Supporting Information

Transformation of a Pd_6 trifacial barrel to a Pd_8 tetrafacial barrel by C_{70} as guest and oxidative photolysis of alkenes using the C_{70} encapsulated barrel under red light

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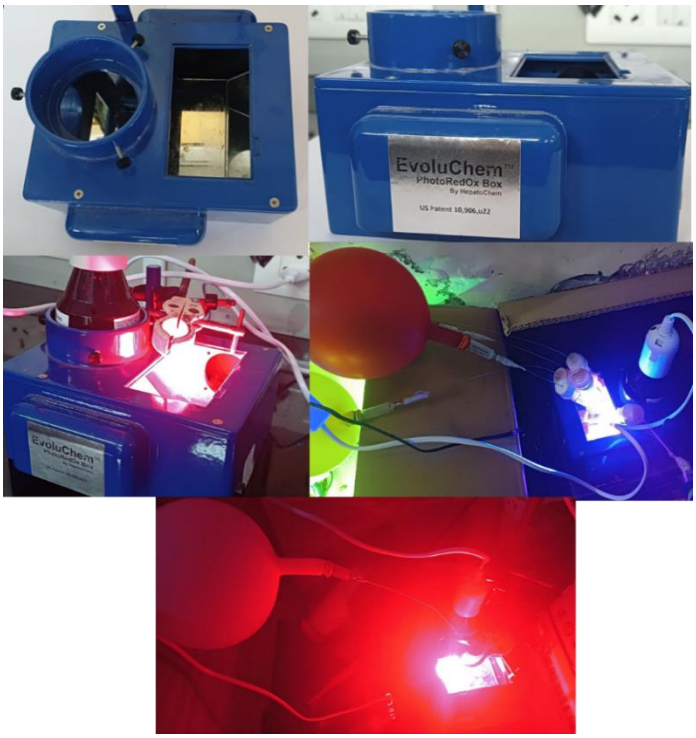
1. Materials and methods

All the chemicals were purchased from commercially available sources and used without further purification. NMR spectra were recorded on Bruker 400 MHz and 500 MHz NMR spectrometers in DMSO-d_6 and $CDCl_3$. Electron-spray ionization mass spectra (ESI-MS) were recorded using Agilent 6538 Ultra-High Definition (UHD) Accurate Mass Q-TOF spectrometer using standard spectroscopic grade solvents. Electronic absorption spectra were recorded using a LAMBDA 750 UV/Vis spectrophotometer. Emission spectra were recorded using a HORIBA JOBIN YVON made Fluoromax-4 spectrometer.

2. Experimental setup

The photochemical reactions were conducted with 18 W blue LED (390 nm) and red LED (650 nm). The reaction tube was kept inside the *EvoluChem* photoreactor while stirring for 24 h. The room temperature was maintained by cooling with the fans located inside the reactor.



Description of reaction tube: Fisher brand Disposable Borosilicate Glass Tubes (16 ×125 mm) with Threaded End (Fisher Scientific); Kimble Black Phenolic Screw Thread Closures with Open Tops (Fisher Scientific); Thermo Scientific National PTFE/Silicone Septa for Sample Screw Thread Caps (Fisher Scientific).

3. Synthesis and characterization of compounds

3.1 Synthesis of ligand L

4,4'-(9-oxo-9H-fluorene-2,7-diyl)dibenzaldehyde (**P**) was prepared by Suzuki coupling reaction of 2,7-dibromo-9H-fluoren-9-one with (4-formylphenyl)boronic acid following a reported procedure.[S1] ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 10.08 (s, 2H), 8.03 – 7.97 (m, 6H), 7.86 – 7.77 (m, 6H), 7.70 (d, *J* = 7.8 Hz, 2H) ppm. To a 20 mL ethanol solution of 4-acetylpyridine (0.97 g, 0.008 mol), potassium hydroxide (0.224 g, 0.004 mol) was added after grinding. After 10 minutes, 4,4'-(9-oxo-9H-fluorene-2,7-diyl)dibenzaldehyde (0.38 g, 0.001 mol) was added and the reaction mixture was stirred for 12 h. The solution was cooled down to 0 ºC and 20 mL concentrated ammonia was added to the reaction mixture and heated at 65 ºC for 24 h. After cooling down the solution to room temperature, it was filtered, and the precipitate was washed thoroughly with ethanol and methanol. After drying, the precipitate was washed thoroughly with dichloromethane and then dried in vacuum to obtain pure **L**. Yield: (254 mg, ~32%). ^{1}H-NMR (400 MHz, DMSO-*d*$_6$, 10 µL CF_3COOH): δ = 9.11 (d, 8H), 8.98 (d, 8H), 8.86 (s, 4H), 8.27 (d, 4H), 8.00 – 7.90 (m, 10H) ppm. ^{13}C-NMR (125 MHz, DMSO-*d*$_6$): δ = 192.54, 151.76, 150.20, 143.62, 142.95, 140.32, 139.96, 134.81, 134.49, 133.56, 128.13, 127.02, 124.12, 123.82, 121.99, 121.83, 121.58 ppm. ESI-MS (MeOH-$CHCl_3$) m/z = 795.3428 ($[M+H]^+$).

3.2 Synthesis of trifacial barrel M1

To a 0.5 mL dimethyl sulfoxide solution of *cis*-[(tmeda)Pd(ONO_2)$_2$] (8.7 mg, 0.0252 mmol) taken in a 4 mL glass vial, solid **L** (10.0 mg, 0.0126 mmol) was added, and the mixture was stirred at 70 ºC for 24 h. A clear yellowish-red solution was obtained and the addition of 10 mL ethyl acetate to it afforded a yellow precipitate. The precipitate was washed thoroughly with diethyl ether and dried in vacuum. Yield: 16.4 mg (~88%). ^{1}H-NMR (400 MHz, DMSO-*d*$_6$): δ = 9.49 (d, *J* = 6.3 Hz, 4H), 9.37 (d, *J* = 5.9 Hz, 4H), 8.87 (d, *J* = 6.4 Hz, 4H), 8.74 (d, *J* = 6.0 Hz, 4H), 8.68 (s, 4H), 8.10 (d, *J* = 7.9 Hz, 4H), 8.06 (d, *J* = 7.5 Hz, 2H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.93 – 7.87 (m, 6H), 3.10 (s, 8H), 2.73 (s, 24H) ppm. ^{13}C-NMR (125 MHz, DMSO-*d*$_6$): δ = 151.60, 151.05, 150.48, 147.30, 142.98, 140.46, 135.57, 134.42, 133.90, 128.23, 127.24, 123.75, 122.24, 122.10, 120.64 ppm. ESI-MS (CH_3CN) m/z = 1219.9336 [**M1**-4PF_6]$^{4+}$(calc. 1219.9440), 946.9544 [**M1**-5PF_6]$^{5+}$(calc. 946.9620), and 764.9654 [**M1**-6PF_6]$^{6+}$(calc. 764.9740).

3.3 Synthesis of $(C_{70})_3$@M2

To a 0.5 mL dimethyl sulfoxide solution of **M1** (10 mg, 0.0022 mmol), 4 equivalents of C_{70} (7.4 mg, 0.0088 mmol) was added and the mixture was stirred at 70 ºC for 12 h. The reaction mixture was centrifuged, and the clear dark-brown solution was decanted. Dark-brown precipitate was obtained by treating the solution with 10 mL of ethyl acetate. The solid obtained was thoroughly washed with diethyl ether and dried in vacuum. Yield: 9.2 mg (~65%). ^{1}H-NMR (500 MHz, DMSO-*d*$_6$): δ = 9.54 (s, 4H), 9.46 (d, *J* = 6.0 Hz, 4H), 8.63 (d, *J* = 6.3 Hz, 4H), 8.58 (s, 4H), 8.42 (s, 4H), 7.98 (m, 12H), 7.92 (d, *J* = 7.2 Hz, 2H), 3.08 (s, 8H) 2.79 (s, 24H) ppm. ^{13}C-NMR (125 MHz, DMSO-*d*$_6$): δ = 152.82, 151.70, 149.04, 146.29, 145.62, 143.40, 140.47, 134.43, 128.81, 128.39, 127.26, 121.98 ppm. ESI-MS (CH_3CN) m/z = 1815.3732 [$(C_{70})_3$@ **M2**-5PF_6]$^{5+}$(calc. 1815.4040), 1488.6732 [$(C_{70})_3$@**M2**-6PF_6]$^{6+}$(calc.

1488.6780), 1255.2926 $[(C_{70})_3$@**M2**-$7PF_6]^{7+}$(calc. 1255.3020), and 1080.2664 $[(C_{70})_3$@**M2**-$8PF_6]^{8+}$(calc. 1080.2620).

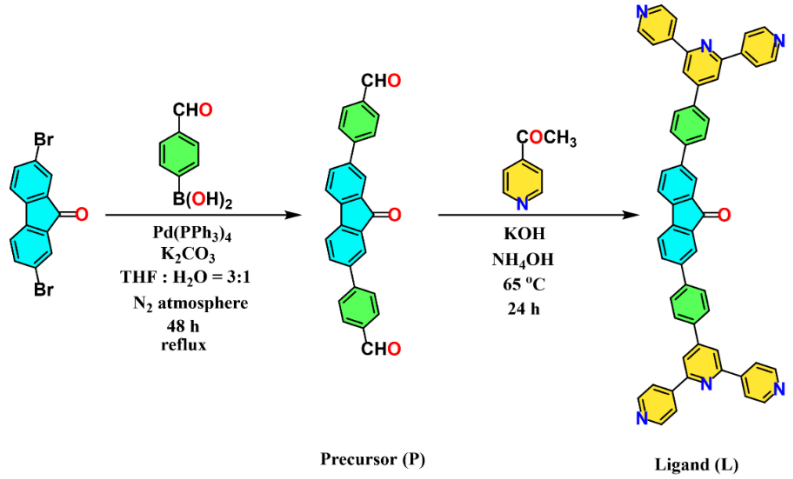
3.4 Synthesis of $(C_{60})_3$@M2

To a 0.5 mL dimethyl sulfoxide solution of **M1** (10 mg, 0.0022 mmol), 4 equivalents of C_{60} (6.3 mg, 0.0088 mmol) were added and the mixture was stirred at 70 ºC for 12 h. The reaction mixture was centrifuged, and clear brown solution was decanted. Brown precipitate was obtained by treating the brown solution with 10 mL of ethyl acetate. The solid obtained was thoroughly washed with diethyl ether and dried in vacuum. Yield: 9.8 mg. Presence of both the free trifacial barrel (**M1**) and **$(C_{60})_3$@M2** was detected in the product from ESI-MS and NMR analyses. ^{1}H-NMR (500 MHz, DMSO-d_6): δ = 9.55 (s), 9.49 (d, *J* = 6.1 Hz), 9.44 (s), 9.37 (d, *J* = 5.9 Hz), 8.87 (d, *J* = 6.4 Hz), 8.73 (d, *J* = 5.8 Hz), 8.69 (s), 8.60 (s), 8.47 (s), 8.11 (d, *J* = 7.9 Hz), 8.06 (d, *J* = 7.5 Hz), 8.03 – 7.97 (m), 7.98 – 7.84 (m), 3.09 (s), 2.80 (s) ppm. ^{13}C-NMR (125 MHz, DMSO-d_6): δ = 151.67, 151.09, 150.58, 147.35, 143.06, 141.31, 140.48, 135.64, 134.45, 133.95, 129.36, 128.25, 127.26, 123.76, 122.11 ppm. ESI-MS (CH_3CN) m/z = 1743.3881 $[(C_{60})_3$@**M2**-$5PF_6]^{5+}$(calc. 1743.4040), 1428.6888 $[(C_{60})_3$@**M2**-$6PF_6]^{6+}$(calc. 1428.6780), 1203.8889 $[(C_{60})_3$@**M2**-$7PF_6]^{7+}$(calc. 1203.8760), 1219.9545 [**M1**-$4PF_6]^{4+}$(calc. 1219.9440), and 946.9792 [**M1**-$5PF_6]^{5+}$(calc. 946.9620).

4. Optimization methods

All theoretical calculations were performed using Gaussian 09 package.[S2] DFT optimizations and single-point energy calculations of trifacial barrel **M1** and trifacial tube were carried out using the hybrid B3LYP functional with a mixed basis set of LanL2DZ (for Pd atom) and 3-21G (for C, H, N and O atoms). The geometries of tetrafacial barrel **M2**, tetrafacial tube, **$(C_{70})_3$@M2**, **$(C_{60})_3$@M2**, and $(C_{70})_3$@Tetrafacial tube were optimized using PM6 semi-empirical method. No symmetry constraints were used during optimization.

5. Schemes and figures



Scheme S1 Schematic representation for the synthesis of ligand **L**.

