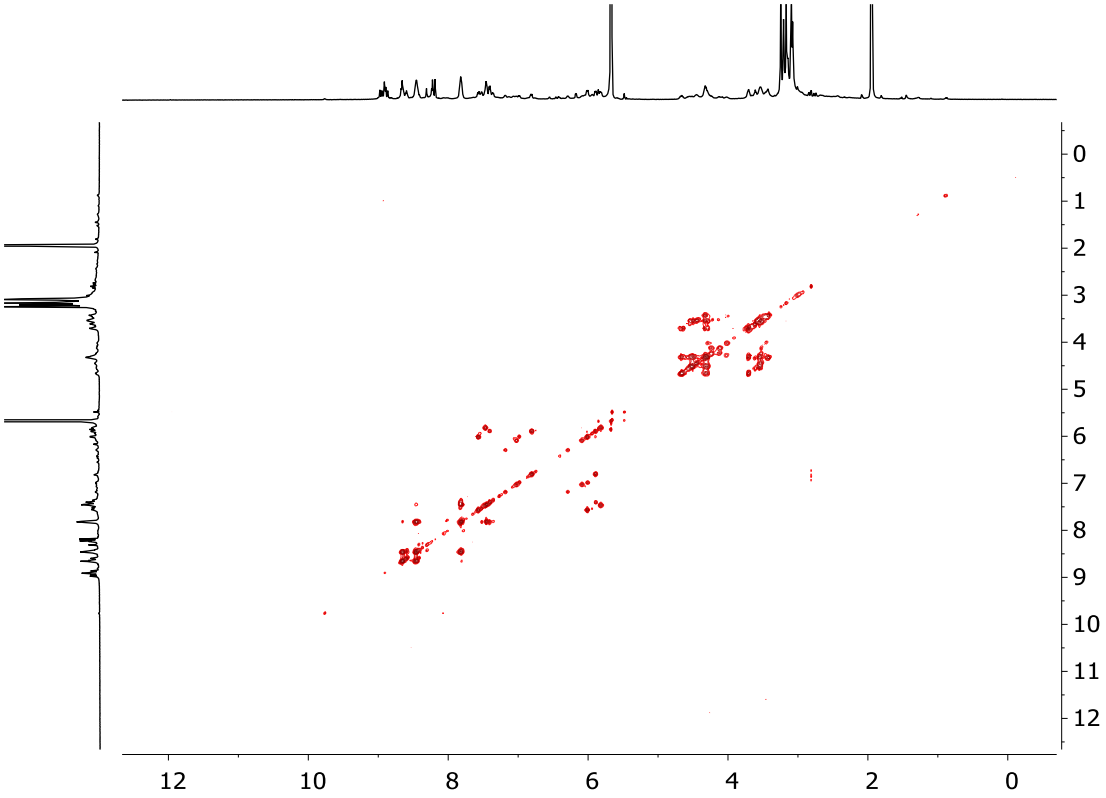


Figure S16. ^{1}H-^{1}H COSY spectrum (500 MHz, 298 K, CD_3CN) of [C_{60} ⊂ **1**]. The sample was measured 1 day after the addition of $AgNTf_2$.

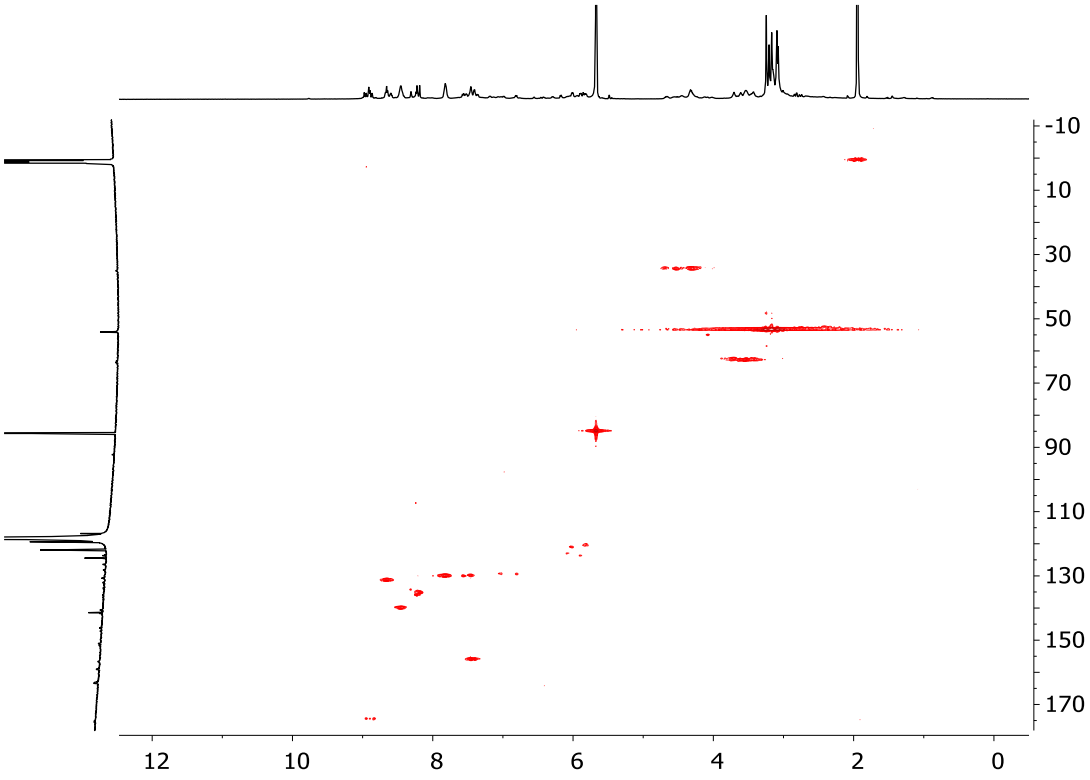


Figure S17. HSQC spectrum (500 MHz, 298 K, CD_3CN) of [C_{60} ⊂ **1**]. The sample was measured 1 day after the addition of $AgNTf_2$.

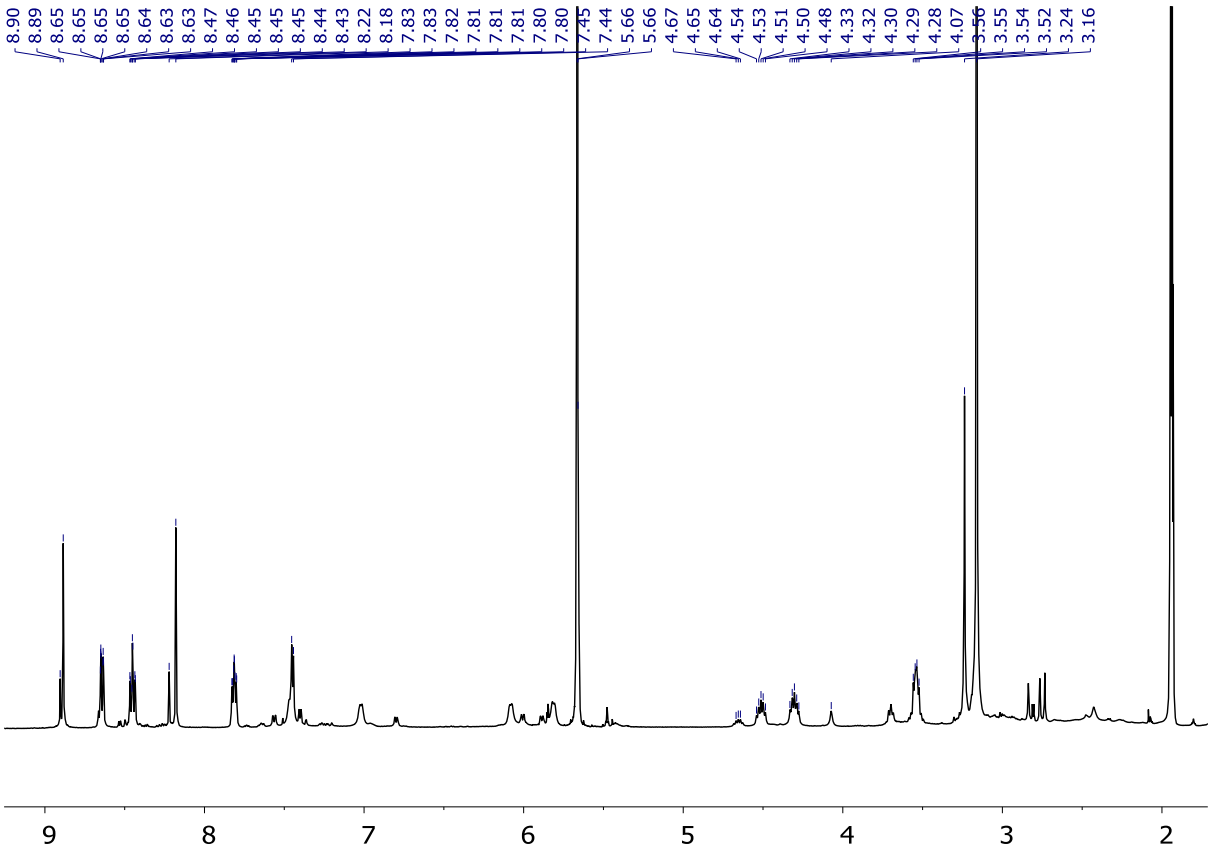


Figure S18. ^{1}H NMR (500 MHz, 298 K, CD_3CN) of C_{60}⊂**1**. The sample was measured 10 days after the addition of $AgNTf_2$.

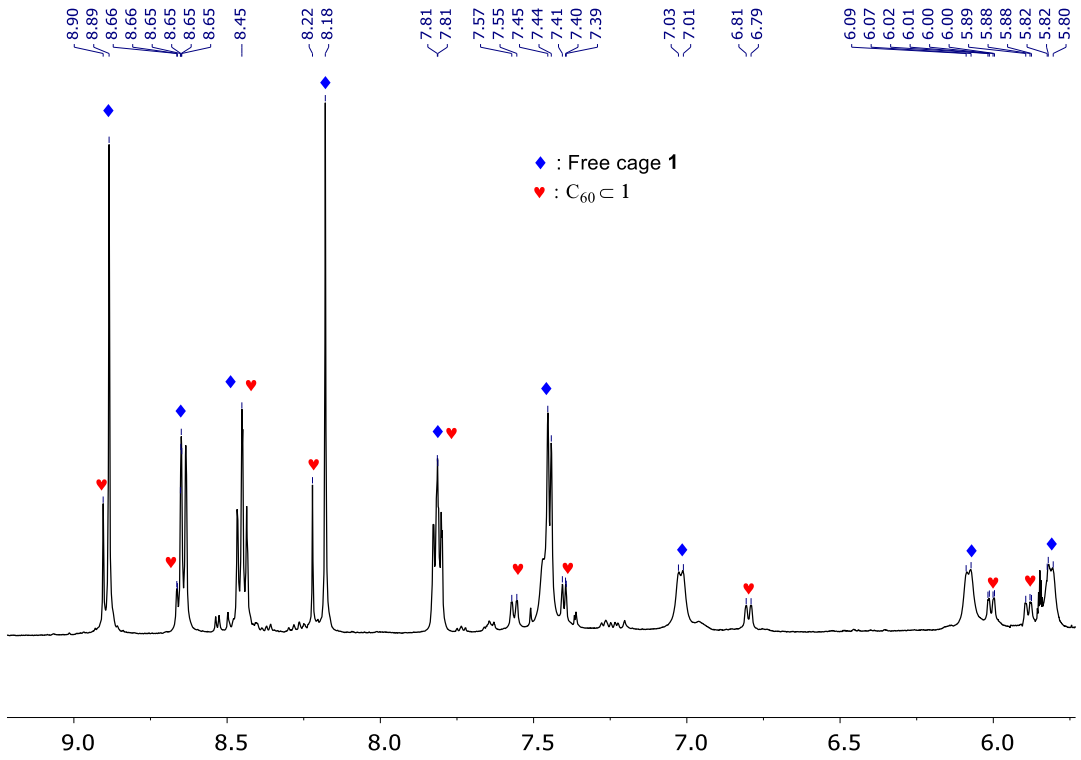


Figure S19. Aromatic region of the ^{1}H NMR (500 MHz, 298 K, CD_3CN) of C_{60}⊂**1**. The sample was measured 10 days after the addition of $AgNTf_2$.

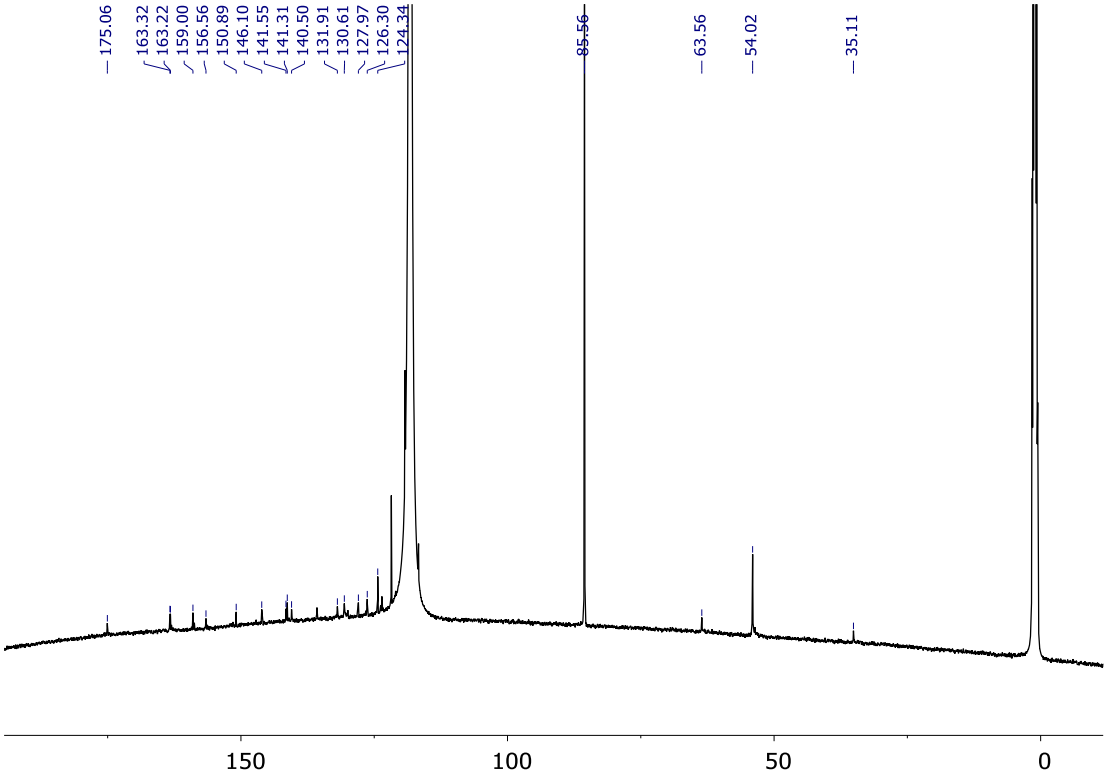


Figure S20. ^{13}C NMR (126 MHz, 298 K, CD_3CN) of C_{60}⊂**1**. The sample was measured 10 days after the addition of $AgNTf_2$.

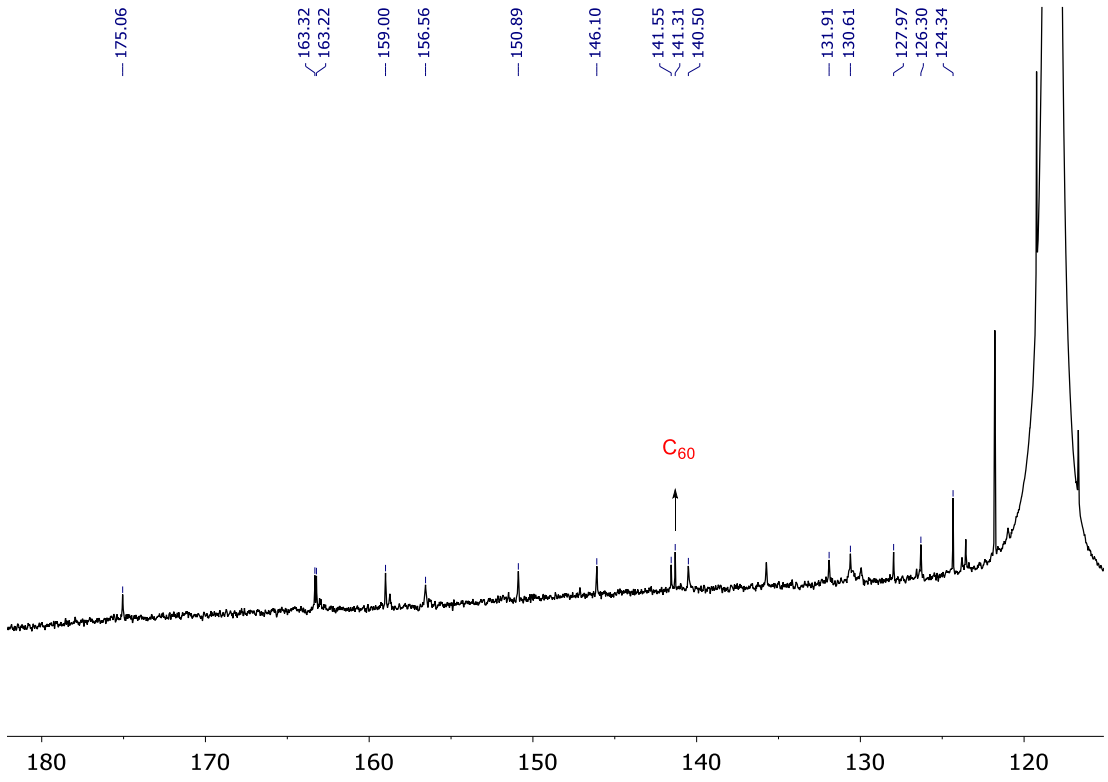


Figure S21. Aromatic region of the ^{13}C NMR (126 MHz, 298 K, CD_3CN) of C_{60}⊂**1**. The sample was measured 10 days after the addition of $AgNTf_2$.

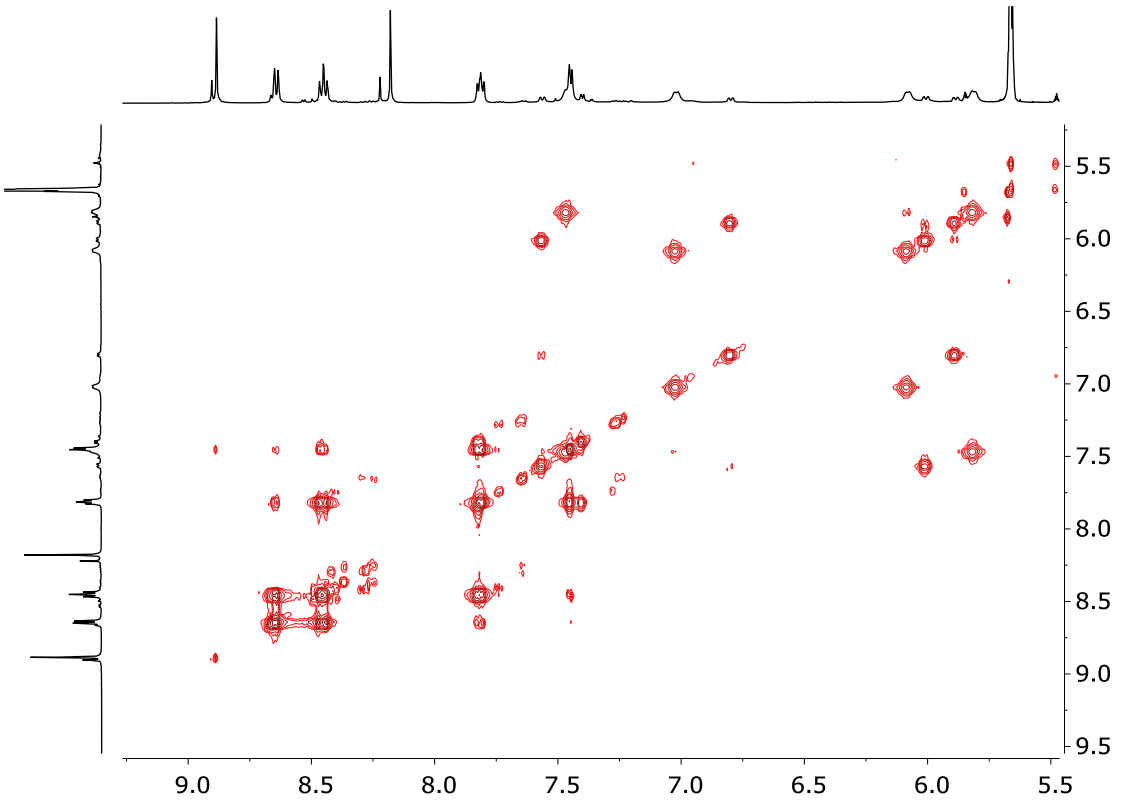


Figure S22. ^{1}H-^{1}H COSY spectrum (500 MHz, 298 K, CD_3CN) of [C_{60} ⊂ **1**]. The sample was measured 10 days after the addition of $AgNTf_2$.

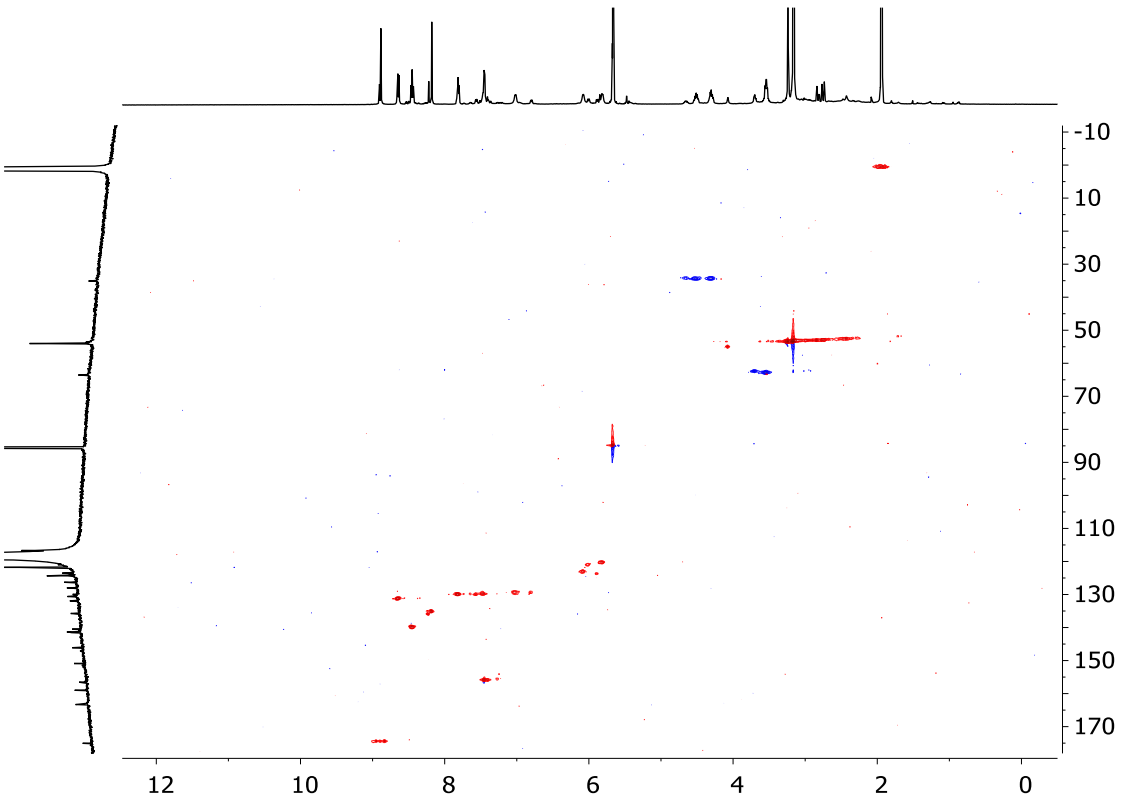


Figure S23. HSQC spectrum (500 MHz, 298 K, CD_3CN) of [C_{60} ⊂ **1**]. The sample was measured 10 days after the addition of $AgNTf_2$.

