Supporting Information

Formation of a Pd_{16} Molecular Basket Architecture of Reduced Symmetry and Angular Deviation in Fluorenone-Scaffold to Govern the Host-Guest Chemistry of Pd_6 Trifacial Tubes

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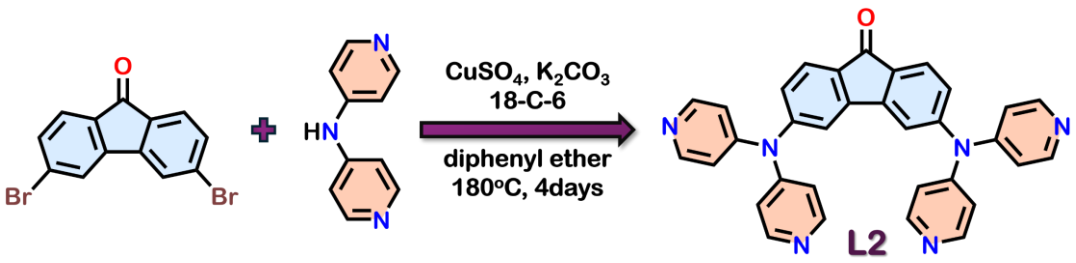
1. Materials and Methods

All the chemicals and solvents were purchased from different commercially available sources and directly used without further purification. NMR studies were performed on Bruker 400 MHz and 500 MHz spectrometers. The chemical shifts (δ) in the ^{1}H NMR spectra were reported in ppm relative to the tetramethylsilane (TMS), which was used as an internal standard (δ = 0.00 ppm) for $CDCl_3$ or the resonance of the proton resulting from partial deuteriation of the NMR solvent: D_2O (δ = 4.79 ppm). Electrospray ionization mass spectra were recorded using Agilent 6538 Ultra-High Definition (UHD) Accurate Mass Q-TOF spectrometer along with the use of standard spectroscopic grade solvents.

2. Synthetic procedures

2.1. Synthesis of ligand L2

Ligand **L2** was synthesized following standard copper-catalyzed Ullmann coupling procedures.[S1] 3,6-dibromo-9*H*-fluoren-9-one (1 g, 2.95 mmol) and bis(4-pyridyl) amine (1.52 g, 8.87 mmol), anhydrous $CuSO_4$ (0.25 g, 1.47 mmol) and K_2CO_3 (1.63 g, 11.8 mmol) were taken in a two-neck round-bottom flask containing diphenyl ether (40 mL). The reaction mixture was degassed with N_2 and stirred at 50 °C for 30 minutes, followed by the addition of 18-Crown-6 (0.01g, 0.05 mmol). Finally, it was stirred vigorously at 180 ºC for 4 days under the N_2 atmosphere. After completion of the reaction, the solvent was removed under reduced pressure. The crude product was first purified by column chromatography using silica as the stationary phase and THF/$CHCl_3$ (1:1) as eluent to extract the product and bis(4-pyridyl) amine mixture. Further purification by column chromatography using neutral alumina as the stationary phase with MeOH/$CHCl_3$ (1:99) as the eluent afforded pure product yellow solid. Yield = 650 mg (42%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) = 8.48 (dd, 8H, J = 6.36 Hz), 7.72 (d, 2H, J = 8.08 Hz), 7.18 (d, 2H, J = 1.79 Hz), 7.10 (dd, 2H, J = 8.09 Hz), 6.99 (dd, 8H, J = 6.33 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 190.48, 151.91, 151.41, 150.42, 145.50, 132.01, 127.26, 126.36, 118.54, 117.65. HRMS (ESI): $C_{33}H_{22}N_6O$ (**L2**), $[L2+H^+]^+$ = 519.2090.



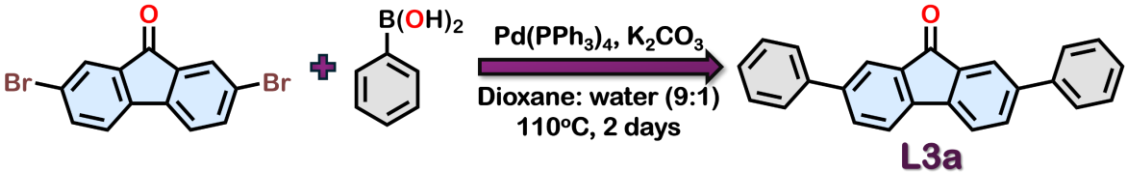
Scheme S1. Synthetic route for the preparation of the ligand **L2**.

2.2. Synthesis of Ligand L3

The ligand was synthesized in three steps.

Synthesis of Precursor L3a

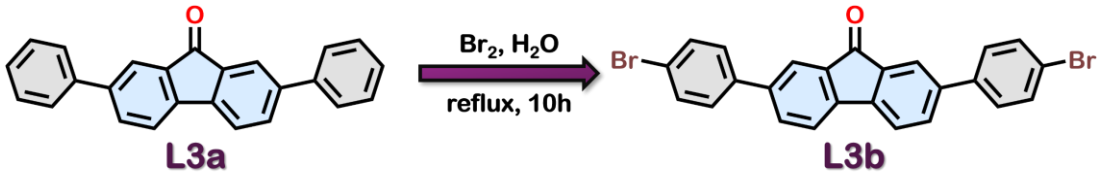
The precursor **L3a** was synthesized by slight modification of a reported procedure.[S2] 2,7-dibromo-9*H*-fluoren-9-one (1 g, 2.96 mmol), phenylboronic acid (903 mg, 7.04 mmol) and K_2CO_3 (4 g, 29.6 mmol) were taken in a 250 mL double-neck round bottom flask. 45 mL of 1,4-dioxane and 5 mL of water were added. Then, the reaction mixture was degassed under a nitrogen atmosphere. $Pd(PPh_3)_4$ (345.9 mg, 0.29 mmol) was added to the reaction mixture and refluxed under an inert atmosphere for 48 h. After the completion of the reaction, the mixture was evaporated. Further, the reaction mixture was extracted with chloroform and dried over anhydrous Na_2SO_4. The crude product was purified by column chromatography using silica gel as the stationary phase and DCM/Hexane (1:1) as eluent to afford yellow solid. Yield = 767 mg (78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, 1H, J = 1.43 Hz), 7.74 (dd, 1H, J = 7.81 Hz), 7.60 (t, 3H, J = 16.61 Hz) 7.46 (t, 2H, J = 15.04 Hz), 7.37 (t, 1H, J = 14.89 Hz).



Scheme S2. Synthetic route for the preparation of the precursor **L3a**.

Synthesis of Precursor L3b

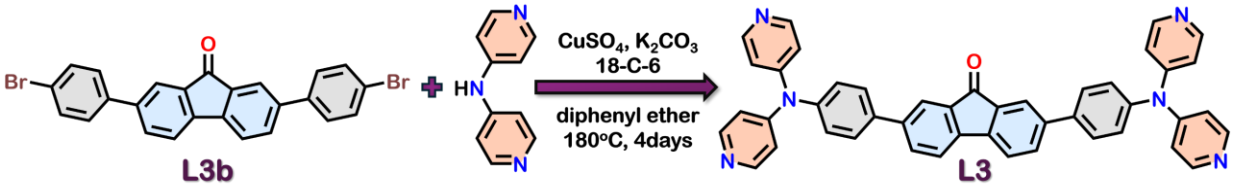
The precursor **L3b** was synthesized following a reported procedure.[S3] The product of the first step, **L3a** (2,7-diphenyl-9H-fluoren-9-one) (0.3g, 0.9 mmol), was brominated using Br_2 (0.2ml, 3.9 mmol) in water (10 ml). The reaction mixture was refluxed and stirred for 10 h. The reaction mixture was cooled to room temperature and washed with water to obtain a yellow solid. Yield= 376 mg (85%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.88 (bs, 1H), 7.71 (d, 1H, J = 7.66 Hz), 7.60 (t, 3H, J = 16.45 Hz) 7.48 (d, 2H, J = 8.47 Hz).



Scheme S3. Synthetic route for the preparation of the precursor **L3b**.

Synthesis of Ligand L3

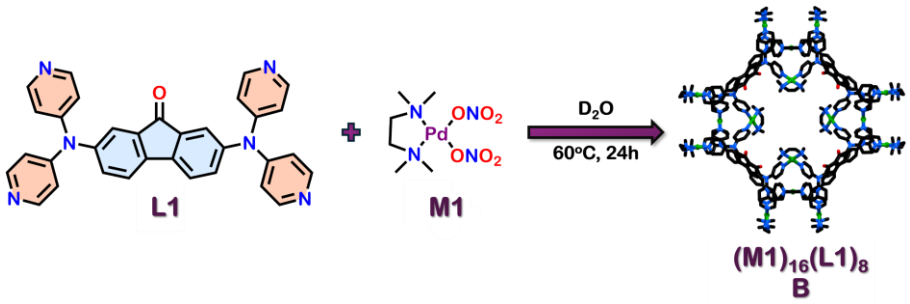
Ligand **L3** was synthesized following standard copper-catalyzed Ullmann coupling procedures.[S1] The product of second step **L3b** 2,7-bis(4-bromophenyl)-9*H*-fluoren-9-one (500 mg, 1.02 mmol), and bis(4-pyridyl)amine (524 mg, 3.06 mmol), anhydrous $CuSO_4$ (81 mg, 0.51 mmol), and K_2CO_3 (564 mg, 4.08 mmol) were taken in a two-neck round-bottom flask containing diphenyl ether (40 mL). The reaction mixture was degassed with N_2 and stirred at 50 °C for 30 minutes, followed by the addition of 18-Crown-6 (0.015g, 0.05 mmol). Finally, it was stirred vigorously at 180 °C for 4 days under N_2 atmosphere. After completion of the reaction, the solvent was removed under reduced pressure. The crude product was first purified by column chromatography using neutral alumina as the stationary phase and THF/$CHCl_3$ (1:1) as eluent to extract the product and bis(4-pyridyl) amine mixture. Further purification by column chromatography using neutral alumina as the stationary phase with MeOH/$CHCl_3$ (1:49) as the eluent afforded pure yellow solid. Yield = 120 mg (18 %). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) = 8.45 (d, 8H, J = 5.52 Hz), 7.95 (s, 2H), 7.77 (d, 2H, J = 7.83 Hz), 7.65 (t, 6H, J = 18.11 Hz), 7.27 (d, 4H, J = 8.06 Hz), 7.01 (d, 8H, J = 6.06 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 193.41, 152.62, 149.84, 143.49, 143.10, 140.91, 139.09, 135.43, 133.43, 128.96, 127.97, 123.07, 121.27, 116.63. HRMS (ESI): $C_{45}H_{30}N_6O$ (L3), $[L3+H^+]^+$ = 671.3247.



Scheme S4. Synthetic route for the preparation of the ligand **L3**.

2.3.Synthesis of Molecular Basket B

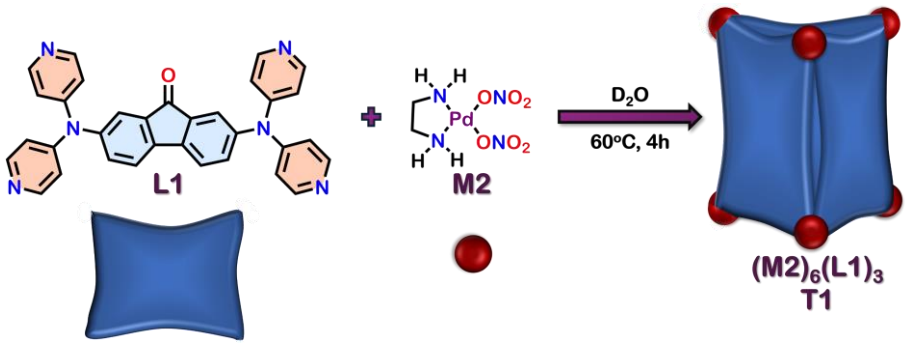
The solid donor **L1** (0.01 mmol, 5.18 mg) was added to a solution of *cis*-[(tmed)Pd(NO_3)$_2$] **(M1)** acceptor (0.02 mmol, 6.93 mg) in 0.5 mL of D_2O. The resulting mixture was stirred at 60 °C for 24 hours to give a clear, amber-colored solution. ^{1}H NMR (400 MHz, D_2O, 298 K): δ 9.01 (s, 1 H), 8.92 (d, 1H), 8.83 (t, 2 H), 8.76 (s, 1H), 8.74 (d, 2H), 8.72 (s, 1H), 8.69 (d, 1H), 8.65 (s, 1H), 7.94 (d, 1H), 7.82 (d, 2H), 7.78 (bs, 2H), 7.76 (s, 1H), 7.60 (d, 1H), 7.41 (s, 1H), 6.24 (m, 3H), 6.70 (s, 1H), 3.17 (s, 4H), 3.07 (s, 2H), 2.89 (m, 9H), 2.82 (m, 7H), 2.78 (m,8 H), 2.44 (s, 2H). ESI-MS (CH_3CN) *m/z* =1913.1742 [**B.**26PF_6]$^{6+}$(calc. 1913.1907), 1619.1538 [**B.**25PF_6]$^{7+}$ (calc. 1619.1686), 1398.6333 [**B.**24PF_6]$^{8+}$ (calc.1398.6520), 1227.1254 [**B.**23PF_6]$^{9+}$ (calc. 1227.1390), 1089.9237 [**B.**22PF_6]$^{10+}$ (calc. 1089.9287), 977.6564 [**B.**21PF_6]$^{11+}$ (calc. 977.6657), and 884.1113 [**B.**21PF_6]$^{12+}$(calc. 884.1132).



Scheme S5. Schematic representation of the synthesis of molecular basket **B**.

2.4. Synthesis of T1

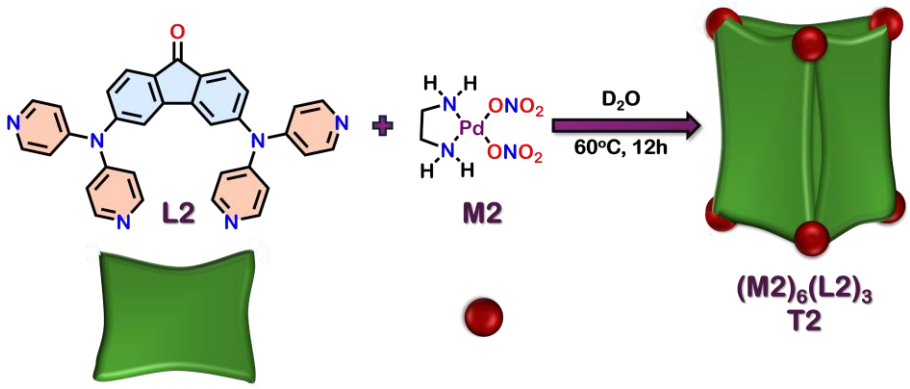
T1 was synthesized following the same procedure as our earlier report. [S1]



Scheme S6. Schematic representation for the formation of trifacial tube **T1**.

2.5. Synthesis of T2

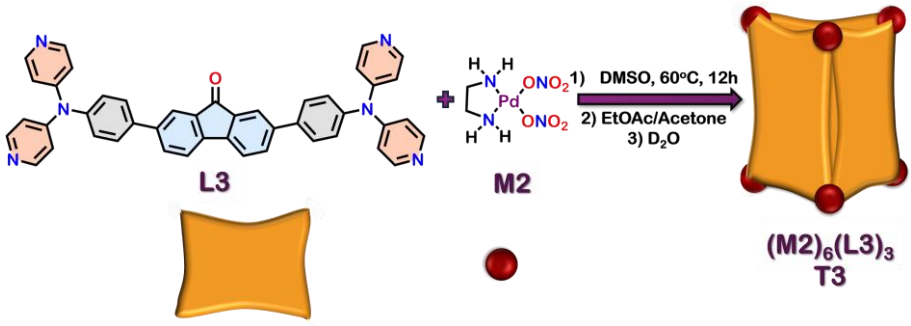
The solid donor **L2** (0.01 mmol, 5.18 mg) was added to a solution of *cis*-[(en)Pd(NO_3)$_2$] **(M2)** acceptor (0.02 mmol, 5.77 mg) in 0.5 ml of D_2O. The resulting mixture was stirred at 60 °C for 12 h to give an almost clear lime colored solution. The solution was centrifuged to remove the inconsistencies, and the NMR was recorded. ^{1}H NMR (400 MHz, D_2O, 298 K): δ 8.25 (d, 8H, J = 6.90 Hz), 7.88 (d, 2H, J = 7.88 Hz), 7.39 (dd, 2H, J = 7.99 Hz), 7.27 (d, 2H, J = 1.54 Hz), 7.08 (d, 8H, J = 6.93 Hz), 2.84 (s, 8H). ESI-MS (CH_3CN) *m/z* = 1286.3477 [**T2.**9PF_6]$^{3+}$ (calc. 1286.3601), 928.5203 [**T2.**8PF_6]$^{4+}$ (calc. 928.5290), 713.8323 [**T2.**7PF_6]$^{5+}$ (calc. 713.8304).



Scheme S7. Schematic representation for the formation of trifacial tube **T2**.

2.6. Synthesis of T3

The solid donor **L3** (0.01 mmol, 6.77 mg) was added to a solution of *cis*-[(en)Pd(NO_3)$_2$] **(M1)** acceptor (0.02 mmol, 5.77 mg) in 0.5 mL of dimethyl sulfoxide (DMSO). The resulting mixture was stirred at 60 °C for 12 h to give a clear orange solution. Then, the reaction mixture was centrifuged, and the solution was treated with excess ethyl acetate (12 mL) to obtain a dark orange solid. It was further washed with acetone and dried under a vacuum which afforded an orange solid. The precipitate was dissolved in DMSO and the diffusion of 1,4-dioxane vapours into the DMSO solution afforded orange crystals. The crystals were dissolved in D_2O and ^1H NMR was recorded. ^1H NMR (400 MHz, D_2O, 298 K): δ 8.80 (d, 4H, J = 5.61 Hz), 8.22 (d, 8H, J = 6.43 Hz), 7.81 (d, 6H, J = 6.80 Hz), 7.53 (d, 2H, J =7.88 Hz), 7.32 (s, 2H), 7.17 (d, 8H, J = 5.91 Hz), 2.87 (s, 8H). ESI-MS (CH_3CN) *m/z* = 1042.5726 [**T3.**8PF_6]$^{4+}$ (calc. 1042.5760), 805.0678 [**T3.**7PF_6]$^{5+}$ (calc. 806.0650), 646.7214 [**T3.**6PF_6]$^{6+}$ (calc. 646.7292).



Scheme S8. Schematic representation of the synthesis of trifacial tube **T3**.

3. Host-guest studies

The host-guest studies were conducted with the in-situ formed solution of **T1/T2** in D_2O. In a clean 4 mL glass vial, the solid donor **Lx** (x = 1, 2) (0.005 mmol, 2.59 mg) was added to a solution of *cis*-[(en)Pd(NO_3)$_2$] **(M2)** acceptor (0.01 mmol, 2.88 mg) in 0.5 mL of D_2O. The resulting mixture was stirred at 60 °C for 4 hours to give an almost clear solution of **T1/T2**. The solution was centrifuged, and the clear supernatant was treated with excess guest (**G1**/**G2**)

and stirred for 12 h at room temperature under dark conditions. The resultant solution was then subjected to centrifugation and characterised by ^{1}H NMR spectroscopy. For host-guest studies using **G3** as a guest, 2 equivalents of **G3** were added with respect to **T1/T2** since G3 has high solubility in aqueous media.

4. X-ray data collection and structure refinement

Single crystals were obtained by diffusion of acetone into aqueous solutions of **T3** or **B**. Single crystal X-ray diffraction data of the crystals obtained were collected with a monochromatic wavelength of 0.7000 Å at the XRD1 beamline of the Elettra synchrotron, Trieste (Italy), employing the rotating-crystal method and a Dectris Pilatus 2M area detector. Measurements were performed at 100(2) K using a nitrogen stream cryo-cooler, with paratone as a cryo-protectant. Diffraction data were indexed and integrated using the XDS package,[S4] while scaling was carried out with XSCALE.[S5] The structures were solved using the SHELXT package[S6] and structure refinement was performed by the full-matrix least-squares (FMLS) method with SHELXL-19/3,[S7] operating through either the WinGX GUI[S8] or the ShelXle Qt5 GUI.[S9] Non-hydrogen atoms were refined anisotropically, with the exception of the C and N atoms of **B** with less than full occupancy factors (see below for details), while hydrogen atoms were included at calculated positions and refined using a riding model. Crystallographic data and refinement details are reported in Table S1.

T3 crystallized in the hexagonal P6/m space group with one sixth of a Pd_6L_3 cage structure (PdL0.5) in the asymmetric unit (ASU). The final model contains one Pd(II) ion, an associated ethylenediamine ligand, one half of ligand **L3** and a total of five sixths of a nitrate ion in the ASU (Figure S1a), while six ASUs combine to form a regular equilateral triangular prism with Pd(II) ions at the vertices (Figure S1b). The Pd···Pd distances which define the base, and the length of the prism are 10.962 Å (triangular faces) and 23.246 Å (length of the rectangular faces). The **L3** ligands lie on the rectangular faces with the carbonyl groups directed inwards, while the triangular faces are open and contain nitrate anions (Figure S2a). The carbonyl group of **L3** in the asymmetric unit lies on a mirror plane, with the second half of the ligand completed by reflection through this plane. The C and O atoms of the carbonyl group were therefore refined with 0.5 occupancy factors. The cage structure of **T3** is analogous to that previously reported for **T1**. As might be expected, the main difference between the two structures is the of the rectangular faces of the prisms.

The nitrate ions which were identified in the electron density were refined in two positions, both associated with symmetry elements of the structure. In the first case, the nitrogen atom is located on a three-fold axis which coincides with the central axis of the trifacial barrel (Figure S2a), at a distance of 0.686 Å outside each triangular prism face defined by the Pd(II) ions. This atom was refined at one third occupancy, while the single bound oxygen atom was refined at full occupancy. For the other nitrate position identified, the nitrate ion lies across a mirror plane, with the nitrogen atom and an oxygen are located on a mirror plane (refined at 0.5 occupancy) and another oxygen atom bound to the nitrogen atom refined at full occupancy. Full nitrate ions are generated, respectively, by rotation around the three-fold axis and reflection through the plane.

The nitrate ions positioned across the mirror plane are important to the packing of the trifacial barrels as they bridge adjacent barrels in three positions (Figure S2b), resulting in alignment of the barrels parallel to the crystallographic *c*-axis and, consequently, the creation of channels in this direction (Figure S2a). Various bridging interactions between the nitrate ions and H atoms of both L and diethylamine ligands are present. These include two symmetric interactions (one to each trifacial barrel) between the nitrate oxygen atoms which do not lie on the mirror plane and -NH groups of the ethylenediamine ligands (NH···O distance = 2.297 Å and N···H···O angle = 167.66°); and two analogous symmetric interactions between the same oxygen atoms and aromatic -CH moieties of pyridyl groups (CH···O distance = 2.425 Å and C···H···O angle = 162.87°).

The cell also contained residual electron density attributed to the remaining disordered nitrate counterions and water solvent molecules. This was not modelled but was accounted for using the Platon squeeze tool.[S7] The residual electron density of 1875 electrons/cell in a total potential solvent accessible void volume of 8507 $Å^3$ (59.3% of the cell volume) can be attributed to 7 nitrate ions and ca. 71 water molecules per cage, with a calculated crystal density of 1.17 g cm^{-3}.

An AFIX 66 restraint was used to maintain the hexagonal geometry of one of the coordinating pyridyl rings and SIMU restraints were applied to all anisotropic thermal factors.

It should be noted that the quality of the data for **T3** is rather poor, characterised by weak diffraction and low resolution, as well as disorder observed for the nitrate counter ions and water solvent molecules. This resulted in a number of refinement problems, especially a high final value of R. However, the final model of the cage confirms the desired chemical structure without ambiguity. This is clearly illustrated in Figure S3, in which there is a very good correspondence between the observed electron density maps (Fo) and the model.

B crystallized in the I -4m2 space group, with a total of one eight of a $Pd_{16}L_8$ superstructure (Pd_2L) in the asymmetric unit (ASU, Figure S1c). In the final model, one of the Pd(II) ions in the ASU is present in a general position at full occupancy, while two Pd(II) sites lie on mirror planes with 0.5 occupancy. In addition, one these Pd(II) sites on the mirror plane shows a two-position statistical disorder (0.25:0.25 occupancy factors), however both positions lie on the mirror plane. Therefore, overall, the ASU was refined with one Pd(II) at full occupancy, one with a 0.5 occupancy factor and two with 0.25 occupancy factors.
The Pd(II) ions also have associated tetramethylethylenediamine (tmeda) ligands (Figure S1c). The Pd(II) ion at full occupancy is complexed a full tmeda ligand, while those which lie on a mirror plane have only one half of each of the tmeda ligands, the other half of each being generated by reflection through the mirror plane. However, the electron density of tmeda associated with one of the Pd(II) ions refined at 0.25 occupancy could not be identified clearly in the electron density maps, and was not included in the final model. The other half-tmeda ligand, with the atoms at 0.5 occupancy, was refined isotropically.
Consistently with the two above-discussed, two-position statistical disorder of the Pd(II) ions, the pyridyl group of the ligand **L** complexed to this Pd(II) was also refined with a two-position disorder of all six members of the ring. Each position was refined isotropically with a 0.5

occupancy factor and AFIX 66 instructions were used to maintain the hexagonal geometry of each position.

A $Pd_{16}L_8$ superstructure is completed by seven symmetry-related asymmetric units generated by symmetry operations involving reflections, two-fold axes and four-fold axes (Figure S1d). In this superstructure, the Pd(II) ions form four slighted distorted tetrahedra and the superstructure is composed of four of these tetrahedra which are connected by the eight **L** ligands (Figure S4)

The cell also contained residual electron density attributed to disordered nitrate counterions, the partial tmeda ligand which could not be located and water solvent molecules. This was not modelled but was accounted for using the Platon squeeze tool.[S10] The residual electron density of 7613 electrons/cell in a total potential solvent accessible void volume of 21911 $Å^3$ (61.5% of the cell volume) can be attributed to 32 nitrate ions and ca. 266 molecules per cage, with a calculated crystal density of 1.35 g cm^{-3}.

For one of the tmeda ligands, a DFIX restraint was applied to the C-C bond distance and SIMU restraints were applied its anisotropic thermal factors. Finally, B was refined as a perfect inversion twin.

Table S1. Crystallographic data and refinement parameters of **T3** and **B**.

Identification code	**T3**	**B**
Empirical formula	6 $Pd(C_2H_8N_2)^{2+}$, 3 ($C_{45}H_{30}N_6O$), 12 NO_3^-, 71 H_2O	16 $Pd(C_6H_{16}N_2)^{2+}$, 8 ($C_{33}H_{22}N_6O$), 32 NO_3^-, 266 H_2O
Formula weight	5034.19	14484.16
Temperature / K	100(2)	100(2)
Crystal system	Hexagonal	Tetragonal
Space group	P6/m	I-4m2
a (Å)	23.25(3)	42.860 (10)
b (Å)	23.45(3)	42.860 (10)
c (Å)	30.61(4)	19.405(1)
α (°)	90	90
β (°)	90	90
γ (°)	120	90
Volume ($Å^3$)	14334(42)	35647(16)
Z	2	2
ρ_{calc} (g/cm^3)	1.17	1.35
μ (mm^{-1})	0.386	0.403
F(000)	3370	7640
Crystal size/mm	0.08 x 0.04 x 0.01	0.1 × 0.05 × 0.02
Radiation	synchrotron (λ = 0.700)	synchrotron (λ = 0.700)
2Θ range for data collection (°)	1.31 to 31.322	1.324 to 59.532

Index ranges	-17≤ h≤17, -17≤ k ≤17, -23 ≤ l ≤ 23	-60≤ h≤60, -60≤ k ≤60, -25 ≤ l ≤ 25
Reflections collected	40807	331675
Independent reflections	2152 [R_{int} = 0.1611, R_{sigma} = 0.0450]	26766 [R_{int} = 0.0397, R_{sigma} = 0.0164]
Data Completeness (%)	91.0	98.1
Data/restraints/parameters	2152/240/304	26766/43/489
Goodness-of-fit on F^2	1.798	1.089
Final R indexes [I>=2σ (I)]	R_1[a] = 0.1442, wR_2[b] = 0.3820	R_1[a] = 0.0629, wR_2[b] = 0.1750
Final R indexes [all data]	R_1[a] = 0.2015, wR_2[b] = 0.4424	R_1[a] = 0.0651, wR_2[b] = 0.1785
CCDC No.	2410383	2361330

[a]$R_1=\Sigma\big|\,|F_o|-|F_c|\,\big|/\Sigma|F_o|$, [b]$wR_2=[\Sigma\{w(F_o^2-F_c^2)^2\}/\Sigma\{w(F_o^2)^2\}]^{1/2}$.

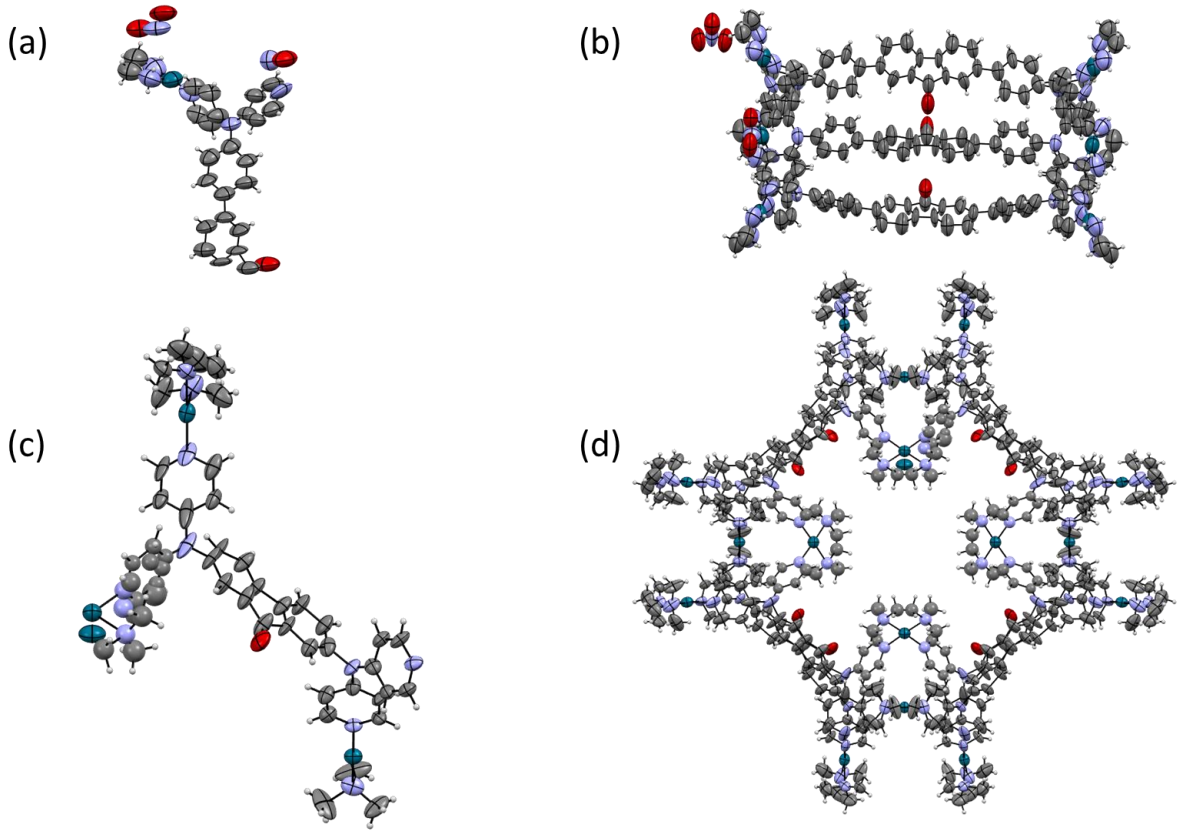


Figure S1. ORTEP diagrams (a) of the asymmetric unit **T3**; (b) of the full Pd_6L_3 cage structure of T3, composed of six asymmetric units, as viewed along the crystallographic *b*-axis; (c) of the asymmetric unit of **B** and (d) of the full $Pd_{16}L_8$ structure of **B**, composed of eight asymmetric

units, as viewed along the crystallographic *c*-axis. Elipsoids at 50% probability. Colours: Pd: green carbon: grey, nitrogen: blue, oxygen: red.

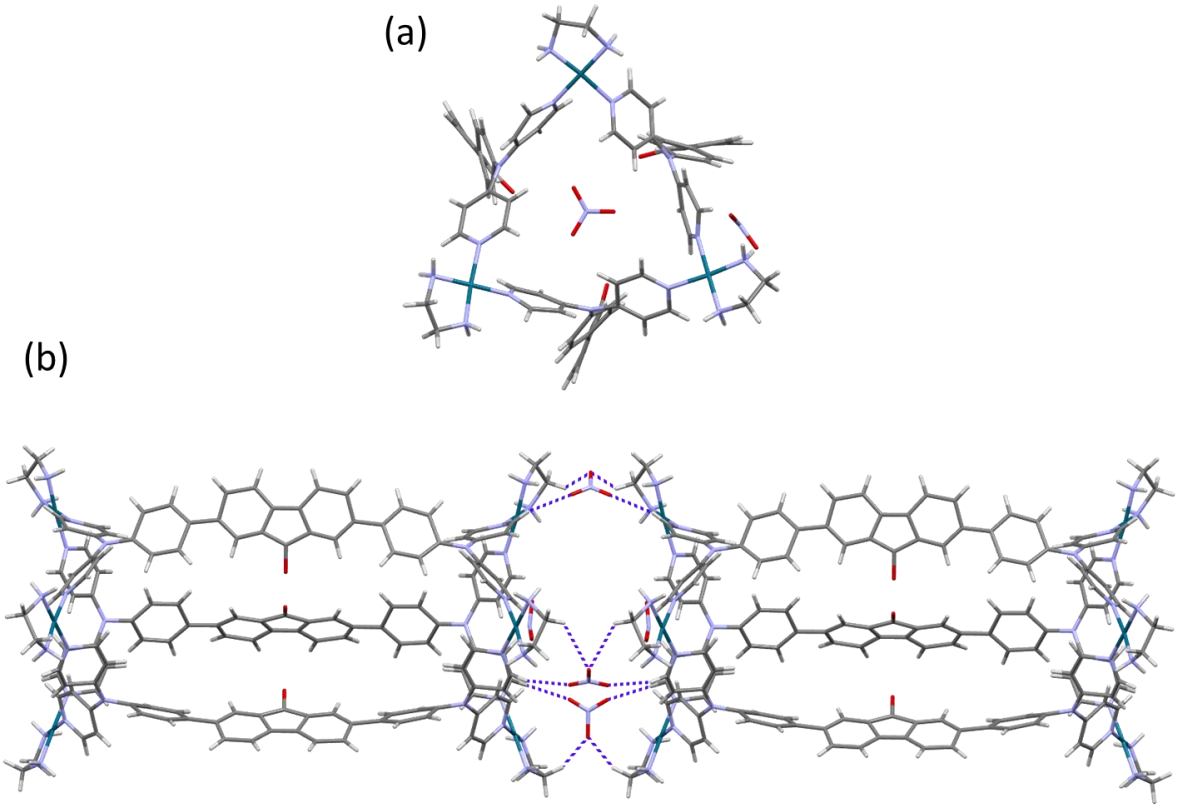


Figure S2. (a) view along the crystallographic *c*-axis of **T3**. The Pd atoms define equilateral triangular prisms which are arranged as parallel channels along the *c*-axis. Each Pd_6L_3 cage contains two nitrate ions located on the central axis; (b) view along the crystallographic *b*-axis of **T3**. Consecutive cages are bridged by three nitrate ions.

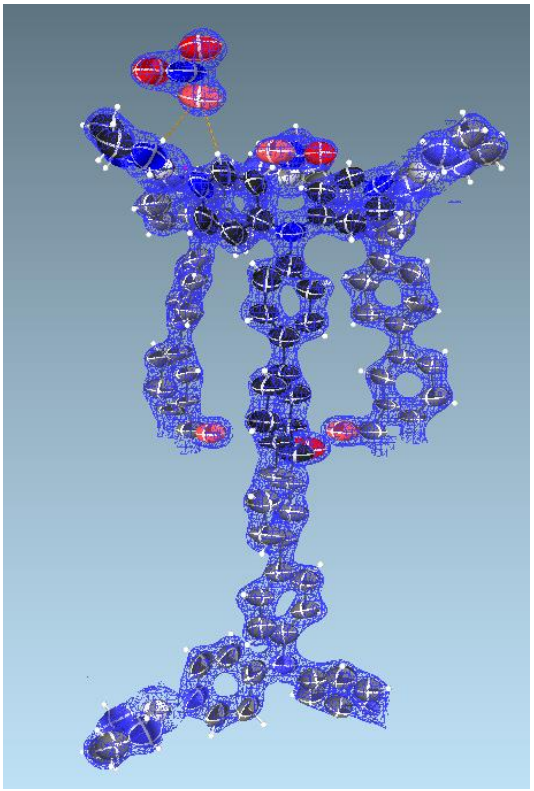


Figure S3. Correspondence between the observed electron density maps (Fo) and the model for **T3**. The black spheres represent the carbon atoms in the asymmetric unit, while blue (nitrogen), red (oxygen) and white (Pd) spheres bonded to these atoms are also in the asymmetric unit. The grey atoms are carbon atoms generated by symmetry, as are the atoms bonded to these grey atoms.

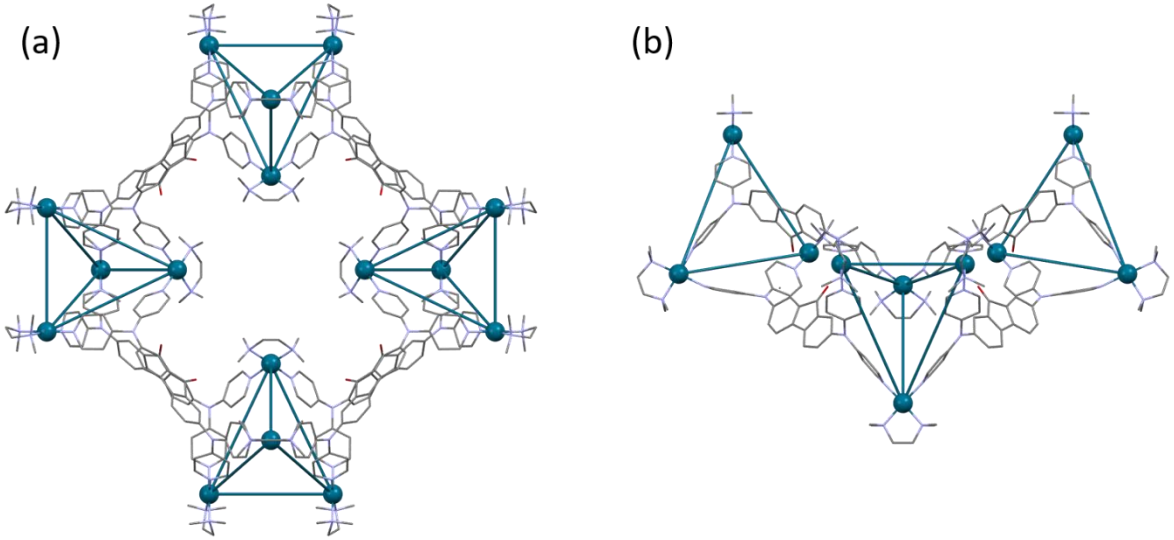


Figure S4. Views (a) along the crystallographic *c*-axis and (b) along the crystallographic *a*-axis of **B**, showing the four tetrahedra of Pd(II) ions which compose the $Pd_{16}L_8$ superstructure. To highlight this arrangement, the Pd(II) ions are included as green ellipsoids, while the tmeda and **L** ligands are included as wireframe structures. Disordered atoms have been removed for clarity.