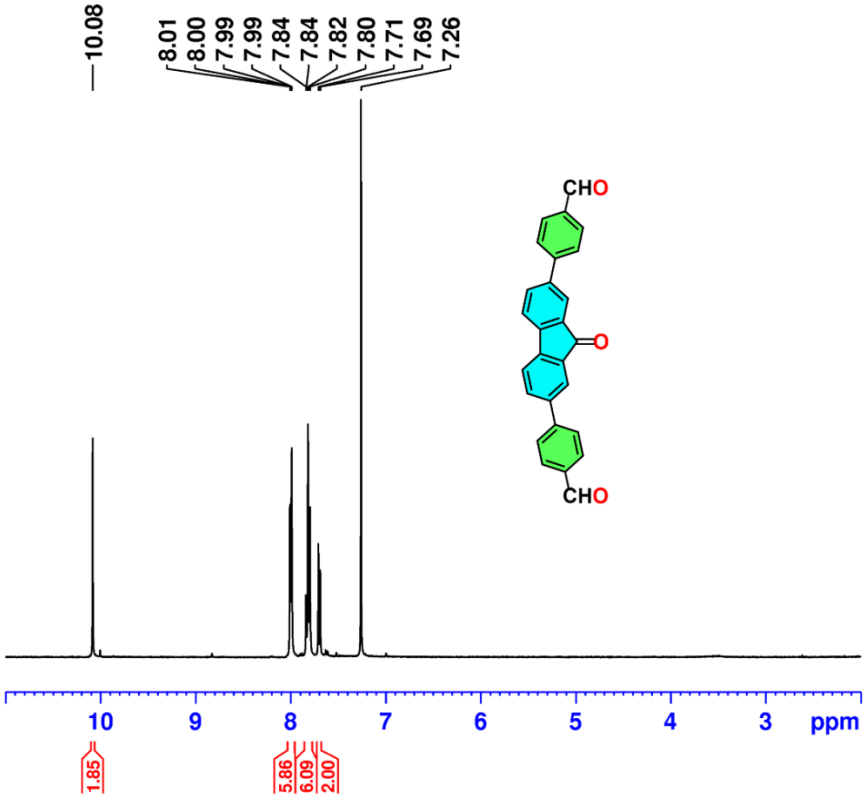


Fig. S1 ^{1}H-NMR spectrum of aldehyde **P** ($CDCl_3$, 298 K).

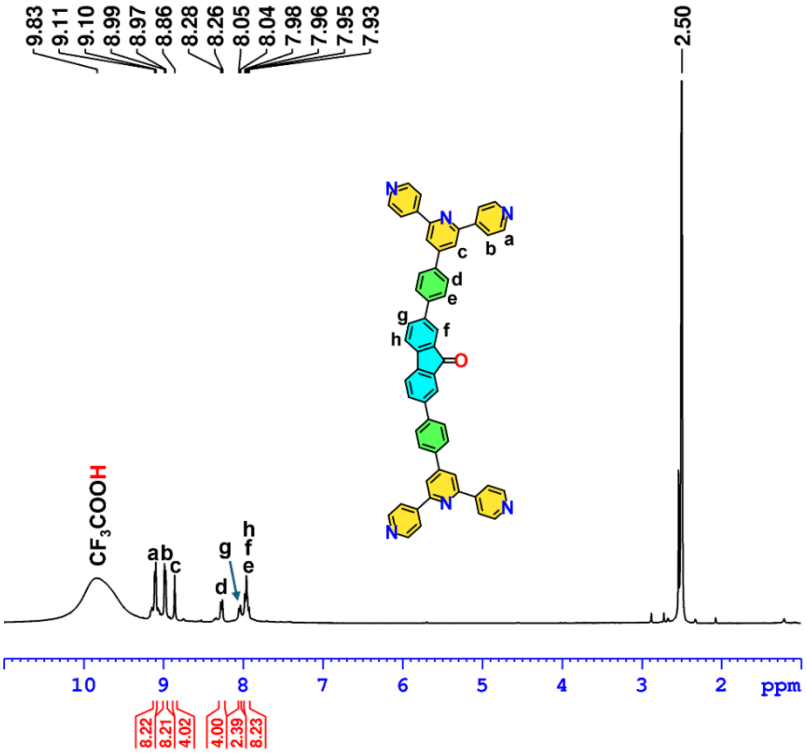


Fig. S2 ^{1}H-NMR spectrum of ligand **L** (DMSO-d_6, 10 μL CF_3COOH, 298 K).

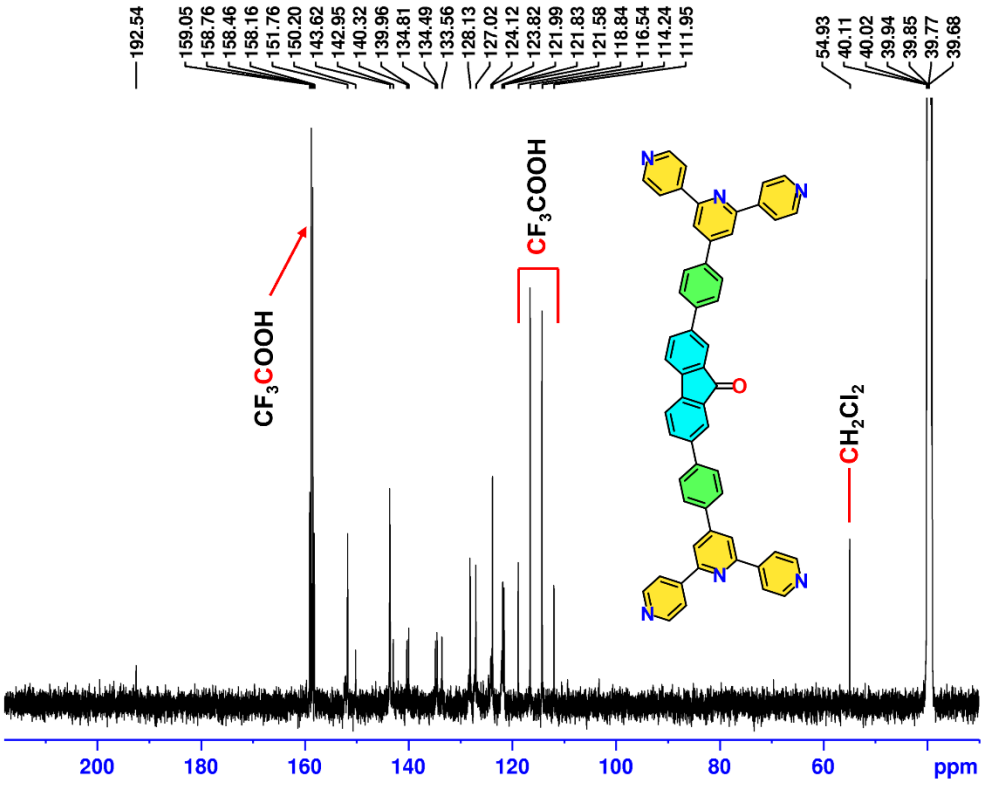


Fig. S3 ^{13}C-NMR spectrum of ligand **L** (DMSO-d_6, 10 μL CF_3COOH, 298 K).

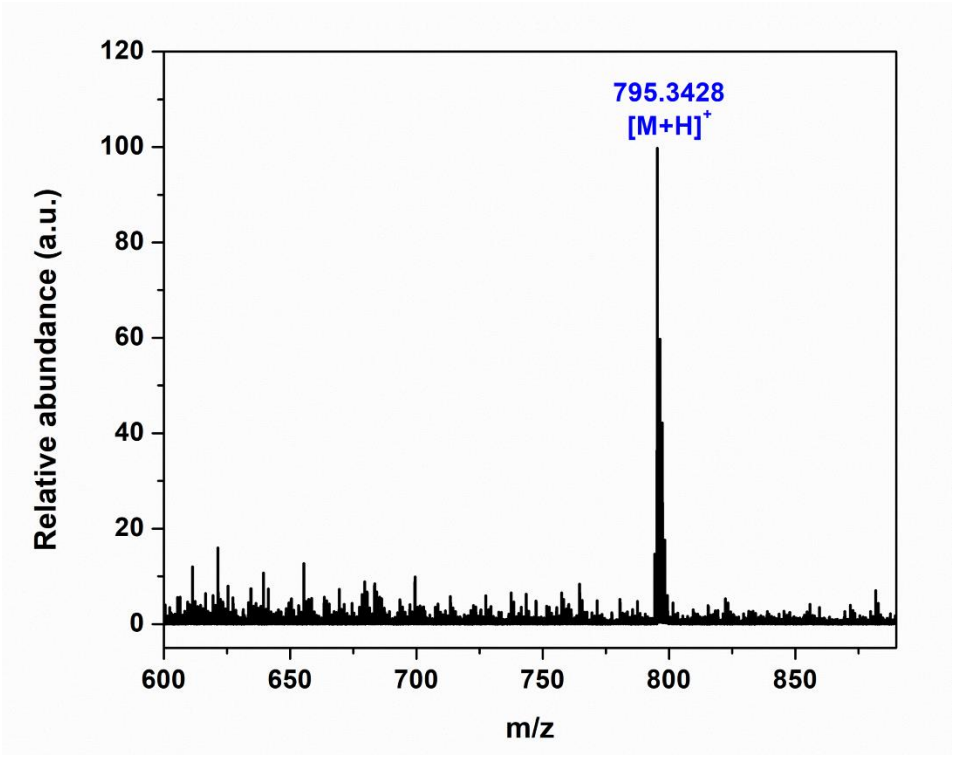


Fig. S4 ESI-MS spectrum of ligand **L** in MeOH-$CHCl_3$ mixture.

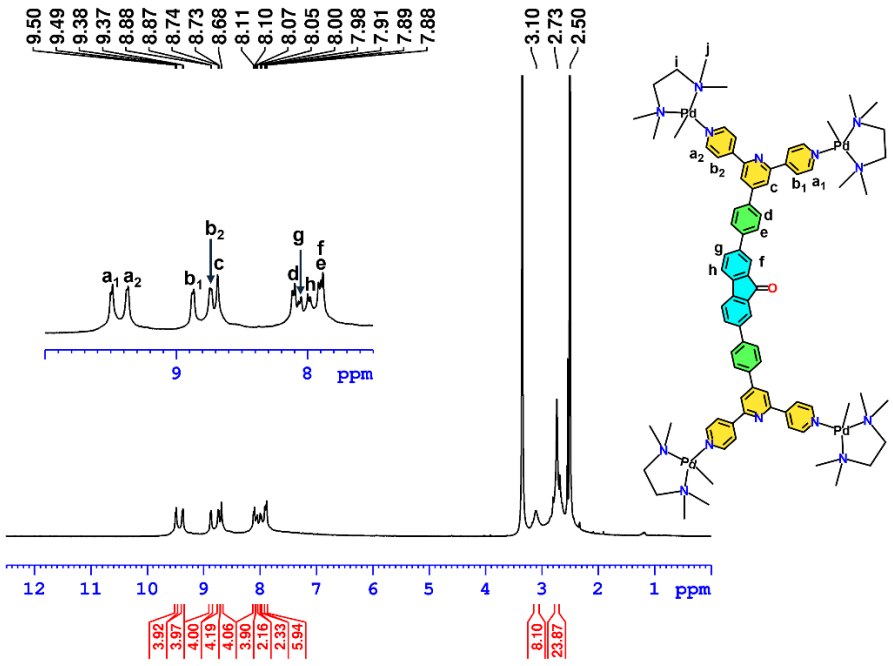


Fig. S5 ^{1}H-NMR spectrum of **M1** (DMSO-d_6, 298 K). Inset: Expanded aromatic region.

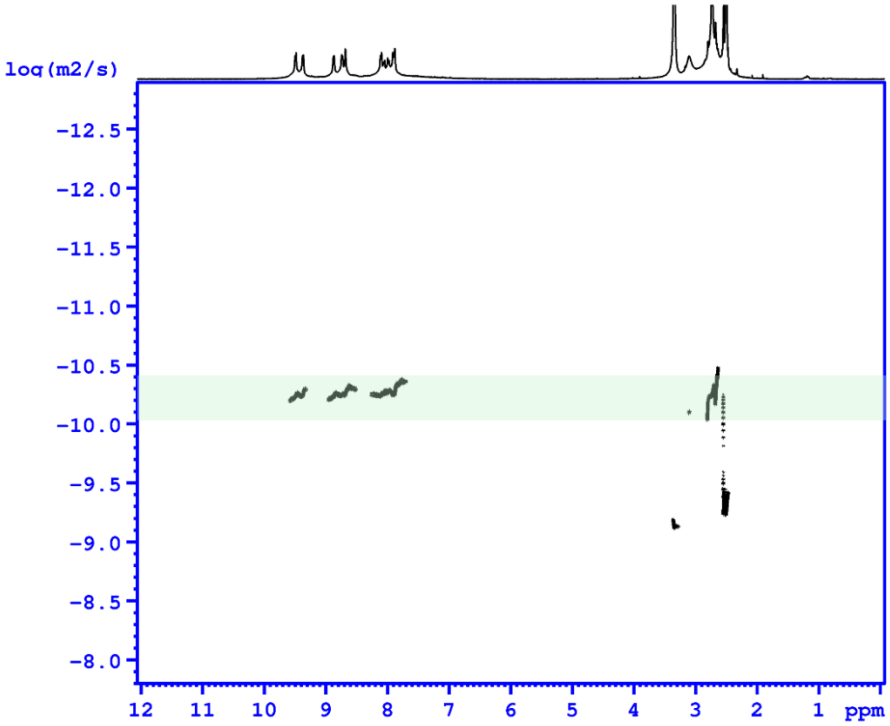


Fig. S6 ^{1}H DOSY NMR spectrum of **M1** (DMSO-d_6, 298 K).

Diffusion coefficient (D) = 5.37×10^{-11} m^2/s; Solvodynamic radius = 20.4 Å.