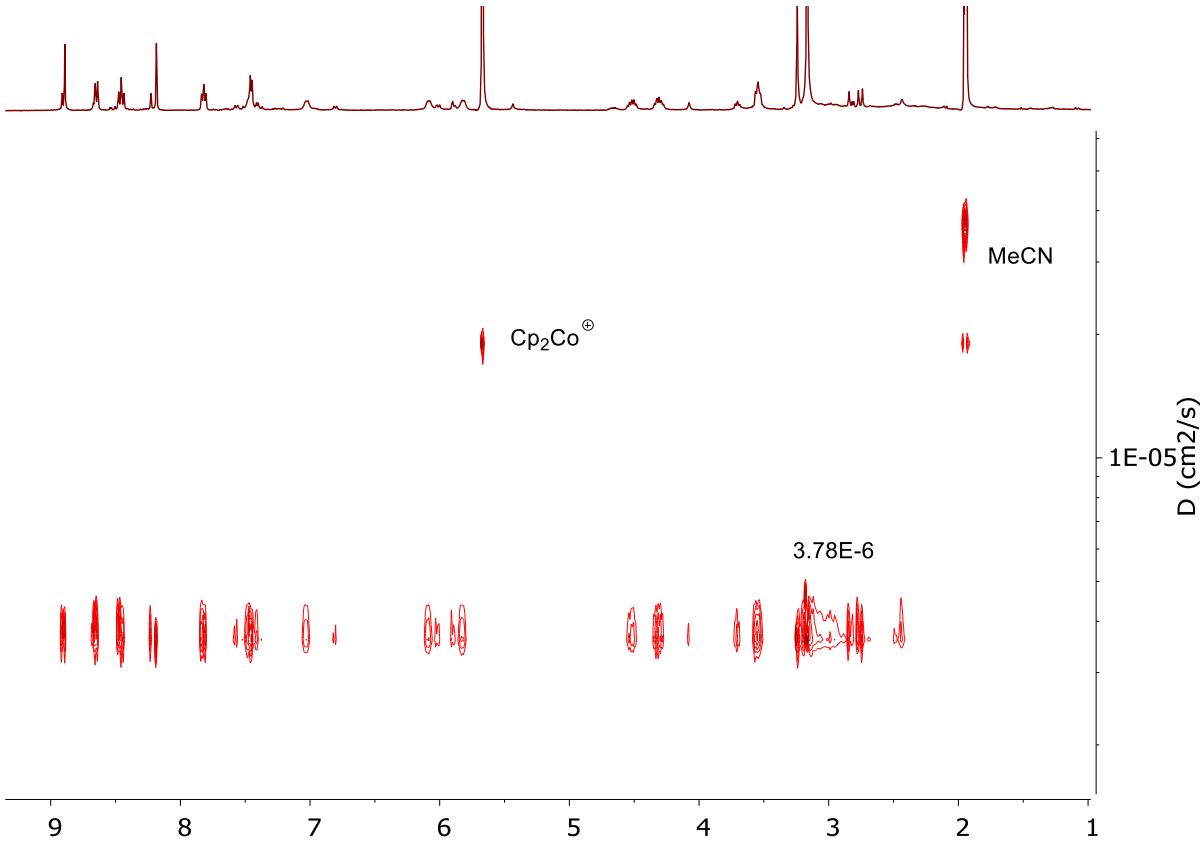


Figure S24. ^{1}H DOSY NMR (400 MHz, 298 K, CD_3CN) of C_{60}⊂**1**. The sample was measured 10 days after the addition of $AgNTf_2$. Vertical axis corresponds to the diffusion coefficient *D* (in $cm^2\ s^{-1}$).

5. Electrochemistry

Electrochemical experiments were performed with a SP-150 potentiostat manufactured by BioLogic. Measurements were conducted under Ar atmosphere with a glassy carbon working electrode (diameter 3 mm) and a platinum auxiliary electrode at a scan rate of 50 mV s^{-1}. A silver wire was used as reference electrode. All three electrodes were immersed in a CH_3CN solution (3 mL) containing $TBANTf_2$ (0.1 M) as a supporting electrolyte and Cage **1** or ligand **A** (0.001 M). In all cases, ferrocene was used as an internal standard, and all reduction potentials are reported with respect to the $E_{1/2}$ of the Fc/Fc^+ redox couple.

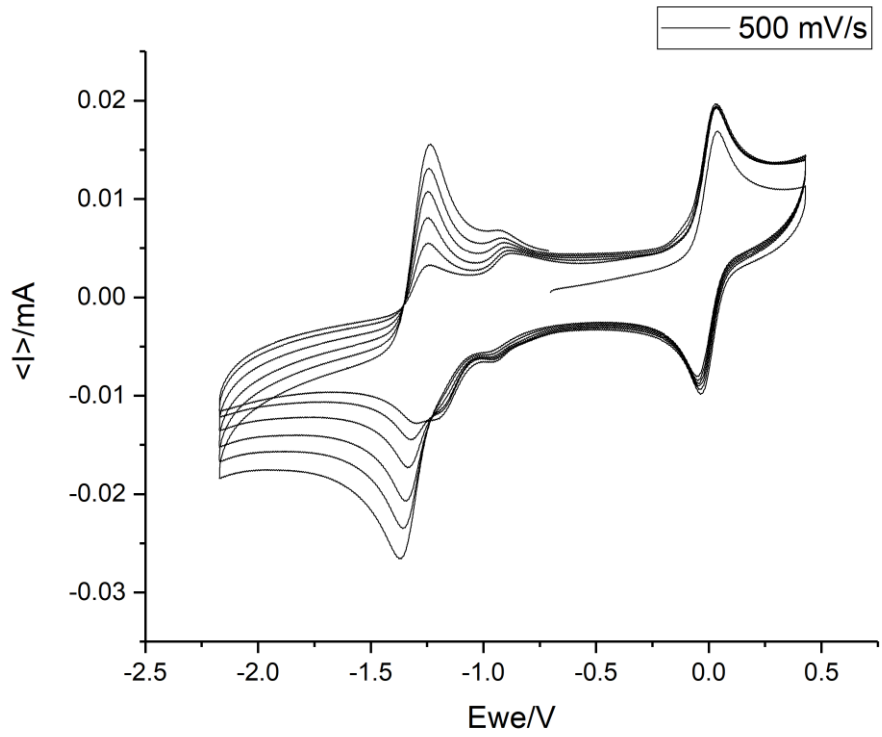


Figure S25. Cyclic voltammetry (three scans) of ligand **A** in MeCN (0.1 M $n$$Bu_4N^+Tf_2N^-$) at room temperature. The intensity of signals decreased after each cycle.

6. VOIDOO calculations

In order to determine the size of the inner cavity of **1**, VOIDOO calculations based on the crystal structure of **1** were performed based on the crystal structure.[2] A virtual probe with a radius of 1.4 Å (default, water-sized) was employed, and the following parameters were changed from their default settings:

Maximum number of volume-refinement cycles: 30

Minimum size of secondary grid: 3

Grid for plot files: 0.2

Primary grid spacing: 0.1

Plot grid spacing: 0.1

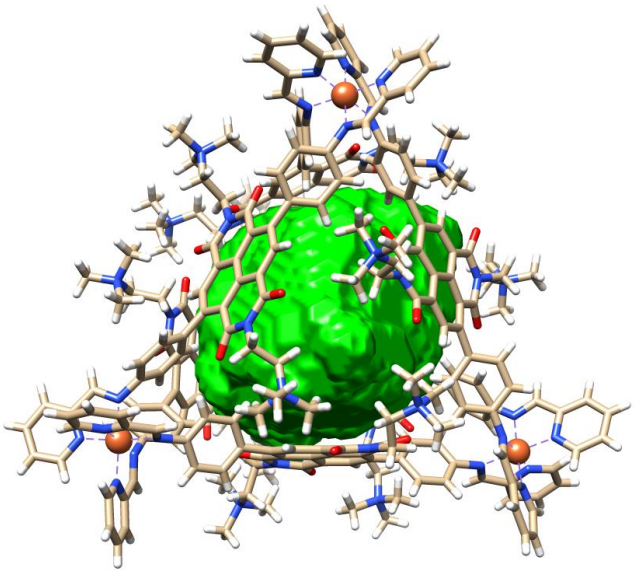


Figure S26. Void volume of **1** (1100 $Å^3$) calculated by VOIDOO.

7. Host-guest chemistry

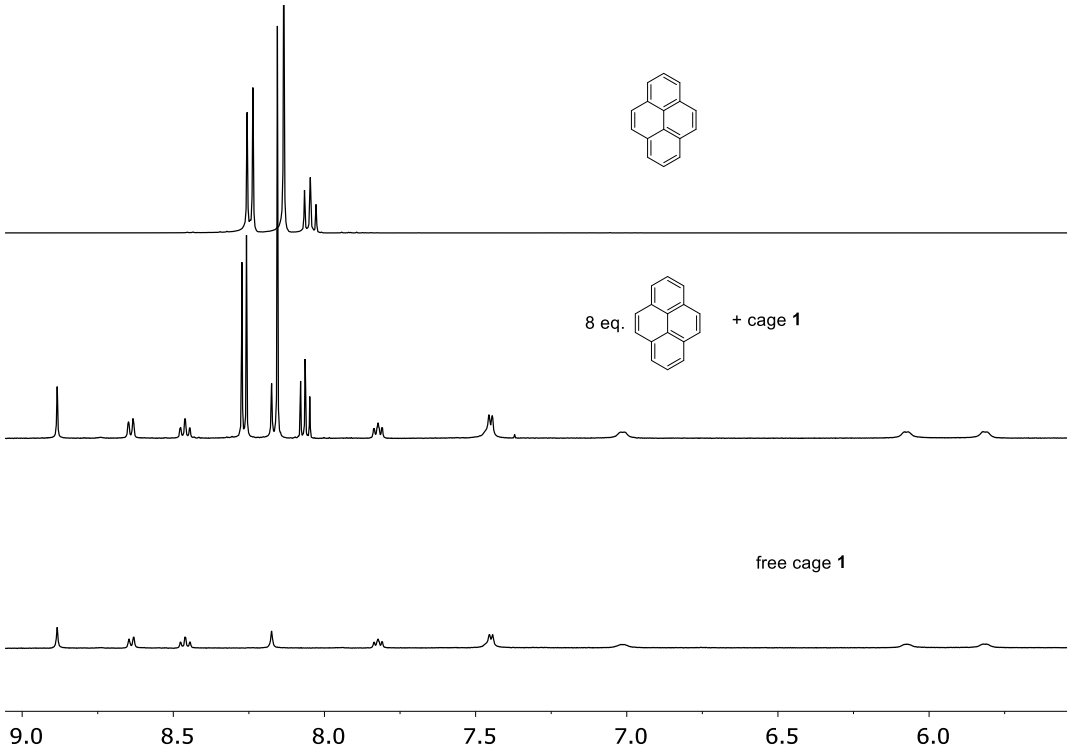


Figure S27. Aromatic region of the ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) for pyrene (top), [Pyrene ⊂**1**] (middle), cage **1** (bottom).

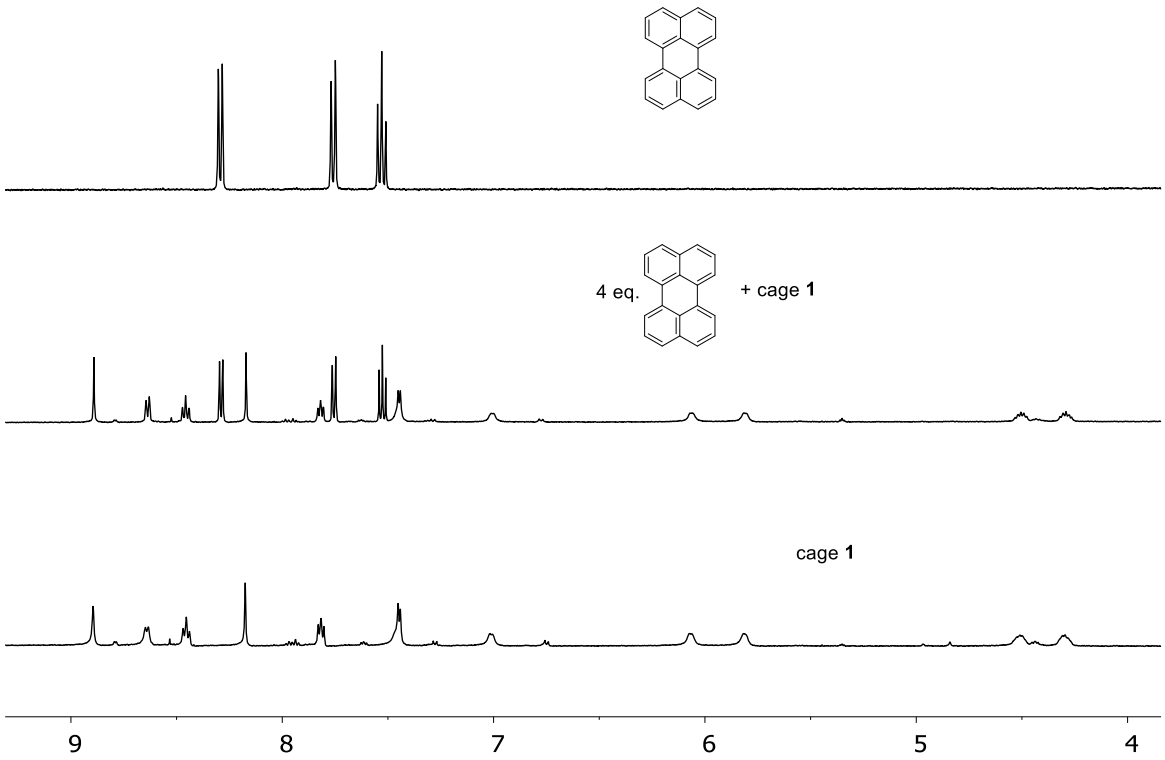


Figure S28. Aromatic region of the ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) for perylene (top), Perylene with **1** (middle), cage **1** (bottom).

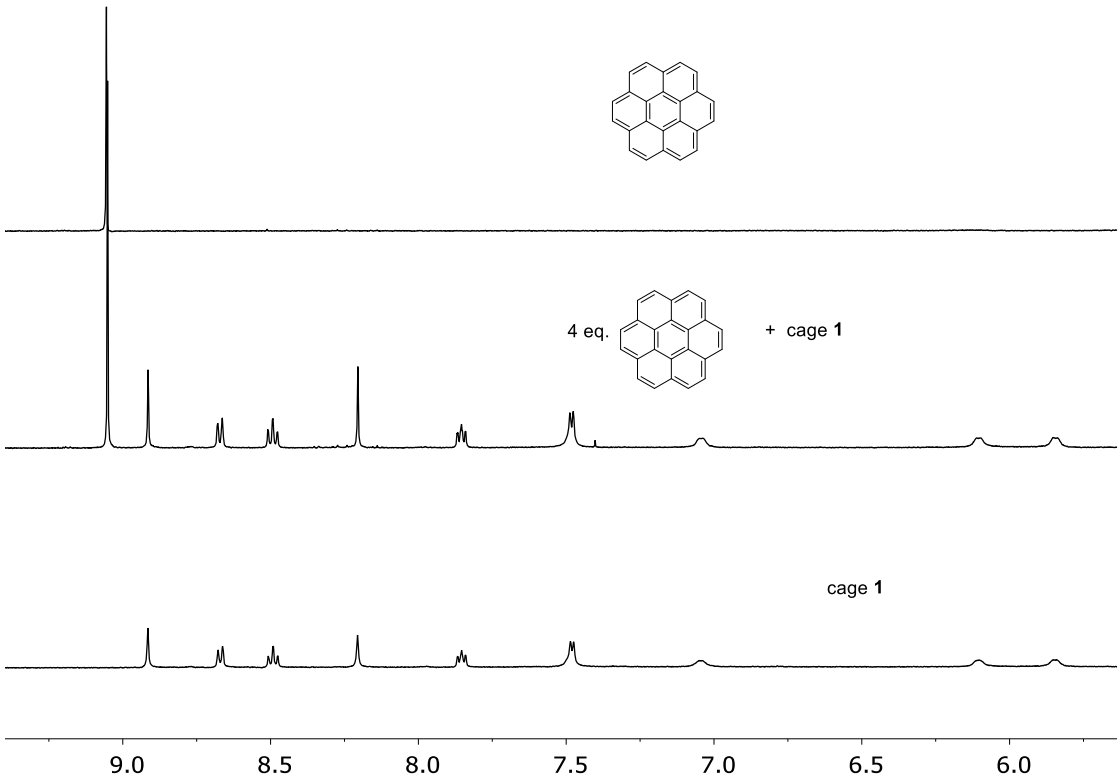


Figure S29. Aromatic region of the ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) for coronene (top), Coronene with **1** (middle), cage **1** (bottom).

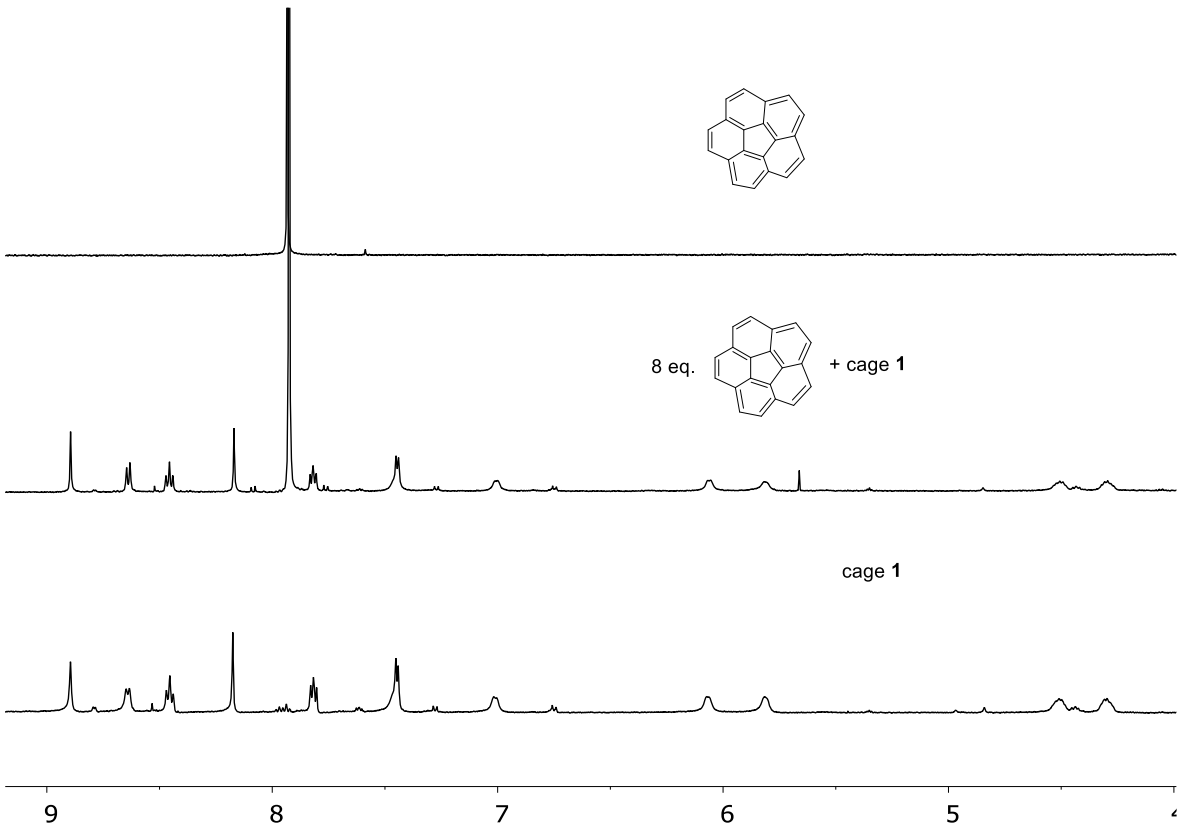


Figure S30. Aromatic region of the ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) for Corannulene (top), Corannulene with **1** (middle), cage **1** (bottom).

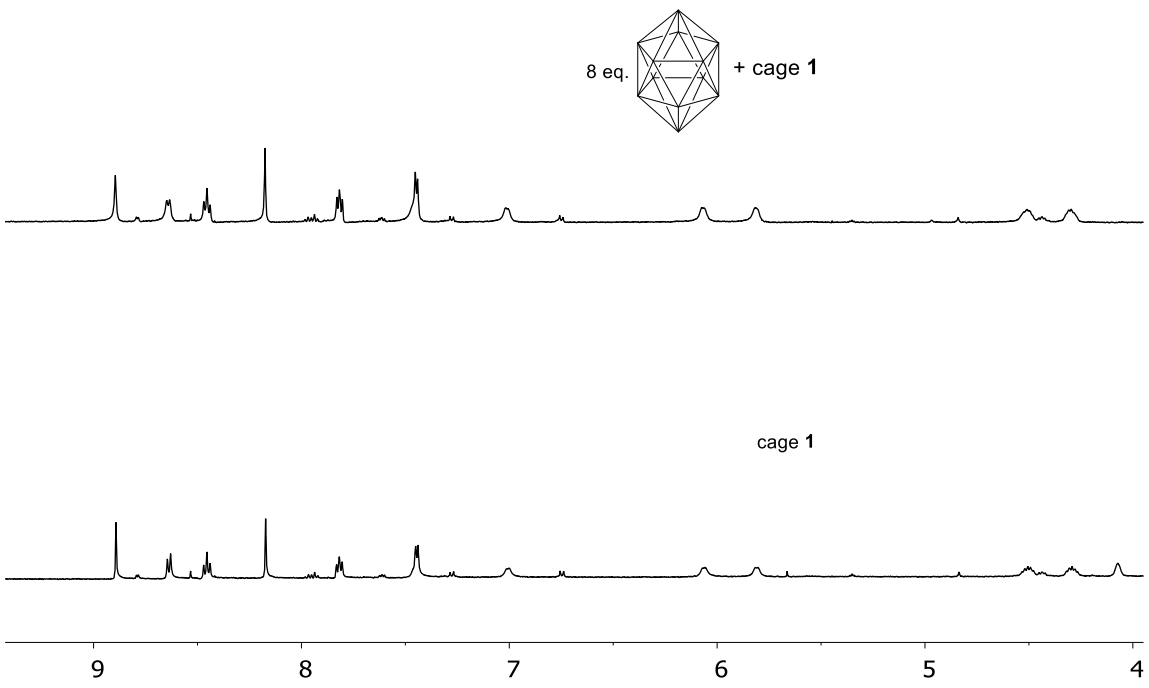


Figure S31. Aromatic region of the ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) for *ortho*-carborane with **1** (top), cage **1** (bottom).