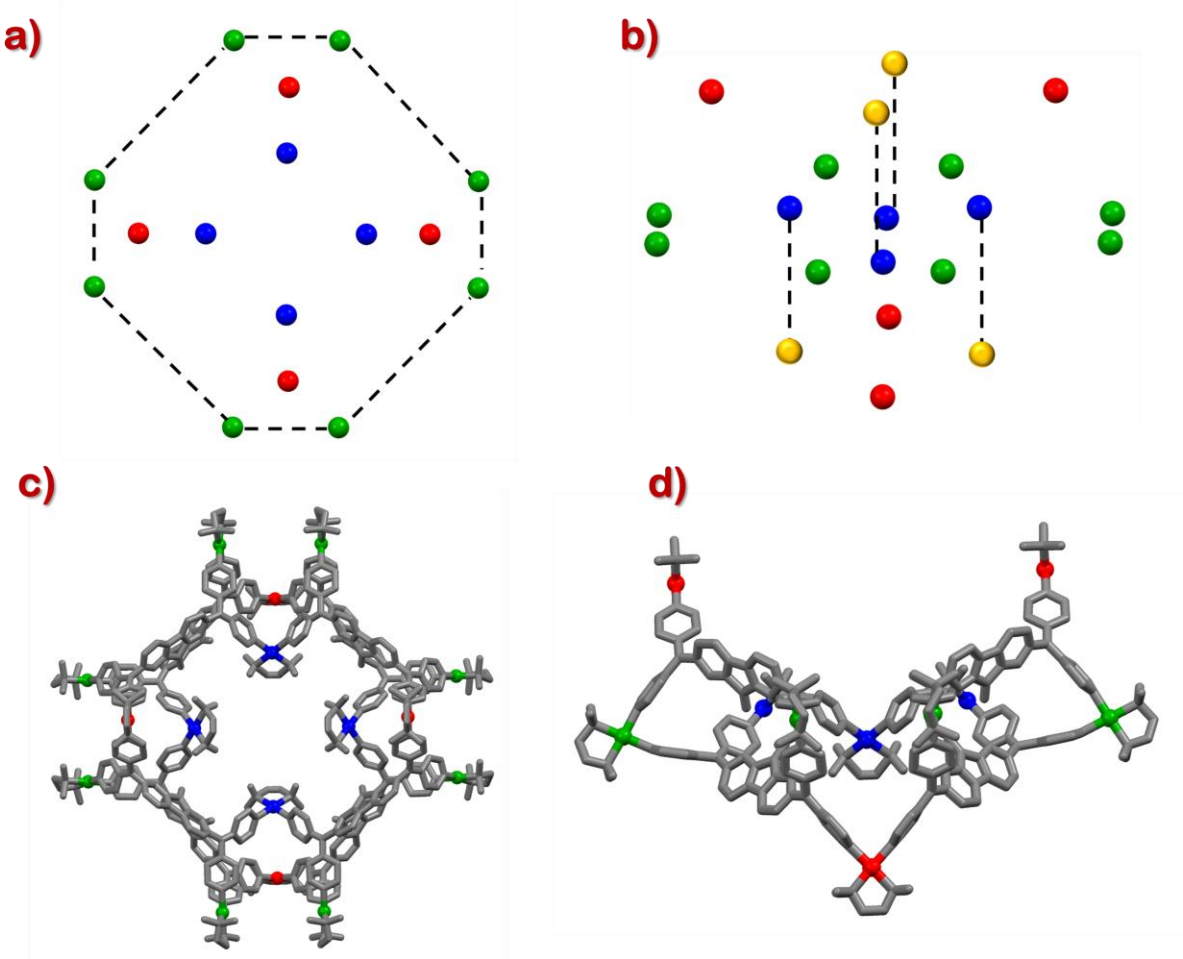


Figure S5. The arrangement of 16 Pd(II) acceptors in the crystal structure of **B**: (a) top view, (b) side view. The structure can be described as a distorted square gyrobicupola architecture (Johnson polyhedron, J_{29}) with respect to the arrangement of Pd(II) acceptors at the vertices. The green atoms form the octagonal base and eight vertices of square gyrobicupola, the red atoms are at their expected vertex positions as expected in a square gyrobicupola arrangement whereas the blue atoms are displaced from their expected vertex position and pushed inwards (yellow atoms are dummy atoms which shows the position of the blue atoms in an ideal gyrobicupola arrangement). The crystal structure of B where only the "Pd" atoms are highlighted with green, red or blue colours as described earlier: (c) top view (d) side view.

5. Spectral section

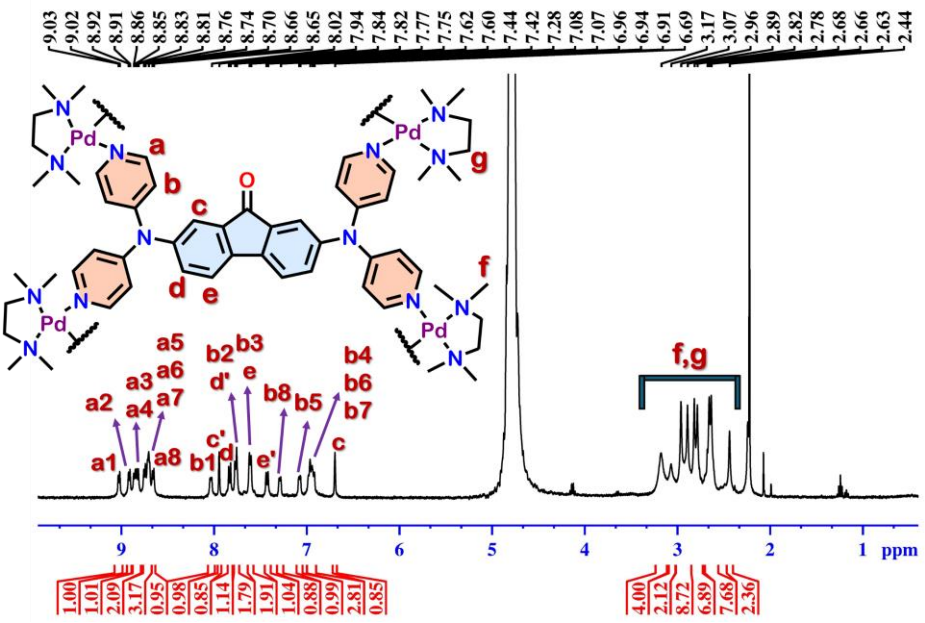


Figure S6. ^{1}H NMR spectrum of **B** (D_2O, 298 K).

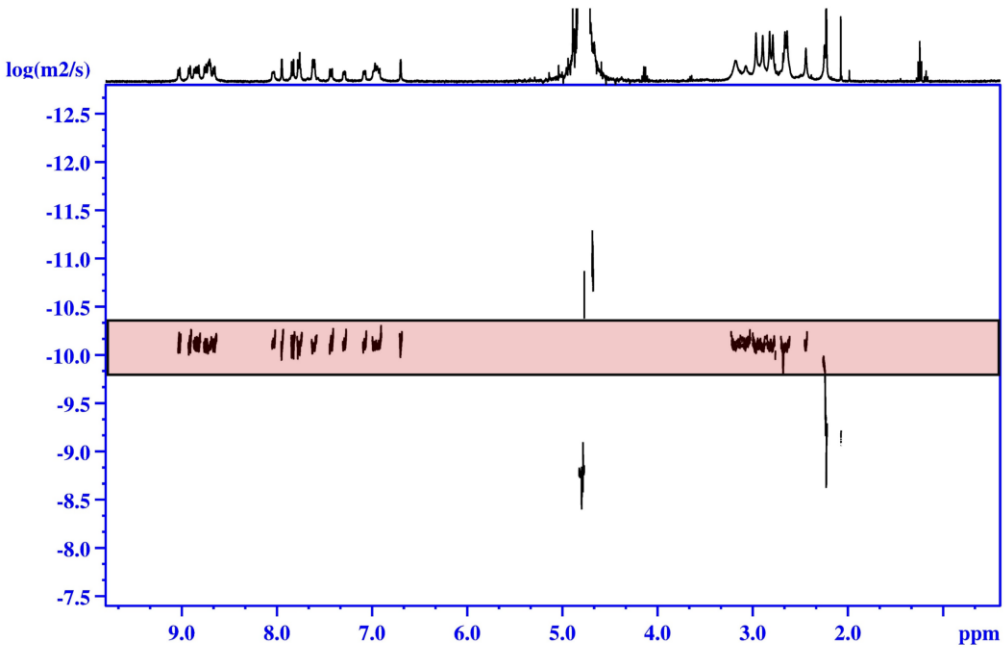


Figure S7. ^{1}H DOSY NMR spectrum of **B** (D_2O, 298 K).

Diffusion coefficient, D = 8.91 × 10^{-11} m^2 /s and hydrodynamic radius, r = 27.8 Å.

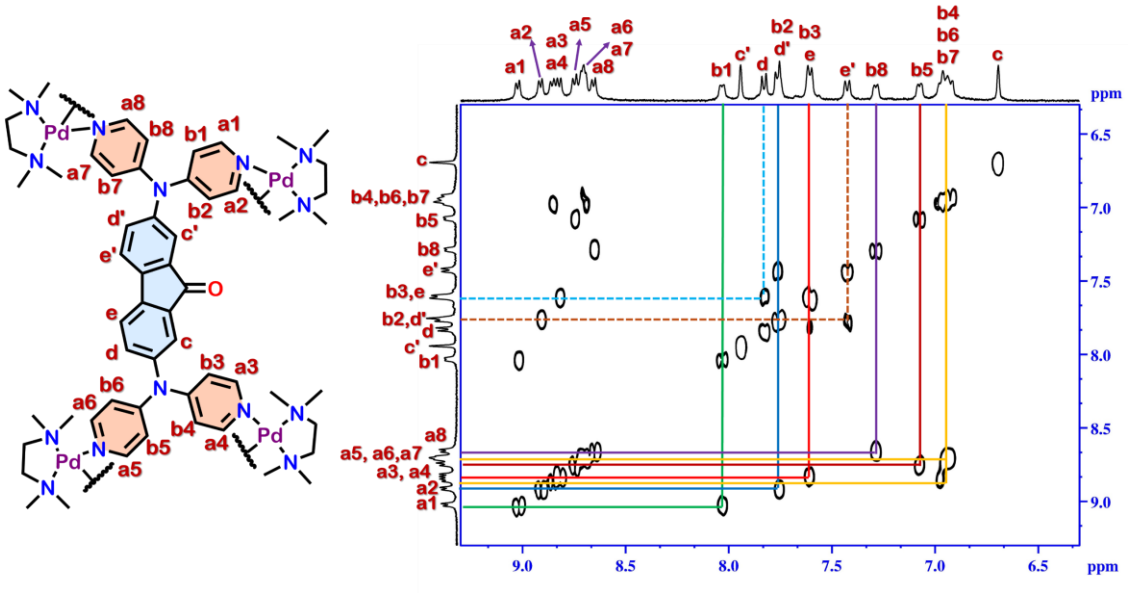


Figure S8. ^{1}H-^{1}H COSY NMR spectrum of **B** (D_2O, 298 K).

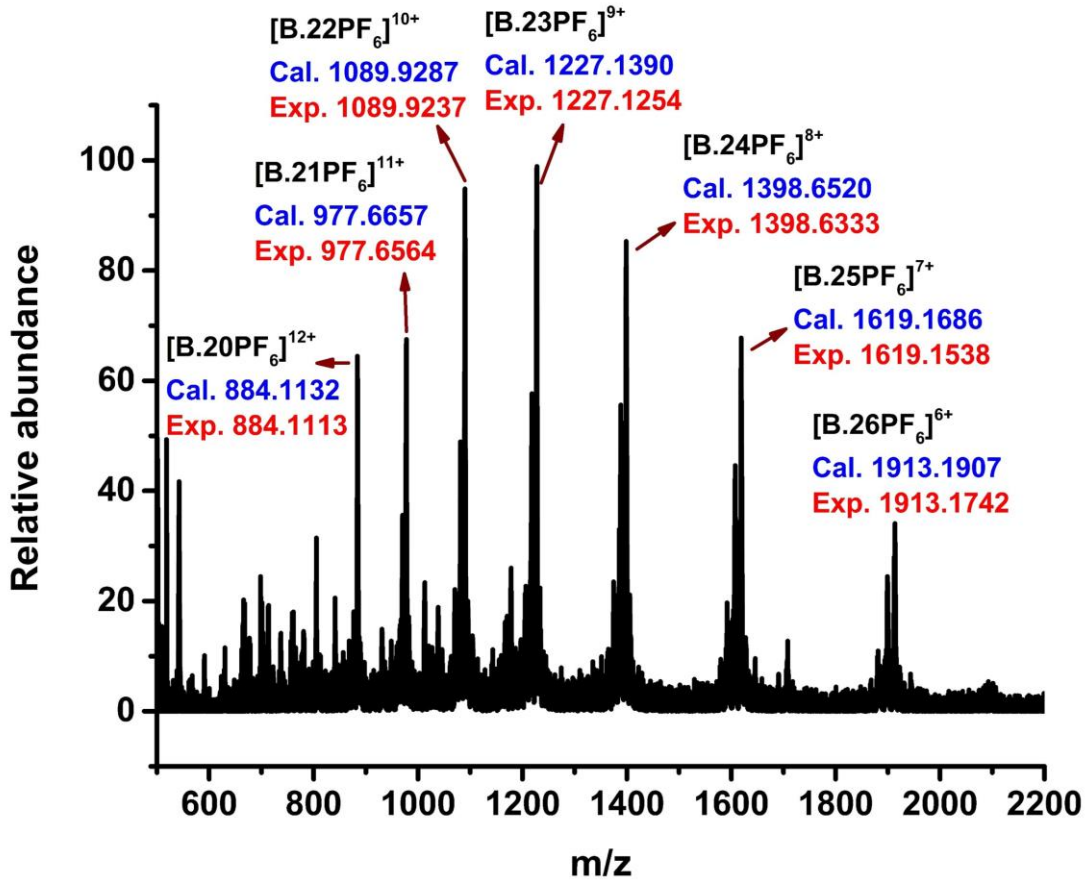


Figure S9. ESI-MS of PF_6^- analogue of **B** in CH_3CN.

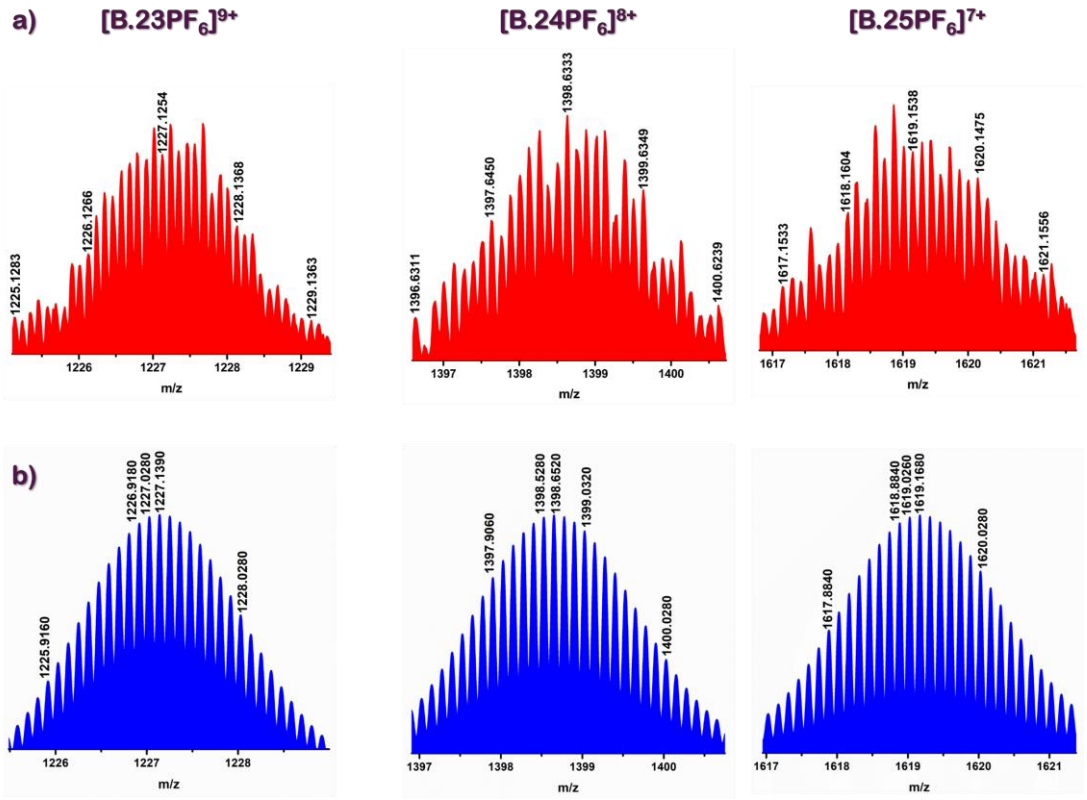


Figure S10. (a) Experimental (red) and (b) calculated (blue) isotopic patterns of the fragments $[\mathbf{B}.23PF_6]^{9+}$, $[\mathbf{B}.24PF_6]^{8+}$ and $[\mathbf{B}.25PF_6]^{7+}$.

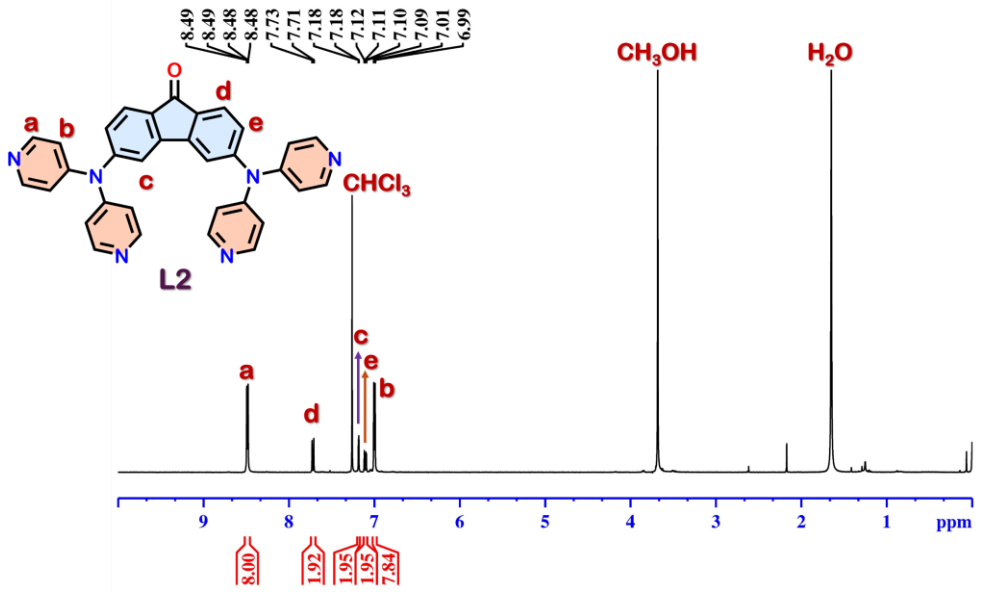


Figure S11. ^{1}H NMR spectrum of the ligand **L2** ($CDCl_3$, 298 K).

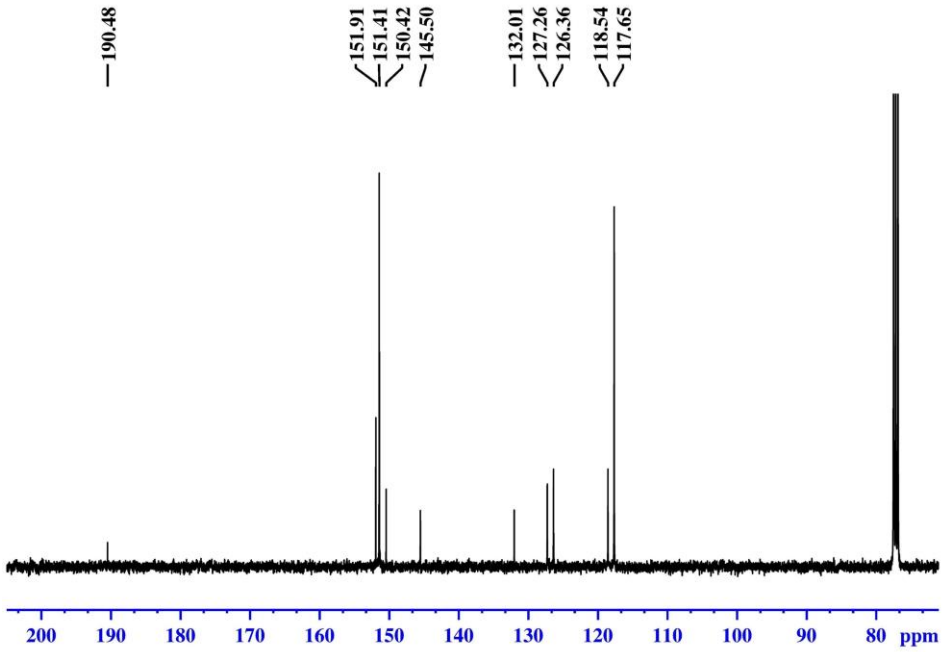


Figure S12. ^{13}C NMR spectrum of the ligand **L2** ($CDCl_3$, 298 K).

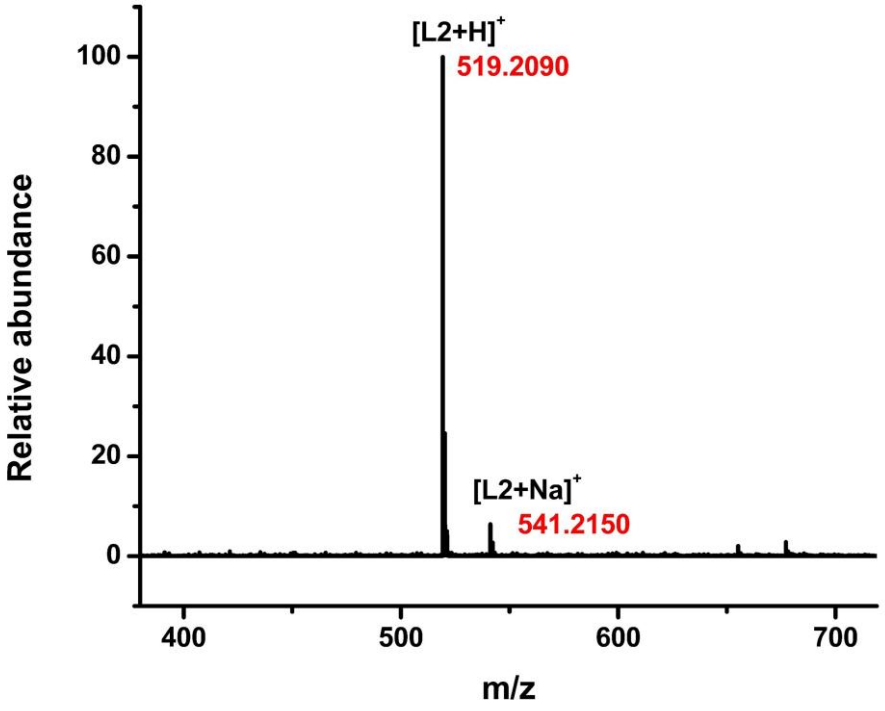


Figure S13. ESI-MS of ligand **L2** in MeOH.

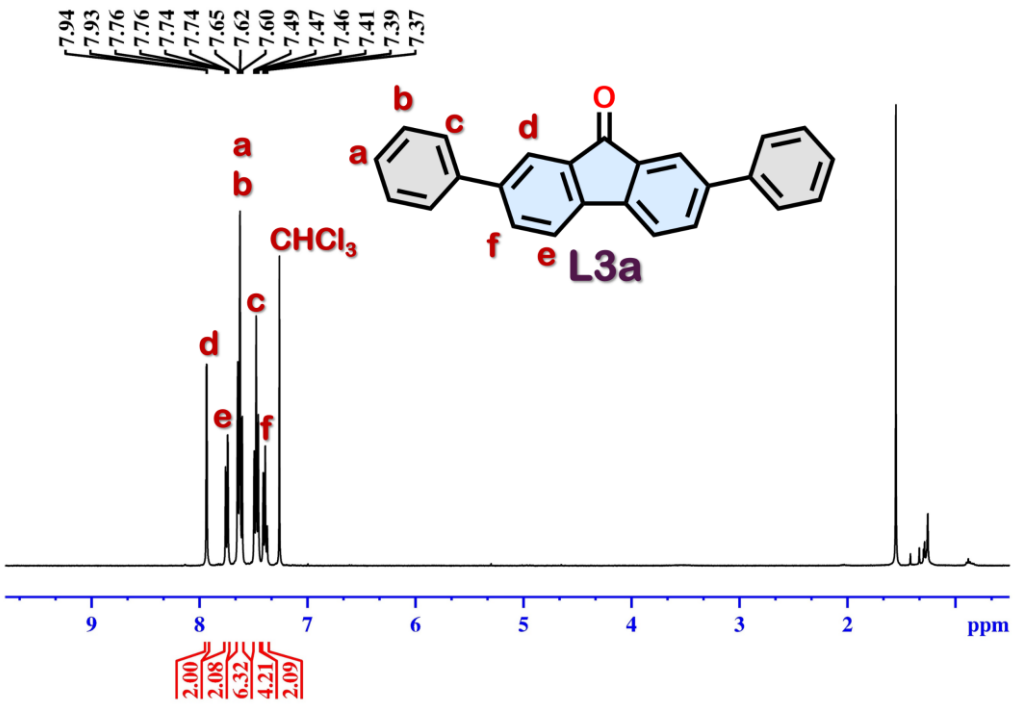


Figure S14. ^{1}H NMR spectrum of the precursor **L3a** ($CDCl_3$, 298 K).

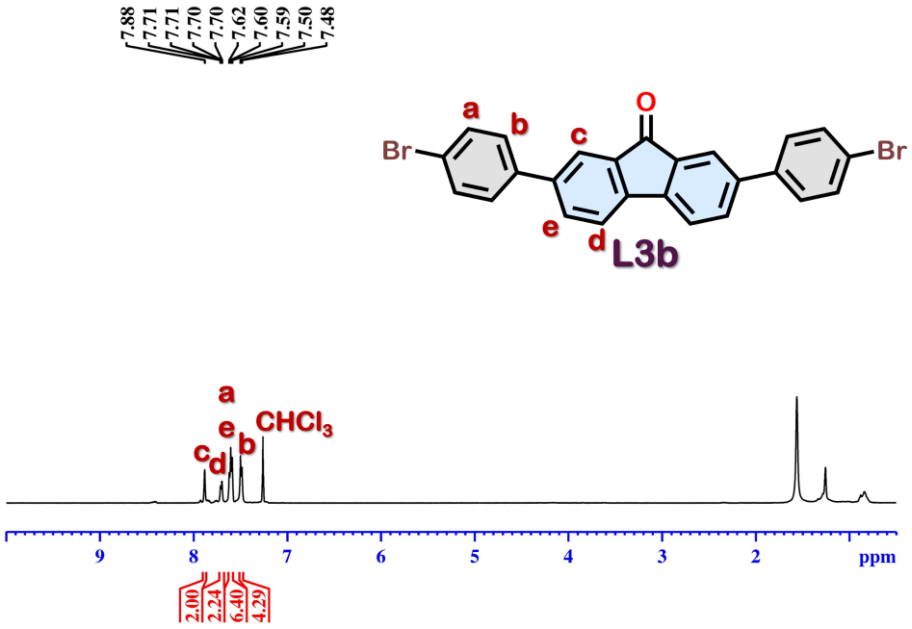


Figure S15. ^{1}H NMR spectrum of the precursor **L3b** ($CDCl_3$, 298 K).

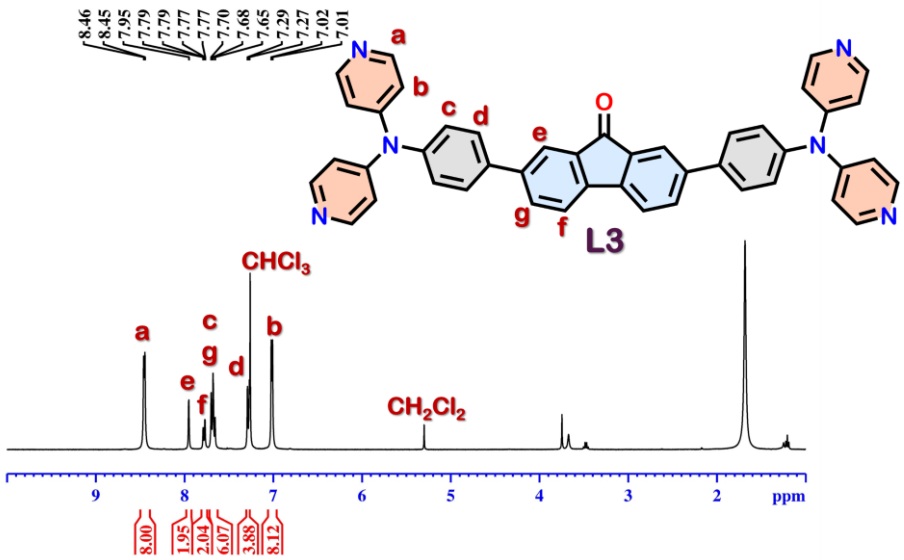


Figure S16. ^{1}H NMR spectrum of the ligand **L3** ($CDCl_3$, 298 K).

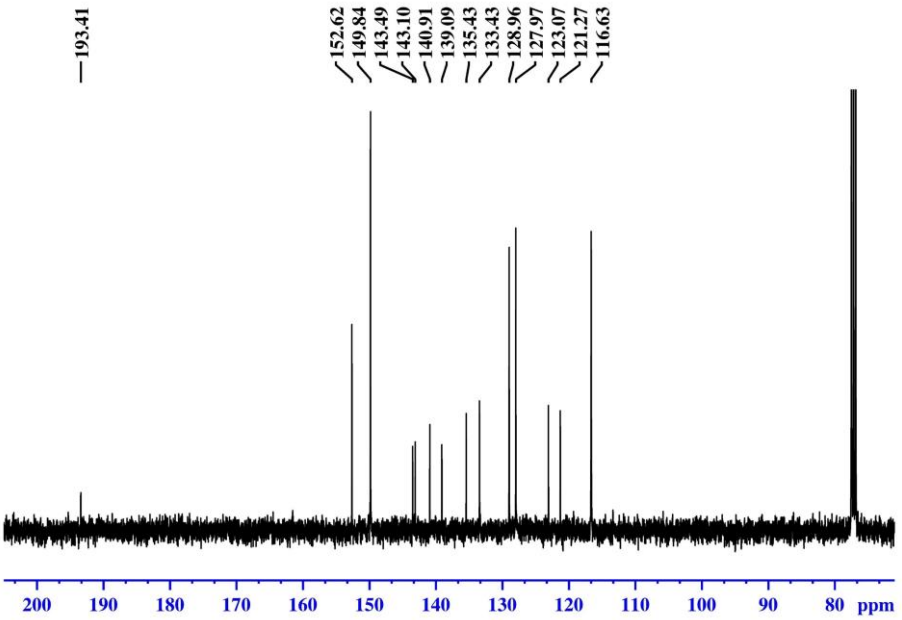


Figure S17. ^{13}C NMR spectrum of the ligand **L3** ($CDCl_3$, 298 K).

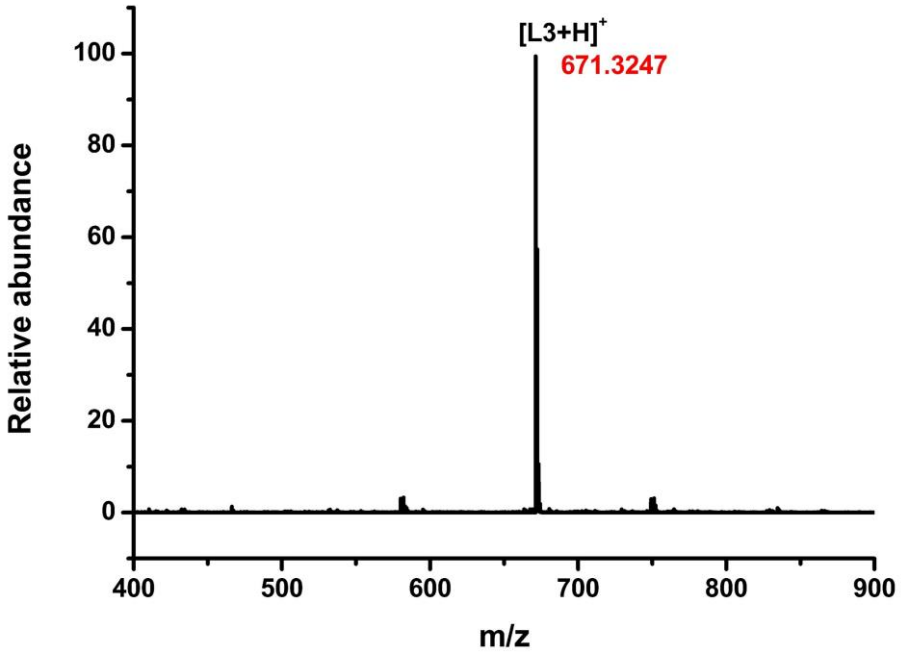


Figure S18. ESI-MS of ligand **L3** in MeOH.

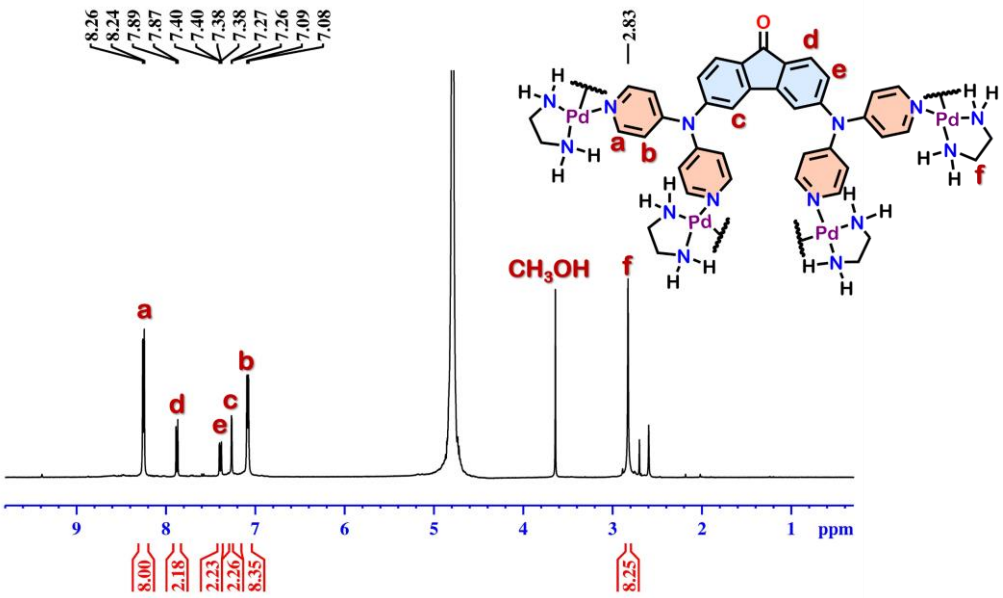


Figure S19. ^{1}H NMR spectrum of **T2** (D_2O, 298 K).

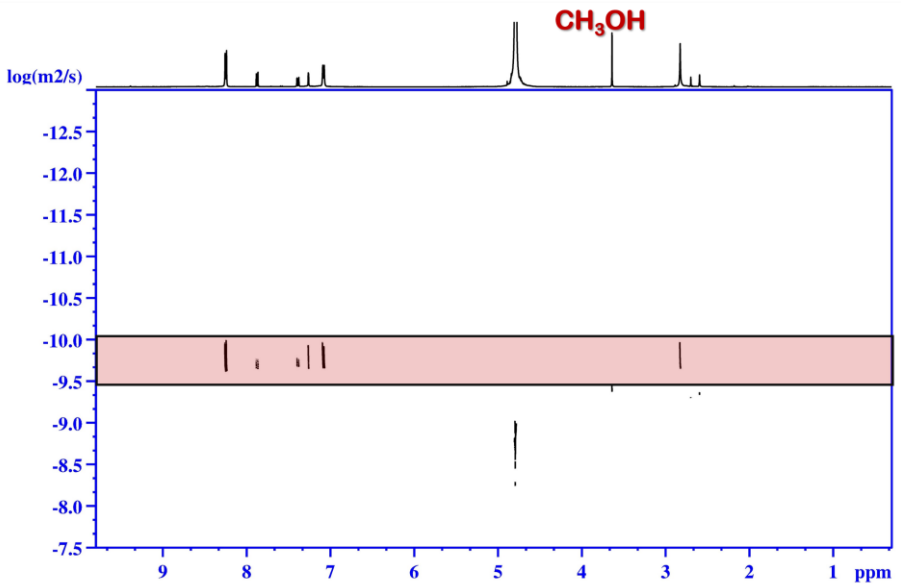


Figure S20. ^{1}H DOSY NMR spectrum of **T2** (D_2O, 298 K).