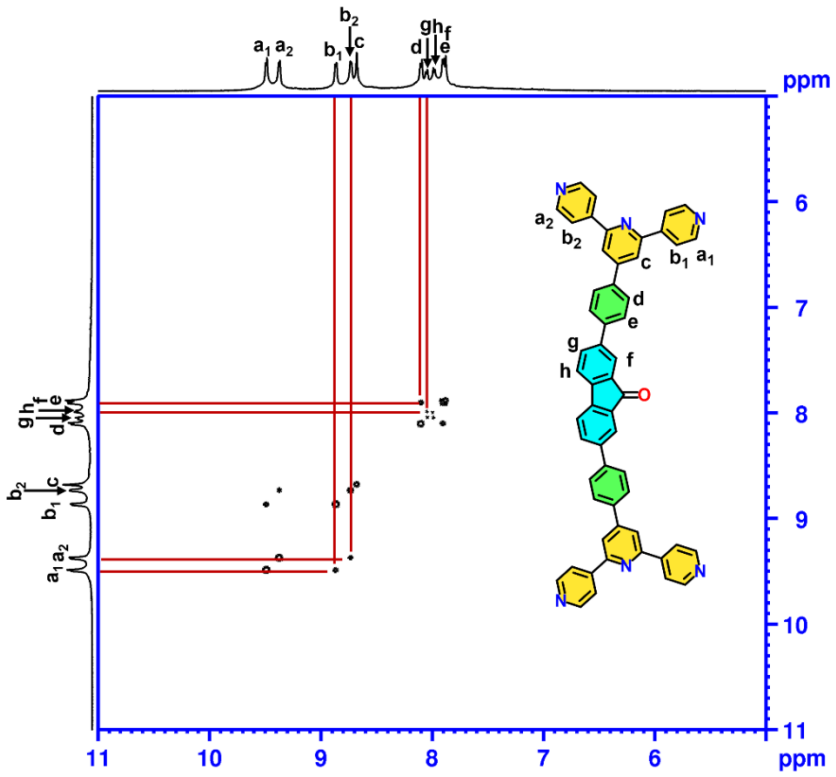


Fig. S7 ^{1}H-^{1}H COSY NMR spectrum of **M1** (DMSO-d_6, 298 K).

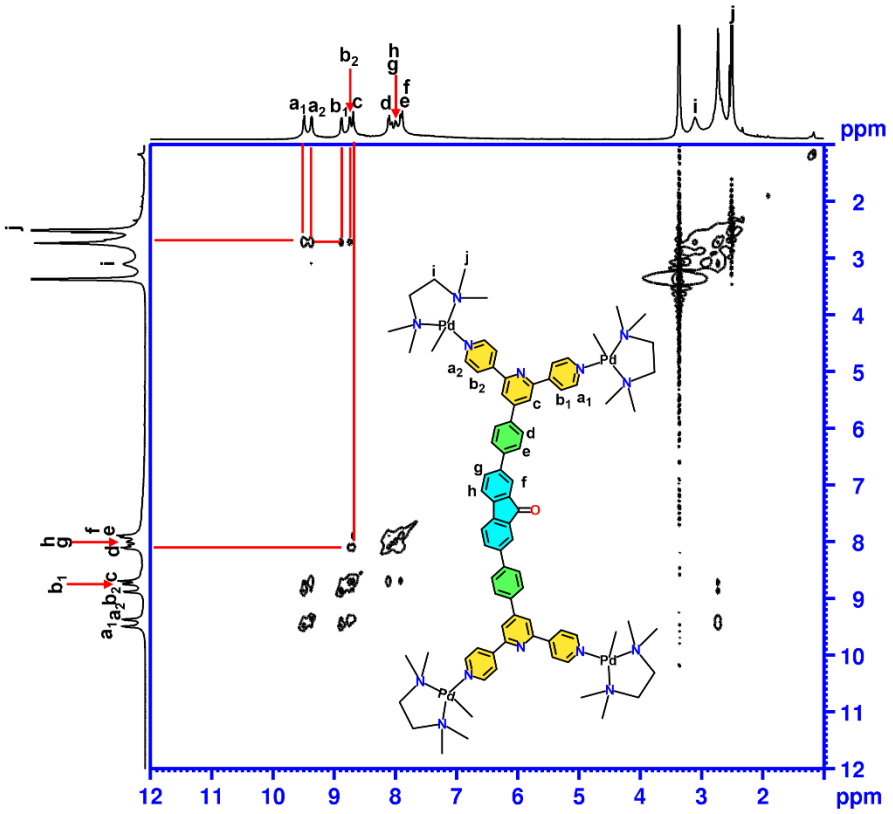
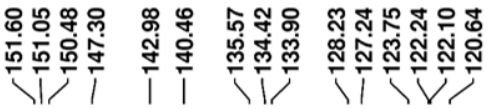


Fig. S8 ^{1}H-^{1}H NOESY NMR spectrum of **M1** (DMSO-d_6, 298 K).



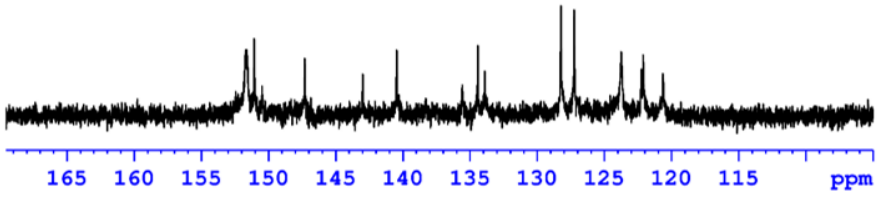


Fig. S9 ^{13}C-NMR spectrum of **M1** (DMSO-d_6, 298 K).

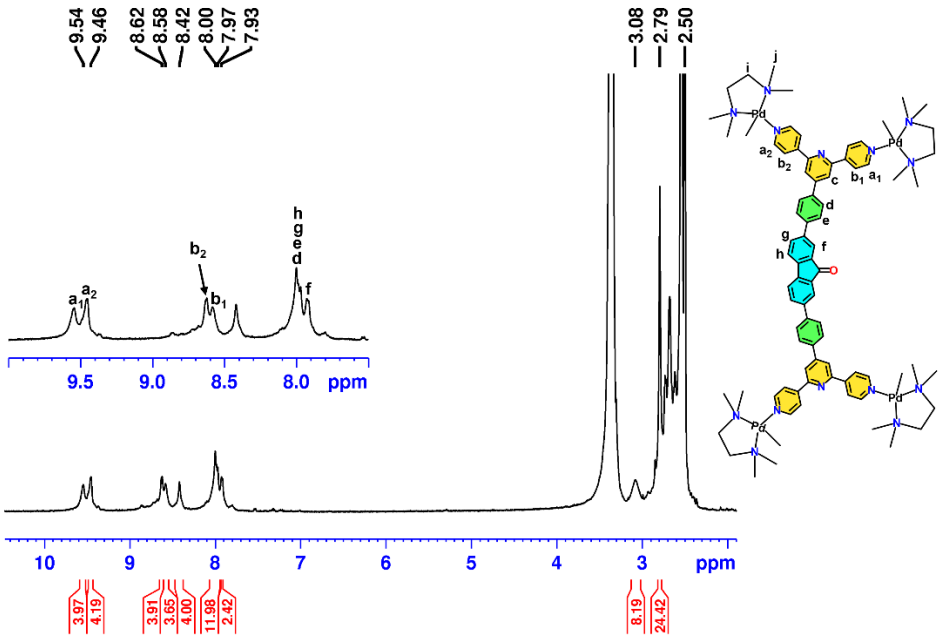


Fig. S10 ^{1}H-NMR spectrum of **(C$_{70}$)$_3$@M2** (DMSO-*d*$_6$, 298 K). Inset: Expanded aromatic region.

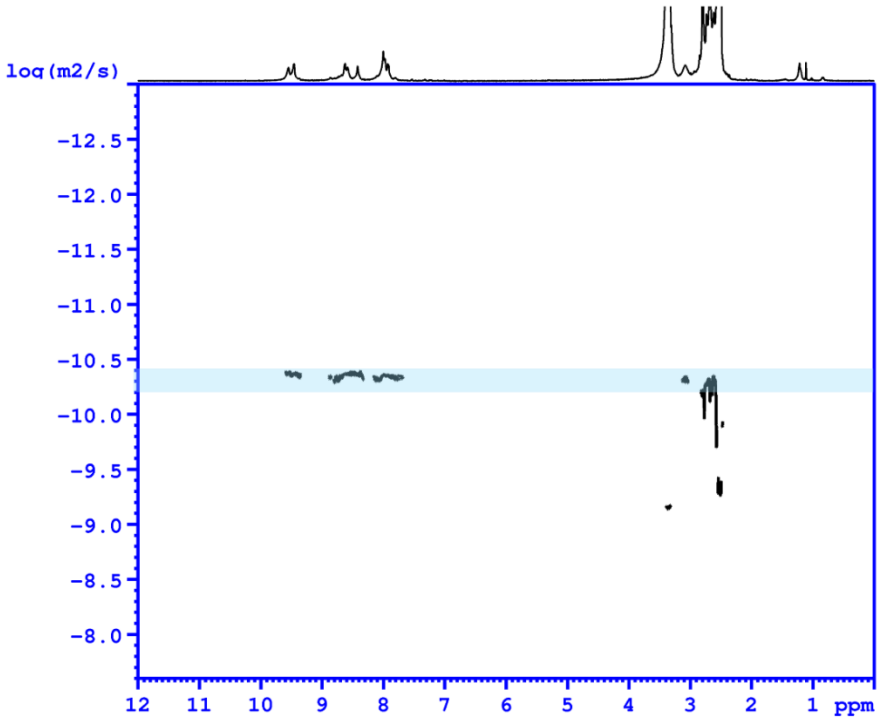


Fig. S11 ^{1}H DOSY NMR spectrum of **(C$_{70}$)$_3$@M2** (DMSO-*d*$_6$, 298 K).

Diffusion Coefficient (D) = 4.37 × 10^{-11} m^2/s; Solvodynamic radius = 25.1 Å.

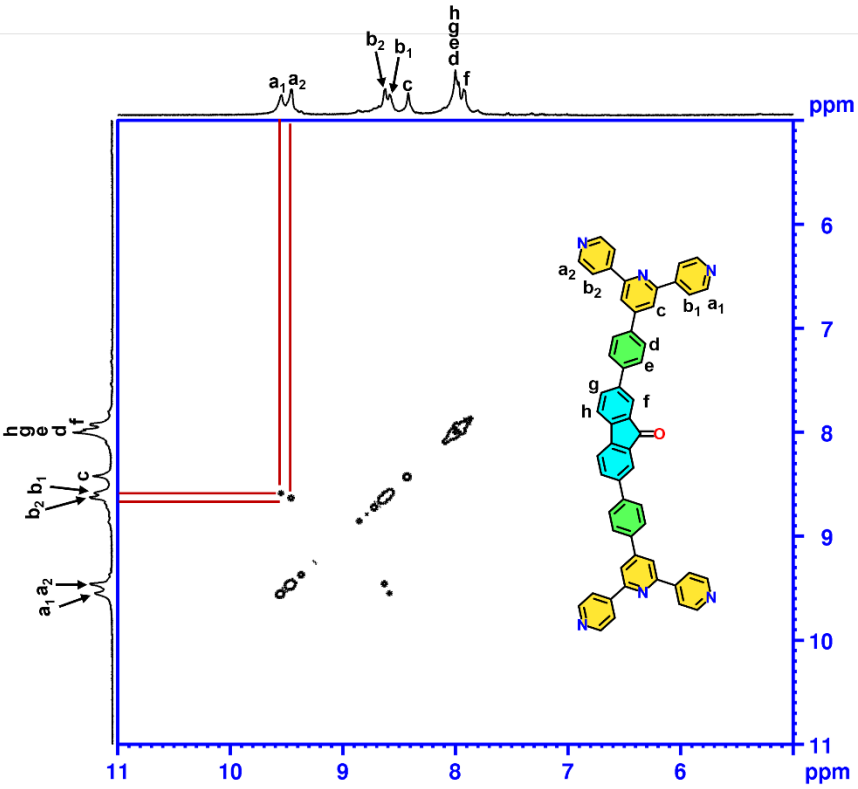


Fig. S12 ^{1}H-^{1}H COSY NMR spectrum of **$(C_{70})_3$@M2** (DMSO-d_6, 298 K).

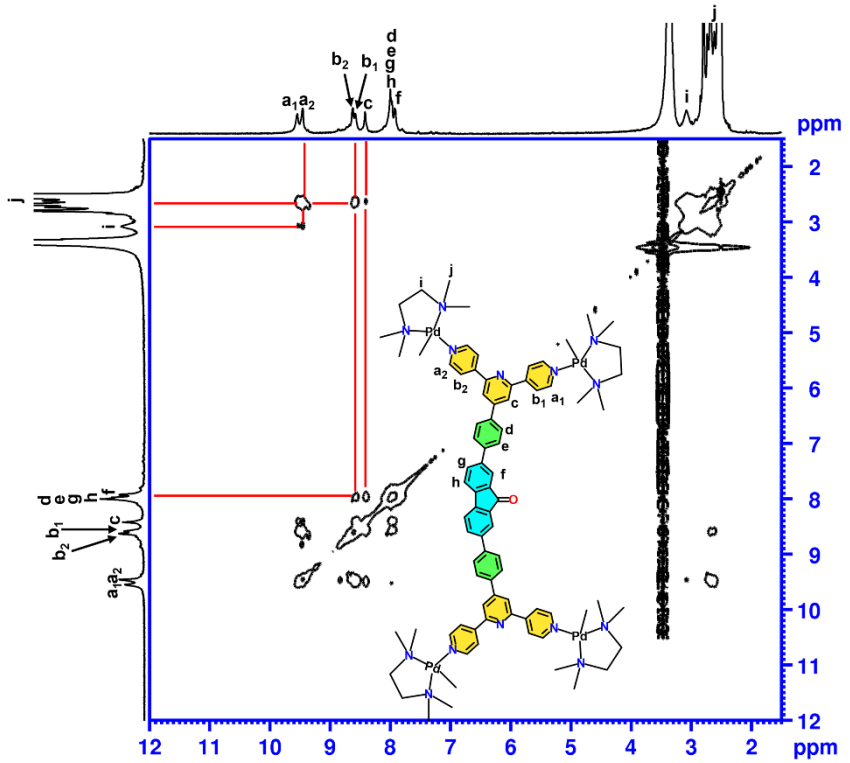


Fig. S13 ^{1}H-^{1}H NOESY NMR spectrum of **$(C_{70})_3$@M2** (DMSO-d_6, 298 K).