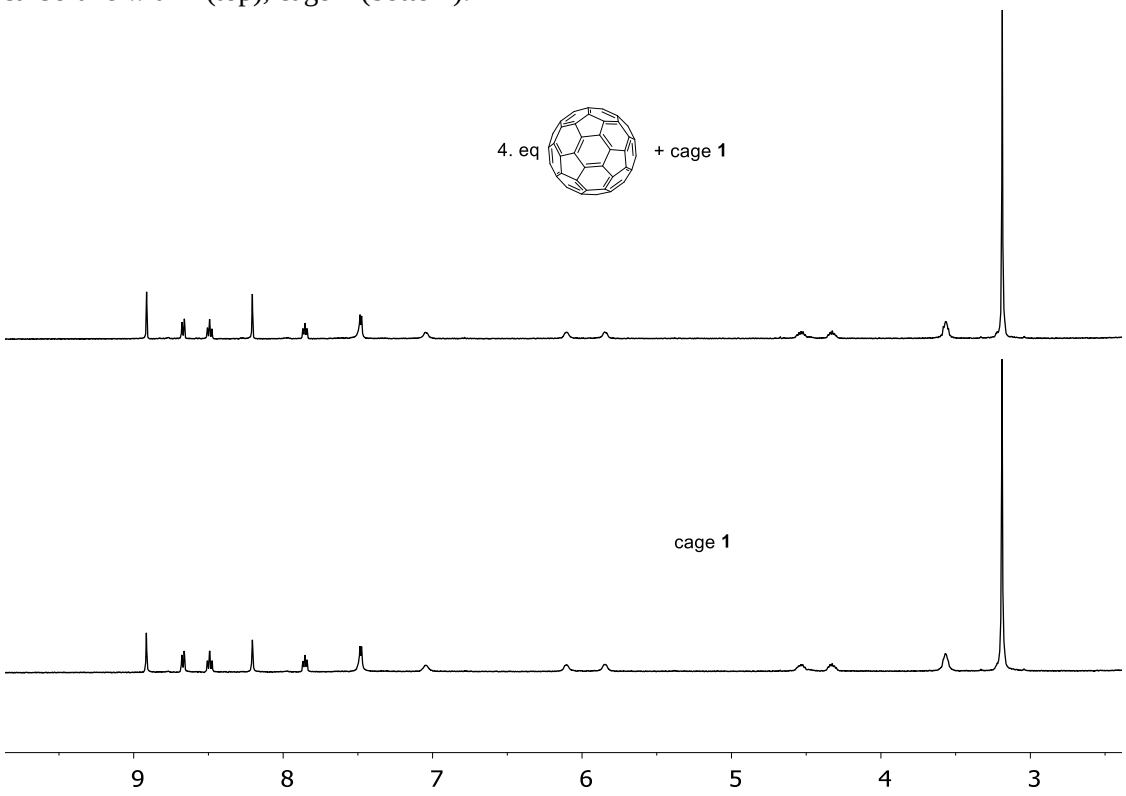


Figure S32. Aromatic region of the ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) for C_{60} with **1** (top), cage **1** (bottom).

8. Titrations

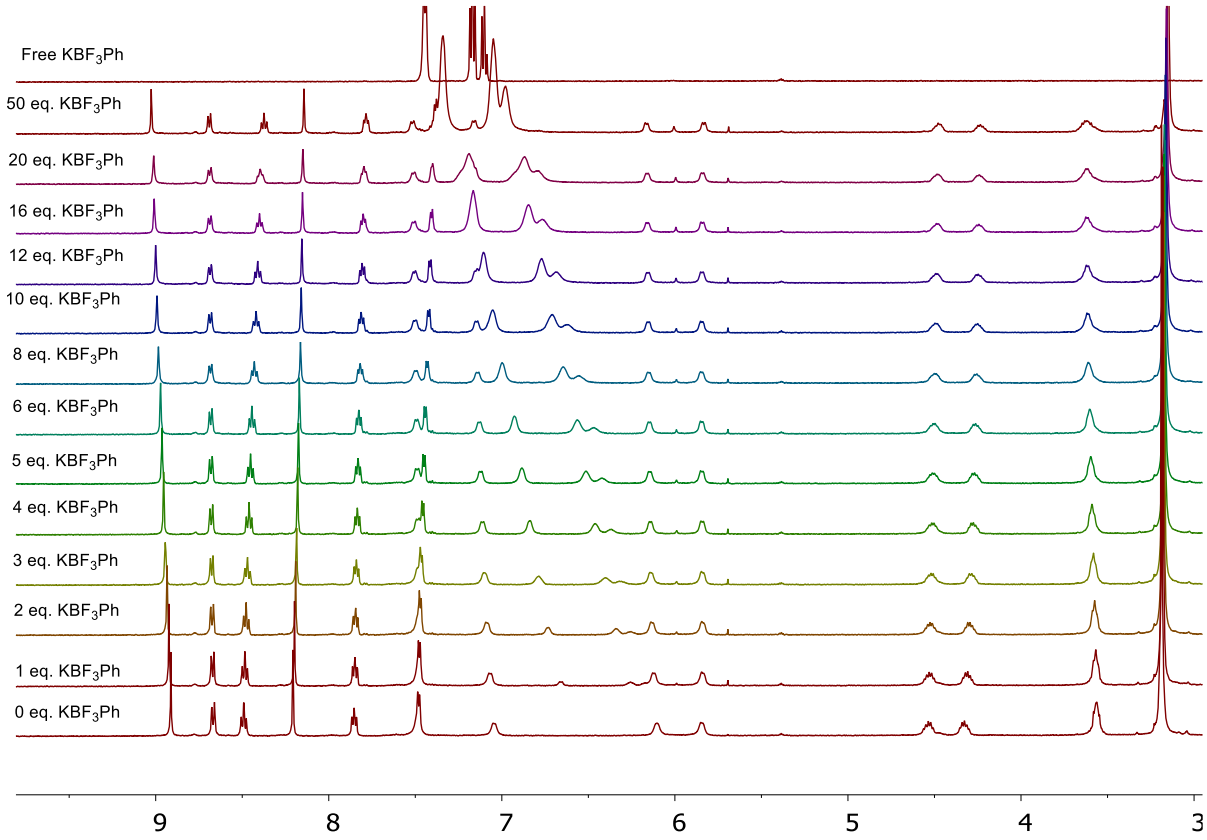


Figure S33. ^{1}H NMR titration (400 MHz, 298 K) of KBF_3Ph into a solution of **1** (0.17 mM) in CD_3CN (equivalents of anion added are labelled on individual spectra)

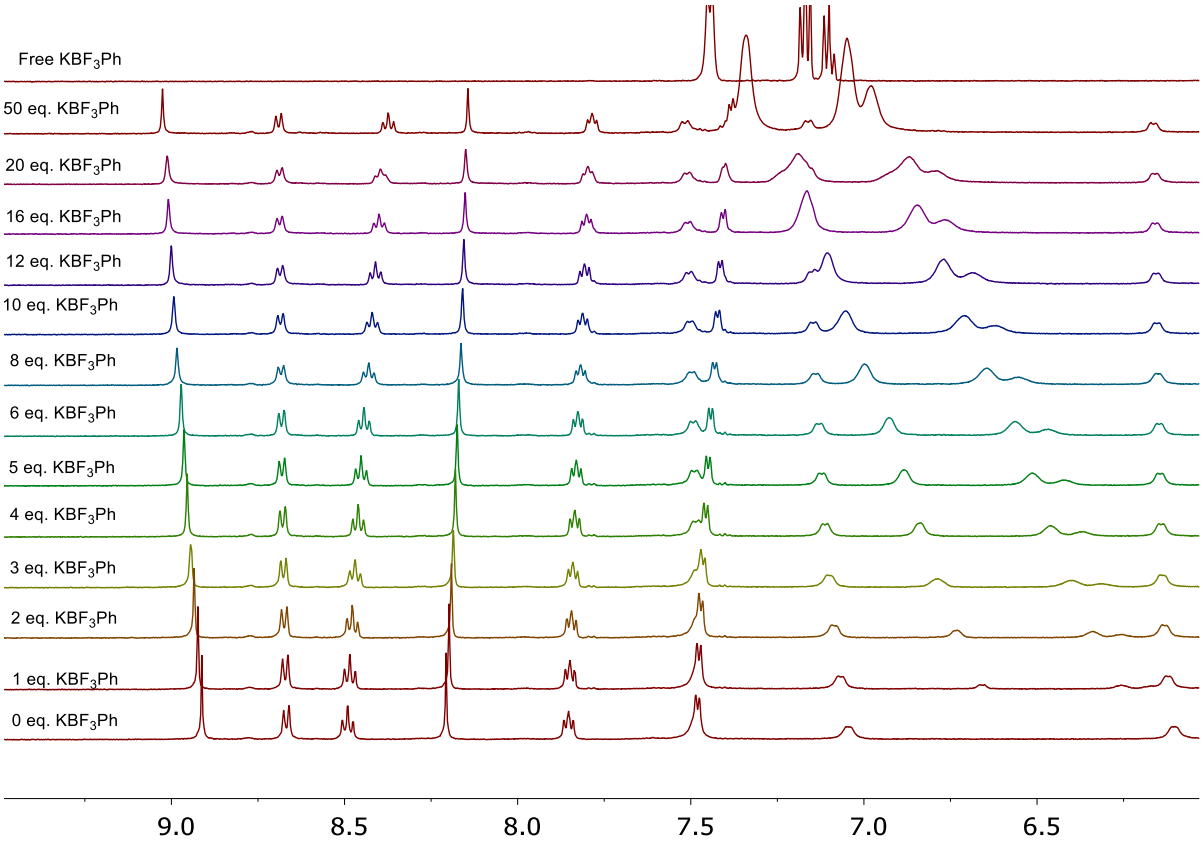


Figure S34. ^{1}H NMR titration (400 MHz, 298 K) of KBF_3Ph into a solution of **1** in CD_3CN (equivalents of anion are labelled on individual spectra)

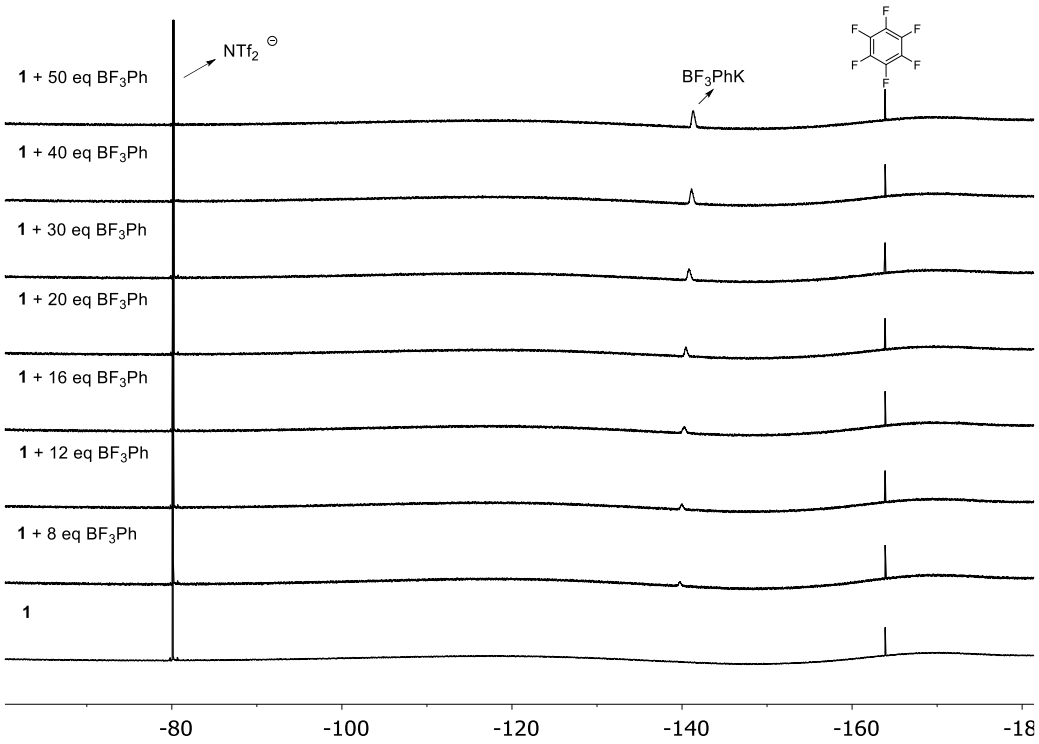


Figure S35. ^{19}F NMR titration (376 MHz, 298 K) of KBF_3Ph into a solution of **1** in CD_3CN, with hexaflurobenzene in a capillary as external standard. (Equivalents of anion are labelled on individual spectra).

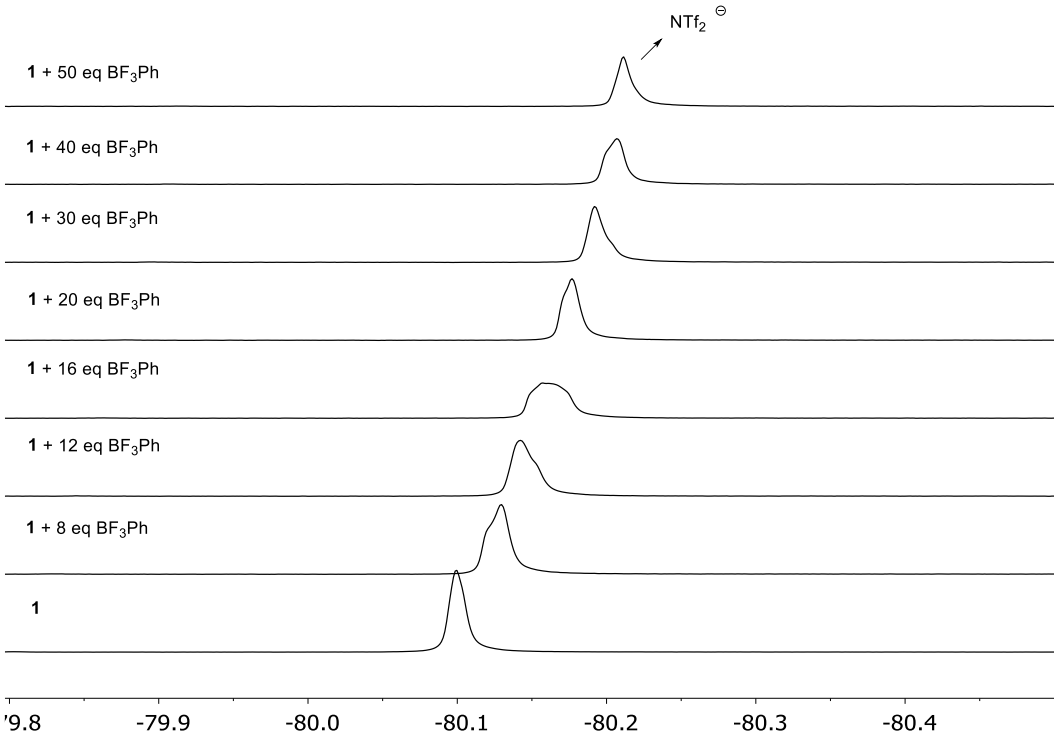


Figure S36. Expansion of the triflimide signal during the ^{19}F NMR titration (376 MHz, 298 K) of KBF_3Ph into a solution of **1** in CD_3CN.

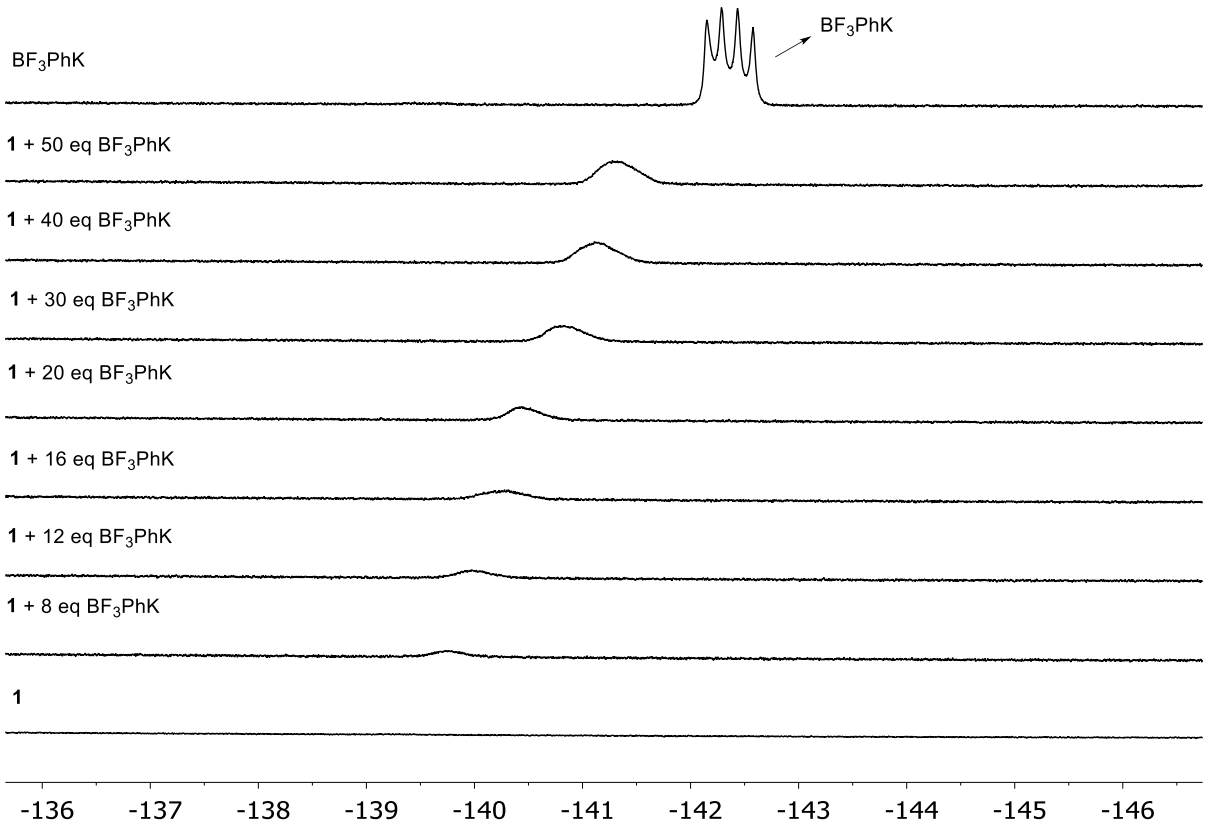


Figure S37. Expansion of the KBF_3Ph signal of ^{19}F NMR titration (376 MHz, 298 K) of KBF_3Ph into a solution of **1** in CD_3CN.