Diffusion coefficient, D = 1.78 ×10^{-10} m^2/s and hydrodynamic radius, r = 13.8 Å

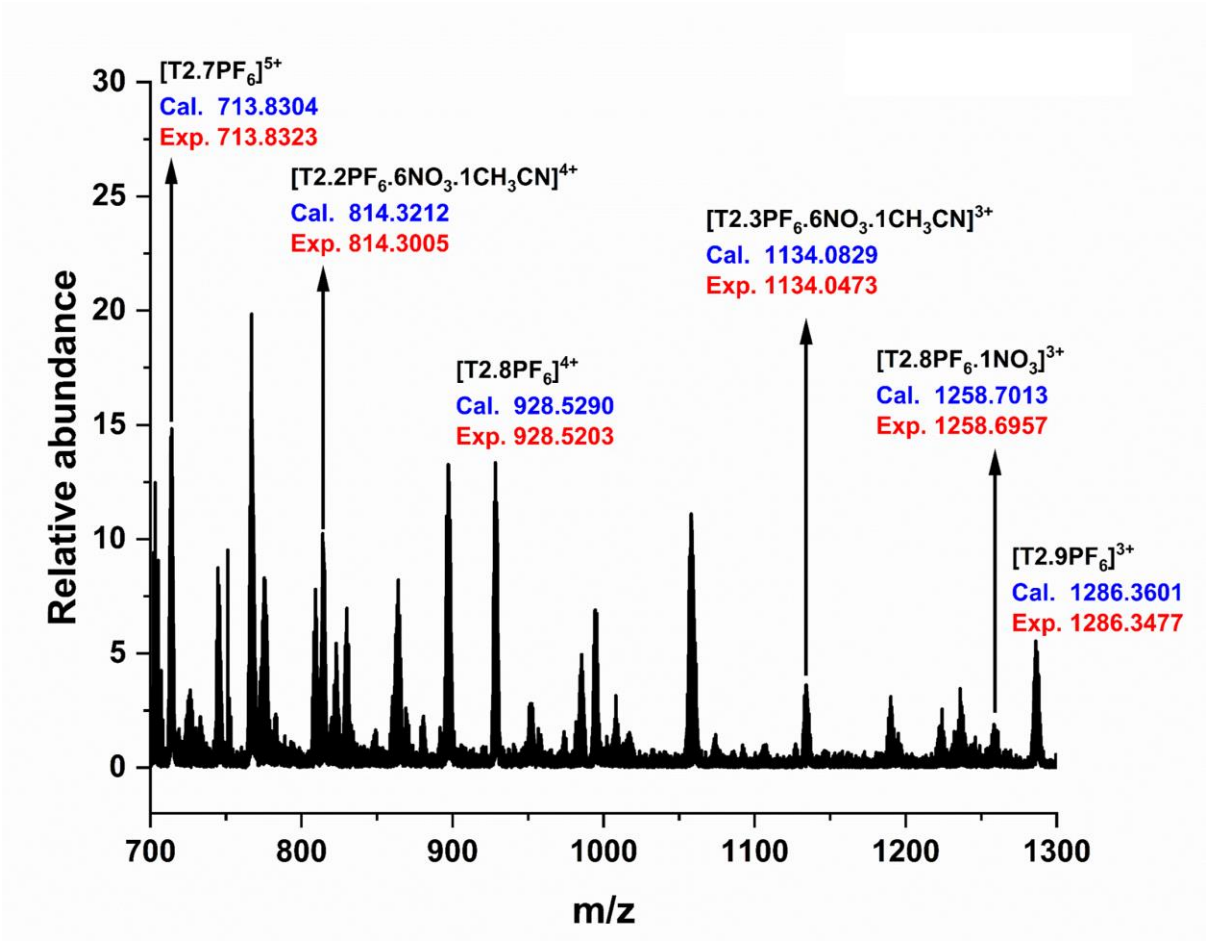


Figure S21. ESI-MS of PF_6^- analogue of **T2** in CH_3CN.

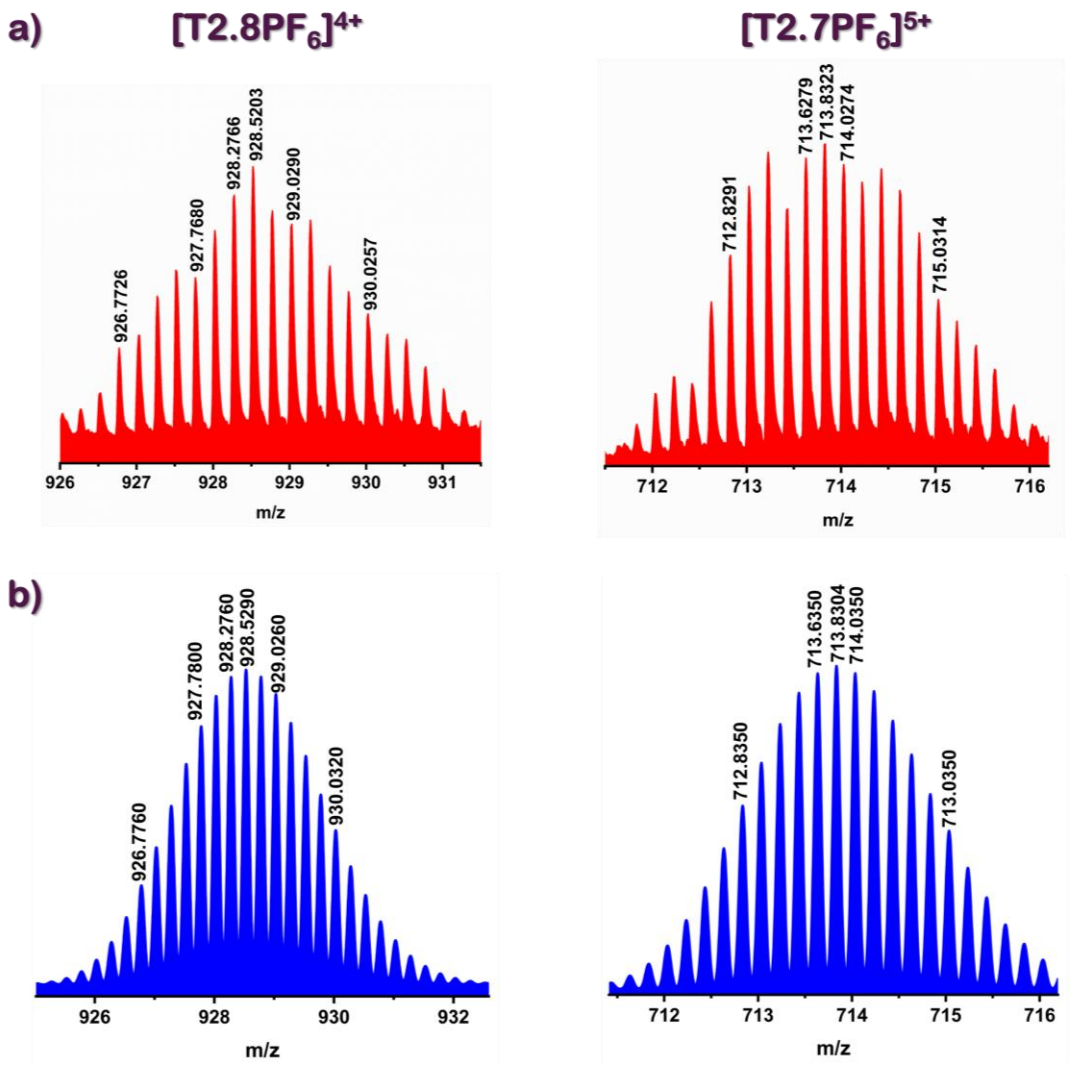


Figure S22. (a) Experimental (red) and (b) calculated (blue) isotopic patterns of the fragments $[\mathbf{T2}.8PF_6]^{4+}$ and $[\mathbf{T2}.7PF_6]^{5+}$.

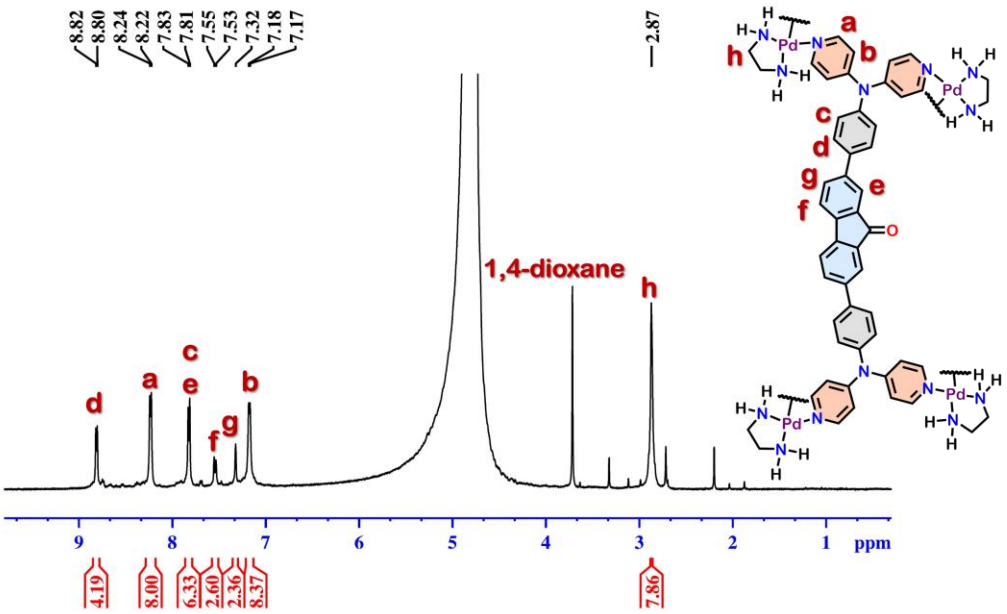


Figure S23. ^{1}H NMR spectrum of **T3** (D_2O, 298 K).

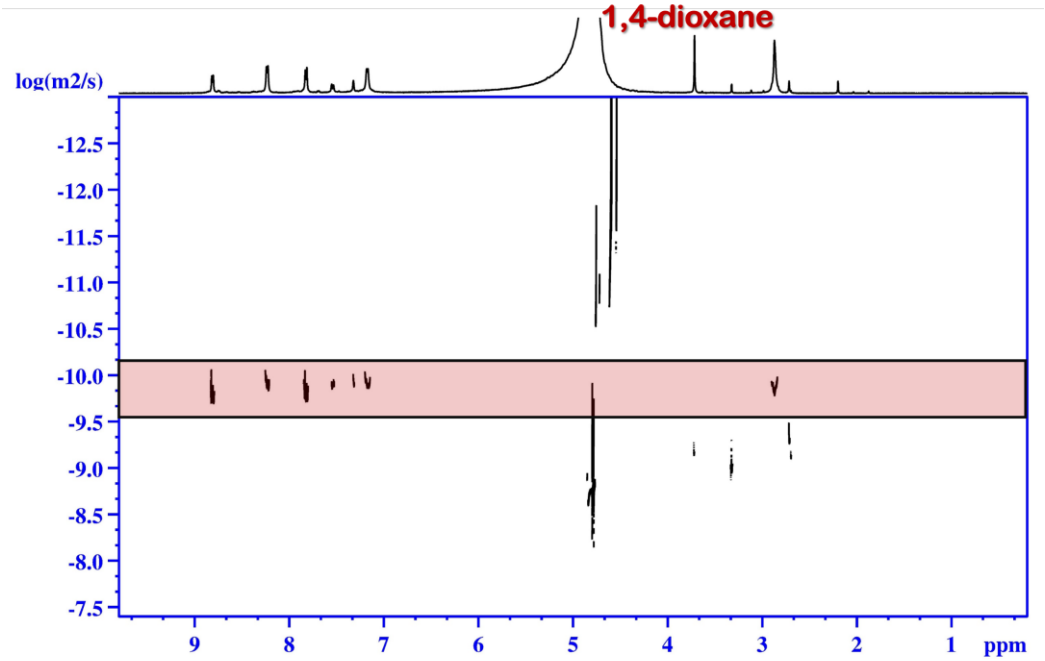


Figure S24. ^{1}H DOSY NMR spectrum of **T3** (D_2O, 298 K).

Diffusion coefficient, D = 1.41 × 10^{-10} m^2 /s and hydrodynamic radius, r = 17.4 Å.

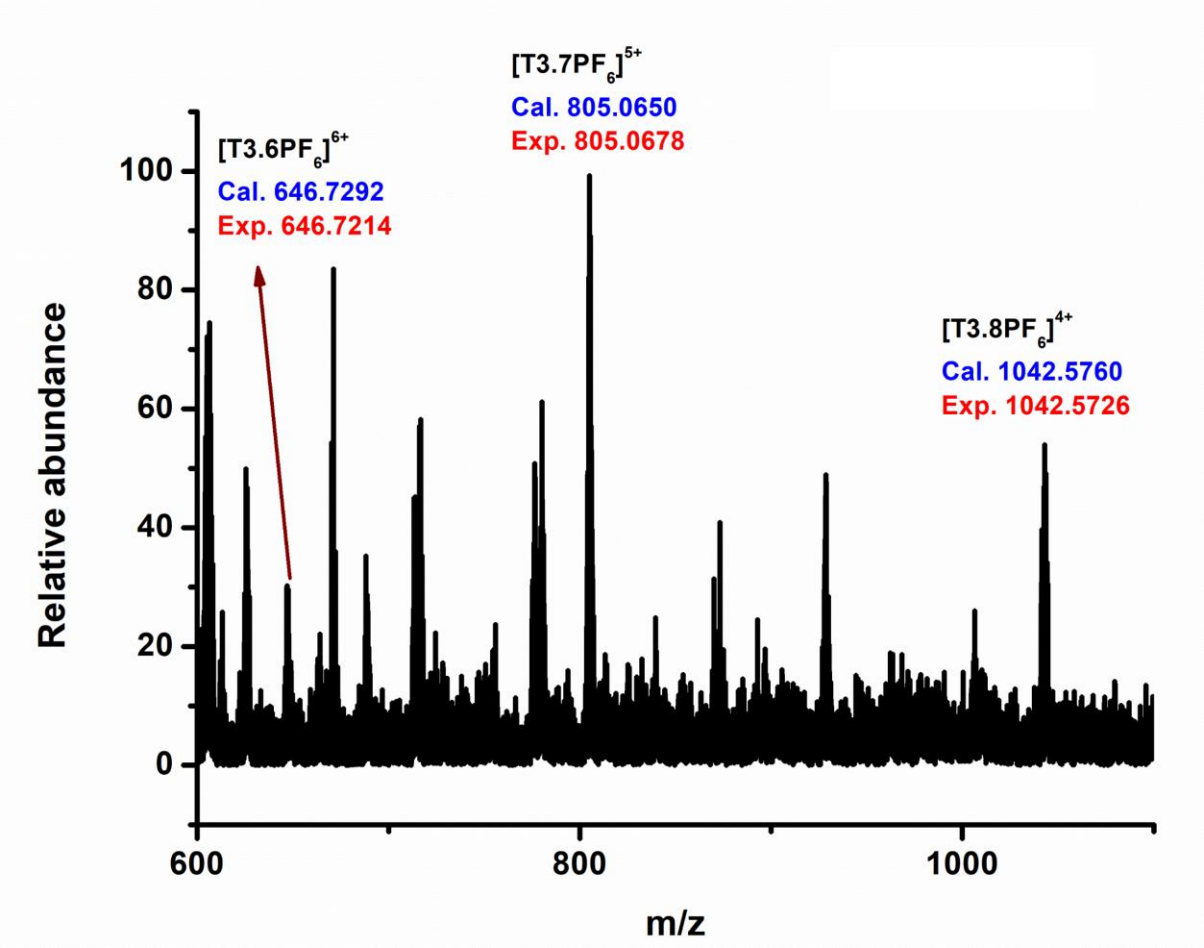


Figure S25. ESI-MS of PF_6^- analogue of **T3** in CH_3CN.

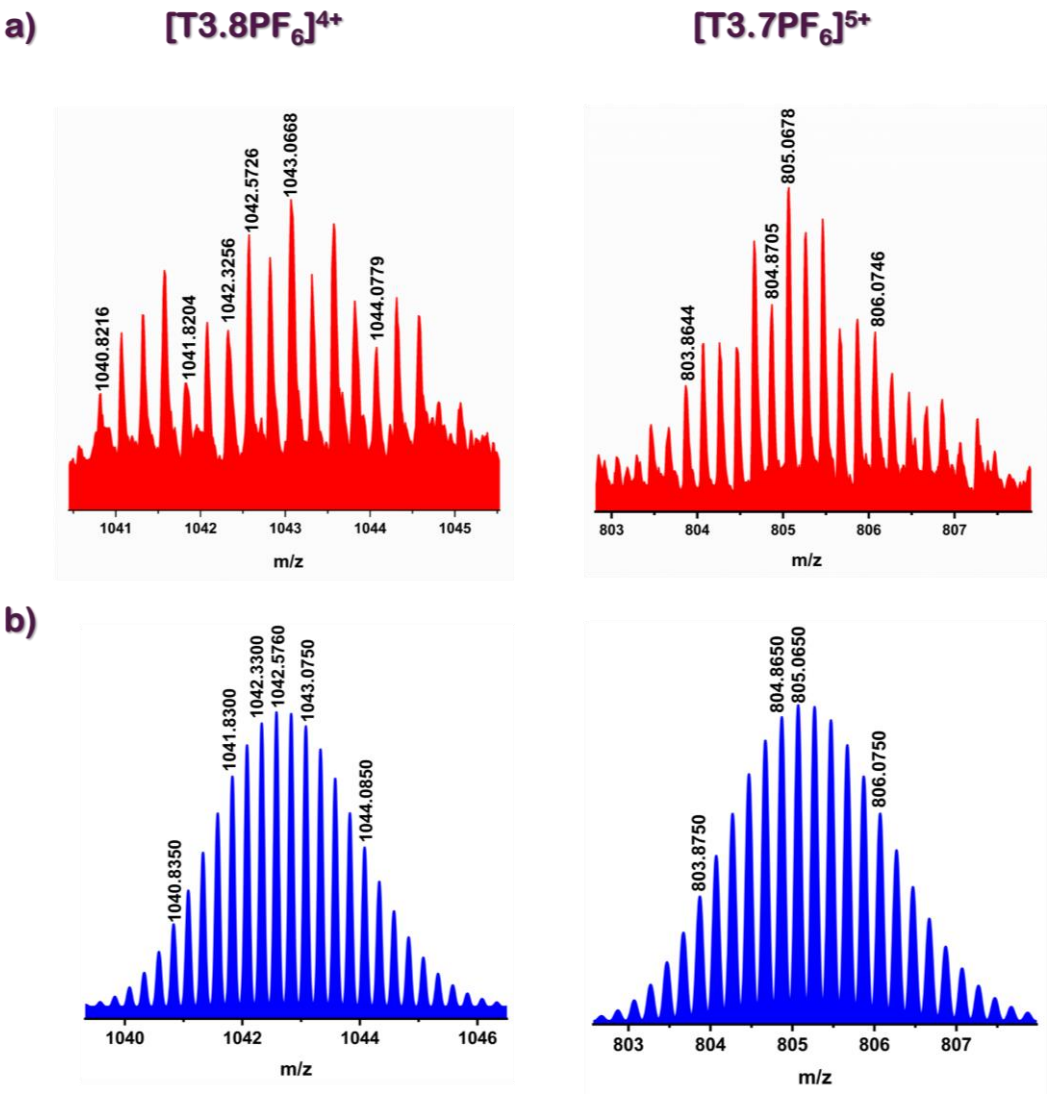
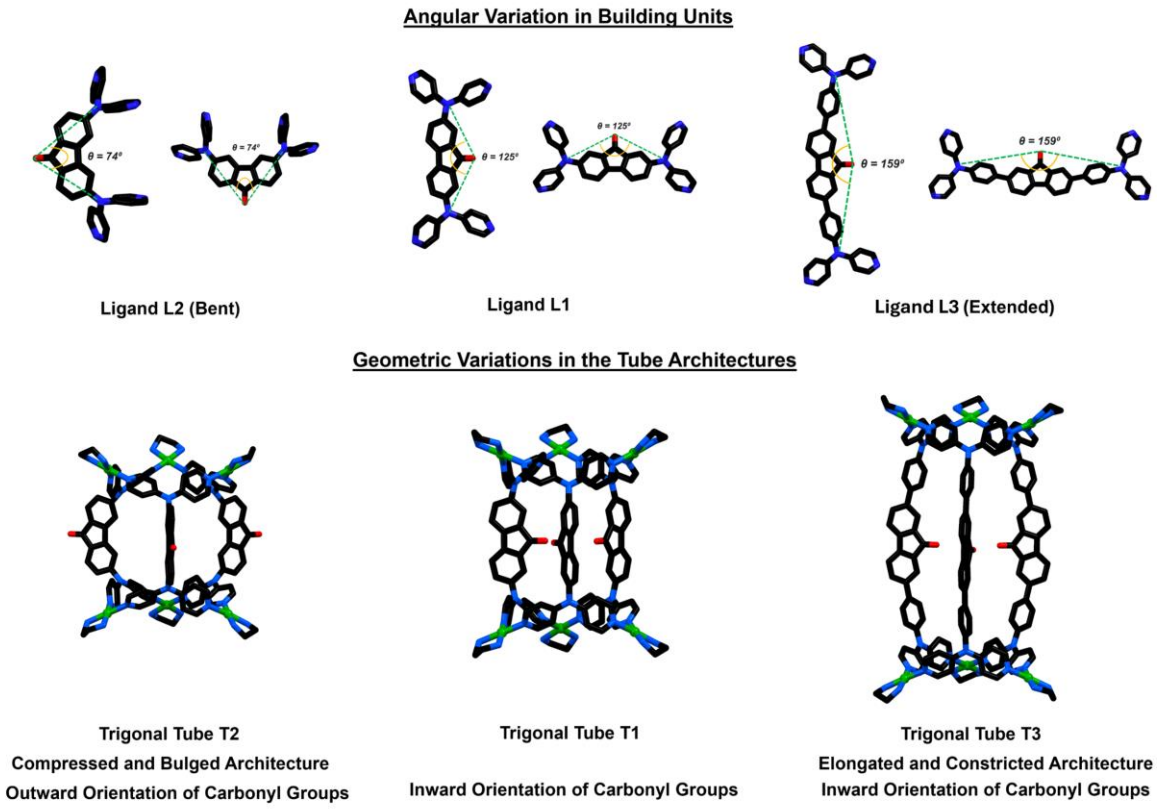


Figure S26. (a) Experimental (red) and (b) calculated (blue) isotopic patterns of the fragments $[\mathbf{T3}.8PF_6]^{4+}$ and $[\mathbf{T3}.7PF_6]^{5+}$.



Scheme S9. Schematic representation of how the angular modulation of the ligands via change in dipyridyl amine binding sites to the central core (**L1** to **L2**) or extension in ligand length (**L1** to **L3**) leads to the formation of trifacial tubes (**T1**/**T2**/**T3**) of different cavity shapes and sizes upon self-assembly with **M2** which eventually affect their guest binding abilities. The angles (ɵ) being referred to is the angle subtended by the two dipyridyl amine nitrogen atoms to the central oxygen atom of the fluorenone core.

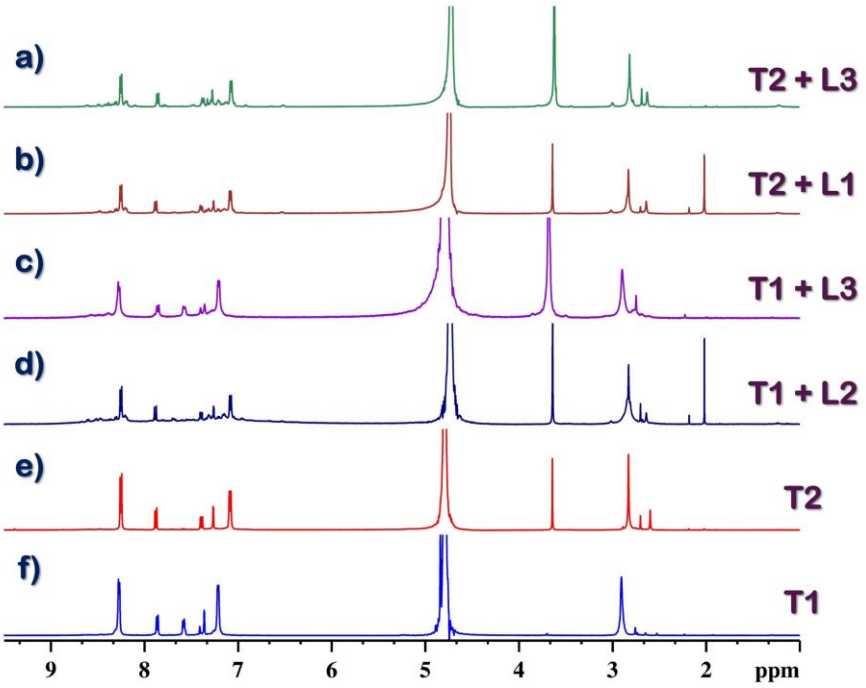


Figure S27. Stacked ^{1}H NMR spectra: (a) after addition of equivalent amount (3 equivalents with respect to **T2**) of **L3** to solution of **T2**, (b) after addition of equivalent amount of **L1** (3 equivalents with respect to **T2**) to solution of **T2**, (c) after addition of equivalent amount of **L3** (3 equivalents with respect to **T1**) to solution of **T1**, (d) after addition of equivalent amount of **L2** (3 equivalents with respect to **T1**) to solution of **T1**, (e) **T2**, and (f) **T1**. All the spectra were recorded in D_2O at 298 K. The addition of equivalent amount (3 equivalents) of **L2** to **T1** leads to formation of **T2** via the displacement of **L1** by **L2** (d). The addition of **L1** (b) or **L3** (a) to **T2** leads to no change NMR indicating **T2** remains intact. These experiments indicate that in aqueous media **T2** is the most stable tube architecture.

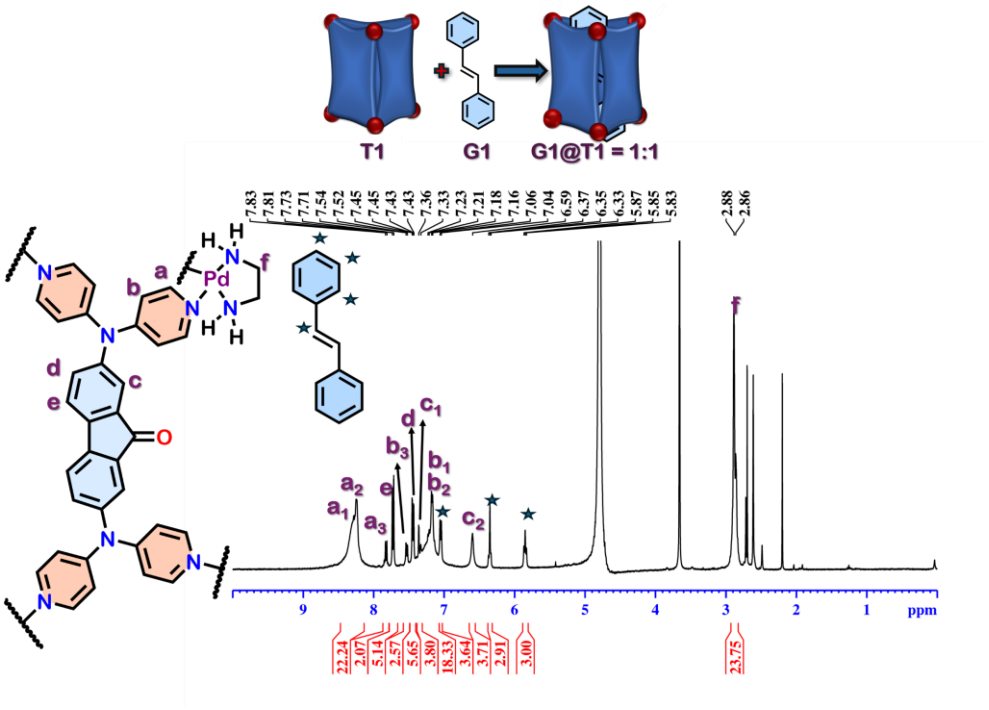


Figure S28. ^{1}H NMR spectrum of **G1**@**T1** (D_2O, 298 K). **G1** peaks are designated by blue star marks (★).

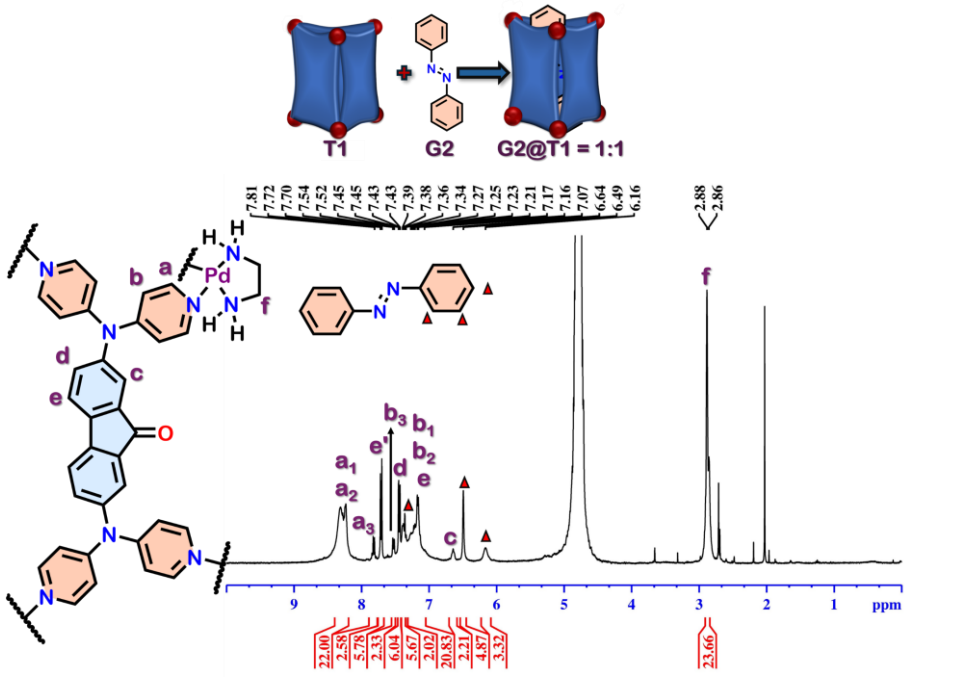


Figure S29. ^{1}H NMR spectrum of **G2**@**T1** (D_2O, 298 K). **G2** peaks are designated by red triangle marks (▲).

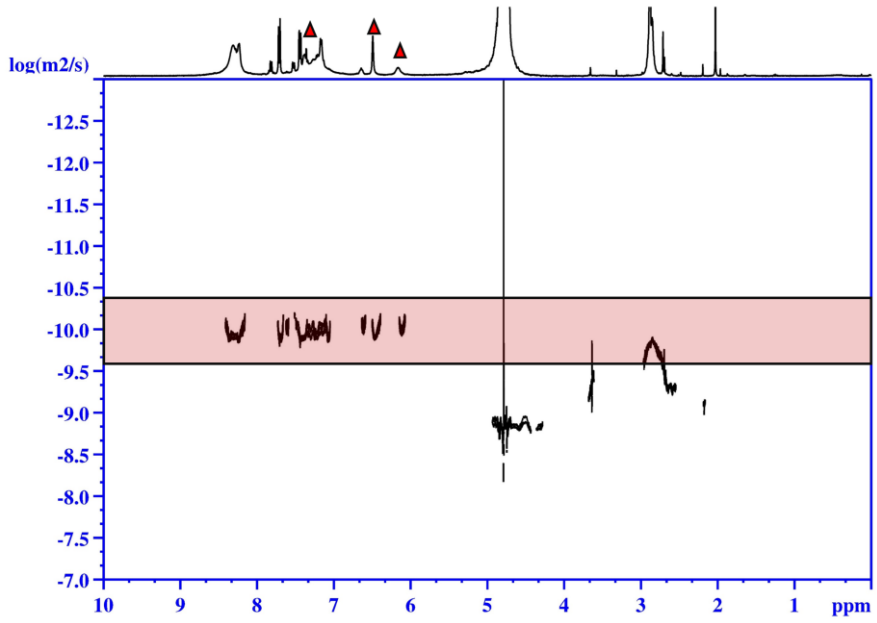


Figure S30. ^{1}H DOSY NMR spectrum of **G2@T1** (D_2O, 298 K).

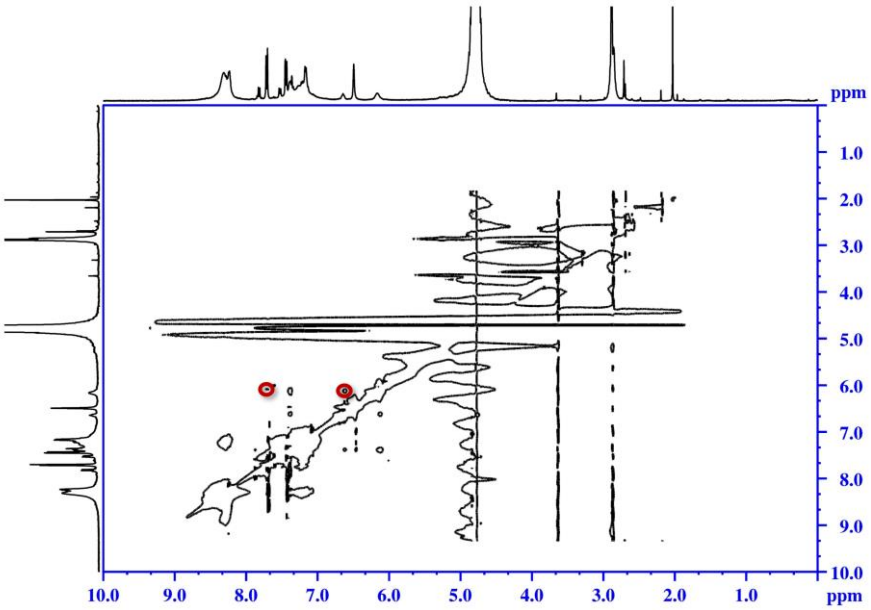


Figure S31. ^{1}H-^{1}H NOESY NMR spectrum of **G2@T1** (D_2O, 298 K). The through space correlations between host and guest protons are depicted by red circles.

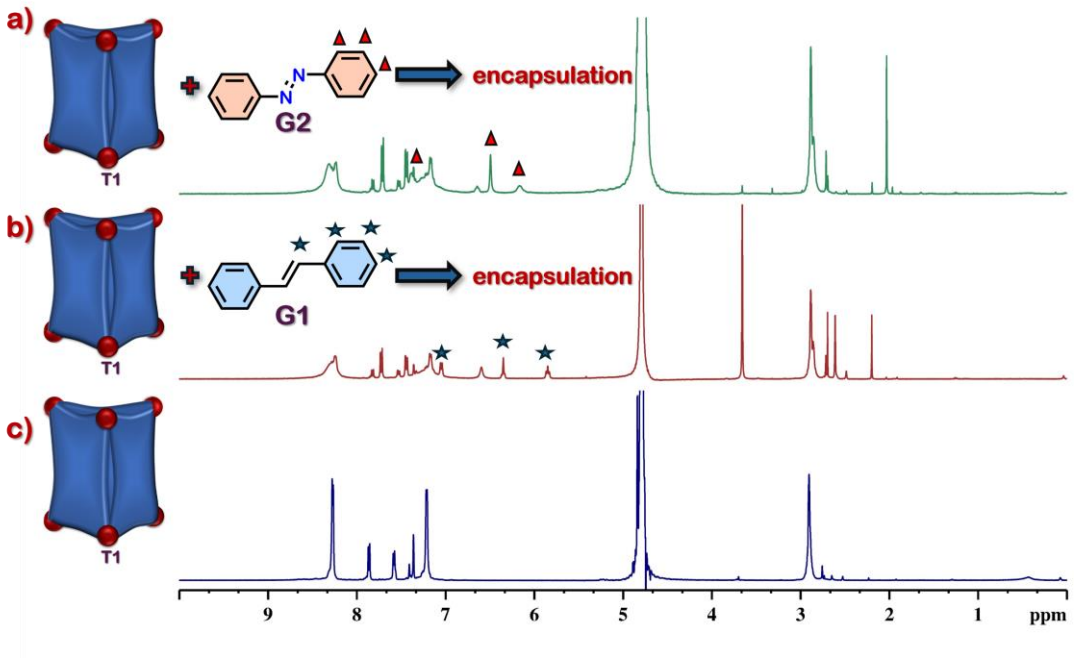


Figure S32. Stacked ^{1}H NMR spectrum of (a) **G2@T1** (b) **G1**@**T1** (c) **T1**, recorded in D_2O at 298 K. The stacked plot shows the encapsulation of 1 molecule of **G1** or **G2** by **T1** forming 1:1 host-guest complexes, **G2@T1** and **G1@T1**, respectively.

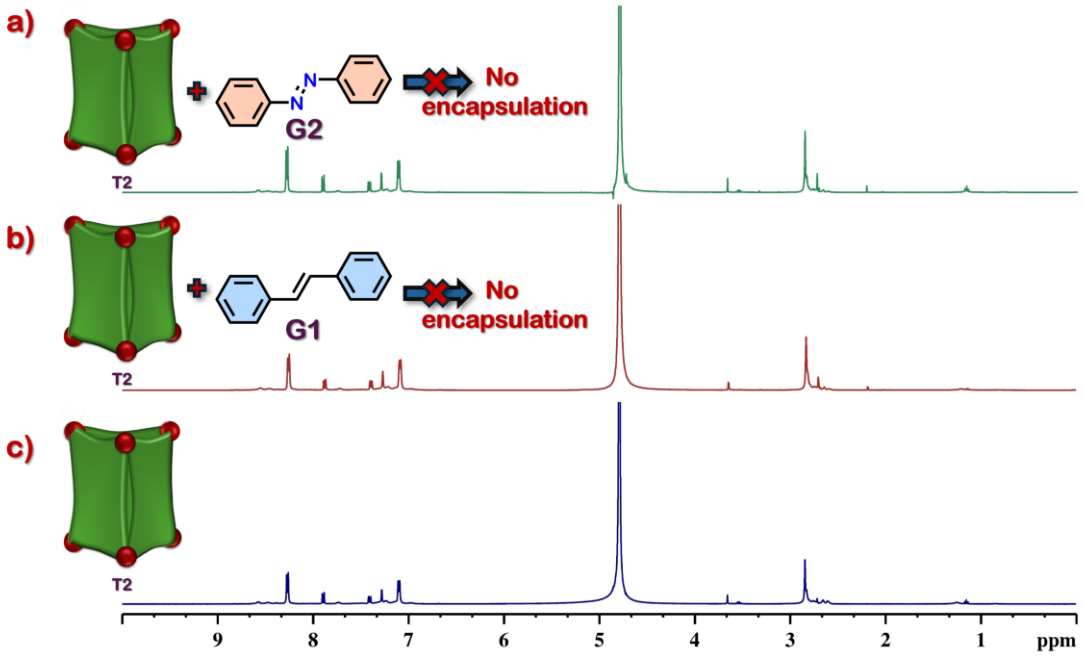


Figure S33. Stacked ^{1}H NMR spectrum of (a) after addition of excess of **G2** to **T2** (b) after addition of excess of **G1** to **T2** (c) **T2**, recorded in D_2O at 298 K. The stacked plot shows no encapsulation of **G1** and **G2** by **T2.**

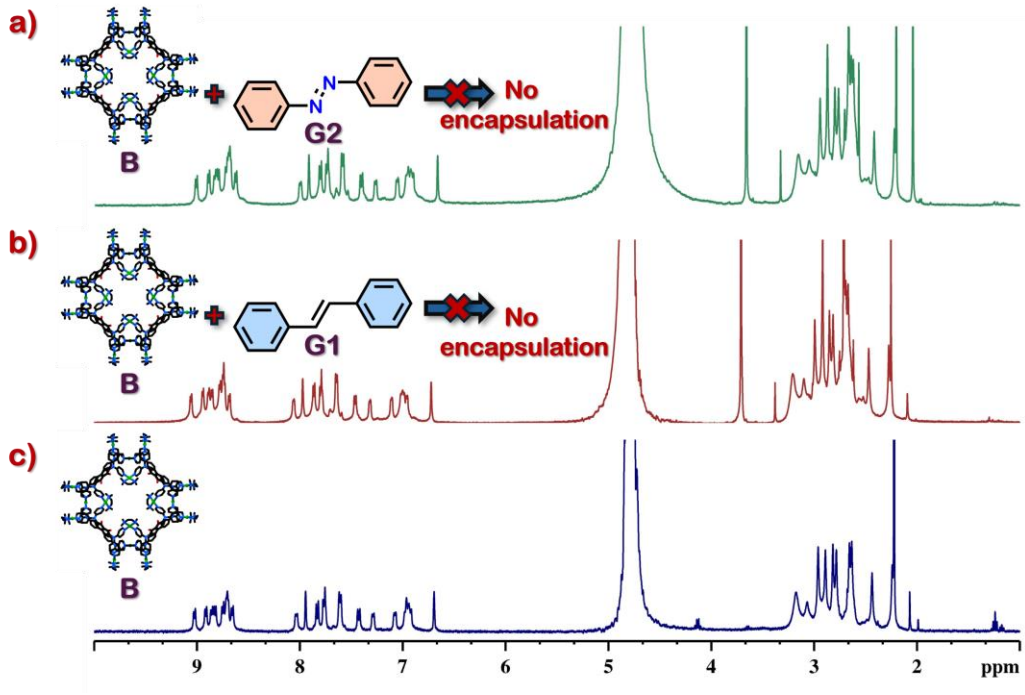


Figure S34. Stacked ^{1}H NMR spectrum of (a) after the addition of an excess of **G2** to **B**, (b) after the addition of an excess of **G1** to **B** (c) **B**, recorded in D_2O at 298 K. The stacked plot shows no encapsulation of **G1** and **G2** by **B** due to presence of hollow, open cavity.