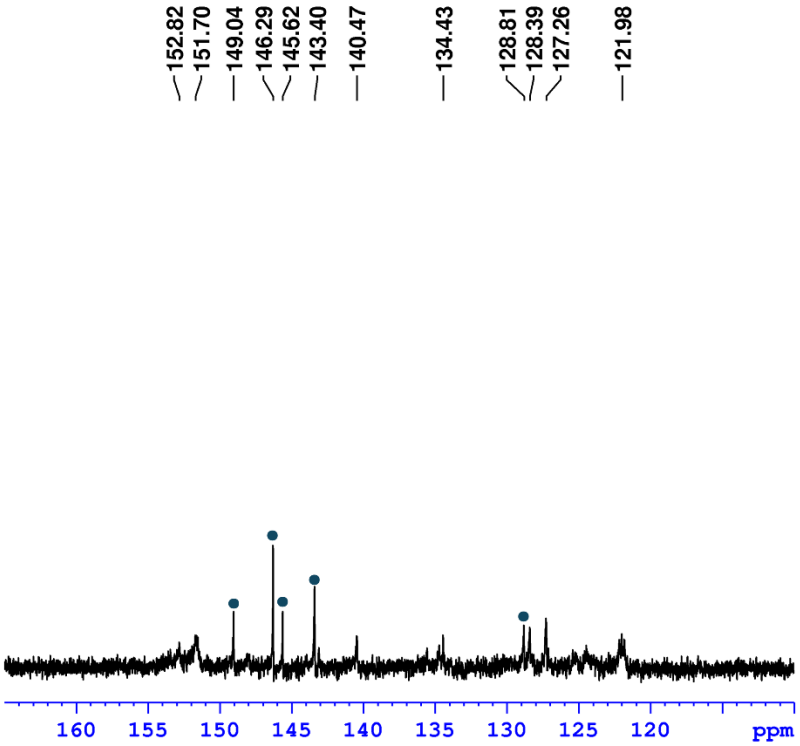


Fig. S14 ^{13}C-NMR spectrum of **$(C_{70})_3$@M2** (DMSO-d_6, 298 K). **C_{70}** characteristic peaks are marked with blue circles (.).

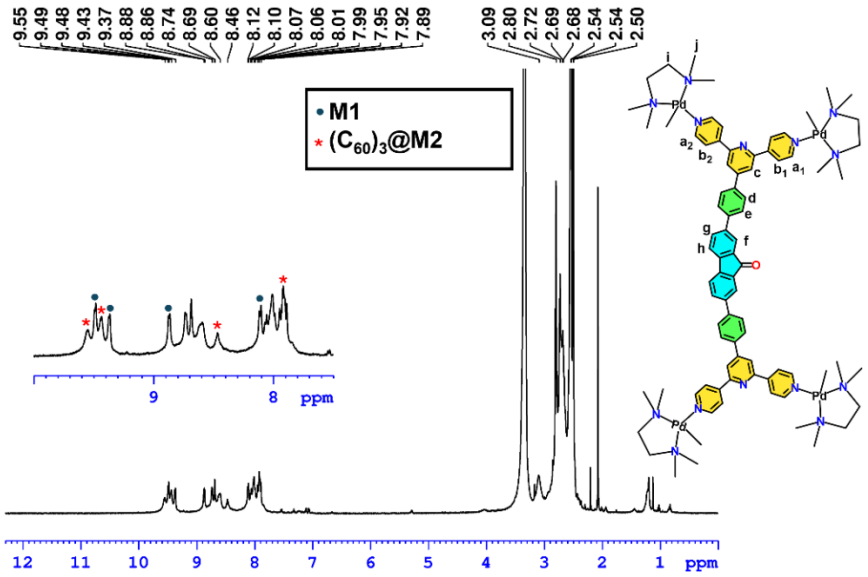


Fig. S15 ^{1}H-NMR spectrum of mixture of **M1** and **$(C_{60})_3$@M2** after treating **M1** with excess of **C_{60}** (DMSO-d_6, 298 K). Peaks marked with red asterisk marks (*) correspond to **$(C_{60})_3$@M2** whereas peaks marked with blue circles (.) correspond to **M1**. Inset: Expanded aromatic region.

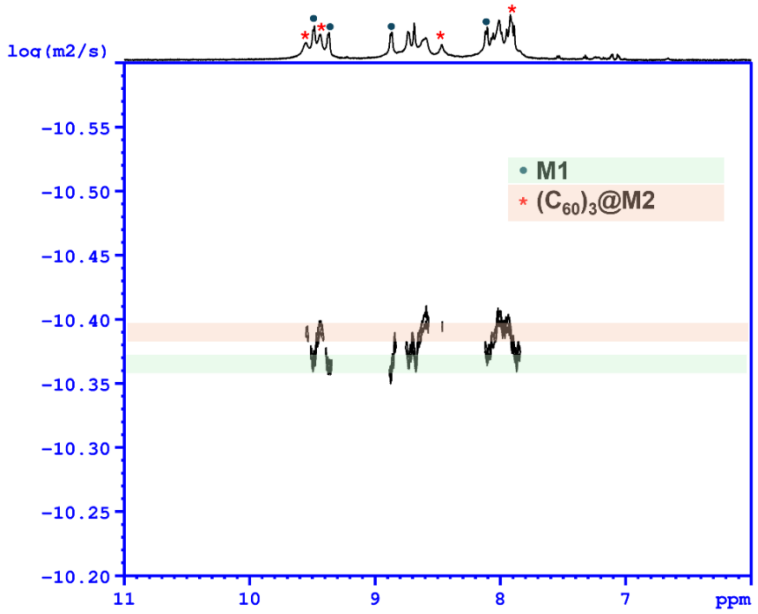


Fig. S16 ^{1}H DOSY NMR spectrum of mixture of **M1** and **(C60)3@M2** after treating **M1** with excess of **C60** (DMSO-*d6*, 298 K). Peaks marked with red asterisk marks (*) correspond to **(C60)3@M2** whereas peaks marked with blue circles (.) correspond to **M1**. **(C60)3@M2** has smaller diffusion coefficient and hence a larger solvo-dynamic radii compared to **M1**.

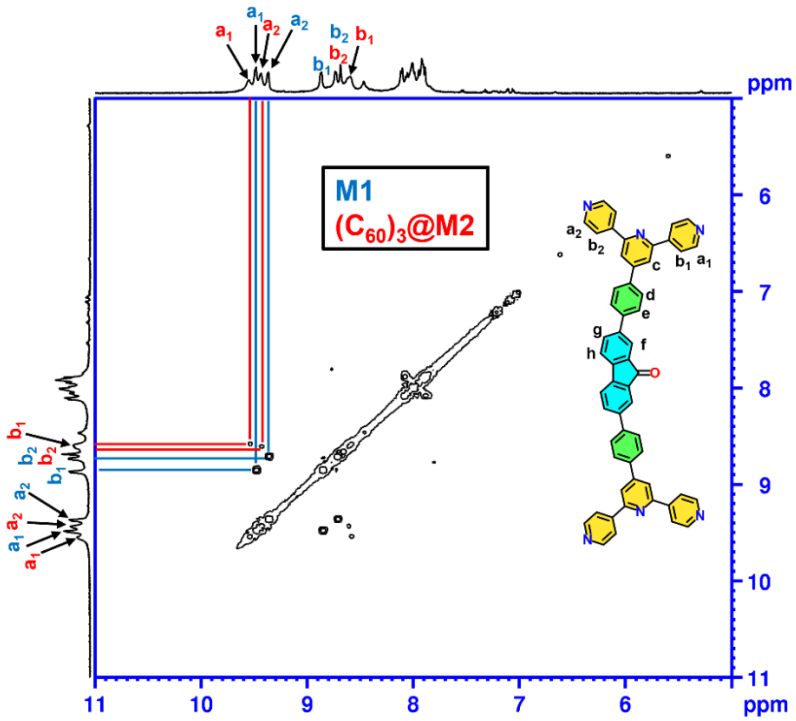


Fig. S17 ^{1}H-^{1}H COSY NMR spectrum of mixture of **M1** and **(C60)3@M2** after treating **M1** with excess of **C60** (DMSO-*d6*, 298 K). Peaks marked with red labels correspond to **(C60)3@M2** whereas peaks marked with blue labels correspond to **M1**.

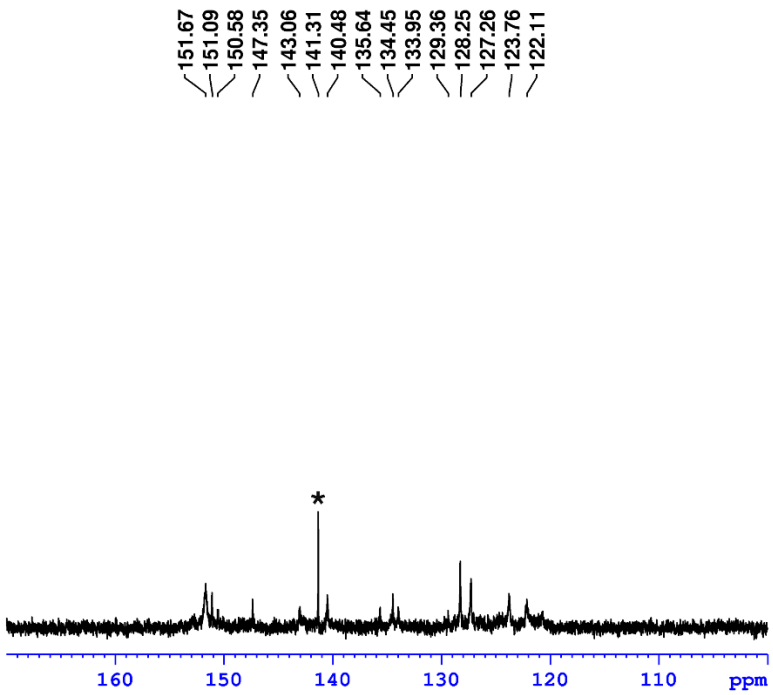


Fig. S18 ^{13}C-NMR spectrum of mixture of **M1** and **$(C_{60})_3$@M2** after treating **M1** with excess of **C_{60}** (DMSO-d_6, 298 K).**C_{60}** characteristic peak is marked with black asterisk mark.

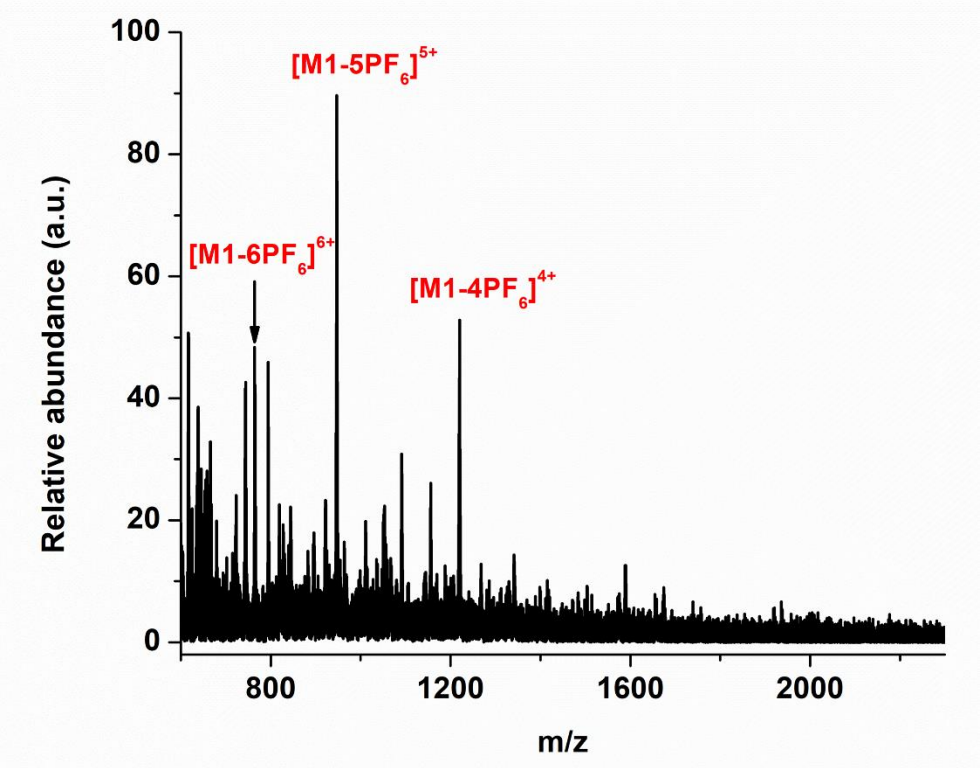


Fig. S19 Full ESI-MS of **M1** in CH_3CN.