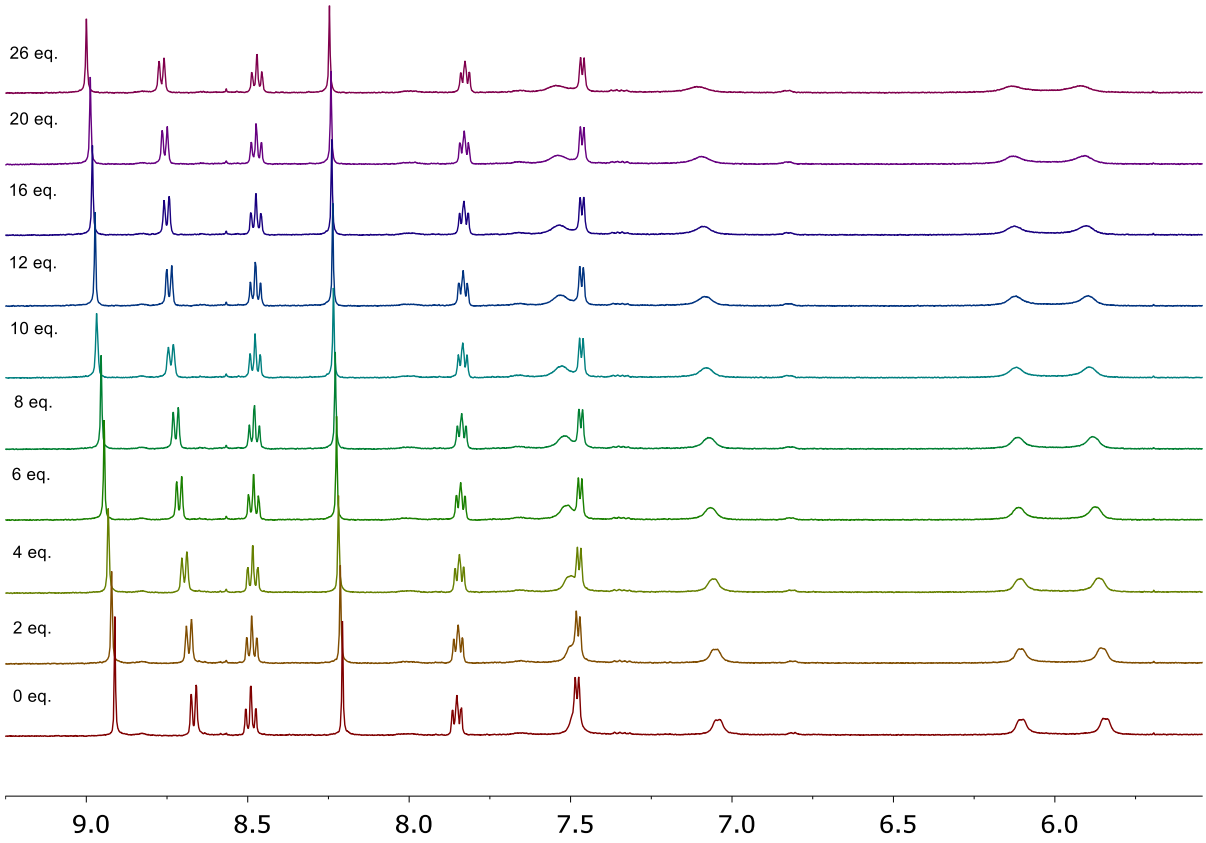


Figure S38. ^{1}H NMR titration (400 MHz, 298 K) of $TBABF_4$ into a solution of **1** in CD_3CN (equivalents of anion are labelled on individual spectra)

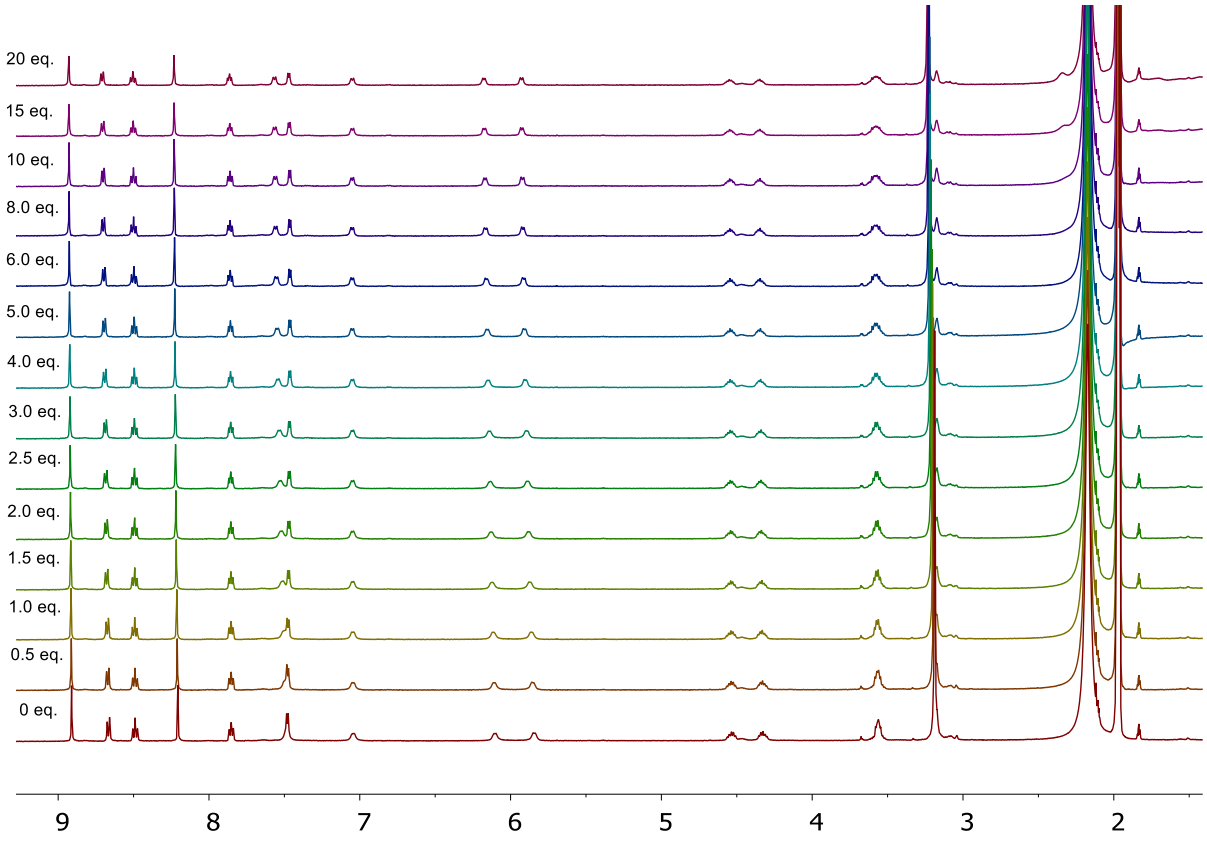


Figure S39. ^{1}H NMR titration (400 MHz, 298 K) of cesium carborane into a solution of **1** in CD_3CN (equivalents of anion are labelled on individual spectra)

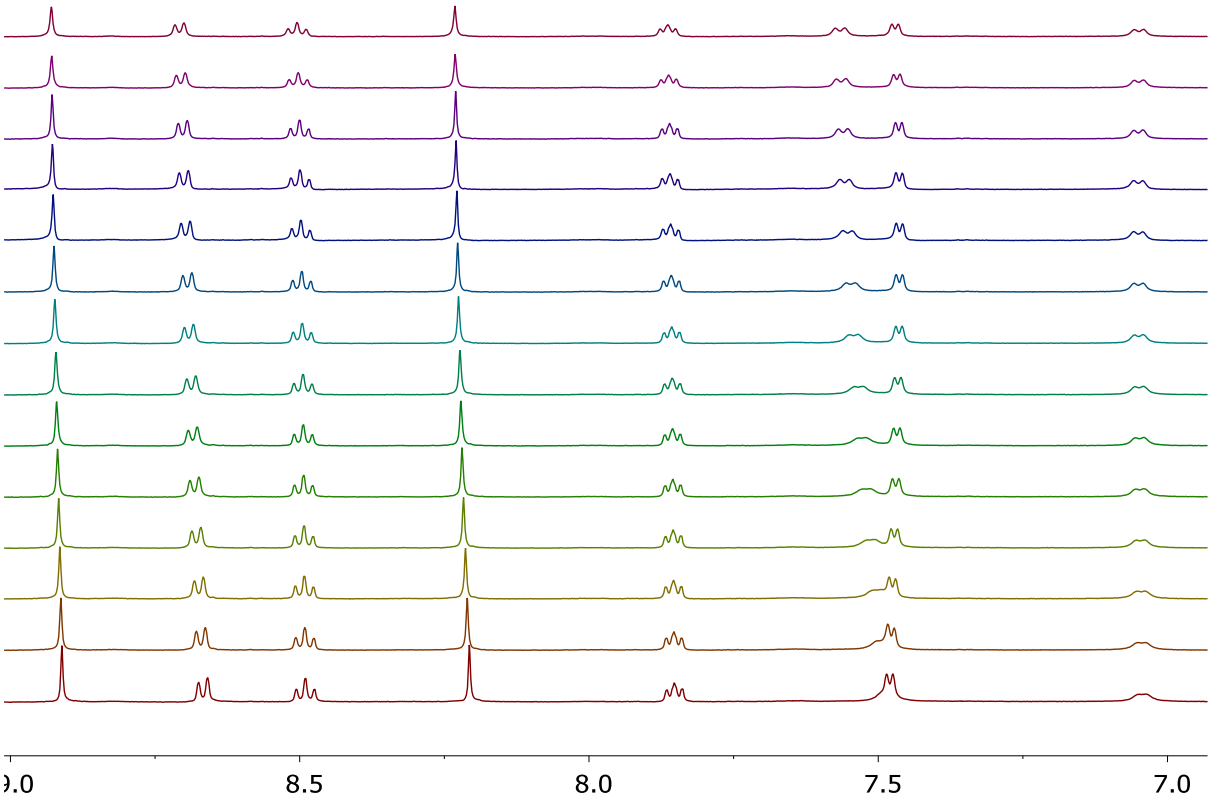


Figure S40. ^{1}H NMR titration (400 MHz, 298 K) of cesium carborane into a solution of **1** in CD_3CN (equivalents of anion are labelled on individual spectra)

9. Redox-switching experiment of cage 1

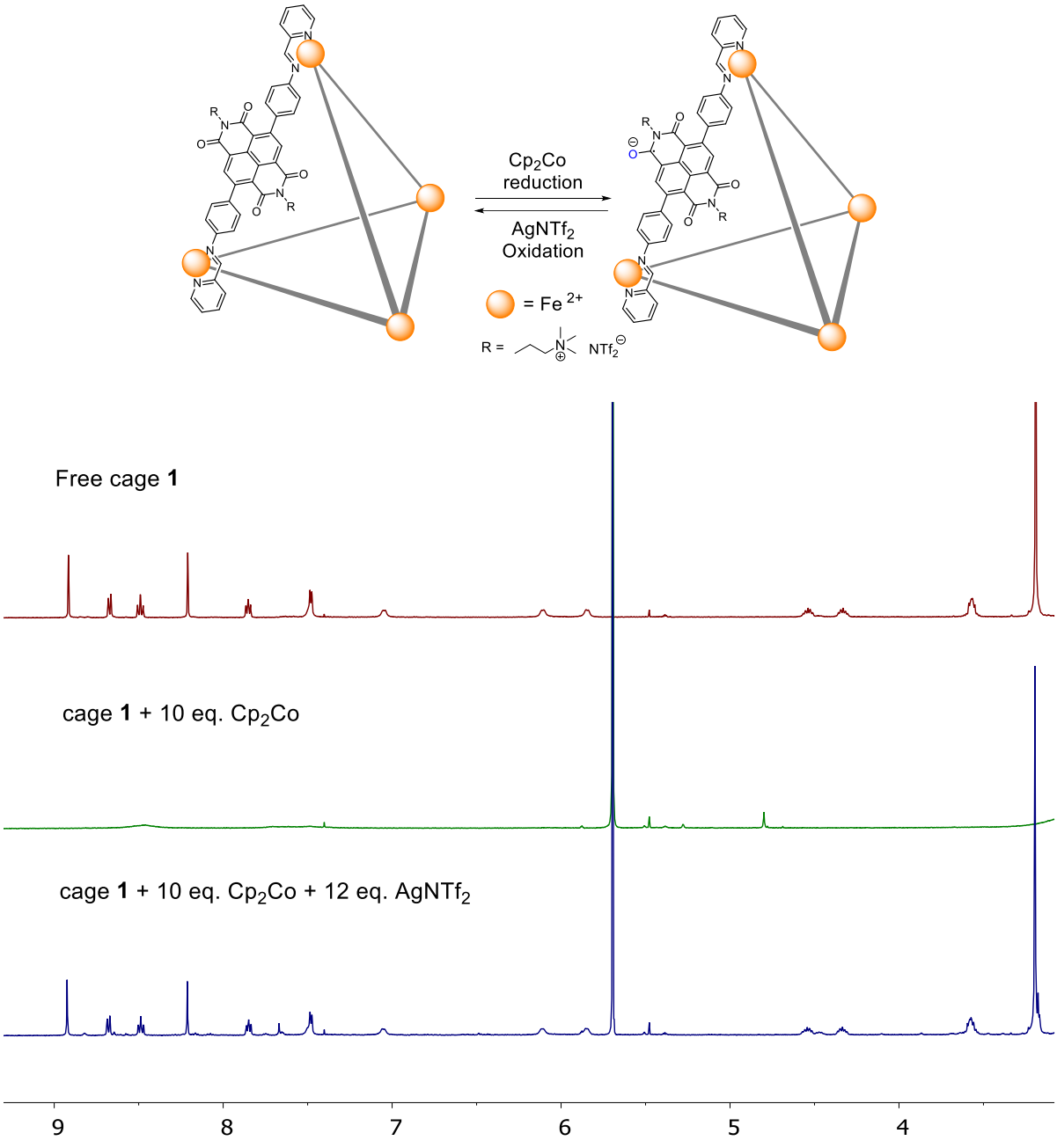


Figure S41. Control experiments of cage **1** upon the addition of Cp_2Co and $AgNTf_2$, showing loss of signals in the ^1H NMR spectrum (500 MHz, 298 K, CD_3CN) in the presence of Cp_2Co and the recovery of **1** with the addition of $AgNTf_2$.

10. Phase transfer of cage 1 by anion exchange

Cage **1** (1 mg, 0.094 mmol) was dissolved in CD_3CN (0.4 mL). Its ^1H NMR spectrum was recorded. EtOAc (0.3 mL) was then added into the solution. This combined solution was then added to a Na_2SO_4 (0.5 mg, 2.6 mmol) solution in D_2O (0.6 mL) to form a bilayer (organic phase: red; water phase: colourless). After shaking, the red organic phase became light brown, and the water solution turned red. The presence of cage **1** was confirmed by ^1H NMR in D_2O.

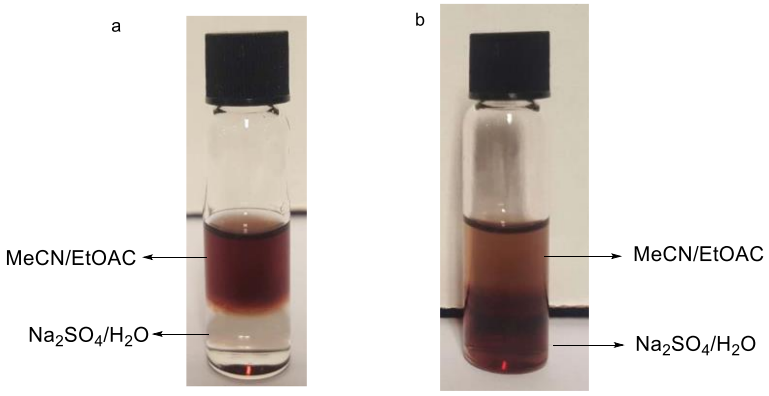


Figure 42. (a) the formation of bilayer phase; (b) phase-transfer after shaking.

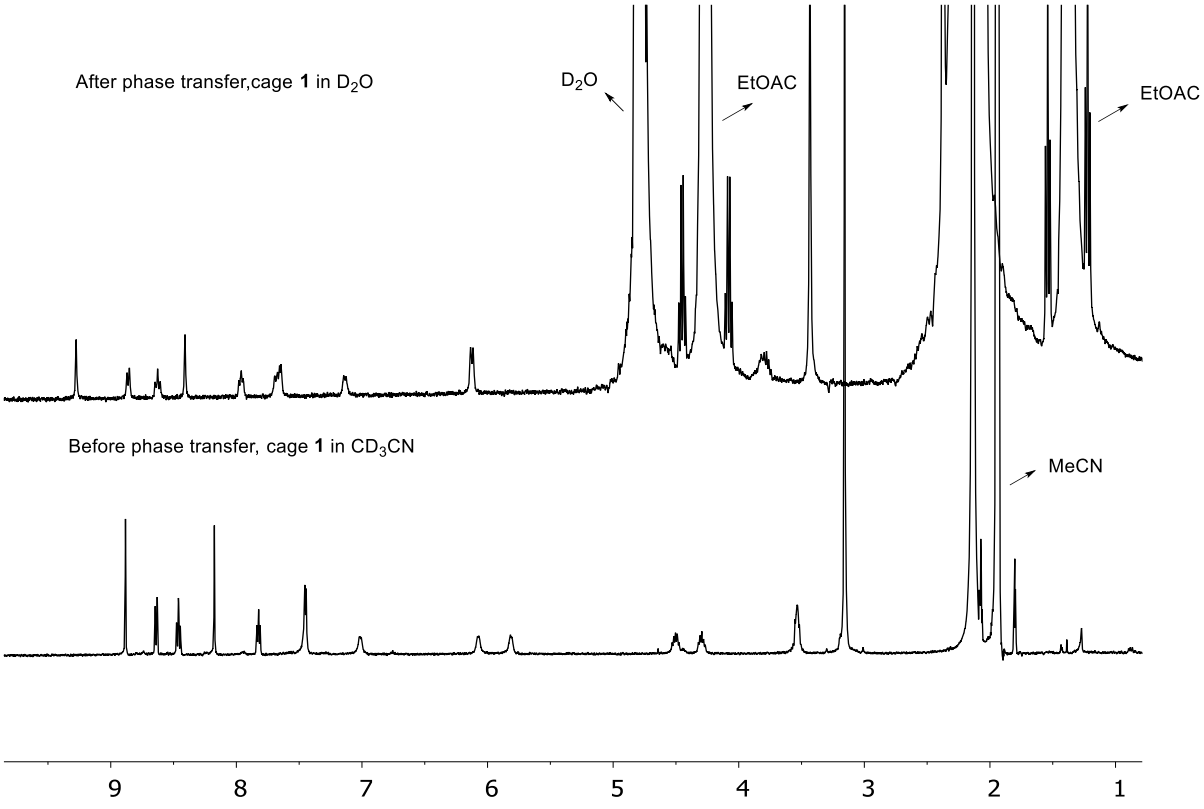


Figure S43. ^1H NMR (500 MHz) of cage **1** before phase transfer (bottom, in CD_3CN) and after phase transfer (top, in D_2O)

Cage **1** (2 mg, 0.00019 mmol, 1 equiv) and C_{60} (0.5 mg, 0.00076 mmol, 4 equiv) were mixed in CD_3CN (0.5 mL). Cp_2Co (0.4 mg, 0.0019 mmol, 10 equiv) was added into the mixture at room temperature. The reaction was kept at room temperature overnight. Then $AgNTf_2$ (1.1 mg, 0.0029 mmol, 15 equiv) was added to the mixture, and the formation of $C_{60} \subset$ **1** was characterized by NMR spectroscopy. EtOAc (0.3 mL) was then added into the solution. This solution was then added to a Na_2SO_4 (1 mg, 5.2 mmol) D_2O (0.6 mL) solution to form a bilayer (organic phase: red; water phase: colorless). After shaking, the red organic phase became light brown, and the water solution turned red. The presence of cage **1** containing no C_{60} was confirmed by ^1H NMR in D_2O (Figure S44). C_{60} can be recovered by filtration of the bilayer liquid through a filter paper.

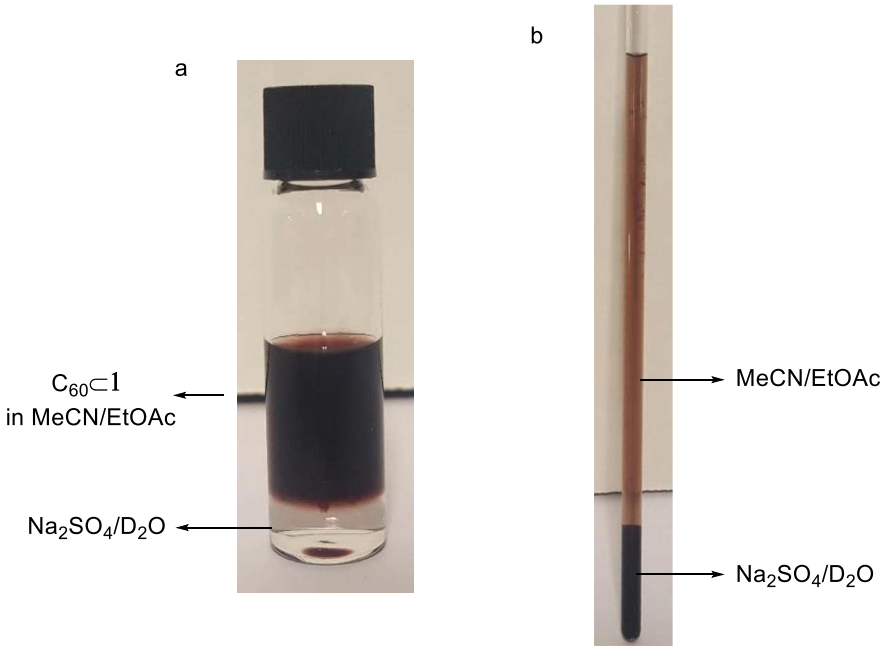


Figure S44. (a) The formation of bilayer phase for $C_{60} \subset$ **1** ; (b) phase-transfer after shaking.

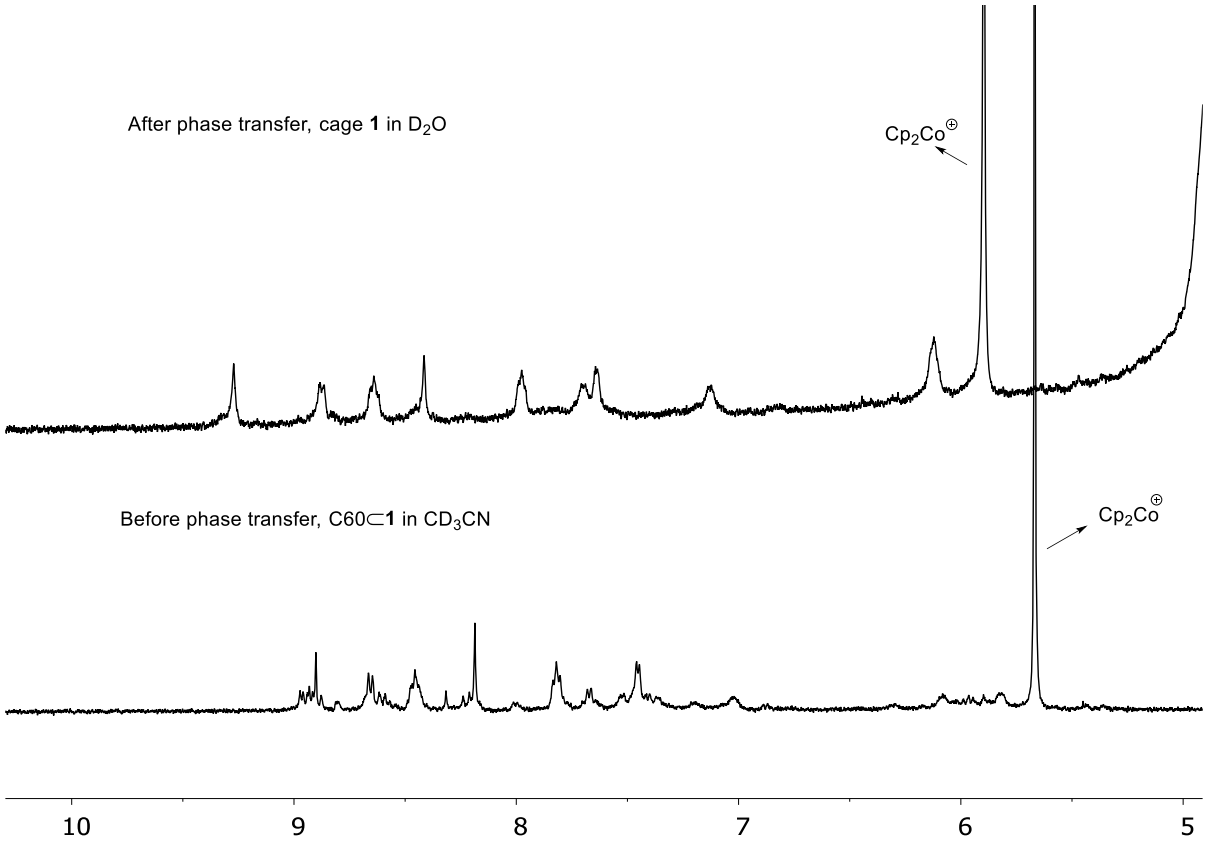


Figure S45. ^{1}H NMR (500 MHz) of $C_{60} \subset$ **1** before phase transfer (bottom, in CD_3CN) and after phase transfer (top, in D_2O)

11. X-ray crystallography

Crystals of $[Fe_4L_6]\cdot 8.2CB_{11}H_{12}\cdot 3NTf_2\cdot 4.5CH_3CN$ [+8.8 anions + solvent] were grown by vapour diffusion of diethyl ether into an acetonitrile solution of $[Fe_4L_6]\cdot 20NTf_2$ **1** containing excess $CsCB_{11}H_{12}$. Data were collected at Beamline I19 of Diamond Light Source employing silicon double crystal monochromated synchrotron radiation (0.6889 Å) with ω and ψ scans at 100(2) K.[3] Data integration and reduction were undertaken with Xia2.[4-6] Subsequent computations were carried out using the WinGX-32 graphical user interface.[7] Multi-scan empirical absorption corrections were applied to the data using the AIMLESS[8] tool in the CCP4 suite.[9] The structure was solved by direct methods using SHELXT[10] then refined and extended with SHELXL.[11] In general, non-hydrogen atoms with occupancies greater than 0.5 were refined anisotropically. Carbon-bound hydrogen atoms were included in idealised positions and refined using a riding model. Disorder was modelled using standard crystallographic methods including constraints, restraints and rigid bodies where necessary.