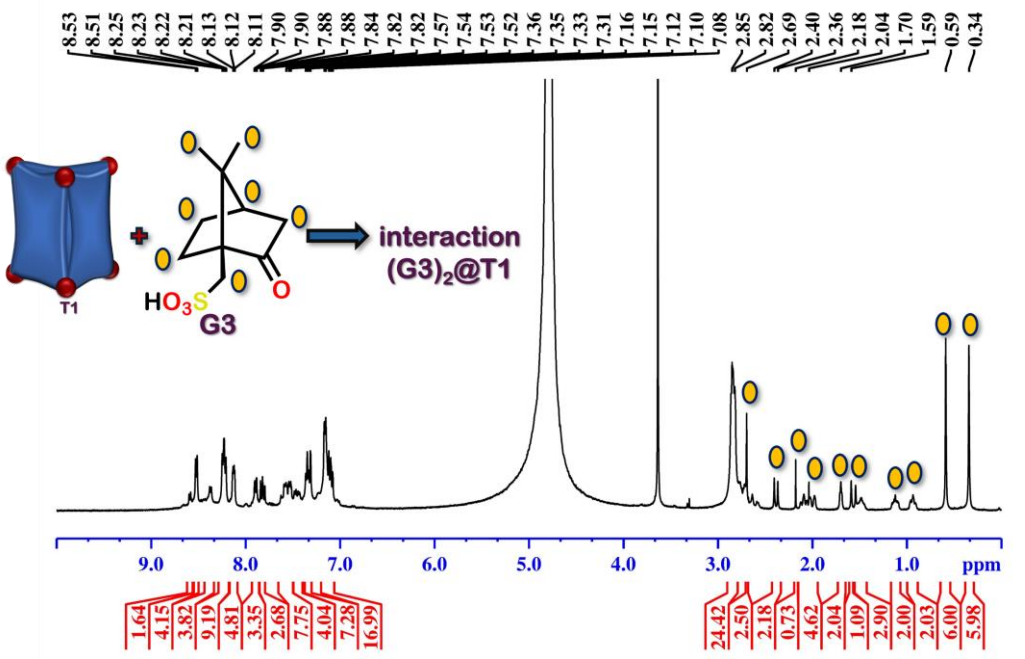


Figure S35. ^{1}H NMR spectrum of **G3@T1** (D_2O, 298 K). **G3** peaks are designated by yellow circles (○). The de-symmetrization of **T1** NMR and the upfield shifts of protons of **G3** indicate interaction with **T1**. The host-guest stoichiometry was found to be 1:2 from NMR integrations.

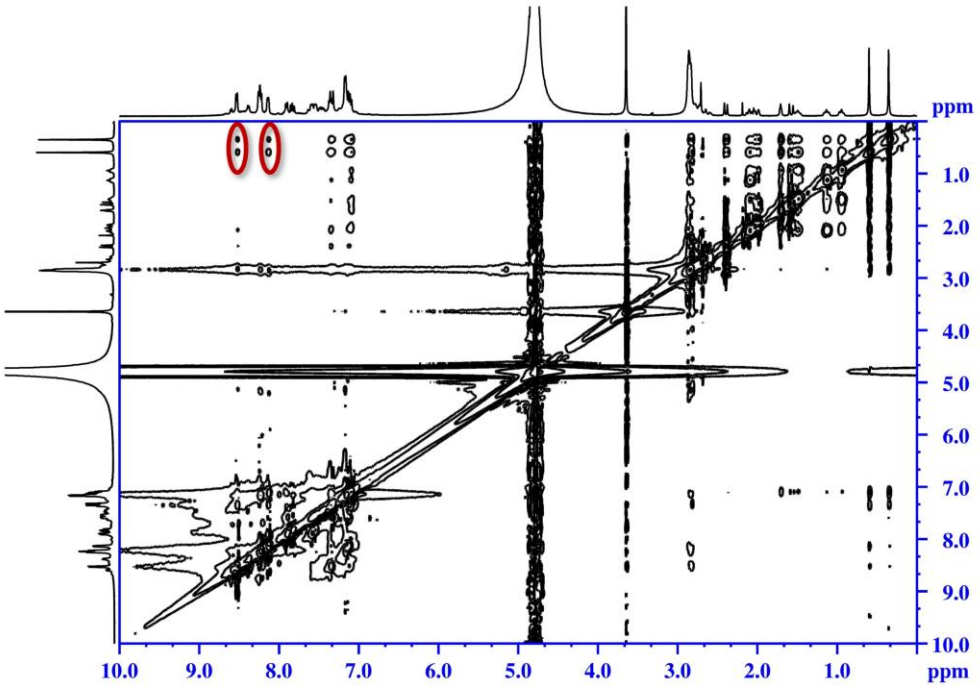


Figure S36. ^{1}H-^{1}H NOESY NMR spectrum of (**G3**)$_2$**@T1** (D_2O, 298 K). The marked peaks display through space correlation between host **T1** protons and guest **G3** protons.

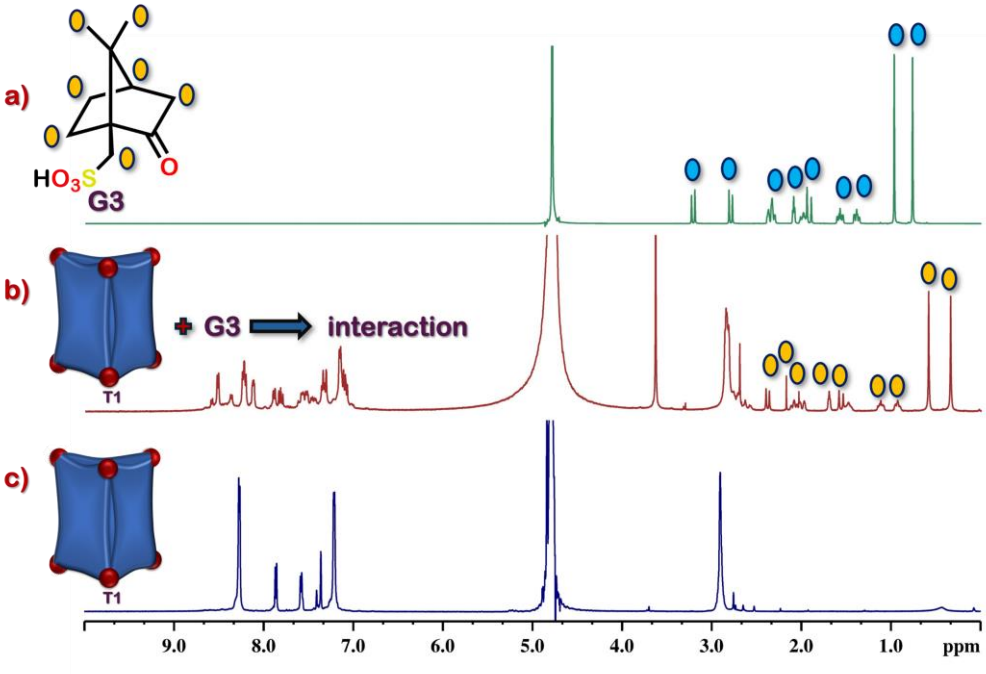


Figure S37. Stacked ^{1}H NMR spectra of (a) **G3**, (b) (**G3**)$_2$@**T1**, (c) **T1**, recorded in D_2O at 298 K. The stacked plot shows the encapsulation of two molecule of **G3** by **T1** forming 1:2 host-guest complexes.

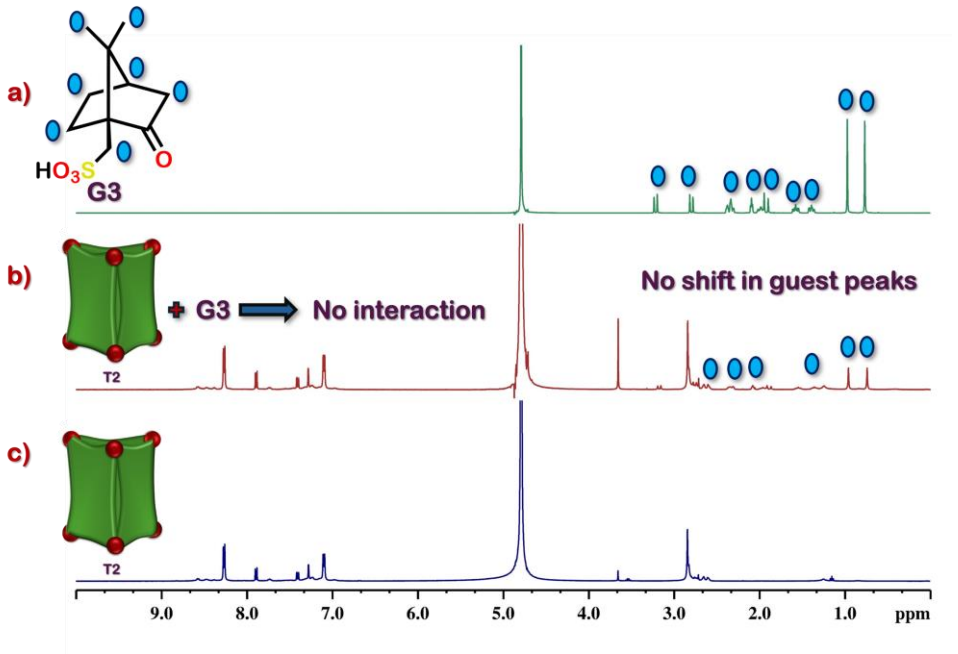


Figure S38. Stacked ^{1}H NMR spectra of (a) **G3**, (b) after addition of 2 equivalents of **G3** to aqueous solution of **T2**, (c) **T2**, recorded in D_2O at 298 K. The stacked plot shows no encapsulation/interactions of **G3** with **T2**.

6. NMR Titrations to determine Association Constants

The NMR Titrations of **T1** with **G1**, **G2** and **G3**, respectively were carried out and the apparent association constants (K_a) were calculated using Hill's equation.

To carry out the titrations, solutions of host **T1** (c =1.287 mM) in D_2O were prepared, gradually titrated with guest solutions of high concentration (**G1** and **G2** in CD_3OD ; **G3** in D_2O; c =12.87 mM) and the changes in the ^{1}H NMR was monitored.

The **T1** peaks showed shifts upon gradual addition of **G1/G2** and showed saturation when upto 1 equivalent of respective guest **G1/G2** were added indicating formation of 1:1 complex. In case of addition of guest **G3**, saturation was observed after addition of upto 2 equivalents of **G3** indicating formation of 1:2 complex.

From these data, the apparent association constants (K_a) were calculated using Hill's equation:

$$\log\left(\frac{\theta}{1-\theta}\right) = n\log[G] + n\log Ka$$

where, $\theta = \left(\frac{\Delta\delta}{\delta sat - \delta cage}\right)$ n = Hill's coefficient

The apparent association constants (K_a) and Hill's coefficient (n) determined by this fit are given in Table S2 and Figures S39-S44.

Table S2. Determination of Ka from Hill's Plot

Guest	Host	n	Ka (M^{-1})
G1	**T1**	2.16	1958.85
G2	**T1**	1.76	2462.55
G3	**T1**	2.43	1021.11

Similarly, solutions of **T2** in D_2O (c =1.287 mM) were also titrated with solutions of **G1**, **G2** (in CD_3OD) and **G3** (in D_2O). The ^1H NMR showed no changes confirming no affinity of **T2** for all the guests (Figures S45-S47).

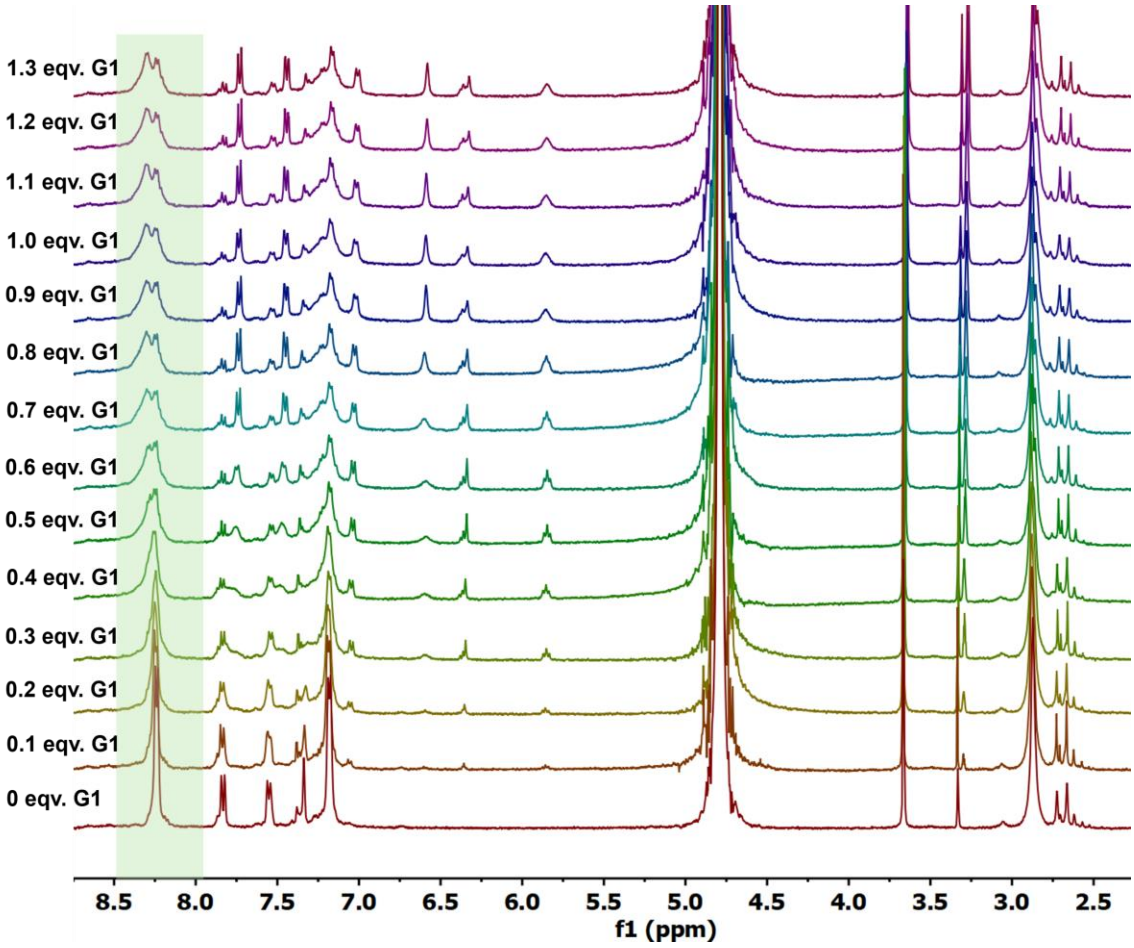


Figure S39. ^1H NMR titration of **T1** (in D_2O) (1.287 mM) with **G1** (in CD_3OD).

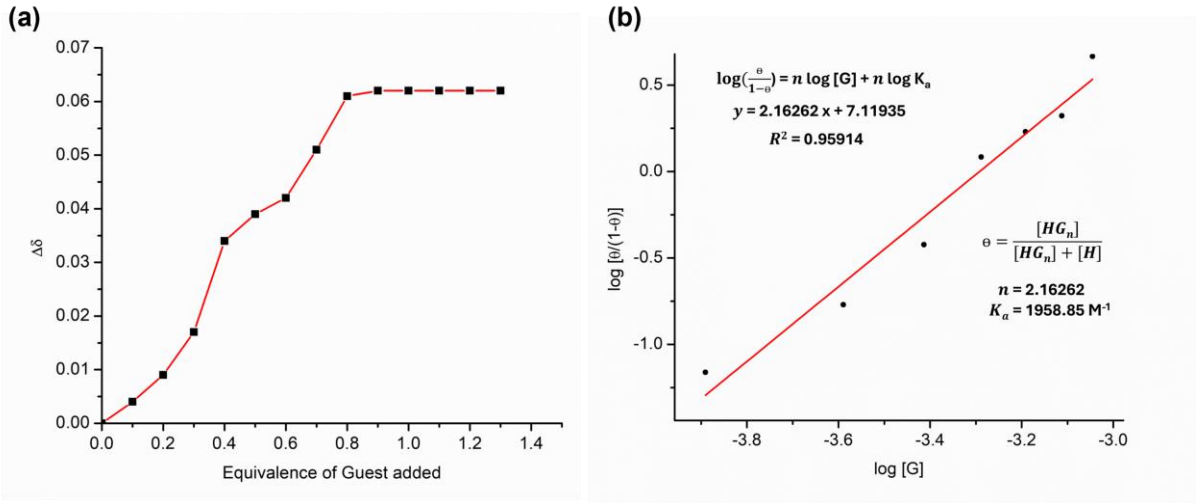


Figure S40. ^{1}H NMR titration: (a) Plot of change in ppm value (Δδ) against equivalents of guest (**G1**) added to **T1**. (b) Hill's plot to determine association constant (K_a).

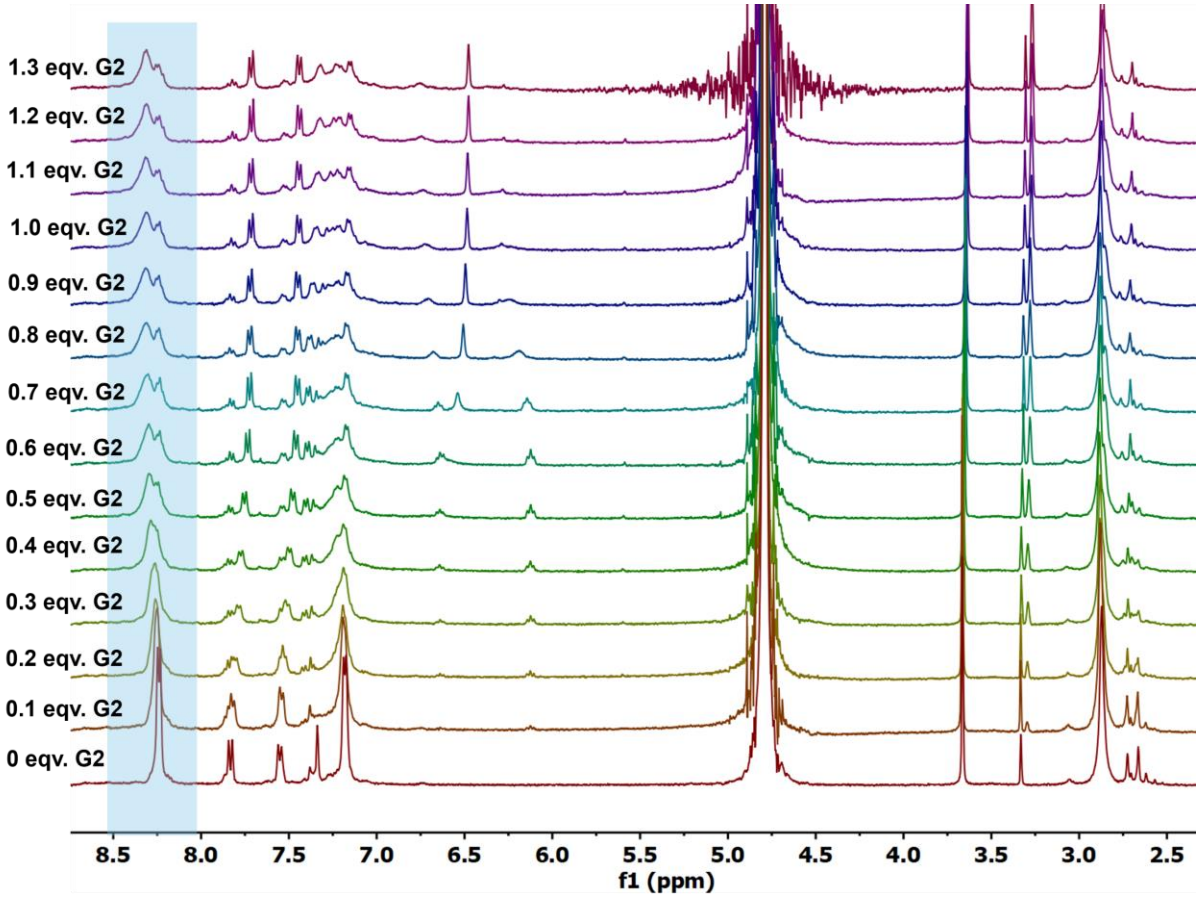


Figure S41. ^{1}H NMR titration of **T1**(in D_2O) (1.287 mM) with **G2** (in CD_3OD).

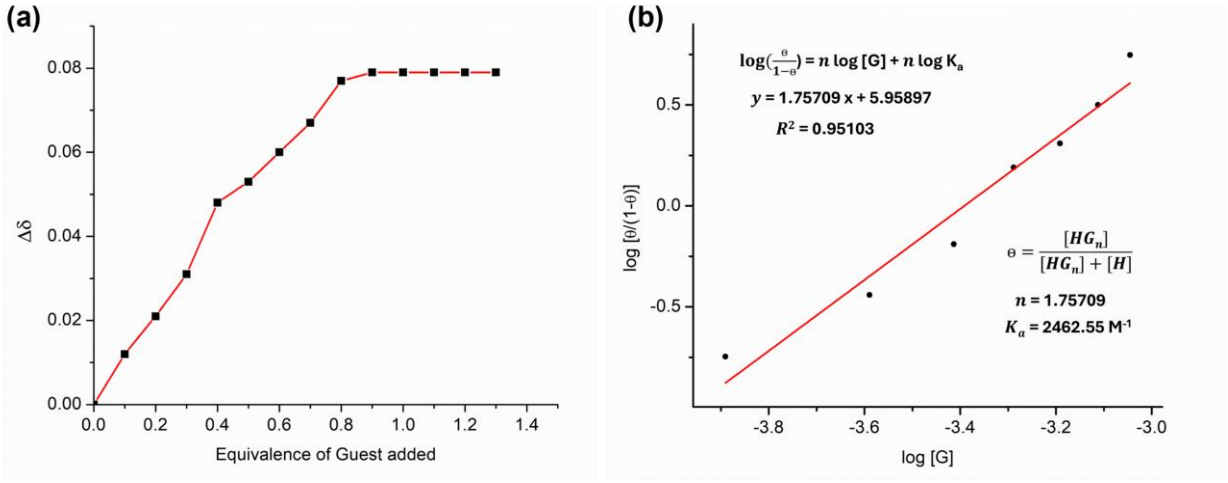


Figure S42. ^{1}H NMR titration: (a) Plot of change in ppm value (Δδ) against equivalents of guest (**G2**) added to **T1**. (b) Hill's plot to determine association constant (K_a).

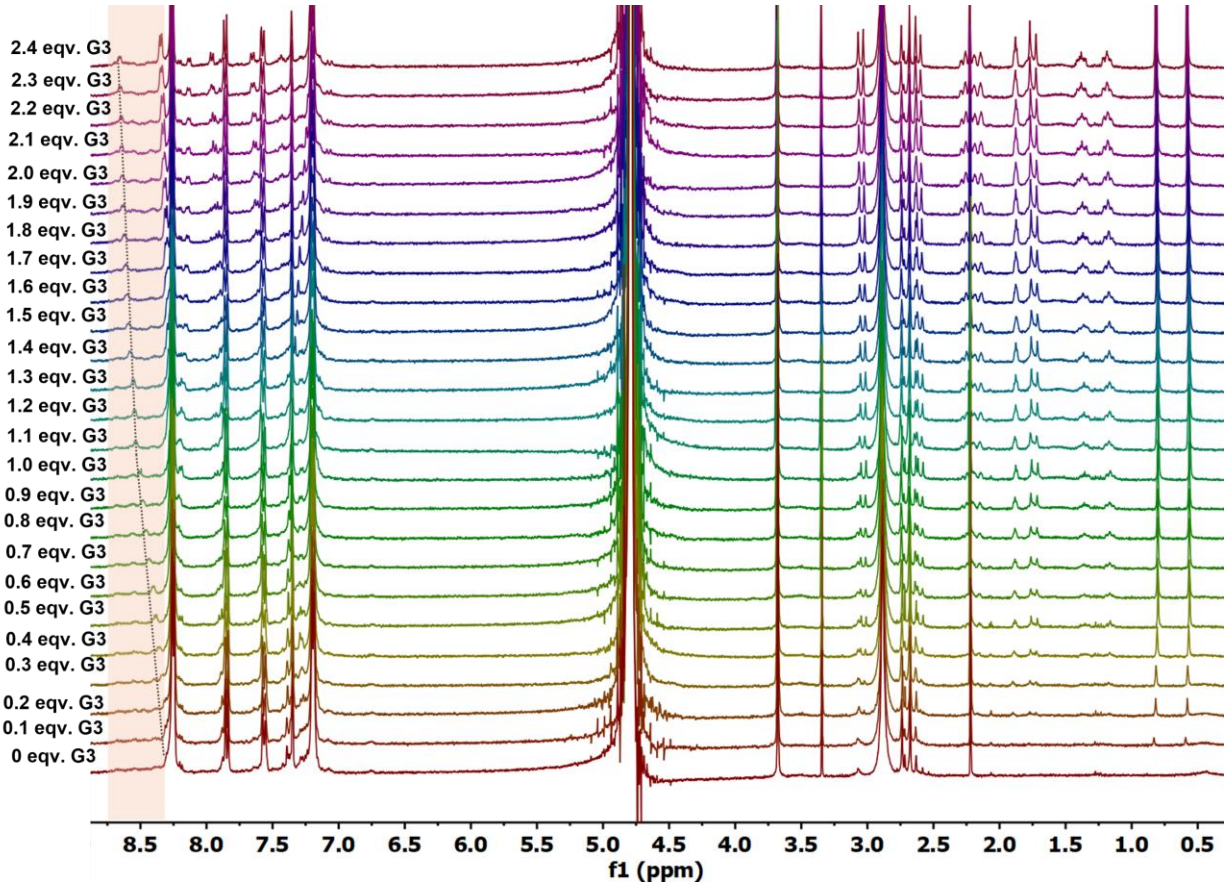


Figure S43. ^{1}H NMR titration of **T1**(in D_2O) (1.287 mM) with **G3** (in D_2O).

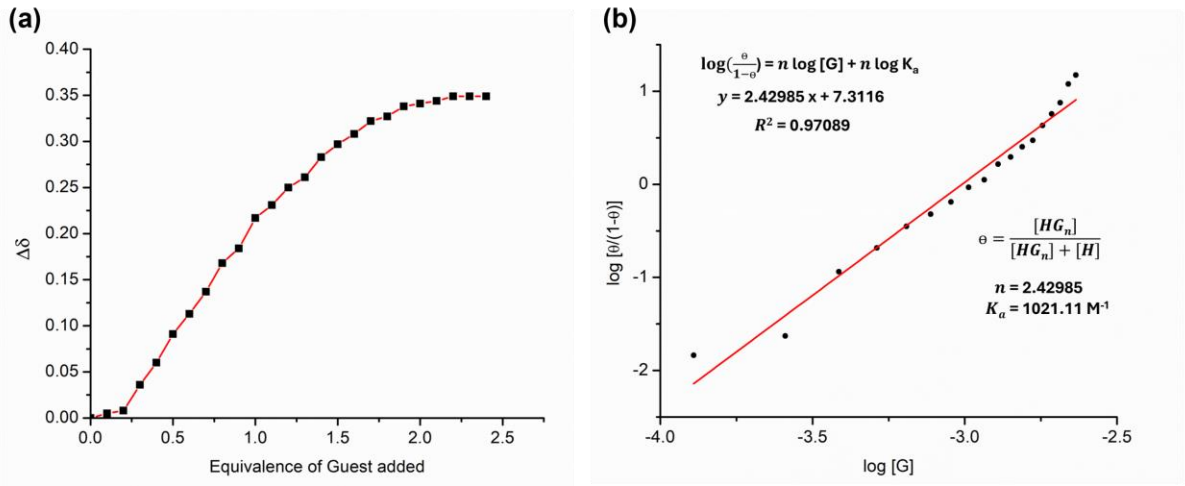


Figure S44. ^{1}H NMR titration: (a) Plot of change in ppm value (Δδ) against equivalents of guest (**G3**) added to **T1**. (b) Hill's plot to determine association constant (K_a).

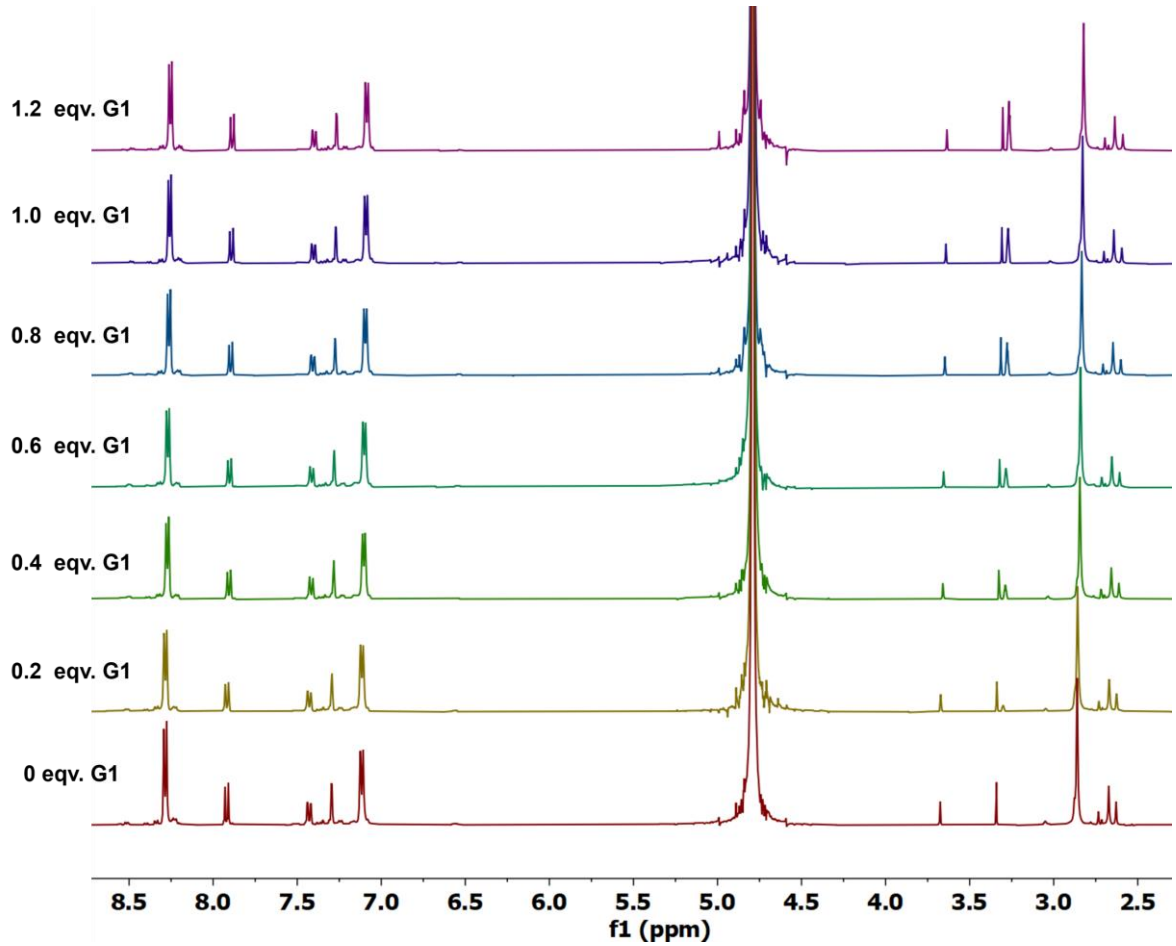


Figure S45. ^{1}H NMR titration of **T2** (in D_2O) (1.287 mM) with **G1** (in CD_3OD). No changes in ^{1}H NMR was observed upon guest addition indicating no binding of **G1**.

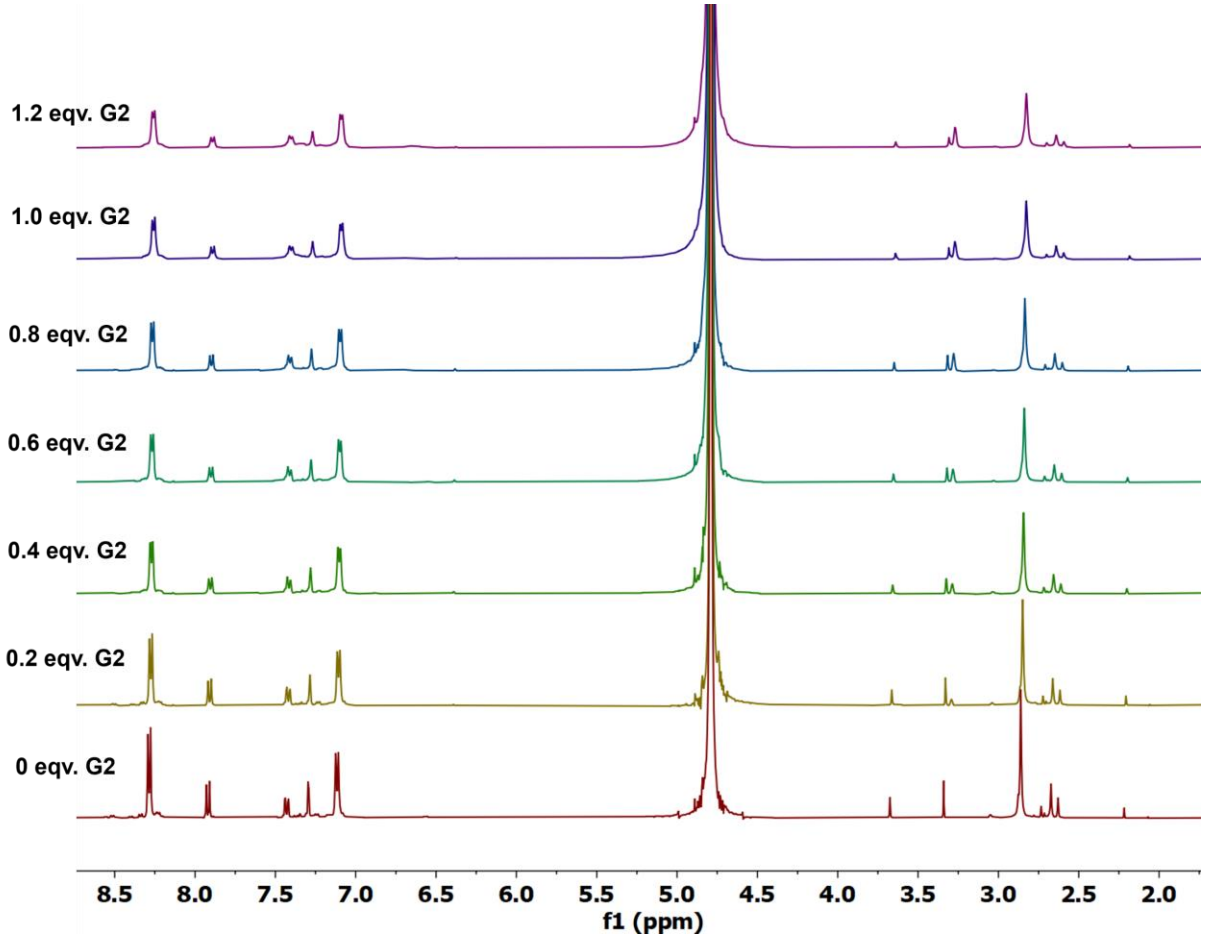


Figure S46. ^{1}H NMR titration of **T2** (in D_2O) (1.287 mM) with **G2** (in CD_3OD). No changes in ^{1}H NMR was observed upon guest addition indicating no binding of **G2**.