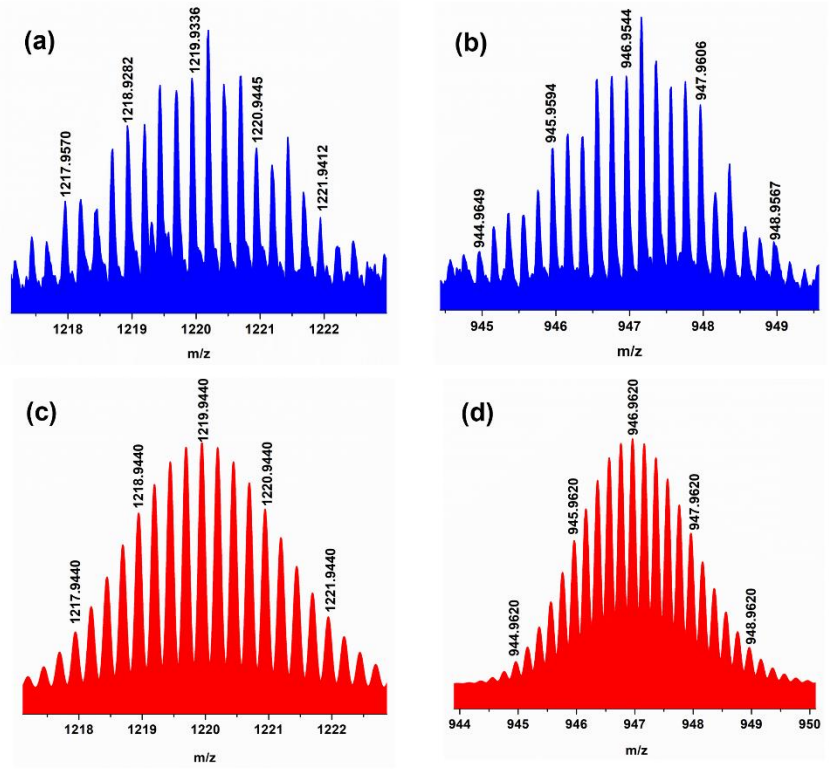


Fig. S20 (a) Experimental (blue) and (c) calculated (red) isotopic patterns of [**M1**-4PF_6]$^{4+}$ fragment; (b) Experimental (blue) and (d) calculated (red) isotopic patterns of [**M1**-5PF_6]$^{5+}$ fragment in ESI-MS.

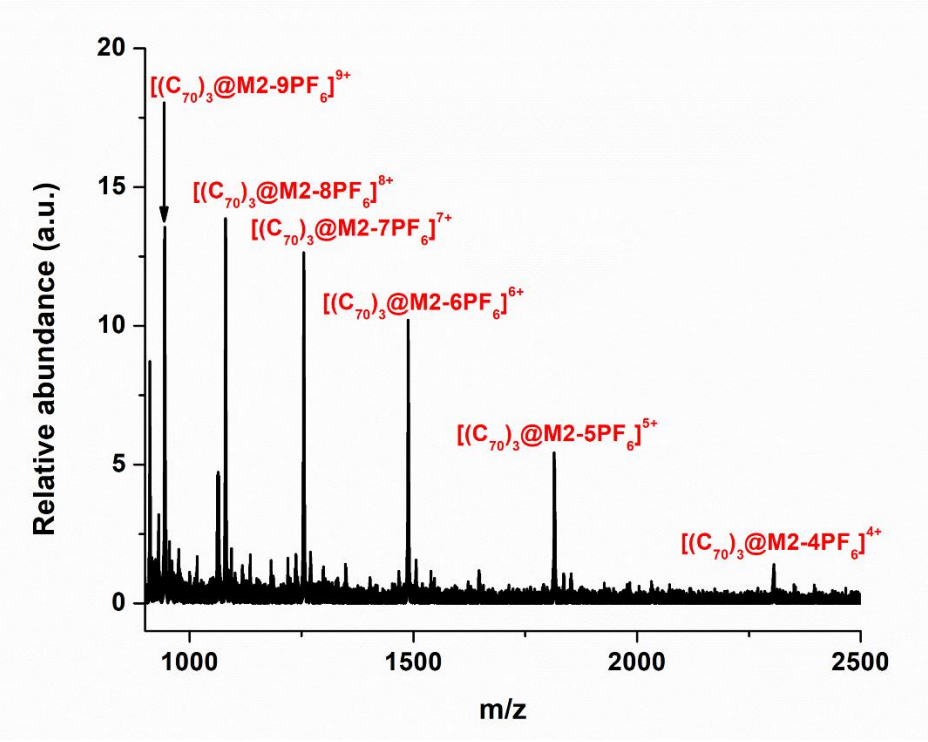


Fig. S21 Full ESI-MS of **$(C_{70})_3$@M2** in CH_3CN.

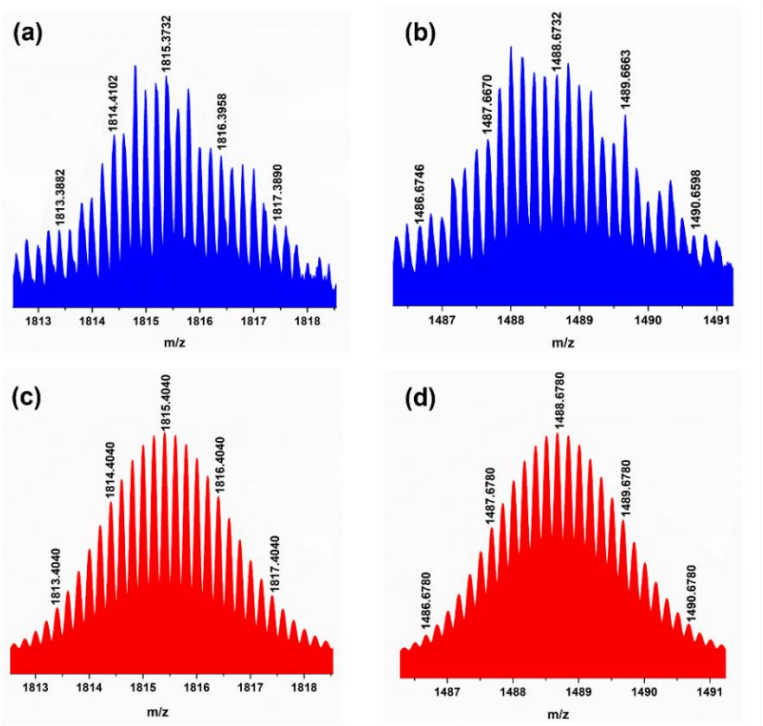


Fig. S22 (a) Experimental (blue) and (c) calculated (red) isotopic patterns of [**(C$_{70}$)$_3$@M2**-5PF$_6$]$^{5+}$ fragment; (b) Experimental (blue) and (d) calculated (red) isotopic patterns of [**(C$_{70}$)$_3$@M2**-6PF$_6$]$^{6+}$ fragment in ESI-MS.

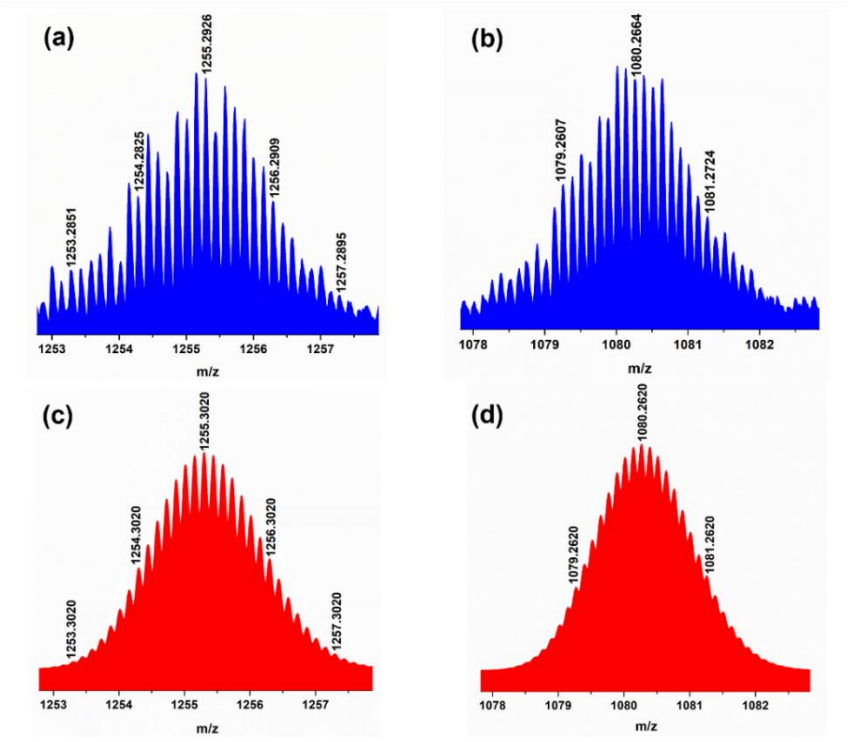


Fig. S23 (a) Experimental (blue) and (c) calculated (red) isotopic patterns of [**(C$_{70}$)$_3$@M2**-7PF$_6$]$^{7+}$ fragment; (b) Experimental (blue) and (d) calculated (red) isotopic patterns of [**(C$_{70}$)$_3$@M2**-8PF$_6$]$^{8+}$ fragment in ESI-MS.

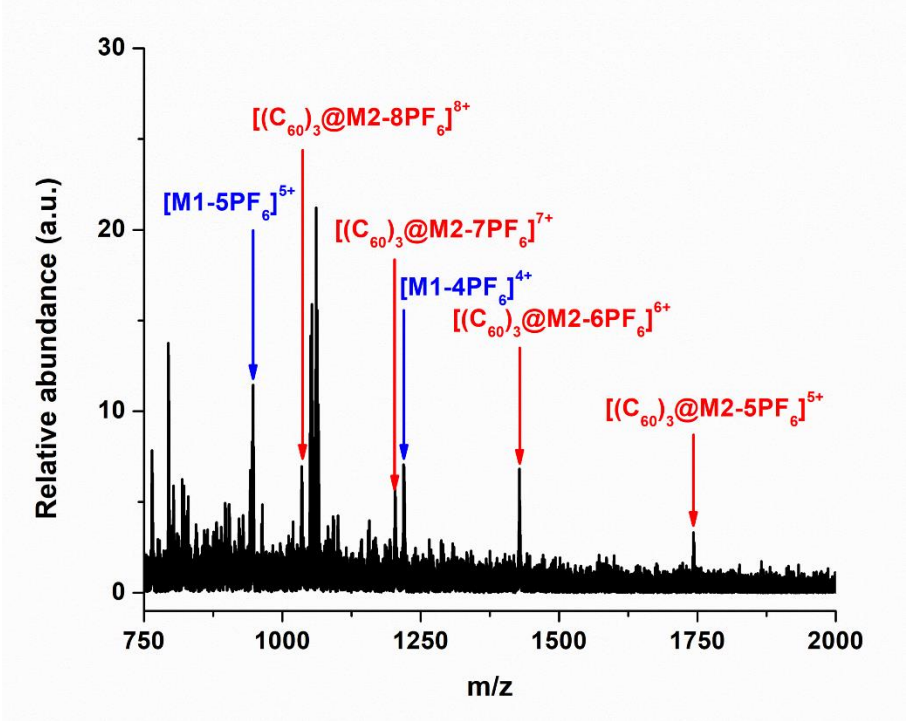


Fig. S24 Full ESI-MS of mixture of **M1** and **$(C_{60})_3$@M2** in CH_3CN.

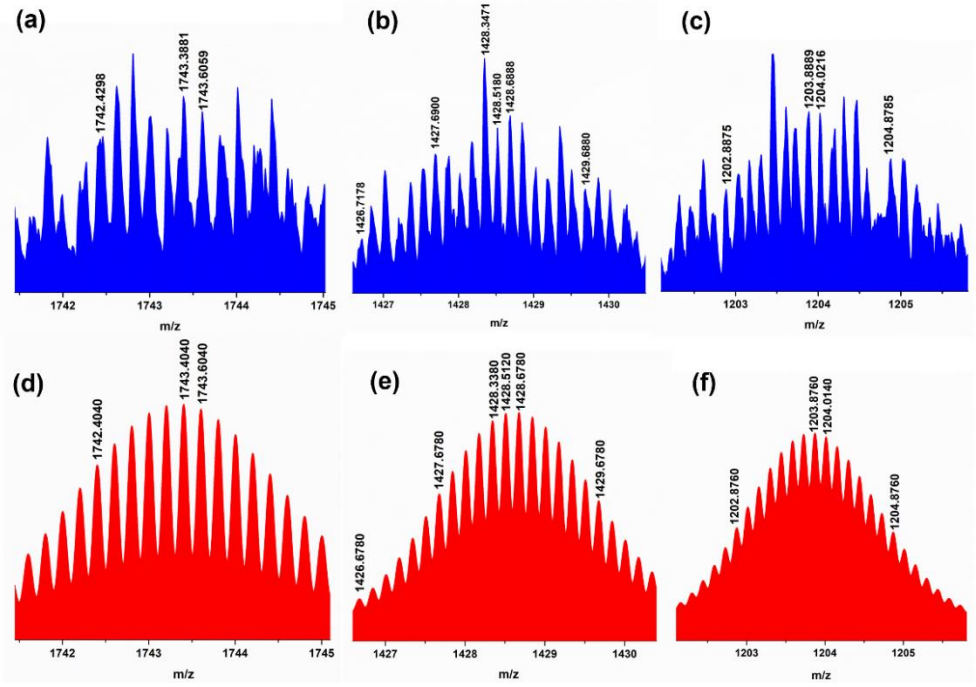


Fig. S25 (a) Experimental (blue) and (d) calculated (red) isotopic patterns of [**$(C_{60})_3$@M2**-$5PF_6$]$^{5+}$ fragment; (b) Experimental (blue) and (e) calculated (red) isotopic patterns of [**$(C_{60})_3$@M2**-$6PF_6$]$^{6+}$ fragment; (c) Experimental (blue) and (f) calculated (red) isotopic patterns of [**$(C_{60})_3$@M2**-$7PF_6$]$^{7+}$ fragment in ESI-MS.