The crystals employed in this study were small and weakly diffracting, immediately losing solvent after removal from the mother liquor. Rapid handling prior to flash cooling in the cryostream was required to collect data. Despite these measures and the use of synchrotron radiation few reflections at greater than 0.95 Å resolution were observed and the data were trimmed accordingly. Nevertheless, the quality of the data is far more than sufficient to establish the connectivity of the structure. The asymmetric unit was found to contain one complete Fe_4L_6 assembly and associated counterions and solvent molecules.

Due to the less than ideal resolution, bond lengths and angles within pairs of organic ligands were restrained to be similar to each other and thermal parameter restraints (SIMU, RIGU, ISOR) were applied to all atoms except for iron. DFIX and DANG restraints were also applied to some atoms within the organic ligands.

The anions within the structure show significant evidence of disorder. Two triflimide anions were modelled as disordered over two locations and many anions were modelled with partial occupancy. The occupancies of the disordered anions were allowed to refine freely and then fixed at the obtained values. Some lower occupancy disordered atoms were modelled with isotropic thermal parameters and bond length restraints were applied to facilitate realistic modelling of the disordered triflimide anions. The $CB_{11}H_{12}^-$ anions were modelled as rigid groups; for these anions the carbon site could not be clearly discerned from the electron density map so all atoms of the $CB_{11}H_{12}^-$ anions were modelled as boron.

Further reflecting the solvent loss and poor diffraction properties there is a significant amount of void volume in the lattice containing smeared electron density from disordered solvent and 8.8 unresolved anions per Fe_4L_4 tetrahedron (required in order to achieve charge balance). Consequently the SQUEEZE[12] function of PLATON[13] was employed to remove the contribution of the electron density associated with these remaining anions and further highly disordered solvent, which gave a potential solvent accessible void of 12998 $Å^3$ per unit cell (a total of approximately 3818 electrons). Since the

remaining anions could not be assigned conclusively to triflimide or $CB_{11}H_{12}^-$ they were not included in the formula. Similarly diffuse solvent molecules could not be assigned to acetonitrile or diethyl ether. Consequently, the molecular weight and density given above are underestimated.

CheckCIF gives 6 A and 10 B level alerts. These alerts (both A and B level) result from the poor diffraction properties (low resolution) and thermal motion and/or unresolved disorder of some anions and solvent molecules (large average Ueqs, short contacts).

Crystallographic data have been deposited with the CCDC (CCDC 1935513).

Formula $C_{311.20}H_{387.90}B_{90.20}F_{18}Fe_4N_{55.50}O_{36}S_6$, *M* 7214.87, Monoclinic, space group C c (#9), *a* 33.3570(2), *b* 32.3478(3), *c* 45.8124(3) Å, β 102.3200(10), *V* 48294.4(6) $Å^3$, D_c 0.992 g cm^{-3}, *Z* 4, crystal size 0.040 by 0.030 by 0.030 mm, colour purple, habit block, temperature 100(2) Kelvin, λ(Synchrotron) 0.6889 Å, μ(Synchrotron) 0.188 mm^{-1}, $T(\text{Analytical})_{min,max}$ 0.97710440761, 1.0, $2\theta_{max}$ 42.52, *hkl* range -34 32, -30 34, -48 47, *N* 89539, N_{ind} 51296(R_{merge} 0.0565), N_{obs} 34171(I > 2σ(I)), N_{var} 4647, residuals* *R*1(*F*) 0.1030, *wR*2(F^2) 0.2822, GoF(all) 1.027, $\Delta\rho_{min,max}$ -0.336, 0.610 e^- $Å^{-3}$.

*$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ for $F_o > 2\sigma(F_o)$; $wR2 = (\Sigma w(F_o^2 - F_c^2)^2/\Sigma(wF_c^2)^2)^{1/2}$ all reflections

$w=1/[\sigma^2(F_o^2)+(0.2000P)^2]$ where $P=(F_o^2+2F_c^2)/3$

12. Geometry optimized models

Cage $C_{60}\subset$**1** is comprised of four vertices with metal centers having either in Λ or Δ stereochemical configuration. The mixture of Λ and Δ configurations can give rise to five diastereomers including two pairs of enantiomers: ΛΛΛΛ (*T*-symmetric), ΛΛΛΔ (C_3-symmetric), ΛΛΔΔ (S_4-symmetric), ΛΔΔΔ (C_3-symmetric) and ΔΔΔΔ (*T*-symmetric). PM3 geometry optimized models of three diastereomers (ΔΔΔΔ, ΛΔΔΔ and ΛΛΔΔ) including C_{60} are shown below (Figure S45 and Tables S1-S3). The ΔΔΔΔ diastereomer is based on the free cage crystal structure while the other diastereomers were generated by inverting the stereo-configuration of one or two vertices from Δ to Λ. Note that modelling was performed in the absence of anions which led, in a first modelling attempt, to extreme ionic repulsion between the trimethylammonium moieties which is not observed in the crystal structure due to charge stabilization by counter-anions; therefore, the trimethylammonium moieties were replaced by *tert*-butyl moieties to avoid ionic repulsion and reduce calculation time.

Geometry optimized structures were modelled with semi-empirical methods using PM3 models using SCIGRESS software (Fujitsu Limited, Tokyo, Japan, 2013) version FJ 2.6 (EU 3.1.9) Build 5996.8255.20141202. The Cartesian coordinates for all models are given below.

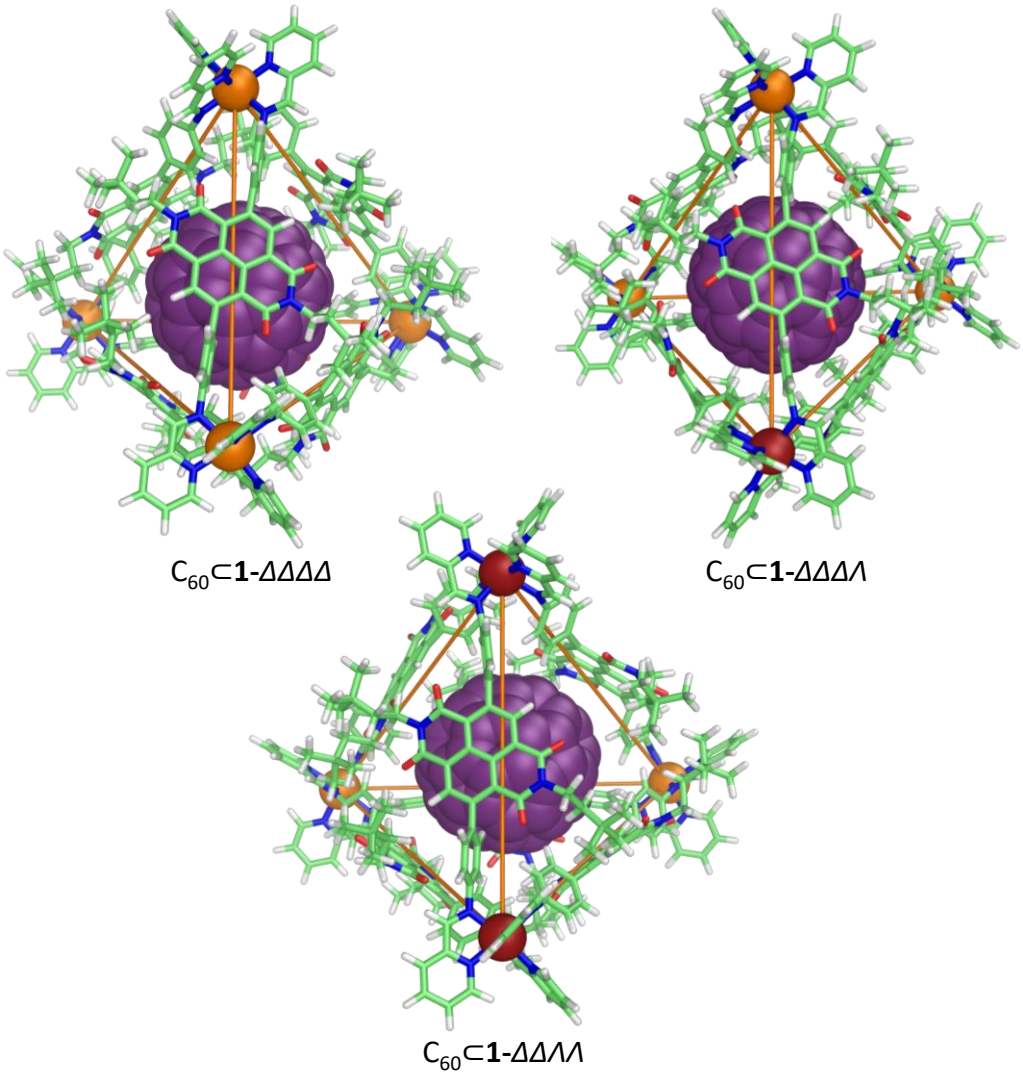


Figure S46. PM3-optimized structures of the three diastereomers of C_{60}⊂**1**. Fe^{II} centers with *Δ* and *Λ* stereochemistry are colored orange and dark red, respectively.

Table S1. Cartesian coordinates (in Å) for the PM3 model of the tert-butyl derivative of C60⊂1-ΔΔΔΔ.

Fe	12.223332	7.366899	28.651222	H	15.150004	3.030149	29.695315
Fe	2.833352	16.559087	14.474671	C	14.533093	3.116423	27.617464
Fe	21.839562	14.056179	13.605780	H	15.013169	2.166092	27.343525
Fe	14.501821	26.397077	26.245224	C	13.831027	3.851390	26.658550
O	8.291000	11.133352	25.446344	H	13.751150	3.489175	25.624721
O	4.274299	12.838143	24.122589	C	13.222613	5.049335	27.031707
O	9.538264	9.119409	18.774730	C	12.433282	5.847152	26.082275
O	6.351285	12.031637	17.340867	H	12.360810	5.515822	25.017984
N	13.308106	5.530192	28.326942	C	11.003249	7.684246	25.642504
N	11.840824	6.919255	26.549034	C	9.664251	7.322492	25.468814
N	2.762896	16.352427	16.639342	H	9.230548	6.473123	26.011185
N	1.403276	18.073675	15.044188	C	8.875504	8.033978	24.570860
N	6.253689	11.960438	24.868575	H	7.827111	7.747835	24.420106
N	8.009964	10.643627	18.021753	C	9.422577	9.099787	23.854200
C	6.258077	14.313117	27.963075	C	10.756925	9.465835	24.048155
C	8.310452	8.628206	14.722797	H	11.180810	10.309988	23.488932
C	13.990051	4.803689	29.247412	C	11.553018	8.760998	24.943196
H	14.019838	5.219889	30.264382	H	12.611801	9.037675	25.070478
C	14.611284	3.593645	28.920756	C	4.879669	13.623533	19.088784

C	3.634482	13.268211	18.564886	C	8.252397	9.705482	13.642301
H	3.195165	12.291634	18.805568	H	8.594828	9.311228	12.674978
C	2.942274	14.156379	17.748115	H	7.228671	10.078365	13.504026
H	1.956750	13.873218	17.360154	H	8.891886	10.566588	13.885873
C	3.501916	15.405016	17.458003	O	19.081702	18.905819	15.964104
C	4.758313	15.757622	17.957270	O	15.904834	21.999234	16.925957
H	5.201863	16.741844	17.736199	O	21.391793	19.240749	22.694353
C	5.443512	14.860961	18.769800	O	18.192871	22.306499	23.659648
H	6.423530	15.139686	19.174932	N	23.338633	12.584639	14.116929
C	1.971118	17.205690	17.239577	N	22.230004	14.467229	15.707004
H	1.844827	17.258134	18.335125	N	14.595025	26.366935	24.062761
C	1.195969	18.136775	16.409027	N	13.453424	28.203795	25.688635
C	0.278386	19.026521	16.968265	N	17.380108	20.320788	16.455027
H	0.131028	19.059666	18.056763	N	19.898908	20.900747	23.173182
C	-0.454541	19.865775	16.126559	C	16.871217	21.116824	12.692621
H	-1.187025	20.568875	16.547784	C	20.353045	19.732857	26.830488
C	-0.255122	19.795234	14.752065	C	23.945399	11.691592	13.295685
H	-0.826577	20.438811	14.068112	H	23.607726	11.690730	12.250018
C	0.680019	18.891180	14.237930	C	24.947750	10.830063	13.753590
H	0.867947	18.794513	13.159171	H	25.421244	10.124110	13.057160
C	5.361594	12.384083	23.820173	C	25.337993	10.882009	15.086743
C	7.463710	11.273800	24.555626	H	26.125718	10.214095	15.463875
C	7.668485	10.775014	23.163073	C	24.724976	11.799872	15.943759
C	8.614142	9.818336	22.852345	H	25.023812	11.864181	16.999616
C	8.880511	9.499865	21.494764	C	23.735740	12.643638	15.440538
H	9.635259	8.726189	21.271257	C	23.093723	13.665918	16.277749
C	8.241064	10.163711	20.475179	H	23.376526	13.728636	17.345972
C	8.647067	9.898487	19.069523	C	21.651497	15.543095	16.492372
C	6.915049	11.523560	18.299020	C	22.338080	16.756864	16.598890
C	6.546138	11.814358	19.716904	H	23.319156	16.897101	16.128584
C	5.575817	12.742330	20.048304	C	21.775440	17.799530	17.326455
C	5.189780	12.921250	21.405045	H	22.308997	18.754228	17.414995
H	4.364712	13.613516	21.637443	C	20.534028	17.629930	17.943485
C	5.825596	12.240576	22.412173	C	19.861772	16.409879	17.844247
C	6.908835	11.370667	22.112512	H	18.894525	16.272766	18.342916
C	7.223389	11.114549	20.762119	C	20.417379	15.360041	17.120484
C	5.972788	12.393087	26.275348	H	19.892701	14.392224	17.065882
H	4.910151	12.155402	26.498014	C	16.646598	23.508687	21.716383
H	6.578752	11.777837	26.972534	C	17.185731	24.787112	21.878499
C	6.245655	13.879696	26.484922	H	18.139812	25.047723	21.402955
H	5.473116	14.471890	25.944736	C	16.510775	25.734372	22.641037
H	7.215492	14.166056	26.028598	H	16.936349	26.739356	22.749392
C	5.125626	13.660629	28.754271	C	15.294673	25.395300	23.242778
H	4.157458	13.795211	28.252839	C	14.744175	24.123217	23.075078
H	5.040347	14.102174	29.756728	H	13.768194	23.866643	23.517824
H	5.285660	12.582370	28.887586	C	15.425067	23.183190	22.309790
C	6.064328	15.830778	28.008207	H	14.997881	22.182835	22.172375
H	6.785541	16.347912	27.361384	C	13.973444	27.356792	23.472553
H	6.195814	16.218525	29.026688	H	13.910405	27.474176	22.375332
H	5.057154	16.116860	27.674125	C	13.344712	28.377585	24.321255
C	7.598066	13.958847	28.608130	C	12.698163	29.486578	23.774923
H	7.829115	12.890481	28.499081	H	12.620394	29.600838	22.684336
H	7.586903	14.187432	29.682461	C	12.160515	30.451406	24.629948
H	8.439616	14.524943	28.168137	H	11.651826	31.334235	24.218116
C	8.388851	10.346819	16.602191	C	12.284303	30.286814	26.005181
H	9.493257	10.181523	16.553188	H	11.880339	31.036955	26.699094
H	8.191218	11.248811	15.986733	C	12.933550	29.154091	26.506608
C	7.667887	9.130900	16.029509	H	13.058538	28.982948	27.585606
H	7.673816	8.297669	16.762891	C	16.843313	21.329424	17.322100
H	6.600639	9.367648	15.845881	C	18.541501	19.575494	16.832814
C	9.763317	8.223239	14.970601	C	18.999038	19.611018	18.253187
H	10.276203	7.967379	14.033988	C	19.947474	18.728347	18.735338
H	10.327147	9.043605	15.446464	C	20.413740	18.840895	20.071157
H	9.827813	7.351969	15.635018	H	21.188475	18.129903	20.426338
C	7.526709	7.405303	14.242729	C	19.919137	19.809960	20.909791
H	6.479529	7.656963	14.028757	C	20.472970	19.928578	22.286119
H	7.528636	6.603428	14.993938	C	18.757850	21.664138	22.784176
H	7.962120	6.992433	13.322565	C	18.315070	21.646278	21.358296

C	17.336034	22.500821	20.887451	C	16.452984	8.236122	25.541935
C	16.898467	22.414524	19.539739	H	17.255430	7.591783	25.162315
H	16.117437	23.112497	19.190837	C	16.052044	9.359531	24.815601
C	17.413776	21.465813	18.690062	C	15.038029	10.187155	25.303163
C	18.445435	20.591142	19.132273	H	14.737320	11.079445	24.740091
C	18.895365	20.692858	20.466604	C	14.408264	9.888353	26.506703
C	16.847092	20.188801	15.062528	H	13.627656	10.560981	26.896705
H	16.860222	19.109893	14.798850	C	18.709468	11.057352	17.471121
H	15.773145	20.496918	15.044297	C	18.204011	12.215282	16.873543
C	17.619975	21.008628	14.034259	H	17.385256	12.767149	17.352060
H	18.621495	20.565476	13.860138	C	18.735474	12.677643	15.674990
H	17.802673	22.033994	14.416423	H	18.315884	13.578426	15.201790
C	16.615751	19.733146	12.097272	C	19.779586	11.971190	15.072279
H	16.217439	19.811641	11.076847	C	20.274384	10.797906	15.650748
H	15.881379	19.156868	12.687365	H	21.077051	10.224374	15.170575
H	17.538783	19.139383	12.049333	C	19.735997	10.343444	16.850398
C	17.737852	21.918693	11.720414	H	20.123700	9.424846	17.307486
H	18.688606	21.409937	11.514703	C	19.983159	11.911994	12.705623
H	17.973561	22.915132	12.118220	H	19.233266	11.103971	12.639413
H	17.225226	22.063418	10.759730	C	20.604206	12.383214	11.460435
C	15.542193	21.841283	12.895657	C	20.294381	11.809824	10.226982
H	15.698021	22.889258	13.185103	H	19.560063	10.995363	10.162869
H	14.951086	21.361431	13.693501	C	20.935307	12.279125	9.078491
H	14.938836	21.835961	11.979117	H	20.707527	11.837219	8.097450
C	20.378044	20.957229	24.590743	C	21.868966	13.304141	9.189634
H	20.287231	22.002791	24.950419	H	22.391552	13.686517	8.301251
H	21.470104	20.718888	24.620001	C	22.145155	13.848983	10.447360
C	19.618371	19.996521	25.503164	H	22.879643	14.654059	10.585738
H	18.605335	20.392615	25.717001	C	14.915752	8.874761	19.734248
H	19.463679	19.023211	24.993719	C	14.961277	8.473386	22.190383
C	20.536453	21.030759	27.614579	C	16.184275	9.320388	22.302946
H	21.224327	21.718348	27.104095	C	16.703214	9.683860	23.531735
H	20.954692	20.833408	28.611687	C	17.920230	10.410133	23.605714
H	19.581622	21.554437	27.752594	H	18.313456	10.690068	24.606259
C	21.717094	19.101184	26.557651	C	18.600056	10.753958	22.461980
H	21.614287	18.103737	26.108986	C	19.923797	11.421893	22.577031
H	22.301375	18.993661	27.480583	C	19.923395	11.753865	20.108269
H	22.302361	19.719104	25.856000	C	18.691403	10.918175	19.986614
C	19.510955	18.765589	27.663292	C	18.141544	10.601935	18.756915
H	19.350723	17.811497	27.141728	C	16.934378	9.855512	18.685105
H	18.521185	19.184743	27.894219	H	16.523632	9.590377	17.686268
H	20.001193	18.535222	28.618523	C	16.270350	9.484741	19.831109
O	14.468084	7.862754	23.127806	C	16.837882	9.750320	21.108980
O	14.281956	8.825541	18.694138	C	18.051774	10.464572	21.180486
O	20.485701	11.608956	23.640865	C	12.998513	7.640845	20.842005
O	20.423878	12.366301	19.174126	H	12.385914	7.867849	21.747548
N	12.822361	7.678826	30.714595	H	12.415434	8.029166	19.979452
N	14.120695	8.414514	28.454682	C	13.198787	6.133090	20.716782
N	20.353454	12.467271	13.832440	H	13.969139	5.778473	21.431702
N	21.525215	13.407032	11.571114	H	13.582953	5.882655	19.706869
N	14.287057	8.396528	20.932527	C	11.377984	5.621995	22.381842
N	20.574848	11.857613	21.374016	H	10.420038	5.113418	22.551567
C	11.898522	5.347913	20.970465	H	11.221701	6.704500	22.531479
C	23.040751	14.848319	21.496777	H	12.073032	5.290672	23.176350
C	12.194569	7.264333	31.843575	C	12.197430	3.856557	20.814528
H	11.244867	6.731045	31.701580	H	12.963595	3.519965	21.524506
C	12.730142	7.498312	33.114587	H	12.559792	3.627413	19.802425
H	12.195262	7.142690	34.007762	H	11.297865	3.250369	20.983422
C	13.940344	8.173116	33.234164	C	10.830715	5.741777	19.949042
H	14.377971	8.362838	34.226015	H	11.216036	5.668982	18.922404
C	14.600237	8.602566	32.080413	H	10.481246	6.774206	20.097111
H	15.560181	9.130535	32.151391	H	9.952292	5.086166	20.015798
C	14.028652	8.343067	30.835771	C	21.883065	12.577946	21.474645
C	14.693448	8.736212	29.587585	H	22.481587	12.380086	20.553688
H	15.652751	9.277410	29.656259	H	22.464257	12.136905	22.312780
C	14.799280	8.750177	27.215100	C	21.716173	14.083624	21.669848
C	15.825510	7.926162	26.743136	H	20.976864	14.487443	20.947848
H	16.151421	7.044386	27.309410	H	21.304555	14.292890	22.678843