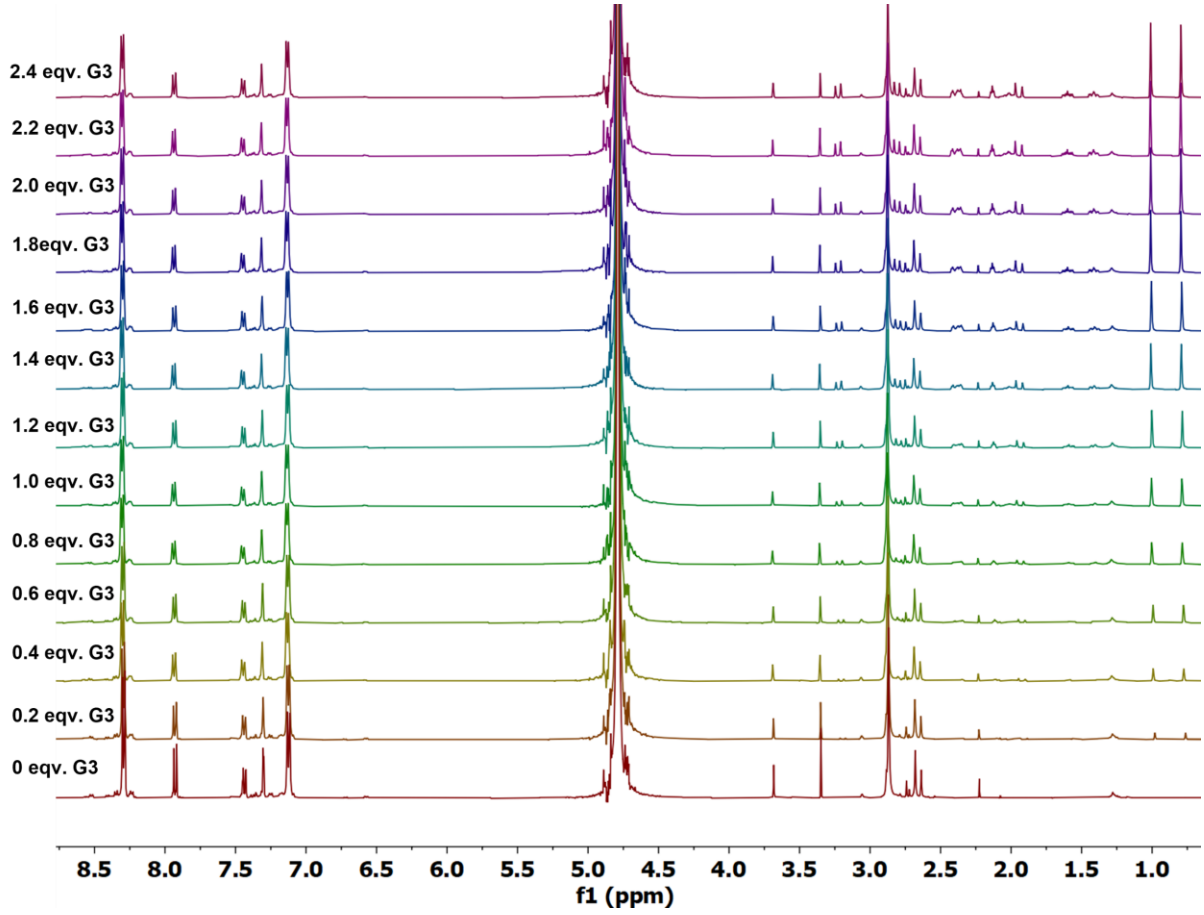


Figure S47. ^{1}H NMR titration of **T2** (in D_2O) (1.287 mM) with **G3** (in D_2O). No changes in ^{1}H NMR was observed upon guest addition indicating no binding of **G3**.

7. Computational Studies

DFT optimizations of all the assemblies **T1**, **T2** and **T3** were carried out using the Gaussian 09 package.[S11] Single-point energies of **T1**, **T2**, and **T3** were calculated using the hybrid B3LYP functional with a mixed basis set of LanL2DZ (for Pd atom) and 6-31G(d) (for C, H, N and O atoms) (Table S3).

The geometries of **(G3)$_2$@T1** and **(G3)$_2$@T2** were optimized using PM6 semi-empirical method using the Gaussian 09 package.[S11]

Table S3. Single Point Energies of **T1**, **T2**, and **T3**

Species	Method	Basis set	Total energy (a.u.)	Total energy (kcal/mol)
T1	DFT/B3LYP	LanL2DZ/6-31G(d)	-6922.16138971	-4343725.49
T2	DFT/B3LYP	LanL2DZ/6-31G(d)	-6922.04096304	-4343649.92
T3	DFT/B3LYP	LanL2DZ/6-31G(d)	-8308.87662836	-5213903.17

7.1 DFT Optimized Structures

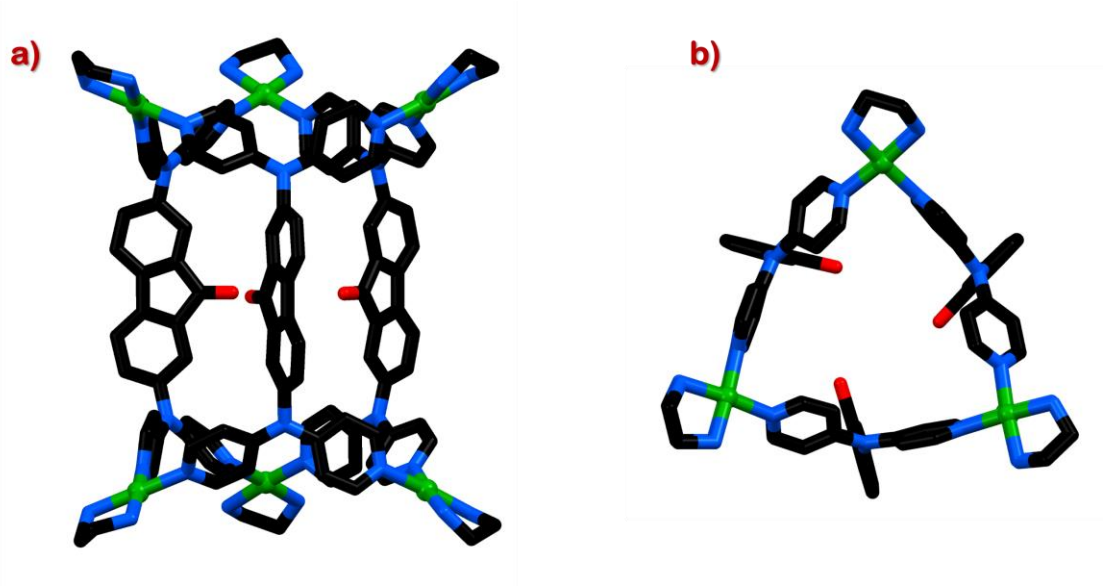


Figure S48. DFT optimized structure of **T1**: (a) side view (b) top view. Color codes: carbon (black), nitrogen (blue), oxygen (red) and palladium (green). Hydrogen atoms were omitted for clarity.

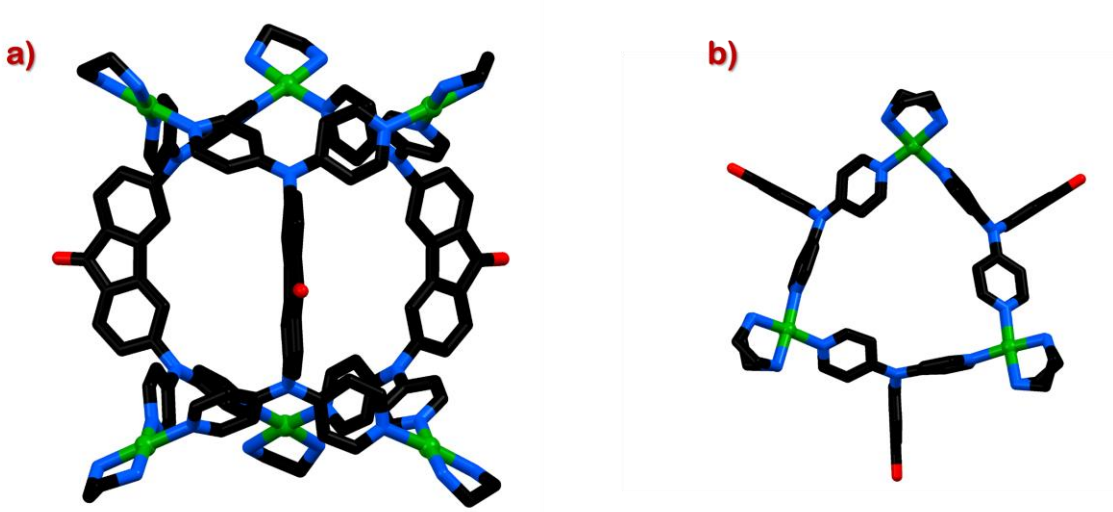


Figure S49. DFT optimized structure of **T2**: (a) side view (b) top view. Color codes: carbon (black), nitrogen (blue), oxygen (red) and palladium (green). Hydrogen atoms were omitted for clarity.

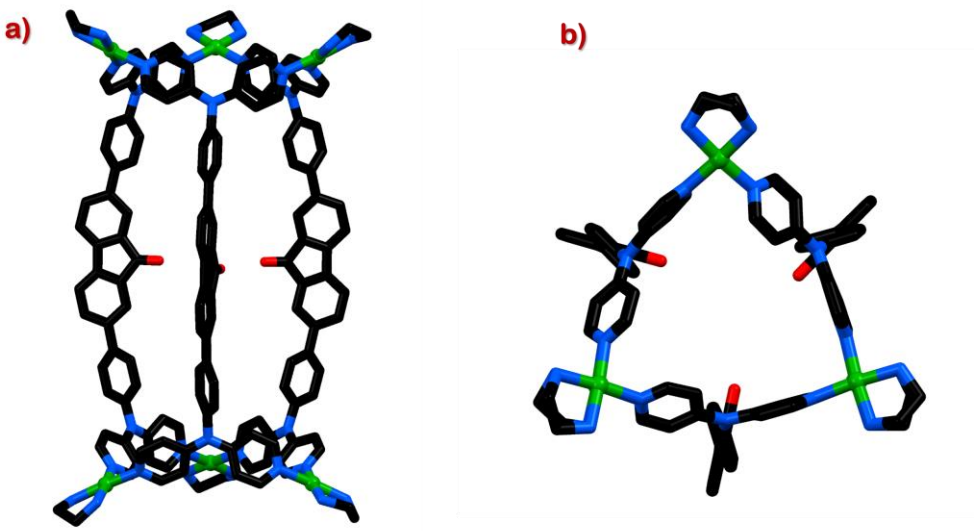


Figure S50. DFT optimized structure of **T3**: (a) side view (b) top view. Color codes: carbon (black), nitrogen (blue), oxygen (red) and palladium (green). Hydrogen atoms were omitted for clarity.

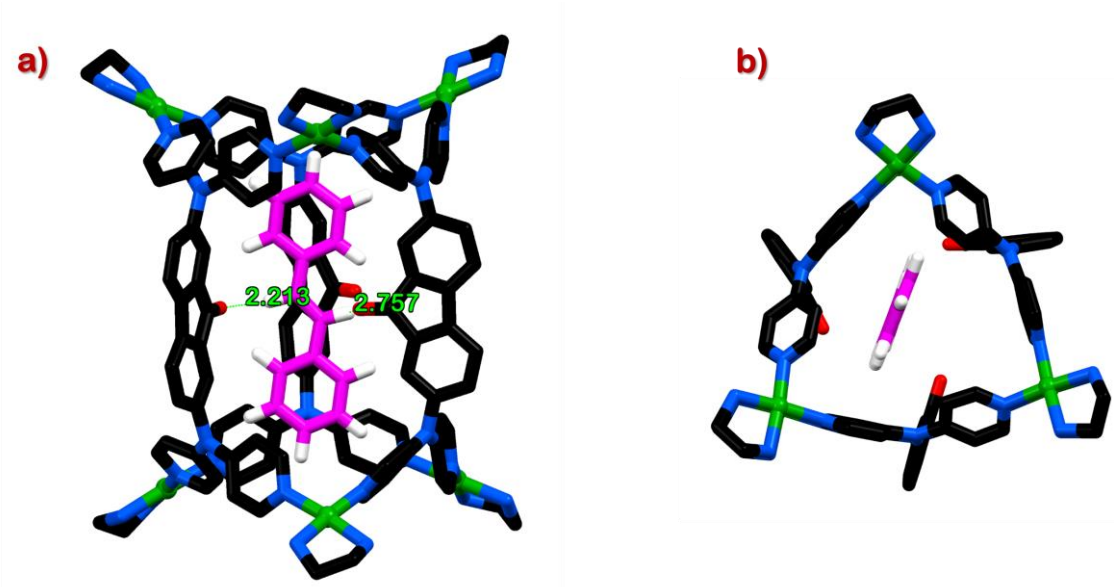


Figure S51. DFT optimized structure of **G1@T1**: (a) side view, (b) top view. Color codes for host **T1**: carbon (black), nitrogen (blue), oxygen (red) and palladium (green). Color codes for guest **G1**: magenta (carbon), hydrogen (white). Hydrogen atoms of host **T1** were omitted for clarity. The labelled interactions depict the H-bonding interactions between the alkene protons of **G1** and fluorenone oxygen atoms of **T1**.

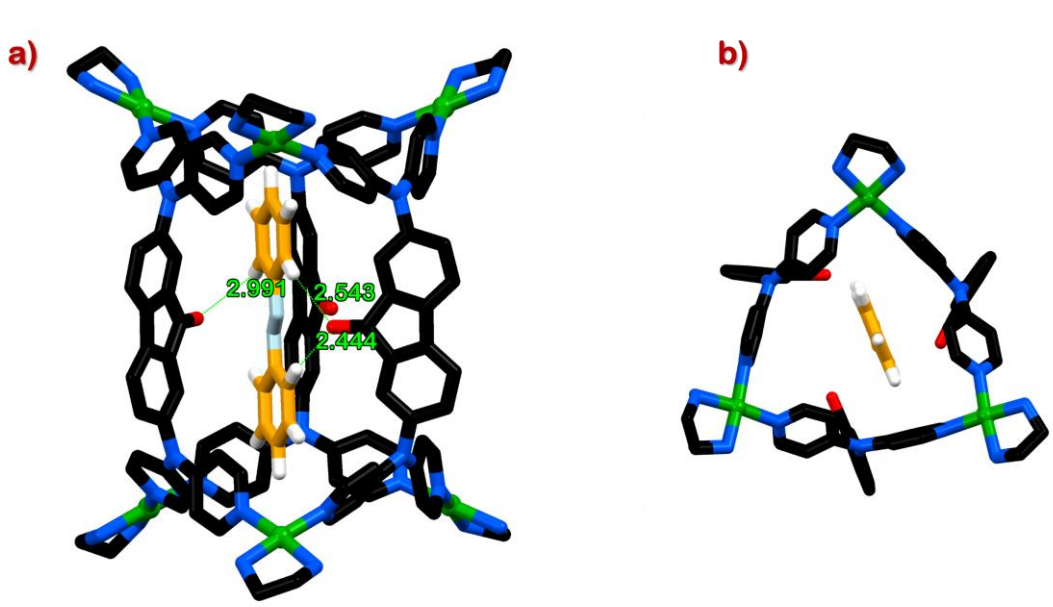


Figure S52. DFT optimized structure of **G2@T1**: (a) side view (b) top view. Color codes for host **T1**: carbon (black), nitrogen (blue), oxygen (red) and palladium (green). Color codes for guest **G2**: carbon (orange), nitrogen (light blue), hydrogen (white). Hydrogen atoms of host **T1** were omitted for clarity. The labelled interactions depict the H-bonding interactions between the phenyl protons of **G2** and fluorenone oxygen atoms of **T1**.

7.2 PM6 Optimized Structures

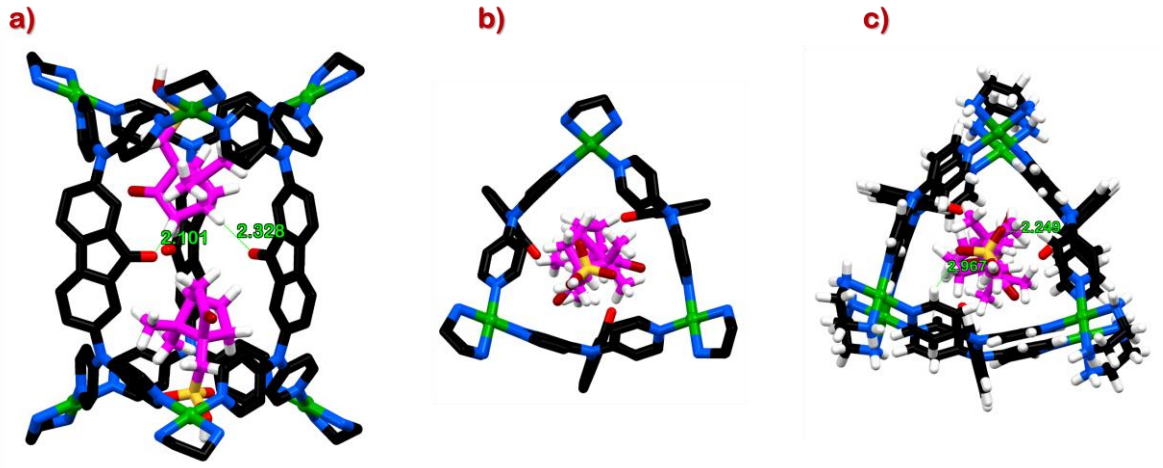


Figure S53. PM6 optimized structure of **(G3)$_2$@T1**: (a) side view, (b) top view. Color codes for host **T1**: carbon (black), nitrogen (blue), oxygen (red) and palladium (green). Color codes for guest **G3**: carbon (magenta), oxygen (brown), sulphur (yellow), hydrogen (white). Hydrogen atoms of host **T1** were omitted for clarity. The labelled interactions in (a) depict the H-bonding interactions between the aliphatic protons of **G3** and fluorenone

oxygen atoms of **T1**. (c) top view, showing the H-bonding interactions between aromatic protons of host (**T1**) and sulphonic acid oxygen atoms of **G3**.

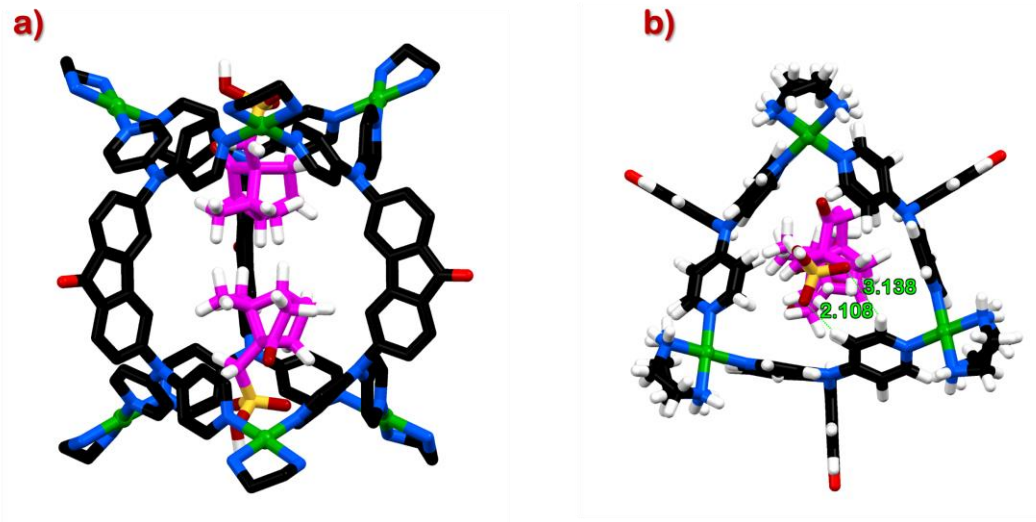


Figure S54. Possible PM6 optimized structure of **(G3)$_2$@T2**: (a) side view (b) top view. Color codes for host **T2**: carbon (black), nitrogen (blue), oxygen (red) and palladium (green). Color codes for guest **G3**: carbon (magenta), oxygen (brown), sulphur (yellow), hydrogen (white). Hydrogen atoms of host **T2** in (a) were omitted for clarity. (b) top view, showing the H-bonding interactions between aromatic protons of host (**T2**) and sulphonic acid oxygen atoms of **G3**. No H-bonding interactions are possible with the fluorenone oxygen atoms of host (**T2**) leading to poor stability and non-existence of **(G3)$_2$@T2**.

Table S4. Relative energies of **(G3)$_2$@T1** and **(G3)$_2$@T2**

Species	Method	Total energy (a.u.)	Total energy (kcal/mol)
(G3)$_2$@T1	PM6	5.56192662	3490.1646
(G3)$_2$@T2	PM6	5.67464836	3560.8986

8. Calculation of Hydrodynamic Radii from DOSY experiments

The ^{1}H-DOSY NMR spectra for **T1**, **T2**, **T3**, and **B** were recorded, and the corresponding hydrodynamic radii (r) were calculated from the diffusion coefficient (D) values using the Stokes-Einstein equation:

$$r = \frac{k_B T}{6\pi\eta D}$$

[where r: hydrodynamic radius; D: diffusion coefficient; η: coefficient of viscosity; k_B: Boltzmann constant; T: temperature in Kelvin scale].

Table S5. Hydrodynamic Radii of **T1**, **T2**, **T3**, and **B**.

Compound	Diffusion Coefficient (m^2/s)	Hydro-dynamic radii (Å)	Non-solvated radii (from Crystal structures or DFT optimized structures)
T1	1.69×10^{-10}	14.4	13.3
T2	1.78×10^{-10}	13.8	13.1
T3	1.41×10^{-10}	17.4	16.3
B	8.91×10^{-11}	27.8	19.8

The DOSY experiments were conducted at room temperature (T = 298 K) in D_2O. The coefficient of viscosity of D_2O at 298 K, η = 0.89 centipoise; Boltzmann constant (kB) = 1.38 x 10^{-23} $m^2kgs^{-2}K^{-1}$.

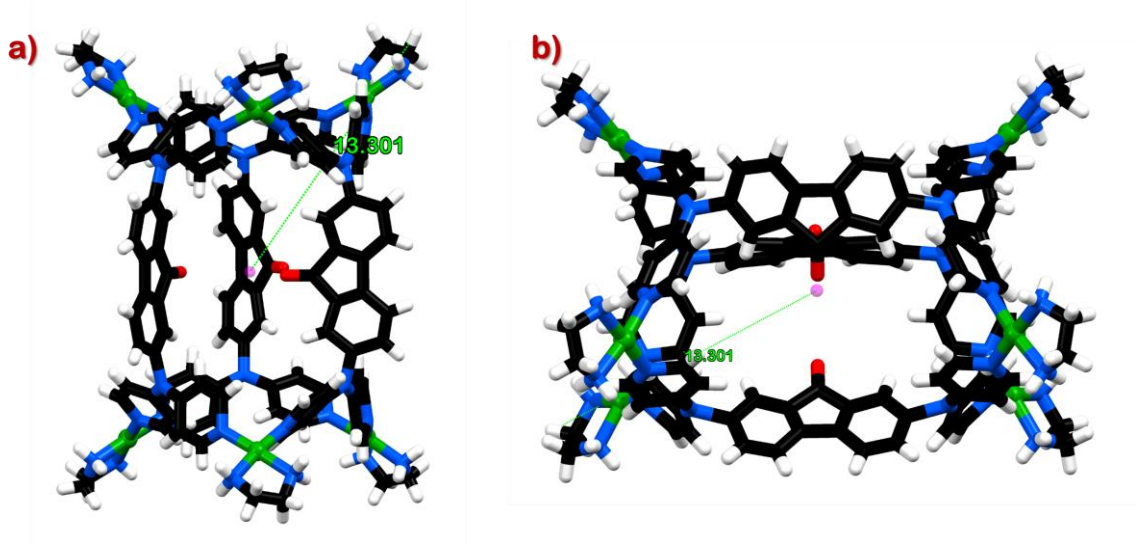


Figure S55. Non-solvated radii of **T1** from SC-XRD structure.

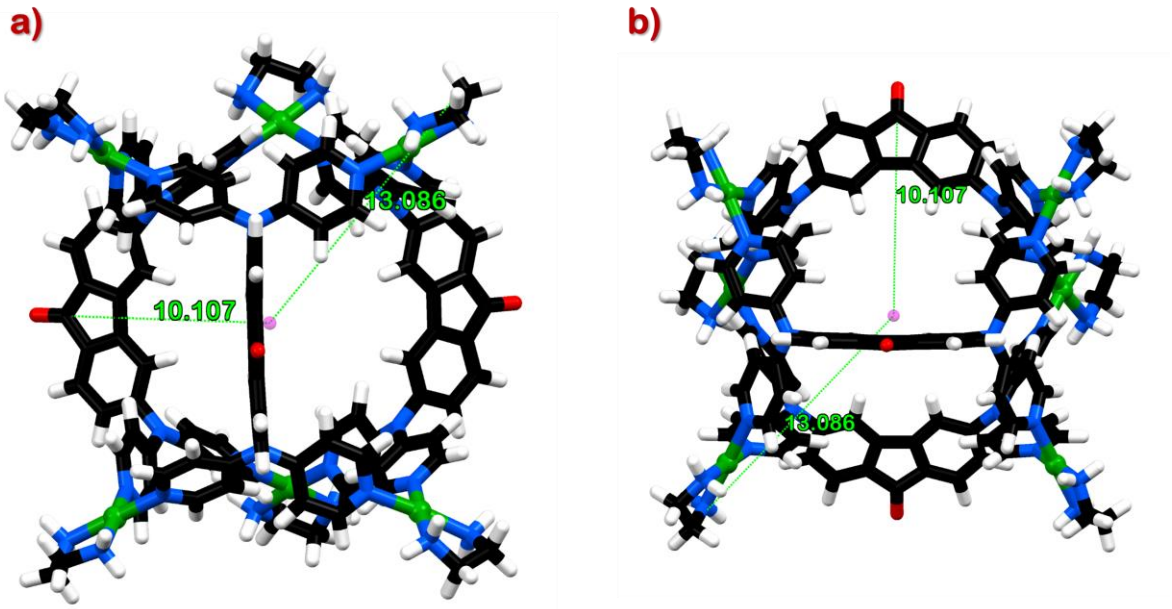


Figure S56. Non-solvated radii of **T2** from DFT optimized structure.

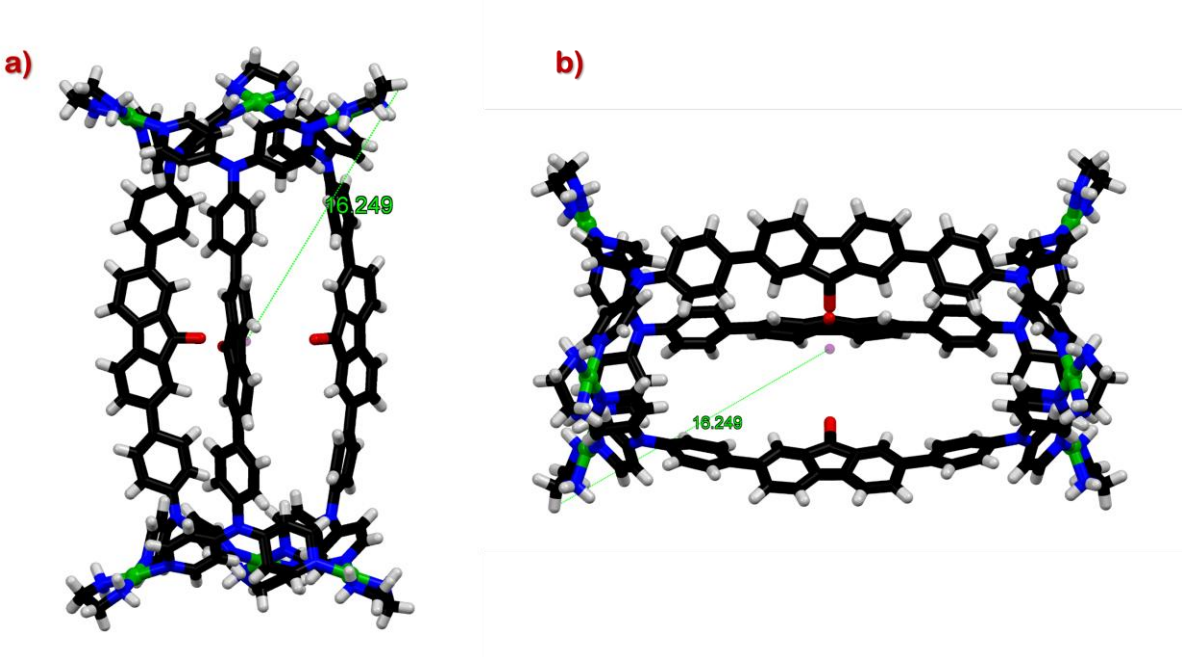


Figure S57. Non-solvated radii of **T3** from SC-XRD structure.

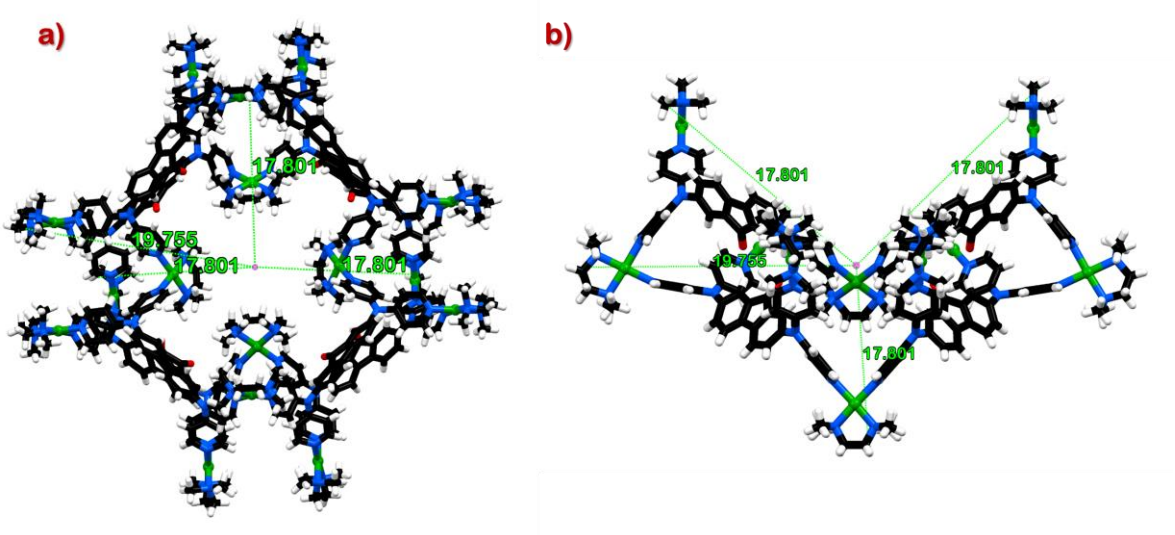


Figure S58. Non-solvated radii of **B** from SC-XRD structure.

9. Cage Cavity Volume Calculations

The volumes of the cavities enclosed by the cages trifacial tubes **T1**, **T2**, **T3** and molecular basket **B** were calculated from the SC-XRD structures of **T1**, **T3** and **B** and from the DFT optimized structure of **T2** using the MOLOVOL software following the two-probe model.[S12]

Table S6. Cage Cavity Volume Calculations

Cage	No. of Cavities	Cavity Types	Occupied Volume[#] ($Å^3$)	Accessible Volume[##] ($Å^3$)
T1	1	Tunnel	461.880	100.008
T2	10	Tunnel	28.512	1.576
		Tunnel	28.408	1.632
		Isolated	3.424	0.008
		Isolated	3.408	0.008
		Isolated	3.328	0.008
		Pocket	3.184	0.020
		Pocket	3.152	0.032
		Isolated	3.048	0.008
		Isolated	3.032	0.008
		Pocket	3.008	0.020
			Net = 82.504	Net = 3.32
T3	3	Tunnel	153.360	29.000
		Tunnel	152.544	29.416

		Pocket	20.472 Net = 326.376	3.248 Net = 61.664
B	43	Tunnel	234.304	38.176
		Tunnel	234.304	38.176
		Tunnel	230.192	37.664
		Tunnel	224.816	37.664
		Isolated	21.792	0.384
		Isolated	21.792	0.384
		Isolated	20.992	0.384
		Isolated	20.992	0.384
		Pocket	13.752	0.48
		Pocket	13.752	0.48
		Pocket	12.88	0.432
		Pocket	12.88	0.432
		Pocket	12.744	0.392
		Pocket	12.744	0.392
		Pocket	12.552	0.424
		Pocket	12.552	0.424
		Pocket	10.528	0.24
		Pocket	10.48	0.224
		Pocket	9.552	0.168
		Pocket	9.552	0.168
		Pocket	7.944	0.136
		Pocket	7.944	0.136
		Pocket	7.328	0.12
		Pocket	7.328	0.12
		Pocket	7.32	0.104
		Pocket	7.32	0.104
		Pocket	6.464	0.072
		Pocket	6.464	0.072
		Pocket	6.344	0.088
		Pocket	6.344	0.088
		Pocket	6.296	0.072
		Pocket	6.296	0.072
		Pocket	5.872	0.08
		Pocket	5.872	0.08
		Pocket	5.856	0.144
		Pocket	5.744	0.048
		Pocket	5.744	0.048
		Pocket	5.6	0.04
		Pocket	5.6	0.04
		Pocket	5.04	0.02

		Pocket Isolated Isolated	5.024 0.472 0.472 Net = 1287.84	0.02 0.008 0.008 Net = 159.192

Probe occupied volume corresponds to empty space as defined by the molecular surface (similar to the Connolly surface). This occupied volume is typically the volume reported for cavities in cage compounds.

Probe accessible volume corresponds to empty space as defined by the surface accessible to its core (similar to the Lee-Richards surface).

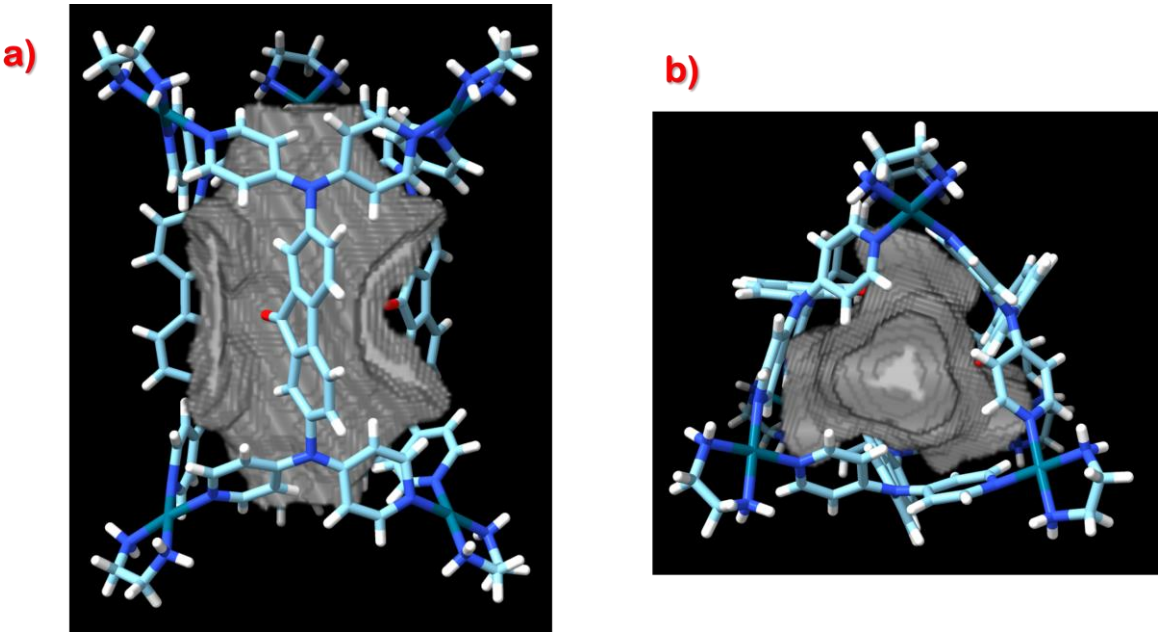


Figure S59. Representation of the cavity volume of **T1** calculated using MOLOVOL. The cavity is represented by grey colour block: (a) side view and (b) top view.

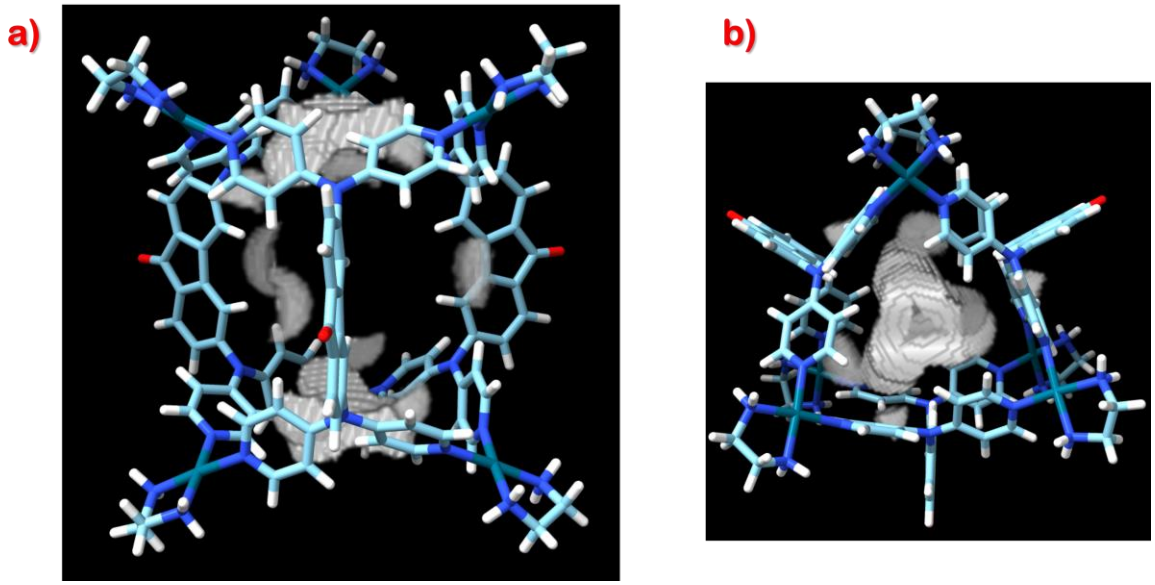


Figure S60. Representation of the cavity volume of **T2** calculated using MOLOVOL. The cavity is represented by grey colour block: (a) side view and (b) top view.