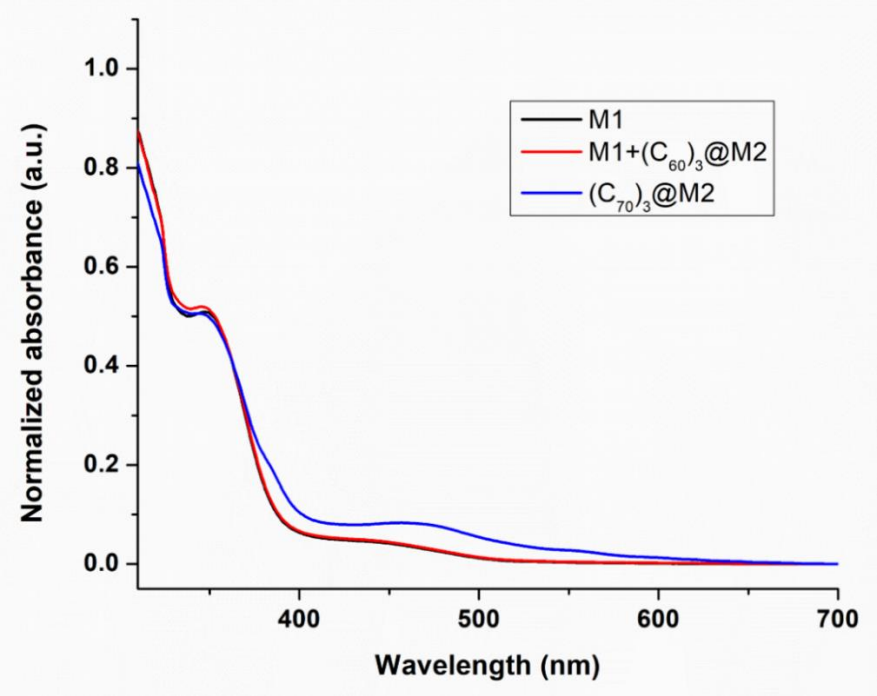


Fig. S26 Normalized absorption spectra of **M1**, **$(C_{70})_3$@M2** and **$(C_{60})_3$@M2** in dimethyl sulfoxide.

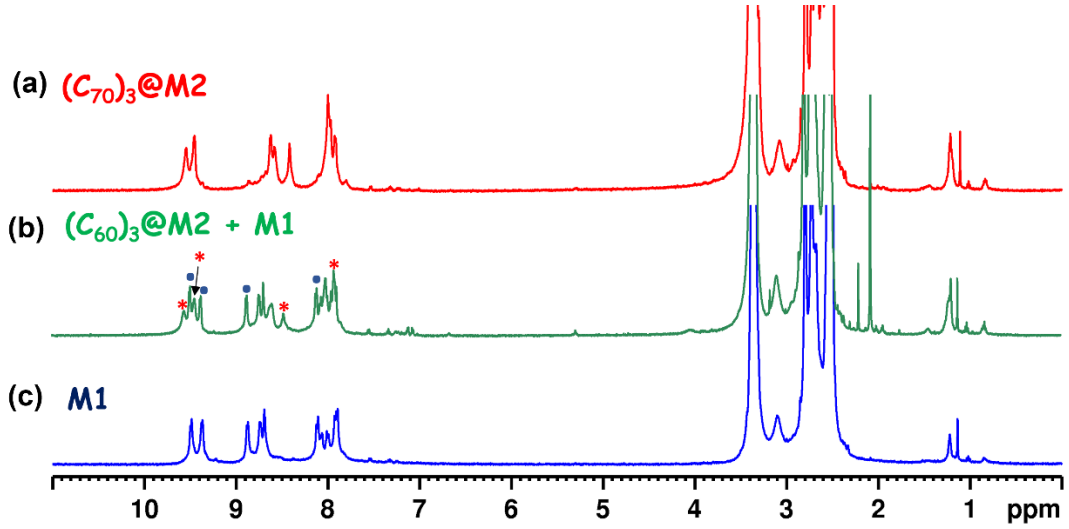


Fig. S27 Stacked ^{1}H NMR of (a) **$(C_{70})_3$@M2**, (b) mixture of **M1**and **$(C_{60})_3$@M2**, (c) **M1** in DMSO-d_6 at 298 K.

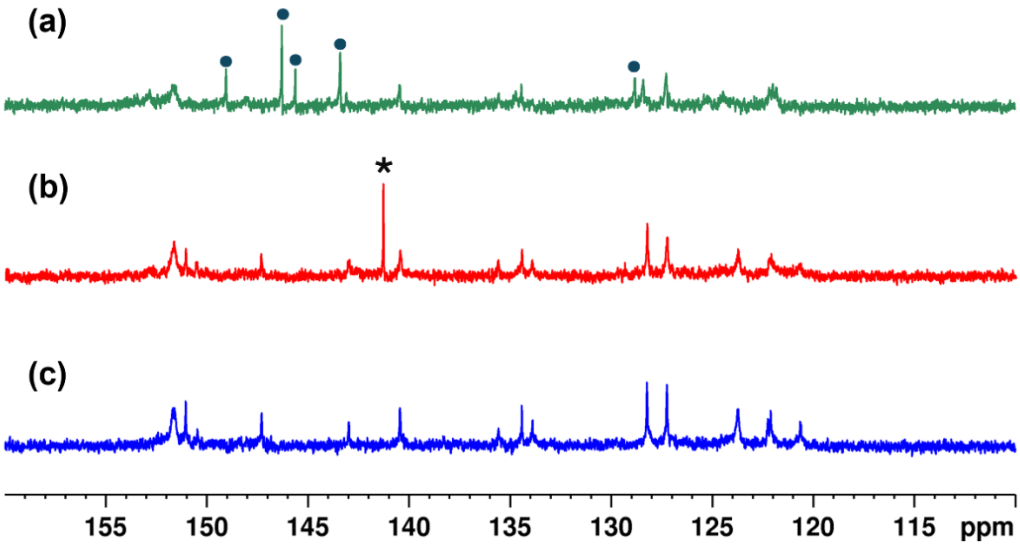


Fig. S28 Stacked ^{13}C NMR of (a) **$(C_{70})_3$@M2**, (b) mixture of **M1**and **$(C_{60})_3$@M2**, (c) **M1** in DMSO-d_6 at 298 K.

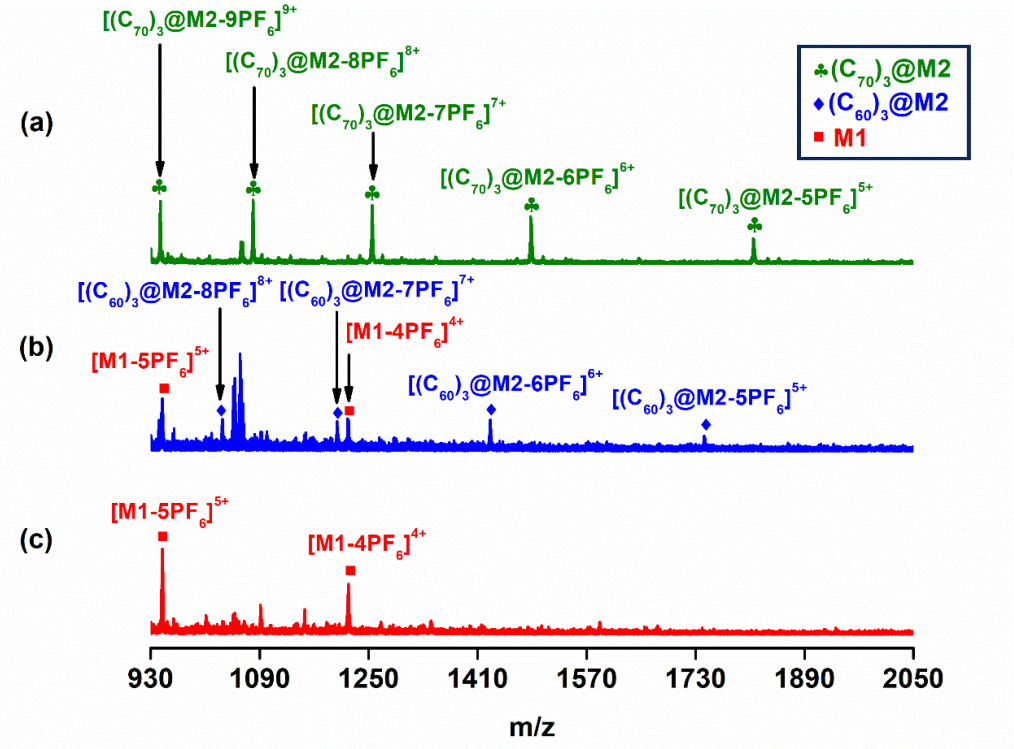


Fig. S29 Stacked ESI-MS: (a) **$(C_{70})_3$@M2**, (b) mixture of **M1** and **$(C_{60})_3$@M2**, (c) **M1** in acetonitrile.

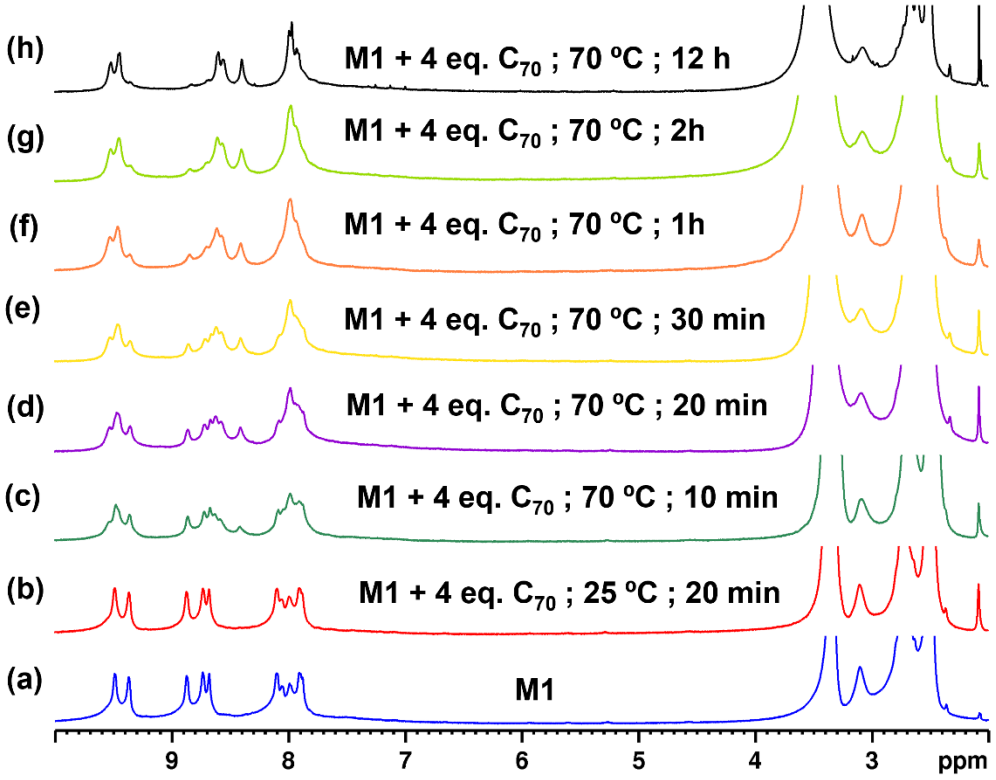


Fig. S30 Time and temperature dependent changes in ^{1}H NMR of **M1** (in DMSO-d_6) upon addition of excess of **C$_{70}$** (4 equivalents with respect to **M1**) to solution of **M1**: (a) **M1** (b) **M1** + 4 eq. **C$_{70}$**, 20 min stirring at 25 ºC; **M1** + 4 eq. **C$_{70}$**, stirring at 70 ºC for (c) 10 min (d) 20 min, (e) 30 min (f) 1 h (g) 2 h (h) 12 h (corresponding to **(C$_{70}$)$_3$@M2**). The NMR of **M1** remains intact upon stirring with excess **C$_{70}$** guest at 25 ºC indicating no encapsulation. Heating the sample at 70 ºC leads to gradual appearance of peaks corresponding to **(C$_{70}$)$_3$@M2** within 10 min and conversion of **M1** to **(C$_{70}$)$_3$@M2** is almost complete within 2 h. These experiments concludes that **M1** instantly converts to **(C$_{70}$)$_3$@M2** upon heating in presence **C$_{70}$** without involvement of any detectable intermediates [**M2**/**M1** binding 1 or 2 **C$_{70}$** molecule/(s)]. All spectra were recorded at 298 K.