C	24.069234	14.385844	22.526983	C	13.522201	15.130352	28.379137
H	24.974647	15.007642	22.492372	C	12.233918	14.630458	28.409566
H	23.667240	14.446260	23.547140	C	11.125868	15.514413	28.304243
H	24.380812	13.346916	22.353526	H	10.096625	15.097473	28.350756
C	22.771913	16.338772	21.710412	C	11.319962	16.863835	28.125445
H	23.691157	16.927686	21.595599	C	10.143309	17.762734	27.983802
H	22.381670	16.535431	22.718496	C	11.682683	19.666159	27.513192
H	22.036493	16.737576	20.990871	C	12.853010	18.800913	27.840956
C	23.591162	14.635140	20.087995	C	14.142966	19.299222	27.874948
H	22.949218	15.102849	19.327685	C	15.226730	18.441614	28.206633
H	23.652336	13.560261	19.848354	H	16.238137	18.872102	28.301349
H	24.597388	15.062701	19.985790	C	15.026198	17.098374	28.409645
O	14.677351	13.051042	28.089043	C	13.723650	16.541243	28.291720
O	17.232241	16.655814	29.198812	C	12.632989	17.410688	28.089927
O	8.999389	17.407245	28.200299	C	17.216434	13.926312	28.745735
O	11.781568	20.842555	27.192316	H	17.754966	14.197022	29.679090
N	10.323939	6.451901	29.114361	H	16.914419	12.860295	28.854453
N	10.906313	9.095804	28.892420	C	18.134572	14.068936	27.534171
N	15.749417	24.650525	26.667661	H	18.592277	15.080278	27.521271
N	16.496827	27.218157	26.182380	H	17.551328	13.985757	26.594920
N	16.005069	14.802619	28.648115	C	20.259274	13.408725	26.426190
N	10.369364	19.103653	27.514901	H	21.033801	12.639440	26.303152
C	19.255324	13.013021	27.509209	H	20.766622	14.350482	26.676561
C	7.640335	21.800879	28.116815	H	19.771571	13.542667	25.451109
C	10.050479	5.134421	29.288986	C	19.988118	12.946002	28.848792
H	10.887670	4.441481	29.123389	H	20.898063	12.334546	28.771353
C	8.780164	4.687107	29.666936	H	19.363915	12.497888	29.633530
H	8.597489	3.612394	29.803598	H	20.289814	13.944484	29.190691
C	7.762160	5.612465	29.870866	C	18.667683	11.640633	27.183132
H	6.757748	5.279472	30.169666	H	19.404411	10.843164	27.351088
C	8.029988	6.972799	29.701329	H	17.790965	11.434830	27.817709
H	7.242746	7.721120	29.865516	H	18.346224	11.563431	26.128668
C	9.314148	7.371227	29.328853	C	9.186818	19.979576	27.238706
C	9.664112	8.789207	29.171920	H	8.381453	19.344788	26.812343
H	8.864497	9.538159	29.306541	H	9.453482	20.711334	26.438696
C	11.258530	10.501044	28.773321	C	8.683420	20.725093	28.470333
C	11.550527	11.246012	29.920399	H	8.237830	20.012495	29.194382
H	11.509648	10.791382	30.917535	H	9.528949	21.209989	28.999989
C	11.879682	12.591712	29.798116	C	7.197628	22.485529	29.410449
H	12.104375	13.181237	30.696383	H	6.473164	23.286036	29.208260
C	11.914501	13.194445	28.538036	H	6.717353	21.773444	30.095179
C	11.621353	12.442510	27.398297	H	8.046845	22.935457	29.942642
H	11.645974	12.914368	26.408769	C	6.417772	21.173900	27.450205
C	11.295300	11.094458	27.509453	H	6.650835	20.786824	26.448433
H	11.044800	10.518570	26.603870	H	5.609002	21.908614	27.332758
C	14.509659	20.696742	27.566594	H	6.021223	20.340631	28.045680
C	14.574682	21.657515	28.577725	C	8.254681	22.841647	27.181626
H	14.317444	21.387910	29.609853	H	9.047531	23.416531	27.681362
C	14.973088	22.958220	28.282865	H	7.499177	23.553476	26.825347
H	15.034488	23.696797	29.090646	H	8.708359	22.358826	26.298617
C	15.310269	23.296400	26.969109	O	5.270185	19.062174	19.830560
C	15.242104	22.341509	25.950222	O	5.724075	21.335538	23.744300
H	15.519708	22.598553	24.914266	O	10.854399	22.523265	17.174702
C	14.840474	21.045667	26.254223	O	11.650489	24.398060	21.231812
H	14.791569	20.294167	25.457650	N	2.860251	17.011212	12.362541
C	17.036375	24.887875	26.616887	N	4.316091	18.153728	14.340417
H	17.808453	24.110321	26.753382	N	12.562165	25.477886	26.539923
C	17.481697	26.267099	26.374361	N	14.192953	26.602228	28.370489
C	18.834498	26.606947	26.367133	N	5.383898	20.251888	21.760742
H	19.600864	25.834337	26.518387	N	11.368591	23.350795	19.240615
C	19.199944	27.941238	26.171245	C	3.517534	17.378703	23.573074
H	20.261309	28.228746	26.166451	C	13.723372	26.147683	17.950348
C	18.209268	28.900395	25.992464	C	2.081456	16.484619	11.384122
H	18.470847	29.957644	25.848032	H	1.359253	15.718676	11.702302
C	16.865974	28.510868	26.001567	C	2.188751	16.896392	10.051528
H	16.047343	29.231825	25.868988	H	1.536823	16.449928	9.288227
C	16.170504	16.225829	28.789744	C	3.117695	17.873030	9.710784
C	14.725208	14.243694	28.360312	H	3.215645	18.209345	8.669596

C	3.922341	18.429853	10.707843	H	3.669246	16.035641	21.854906
H	4.657767	19.208956	10.462586	H	2.731004	17.511580	21.547828
C	3.774914	17.991861	12.024272	C	12.620815	23.980210	18.711926
C	4.555721	18.575630	13.123853	H	13.043276	23.313144	17.930363
H	5.304534	19.355349	12.882118	H	13.382884	24.010568	19.528406
C	5.026965	18.788796	15.436020	C	12.401913	25.384609	18.157926
C	6.172950	18.185786	15.956744	H	11.857401	25.333588	17.193271
H	6.549960	17.235514	15.546794	H	11.757064	25.975950	18.840873
C	6.871735	18.822376	16.977672	C	14.629609	25.406860	16.970161
H	7.782315	18.361731	17.381333	H	15.010700	24.467523	17.397396
C	6.429521	20.048505	17.478389	H	15.500159	26.017529	16.695041
C	5.265634	20.631508	16.969849	H	14.096739	25.157353	16.042406
H	4.911733	21.591559	17.367104	C	13.397717	27.526862	17.378300
C	4.562350	20.004755	15.947218	H	12.725814	28.092191	18.039004
H	3.664659	20.486252	15.539387	H	12.908867	27.448169	16.397836
C	10.237619	23.683631	23.498541	H	14.308467	28.126883	17.243378
C	9.981517	25.003334	23.876450	C	14.447744	26.313115	19.284780
H	9.183108	25.572216	23.384006	H	15.430755	26.782617	19.149479
C	10.738578	25.599421	24.879893	H	14.602593	25.333021	19.770035
H	10.520259	26.632295	25.177810	H	13.873619	26.936886	19.983783
C	11.751419	24.865771	25.503493	O	8.769418	17.665061	13.652478
C	12.011349	23.542554	25.134602	O	12.906525	19.495831	13.414318
H	12.789591	22.951588	25.645261	O	11.662059	11.158684	13.282888
C	11.248887	22.956593	24.131281	O	15.809354	12.974713	13.295395
H	11.439462	21.915241	23.845899	N	1.419855	14.929127	14.350275
C	12.129620	25.469937	27.775880	N	4.104668	14.855647	14.022608
H	11.172822	25.017226	28.089106	N	20.504883	15.728459	13.165135
C	12.975623	26.102554	28.797383	N	23.216158	15.655193	13.135838
C	12.570822	26.206766	30.127605	N	10.834296	18.590621	13.733017
H	11.599100	25.804864	30.444584	N	13.756735	12.050012	13.071535
C	13.413206	26.836316	31.047675	C	8.866142	21.816706	12.871125
H	13.108885	26.933254	32.099883	C	15.042972	8.598138	14.269596
C	14.634392	27.343840	30.617922	C	0.069810	14.981177	14.473569
H	15.312120	27.848613	31.321029	H	-0.355870	15.964387	14.713754
C	14.999087	27.214030	29.273741	C	-0.730521	13.847597	14.300117
H	15.949730	27.604808	28.885241	H	-1.821963	13.927889	14.405114
C	6.139672	21.122376	22.619630	C	-0.135037	12.630154	13.988959
C	5.824608	19.972012	20.432317	H	-0.749646	11.728921	13.845018
C	6.933510	20.783392	19.846228	C	1.253904	12.562048	13.854642
C	7.228525	20.757229	18.496830	H	1.744469	11.611148	13.603637
C	8.383688	21.423831	18.007601	C	2.010679	13.719545	14.035732
H	8.605483	21.374530	16.927609	C	3.472224	13.717174	13.887928
C	9.226632	22.094507	18.860662	H	3.972733	12.758325	13.670715
C	10.495255	22.666238	18.331272	C	5.548743	14.880663	13.869067
C	10.953538	23.632843	20.581704	C	6.351283	14.847511	15.012164
C	9.743607	22.952197	21.129678	H	5.906143	14.769821	16.016064
C	9.412003	23.022718	22.469700	C	7.733675	14.884966	14.872398
C	8.218562	22.416508	22.942917	H	8.368679	14.849884	15.764543
H	7.957242	22.525250	24.009084	C	8.312561	14.958087	13.603537
C	7.399610	21.714808	22.092860	C	7.503497	14.983370	12.465354
C	7.744136	21.568326	20.721298	H	7.956715	15.032900	11.467126
C	8.905549	22.210846	20.241737	C	6.118332	14.944327	12.594148
C	4.229797	19.498279	22.345682	H	5.493819	14.950881	11.692142
H	3.565577	19.125708	21.530179	C	16.270926	15.683442	13.168257
H	3.618387	20.213668	22.936437	C	16.966105	15.543468	11.964634
C	4.676972	18.324684	23.213925	H	16.417565	15.422312	11.023045
H	5.463736	17.738727	22.695423	C	18.356607	15.557708	11.957549
H	5.141015	18.698295	24.150598	H	18.890788	15.458393	11.004956
C	2.407592	18.128414	24.306891	C	19.051160	15.715842	13.161365
H	1.894958	18.842486	23.648253	C	18.362909	15.868408	14.367293
H	2.803465	18.691008	25.163352	H	18.906397	16.033175	15.312454
H	1.646963	17.435026	24.689853	C	16.972565	15.851477	14.364302
C	4.059848	16.282501	24.490212	H	16.427767	15.976926	15.307463
H	3.280188	15.547916	24.737015	C	21.116721	16.849342	12.876728
H	4.434197	16.694304	25.438505	H	20.590530	17.795130	12.659291
H	4.887014	15.733866	24.018013	C	22.583994	16.846363	12.829625
C	2.955639	16.740362	22.304105	C	23.305030	17.984744	12.470741
H	2.030072	16.188195	22.511108	H	22.781241	18.921560	12.234933

C	24.698869	17.914630	12.405075	C	14.006278	13.987857	18.080758
H	25.284392	18.800541	12.116966	C	10.455766	16.877571	18.520525
C	25.334975	16.713882	12.699557	C	9.741156	15.880195	19.307124
H	26.429560	16.630737	12.645421	C	10.094373	14.545464	19.215672
C	24.569501	15.600429	13.061197	C	13.307928	15.006998	17.457355
H	25.027498	14.629571	13.297086	C	11.858126	15.082970	17.586878
C	12.240911	18.476441	13.469524	C	11.487540	16.489112	17.683639
C	9.972974	17.456819	13.602608	C	12.543162	16.781315	24.278659
C	10.569748	16.094253	13.473283	C	11.845130	17.800937	23.656144
C	9.783768	14.956860	13.475670	C	13.992481	16.705765	24.150758
C	10.385208	13.675268	13.376726	C	9.960745	17.824289	20.623212
H	9.736695	12.783529	13.373453	C	9.434823	16.465511	20.606388
C	11.749887	13.540582	13.296382	C	15.267592	14.273586	18.753590
C	12.334789	12.173829	13.221011	C	13.833577	16.366243	17.474625
C	14.608418	13.188009	13.205666	C	10.084988	16.224844	22.968215
C	14.009566	14.556155	13.223940	C	10.583743	17.515582	22.983718
C	14.794710	15.694014	13.195333	C	9.496032	15.686380	21.748301
C	14.189419	16.977808	13.233975	C	10.520444	18.335876	21.780955
H	14.842076	17.874276	13.175867	C	15.031152	16.637718	18.113163
C	12.826554	17.114122	13.343442	C	14.099499	12.956391	22.471839
C	11.988473	15.964548	13.367551	C	13.509693	12.419863	21.251915
C	12.588480	14.688741	13.290443	C	12.060147	12.493604	21.381024
C	10.234830	19.947506	13.932726	C	11.753150	13.077635	22.681042
H	9.358668	19.856574	14.619888	C	13.013816	13.363716	23.354791
H	10.974251	20.580647	14.468863	C	15.258228	13.710582	22.404697
C	9.801608	20.616842	12.631534	C	15.888649	13.965892	21.116006
H	9.281264	19.889878	11.973960	C	15.329082	13.455291	19.958413
H	10.691673	20.957863	12.063365	C	14.108094	12.662989	20.028130
C	8.516284	22.432351	11.516078	C	11.284220	12.809019	20.279214
H	8.040032	21.701076	10.849534	C	10.159494	13.725450	20.418529
H	9.412225	22.810994	11.006110	C	9.867923	14.280656	21.651871
H	7.822768	23.276301	11.630302	C	10.685625	13.948876	22.812136
C	9.551878	22.875375	13.732980	C	11.914205	13.062615	18.989885
H	8.957086	23.797689	13.775320	C	13.290709	12.991319	18.867369
H	10.539313	23.138977	13.331224	C	13.142365	14.506504	24.124924
H	9.693632	22.529137	14.766507	C	12.017549	15.422067	24.263489
C	7.584681	21.354055	13.562192	C	10.820651	15.151005	23.624542
H	6.942252	22.205097	13.820359	C	15.394388	14.912052	23.218112
H	7.819589	20.809549	14.494745	C	14.363302	15.299417	24.055560
H	6.998515	20.674301	12.926947	C	15.766664	15.564522	18.770066
C	14.362383	10.684537	12.973800	C	16.415619	15.324616	21.132465
H	15.245958	10.748854	12.307346	C	16.356619	16.103014	19.989639
H	13.644138	9.996316	12.463300	C	16.110159	15.909777	22.432048
C	14.743956	10.106938	14.334038	C	12.708181	17.282243	17.613412
H	15.627706	10.639233	14.740441	C	10.591844	18.078983	19.334254
H	13.926832	10.267969	15.067581	C	12.559987	18.798720	22.871219
C	13.808365	7.842451	13.776893	C	11.741419	19.129019	21.711511
H	14.012113	6.770059	13.667274	C	12.340875	19.369896	20.488029
H	12.958930	7.952526	14.467041	C	11.751387	18.831423	19.268486
H	13.479972	8.228585	12.797353	C	12.836851	18.423293	18.386084
C	16.218546	8.318458	13.335882	C	15.757990	17.244914	22.523699
H	15.984681	8.590573	12.297507	C	14.671965	17.653899	23.406005
H	16.481520	7.251128	13.337432	C	13.936952	18.727313	22.749357
H	17.111765	8.881812	13.635130	C	14.568026	18.981377	21.460105
C	15.394381	8.116537	15.678125	C	13.790610	19.293835	20.358896
H	15.821351	7.104676	15.658872	C	14.096934	18.708469	19.060018
H	16.127836	8.775427	16.177872	C	15.164791	17.838693	18.927755
H	14.502473	8.083529	16.317535	C	15.982939	17.508033	20.086968
C	11.179333	14.135966	18.332996	C	15.692394	18.064563	21.320570

Table S2. Cartesian coordinates (in Å) for the PM3 model of the *tert*-butyl derivative of C_{60}⊂**1**-ΛΔΔΔ.

Fe	12.340419	7.448859	28.676333	C	8.522160	9.949648	19.169245
Fe	2.765935	16.363929	14.398839	C	6.794602	11.577813	18.401098
Fe	21.703489	14.010424	13.477607	C	6.441234	11.886420	19.817544
Fe	14.435139	26.611082	26.493994	C	5.461151	12.806527	20.142625
O	8.280665	11.306292	25.541767	C	5.110349	13.023100	21.502552
O	4.263658	13.025792	24.234938	H	4.282698	13.711679	21.735407
O	9.371727	9.128290	18.868661	C	5.781730	12.382030	22.513437
O	6.216581	12.065667	17.439976	C	6.861835	11.506795	22.215735
N	13.545781	5.704297	28.265265	C	7.145884	11.217610	20.865144
N	11.962613	7.097022	26.557076	C	5.915261	12.498392	26.386724
N	2.554923	16.170363	16.558361	H	4.900758	12.088252	26.578655
N	1.216079	17.797292	14.846830	H	6.610147	11.961276	27.075502
N	6.267380	12.189777	24.964126	C	5.957146	13.990390	26.711317
N	7.895292	10.706652	18.123340	H	5.094613	14.515062	26.245421
C	5.946390	14.241596	28.231626	H	6.862675	14.464382	26.280015
C	8.014502	8.909959	14.680823	C	4.777788	13.519856	28.903899
C	14.291765	4.976927	29.134082	H	3.828213	13.747293	28.401001
H	14.307445	5.334410	30.173150	H	4.675357	13.822145	29.955257
C	14.991663	3.835860	28.728841	H	4.906833	12.428899	28.894026
H	15.581887	3.268066	29.461778	C	5.787260	15.739026	28.488223
C	14.927544	3.430009	27.400361	H	6.617739	16.336860	28.075540
H	15.470559	2.534982	27.064886	H	5.741568	15.955643	29.565538
C	14.159036	4.166208	26.495627	H	4.859099	16.124877	28.039430
H	14.088676	3.861612	25.442258	C	7.264309	13.748585	28.827944
C	13.473257	5.293489	26.947363	H	7.431565	12.692147	28.557756
C	12.623302	6.086291	26.049292	H	7.264568	13.826596	29.922072
H	12.570853	5.789895	24.976034	H	8.128676	14.323339	28.450198
C	11.089554	7.857281	25.676137	C	8.277042	10.437020	16.700601
C	9.729656	7.540604	25.605227	H	9.359114	10.164136	16.654908
H	9.305981	6.726808	26.206512	H	8.180851	11.386916	16.133445
C	8.903693	8.247519	24.736369	C	7.451107	9.331825	16.050985
H	7.839480	7.990692	24.667783	H	7.420604	8.438531	16.707846
C	9.429373	9.271031	23.944585	H	6.398177	9.657497	15.928881
C	10.785801	9.594835	24.037533	C	9.439913	8.383673	14.838365
H	11.199159	10.405798	23.423091	H	9.905747	8.191997	13.863428
C	11.620387	8.889644	24.897260	H	10.070914	9.109403	15.378216
H	12.693542	9.137323	24.942644	H	9.459289	7.444801	15.407573
C	4.724219	13.632350	19.164836	C	7.129258	7.796072	14.119433
C	3.458584	13.247644	18.716415	H	6.099206	8.142036	13.961438
H	3.022283	12.297680	19.049045	H	7.088867	6.932077	14.796438
C	2.742277	14.072813	17.854822	H	7.509546	7.437162	13.153523
H	1.741227	13.767229	17.526286	C	8.005928	10.084671	13.703968
C	3.299344	15.286748	17.440966	H	8.279795	9.756815	12.691827
C	4.570388	15.671470	17.874770	H	7.012795	10.549423	13.644906
H	5.009643	16.632039	17.564011	H	8.722468	10.866412	13.996098
C	5.278109	14.841236	18.736336	O	19.059629	19.171208	16.323065
H	6.269566	15.148235	19.089513	O	16.172287	22.232116	17.997295
C	1.652424	16.960084	17.084801	O	21.476291	18.053201	22.950997
H	1.428174	16.999775	18.164122	O	19.678659	22.037320	24.218308
C	0.888263	17.838508	16.189338	N	23.088662	12.439620	14.003998
C	-0.130930	18.662156	16.667279	N	22.131887	14.434201	15.559001
H	-0.375377	18.678505	17.738311	N	13.692602	26.693053	24.418877
C	-0.841637	19.458151	15.765709	N	15.639584	28.168635	25.623516
H	-1.653156	20.108701	16.122460	N	17.452918	20.517300	17.199432
C	-0.517054	19.412976	14.414315	N	20.598754	20.045886	23.642033
H	-1.065314	20.024658	13.684185	C	16.291738	21.645136	13.662817
C	0.515255	18.573640	13.982565	C	20.882627	18.660730	27.235110
H	0.802681	18.499189	12.924270	C	23.609293	11.476523	13.202857
C	5.347118	12.566712	23.925269	H	23.259486	11.474752	12.160928
C	7.452105	11.457150	24.654047	C	24.542224	10.548288	13.676724
C	7.643077	10.935745	23.265918	H	24.946370	9.784949	12.997416
C	8.585846	9.973759	22.957683	C	24.952314	10.606853	15.004203
C	8.819072	9.623395	21.600437	H	25.685611	9.885941	15.392586
H	9.566997	8.843904	21.376857	C	24.428436	11.596071	15.839938
C	8.155499	10.258014	20.577891	H	24.740936	11.665934	16.891188