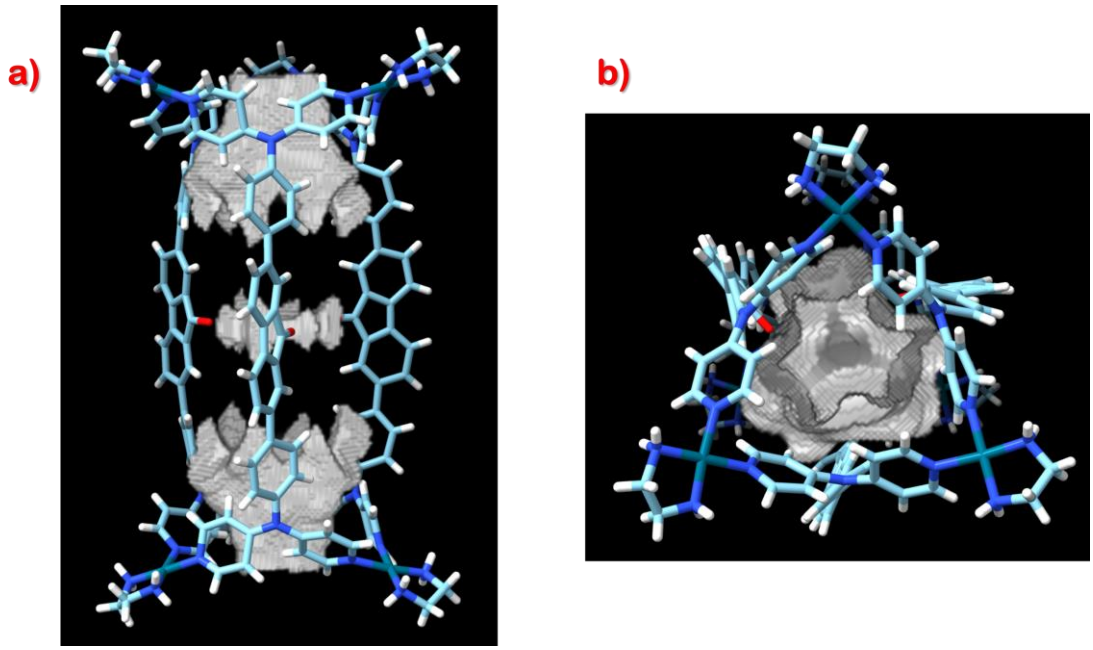


Figure S61. Representation of the cavity volume of **T3** calculated using MOLOVOL. The cavity is represented by grey colour block: (a) side view and (b) top view.

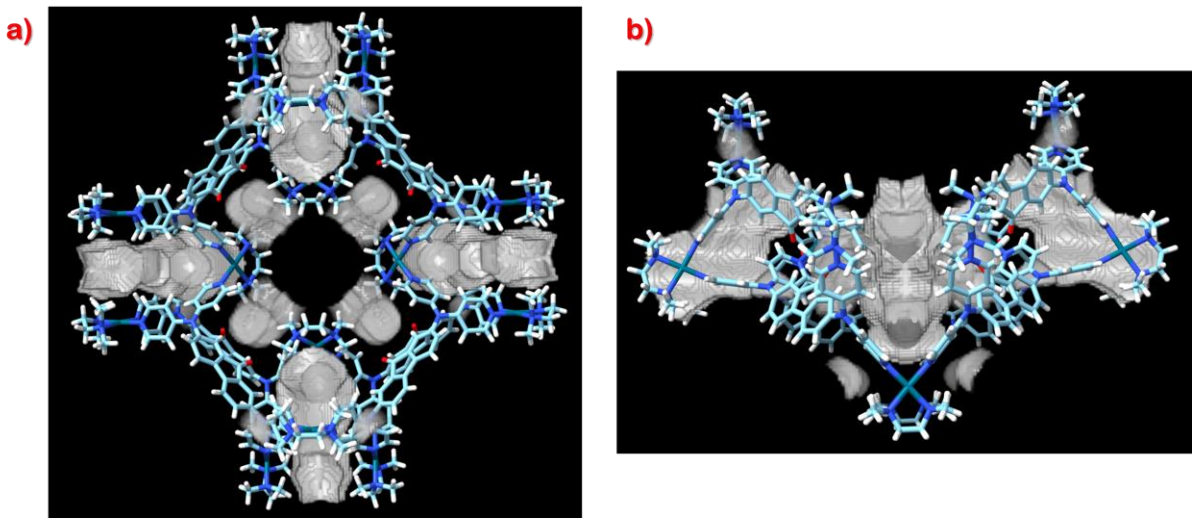


Figure S62. Representation of the cavity volume of **B** calculated using MOLOVOL. The cavity is represented by grey colour block: (a) top view and (b) side view.

10. Coordinates of DFT Optimized Structures

10.1 T1

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	46	0	-7.53818	6.112748	2.170084
2	8	0	0.000077	2.58978	-0.75023
3	6	0	0.000077	3.182579	-1.8132
4	6	0	-1.19018	3.627033	-2.61282
5	6	0	-2.53581	3.404347	-2.3543
6	1	0	-2.83938	2.85361	-1.46822
7	6	0	-3.47959	3.88519	-3.27892
8	7	0	-4.89909	3.601624	-3.07466
9	6	0	-5.49946	2.613323	-3.88693
10	6	0	-4.72284	1.598937	-4.48575
11	1	0	-3.64748	1.571019	-4.36366
12	6	0	-5.33311	0.601503	-5.23195
13	1	0	-4.73529	-0.18798	-5.67314
14	7	0	-6.66854	0.536058	-5.43552
15	6	0	-7.41527	1.544724	-4.927
16	1	0	-8.48078	1.522004	-5.132
17	6	0	-6.88129	2.584407	-4.17427
18	1	0	-7.54923	3.370233	-3.84082
19	6	0	-5.55539	4.201992	-1.97987
20	6	0	-5.11763	5.438537	-1.45889

21	1	0	-4.31402	5.992239	-1.92995
22	6	0	-5.7247	5.977036	-0.33108
23	1	0	-5.38523	6.930837	0.059949
24	7	0	-6.74309	5.371802	0.326872
25	6	0	-7.18767	4.200886	-0.18149
26	1	0	-8.01131	3.726291	0.340486
27	6	0	-6.63494	3.595451	-1.30019
28	1	0	-7.04243	2.643753	-1.6158
29	6	0	-3.05514	4.592389	-4.41448
30	1	0	-3.79062	4.97562	-5.11633
31	6	0	-1.68818	4.812256	-4.66518
32	1	0	-1.39675	5.363096	-5.55457
33	6	0	-0.74744	4.313114	-3.76429
34	7	0	-8.50306	7.757793	1.289177
35	1	0	-7.95996	8.211249	0.5496
36	1	0	-9.35175	7.407639	0.83164
37	6	0	-8.88344	8.773586	2.344043
38	1	0	-9.64601	9.455444	1.952814
39	1	0	-7.98999	9.359843	2.57718
40	6	0	-9.38312	8.009683	3.552225
41	1	0	-9.56761	8.673839	4.403328
42	1	0	-10.3094	7.469984	3.335362
43	7	0	-8.32802	6.985722	3.910172
44	1	0	-8.7113	6.313704	4.58028
45	1	0	-7.55433	7.448889	4.399174
46	6	0	1.190334	3.626999	-2.61284
47	6	0	2.535959	3.40428	-2.35434
48	1	0	2.839527	2.853541	-1.46826
49	6	0	3.479736	3.885095	-3.27898
50	7	0	4.899235	3.601513	-3.07471
51	6	0	5.499592	2.613181	-3.88696
52	6	0	4.722959	1.598739	-4.48569
53	1	0	3.647609	1.570789	-4.36352
54	6	0	5.33321	0.60129	-5.23187
55	1	0	4.735396	-0.18824	-5.67298
56	7	0	6.668636	0.535892	-5.43555
57	6	0	7.415361	1.544613	-4.92714
58	1	0	8.480851	1.52193	-5.13222
59	6	0	6.881401	2.584305	-4.17441
60	1	0	7.54933	3.370176	-3.84106
61	6	0	5.555545	4.201909	-1.97994
62	6	0	5.117849	5.438525	-1.45908
63	1	0	4.314317	5.992259	-1.93022

64	6	0	5.724891	5.977059	-0.33128
65	1	0	5.385471	6.930915	0.059666
66	7	0	6.743171	5.37178	0.326805
67	6	0	7.187694	4.20079	-0.18144
68	1	0	8.011244	3.726158	0.340631
69	6	0	6.635005	3.59533	-1.30015
70	1	0	7.042432	2.643574	-1.61566
71	6	0	3.055293	4.592298	-4.41453
72	1	0	3.790771	4.975509	-5.1164
73	6	0	1.688337	4.8122	-4.66521
74	1	0	1.396909	5.363045	-5.5546
75	6	0	0.747593	4.313091	-3.7643
76	46	0	-7.53883	-1.17667	-6.37847
77	8	0	0.000041	-1.94534	-1.86932
78	6	0	0.000024	-3.16229	-1.85056
79	6	0	-1.19024	-4.07698	-1.83539
80	6	0	-2.53584	-3.74164	-1.77183
81	1	0	-2.83927	-2.69886	-1.73816
82	6	0	-3.4797	-4.78272	-1.72555
83	7	0	-4.89915	-4.4639	-1.58193
84	6	0	-5.49942	-4.67301	-0.31985
85	6	0	-4.72255	-4.68532	0.85789
86	1	0	-3.6471	-4.56644	0.820843
87	6	0	-5.33266	-4.83276	2.094882
88	1	0	-4.73464	-4.82091	2.999063
89	7	0	-6.66816	-4.97546	2.253597
90	6	0	-7.41518	-5.03859	1.125954
91	1	0	-8.48074	-5.20434	1.248334
92	6	0	-6.8814	-4.90651	-0.15087
93	1	0	-7.54957	-5.01013	-0.998
94	6	0	-5.55537	-3.81562	-2.64917
95	6	0	-5.11842	-3.9834	-3.98071
96	1	0	-4.31552	-4.66896	-4.22493
97	6	0	-5.72543	-3.27569	-5.01085
98	1	0	-5.38665	-3.41447	-6.03254
99	7	0	-6.7429	-2.40228	-4.81537
100	6	0	-7.18657	-2.25622	-3.54692
101	1	0	-8.00933	-1.56591	-3.3966
102	6	0	-6.6339	-2.92258	-2.46338
103	1	0	-7.0405	-2.71925	-1.48118
104	6	0	-3.05531	-6.11977	-1.76989
105	1	0	-3.79083	-6.91918	-1.75057
106	6	0	-1.68836	-6.44693	-1.83487

107	1	0	-1.39702	-7.49262	-1.8669
108	6	0	-0.74754	-5.41724	-1.85341
109	7	0	-8.50686	-2.76184	-7.3601
110	1	0	-7.96404	-3.6292	-7.38434
111	1	0	-9.3543	-2.98277	-6.826
112	6	0	-8.8906	-2.35616	-8.76634
113	1	0	-9.6546	-3.03549	-9.15916
114	1	0	-7.99882	-2.44804	-9.39292
115	6	0	-9.38921	-0.92758	-8.70783
116	1	0	-9.57611	-0.52266	-9.70814
117	1	0	-10.3139	-0.84482	-8.12952
118	7	0	-8.33171	-0.10615	-8.003
119	1	0	-8.71374	0.810526	-7.75539
120	1	0	-7.55948	0.084965	-8.65058
121	6	0	1.19026	-4.07701	-1.83539
122	6	0	2.535873	-3.74172	-1.77185
123	1	0	2.839336	-2.69895	-1.73818
124	6	0	3.479699	-4.78283	-1.72557
125	7	0	4.899167	-4.46406	-1.58199
126	6	0	5.499458	-4.67318	-0.31992
127	6	0	4.722636	-4.68537	0.857856
128	1	0	3.647201	-4.5664	0.82085
129	6	0	5.3328	-4.83276	2.09483
130	1	0	4.734823	-4.82079	2.999039
131	7	0	6.66829	-4.97555	2.253494
132	6	0	7.415254	-5.03882	1.125822
133	1	0	8.480806	-5.20463	1.248164
134	6	0	6.881425	-4.90678	-0.15098
135	1	0	7.549557	-5.01048	-0.99814
136	6	0	5.555391	-3.81579	-2.64923
137	6	0	5.118367	-3.9835	-3.98076
138	1	0	4.315404	-4.66898	-4.22497
139	6	0	5.725382	-3.27578	-5.0109
140	1	0	5.386548	-3.4145	-6.03258
141	7	0	6.742932	-2.40246	-4.81542
142	6	0	7.186666	-2.25648	-3.54699
143	1	0	8.009489	-1.56624	-3.39668
144	6	0	6.633984	-2.92283	-2.46345
145	1	0	7.040639	-2.71957	-1.48126
146	6	0	3.055268	-6.11986	-1.76991
147	1	0	3.79076	-6.91929	-1.7506
148	6	0	1.688312	-6.44698	-1.83488
149	1	0	1.396938	-7.49266	-1.8669

150	6	0	0.747515	-5.41726	-1.85341
151	46	0	-7.53825	-4.93567	4.208345
152	8	0	0.000007	-0.6464	2.618794
153	6	0	0.00002	-0.0215	3.663217
154	6	0	-1.19022	0.449047	4.447776
155	6	0	-2.53584	0.336355	4.125708
156	1	0	-2.83937	-0.15617	3.205978
157	6	0	-3.47961	0.897192	5.004127
158	7	0	-4.89908	0.862077	4.656421
159	6	0	-5.49935	2.059593	4.206313
160	6	0	-4.72262	3.08498	3.62666
161	1	0	-3.64732	2.992813	3.541056
162	6	0	-5.33273	4.229934	3.135807
163	1	0	-4.73488	5.006432	2.672199
164	7	0	-6.66807	4.439401	3.181395
165	6	0	-7.41491	3.495008	3.801071
166	1	0	-8.48033	3.684264	3.884179
167	6	0	-6.88111	2.323217	4.325138
168	1	0	-7.54909	1.641738	4.839175
169	6	0	-5.55531	-0.38628	4.628846
170	6	0	-5.11803	-1.45552	5.439733
171	1	0	-4.31489	-1.32427	6.155294
172	6	0	-5.72493	-2.70156	5.341952
173	1	0	-5.38581	-3.51701	5.972756
174	7	0	-6.74267	-2.96897	4.488142
175	6	0	-7.18676	-1.94345	3.727724
176	1	0	-8.00977	-2.15842	3.05504
177	6	0	-6.63416	-0.67185	3.762947
178	1	0	-7.04111	0.077203	3.096098
179	6	0	-3.05515	1.527544	6.184068
180	1	0	-3.79064	1.944037	6.866705
181	6	0	-1.68821	1.63487	6.499786
182	1	0	-1.39679	2.130063	7.421322
183	6	0	-0.74747	1.10381	5.617337
184	7	0	-8.50361	-4.99427	6.073216
185	1	0	-7.96002	-4.58129	6.835787
186	1	0	-9.35156	-4.42187	5.998724
187	6	0	-8.88584	-6.41527	6.425357
188	1	0	-9.64893	-6.41644	7.21097
189	1	0	-7.99324	-6.91129	6.817197
190	6	0	-9.38551	-7.07918	5.159459
191	1	0	-9.5713	-8.14812	5.309048
192	1	0	-10.3111	-6.62048	4.799959

193	7	0	-8.32966	-6.87846	4.094218
194	1	0	-8.71275	-7.12246	3.177017
195	1	0	-7.55672	-7.53431	4.251257
196	6	0	1.190284	0.449027	4.447757
197	6	0	2.535897	0.336316	4.125665
198	1	0	2.839403	-0.15621	3.205928
199	6	0	3.479688	0.897138	5.004069
200	7	0	4.899145	0.862023	4.65633
201	6	0	5.499409	2.059547	4.206234
202	6	0	4.722658	3.084989	3.626714
203	1	0	3.647347	2.992861	3.541214
204	6	0	5.332753	4.229958	3.135876
205	1	0	4.734875	5.006503	2.672378
206	7	0	6.668105	4.439376	3.181332
207	6	0	7.414977	3.494916	3.800862
208	1	0	8.480415	3.684132	3.883864
209	6	0	6.881192	2.323117	4.324928
210	1	0	7.549207	1.641582	4.838849
211	6	0	5.555376	-0.38633	4.628719
212	6	0	5.118074	-1.45561	5.439546
213	1	0	4.314904	-1.3244	6.155076
214	6	0	5.725007	-2.70163	5.341749
215	1	0	5.385878	-3.51712	5.972511
216	7	0	6.742802	-2.969	4.48799
217	6	0	7.18691	-1.94343	3.727634
218	1	0	8.009968	-2.15836	3.054995
219	6	0	6.634282	-0.67185	3.762865
220	1	0	7.04126	0.07724	3.096074
221	6	0	3.05526	1.52749	6.184021
222	1	0	3.790764	1.943972	6.866645
223	6	0	1.688319	1.634836	6.499762
224	1	0	1.396927	2.130032	7.421304
225	6	0	0.747555	1.103795	5.617326
226	46	0	7.538131	6.112785	2.170049
227	7	0	8.505164	7.75639	1.288821
228	1	0	7.962632	8.210437	0.549191
229	1	0	9.353383	7.405055	0.831312
230	6	0	8.886905	8.771831	2.343528
231	1	0	9.650238	9.452735	1.952127
232	1	0	7.994186	9.359175	2.57674
233	6	0	9.38585	8.007425	3.551692
234	1	0	9.571293	8.671423	4.402712
235	1	0	10.31147	7.466603	3.334706

236	7	0	8.329598	6.984742	3.909911
237	1	0	8.712274	6.31224	4.579885
238	1	0	7.556624	7.448832	4.399162
239	46	0	7.538921	-1.17685	-6.37849
240	7	0	8.505395	-2.76234	-7.36115
241	1	0	7.962273	-3.62953	-7.3848
242	1	0	9.353326	-2.98353	-6.82794
243	6	0	8.887782	-2.35682	-8.7678
244	1	0	9.651245	-3.03633	-9.16137
245	1	0	7.995349	-2.44856	-9.39346
246	6	0	9.386722	-0.92832	-8.70992
247	1	0	9.572663	-0.52352	-9.71046
248	1	0	10.31203	-0.84569	-8.13256
249	7	0	8.330097	-0.10666	-8.00406
250	1	0	8.712498	0.810013	-7.75702
251	1	0	7.557175	0.084435	-8.65083
252	46	0	7.538487	-4.93565	4.208194
253	7	0	8.50239	-4.99489	6.073803
254	1	0	7.958479	-4.58158	6.835967
255	1	0	9.350752	-4.42301	5.999957
256	6	0	8.883474	-6.41613	6.426241
257	1	0	9.64606	-6.41776	7.212346
258	1	0	7.990304	-6.91155	6.817529
259	6	0	9.383513	-7.08043	5.160697
260	1	0	9.568491	-8.14949	5.310461
261	1	0	10.30963	-6.62237	4.801756
262	7	0	8.328463	-6.87906	4.09479
263	1	0	8.71192	-7.12347	3.17785
264	1	0	7.554932	-7.5343	4.251457

10.2 T2

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	3.093165	-6.0026	0.427062
2	6	0	3.487587	-7.34398	0.358976
3	6	0	2.520503	-8.35391	0.36189
4	6	0	1.187386	-7.98021	0.412905
5	6	0	0.757214	-6.63483	0.474266
6	6	0	1.730925	-5.62455	0.494286
7	1	0	4.542258	-7.59866	0.306541

8	1	0	2.793789	-9.40498	0.316995
9	1	0	1.469033	-4.5706	0.548417
10	6	0	-1.18575	-7.9796	0.41322
11	6	0	-2.51905	-8.35266	0.362628
12	6	0	-3.48559	-7.34224	0.359304
13	6	0	-3.09054	-6.00098	0.426123
14	6	0	-1.72812	-5.62356	0.493305
15	6	0	-0.75492	-6.63442	0.474136
16	1	0	-2.79289	-9.40361	0.318256
17	1	0	-4.54038	-7.59644	0.307235
18	1	0	-1.46562	-4.56972	0.546826
19	6	0	0.000582	-8.89616	0.384962
20	8	0	0.000257	-10.102	0.336053
21	7	0	-4.16253	-4.99492	0.386136
22	7	0	4.164947	-4.99645	0.38883
23	6	0	-4.75989	-4.7628	-0.87953
24	6	0	-3.96987	-4.72707	-2.04691
25	6	0	-6.14936	-4.60682	-1.06931
26	6	0	-4.5532	-4.46711	-3.27997
27	1	0	-2.90166	-4.90086	-1.99923
28	6	0	-6.65735	-4.35533	-2.33858
29	1	0	-6.85157	-4.71332	-0.25099
30	7	0	-5.87935	-4.25165	-3.44129
31	1	0	-3.94183	-4.42135	-4.17447
32	1	0	-7.72814	-4.24486	-2.47945
33	6	0	-4.72232	-4.52496	1.585604
34	6	0	-4.44407	-5.13305	2.830204
35	6	0	-5.56041	-3.38611	1.640493
36	6	0	-5.00928	-4.63262	3.997433
37	1	0	-3.81042	-6.00896	2.898054
38	6	0	-6.09067	-2.95855	2.846506
39	1	0	-5.80819	-2.82415	0.749258
40	7	0	-5.8353	-3.55892	4.031064
41	1	0	-4.79507	-5.11746	4.944338
42	1	0	-6.74519	-2.09487	2.872595
43	6	0	4.722575	-4.52669	1.589792
44	6	0	4.455867	-5.14482	2.831733
45	6	0	5.547446	-3.37854	1.64755
46	6	0	5.019451	-4.64407	3.999733
47	1	0	3.833684	-6.02915	2.896873
48	6	0	6.07535	-2.95009	2.854195
49	1	0	5.785974	-2.80993	0.757938
50	7	0	5.830938	-3.55952	4.036626

51	1	0	4.817732	-5.13932	4.943766
52	1	0	6.718646	-2.07821	2.882881
53	6	0	4.76437	-4.76233	-0.87501
54	6	0	3.978226	-4.73415	-2.04532
55	6	0	6.153484	-4.5971	-1.06041
56	6	0	4.564254	-4.47276	-3.27674
57	1	0	2.911032	-4.91496	-2.00123
58	6	0	6.664311	-4.34568	-2.32842
59	1	0	6.853533	-4.69697	-0.23942
60	7	0	5.889753	-4.24922	-3.43415
61	1	0	3.955766	-4.43289	-4.17351
62	1	0	7.734898	-4.2297	-2.46533
63	6	0	3.092095	2.632091	-5.41124
64	6	0	3.486332	3.362096	-6.53869
65	6	0	2.519109	3.864766	-7.4145
66	6	0	1.186038	3.633536	-7.11631
67	6	0	0.756054	2.907278	-5.98206
68	6	0	1.729902	2.38463	-5.11739
69	1	0	4.540973	3.534984	-6.73307
70	1	0	2.792252	4.429505	-8.30215
71	1	0	1.468128	1.810518	-4.23184
72	6	0	-1.1871	3.632718	-7.11569
73	6	0	-2.52046	3.862988	-7.41329
74	6	0	-3.48686	3.360136	-6.53671
75	6	0	-3.09163	2.631277	-5.40887
76	6	0	-1.72914	2.384516	-5.11576
77	6	0	-0.75609	2.907002	-5.98149
78	1	0	-2.79444	4.427198	-8.30101
79	1	0	-4.5417	3.53222	-6.73068
80	1	0	-1.46647	1.810991	-4.23008
81	6	0	-0.00089	4.11594	-7.89524
82	8	0	-0.00139	4.761624	-8.91483
83	7	0	-4.16351	2.162397	-4.51772
84	7	0	4.164007	2.162164	-4.52091
85	6	0	-4.76148	3.14218	-3.68403
86	6	0	-3.97207	4.136161	-3.06999
87	6	0	-6.15096	3.227561	-3.45369
88	6	0	-4.55589	5.073928	-2.22853
89	1	0	-2.90396	4.182565	-3.24472
90	6	0	-6.65944	4.200868	-2.60137
91	1	0	-6.85286	2.571474	-3.95467
92	7	0	-5.88196	5.104834	-1.96078
93	1	0	-3.945	5.826431	-1.74217

94	1	0	-7.73023	4.266792	-2.43487
95	6	0	-4.72257	0.888319	-4.71055
96	6	0	-4.44358	0.114684	-5.8594
97	6	0	-5.56053	0.270873	-3.7519
98	6	0	-5.00815	-1.14664	-6.00984
99	1	0	-3.80989	0.494217	-6.6517
100	6	0	-6.09025	-0.98753	-3.9849
101	1	0	-5.80869	0.761541	-2.81962
102	7	0	-5.83424	-1.71297	-5.0971
103	1	0	-4.79341	-1.72417	-6.90311
104	1	0	-6.74487	-1.44235	-3.25031
105	6	0	4.72157	0.887203	-4.71469
106	6	0	4.454727	0.120866	-5.87105
107	6	0	5.546462	0.262974	-3.74935
108	6	0	5.018355	-1.14098	-6.02164
109	1	0	3.832447	0.506709	-6.66936
110	6	0	6.074512	-0.99613	-3.98191
111	1	0	5.784934	0.748943	-2.81202
112	7	0	5.830058	-1.7152	-5.10103
113	1	0	4.816554	-1.71085	-6.92258
114	1	0	6.717975	-1.45705	-3.24141
115	6	0	4.763589	3.139698	-3.68645
116	6	0	3.977587	4.139641	-3.07753
117	6	0	6.152678	3.21735	-3.45033
118	6	0	4.563676	5.075604	-2.23574
119	1	0	2.910475	4.192154	-3.25654
120	6	0	6.663549	4.18992	-2.59881
121	1	0	6.852703	2.555953	-3.9469
122	7	0	5.88909	5.099777	-1.96301
123	1	0	3.955332	5.832777	-1.75341
124	1	0	7.734102	4.250253	-2.42961
125	6	0	3.091422	3.371041	4.984845
126	6	0	3.485568	3.98283	6.180611
127	6	0	2.518257	4.490145	7.053634
128	6	0	1.185213	4.347289	6.704272
129	6	0	0.755318	3.727699	5.508376
130	6	0	1.729258	3.240035	4.623603
131	1	0	4.540198	4.064882	6.427537
132	1	0	2.791317	4.976823	7.986393
133	1	0	1.467595	2.759898	3.683748
134	6	0	-1.18792	4.346979	6.703188
135	6	0	-2.5213	4.489563	7.051349
136	6	0	-3.48765	3.981424	6.177782

137	6	0	-3.09235	3.368733	4.982861
138	6	0	-1.72985	3.23832	4.622627
139	6	0	-0.75684	3.727212	5.507817
140	1	0	-2.79533	4.976525	7.983672
141	1	0	-4.5425	4.063265	6.423785
142	1	0	-1.46716	2.757734	3.683281
143	6	0	-0.00178	4.7809	7.511287
144	8	0	-0.00234	5.341412	8.58007
145	7	0	-4.16415	2.830965	4.131438
146	7	0	4.163409	2.835086	4.132735
147	6	0	-4.76158	1.618832	4.563118
148	6	0	-3.97178	0.590295	5.116788
149	6	0	-6.15099	1.376168	4.521989
150	6	0	-4.55515	-0.60755	5.508117
151	1	0	-2.9037	0.718738	5.244288
152	6	0	-6.65902	0.151213	4.938788
153	1	0	-6.85318	2.137848	4.204422
154	7	0	-5.88116	-0.85532	5.401156
155	1	0	-3.94394	-1.4048	5.916533
156	1	0	-7.72975	-0.0263	4.912819
157	6	0	-4.72387	3.634819	3.124687
158	6	0	-4.44618	5.016862	3.029522
159	6	0	-5.56133	3.112845	2.110509
160	6	0	-5.01142	5.777561	2.012589
161	1	0	-3.813	5.513638	3.754535
162	6	0	-6.09177	3.943589	1.13739
163	1	0	-5.80852	2.059915	2.069018
164	7	0	-5.83699	5.269762	1.065575
165	1	0	-4.79765	6.84013	1.959354
166	1	0	-6.74592	3.534328	0.376076
167	6	0	4.720871	3.64048	3.125493
168	6	0	4.453885	5.025051	3.039989
169	6	0	5.545812	3.116685	2.102231
170	6	0	5.017462	5.786443	2.022506
171	1	0	3.831508	5.523406	3.773259
172	6	0	6.073809	3.947696	1.128113
173	1	0	5.784333	2.061958	2.05438
174	7	0	5.829238	5.276406	1.064912
175	1	0	4.815487	6.851584	1.97943
176	1	0	6.717264	3.536844	0.358711
177	6	0	4.763287	1.623793	4.562032
178	6	0	3.977632	0.596253	5.123644
179	6	0	6.15242	1.380765	4.510927

180	6	0	4.564071	-0.60065	5.513077
181	1	0	2.910506	0.724719	5.258817
182	6	0	6.663651	0.157141	4.927283
183	1	0	6.852234	2.141665	4.18636
184	7	0	5.889514	-0.84863	5.39736
185	1	0	3.955969	-1.39713	5.927665
186	1	0	7.734238	-0.01933	4.894706
187	6	0	-8.65863	-3.14912	8.062661
188	6	0	-8.12482	-4.53933	7.790549
189	1	0	-9.56027	-2.93964	7.479963
190	1	0	-8.8978	-3.0071	9.122087
191	1	0	-7.25799	-4.77005	8.416401
192	1	0	-8.88611	-5.30693	7.966269
193	7	0	-7.59395	-2.16357	7.632777
194	1	0	-6.85646	-2.12637	8.344781
195	7	0	-7.67139	-4.57723	6.346582
196	1	0	-8.49062	-4.66849	5.735932
197	46	0	-6.70779	-2.78116	5.830744
198	1	0	-7.11278	-5.41895	6.183291
199	1	0	-7.98852	-1.21973	7.597354
200	6	0	8.669374	8.616846	0.045249
201	6	0	8.105289	8.953828	-1.31836
202	1	0	9.563485	7.991181	-0.02806
203	1	0	8.930207	9.517461	0.611334
204	1	0	7.23896	9.617634	-1.24654
205	1	0	8.851261	9.436772	-1.9586
206	7	0	7.613767	7.823552	0.787008
207	1	0	6.901512	8.468896	1.143906
208	7	0	7.639912	7.658226	-1.94782
209	1	0	8.451186	7.159032	-2.32723
210	46	0	6.707032	6.441424	-0.51047
211	1	0	7.03529	7.857649	-2.74969
212	1	0	8.029493	7.378535	1.610021
213	6	0	-8.12642	9.015831	0.034403
214	6	0	-8.65962	8.556602	-1.30592
215	1	0	-7.25936	9.672965	-0.07824
216	1	0	-8.88788	9.55195	0.610942
217	1	0	-9.56135	7.947282	-1.19651
218	1	0	-8.89842	9.403177	-1.95864
219	7	0	-7.67366	7.784103	0.789349
220	1	0	-8.49322	7.300939	1.173063
221	7	0	-7.59466	7.691569	-1.94404
222	1	0	-6.85695	8.289612	-2.3318

223	46	0	-6.70921	6.439599	-0.50791
224	1	0	-7.98884	7.189079	-2.74397
225	1	0	-7.1156	8.063357	1.600393
226	6	0	-8.12129	-4.47961	-7.82725
227	6	0	-8.65496	-5.41079	-6.75968
228	1	0	-7.25382	-4.90559	-8.33946
229	1	0	-8.8823	-4.24848	-8.5803
230	1	0	-9.55702	-5.01152	-6.28721
231	1	0	-8.89335	-6.39941	-7.16658
232	7	0	-7.66918	-3.20988	-7.13772
233	1	0	-8.48896	-2.63608	-6.91175
234	7	0	-7.59056	-5.53071	-5.69089
235	1	0	-6.85242	-6.16516	-6.01467
236	46	0	-6.70594	-3.66072	-5.32393
237	1	0	-7.98503	-5.9726	-4.85609
238	1	0	-7.11073	-2.64709	-7.78471
239	6	0	8.106687	-3.33265	8.412955
240	6	0	8.671643	-4.34462	7.43936
241	1	0	7.240468	-3.72738	8.951636
242	1	0	8.852266	-3.0192	9.151521
243	1	0	9.565436	-3.96752	6.934194
244	1	0	8.933267	-5.28497	7.936241
245	7	0	7.640708	-2.14002	7.605606
246	1	0	8.451682	-1.56142	7.363009
247	7	0	7.616229	-4.59118	6.381486
248	1	0	6.904427	-5.2234	6.762005
249	46	0	6.708277	-2.77708	5.833111
250	1	0	8.03229	-5.08121	5.584627
251	1	0	7.035723	-1.54559	8.179158
252	6	0	8.107851	-5.61727	-7.09342
253	6	0	8.672222	-4.26769	-7.48237
254	1	0	7.242152	-5.8868	-7.70517
255	1	0	8.853938	-6.41315	-7.19104
256	1	0	9.565568	-4.01837	-6.90269
257	1	0	8.934356	-4.22744	-8.54504
258	7	0	7.640983	-5.51509	-5.6571
259	1	0	8.451587	-5.59449	-5.03427
260	7	0	7.61602	-3.22898	-7.16727
261	1	0	6.904452	-3.24289	-7.90527
262	46	0	6.708063	-3.6619	-5.32217
263	1	0	8.031438	-2.29358	-7.19303
264	1	0	7.035946	-6.30919	-5.42983

10.3 T3

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstrom)		
			X	Y	Z
1	8	0	-0.00053	-3.18574	1.638683
2	6	0	-0.00087	-4.39418	1.792251
3	6	0	1.18689	-5.30245	1.897871
4	6	0	2.529769	-4.97505	1.843979
5	1	0	2.814	-3.93143	1.743157
6	6	0	3.497875	-5.99768	1.955192
7	7	0	9.095058	-4.56798	1.694055
8	6	0	9.613674	-3.8859	2.809206
9	6	0	8.743209	-3.23881	3.714538
10	1	0	7.669513	-3.29137	3.588777
11	6	0	9.256017	-2.51433	4.776603
12	1	0	8.580791	-2.01569	5.462099
13	7	0	10.58102	-2.37834	5.01722
14	6	0	11.42243	-3.06114	4.206287
15	1	0	12.48176	-3.00055	4.432944
16	6	0	10.98928	-3.82303	3.128843
17	1	0	11.73072	-4.37985	2.569045
18	6	0	9.776768	-4.72032	0.476092
19	6	0	10.8885	-3.93745	0.090633
20	1	0	11.31463	-3.18694	0.742055
21	6	0	11.4476	-4.09038	-1.16736
22	1	0	12.30525	-3.4903	-1.44822
23	7	0	10.97763	-4.95172	-2.09533
24	6	0	9.925372	-5.72585	-1.73209
25	1	0	9.556914	-6.43161	-2.46889
26	6	0	9.318829	-5.64818	-0.48803
27	1	0	8.483838	-6.30406	-0.27492

28	6	0	3.047538	-7.32277	2.128638
29	1	0	3.770144	-8.13096	2.193834
30	6	0	1.684635	-7.65015	2.184008
31	1	0	1.390776	-8.68785	2.309626
32	6	0	0.742195	-6.63115	2.063094
33	6	0	-0.74521	-6.6307	2.063373
34	6	0	-1.68823	-7.64912	2.184691
35	1	0	-1.39496	-8.68699	2.310241
36	6	0	-3.05096	-7.32089	2.129871
37	1	0	-3.77404	-8.12863	2.195436
38	6	0	-3.50053	-5.99554	1.956537
39	7	0	-9.09654	-4.56054	1.699589
40	6	0	-9.78004	-4.71331	0.482619
41	6	0	-10.8913	-3.92954	0.097589
42	1	0	-11.3151	-3.17715	0.748319
43	6	0	-11.453	-4.08404	-1.1591
44	1	0	-12.3103	-3.48314	-1.43944
45	7	0	-10.9857	-4.94742	-2.08626
46	6	0	-9.933	-5.72147	-1.72405
47	1	0	-9.56549	-6.42727	-2.46151
48	6	0	-9.32436	-5.64278	-0.48105
49	1	0	-8.48931	-6.29879	-0.26858
50	6	0	-9.61259	-3.87668	2.814805
51	6	0	-8.73963	-3.23275	3.720031
52	1	0	-7.66617	-3.28914	3.594037
53	6	0	-9.24945	-2.50673	4.782535
54	1	0	-8.57213	-2.01078	5.467964
55	7	0	-10.5737	-2.36576	5.023182
56	6	0	-11.418	-3.04467	4.211888
57	1	0	-12.4773	-2.97799	4.437729
58	6	0	-10.9879	-3.80858	3.134621

59	1	0	-11.7316	-4.36244	2.574928
60	6	0	-2.53184	-4.97352	1.844888
61	1	0	-2.81548	-3.92972	1.744157
62	6	0	-1.18915	-5.30173	1.898285
63	6	0	4.947178	-5.66873	1.878166
64	6	0	5.3945	-4.5931	1.081603
65	6	0	5.925454	-6.39283	2.590662
66	6	0	6.739831	-4.24082	1.017653
67	1	0	4.677462	-4.03177	0.491559
68	6	0	7.280356	-6.05716	2.524737
69	1	0	5.628211	-7.22131	3.225656
70	6	0	7.68897	-4.97183	1.742354
71	1	0	7.053487	-3.40265	0.40059
72	1	0	8.007816	-6.63521	3.087694
73	6	0	-4.94965	-5.6656	1.880217
74	6	0	-5.92804	-6.38871	2.59357
75	6	0	-5.39662	-4.58984	1.083641
76	6	0	-7.28269	-6.0518	2.528658
77	1	0	-5.63104	-7.21728	3.228571
78	6	0	-6.74168	-4.23635	1.020667
79	1	0	-4.67952	-4.02931	0.492917
80	6	0	-7.6909	-4.96624	1.746389
81	1	0	-8.01021	-6.62892	3.092493
82	1	0	-7.05506	-3.39799	0.403716
83	6	0	12.84279	-0.76906	9.056057
84	6	0	12.21671	-2.14615	9.154208
85	1	0	13.83455	-0.81093	8.596559
86	1	0	12.94474	-0.3022	10.04113
87	1	0	12.85979	-2.84215	9.702676
88	1	0	11.24632	-2.11115	9.657651
89	7	0	11.96154	0.073806	8.164987

90	7	0	11.98261	-2.64599	7.748291
91	46	0	11.2695	-1.07561	6.546253
92	8	0	-0.00149	1.05213	-3.26728
93	6	0	-0.00151	0.966984	-4.48251
94	6	0	-1.1904	0.894941	-5.39386
95	6	0	-2.53442	0.901602	-5.0643
96	1	0	-2.82183	0.999253	-4.02117
97	6	0	-3.50011	0.814982	-6.09174
98	7	0	-9.12221	0.755075	-4.73872
99	6	0	-9.68235	1.975629	-4.31288
100	6	0	-8.86974	2.962012	-3.71256
101	1	0	-7.80242	2.812796	-3.60742
102	6	0	-9.43503	4.130372	-3.22863
103	1	0	-8.81498	4.874207	-2.74143
104	7	0	-10.7591	4.402975	-3.3113
105	6	0	-11.5342	3.503191	-3.96101
106	1	0	-12.5848	3.74892	-4.07596
107	6	0	-11.0448	2.309765	-4.47528
108	1	0	-11.7268	1.668063	-5.02041
109	6	0	-9.79444	-0.47367	-4.67818
110	6	0	-10.9782	-0.6876	-3.93448
111	1	0	-11.4711	0.11173	-3.39844
112	6	0	-11.5305	-1.95453	-3.84858
113	1	0	-12.4458	-2.10296	-3.28633
114	7	0	-10.988	-3.04783	-4.42805
115	6	0	-9.86928	-2.85396	-5.16888
116	1	0	-9.44477	-3.72648	-5.65389
117	6	0	-9.26467	-1.61616	-5.32308
118	1	0	-8.37495	-1.54576	-5.93617
119	6	0	-3.0474	0.733988	-7.42492
120	1	0	-3.76862	0.642563	-8.23171