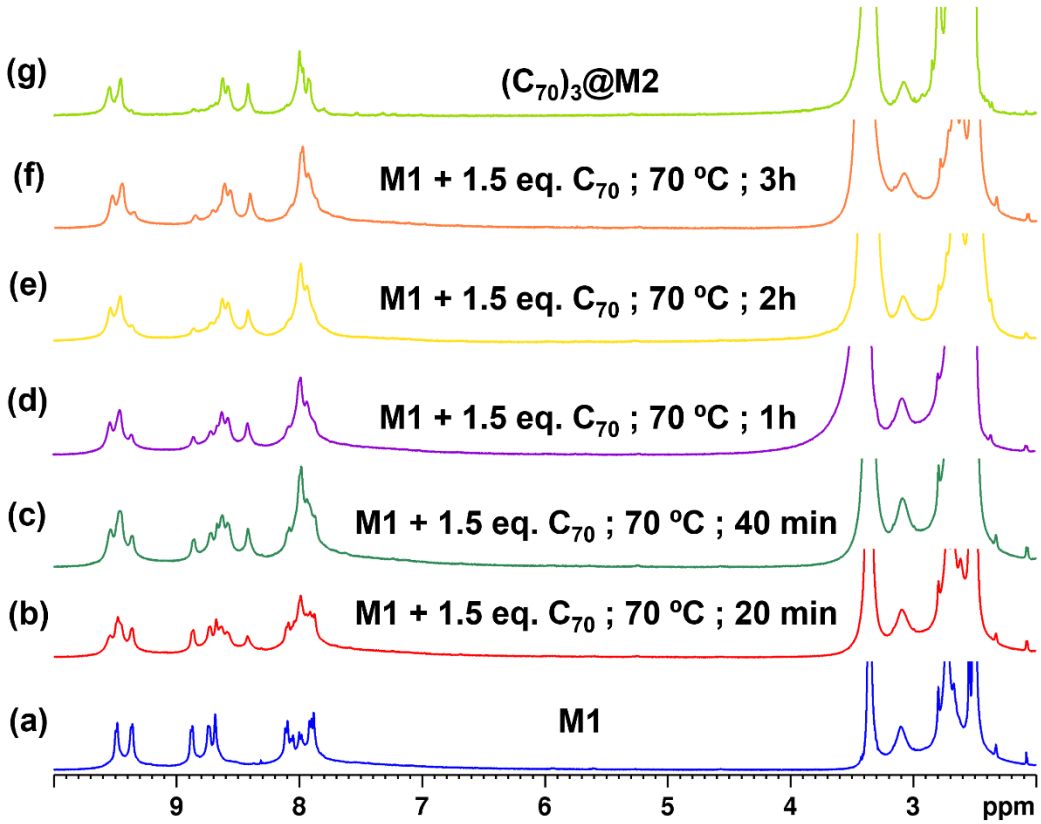


Fig. S31 Time dependent changes in ^{1}H NMR of **M1** (in DMSO-d_6) upon addition of 1.5 equivalents of $\mathbf{C_{70}}$ (1.5 equivalents with respect to **M1**/2 equivalents with respect to transformed **M2**) to solution of **M1**: (a) **M1** ; **M1** + 1.5 eq. $\mathbf{C_{70}}$, stirring at 70 ºC for (b) 20 min (c) 40 min, (d) 1 h (e) 2 h (f) 3 h; (g) $\mathbf{(C_{70})_3}$**@M2**. Heating the sample at 70 ºC leads to gradual appearance of peaks corresponding to $\mathbf{(C_{70})_3}$**@M2** within 20 min and conversion of **M1** to $\mathbf{(C_{70})_3}$**@M2** is almost complete within 3 h even in presence of less amount of guest $\mathbf{C_{70}}$ (2 equivalents with respect to transformed **M2**). These experiments concludes that **M1** instantly converts to $\mathbf{(C_{70})_3}$**@M2** upon heating in presence $\mathbf{C_{70}}$ without involvement of any detectable intermediates even when the amount of guest is lesser than required to form $\mathbf{(C_{70})_3}$**@M2**. This also indicates that **M1** instantly degrades in presence of $\mathbf{C_{70}}$ at 70 ºC and forms thermodynamically stable $\mathbf{(C_{70})_3}$**@M2** without involvement of any detectable intermediates [**M2**/**M1** binding 1 or 2 $\mathbf{C_{70}}$ molecule/(s)]. All spectra were recorded at 298 K.

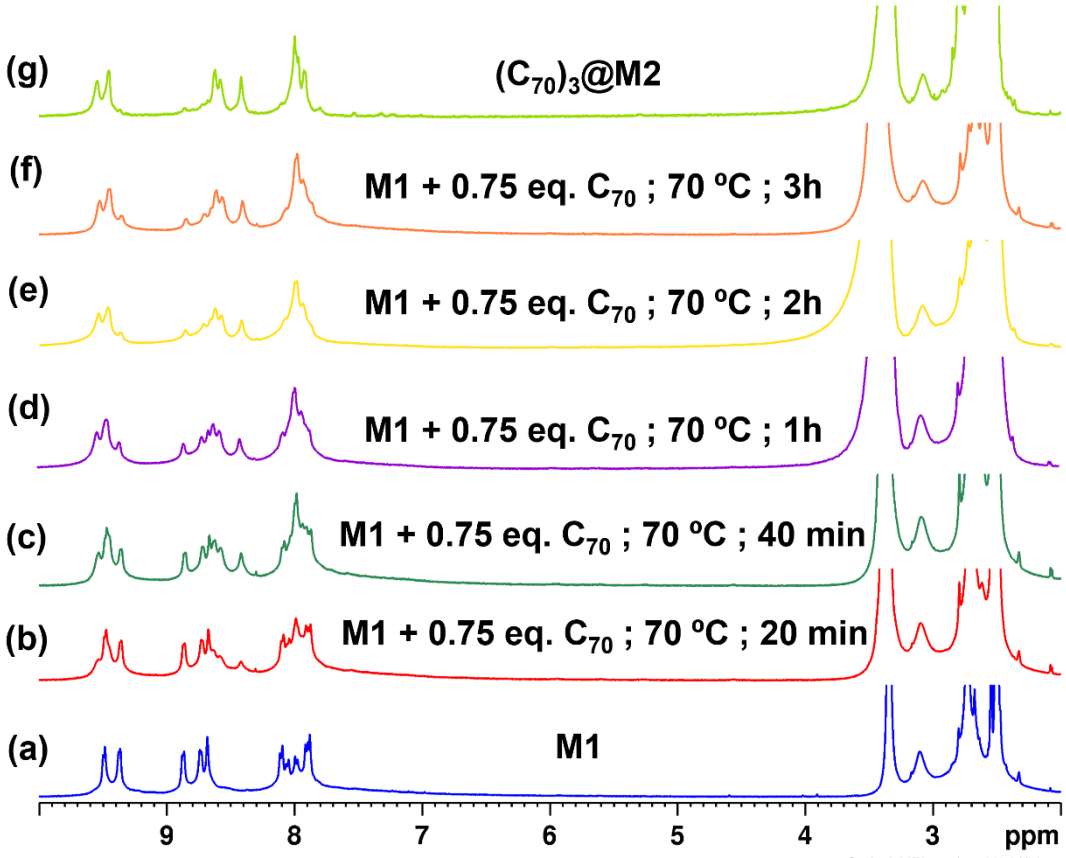


Fig. S32 Time dependent changes in ^{1}H NMR of **M1** (in DMSO-d_6) upon addition of 0.75 equivalents of **C70** (0.75 equivalents with respect to **M1**/1 equivalent with respect to transformed **M2**) to solution of **M1**: (a) **M1** ; **M1** + 0.75 eq. **C70**, stirring at 70 ºC for (b) 20 min (c) 40 min, (d) 1 h (e) 2 h (f) 3 h; (g) **(C70)3@M2**. Heating the sample at 70 ºC leads to gradual appearance of peaks corresponding to **(C70)3@M2** within 20 min and conversion of **M1** to **(C70)3@M2** is almost complete within 3h even in presence of less amount of guest **C70** (1 equivalent with respect to transformed **M2**). These experiments concludes that **M1** instantly converts to **(C70)3@M2** upon heating in presence **C70** without involvement of any detectable intermediates even when the amount of guest is lesser than required to form **(C70)3@M2**. This also indicates that **M1** instantly degrades in presence of **C70** at 70 ºC and forms thermodynamically stable **(C70)3@M2** without involvement of any detectable intermediates [**M2**/**M1** binding 1 or 2 **C70** molecule/(s)]. All spectra were recorded at 298 K.

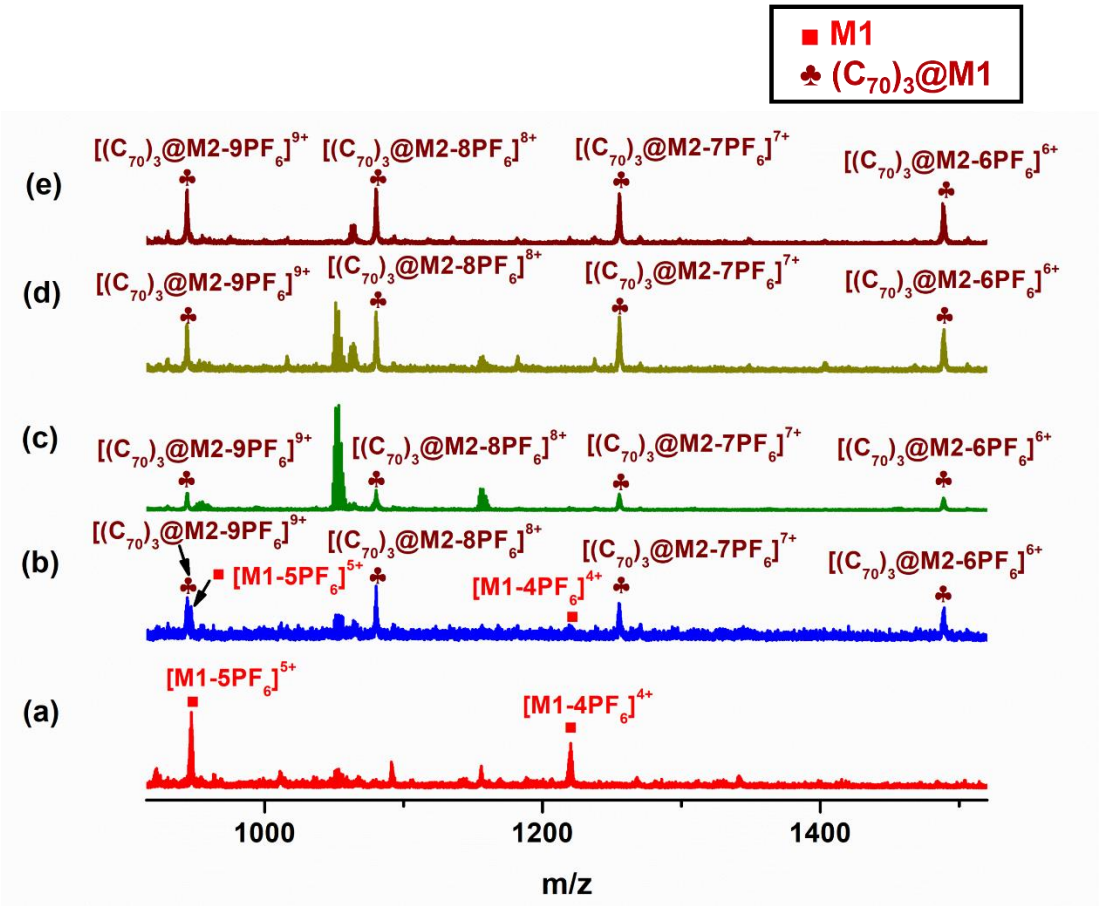


Fig. S33 ESI-MS recorded in acetonitrile after addition of different equivalents of **C_{70}** to **M1** in DMSO followed by stirring at 70 ºC for different time intervals and conversion to PF_6^- analogues; (a) **M1** (b) **M1** + 0.75 eq. **C_{70}** stirring at 70 ºC for 10 min (c) **M1** + 0.75 eq. **C_{70}**, stirring at 70 ºC for 1 h (d) **M1** + 1.5 eq. **C_{70}**, stirring at 70 ºC for 1 h; (e) **$(C_{70})_3$@M2**. These experiments concludes that **M1** instantly converts to **$(C_{70})_3$@M2** upon heating in presence **C_{70}** without involvement of any detectable intermediates even when the amount of guest is lesser than required to form **$(C_{70})_3$@M2**. Even when 0.75 equivalents of **C_{70}** (1 equivalent with respect to transformed **M2**) was added to **M1** and stirred at 70 ºC for 10 min, peaks corresponding to **$(C_{70})_3$@M2** were obtained with very less intense peaks for **M1**. However, no other compositions of **M1**/**M2** with **C_{70}** were detected from ESI-MS analyses. This also indicates that **M1** instantly degrades in presence of **C_{70}** at 70 ºC and forms thermodynamically stable **$(C_{70})_3$@M2** without involvement of any detectable intermediates [**M2**/**M1** binding 1 or 2 **C_{70}** molecule/(s)]. The less intense unassigned peaks in the mass spectra do not correspond to isotopic distributions of any composition of host or host-guest complex. These are +1 or +2 charged fragments generated under ionization conditions.