C	23.505221	12.503388	15.321209	C	21.180383	19.874506	25.011840
C	22.943294	13.585350	16.140064	H	21.504234	20.866840	25.389932
H	23.227838	13.647766	17.215773	H	22.108141	19.254077	24.949940
C	21.601459	15.525230	16.360028	C	20.194091	19.217884	25.975641
C	22.278242	16.747427	16.402434	H	19.412976	19.944393	26.276918
H	23.196178	16.907685	15.824165	H	19.658958	18.384144	25.475452
C	21.798098	17.767422	17.218022	C	21.617284	19.767089	27.989077
H	22.331820	18.724591	17.268517	H	22.471394	20.151411	27.414600
C	20.645594	17.567195	17.980078	H	22.009262	19.399506	28.947089
C	19.953387	16.356119	17.901475	H	20.952897	20.613629	28.205546
H	19.040875	16.204930	18.492194	C	21.867349	17.561073	26.844347
C	20.429796	15.329195	17.095924	H	21.343148	16.675752	26.445396
H	19.900383	14.363430	17.071477	H	22.464612	17.232745	27.704813
C	10.892097	24.292410	22.341916	H	22.562129	17.915856	26.065372
C	10.613870	25.644789	22.556288	C	19.809202	18.069308	28.149540
H	9.699638	26.090570	22.144863	H	19.213740	17.291785	27.638194
C	11.512905	26.439787	23.260431	H	19.110782	18.838753	28.504137
H	11.299234	27.508672	23.388755	H	20.259795	17.599545	29.035030
C	12.687268	25.872506	23.766709	O	14.608930	7.980328	23.276645
C	12.938591	24.507454	23.610163	O	14.594777	8.395165	18.773608
H	13.846707	24.048771	24.039104	O	20.395707	12.138246	23.618498
C	12.041148	23.722415	22.895542	O	20.639811	12.188144	19.107438
H	12.249958	22.656541	22.748823	N	12.928502	7.707392	30.741786
C	14.260756	27.630105	23.699553	N	14.178371	8.621538	28.515196
H	13.998804	27.829179	22.645124	N	20.112086	12.533077	13.755122
C	15.301389	28.461016	24.315614	N	21.287460	13.357774	11.456141
C	15.919352	29.495717	23.613252	N	14.437773	8.381367	21.051444
H	15.632575	29.710418	22.574517	N	20.657733	11.959087	21.358979
C	16.901841	30.258089	24.249818	C	12.064869	5.316310	21.186080
H	17.396836	31.081313	23.714416	C	23.536888	14.521149	20.987462
C	17.241612	29.967489	25.566552	C	12.332386	7.203545	31.851671
H	18.008674	30.554474	26.091250	H	11.436844	6.589137	31.682858
C	16.594569	28.919100	26.229025	C	12.833539	7.446597	33.134678
H	16.826528	28.659155	27.271235	H	12.325588	7.017676	34.009977
C	17.091821	21.460935	18.217143	C	13.974043	8.227529	33.286731
C	18.638645	19.720826	17.328887	H	14.381931	8.429633	34.287409
C	19.250652	19.564034	18.679876	C	14.603627	8.746163	32.152802
C	20.190601	18.587305	18.944625	H	15.511871	9.356930	32.249242
C	20.747441	18.462713	20.245525	C	14.070712	8.470753	30.893566
H	21.492670	17.659558	20.429203	C	14.717835	8.945088	29.663387
C	20.358270	19.301338	21.259718	H	15.644459	9.536430	29.759172
C	20.864900	19.061875	22.639394	C	14.863424	8.997979	27.291450
C	19.759860	21.170942	23.362657	C	15.981597	8.265370	26.877566
C	19.032297	21.233293	22.056648	H	16.377152	7.442272	27.485557
C	18.010808	22.138416	21.828724	C	16.605182	8.587526	25.678573
C	17.410420	22.223835	20.547111	H	17.476255	8.010884	25.343882
H	16.611051	22.962102	20.386845	C	16.114263	9.634810	24.893612
C	17.806050	21.397389	19.521768	C	15.022881	10.386252	25.332723
C	18.836966	20.439789	19.730486	H	14.654724	11.226745	24.729311
C	19.417096	20.339977	21.012967	C	14.392473	10.071498	26.533358
C	16.704885	20.511087	15.904079	H	13.541712	10.679887	26.879966
H	16.756656	19.484550	15.484827	C	18.688902	11.128172	17.484598
H	15.624338	20.701510	16.113181	C	18.183874	12.315014	16.946153
C	17.213138	21.531275	14.892161	H	17.425455	12.888748	17.495776
H	18.237019	21.267381	14.558837	C	18.631946	12.773612	15.711811
H	17.293727	22.531432	15.365362	H	18.208558	13.694799	15.280629
C	16.238217	20.325462	12.893294	C	19.596796	12.038427	15.020121
H	15.743660	20.458658	11.920830	C	20.083228	10.833017	15.537116
H	15.672704	19.543726	13.430762	H	20.814553	10.232521	14.981982
H	17.245094	19.931402	12.702575	C	19.626119	10.379706	16.769960
C	16.861280	22.724683	12.740182	H	20.006786	9.436286	17.180501
H	17.864841	22.458891	12.382656	C	19.640664	12.024168	12.644985
H	16.937042	23.694007	13.251819	H	18.822245	11.279572	12.612205
H	16.223437	22.870035	11.857849	C	20.252492	12.444831	11.377298
C	14.882890	22.047750	14.091634	C	19.837417	11.915486	10.155490
H	14.855648	23.072888	14.502065	H	19.010345	11.193480	10.117568
H	14.499774	21.375562	14.877376	C	20.492829	12.307158	8.985997
H	14.182495	22.011418	13.247260	H	20.183948	11.896233	8.014216

C	21.544709	13.213305	9.065497	C	10.319905	5.047343	29.203744
H	22.084168	13.528251	8.161398	H	11.192022	4.418270	28.977089
C	21.919993	13.723116	10.312572	C	9.087044	4.501986	29.576421
H	22.747101	14.437985	10.425951	H	8.971017	3.411277	29.646466
C	15.117182	8.709136	19.828416	C	8.021445	5.349358	29.860304
C	15.091328	8.556801	22.312242	H	7.046331	4.938014	30.158157
C	16.277461	9.459806	22.390914	C	8.203031	6.731393	29.769116
C	16.754735	9.936455	23.598462	H	7.376332	7.418882	29.994591
C	17.922792	10.742994	23.637259	C	9.451097	7.229012	29.395087
H	18.259795	11.151391	24.614902	C	9.710502	8.671564	29.292025
C	18.621539	11.016159	22.484379	H	8.872058	9.366692	29.466435
C	19.919131	11.740975	22.570537	C	11.205986	10.473340	28.860480
C	20.049543	11.749363	20.085422	C	11.456874	11.256827	29.990369
C	18.764393	10.994556	20.006983	H	11.437091	10.823177	30.997538
C	18.187977	10.664891	18.794155	C	11.714444	12.615402	29.835667
C	17.011683	9.871790	18.755338	H	11.904254	13.237916	30.718779
H	16.602314	9.580552	17.765492	C	11.716323	13.186853	28.561180
C	16.391447	9.473503	19.914498	C	11.480568	12.391824	27.437176
C	16.932414	9.836909	21.179786	H	11.478504	12.841090	26.436696
C	18.118237	10.600571	21.219076	C	11.224940	11.033723	27.580872
C	13.158640	7.607708	20.989948	H	11.009003	10.423856	26.689071
H	12.548520	7.857286	21.891562	C	13.184794	21.023006	28.054552
H	12.575690	7.973700	20.117947	C	13.195498	21.881367	29.156655
C	13.360564	6.097715	20.902274	H	13.184327	21.470556	30.174301
H	14.138285	5.766579	21.620777	C	13.167901	23.260061	28.966449
H	13.737689	5.820903	19.896531	H	13.131196	23.921968	29.841190
C	11.572567	5.612515	22.600764	C	13.146878	23.779386	27.667081
H	10.608049	5.128306	22.797851	C	13.213932	22.925384	26.564965
H	11.448791	6.699286	22.753686	H	13.215233	23.330805	25.538368
H	12.285906	5.258563	23.365312	C	13.233067	21.550364	26.761862
C	12.365162	3.822439	21.060044	H	13.254381	20.879820	25.895207
H	13.158865	3.509087	21.751438	C	11.910736	25.784097	27.852644
H	12.691126	3.565023	20.043155	H	11.099968	25.241632	28.371188
H	11.475647	3.217440	21.282190	C	11.745051	27.227511	27.646776
C	10.973790	5.689943	20.184229	C	10.605445	27.898016	28.092314
H	11.334236	5.601709	19.150638	H	9.799700	27.348083	28.598065
H	10.623252	6.722701	20.327488	C	10.505884	29.277103	27.893897
H	10.100236	5.031763	20.285565	H	9.617998	29.823823	28.242822
C	22.052150	12.497725	21.428053	C	11.543504	29.949157	27.257396
H	22.651234	12.032444	20.608381	H	11.493444	31.035303	27.095435
H	22.516952	12.153916	22.376695	C	12.664158	29.232466	26.824694
C	22.119599	14.018524	21.319403	H	13.508946	29.723480	26.321799
H	21.423146	14.383910	20.536675	C	15.579106	16.762863	28.835534
H	21.783759	14.485464	22.267850	C	14.404916	14.589765	28.487028
C	24.524820	14.116103	22.081358	C	13.097238	15.309534	28.442148
H	25.507186	14.580374	21.919391	C	11.887103	14.641951	28.390328
H	24.172220	14.427359	23.073768	C	10.691701	15.352477	28.089544
H	24.677668	13.028916	22.109111	H	9.736931	14.795794	27.992732
C	23.501866	16.047517	20.904991	C	10.723298	16.706819	27.877644
H	24.450498	16.446833	20.522487	C	9.547493	17.408019	27.297066
H	23.331786	16.493419	21.895687	C	10.574727	19.560829	27.992866
H	22.696849	16.413550	20.243501	C	11.898182	18.869997	28.098266
C	24.005926	13.947759	19.651494	C	13.091628	19.559129	28.217798
H	23.389536	14.304253	18.808372	C	14.294768	18.850626	28.468172
H	23.940775	12.846207	19.654757	H	15.226022	19.419917	28.604675
H	25.047470	14.224304	19.442250	C	14.304414	17.477891	28.558790
O	14.505872	13.376214	28.365618	C	13.105369	16.737501	28.377773
O	16.595558	17.326700	29.197986	C	11.913310	17.444823	28.126628
O	8.696778	16.833898	26.637374	C	16.942643	14.648397	28.607859
O	10.393696	20.723081	28.313998	H	17.513007	14.965590	29.507014
N	10.509983	6.387285	29.107676	H	16.809317	13.544064	28.695790
N	10.925932	9.055181	28.991694	C	17.730882	14.952162	27.335175
N	13.007902	25.205838	27.428915	H	18.092481	16.008468	27.350517
N	12.773814	27.892356	27.006963	H	17.079014	14.861768	26.442927
N	15.612239	15.339568	28.626035	C	19.720531	14.491206	25.916834
N	9.464908	18.830880	27.452972	H	20.552062	13.809066	25.691955
C	18.948847	14.026395	27.152011	H	20.153116	15.497194	26.064537
C	5.783667	19.767277	28.200770	H	19.077948	14.532088	25.027798

C	19.877762	14.114619	28.363251	H	16.262638	21.391950	23.715269
H	20.818686	13.577367	28.181182	C	16.883625	25.128887	27.278427
H	19.420439	13.676696	29.260434	H	17.777821	24.482512	27.316096
H	20.134215	15.160092	28.593229	C	16.527361	25.879592	28.488879
C	18.498217	12.577557	26.957911	C	17.312151	25.822771	29.640556
H	19.323665	11.877630	27.145070	H	18.215785	25.198540	29.666380
H	17.681089	12.330553	27.655971	C	16.938236	26.576355	30.756052
H	18.140035	12.375009	25.932589	H	17.547311	26.549148	31.671318
C	8.128118	19.481351	27.300975	C	15.794214	27.364151	30.693486
H	7.692101	19.180982	26.317820	H	15.482361	27.971420	31.555096
H	8.234635	20.590853	27.250604	C	15.037220	27.386214	29.517186
C	7.160918	19.116277	28.423664	H	14.129640	27.998347	29.419578
H	7.029688	18.008412	28.481048	C	6.913868	21.397040	22.427638
H	7.560899	19.434101	29.406812	C	6.196759	20.161057	20.391471
C	4.852445	19.352187	29.338949	C	7.197133	20.910651	19.575901
H	3.856141	19.797217	29.214790	C	7.267748	20.773670	18.204512
H	4.725857	18.259870	29.375882	C	8.300669	21.419441	17.471198
H	5.238447	19.674489	30.314991	H	8.329932	21.278104	16.368079
C	5.202665	19.279628	26.877830	C	9.248292	22.178076	18.113091
H	5.882041	19.488183	26.026875	C	10.381193	22.739136	17.327184
H	4.231956	19.747839	26.643452	C	11.183578	23.895972	19.381392
H	5.038095	18.185718	26.883960	C	10.097440	23.249528	20.181358
C	5.921204	21.287894	28.187058	C	9.972086	23.455965	21.544128
H	6.185198	21.673683	29.180666	C	8.915438	22.840568	22.263585
H	4.985705	21.772643	27.880326	H	8.823841	23.040693	23.341642
H	6.714081	21.604203	27.489277	C	8.013741	22.015539	21.635520
O	5.552992	19.216195	19.959764	C	8.123424	21.772597	20.238884
O	6.777842	21.573056	23.626705	C	9.159882	22.402528	19.516499
O	10.542006	22.495104	16.141424	C	4.813380	19.985163	22.506237
O	11.977040	24.694426	19.853786	H	4.012302	19.712826	21.777733
N	2.898904	16.818086	12.283155	H	4.394045	20.794674	23.140328
N	4.170622	18.000862	14.351453	C	5.165126	18.766967	23.357873
N	16.134311	25.266771	26.211976	H	5.927322	18.140664	22.852593
N	15.385805	26.657073	28.427422	H	5.626077	19.092621	24.323033
N	5.974431	20.553004	21.749833	C	2.853616	18.699561	24.377950
N	11.351330	23.543968	18.002877	H	2.429040	19.475350	23.726604
C	3.934397	17.889941	23.663602	H	3.253010	19.201906	25.276988
C	13.184048	26.288938	15.953382	H	2.024662	18.055314	24.701252
C	2.204902	16.265703	11.257019	C	4.368516	16.736441	24.569260
H	1.511138	15.456534	11.523722	H	3.538190	16.040673	24.754798
C	2.361042	16.707877	9.938720	H	4.715770	17.100126	25.553836
H	1.778040	16.239541	9.132815	H	5.188319	16.155726	24.125136
C	3.251245	17.740104	9.662730	C	3.365172	17.318423	22.365902
H	3.384673	18.100437	8.632537	H	2.421752	16.786901	22.543919
C	3.970439	18.322006	10.709433	H	4.062108	16.612182	21.895362
H	4.676455	19.143650	10.519092	H	3.168844	18.125729	21.640473
C	3.775889	17.852076	12.007561	C	12.441654	24.191191	17.201564
C	4.474017	18.443780	13.154732	H	12.767324	23.477579	16.413750
H	5.233440	19.242033	12.979326	H	13.337033	24.348254	17.850133
C	4.857090	18.623202	15.471312	C	12.010255	25.518660	16.586291
C	6.042827	18.051364	15.938854	H	11.231319	25.350122	15.815280
H	6.423221	17.104471	15.522049	H	11.542453	26.163700	17.358209
C	6.787889	18.729529	16.895772	C	13.780301	25.507577	14.784819
H	7.739586	18.307567	17.240392	H	14.265375	24.571153	15.110689
C	6.352976	19.967523	17.375116	H	14.543150	26.100498	14.262050
C	5.119556	20.484639	16.972736	H	13.010594	25.239398	14.049224
H	4.758407	21.434874	17.384460	C	12.651383	27.622727	15.426316
C	4.365772	19.813139	16.016293	H	12.197988	28.223386	16.225991
H	3.417859	20.245778	15.674136	H	11.888105	27.471650	14.651449
C	17.450668	23.001954	22.886827	H	13.457275	28.222698	14.981735
C	17.804633	24.348412	22.990434	C	14.263355	26.559055	16.999561
H	18.479493	24.797846	22.251225	H	15.158103	27.002844	16.544590
C	17.340783	25.111856	24.059311	H	14.565324	25.626693	17.505115
H	17.660822	26.157011	24.151396	H	13.905296	27.250359	17.773509
C	16.521274	24.520269	25.024146	O	8.922626	17.632023	14.418156
C	16.107201	23.192221	24.886529	O	12.666078	19.576265	12.712657
H	15.457806	22.720188	25.638067	O	11.869763	11.251999	13.316769
C	16.566197	22.441002	23.812860	O	15.937850	13.230582	13.299546

N	1.456408	14.649721	14.221602	H	10.761813	20.793974	13.467979
N	4.163100	14.727217	14.068002	C	9.044361	20.113458	12.311194
N	20.512331	15.782200	13.022554	H	8.463824	19.177510	12.173592
N	23.200359	15.474306	12.953876	H	9.607483	20.261945	11.367164
N	10.718537	18.654060	13.479472	C	7.121103	21.310524	11.280685
N	13.919584	12.232205	13.087640	H	6.546163	20.376827	11.184523
C	8.053905	21.277475	12.493857	H	7.682238	21.451036	10.347021
C	15.669099	8.930334	14.121009	H	6.398621	22.134145	11.356307
C	0.100341	14.622451	14.242624	C	8.797123	22.608534	12.580848
H	-0.399840	15.590875	14.380647	H	8.097379	23.455402	12.586434
C	-0.616579	13.431044	14.090824	H	9.471023	22.744423	11.724189
H	-1.715435	13.448222	14.109873	H	9.402212	22.676303	13.495606
C	0.072404	12.236155	13.913677	C	7.215264	21.073450	13.754560
H	-0.474705	11.289962	13.793107	H	6.560695	21.935196	13.940039
C	1.469015	12.249258	13.882844	H	7.853959	20.939568	14.652903
H	2.032535	11.317929	13.735987	H	6.569070	20.181379	13.666451
C	2.139889	13.462922	14.033027	C	14.579544	10.897410	12.961567
C	3.605345	13.545949	13.973187	H	15.511557	11.002665	12.356187
H	4.173439	12.609145	13.840029	H	13.926023	10.207636	12.375168
C	5.609684	14.817886	13.956555	C	14.913512	10.258970	14.307727
C	6.407870	14.644554	15.090226	H	15.528382	10.944294	14.925451
H	5.959256	14.441239	16.076271	H	13.986597	10.069292	14.886215
C	7.791981	14.705950	14.963286	C	14.819325	7.961664	13.298829
H	8.423384	14.554021	15.846347	H	15.379412	7.055809	13.033567
C	8.376897	14.954592	13.719789	H	13.924275	7.647652	13.852603
C	7.570482	15.142691	12.594637	H	14.473641	8.435076	12.365010
H	8.027018	15.335112	11.615996	C	17.001834	9.185327	13.417171
C	6.186319	15.072268	12.708390	H	16.853124	9.777083	12.497681
H	5.565843	15.198817	11.812771	H	17.495212	8.245285	13.139435
C	16.288056	15.940037	13.131010	H	17.694190	9.748702	14.060172
C	16.948671	15.891225	11.900871	C	15.935810	8.316207	15.494164
H	16.373415	15.869339	10.966882	H	16.520174	7.390970	15.404623
C	18.337961	15.859758	11.857318	H	16.499099	9.002846	16.149642
H	18.845619	15.824500	10.885379	H	15.000195	8.067474	16.013903
C	19.064163	15.876712	13.052504	C	11.234573	14.049021	18.431846
C	18.412491	15.968795	14.284521	C	14.055342	13.905980	18.114291
H	18.985471	16.029617	15.223599	C	10.499218	16.791917	18.531621
C	17.022379	16.004815	14.317332	C	9.810488	15.822039	19.373511
H	16.504200	16.075540	15.281096	C	10.168925	14.486257	19.324639
C	21.209173	16.834451	12.673972	C	13.335246	14.896590	17.469962
H	20.761446	17.810305	12.418440	C	11.888550	14.969972	17.632567
C	22.670638	16.703871	12.608485	C	11.511752	16.376629	17.684372
C	23.483166	17.760247	12.197536	C	12.729768	16.930439	24.235200
H	23.039789	18.728792	11.928421	C	12.009540	17.921237	23.591221
C	24.864824	17.567356	12.125077	C	14.176055	16.857555	24.074023
H	25.521365	18.386198	11.798030	C	10.049953	17.817317	20.607384
C	25.397895	16.328225	12.462535	C	9.532448	16.455873	20.656528
H	26.480975	16.148382	12.406109	C	15.331655	14.223636	18.742838
C	24.543327	15.299927	12.873621	C	13.852152	16.258137	17.421134
H	24.918171	14.302967	13.144211	C	10.243480	16.310234	23.007920
C	12.103864	18.570836	13.105245	C	10.734025	17.603276	22.961757
C	9.997621	17.480335	13.854432	C	9.626976	15.721803	21.825758
C	10.598787	16.142257	13.585154	C	10.635335	18.376059	21.730198
C	9.846703	14.983559	13.584986	C	15.063785	16.560229	18.018294
C	10.489454	13.724692	13.450402	C	14.264045	13.046063	22.538193
H	9.871058	12.811328	13.445189	C	13.647288	12.459631	21.354972
C	11.857460	13.636974	13.348714	C	12.201113	12.530287	21.517815
C	12.495137	12.295858	13.256933	C	11.923097	13.162558	22.801404
C	14.728722	13.401753	13.218492	C	13.198419	13.481183	23.432144
C	14.078150	14.745232	13.234707	C	15.415468	13.803907	22.412907
C	14.812743	15.917010	13.180633	C	16.012152	14.012235	21.099570
C	14.154754	17.175593	13.155970	C	15.427472	13.453682	19.976906
H	14.763945	18.100142	13.066920	C	14.213632	12.658102	20.107843
C	12.784735	17.251026	13.233076	C	11.396075	12.798911	20.424476
C	12.009150	16.067215	13.380189	C	10.269331	13.713705	20.556442
C	12.654756	14.815404	13.319479	C	10.005177	14.314982	21.774194
C	10.011909	19.974224	13.484526	C	10.854194	14.033149	22.924892
H	9.459027	20.090600	14.448534	C	11.992494	13.005719	19.110991

C	13.365794	12.936664	18.956454	C	11.849002	19.172470	21.599213
C	13.339430	14.654327	24.153127	C	12.416043	19.369254	20.352370
C	12.212520	15.568837	24.284649	C	11.799632	18.781066	19.169968
C	11.001937	15.266764	23.686637	C	12.865305	18.343798	18.277003
C	15.565529	15.036192	23.175898	C	15.896369	17.341936	22.382679
C	14.553267	15.450482	24.023608	C	14.830503	17.779087	23.275653
C	15.822153	15.517248	18.697409	C	14.072338	18.821739	22.596131
C	16.531316	15.372994	21.050627	C	14.669043	19.028890	21.282621
C	16.439424	16.105825	19.880000	C	13.862513	19.295031	20.190265
C	16.254514	16.006273	22.333717	C	14.140028	18.661338	18.907742
C	12.725201	17.173065	17.552873	C	15.209747	17.792462	18.782194
C	10.647307	18.025095	19.294285	C	16.059017	17.511538	19.932617
C	12.698568	18.891482	22.749990	C	15.795001	18.113271	21.150659

Table S3. Cartesian coordinates (in Å) for the PM3 model of the *tert*-butyl derivative of C_{60}⊂**1**-ΛΛΔΔ.