121	6	0	-1.68452	0.728199	-7.75468
122	1	0	-1.3883	0.654509	-8.79667
123	6	0	-0.74475	0.804681	-6.72936
124	6	0	0.741694	0.805379	-6.72943
125	6	0	1.681452	0.729729	-7.75483
126	1	0	1.385219	0.655729	-8.79679
127	6	0	3.044358	0.736762	-7.42518
128	1	0	3.765577	0.645949	-8.23204
129	6	0	3.49711	0.818247	-6.09205
130	7	0	9.118904	0.763838	-4.73745
131	6	0	9.791533	-0.46481	-4.67595
132	6	0	10.97284	-0.67926	-3.92851
133	1	0	11.46293	0.119334	-3.38887
134	6	0	11.52625	-1.94577	-3.84348
135	1	0	12.43977	-2.09419	-3.27836
136	7	0	10.98682	-3.03832	-4.42675
137	6	0	9.869545	-2.84436	-5.16987
138	1	0	9.446728	-3.71699	-5.65646
139	6	0	9.264309	-1.60678	-5.32385
140	1	0	8.376039	-1.53619	-5.93903
141	6	0	9.677909	1.984761	-4.31153
142	6	0	8.863099	2.973718	-3.71833
143	1	0	7.795003	2.82621	-3.61905
144	6	0	9.426934	4.142692	-3.2339
145	1	0	8.804789	4.888601	-2.75251
146	7	0	10.75172	4.412909	-3.30874
147	6	0	11.52985	3.510271	-3.95098
148	1	0	12.58227	3.753168	-4.0567
149	6	0	11.04174	2.316913	-4.46658
150	1	0	11.72631	1.673399	-5.00631
151	6	0	2.531401	0.904077	-5.06455

152	1	0	2.818783	1.002094	-4.02144
153	6	0	1.187368	0.896113	-5.39398
154	6	0	-4.95171	0.796211	-5.76459
155	6	0	-5.41131	0.209489	-4.56624
156	6	0	-5.92198	1.356023	-6.62121
157	6	0	-6.76304	0.193901	-4.23109
158	1	0	-4.69945	-0.25859	-3.89411
159	6	0	-7.28167	1.335468	-6.30243
160	1	0	-5.61483	1.832274	-7.54677
161	6	0	-7.70504	0.75684	-5.10111
162	1	0	-7.08695	-0.26564	-3.30067
163	1	0	-8.00321	1.771682	-6.98744
164	6	0	4.948728	0.800732	-5.76488
165	6	0	5.918718	1.360821	-6.62166
166	6	0	5.408595	0.215048	-4.56614
167	6	0	7.278389	1.34161	-6.30261
168	1	0	5.611364	1.836323	-7.54754
169	6	0	6.760245	0.200895	-4.23068
170	1	0	4.697025	-0.25323	-3.89384
171	6	0	7.701945	0.764138	-5.10081
172	1	0	7.999671	1.778186	-6.98767
173	1	0	7.084339	-0.25763	-3.29982
174	1	0	12.45922	0.921462	7.88099
175	1	0	11.14541	0.397249	8.693993
176	1	0	11.34969	-3.45004	7.761672
177	1	0	12.86557	-2.99117	7.358863
178	6	0	13.28753	8.059593	-3.80026
179	6	0	12.8051	8.812711	-2.57645
180	1	0	14.24128	7.557938	-3.61268
181	1	0	13.4176	8.727775	-4.65785
182	1	0	13.55459	9.529158	-2.22463

183	1	0	11.88057	9.36028	-2.78107
184	7	0	12.26497	6.99416	-4.1162
185	7	0	12.50531	7.796689	-1.50014
186	46	0	11.57193	6.108326	-2.33879
187	1	0	12.65034	6.330899	-4.79309
188	1	0	11.45586	7.419737	-4.58057
189	1	0	11.97302	8.235236	-0.7445
190	1	0	13.38162	7.481468	-1.07124
191	6	0	-12.6944	8.395697	-3.87916
192	6	0	-13.3699	8.470773	-2.52452
193	1	0	-11.7752	8.988021	-3.90373
194	1	0	-13.3516	8.754363	-4.67808
195	1	0	-13.5864	9.50511	-2.23821
196	1	0	-14.3101	7.911956	-2.51229
197	7	0	-12.3141	6.953783	-4.12133
198	7	0	-12.4447	7.83045	-1.51618
199	46	0	-11.5697	6.10679	-2.34589
200	1	0	-11.6439	6.892321	-4.89246
201	1	0	-13.1425	6.433174	-4.42606
202	1	0	-12.9532	7.631877	-0.65048
203	1	0	-11.7078	8.495885	-1.26275
204	6	0	-13.7003	-6.23687	-5.95027
205	6	0	-13.1456	-7.39156	-5.1396
206	1	0	-14.6107	-5.83101	-5.49988
207	1	0	-13.9351	-6.54138	-6.97541
208	1	0	-13.8898	-8.18359	-5.00693
209	1	0	-12.2644	-7.82988	-5.61692
210	7	0	-12.6641	-5.13824	-5.95376
211	7	0	-12.7146	-6.8471	-3.79846
212	46	0	-11.798	-4.9704	-4.04611
213	1	0	-13.0814	-4.26202	-6.27788

214	1	0	-11.9285	-5.36387	-6.6309
215	1	0	-12.1264	-7.531	-3.31557
216	1	0	-13.5362	-6.71852	-3.19929
217	6	0	-12.2266	-0.7923	9.351893
218	6	0	-12.8267	-2.09689	8.866213
219	1	0	-11.255	-0.95052	9.828757
220	1	0	-12.8819	-0.29186	10.07219
221	1	0	-12.9176	-2.82509	9.678757
222	1	0	-13.82	-1.94535	8.433983
223	7	0	-12.0037	0.088722	8.145692
224	7	0	-11.9315	-2.63659	7.776162
225	46	0	-11.2665	-1.06339	6.549429
226	1	0	-11.3869	0.868287	8.388321
227	1	0	-12.8932	0.513295	7.864517
228	1	0	-12.4118	-3.38249	7.266491
229	1	0	-11.1058	-3.07696	8.194623
230	6	0	13.69995	-7.07857	-4.91246
231	6	0	13.13747	-6.52404	-6.2064
232	1	0	14.60821	-6.54948	-4.60998
233	1	0	13.94074	-8.1429	-5.00183
234	1	0	13.87848	-6.55273	-7.01189
235	1	0	12.25762	-7.08509	-6.53432
236	7	0	12.66596	-6.86366	-3.8327
237	7	0	12.70071	-5.10194	-5.9461
238	46	0	11.79256	-4.96429	-4.05469
239	1	0	13.08777	-6.9987	-2.91025
240	1	0	11.93535	-7.5779	-3.9132
241	1	0	12.10334	-4.77317	-6.70898
242	1	0	13.51902	-4.48486	-5.95052
243	8	0	0.000944	2.472882	2.631387
244	6	0	0.001448	3.577061	3.145372

245	6	0	-1.18569	4.409992	3.523413
246	6	0	-2.5278	4.117283	3.363896
247	1	0	-2.81075	3.156877	2.942489
248	6	0	-3.49681	5.056716	3.78068
249	7	0	-9.07913	3.756266	3.014544
250	6	0	-9.61053	2.74961	3.834876
251	6	0	-8.75066	1.921122	4.59209
252	1	0	-7.67849	2.0661	4.57399
253	6	0	-9.27103	0.904915	5.373956
254	1	0	-8.60271	0.278658	5.954237
255	7	0	-10.5943	0.633637	5.463864
256	6	0	-11.4333	1.461185	4.797703
257	1	0	-12.4966	1.278004	4.911551
258	6	0	-10.9948	2.514453	4.005867
259	1	0	-11.7426	3.156218	3.556333
260	6	0	-9.7338	4.300426	1.894552
261	6	0	-10.733	3.626681	1.157022
262	1	0	-11.09	2.646686	1.445482
263	6	0	-11.2514	4.193984	0.002288
264	1	0	-12.0059	3.66662	-0.57068
265	7	0	-10.8503	5.38969	-0.4834
266	6	0	-9.91031	6.058813	0.229899
267	1	0	-9.59999	7.026306	-0.15041
268	6	0	-9.34221	5.561548	1.391684
269	1	0	-8.59187	6.153612	1.901579
270	6	0	-3.04807	6.26093	4.361237
271	1	0	-3.77138	7.009442	4.67151
272	6	0	-1.68525	6.553287	4.521712
273	1	0	-1.39247	7.500257	4.964981
274	6	0	-0.74154	5.621873	4.093199
275	6	0	0.746341	5.621137	4.093289

276	6	0	1.690931	6.551626	4.52189
277	1	0	1.399032	7.498903	4.965088
278	6	0	3.053475	6.257911	4.361591
279	1	0	3.777482	7.005728	4.671915
280	6	0	3.501097	5.053226	3.781141
281	7	0	9.082409	3.747479	3.016252
282	6	0	9.738514	4.291918	1.897288
283	6	0	10.74106	3.620028	1.162608
284	1	0	11.09929	2.640819	1.452131
285	6	0	11.26199	4.188175	0.009295
286	1	0	12.01954	3.662336	-0.56099
287	7	0	10.85952	5.382525	-0.47793
288	6	0	9.914953	6.049429	0.231561
289	1	0	9.601732	7.014841	-0.15222
290	6	0	9.345154	5.551747	1.392333
291	1	0	8.591706	6.142191	1.899483
292	6	0	9.611918	2.739682	3.83654
293	6	0	8.750251	1.912134	4.592767
294	1	0	7.678356	2.058958	4.574179
295	6	0	9.268341	0.894567	5.374424
296	1	0	8.598433	0.269253	5.953899
297	7	0	10.59092	0.620698	5.464492
298	6	0	11.43176	1.447026	4.79912
299	1	0	12.49476	1.260571	4.912383
300	6	0	10.99568	2.502072	4.008258
301	1	0	11.74488	3.142879	3.559812
302	6	0	2.531206	4.114753	3.364245
303	1	0	2.813239	3.154052	2.942897
304	6	0	1.189368	4.40881	3.523574
305	6	0	-4.94423	4.769086	3.589727
306	6	0	-5.37696	3.999903	2.48862

307	6	0	-5.93404	5.227582	4.484035
308	6	0	-6.71869	3.680006	2.303243
309	1	0	-4.65081	3.657127	1.758887
310	6	0	-7.28619	4.923258	4.302108
311	1	0	-5.64795	5.814274	5.351255
312	6	0	-7.67937	4.137879	3.212916
313	1	0	-7.02069	3.076345	1.451139
314	1	0	-8.02222	5.288393	5.013038
315	6	0	4.948264	4.764154	3.590448
316	6	0	5.938373	5.221933	4.484796
317	6	0	5.380463	3.994321	2.489574
318	6	0	7.290272	4.916331	4.303132
319	1	0	5.652705	5.809071	5.351854
320	6	0	6.721931	3.673156	2.30445
321	1	0	4.654107	3.652065	1.759799
322	6	0	7.682884	4.130381	3.214161
323	1	0	8.026526	5.280901	5.014115
324	1	0	7.023526	3.06908	1.452492

10.4 G1@T1

Center Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstrom)**		
			X	**Y**	**Z**
1	46	0	7.595584	6.461286	-0.14795
2	8	0	0.041796	3.168356	1.59647
3	6	0	0.041132	3.057597	2.809718
4	6	0	1.229855	2.9847	3.720104
5	6	0	2.567929	2.843035	3.379295
6	1	0	2.862483	2.767338	2.336967
7	6	0	3.512164	2.756436	4.417417
8	7	0	4.916346	2.507451	4.098824

9	6	0	5.482328	1.277147	4.505567
10	6	0	4.676822	0.137134	4.71279
11	1	0	3.603318	0.182337	4.582778
12	6	0	5.255632	-1.07505	5.060461
13	1	0	4.634614	-1.9528	5.199591
14	7	0	6.588397	-1.24528	5.223488
15	6	0	7.364498	-0.14285	5.089708
16	1	0	8.428828	-0.26467	5.263668
17	6	0	6.862264	1.10907	4.751689
18	1	0	7.553741	1.942723	4.70494
19	6	0	5.583267	3.402155	3.235476
20	6	0	5.202901	4.759128	3.154508
21	1	0	4.441529	5.167975	3.808439
22	6	0	5.807669	5.602043	2.230051
23	1	0	5.506241	6.64308	2.174072
24	7	0	6.776335	5.196197	1.372729
25	6	0	7.173548	3.907647	1.469936
26	1	0	7.960533	3.590311	0.794719
27	6	0	6.616672	3.001565	2.359716
28	1	0	6.980455	1.982761	2.341857
29	6	0	3.095558	2.85804	5.754411
30	1	0	3.832214	2.829882	6.55237
31	6	0	1.733576	2.981646	6.085963
32	1	0	1.449385	3.044271	7.132194
33	6	0	0.788179	3.017833	5.060684
34	7	0	8.571087	7.724288	1.217028
35	1	0	8.023911	7.931639	2.056758
36	1	0	9.406702	7.230218	1.548468
37	6	0	8.983847	9.013626	0.541346
38	1	0	9.751068	9.521367	1.135585
39	1	0	8.103583	9.661321	0.497223

40	6	0	9.489837	8.661021	-0.84157
41	1	0	9.698832	9.556437	-1.43663
42	1	0	10.40352	8.061333	-0.79759
43	7	0	8.423952	7.824886	-1.51539
44	1	0	8.806264	7.391208	-2.35997
45	1	0	7.665612	8.434705	-1.83976
46	6	0	-1.14916	2.990426	3.719593
47	6	0	-2.4881	2.855988	3.379128
48	1	0	-2.78391	2.784882	2.336751
49	6	0	-3.43357	2.773693	4.417089
50	7	0	-4.84022	2.540312	4.098354
51	6	0	-5.42512	1.319311	4.506859
52	6	0	-4.63856	0.167664	4.720985
53	1	0	-3.56369	0.195735	4.597021
54	6	0	-5.23814	-1.03502	5.067371
55	1	0	-4.63125	-1.92188	5.211374
56	7	0	-6.57419	-1.18483	5.222839
57	6	0	-7.33216	-0.07046	5.083607
58	1	0	-8.39915	-0.17537	5.25225
59	6	0	-6.80868	1.172888	4.746875
60	1	0	-7.48701	2.016949	4.695147
61	6	0	-5.49626	3.444266	3.235883
62	6	0	-5.10431	4.798164	3.160667
63	1	0	-4.34216	5.198866	3.81875
64	6	0	-5.69812	5.648504	2.235757
65	1	0	-5.38765	6.687067	2.183324
66	7	0	-6.66655	5.252537	1.373663
67	6	0	-7.07542	3.96724	1.466218
68	1	0	-7.86165	3.658141	0.786362
69	6	0	-6.52953	3.054417	2.355525
70	1	0	-6.89681	2.037255	2.330196

71	6	0	-3.01582	2.870959	5.754003
72	1	0	-3.75248	2.846433	6.552063
73	6	0	-1.65318	2.987173	6.085523
74	1	0	-1.36861	3.047189	7.131807
75	6	0	-0.7076	3.020685	5.0604
76	46	0	7.415041	-3.19045	5.590878
77	8	0	-0.03662	-3.11603	1.675036
78	6	0	-0.0368	-4.14582	1.017552
79	6	0	1.149452	-4.92005	0.543773
80	6	0	2.487285	-4.55895	0.601739
81	1	0	2.780306	-3.60393	1.024973
82	6	0	3.440762	-5.4356	0.058179
83	7	0	4.844864	-5.03377	0.027923
84	6	0	5.430714	-4.75828	-1.23204
85	6	0	4.647207	-4.33396	-2.32461
86	1	0	3.572297	-4.23591	-2.23815
87	6	0	5.251349	-4.00902	-3.53149
88	1	0	4.649582	-3.6614	-4.36356
89	7	0	6.586377	-4.07996	-3.73736
90	6	0	7.340308	-4.55019	-2.71487
91	1	0	8.40613	-4.65111	-2.89287
92	6	0	6.812393	-4.90301	-1.47792
93	1	0	7.484026	-5.30398	-0.72701
94	6	0	5.482671	-4.69969	1.241528
95	6	0	5.083398	-5.28168	2.464381
96	1	0	4.32911	-6.05936	2.49558
97	6	0	5.661846	-4.86854	3.658856
98	1	0	5.345342	-5.321	4.593141
99	7	0	6.620873	-3.9128	3.733765
100	6	0	7.035958	-3.37723	2.56403
101	1	0	7.815031	-2.62535	2.624025

102	6	0	6.505952	-3.72878	1.331104
103	1	0	6.88607	-3.22264	0.453354
104	6	0	3.027436	-6.65908	-0.49323
105	1	0	3.767074	-7.35237	-0.88384
106	6	0	1.663285	-7.00626	-0.56158
107	1	0	1.385369	-7.95786	-1.00492
108	6	0	0.710187	-6.11955	-0.05938
109	7	0	8.356234	-5.00985	6.060543
110	1	0	7.805305	-5.83937	5.824347
111	1	0	9.204917	-5.07155	5.487601
112	6	0	8.73477	-5.04536	7.524867
113	1	0	9.48673	-5.82193	7.701116
114	1	0	7.837052	-5.30547	8.092996
115	6	0	9.252761	-3.67138	7.894252
116	1	0	9.437889	-3.58433	8.970221
117	1	0	10.18267	-3.43461	7.369281
118	7	0	8.211406	-2.66236	7.461786
119	1	0	8.607211	-1.71929	7.498823
120	1	0	7.436834	-2.66101	8.134268
121	6	0	-1.22417	-4.91649	0.542739
122	6	0	-2.56038	-4.55129	0.603131
123	1	0	-2.8494	-3.59599	1.028121
124	6	0	-3.51746	-5.42464	0.060916
125	7	0	-4.91978	-5.01629	0.028753
126	6	0	-5.4965	-4.73217	-1.23408
127	6	0	-4.70217	-4.30693	-2.31839
128	1	0	-3.62755	-4.21497	-2.22304
129	6	0	-5.29464	-3.97315	-3.52835
130	1	0	-4.68438	-3.62511	-4.35397
131	7	0	-6.62834	-4.0354	-3.745
132	6	0	-7.3929	-4.50633	-2.73087

133	1	0	-8.45793	-4.59978	-2.91733
134	6	0	-6.87672	-4.86859	-1.49136
135	1	0	-7.5564	-5.27035	-0.74809
136	6	0	-5.55571	-4.67528	1.241014
137	6	0	-5.14454	-5.24201	2.467494
138	1	0	-4.38786	-6.01714	2.501422
139	6	0	-5.71145	-4.81485	3.662341
140	1	0	-5.38413	-5.25437	4.599094
141	7	0	-6.67161	-3.86001	3.734907
142	6	0	-7.10328	-3.34427	2.562231
143	1	0	-7.88559	-2.59551	2.620168
144	6	0	-6.58525	-3.71055	1.32839
145	1	0	-6.97665	-3.21673	0.448744
146	6	0	-3.1087	-6.64987	-0.48992
147	1	0	-3.85107	-7.34084	-0.87948
148	6	0	-1.74565	-7.00187	-0.5593
149	1	0	-1.47169	-7.95509	-1.00164
150	6	0	-0.78901	-6.11766	-0.05936
151	46	0	7.457821	-3.37716	-5.56476
152	8	0	0.041425	0.263021	-2.89459
153	6	0	0.04065	1.196183	-3.6784
154	6	0	1.229216	1.902409	-4.25437
155	6	0	2.571068	1.690237	-3.97098
156	1	0	2.865578	0.92422	-3.2592
157	6	0	3.521366	2.514265	-4.59843
158	7	0	4.935398	2.356256	-4.25971
159	6	0	5.541673	3.334356	-3.44115
160	6	0	4.765798	4.186097	-2.62455
161	1	0	3.684067	4.146595	-2.64149
162	6	0	5.382238	5.086584	-1.76608
163	1	0	4.781117	5.719591	-1.12291

164	7	0	6.724072	5.217307	-1.663
165	6	0	7.475836	4.467026	-2.50401
166	1	0	8.550841	4.611894	-2.46575
167	6	0	6.937627	3.545237	-3.39445
168	1	0	7.615517	3.017445	-4.05514
169	6	0	5.561107	1.131951	-4.58805
170	6	0	5.15082	0.388597	-5.71515
171	1	0	4.39757	0.770388	-6.39442
172	6	0	5.720011	-0.85082	-5.98171
173	1	0	5.400624	-1.41344	-6.85304
174	7	0	6.675947	-1.41472	-5.20344
175	6	0	7.091651	-0.69904	-4.1348
176	1	0	7.862857	-1.14914	-3.51955
177	6	0	6.572126	0.542663	-3.79792
178	1	0	6.949341	1.025815	-2.90605
179	6	0	3.104642	3.500452	-5.50636
180	1	0	3.843679	4.121666	-6.0048
181	6	0	1.738682	3.707425	-5.78151
182	1	0	1.45595	4.483184	-6.48698
183	6	0	0.789744	2.911868	-5.13835
184	7	0	8.439288	-2.82037	-7.33723
185	1	0	7.905584	-2.17465	-7.92518
186	1	0	9.288293	-2.31061	-7.06958
187	6	0	8.821176	-4.04651	-8.13737
188	1	0	9.590951	-3.79128	-8.8735
189	1	0	7.930811	-4.3804	-8.67783
190	6	0	9.308645	-5.09423	-7.15905
191	1	0	9.49364	-6.05428	-7.65269
192	1	0	10.23196	-4.7848	-6.66091
193	7	0	8.243821	-5.25229	-6.09559
194	1	0	8.618055	-5.78967	-5.30903

195	1	0	7.470351	-5.81412	-6.46758
196	6	0	-1.14859	1.900462	-4.25699
197	6	0	-2.49117	1.688337	-3.97555
198	1	0	-2.78799	0.918502	-3.2688
199	6	0	-3.44044	2.517076	-4.59878
200	7	0	-4.85447	2.368401	-4.25613
201	6	0	-5.44735	3.351559	-3.43248
202	6	0	-4.66102	4.17398	-2.59653
203	1	0	-3.58078	4.103539	-2.59711
204	6	0	-5.26515	5.086043	-1.74164
205	1	0	-4.65686	5.697823	-1.08489
206	7	0	-6.60434	5.25441	-1.65872
207	6	0	-7.36411	4.527706	-2.51307
208	1	0	-8.43543	4.700003	-2.48816
209	6	0	-6.83808	3.596508	-3.40135
210	1	0	-7.52039	3.089271	-4.07359
211	6	0	-5.49781	1.155278	-4.58914
212	6	0	-5.09199	0.402909	-5.71203
213	1	0	-4.32566	0.769295	-6.38512
214	6	0	-5.68297	-0.82546	-5.98274
215	1	0	-5.36688	-1.39484	-6.8509
216	7	0	-6.65674	-1.37015	-5.21289
217	6	0	-7.06756	-0.6456	-4.14828
218	1	0	-7.85267	-1.07999	-3.53938
219	6	0	-6.52702	0.58588	-3.80773
220	1	0	-6.90248	1.076068	-2.9191
221	6	0	-3.02204	3.505339	-5.50366
222	1	0	-3.76017	4.130229	-5.99881
223	6	0	-1.65608	3.710019	-5.77981
224	1	0	-1.37228	4.487104	-6.48339
225	6	0	-0.70811	2.911865	-5.13856

226	46	0	-7.46246	6.52166	-0.15383
227	7	0	-8.42366	7.805015	1.201979
228	1	0	-7.87656	8.007595	2.042922
229	1	0	-9.26763	7.324553	1.532305
230	6	0	-8.81489	9.097501	0.519679
231	1	0	-9.57661	9.618925	1.109131
232	1	0	-7.925	9.731938	0.476112
233	6	0	-9.32119	8.746768	-0.8636
234	1	0	-9.51471	9.642764	-1.46299
235	1	0	-10.2439	8.160973	-0.82043
236	7	0	-8.26552	7.892002	-1.53018
237	1	0	-8.6513	7.461512	-2.37478
238	1	0	-7.49676	8.489088	-1.8537
239	46	0	-7.43854	-3.11426	5.593817
240	7	0	-8.41339	-4.91372	6.070347
241	1	0	-7.87934	-5.75374	5.832393
242	1	0	-9.26587	-4.95996	5.501616
243	6	0	-8.78515	-4.93982	7.536556
244	1	0	-9.55162	-5.70096	7.717607
245	1	0	-7.88998	-5.21725	8.10049
246	6	0	-9.27359	-3.55528	7.906898
247	1	0	-9.45153	-3.46344	8.983675
248	1	0	-10.2012	-3.30047	7.386381
249	7	0	-8.21441	-2.56774	7.468068
250	1	0	-8.59107	-1.61689	7.505535
251	1	0	-7.4368	-2.58102	8.136866
252	46	0	-7.47558	-3.31728	-5.5778
253	7	0	-8.43471	-2.74241	-7.35664
254	1	0	-7.88453	-2.10785	-7.94152
255	1	0	-9.27501	-2.21568	-7.09447
256	6	0	-8.83601	-3.96122	-8.1585

257	1	0	-9.59607	-3.69121	-8.89943
258	1	0	-7.94918	-4.31309	-8.69334
259	6	0	-9.35013	-4.99845	-7.18264
260	1	0	-9.55104	-5.95499	-7.6769
261	1	0	-10.2702	-4.67049	-6.69034
262	7	0	-8.29521	-5.17685	-6.11261
263	1	0	-8.68486	-5.70664	-5.3284
264	1	0	-7.53057	-5.75386	-6.47962
265	6	0	-3.04009	1.24527	-0.23687
266	6	0	-2.13145	0.367373	0.386626
267	6	0	-2.66427	-0.6946	1.147182
268	6	0	-4.0408	-0.86783	1.262474
269	6	0	-4.92947	0.006947	0.626891
270	6	0	-4.41938	1.069359	-0.12132
271	1	0	-2.64829	2.077579	-0.81596
272	1	0	-1.99446	-1.3958	1.63549
273	1	0	-4.42899	-1.69254	1.853914
274	1	0	-6.00297	-0.14085	0.71537
275	1	0	-5.09262	1.767923	-0.61135
276	6	0	-0.69594	0.602669	0.218558
277	1	0	-0.45046	1.425752	-0.44394
278	6	0	0.295335	-0.08957	0.813316
279	1	0	0.04586	-0.9138	1.472288
280	6	0	1.734123	0.131984	0.656334
281	6	0	2.293102	1.173795	-0.11104
282	6	0	2.618192	-0.74571	1.314912
283	6	0	3.674384	1.312375	-0.22604
284	1	0	1.643173	1.886337	-0.60621
285	6	0	4.001146	-0.61007	1.193822
286	1	0	2.196298	-1.54441	1.919479
287	6	0	4.538282	0.418388	0.417441

288	1	0	4.082636	2.128861	-0.81569
289	1	0	4.659388	-1.30653	1.706603
290	1	0	5.615182	0.528318	0.316663

10.5 G2@T1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstrom)		
			X	Y	Z
1	46	0	7.525777	6.379579	-1.10737
2	8	0	-0.00016	3.265523	1.149455
3	6	0	0.001862	3.377143	2.362386
4	6	0	1.19148	3.470252	3.268888
5	6	0	2.529947	3.286664	2.95169
6	1	0	2.823794	3.04485	1.934642
7	6	0	3.477146	3.385281	3.985622
8	7	0	4.883468	3.103356	3.704795
9	6	0	5.460807	1.953636	4.291761
10	6	0	4.665738	0.850802	4.670166
11	1	0	3.591145	0.867632	4.541071
12	6	0	5.256606	-0.29067	5.193389
13	1	0	4.643998	-1.14301	5.464996
14	7	0	6.591153	-0.42236	5.375542
15	6	0	7.356821	0.654767	5.077371
16	1	0	8.422315	0.570129	5.265858
17	6	0	6.842447	1.837347	4.557184
18	1	0	7.525609	2.661348	4.384995
19	6	0	5.539816	3.859226	2.710613
20	6	0	5.144713	5.182899	2.419654
21	1	0	4.378901	5.680355	3.003227
22	6	0	5.740934	5.878263	1.374677
23	1	0	5.428495	6.894745	1.158115
24	7	0	6.714095	5.354593	0.58927

25	6	0	7.124154	4.100751	0.884372
26	1	0	7.914487	3.690488	0.265448
27	6	0	6.576862	3.338087	1.905057
28	1	0	6.953252	2.33342	2.045846
29	6	0	3.061946	3.703521	5.288612
30	1	0	3.800162	3.814745	6.077848
31	6	0	1.699326	3.870935	5.599081
32	1	0	1.417087	4.106219	6.62098
33	6	0	0.751292	3.728281	4.585346
34	7	0	8.485324	7.846741	0.048992
35	1	0	7.934203	8.174667	0.846661
36	1	0	9.325254	7.418234	0.452887
37	6	0	8.886204	9.021609	-0.81605
38	1	0	9.646174	9.62302	-0.30585
39	1	0	7.999096	9.644995	-0.96011
40	6	0	9.400013	8.466629	-2.12786
41	1	0	9.600801	9.262394	-2.85311
42	1	0	10.3202	7.891303	-1.9914
43	7	0	8.345286	7.524945	-2.66667
44	1	0	8.735309	6.970193	-3.43327
45	1	0	7.581929	8.069139	-3.08296
46	6	0	-1.18658	3.47396	3.269456
47	6	0	-2.52527	3.293251	2.952075
48	1	0	-2.81962	3.052657	1.934805
49	6	0	-3.47231	3.394705	3.985935
50	7	0	-4.87951	3.116828	3.705756
51	6	0	-5.45766	1.966717	4.291874
52	6	0	-4.66337	0.861353	4.664106
53	1	0	-3.58924	0.876203	4.531077
54	6	0	-5.25453	-0.28065	5.1856
55	1	0	-4.64251	-1.13487	5.452499

56	7	0	-6.58874	-0.4107	5.371262
57	6	0	-7.35342	0.668769	5.079247
58	1	0	-8.41852	0.585328	5.270396
59	6	0	-6.83851	1.852405	4.561686
60	1	0	-7.52064	2.678393	4.394909
61	6	0	-5.53378	3.873626	2.711278
62	6	0	-5.12765	5.192236	2.41196
63	1	0	-4.35659	5.686433	2.991315
64	6	0	-5.718	5.886194	1.362824
65	1	0	-5.39609	6.898167	1.139076
66	7	0	-6.69649	5.366288	0.581585
67	6	0	-7.12015	4.119493	0.887311
68	1	0	-7.9163	3.713261	0.273161
69	6	0	-6.57917	3.358651	1.912543
70	1	0	-6.96541	2.358944	2.060176
71	6	0	-3.05611	3.711978	5.288814
72	1	0	-3.7941	3.825428	6.077941
73	6	0	-1.693	3.875538	5.599507
74	1	0	-1.41027	4.109849	6.621493
75	6	0	-0.74542	3.730469	4.585756
76	46	0	7.438555	-2.28567	6.016065
77	8	0	0.009112	-2.73755	2.032762
78	6	0	0.008276	-3.86622	1.569139
79	6	0	1.194971	-4.71379	1.239114
80	6	0	2.533605	-4.35185	1.242739
81	1	0	2.827645	-3.34022	1.502873
82	6	0	3.486242	-5.31068	0.860583
83	7	0	4.891951	-4.92258	0.772344
84	6	0	5.480704	-4.84625	-0.51296
85	6	0	4.696494	-4.61088	-1.66101
86	1	0	3.620453	-4.51118	-1.59333

87	6	0	5.300799	-4.47996	-2.9036
88	1	0	4.698018	-4.27748	-3.78166
89	7	0	6.636887	-4.57132	-3.09387
90	6	0	7.392254	-4.86354	-2.00808
91	1	0	8.459237	-4.9831	-2.16659
92	6	0	6.86441	-5.0161	-0.7308
93	1	0	7.537754	-5.28543	0.075254
94	6	0	5.525937	-4.41216	1.924728
95	6	0	5.124085	-4.81139	3.218023
96	1	0	4.371356	-5.57831	3.359217
97	6	0	5.698705	-4.22857	4.341235
98	1	0	5.381974	-4.54251	5.330645
99	7	0	6.654883	-3.26907	4.278668
100	6	0	7.070784	-2.90599	3.044725
101	1	0	7.84741	-2.15063	2.997319
102	6	0	6.545407	-3.43447	1.874352
103	1	0	6.926931	-3.06114	0.932847
104	6	0	3.072623	-6.6086	0.520468
105	1	0	3.812226	-7.35878	0.25496
106	6	0	1.708127	-6.95925	0.506696
107	1	0	1.428778	-7.97146	0.229657
108	6	0	0.755969	-5.99786	0.848133
109	7	0	8.398896	-4.01021	6.736207
110	1	0	7.857424	-4.87068	6.618552
111	1	0	9.248911	-4.14206	6.177282
112	6	0	8.77593	-3.83638	8.191112
113	1	0	9.537157	-4.57145	8.473547
114	1	0	7.88081	-4.02593	8.790413
115	6	0	9.276599	-2.41802	8.365059
116	1	0	9.458419	-2.17925	9.418388
117	1	0	10.20467	-2.24551	7.812539

118	7	0	8.223907	-1.49212	7.795588
119	1	0	8.607744	-0.54805	7.701483
120	1	0	7.447765	-1.40715	8.460884
121	6	0	-1.17942	-4.71113	1.236368
122	6	0	-2.5174	-4.3472	1.241646
123	1	0	-2.80919	-3.33513	1.502465
124	6	0	-3.4719	-5.30495	0.861243
125	7	0	-4.87719	-4.9156	0.771742
126	6	0	-5.46431	-4.84279	-0.51477
127	6	0	-4.67846	-4.6068	-1.66148
128	1	0	-3.60291	-4.50347	-1.59165
129	6	0	-5.28052	-4.47981	-2.9055
130	1	0	-4.67659	-4.27678	-3.78262
131	7	0	-6.61589	-4.57561	-3.09835
132	6	0	-7.37263	-4.8683	-2.01374
133	1	0	-8.43893	-4.99118	-2.17422
134	6	0	-6.84696	-5.01726	-0.73506
135	1	0	-7.52115	-5.28734	0.07003
136	6	0	-5.51308	-4.40397	1.922295
137	6	0	-5.10841	-4.79599	3.217057
138	1	0	-4.35153	-5.55828	3.360934
139	6	0	-5.68571	-4.2121	4.338349
140	1	0	-5.36676	-4.5206	5.328766
141	7	0	-6.64744	-3.25835	4.27276
142	6	0	-7.06583	-2.90227	3.037558
143	1	0	-7.84695	-2.15168	2.987794
144	6	0	-6.53791	-3.43195	1.868965
145	1	0	-6.92117	-3.06342	0.926321
146	6	0	-3.06027	-6.60388	0.522427
147	1	0	-3.80125	-7.3532	0.258338
148	6	0	-1.69641	-6.95694	0.508373

149	1	0	-1.41899	-7.97019	0.233223
150	6	0	-0.74252	-5.99653	0.847591
151	46	0	7.501614	-4.15698	-5.00988
152	8	0	0.024151	-0.3409	-2.99886
153	6	0	0.021189	0.522554	-3.85661
154	6	0	1.209534	1.175177	-4.50059
155	6	0	2.553264	1.010257	-4.1941
156	1	0	2.853577	0.333147	-3.39968
157	6	0	3.49746	1.76692	-4.91059
158	7	0	4.912078	1.673777	-4.55106
159	6	0	5.508294	2.769993	-3.89081
160	6	0	4.72319	3.727584	-3.21108
161	1	0	3.64187	3.676131	-3.2227
162	6	0	5.329486	4.752601	-2.49758
163	1	0	4.721149	5.468708	-1.95644
164	7	0	6.669901	4.91123	-2.41585
165	6	0	7.429935	4.051035	-3.13556
166	1	0	8.503376	4.210976	-3.12037
167	6	0	6.902081	3.000493	-3.87716
168	1	0	7.58626	2.387026	-4.4517
169	6	0	5.555014	0.42409	-4.70286
170	6	0	5.155117	-0.47859	-5.71091
171	1	0	4.396776	-0.20827	-6.43647
172	6	0	5.740856	-1.73591	-5.79722
173	1	0	5.428937	-2.42233	-6.57779
174	7	0	6.703932	-2.1691	-4.94739
175	6	0	7.110921	-1.30133	-3.99443
176	1	0	7.888794	-1.64767	-3.32299
177	6	0	6.574591	-0.03126	-3.83866
178	1	0	6.94631	0.580932	-3.0273
179	6	0	3.075035	2.634574	-5.92988

180	1	0	3.810061	3.198112	-6.49789
181	6	0	1.708717	2.796524	-6.22708
182	1	0	1.419565	3.480859	-7.01921
183	6	0	0.766016	2.074792	-5.49401
184	7	0	8.473608	-3.87489	-6.85122
185	1	0	7.934437	-3.32987	-7.52926
186	1	0	9.320848	-3.32599	-6.66902
187	6	0	8.85863	-5.20796	-7.45458
188	1	0	9.622935	-5.06569	-8.22606
189	1	0	7.967248	-5.62576	-7.93125
190	6	0	9.357262	-6.08945	-6.32905
191	1	0	9.545191	-7.11336	-6.66949
192	1	0	10.28138	-5.70237	-5.89026
193	7	0	8.298646	-6.08653	-5.24778
194	1	0	8.680273	-6.49256	-4.38928
195	1	0	7.527338	-6.70406	-5.52348
196	6	0	-1.17008	1.166829	-4.50359
197	6	0	-2.51348	0.996112	-4.19811
198	1	0	-2.81221	0.314134	-3.40736
199	6	0	-3.4602	1.753735	-4.91043
200	7	0	-4.87415	1.658672	-4.54975
201	6	0	-5.46963	2.754384	-3.88699
202	6	0	-4.68535	3.699201	-3.18921
203	1	0	-3.60476	3.634384	-3.18249
204	6	0	-5.2918	4.728158	-2.48144
205	1	0	-4.68461	5.435505	-1.92768
206	7	0	-6.63172	4.901263	-2.42044
207	6	0	-7.38975	4.04961	-3.15223
208	1	0	-8.46183	4.219007	-3.15087
209	6	0	-6.86144	2.99626	-3.88982
210	1	0	-7.54321	2.390024	-4.47493

211	6	0	-5.5195	0.411208	-4.70504
212	6	0	-5.11763	-0.49297	-5.71104
213	1	0	-4.35495	-0.22533	-6.43303
214	6	0	-5.70701	-1.74838	-5.7998
215	1	0	-5.39354	-2.43612	-6.57859
216	7	0	-6.67564	-2.17812	-4.95455
217	6	0	-7.0848	-1.30856	-4.00408
218	1	0	-7.867	-1.65218	-3.33629
219	6	0	-6.54522	-0.04031	-3.84609
220	1	0	-6.91828	0.572906	-3.03617
221	6	0	-3.04054	2.626459	-5.92653
222	1	0	-3.77738	3.190657	-6.49148
223	6	0	-1.67496	2.792644	-6.22449
224	1	0	-1.38809	3.480659	-7.01425
225	6	0	-0.72983	2.071361	-5.4942
226	46	0	-7.49232	6.382002	-1.12654
227	7	0	-8.45418	7.858827	0.014888
228	1	0	-7.90677	8.188902	0.814236
229	1	0	-9.29813	7.435448	0.415824
230	6	0	-8.84525	9.030262	-0.85913
231	1	0	-9.60645	9.637063	-0.3572
232	1	0	-7.95505	9.649791	-1.00073
233	6	0	-9.35238	8.469878	-2.17124
234	1	0	-9.54566	9.262366	-2.90208
235	1	0	-10.2755	7.89853	-2.03764
236	7	0	-8.29747	7.521527	-2.69799
237	1	0	-8.68451	6.964375	-3.46433
238	1	0	-7.5294	8.06081	-3.11196
239	46	0	-7.43616	-2.27513	6.008258
240	7	0	-8.39623	-4.00108	6.725371
241	1	0	-7.85349	-4.86081	6.608184