Fe	12.489452	7.389133	28.822045	C	8.729691	10.132408	20.018803
Fe	2.851060	16.199874	14.290209	C	7.017137	11.520386	18.848984
Fe	21.870376	14.260479	13.400460	C	6.365476	11.826670	20.155751
Fe	14.278786	26.709517	26.393248	C	5.266923	12.660780	20.243529
O	6.756425	11.082151	26.196631	C	4.622002	12.855399	21.494773
O	3.279626	13.009765	23.979602	H	3.712894	13.476478	21.530285
O	9.728136	9.434283	19.933925	C	5.110086	12.284127	22.642220
O	6.594459	11.922187	17.774758	C	6.295129	11.499086	22.603160
N	11.308341	5.598182	28.579099	C	6.894864	11.245237	21.350340
N	12.925461	6.813522	26.758738	C	4.358501	12.443578	26.441166
N	2.659758	16.007540	16.441474	H	3.299988	12.116006	26.367605
N	1.310676	17.644418	14.746224	H	4.795023	11.843724	27.274956
N	5.023523	12.094701	25.142372	C	4.430509	13.938239	26.766763
N	8.223107	10.746920	18.828341	H	3.405515	14.361674	26.701899
C	5.006039	14.259307	28.158767	H	5.016589	14.497435	26.005579
C	9.208328	8.908704	15.553104	C	4.344003	13.393494	29.227450
C	10.533629	4.970950	29.499718	H	3.261571	13.571012	29.275402
H	10.465886	5.453392	30.484799	H	4.759081	13.597773	30.222538
C	9.865818	3.775786	29.212849	H	4.497830	12.323364	29.009827
H	9.250238	3.294610	29.986122	C	4.730328	15.732153	28.465221
C	9.993035	3.207074	27.950384	H	5.149570	16.400002	27.690374
H	9.477130	2.266843	27.707757	H	5.177770	16.028153	29.424711
C	10.790478	3.838771	26.992938	H	3.653385	15.938647	28.528960
H	10.910502	3.403165	25.991419	C	6.515563	14.030532	28.180146
C	11.440596	5.026817	27.327572	H	6.770849	12.980612	27.985107
C	12.315650	5.718557	26.373705	H	6.940824	14.294159	29.158190
H	12.433626	5.277893	25.367933	H	7.025228	14.645479	27.425991
C	13.812839	7.451170	25.799645	C	8.902468	10.461189	17.526663
C	15.021981	6.839052	25.452058	H	10.007730	10.439785	17.686467
H	15.347740	5.911030	25.938201	H	8.725274	11.302129	16.814919
C	15.801179	7.386942	24.439268	C	8.464487	9.149972	16.881456
H	16.732966	6.891320	24.138825	H	8.660780	8.295266	17.562846
C	15.370875	8.535301	23.769378	H	7.372124	9.151896	16.694525
C	14.206815	9.188634	24.182468	C	10.712159	8.814662	15.809618
H	13.890607	10.113343	23.682478	H	11.285862	8.791966	14.872495
C	13.419771	8.646634	25.193584	H	11.066981	9.672196	16.404598
H	12.471450	9.132728	25.470530	H	10.966377	7.899000	16.374347
C	4.674242	13.438948	19.136981	C	8.722773	7.590050	14.952009
C	3.478734	13.025726	18.543554	H	7.642063	7.606646	14.757933
H	3.038218	12.057141	18.811649	H	8.925530	6.742640	15.623954
C	2.827467	13.854397	17.635843	H	9.227201	7.383233	13.998846
H	1.871735	13.532536	17.204607	C	8.910839	10.044390	14.574860
C	3.380581	15.099224	17.319700	H	9.535680	9.976296	13.674309
C	4.607733	15.491541	17.859951	H	7.860716	10.028903	14.254658
H	5.056063	16.463779	17.602985	H	9.095915	11.027925	15.039689
C	5.250020	14.657374	18.768290	O	18.931468	19.129493	16.384388
H	6.199464	14.974146	19.215274	O	15.961063	22.115870	18.064746
C	1.778456	16.814113	16.979758	O	21.507487	18.254903	23.011351
H	1.568985	16.856675	18.062169	O	19.732949	22.296486	24.112713
C	1.013303	17.702299	16.094939	N	23.293704	12.720215	13.924689
C	0.017493	18.545583	16.587682	N	22.119917	14.544352	15.544197
H	-0.202075	18.575764	17.663735	N	13.602800	26.756380	24.301838
C	-0.702046	19.342652	15.694196	N	15.515104	28.246636	25.532933
H	-1.495211	20.008956	16.062620	N	17.308324	20.460829	17.251676
C	-0.410587	19.277814	14.336064	N	20.716901	20.321941	23.580863
H	-0.968378	19.888347	13.612084	C	16.208811	21.646919	13.716160
C	0.600469	18.420495	13.889636	C	21.563417	19.549389	27.280745
H	0.862417	18.330943	12.826087	C	23.935876	11.855472	13.100093
C	4.384097	12.498216	23.924513	H	23.711249	11.953515	12.028829
C	6.253983	11.372979	25.121270	C	24.835128	10.901494	13.587731
C	6.876424	11.003856	23.809378	H	25.341066	10.220596	12.889010
C	8.019101	10.227074	23.735546	C	25.080992	10.828723	14.954441
C	8.584733	9.916516	22.473038	H	25.783142	10.083883	15.354849
H	9.473366	9.269039	22.439219	C	24.433066	11.718003	15.815136
C	8.054403	10.423815	21.310696	H	24.616611	11.684815	16.898092

C	23.552081	12.658347	15.281768	C	21.497618	20.333001	24.859250
C	22.885973	13.656176	16.128668	H	21.854574	21.369001	25.041879
H	23.067513	13.632699	17.228726	H	22.416505	19.707449	24.745133
C	21.546964	15.591251	16.375041	C	20.684869	19.823081	26.045658
C	22.195387	16.828186	16.447328	H	19.896365	20.554628	26.314136
H	23.108535	17.023774	15.871846	H	20.154921	18.885840	25.777685
C	21.693855	17.816230	17.286847	C	22.304949	20.811703	27.715129
H	22.204722	18.784582	17.358264	H	23.063844	21.111552	26.979624
C	20.546951	17.572053	18.046322	H	22.823996	20.655692	28.670745
C	19.886315	16.346170	17.943655	H	21.615672	21.656193	27.846451
H	18.981343	16.158277	18.534562	C	22.569643	18.444463	26.965941
C	20.384139	15.349941	17.110658	H	22.068323	17.472562	26.818159
H	19.874556	14.374875	17.058354	H	23.296903	18.320884	27.778641
C	10.855179	24.288773	22.237135	H	23.127562	18.673817	26.042961
C	10.588411	25.654094	22.369392	C	20.656003	19.093465	28.423356
H	9.697124	26.088984	21.899744	H	20.054132	18.211299	28.141840
C	11.470207	26.473267	23.066542	H	19.958943	19.885542	28.726387
H	11.266895	27.549677	23.132512	H	21.245161	18.815475	29.308683
C	12.616002	25.918015	23.646522	O	14.067825	7.124025	21.753128
C	12.856491	24.544438	23.567272	O	14.134848	8.724048	17.499293
H	13.747520	24.100101	24.044891	O	19.586738	11.424342	23.257308
C	11.974402	23.733804	22.862108	O	20.458859	11.740778	18.820140
H	12.173638	22.659501	22.776711	N	11.834350	7.801454	30.835756
C	14.190583	27.679475	23.580071	N	10.653886	8.510247	28.495875
H	13.957853	27.859325	22.515560	N	20.376345	12.672093	13.431879
C	15.215289	28.519130	24.211196	N	21.670883	13.742002	11.307195
C	15.855654	29.541776	23.511130	N	13.962251	8.022973	19.665777
H	15.599378	29.740866	22.461452	N	20.139547	11.447598	21.040904
C	16.821153	30.311988	24.164012	C	11.659934	5.069543	18.654013
H	17.333319	31.125888	23.630628	C	22.926203	14.126182	21.106280
C	17.122615	30.041004	25.494148	C	12.406839	7.410612	32.001970
H	17.875786	30.634560	26.031755	H	13.355948	6.863407	31.914946
C	16.454361	29.004258	26.153990	C	11.816935	7.682111	33.241105
H	16.656030	28.759407	27.206239	H	12.308109	7.345886	34.165200
C	16.918872	21.389515	18.273770	C	10.609386	8.369928	33.287916
C	18.504402	19.682090	17.386741	H	10.128716	8.587698	34.252605
C	19.125182	19.548467	18.735972	C	10.006668	8.776824	32.094974
C	20.072959	18.582064	19.012482	H	9.049249	9.315819	32.108904
C	20.645576	18.489846	20.309603	C	10.631429	8.481481	30.883531
H	21.364917	17.667465	20.512713	C	10.036401	8.863638	29.596393
C	20.303176	19.384768	21.292882	H	9.087520	9.427807	29.610616
C	20.891705	19.244974	22.654759	C	10.043707	8.881875	27.228801
C	19.799521	21.383216	23.305523	C	9.017912	8.100460	26.689056
C	18.984990	21.338058	22.051779	H	8.685978	7.179902	27.184368
C	17.914922	22.188989	21.840288	C	8.374597	8.519505	25.528324
C	17.265715	22.211193	20.579568	H	7.549705	7.924293	25.117463
H	16.433797	22.914577	20.426384	C	8.747720	9.717634	24.915246
C	17.659922	21.371938	19.564139	C	9.820008	10.456640	25.423614
C	18.720764	20.446840	19.770057	H	10.131389	11.383881	24.926376
C	19.347319	20.406766	21.033151	C	10.469387	10.045036	26.581769
C	16.584530	20.468601	15.942058	H	11.284186	10.657008	26.997848
H	16.663282	19.453607	15.498886	C	18.623083	11.014892	16.902395
H	15.496808	20.634749	16.131411	C	18.289078	12.308361	16.494054
C	17.097208	21.523262	14.967965	H	17.568316	12.898253	17.072601
H	18.136018	21.290116	14.657855	C	18.857223	12.849845	15.346863
H	17.142093	22.513546	15.466619	H	18.559520	13.855020	15.008811
C	16.203743	20.343491	12.917724	C	19.768166	12.088680	14.612201
H	15.740686	20.489570	11.931778	C	20.098971	10.787967	15.007147
H	15.633457	19.540945	13.418823	H	20.796911	10.177681	14.420534
H	17.223112	19.969930	12.753870	C	19.523910	10.253524	16.154824
C	16.782633	22.757647	12.833574	H	19.777811	9.233772	16.469624
H	17.800352	22.518734	12.497695	C	20.063783	12.188873	12.255817
H	16.825881	23.716387	13.368641	H	19.328051	11.380587	12.102848
H	16.165949	22.911223	11.937802	C	20.745329	12.741130	11.078077
C	14.781220	22.015262	14.113815	C	20.492963	12.258275	9.794092
H	14.721202	23.038162	14.525761	H	19.751897	11.462773	9.636763
H	14.395634	21.331255	14.888145	C	21.200892	12.792137	8.714869
H	14.101518	21.965171	13.253176	H	21.019954	12.420853	7.696035

C	22.141149	13.790592	8.944887	C	14.533452	5.057419	29.541871
H	22.718124	14.220488	8.114125	H	13.661355	4.406110	29.389737
C	22.355179	14.246502	10.249554	C	15.781698	4.550021	29.917558
H	23.090941	15.029887	10.479273	H	15.909206	3.468727	30.067724
C	14.669429	8.655585	18.596455	C	16.847593	5.423867	30.101779
C	14.557913	7.915957	20.965332	H	17.835585	5.043117	30.398234
C	15.721939	8.796017	21.296833	C	16.649328	6.794014	29.914704
C	16.121650	9.033355	22.599790	H	17.475733	7.502662	30.063675
C	17.295900	9.787329	22.854760	C	15.384822	7.253268	29.546057
H	17.598468	9.957681	23.898461	C	15.106162	8.684901	29.377755
C	18.054687	10.289364	21.823433	H	15.933786	9.395572	29.547778
C	19.281199	11.075695	22.130112	C	13.620014	10.479918	28.967257
C	19.717100	11.294638	19.685206	C	13.413487	11.221713	30.134998
C	18.426196	10.608271	19.390782	H	13.427239	10.741325	31.121126
C	17.966121	10.450412	18.097095	C	13.225878	12.597240	30.050540
C	16.754461	9.754635	17.847875	H	13.086964	13.185468	30.966320
H	16.427275	9.611538	16.796152	C	13.247496	13.232055	28.806311
C	16.002093	9.256497	18.882151	C	13.406606	12.477559	27.641012
C	16.462957	9.373403	20.223191	H	13.411210	12.975660	26.661277
C	17.656115	10.083681	20.473674	C	13.599770	11.102004	27.716779
C	12.697235	7.282381	19.358400	H	13.769975	10.523270	26.796778
H	12.107648	7.144713	20.296116	C	13.204985	21.203787	28.180758
H	12.077052	7.929481	18.699487	C	13.045544	22.113749	29.228480
C	12.939504	5.924931	18.705669	H	12.992920	21.755876	30.264601
H	13.718809	5.360795	19.257806	C	12.921566	23.473332	28.958592
H	13.330369	6.058890	17.675728	H	12.766229	24.173581	29.789453
C	11.192446	4.753022	20.073449	C	12.971979	23.924671	27.634624
H	10.213447	4.257751	20.070047	C	13.160193	23.020873	26.587800
H	11.106098	5.676728	20.670185	H	13.192268	23.371326	25.542305
H	11.899601	4.091115	20.590336	C	13.275758	21.664116	26.863645
C	11.983119	3.764532	17.926051	H	13.405551	20.953261	26.039203
H	12.810820	3.226817	18.408026	C	11.697203	25.918986	27.676201
H	12.269570	3.948548	16.882123	H	10.868523	25.392370	28.181777
H	11.116065	3.090394	17.916418	C	11.540895	27.355395	27.419968
C	10.548045	5.798201	17.901744	C	10.380317	28.036744	27.788436
H	10.920123	6.267274	16.973908	H	9.546221	27.498210	28.259370
H	10.099626	6.598481	18.509151	C	10.296313	29.412108	27.559361
H	9.737729	5.111684	17.621083	H	9.392163	29.967124	27.848230
C	21.488405	12.032930	21.322876	C	11.370266	30.070199	26.970351
H	22.214329	11.627861	20.576701	H	11.333837	31.153442	26.788001
H	21.835162	11.669033	22.313132	C	12.510002	29.342789	26.612317
C	21.503950	13.560257	21.279099	H	13.382944	29.822439	26.147941
H	20.873052	13.934684	20.446994	C	16.281658	17.523044	29.245204
H	21.059598	13.972857	22.207411	C	15.550109	15.154108	29.011920
C	23.831504	13.670027	22.251171	C	14.133431	15.599901	28.835623
H	24.807396	14.172753	22.209334	C	13.091745	14.698009	28.714659
H	23.384638	13.896952	23.228369	C	11.779095	15.161959	28.440668
H	24.019851	12.588361	22.215099	H	10.970081	14.424721	28.330426
C	22.854638	15.653366	21.130910	C	11.519468	16.500803	28.275797
H	23.827495	16.097618	20.880413	C	10.166930	16.931627	27.826591
H	22.574978	16.019393	22.129315	C	10.879553	19.300192	28.100641
H	22.115554	16.062350	20.419615	C	12.286432	18.854698	28.334268
C	23.523019	13.659152	19.779594	C	13.330772	19.754957	28.434979
H	22.974685	14.061179	18.910443	C	14.634046	19.295326	28.755251
H	23.485431	12.558916	19.704158	H	15.438445	20.035222	28.881943
H	24.571271	13.969669	19.682725	C	14.896242	17.956198	28.912485
O	15.897449	13.987402	28.909067	C	13.858763	16.998326	28.744145
O	17.186093	18.313436	29.455967	C	12.554277	17.458288	28.463286
O	9.291769	16.139265	27.514628	C	17.980057	15.674629	29.508041
O	10.512448	20.457288	28.215028	H	18.434874	16.312163	30.295719
N	14.327406	6.384799	29.351425	H	17.989264	14.634241	29.913198
N	13.890047	9.053389	29.058132	C	18.800280	15.736625	28.220710
N	12.812252	25.332319	27.317144	H	19.097874	16.790699	28.008077
N	12.604788	28.005658	26.824033	H	18.189971	15.409355	27.354696
N	16.562295	16.119931	29.309032	C	20.804621	15.000619	26.943483
N	9.908912	18.330481	27.678415	H	21.695613	14.359256	26.918279
C	20.069797	14.866579	28.278092	H	21.141597	16.037914	26.771622
C	6.239896	19.537318	28.030632	H	20.167463	14.712097	26.097228

C	20.996565	15.335587	29.397659	H	16.297197	21.401106	23.818018
H	21.937645	14.769237	29.395183	C	16.695366	25.224464	27.269246
H	20.537646	15.203079	30.386544	H	17.583435	24.572557	27.343137
H	21.251305	16.400226	29.286602	C	16.308032	25.995081	28.457771
C	19.695542	13.402730	28.499080	C	17.055989	25.947920	29.634263
H	20.587756	12.778482	28.635323	H	17.953759	25.317387	29.696643
H	19.064386	13.292548	29.396597	C	16.652983	26.718578	30.727760
H	19.132019	12.999596	27.647705	H	17.232368	26.698328	31.662086
C	8.543273	18.779875	27.259103	C	15.517878	27.514214	30.619146
H	8.225217	18.136368	26.412409	H	15.184025	28.135037	31.462660
H	8.607286	19.817591	26.851765	C	14.798273	27.526559	29.419483
C	7.510301	18.739009	28.380718	H	13.899475	28.144353	29.284516
H	7.226627	17.688880	28.606911	C	6.890531	21.377809	22.315532
H	7.937525	19.150732	29.317906	C	6.157202	20.155200	20.274254
C	5.258742	19.413610	29.197463	C	7.192296	20.867001	19.467298
H	4.353885	20.010039	29.019596	C	7.288879	20.703436	18.099622
H	4.943168	18.370279	29.345714	C	8.337414	21.338855	17.380043
H	5.702998	19.764210	30.138463	H	8.388528	21.194612	16.280124
C	5.580202	18.982478	26.772063	C	9.274450	22.109232	18.022132
H	6.161224	19.192555	25.855767	C	10.397609	22.688599	17.234864
H	4.579824	19.422429	26.609900	C	11.230772	23.791872	19.305741
H	5.438640	17.882759	26.821829	C	10.108883	23.188151	20.089647
C	6.585061	21.009919	27.819264	C	9.954523	23.427930	21.443746
H	6.933921	21.476756	28.749657	C	8.884056	22.827709	22.154456
H	5.714199	21.577171	27.467014	H	8.774844	23.045900	23.227445
H	7.387274	21.121377	27.070902	C	7.993534	21.990885	21.525555
O	5.472682	19.244500	19.831763	C	8.118759	21.728246	20.133834
O	6.756760	21.551871	23.515296	C	9.172061	22.342751	19.422028
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N	5.945885	20.541466	21.636031	C	2.937988	18.725547	24.430674
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C	3.913608	17.897501	23.596202	H	3.433742	19.151904	25.320696
C	13.203214	26.300154	15.960372	H	2.098073	18.111922	24.783450
C	2.281456	16.052662	11.153594	C	4.372064	16.696223	24.423994
H	1.607607	15.229659	11.430246	H	3.525212	16.044020	24.683211
C	2.426341	16.481112	9.829850	H	4.842054	17.012158	25.374352
H	1.855612	15.987417	9.030497	H	5.103880	16.082862	23.881505
C	3.289925	17.532311	9.540630	C	3.209873	17.395197	22.337095
H	3.414493	17.882282	8.505996	H	2.269376	16.884840	22.582020
C	3.993268	18.145279	10.580063	H	3.838293	16.688101	21.779296
H	4.678182	18.982458	10.379382	H	2.975181	18.234022	21.660936
C	3.811111	17.686515	11.884604	C	12.452261	24.152394	17.116521
C	4.498733	18.312630	13.020189	H	12.742933	23.477257	16.282225
H	5.201675	19.142630	12.808858	H	13.368297	24.255487	17.746721
C	4.921385	18.525517	15.333486	C	12.032237	25.520177	16.586113
C	6.043291	17.919700	15.903661	H	11.227701	25.409797	15.830834
H	6.392210	16.931871	15.561080	H	11.600645	26.131666	17.405155
C	6.772794	18.610283	16.865994	C	13.740024	25.575871	14.728253
H	7.676787	18.155636	17.287883	H	14.208771	24.609726	14.983435
C	6.386279	19.894722	17.255623	H	14.501642	26.179108	14.215405
C	5.212442	20.455458	16.745585	H	12.939656	25.372125	14.004378
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C	4.478807	19.775205	15.779883	H	12.285532	28.241102	16.384220
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C	17.146036	25.190504	24.006041	H	14.621685	25.514020	17.418151
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C	0.183501	14.469713	14.124644	C	9.160098	22.430065	12.196995
H	-0.313748	15.436792	14.283287	H	8.658387	23.390300	12.372056
C	-0.537078	13.284490	13.943418	H	9.577998	22.455325	11.181454
H	-1.635990	13.305313	13.959873	H	10.007084	22.353223	12.899371
C	0.147994	12.091615	13.739940	C	7.469126	21.372240	13.708654
H	-0.402146	11.150732	13.594726	H	6.996858	22.356584	13.820772
C	1.544857	12.100082	13.714421	H	8.161171	21.229618	14.562477
H	2.105481	11.170072	13.547548	H	6.680278	20.611515	13.805363
C	2.219701	13.307115	13.895344	C	14.662518	10.857722	12.629371
C	3.685507	13.387845	13.845572	H	15.595003	11.022604	12.051819
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C	5.688524	14.667952	13.870770	C	14.950190	10.114767	13.930785
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C	7.859886	14.580274	14.903570	C	14.004681	7.942267	13.100985
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H	8.125724	15.212276	11.558505	C	16.430023	8.430898	12.763923
C	6.275756	14.927594	12.628727	H	16.202403	8.764591	11.742274
H	5.664466	15.044880	11.725830	H	16.720096	7.373120	12.702321
C	16.356693	15.910017	13.065947	H	17.305487	8.996081	13.111300
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C	18.426866	15.817675	11.822782	H	16.463492	8.427455	15.494167
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C	22.697621	17.059029	12.766897	C	11.477796	16.604020	18.089186
C	23.458020	18.184528	12.450469	C	12.863027	16.736031	24.628799
H	22.965569	19.133827	12.198913	C	12.197965	17.804381	24.053044
C	24.851588	18.085502	12.449643	C	14.297584	16.576401	24.431323
H	25.467924	18.959991	12.196241	C	10.175610	17.984646	21.115543
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H	25.069848	14.786272	13.327019	C	10.316165	16.345921	23.432244
C	12.149328	18.495099	13.110434	C	10.891377	17.604440	23.439045
C	10.061353	17.370954	13.858454	C	9.637532	15.861445	22.237001
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C	11.938668	13.560860	13.201860	C	11.986724	12.528979	21.708567
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C	14.806162	13.339348	13.103520	C	13.083321	13.310535	23.644119
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C	14.211903	17.114451	13.118995	C	15.234789	13.314022	20.140933
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C	12.076859	15.986357	13.335760	C	10.118710	13.884305	20.853781
C	12.730278	14.742829	13.224585	C	9.919224	14.437336	22.106256
C	10.022369	19.853637	13.442767	C	10.770583	14.040822	23.221227
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C	13.123138	12.987734	19.144533	C	12.080866	19.165641	22.131773
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C	10.759063	18.219950	19.800792	C	16.135828	17.318883	20.285380
C	12.932900	18.769708	23.246183	C	15.938029	17.873100	21.537939

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