242	1	0	-9.245	-4.13355	6.164717
243	6	0	-8.77628	-3.82852	8.179622
244	1	0	-9.53722	-4.5646	8.460186
245	1	0	-7.88211	-4.0174	8.780548
246	6	0	-9.27889	-2.41083	8.353429
247	1	0	-9.46304	-2.17289	9.406542
248	1	0	-10.2061	-2.23906	7.799212
249	7	0	-8.22617	-1.48338	7.786557
250	1	0	-8.61098	-0.53972	7.692341
251	1	0	-7.45143	-1.39786	8.453422
252	46	0	-7.4764	-4.16419	-5.01683
253	7	0	-8.4434	-3.8832	-6.86086
254	1	0	-7.9016	-3.33985	-7.53814
255	1	0	-9.29024	-3.33276	-6.68152
256	6	0	-8.82885	-5.21647	-7.46342
257	1	0	-9.59102	-5.07413	-8.23698
258	1	0	-7.93689	-5.63619	-7.93731
259	6	0	-9.33157	-6.0958	-6.338
260	1	0	-9.52012	-7.11986	-6.67762
261	1	0	-10.2562	-5.70682	-5.90207
262	7	0	-8.27574	-6.09299	-5.25403
263	1	0	-8.66021	-6.49739	-4.39603
264	1	0	-7.50465	-6.71203	-5.52693
265	6	0	-2.77306	1.301795	-0.53035
266	6	0	-1.89717	0.503509	0.215613
267	6	0	-2.40485	-0.41107	1.154883
268	6	0	-3.78209	-0.51757	1.328993
269	6	0	-4.65959	0.281483	0.584813
270	6	0	-4.15198	1.19639	-0.3407
271	1	0	-2.34647	2.00272	-1.24051
272	1	0	-1.70684	-1.02693	1.713209

273	1	0	-4.18208	-1.226	2.050108
274	1	0	-5.73359	0.185669	0.724664
275	1	0	-4.82598	1.827269	-0.91303
276	6	0	1.624513	0.303713	0.563215
277	6	0	2.181718	1.191569	-0.37139
278	6	0	2.457308	-0.46834	1.385368
279	6	0	3.566488	1.28208	-0.48506
280	1	0	1.51784	1.801836	-0.97151
281	6	0	3.843778	-0.38241	1.253724
282	1	0	1.98226	-1.13418	2.099087
283	6	0	4.400627	0.492176	0.317579
284	1	0	4.004365	1.978196	-1.19481
285	1	0	4.489356	-0.9889	1.883341
286	1	0	5.480577	0.568679	0.216574
287	7	0	-0.51408	0.677355	-0.05825
288	7	0	0.236913	0.141157	0.79357

11. Coordinates of PM6 Optimized Structures

11.1 $(G3)_2$@T1

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstrom) X	Y	Z
1	46	0	-7.39686	-6.536	-0.11037
2	8	0	0.005424	-2.49631	1.837196
3	6	0	0.010549	-2.71549	3.024284
4	6	0	-1.17464	-2.84708	3.937226
5	6	0	-2.50941	-2.76624	3.611776
6	1	0	-2.81755	-2.64931	2.565068
7	6	0	-3.46798	-2.84007	4.654685
8	7	0	-4.88156	-2.62828	4.317901
9	6	0	-5.47796	-1.38829	4.718161
10	6	0	-4.68099	-0.24099	4.950851
11	1	0	-3.59093	-0.29527	4.901245
12	6	0	-5.28978	0.9781	5.266873
13	1	0	-4.68331	1.877272	5.461579
14	7	0	-6.64615	1.13582	5.354992
15	6	0	-7.41359	0.012407	5.18826
16	1	0	-8.50529	0.141569	5.294983
17	6	0	-6.87305	-1.24496	4.898867
18	1	0	-7.54321	-2.11272	4.846839

19	6	0	-5.5132	-3.53022	3.409115
20	6	0	-5.02144	-4.84978	3.24023
21	1	0	-4.22289	-5.23654	3.886235
22	6	0	-5.57772	-5.68583	2.269515
23	1	0	-5.19884	-6.71352	2.129701
24	7	0	-6.60479	-5.29941	1.444319
25	6	0	-7.10883	-4.04248	1.635016
26	1	0	-7.95266	-3.75105	0.98508
27	6	0	-6.59571	-3.14767	2.580303
28	1	0	-7.03651	-2.14521	2.634277
29	6	0	-3.05027	-3.06877	5.970027
30	1	0	-3.78489	-3.17196	6.78176
31	6	0	-1.67234	-3.17302	6.287902
32	1	0	-1.38045	-3.36209	7.330473
33	6	0	-0.7254	-3.03923	5.284657
34	7	0	-8.32016	-7.77837	1.308167
35	1	0	-7.7512	-8.02514	2.128202
36	1	0	-9.18279	-7.35214	1.680766
37	6	0	-8.65953	-9.02261	0.530564
38	1	0	-9.40672	-9.67857	1.064668
39	1	0	-7.74852	-9.66747	0.431706
40	6	0	-9.21749	-8.61655	-0.83331
41	1	0	-9.54978	-9.53681	-1.39565
42	1	0	-10.1503	-8.00303	-0.73489
43	7	0	-8.16817	-7.83028	-1.57425
44	1	0	-8.5877	-7.383	-2.3994
45	1	0	-7.44347	-8.46846	-1.93759
46	6	0	1.202946	-2.83024	3.929664
47	6	0	2.534146	-2.72807	3.59691
48	1	0	2.84238	-2.62119	2.549817
49	6	0	3.496409	-2.75062	4.639694
50	7	0	4.89798	-2.49022	4.288536
51	6	0	5.460571	-1.22885	4.669117
52	6	0	4.631969	-0.11558	4.95251
53	1	0	3.543499	-0.2095	4.939177
54	6	0	5.206256	1.120101	5.270131
55	1	0	4.57377	1.990642	5.50837
56	7	0	6.558067	1.330496	5.307484
57	6	0	7.359298	0.241647	5.079303
58	1	0	8.448965	0.412324	5.139839
59	6	0	6.856193	-1.0302	4.784872
60	1	0	7.558262	-1.86646	4.678353
61	6	0	5.539451	-3.37819	3.371238
62	6	0	5.145698	-4.73787	3.285423
63	1	0	4.403078	-5.15083	3.981221
64	6	0	5.729329	-5.57621	2.33291
65	1	0	5.425905	-6.63551	2.256614
66	7	0	6.692718	-5.15448	1.448853
67	6	0	7.089678	-3.85068	1.548343
68	1	0	7.881931	-3.52327	0.848883
69	6	0	6.537549	-2.94901	2.465688
70	1	0	6.89818	-1.91088	2.460107
71	6	0	3.091006	-2.97345	5.959299

72	1	0	3.830707	-3.03914	6.770106
73	6	0	1.717834	-3.11793	6.282388
74	1	0	1.434697	-3.30504	7.327717
75	6	0	0.76435	-3.02134	5.281183
76	46	0	-7.50933	3.059273	5.662945
77	8	0	0.014283	2.829043	1.20498
78	6	0	-0.02862	3.969461	0.807906
79	6	0	-1.24486	4.786739	0.482559
80	6	0	-2.56805	4.408469	0.532126
81	1	0	-2.85633	3.412792	0.888643
82	6	0	-3.5513	5.336981	0.102196
83	7	0	-4.94981	4.889659	0.06521
84	6	0	-5.53136	4.645227	-1.2235
85	6	0	-4.71616	4.278107	-2.321
86	1	0	-3.62322	4.210834	-2.21716
87	6	0	-5.29971	3.963565	-3.551
88	1	0	-4.67518	3.684382	-4.41592
89	7	0	-6.65421	3.973916	-3.75916
90	6	0	-7.43794	4.38533	-2.71521
91	1	0	-8.5258	4.429244	-2.90088
92	6	0	-6.91987	4.739034	-1.46212
93	1	0	-7.60348	5.123046	-0.69408
94	6	0	-5.58792	4.550907	1.290373
95	6	0	-5.09651	5.058224	2.523927
96	1	0	-4.29311	5.805756	2.539146
97	6	0	-5.66408	4.645652	3.728402
98	1	0	-5.29517	5.041629	4.690963
99	7	0	-6.69775	3.741777	3.801305
100	6	0	-7.19134	3.274984	2.616362
101	1	0	-8.03155	2.561481	2.68495
102	6	0	-6.67444	3.64816	1.368676
103	1	0	-7.1473	3.230298	0.475928
104	6	0	-3.17704	6.622024	-0.30138
105	1	0	-3.93428	7.359005	-0.6047
106	6	0	-1.81198	7.003355	-0.33084
107	1	0	-1.55095	8.022759	-0.64782
108	6	0	-0.83888	6.088863	0.038222
109	7	0	-8.44235	4.914297	5.987561
110	1	0	-7.87757	5.746611	5.775305
111	1	0	-9.30382	5.007576	5.42739
112	6	0	-8.78703	4.893638	7.453495
113	1	0	-9.53975	5.68624	7.734527
114	1	0	-7.87976	5.148714	8.059436
115	6	0	-9.33865	3.514036	7.811796
116	1	0	-9.67472	3.508496	8.889244
117	1	0	-10.2684	3.27459	7.233318
118	7	0	-8.28256	2.478657	7.527478
119	1	0	-8.69645	1.538796	7.575797
120	1	0	-7.55866	2.505314	8.2624
121	6	0	1.133856	4.864867	0.488976
122	6	0	2.476647	4.570636	0.547454
123	1	0	2.820316	3.585343	0.88613
124	6	0	3.406696	5.562035	0.138591

125	7	0	4.831314	5.202592	0.102087
126	6	0	5.403247	4.906224	-1.17865
127	6	0	4.58517	4.538395	-2.27553
128	1	0	3.495644	4.549051	-2.1914
129	6	0	5.171006	4.172357	-3.49167
130	1	0	4.547482	3.894483	-4.35689
131	7	0	6.525148	4.133557	-3.68826
132	6	0	7.313673	4.550541	-2.64803
133	1	0	8.404186	4.551636	-2.82604
134	6	0	6.796447	4.95758	-1.41298
135	1	0	7.484506	5.349239	-0.65225
136	6	0	5.464998	4.847276	1.332696
137	6	0	4.978645	5.354887	2.565236
138	1	0	4.181212	6.109139	2.583475
139	6	0	5.538984	4.92615	3.770094
140	1	0	5.166363	5.316704	4.733319
141	7	0	6.564034	4.014433	3.839647
142	6	0	7.060913	3.554664	2.652479
143	1	0	7.903724	2.843631	2.716884
144	6	0	6.544413	3.935351	1.408534
145	1	0	6.996165	3.498723	0.513865
146	6	0	2.955371	6.826232	-0.252
147	1	0	3.668704	7.614539	-0.53491
148	6	0	1.568346	7.118993	-0.29673
149	1	0	1.247357	8.123697	-0.60651
150	6	0	0.64994	6.140337	0.04839
151	46	0	-7.47814	3.270375	-5.60131
152	8	0	0.010189	-0.40883	-2.9811
153	6	0	0.025823	-1.29822	-3.79925
154	6	0	-1.15228	-1.98693	-4.42389
155	6	0	-2.4895	-1.74321	-4.20756
156	1	0	-2.80281	-0.8919	-3.59319
157	6	0	-3.43971	-2.63303	-4.77096
158	7	0	-4.84472	-2.46921	-4.37766
159	6	0	-5.42334	-3.44998	-3.50871
160	6	0	-4.60874	-4.31365	-2.73539
161	1	0	-3.52146	-4.31051	-2.8474
162	6	0	-5.19546	-5.19843	-1.82425
163	1	0	-4.57361	-5.88055	-1.22141
164	7	0	-6.54692	-5.27737	-1.62129
165	6	0	-7.33786	-4.49141	-2.41866
166	1	0	-8.42901	-4.59	-2.27756
167	6	0	-6.8226	-3.60303	-3.36878
168	1	0	-7.52093	-3.05712	-4.01461
169	6	0	-5.48001	-1.22463	-4.67295
170	6	0	-5.08842	-0.46778	-5.80708
171	1	0	-4.34743	-0.86337	-6.5151
172	6	0	-5.67313	0.775671	-6.05461
173	1	0	-5.37163	1.373537	-6.93319
174	7	0	-6.63874	1.325811	-5.24688
175	6	0	-7.03096	0.586981	-4.1663
176	1	0	-7.83053	1.02338	-3.54349
177	6	0	-6.47099	-0.6538	-3.84033

178	1	0	-6.82722	-1.16922	-2.93615
179	6	0	-3.01567	-3.65292	-5.62895
180	1	0	-3.74474	-4.32009	-6.11102
181	6	0	-1.63687	-3.85338	-5.89326
182	1	0	-1.3395	-4.65413	-6.58498
183	6	0	-0.69512	-3.04601	-5.27424
184	7	0	-8.38948	2.611342	-7.37534
185	1	0	-7.81906	2.009689	-7.98305
186	1	0	-9.25091	2.07776	-7.17894
187	6	0	-8.7329	3.886294	-8.09987
188	1	0	-9.47502	3.7255	-8.93513
189	1	0	-7.82171	4.286361	-8.61503
190	6	0	-9.302	4.88736	-7.09513
191	1	0	-9.63455	5.820325	-7.63669
192	1	0	-10.2371	4.504394	-6.60995
193	7	0	-8.26069	5.166434	-6.04355
194	1	0	-8.68666	5.677503	-5.25982
195	1	0	-7.53445	5.792232	-6.42613
196	6	0	1.224151	-2.01164	-4.35193
197	6	0	2.552216	-1.79219	-4.06315
198	1	0	2.846863	-1.00214	-3.36226
199	6	0	3.522206	-2.61846	-4.68636
200	7	0	4.929897	-2.41858	-4.3181
201	6	0	5.531479	-3.4039	-3.46451
202	6	0	4.731208	-4.17159	-2.58417
203	1	0	3.63626	-4.06658	-2.57363
204	6	0	5.33091	-5.05985	-1.68806
205	1	0	4.717455	-5.66711	-1.00145
206	7	0	6.688371	-5.22709	-1.5986
207	6	0	7.457094	-4.53489	-2.49442
208	1	0	8.54726	-4.70492	-2.44572
209	6	0	6.921723	-3.64572	-3.43692
210	1	0	7.593697	-3.18058	-4.16969
211	6	0	5.542673	-1.17625	-4.64272
212	6	0	4.999467	-0.34245	-5.65896
213	1	0	4.180138	-0.70097	-6.29482
214	6	0	5.534441	0.923654	-5.88861
215	1	0	5.126427	1.572488	-6.68337
216	7	0	6.580667	1.443711	-5.16092
217	6	0	7.125934	0.633819	-4.20674
218	1	0	7.968223	1.051195	-3.62302
219	6	0	6.650924	-0.65721	-3.9349
220	1	0	7.177571	-1.23749	-3.17662
221	6	0	3.126794	-3.60395	-5.59576
222	1	0	3.87323	-4.2294	-6.10638
223	6	0	1.754386	-3.82106	-5.87914
224	1	0	1.477589	-4.60416	-6.59892
225	6	0	0.794977	-3.04405	-5.25036
226	46	0	7.527786	-6.44356	-0.05392
227	7	0	8.452531	-7.62956	1.412428
228	1	0	7.887623	-7.84817	2.242899
229	1	0	9.313856	-7.18458	1.766437
230	6	0	8.797621	-8.90116	0.682831

231	1	0	9.545456	-9.53459	1.242805
232	1	0	7.888731	-9.55205	0.605839
233	6	0	9.357874	-8.54444	-0.6936
234	1	0	9.692	-9.48438	-1.22192
235	1	0	10.29045	-7.92743	-0.61629
236	7	0	8.309093	-7.78682	-1.46431
237	1	0	8.728983	-7.37079	-2.30545
238	1	0	7.584302	-8.43831	-1.80432
239	46	0	7.382982	3.276257	5.669951
240	7	0	8.282774	5.133957	6.053189
241	1	0	7.700289	5.961875	5.87335
242	1	0	9.137936	5.262585	5.490074
243	6	0	8.638629	5.069386	7.515046
244	1	0	9.379556	5.865439	7.817438
245	1	0	7.731736	5.288059	8.135735
246	6	0	9.216891	3.688361	7.82232
247	1	0	9.561	3.652434	8.896519
248	1	0	10.14609	3.485365	7.229254
249	7	0	8.176895	2.64465	7.509961
250	1	0	8.607096	1.711165	7.524416
251	1	0	7.457471	2.634539	8.249561
252	46	0	7.36467	3.410038	-5.51274
253	7	0	8.278652	2.754517	-7.28742
254	1	0	7.709454	2.146069	-7.88956
255	1	0	9.145667	2.229608	-7.09423
256	6	0	8.606623	4.030313	-8.01746
257	1	0	9.35024	3.874821	-8.85206
258	1	0	7.690589	4.417443	-8.53358
259	6	0	9.164233	5.042544	-7.0172
260	1	0	9.488367	5.975651	-7.56314
261	1	0	10.10196	4.671029	-6.52823
262	7	0	8.118891	5.316834	-5.9683
263	1	0	8.538976	5.838307	-5.18814
264	1	0	7.386419	5.931808	-6.35569
265	6	0	-1.62628	0.611479	-0.33252
266	6	0	-2.17784	-0.3702	0.729502
267	6	0	-4.07416	0.670809	-0.02007
268	1	0	-0.887	1.325088	0.089069
269	1	0	-1.0848	0.108239	-1.16138
270	6	0	-3.55503	-0.8186	0.101577
271	6	0	-2.6247	0.492641	1.94027
272	1	0	-2.82849	-0.12711	2.82651
273	1	0	-1.83745	1.20976	2.235082
274	6	0	-3.90254	1.209215	1.42967
275	1	0	-4.7816	0.973042	2.056815
276	1	0	-3.79125	2.310004	1.448308
277	1	0	-1.48791	-1.19036	0.980851
278	6	0	-4.38699	-1.71061	1.010233
279	1	0	-4.80645	-1.17905	1.875118
280	1	0	-5.22004	-2.19078	0.47658
281	1	0	-3.76704	-2.53681	1.401376
282	6	0	-3.41268	-1.52731	-1.23812
283	1	0	-2.81716	-2.44483	-1.13044

284	1	0	-4.38982	-1.81832	-1.64357
285	1	0	-2.90599	-0.91724	-1.9998
286	6	0	-2.87844	1.3026	-0.8165
287	8	0	-2.99233	2.157013	-1.6569
288	6	0	-5.39719	0.946046	-0.69503
289	1	0	-5.55322	2.055211	-0.71987
290	1	0	-5.29045	0.706104	-1.7848
291	16	0	-6.75793	0.115939	-0.01393
292	8	0	-7.00619	-1.13242	-0.69436
293	8	0	-6.83235	0.156929	1.425818
294	8	0	-7.92222	1.197123	-0.56761
295	1	0	-8.8655	0.980671	-0.42515
296	6	0	1.73028	-0.70412	-0.29307
297	6	0	2.331437	0.582338	0.322629
298	6	0	4.18614	-0.70027	-0.08173
299	1	0	1.002764	-1.21307	0.376816
300	1	0	1.161823	-0.50799	-1.22655
301	6	0	3.689574	0.748138	-0.47043
302	6	0	2.827499	0.206063	1.744224
303	1	0	3.093051	1.099373	2.329487
304	1	0	2.046258	-0.31504	2.321245
305	6	0	4.06026	-0.69438	1.468961
306	1	0	4.967035	-0.29854	1.962311
307	1	0	3.92079	-1.72079	1.854454
308	1	0	1.654568	1.448372	0.296571
309	6	0	4.578154	1.855671	0.081609
310	1	0	5.071009	1.601168	1.029043
311	1	0	5.363396	2.150841	-0.62928
312	1	0	3.972278	2.750649	0.284506
313	6	0	3.5052	0.978943	-1.96699
314	1	0	2.986081	1.930515	-2.14864
315	1	0	4.466929	1.02717	-2.49157
316	1	0	2.894117	0.206838	-2.46241
317	6	0	2.953696	-1.5566	-0.53381
318	8	0	3.020004	-2.67581	-0.97099
319	6	0	5.484714	-1.21483	-0.65643
320	1	0	5.584075	-2.29705	-0.38303
321	1	0	5.373656	-1.26305	-1.76898
322	16	0	6.896964	-0.30792	-0.21
323	8	0	7.200994	0.729982	-1.16191
324	8	0	6.972747	-0.02366	1.202332
325	8	0	8.009238	-1.5414	-0.49087
326	1	0	8.961738	-1.31066	-0.48741

11.2 $(G3)_2$@T2

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstrom) X	Y	Z
1	6	0	-2.97646	-1.46437	5.72453
2	6	0	-3.37275	-1.68027	7.04409

3	6	0	-2.39668	-1.89328	8.039243
4	6	0	-1.06954	-1.86969	7.663417
5	6	0	-0.64508	-1.6531	6.314877
6	6	0	-1.60976	-1.45471	5.331366
7	1	0	-4.42907	-1.68753	7.334707
8	1	0	-2.68829	-2.06991	9.089297
9	1	0	-1.33725	-1.30142	4.294162
10	6	0	1.299589	-1.90648	7.637806
11	6	0	2.633361	-1.97326	7.984266
12	6	0	3.593702	-1.80403	6.965541
13	6	0	3.175853	-1.58482	5.653461
14	6	0	1.801921	-1.52621	5.291967
15	6	0	0.852963	-1.67992	6.298004
16	1	0	2.942201	-2.15356	9.028605
17	1	0	4.654868	-1.85139	7.232111
18	1	0	1.514682	-1.37319	4.2567
19	6	0	0.12316	-2.05205	8.579207
20	8	0	0.131615	-2.25488	9.750863
21	7	0	4.222512	-1.39495	4.623142
22	7	0	-4.04241	-1.21087	4.727601
23	6	0	4.911093	-0.12169	4.699663
24	6	0	4.14553	1.062633	4.651134
25	6	0	6.311301	0.017657	4.792407
26	6	0	4.790201	2.308294	4.620864
27	1	0	3.054458	1.020652	4.654764
28	6	0	6.88805	1.294195	4.750418
29	1	0	6.962805	-0.85365	4.932179
30	7	0	6.150876	2.44344	4.64493
31	1	0	4.208799	3.243668	4.559895
32	1	0	7.984552	1.415575	4.807045
33	6	0	4.826491	-2.55089	4.053941
34	6	0	4.319167	-3.85234	4.314996
35	6	0	5.869882	-2.46436	3.102471
36	6	0	4.841661	-4.95814	3.644847
37	1	0	3.536565	-4.00837	5.06851
38	6	0	6.347463	-3.61745	2.469727
39	1	0	6.350643	-1.51035	2.862961
40	7	0	5.845943	-4.86492	2.711448
41	1	0	4.461188	-5.9741	3.85051
42	1	0	7.166874	-3.55595	1.731891
43	6	0	-4.69625	-2.34188	4.140768
44	6	0	-4.41385	-3.66854	4.555591
45	6	0	-5.57735	-2.20665	3.046818
46	6	0	-5.00672	-4.75146	3.901451
47	1	0	-3.74958	-3.86453	5.408029
48	6	0	-6.14361	-3.33631	2.440919
49	1	0	-5.84717	-1.22658	2.637437
50	7	0	-5.87391	-4.61219	2.844453
51	1	0	-4.79342	-5.7851	4.22563
52	1	0	-6.83532	-3.21719	1.58745
53	6	0	-4.62868	0.09692	4.7778
54	6	0	-3.79931	1.219946	5.03496
55	6	0	-5.99793	0.365438	4.555393

56	6	0	-4.33639	2.50968	5.015708
57	1	0	-2.74386	1.083554	5.292578
58	6	0	-6.4649	1.685868	4.538848
59	1	0	-6.7295	-0.44666	4.463132
60	7	0	-5.65414	2.769302	4.740726
61	1	0	-3.70718	3.388972	5.235798
62	1	0	-7.53618	1.900717	4.369319
63	6	0	-2.76719	5.736977	-1.63917
64	6	0	-3.14611	7.003608	-2.08346
65	6	0	-2.15701	7.949698	-2.4207
66	6	0	-0.83454	7.577328	-2.29708
67	6	0	-0.42681	6.283121	-1.84488
68	6	0	-1.40478	5.350587	-1.50864
69	1	0	-4.19906	7.290319	-2.17744
70	1	0	-2.43445	8.958662	-2.77247
71	1	0	-1.1469	4.36008	-1.15384
72	6	0	1.533436	7.527872	-2.30436
73	6	0	2.870455	7.841248	-2.4367
74	6	0	3.820627	6.849174	-2.11696
75	6	0	3.389847	5.598669	-1.67653
76	6	0	2.011814	5.278675	-1.52915
77	6	0	1.071793	6.25188	-1.85126
78	1	0	3.189799	8.838691	-2.78588
79	1	0	4.884614	7.08652	-2.22582
80	1	0	1.716418	4.293095	-1.16781
81	6	0	0.368015	8.443328	-2.60967
82	8	0	0.389019	9.565989	-3.0012
83	7	0	4.421345	4.57735	-1.39026
84	7	0	-3.8552	4.786456	-1.30959
85	6	0	5.026864	3.990728	-2.5588
86	6	0	4.194012	3.54614	-3.61392
87	6	0	6.417033	3.803119	-2.71633
88	6	0	4.754462	2.882672	-4.71021
89	1	0	3.11902	3.742063	-3.59474
90	6	0	6.906473	3.112281	-3.83094
91	1	0	7.134107	4.215741	-1.99659
92	7	0	6.094651	2.626892	-4.82033
93	1	0	4.125096	2.538879	-5.54763
94	1	0	7.99089	2.939778	-3.95476
95	6	0	5.089875	4.615438	-0.12637
96	6	0	4.759766	5.57791	0.859777
97	6	0	6.02938	3.624923	0.244792
98	6	0	5.345736	5.512092	2.127323
99	1	0	4.060486	6.394201	0.641642
100	6	0	6.591847	3.633923	1.524669
101	1	0	6.316514	2.819819	-0.44577
102	7	0	6.261382	4.554274	2.481527
103	1	0	5.086335	6.25279	2.903181
104	1	0	7.338232	2.877955	1.816013
105	6	0	-4.46684	4.892274	-0.02611
106	6	0	-3.87078	5.6611	1.011034
107	6	0	-5.61828	4.157972	0.334771
108	6	0	-4.41641	5.657035	2.295448

109	1	0	-2.99814	6.293728	0.807151
110	6	0	-6.12885	4.219277	1.636055
111	1	0	-6.18447	3.555873	-0.38319
112	7	0	-5.53577	4.935336	2.636197
113	1	0	-3.96239	6.259046	3.101087
114	1	0	-7.06362	3.675326	1.886826
115	6	0	-4.54596	4.244519	-2.45947
116	6	0	-3.78425	3.625899	-3.47975
117	6	0	-5.94561	4.249422	-2.625
118	6	0	-4.43263	2.983972	-4.5417
119	1	0	-2.69226	3.670353	-3.45878
120	6	0	-6.52896	3.566103	-3.70118
121	1	0	-6.60117	4.811757	-1.94519
122	7	0	-5.79577	2.908622	-4.6502
123	1	0	-3.85626	2.507905	-5.35181
124	1	0	-7.62841	3.540322	-3.81911
125	6	0	-3.21848	-4.22383	-4.13788
126	6	0	-3.63764	-5.21286	-5.02653
127	6	0	-2.67855	-5.97076	-5.72985
128	6	0	-1.34492	-5.70262	-5.50135
129	6	0	-0.89743	-4.69082	-4.59446
130	6	0	-1.84425	-3.93733	-3.90801
131	1	0	-4.69957	-5.42248	-5.19534
132	1	0	-2.98845	-6.75705	-6.43977
133	1	0	-1.55363	-3.15223	-3.21989
134	6	0	1.024052	-5.72295	-5.50713
135	6	0	2.351719	-6.01505	-5.74276
136	6	0	3.327278	-5.27018	-5.05007
137	6	0	2.931252	-4.26789	-4.16402
138	6	0	1.564461	-3.96063	-3.92324
139	6	0	0.600221	-4.70241	-4.59971
140	1	0	2.64259	-6.80952	-6.45116
141	1	0	4.383758	-5.49803	-5.22514
142	1	0	1.293113	-3.16889	-3.2352
143	6	0	-0.16834	-6.40964	-6.13897
144	8	0	-0.17705	-7.29046	-6.93812
145	7	0	3.996432	-3.53114	-3.44808
146	7	0	-4.26226	-3.47921	-3.4002
147	6	0	4.627157	-4.27377	-2.3833
148	6	0	3.813672	-4.92938	-1.42876
149	6	0	6.024687	-4.38781	-2.2249
150	6	0	4.407033	-5.59916	-0.35351
151	1	0	2.726805	-4.94011	-1.54105
152	6	0	6.548491	-5.05333	-1.10969
153	1	0	6.7199	-3.98331	-2.96969
154	7	0	5.761547	-5.64867	-0.16127
155	1	0	3.792825	-6.13161	0.390413
156	1	0	7.640563	-5.12798	-0.96148
157	6	0	4.671105	-2.47932	-4.1364
158	6	0	4.318343	-2.10438	-5.45817
159	6	0	5.657758	-1.68944	-3.49991
160	6	0	4.952591	-1.02315	-6.07383
161	1	0	3.568137	-2.67126	-6.02416

162	6	0	6.260137	-0.62892	-4.18165
163	1	0	5.97529	-1.90102	-2.46892
164	7	0	5.925698	-0.27482	-5.46039
165	1	0	4.689101	-0.73144	-7.10557
166	1	0	7.048546	-0.02696	-3.69888
167	6	0	-4.89538	-2.37707	-4.04799
168	6	0	-4.51409	-1.96748	-5.35304
169	6	0	-5.84705	-1.56537	-3.38997
170	6	0	-5.0744	-0.82334	-5.92234
171	1	0	-3.79964	-2.55708	-5.94154
172	6	0	-6.38636	-0.44342	-4.03042
173	1	0	-6.18791	-1.77452	-2.36713
174	7	0	-6.0066	-0.04358	-5.28135
175	1	0	-4.78479	-0.50201	-6.93793
176	1	0	-7.15263	0.169583	-3.51565
177	6	0	-4.8879	-4.21452	-2.32846
178	6	0	-4.07048	-4.93391	-1.42331
179	6	0	-6.28049	-4.24521	-2.1028
180	6	0	-4.64697	-5.55049	-0.30791
181	1	0	-2.99596	-5.02804	-1.59704
182	6	0	-6.78554	-4.8697	-0.95587
183	1	0	-6.98585	-3.81043	-2.82084
184	7	0	-5.98849	-5.50015	-0.03866
185	1	0	-4.03034	-6.11635	0.409121
186	1	0	-7.87121	-4.87933	-0.75389
187	6	0	8.402744	-8.74109	1.427889
188	6	0	7.854024	-8.76283	2.853814
189	1	0	9.347439	-8.14238	1.353969
190	1	0	8.713622	-9.78353	1.125465
191	1	0	6.934195	-9.39731	2.936425
192	1	0	8.598388	-9.26574	3.53783
193	7	0	7.357322	-8.15836	0.513525
194	1	0	6.620511	-8.85795	0.333355
195	7	0	7.53952	-7.35144	3.27546
196	1	0	8.412313	-6.85658	3.516796
197	46	0	6.617957	-6.51203	1.584887
198	1	0	6.976594	-7.36375	4.135552
199	1	0	7.775243	-7.94865	-0.40226
200	6	0	-8.80068	1.640666	-8.18195
201	6	0	-8.05852	2.956356	-8.41095
202	1	0	-9.67843	1.770181	-7.49658
203	1	0	-9.25954	1.289303	-9.15182
204	1	0	-7.20172	2.83413	-9.12287
205	1	0	-8.74189	3.692374	-8.92677
206	7	0	-7.84124	0.637647	-7.5971
207	1	0	-7.23164	0.263377	-8.33885
208	7	0	-7.55183	3.464275	-7.08626
209	1	0	-8.32646	3.896717	-6.56148
210	46	0	-6.79124	1.738441	-6.15636
211	1	0	-6.86342	4.213245	-7.2433
212	1	0	-8.36363	-0.16716	-7.22441
213	6	0	8.17362	1.216674	-8.92104
214	6	0	8.807449	2.424154	-8.23168

215	1	0	7.28689	1.509326	-9.54053
216	1	0	8.900997	0.782389	-9.66716
217	1	0	9.719704	2.138723	-7.64646
218	1	0	9.194477	3.144882	-9.0099
219	7	0	7.754918	0.221217	-7.87092
220	1	0	8.583126	-0.28331	-7.51805
221	7	0	7.789266	3.050283	-7.31557
222	1	0	7.107725	3.593192	-7.86867
223	46	0	6.883562	1.407816	-6.37199
224	1	0	8.250827	3.728456	-6.69559
225	1	0	7.14931	-0.49376	-8.29311
226	6	0	8.484939	6.550008	5.653243
227	6	0	8.989625	5.293145	6.360629
228	1	0	7.605349	7.000403	6.181575
229	1	0	9.276345	7.354064	5.69988
230	1	0	9.895178	4.866708	5.856468
231	1	0	9.351207	5.560964	7.396007
232	7	0	8.103507	6.193548	4.240575
233	1	0	8.953257	6.092381	3.663621
234	7	0	7.885885	4.268235	6.376537
235	1	0	7.181368	4.525088	7.085714
236	46	0	7.089229	4.367176	4.430898
237	1	0	8.262615	3.35938	6.673723
238	1	0	7.568169	6.963942	3.820293
239	6	0	-8.13577	-8.77211	1.890885
240	6	0	-8.74186	-7.93286	3.014576
241	1	0	-7.26254	-9.37793	2.246517
242	1	0	-8.88434	-9.54482	1.547961
243	1	0	-9.63572	-7.35283	2.666696
244	1	0	-9.15046	-8.61265	3.817793
245	7	0	-7.70096	-7.85343	0.779444
246	1	0	-8.51991	-7.56918	0.221793
247	7	0	-7.69138	-6.98551	3.53307
248	1	0	-7.03046	-7.49654	4.136257
249	46	0	-6.80245	-6.24277	1.77839
250	1	0	-8.13232	-6.27506	4.132762
251	1	0	-7.07941	-8.3593	0.133261
252	6	0	-7.6344	6.114304	6.79735
253	6	0	-8.22661	6.764687	5.548217
254	1	0	-6.71852	6.65266	7.154122
255	1	0	-8.36164	6.21056	7.655877
256	1	0	-9.16623	6.251445	5.215234
257	1	0	-8.56008	7.816462	5.788851
258	7	0	-7.29347	4.680912	6.483033
259	1	0	-8.15171	4.109586	6.490343
260	7	0	-7.2023	6.719136	4.444977
261	1	0	-6.49182	7.450606	4.595735
262	46	0	-6.41094	4.787701	4.581297
263	1	0	-7.6502	6.938222	3.544369
264	1	0	-6.69178	4.297026	7.224355
265	6	0	-2.74443	-1.70654	-0.76841
266	6	0	-2.0684	-0.31352	-0.74601
267	6	0	-4.19365	0.140357	-0.01554

268	1	0	-2.76313	-2.16282	-1.77762
269	1	0	-2.23756	-2.44497	-0.12551
270	6	0	-2.7159	0.370306	0.523113
271	6	0	-2.67965	0.503101	-1.91272
272	1	0	-2.11611	1.430934	-2.09891
273	1	0	-2.67114	-0.05886	-2.86039
274	6	0	-4.12255	0.795783	-1.42633
275	1	0	-4.31431	1.879349	-1.36755
276	1	0	-4.88293	0.380135	-2.11187
277	1	0	-0.96753	-0.36184	-0.74472
278	6	0	-2.33648	1.839654	0.689849
279	1	0	-2.76357	2.492716	-0.08228
280	1	0	-2.66682	2.241962	1.654043
281	1	0	-1.24221	1.966227	0.642706
282	6	0	-2.40133	-0.36133	1.825298
283	1	0	-1.30843	-0.42257	1.980601
284	1	0	-2.81765	0.163786	2.694887
285	1	0	-2.78827	-1.38454	1.872803
286	6	0	-4.14728	-1.39449	-0.27161
287	8	0	-5.03915	-2.17571	-0.06712
288	6	0	-5.31745	0.584218	0.883749
289	1	0	-5.34069	-0.08367	1.790315
290	1	0	-5.05867	1.583271	1.311137
291	16	0	-6.90837	0.651108	0.143022
292	8	0	-7.46174	1.941486	0.456318
293	8	0	-6.92971	0.182009	-1.2175
294	8	0	-7.6806	-0.45822	1.120237
295	1	0	-8.66563	-0.49149	1.086997
296	6	0	1.758835	2.556382	0.820777
297	6	0	1.162527	1.444551	-0.0782
298	6	0	3.251021	0.631569	0.414347
299	1	0	1.852589	3.532267	0.292708
300	1	0	1.150754	2.774498	1.714533
301	6	0	1.751325	0.120431	0.553088
302	6	0	1.904308	1.525657	-1.43449
303	1	0	1.419617	0.905747	-2.20452
304	1	0	1.923521	2.555784	-1.83494
305	6	0	3.328012	1.015462	-1.09279
306	1	0	3.601366	0.154565	-1.72388
307	1	0	4.096615	1.790232	-1.28237
308	1	0	0.063561	1.480943	-0.1474
309	6	0	1.444595	-1.13619	-0.25656
310	1	0	1.972388	-1.17562	-1.21686
311	1	0	1.71507	-2.05016	0.284934
312	1	0	0.36608	-1.19784	-0.48243
313	6	0	1.298816	-0.10697	1.993827
314	1	0	0.212778	-0.3154	2.030787
315	1	0	1.808038	-0.96472	2.456794
316	1	0	1.47248	0.747431	2.656861
317	6	0	3.117717	1.984968	1.181119
318	8	0	3.912909	2.428708	1.967092
319	6	0	4.330833	-0.26316	0.97901
320	1	0	4.523472	0.051014	2.044161

321	1	0	3.916608	-1.29449	1.111872
322	16	0	5.823268	-0.33109	0.088972
323	8	0	6.054689	-1.67783	-0.37451
324	8	0	6.052613	0.755119	-0.82822
325	8	0	6.889952	-0.08884	1.365408
326	1	0	7.848623	-0.11757	1.166072

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