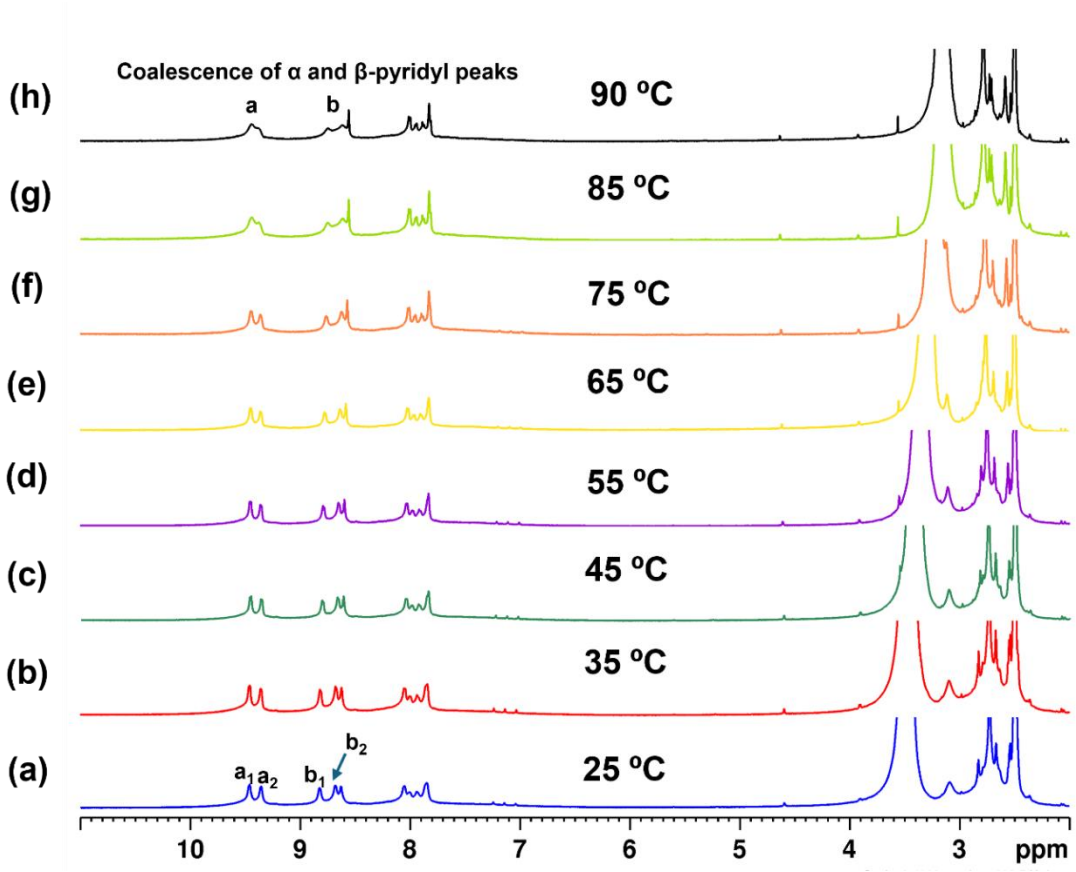


Fig. S34 Variable Temperature (VT) ^{1}H NMR spectra of **M1** (NO_3^- analogue in DMSO-d_6) at: (a) 25 ºC (b) 35 ºC (c) 45 ºC (d) 55 ºC (e) 65 ºC (f) 75 ºC (g) 85 ºC (h) 90 ºC. The α (a_1 and a_2) and β-pyridyl (b_1 and b_2) protons are resolvable at room temperature or slightly elevated temperatures in the NMR timescale due to rigidification upon coordination to the metal acceptors, resulting in two different chemical environments for the pyridyl rings. However, at higher temperatures of 85 ºC or higher the pyridyl protons coalesce into single peaks (a and b) due to faster rotation in the NMR timescale at such high temperatures.

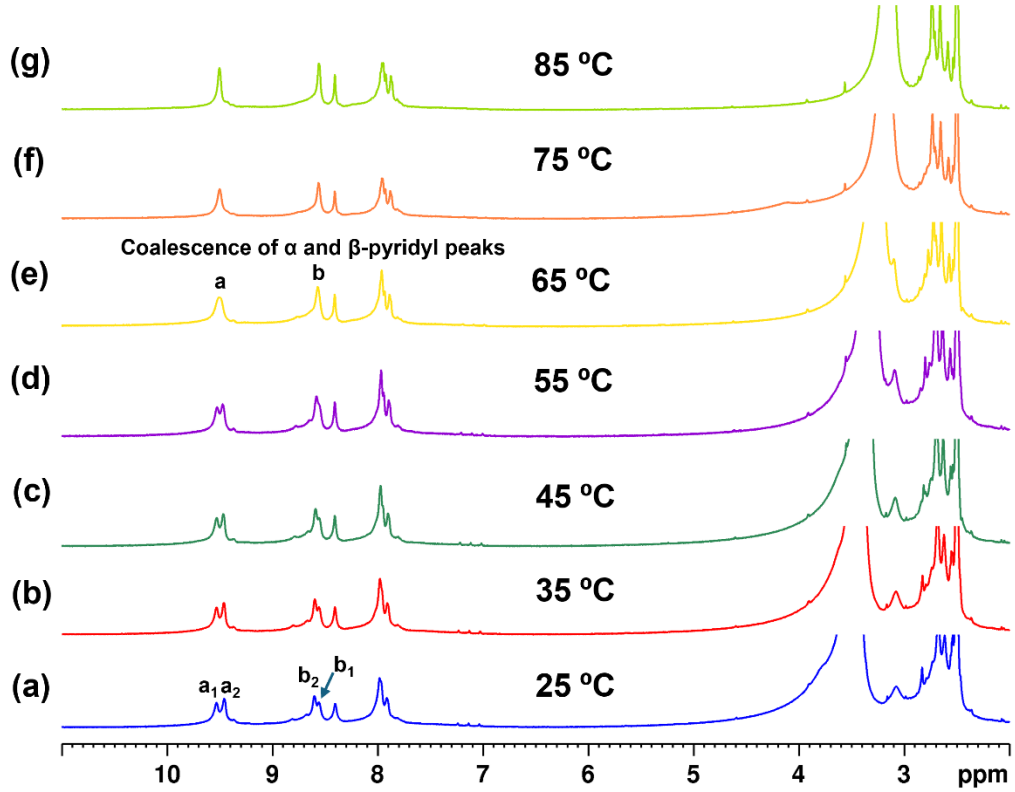


Fig. S35 Variable Temperature (VT) ^{1}H NMR spectra of **(C$_{70}$)$_3$@M2** (NO_3^- analogue in DMSO-d_6) at: (a) 25 ºC (b) 35 ºC (c) 45 ºC (d) 55 ºC (e) 65 ºC (f) 75 ºC (g) 85 ºC. The α (a_1 and a_2) and β-pyridyl (b_1 and b_2) protons are resolvable at room temperature or slightly elevated temperatures in the NMR timescale due to rigidification upon coordination to the metal acceptors, resulting in two different chemical environments for the pyridyl rings. However, at higher temperatures of 65 ºC or higher the pyridyl protons coalesce into single peaks (a and b) due to faster rotation in the NMR timescale at such high temperatures. It is important to mention here that the complex, **(C$_{70}$)$_3$@M2** pyridyl protons coalesce at a temperature (65 ºC) much lower than that for the free cage, **M1** (85 ºC). This indicates that the tetrafacial barrel, **M2** together with the three bound dynamically moving **C$_{70}$** molecules [**(C$_{70}$)$_3$@M2**] within its cavity is conformationally more flexible compared to **M1** as expected. It was not possible to carry out the VT-NMR at temperatures lower than 25 ºC since DMSO freezes at 19 ºC.

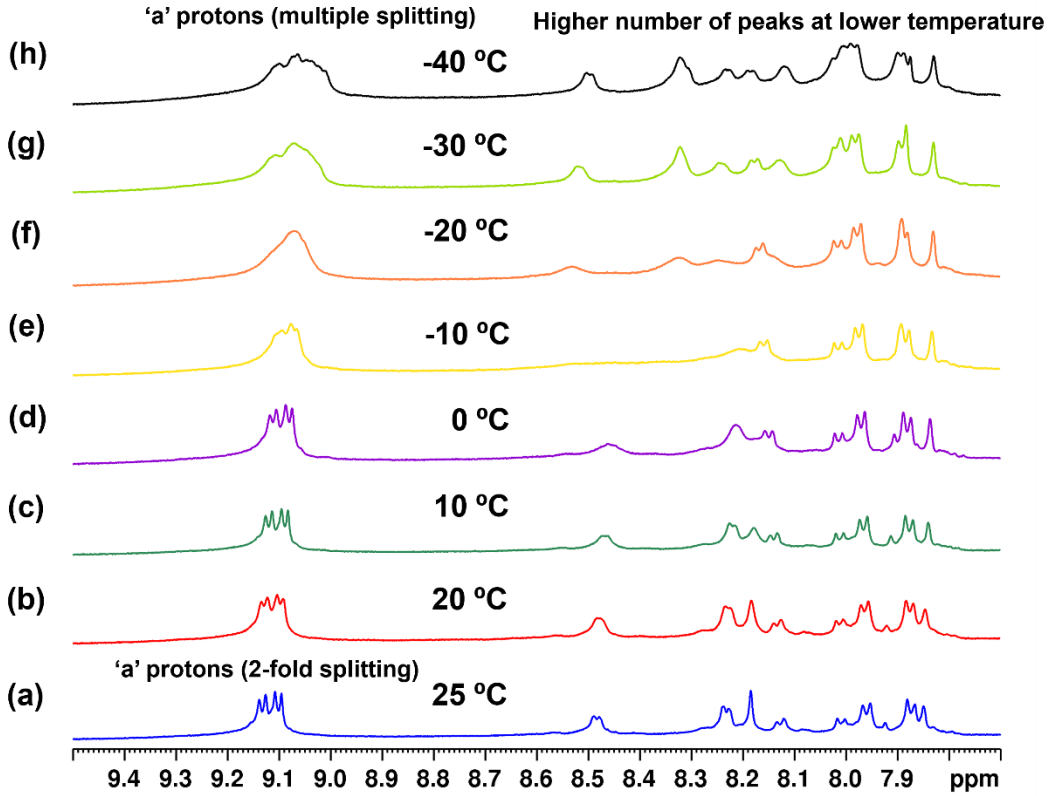


Fig. S36 Low temperature Variable Temperature (VT) ^{1}H NMR spectra of **$(C_{70})_3$@M2** (PF_6^- analogue in CD_3CN) at: (a) 25 ºC (b) 20 ºC (c) 10 ºC (d) 0 ºC (e) -10 ºC (f) - 20 ºC (g) -30 ºC (h) - 40 ºC. At room temperature (25 ºC), the α-pyridyl (a) protons are only doubly split (appear as doublet of doublet) due to high extent of molecular tumbling and free movement of three bound C_{70} molecules within the cavity of **M2**. However, at lower temperatures (-40 ºC), such molecular tumbling and dynamic movement of guests within the cavity are restricted to some extent and the α-pyridyl (a) protons split into a large number of peaks (merged together and appears broad). The other protons also shows higher splitting at such a low temperature (-40 ºC).

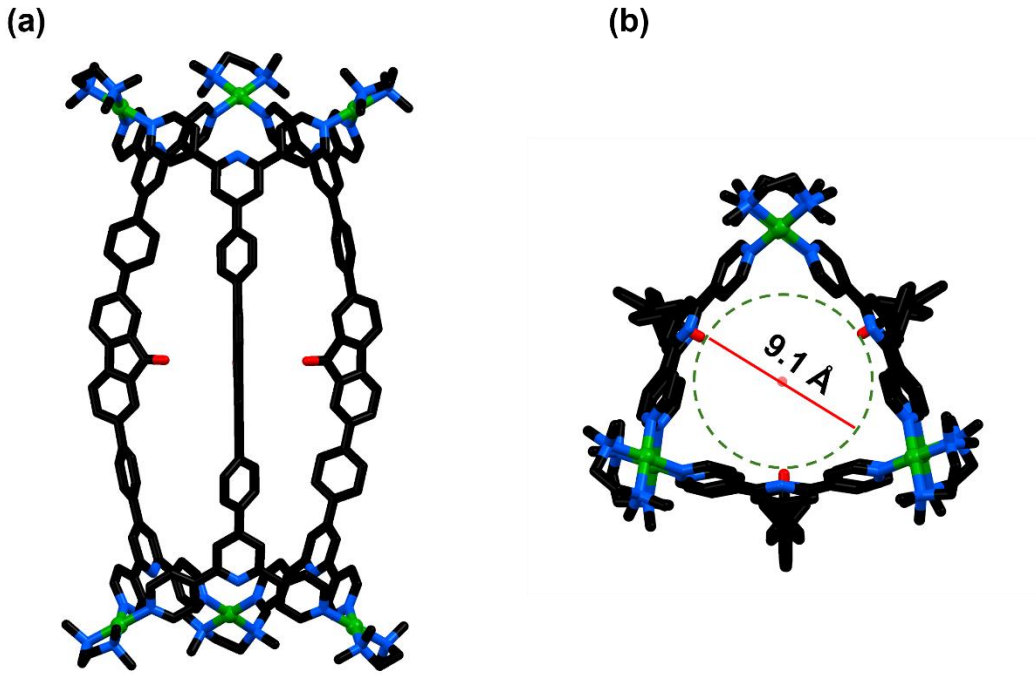


Fig. S37 DFT optimized structure of trifacial tube (isomer of **M1**, where the three ligands are oriented vertically and clipped to six "Pd" acceptors): (a) side view (b) top view. Color codes: carbon (black), nitrogen (blue), oxygen (red) and palladium (green). Hydrogen atoms are omitted for clarity.

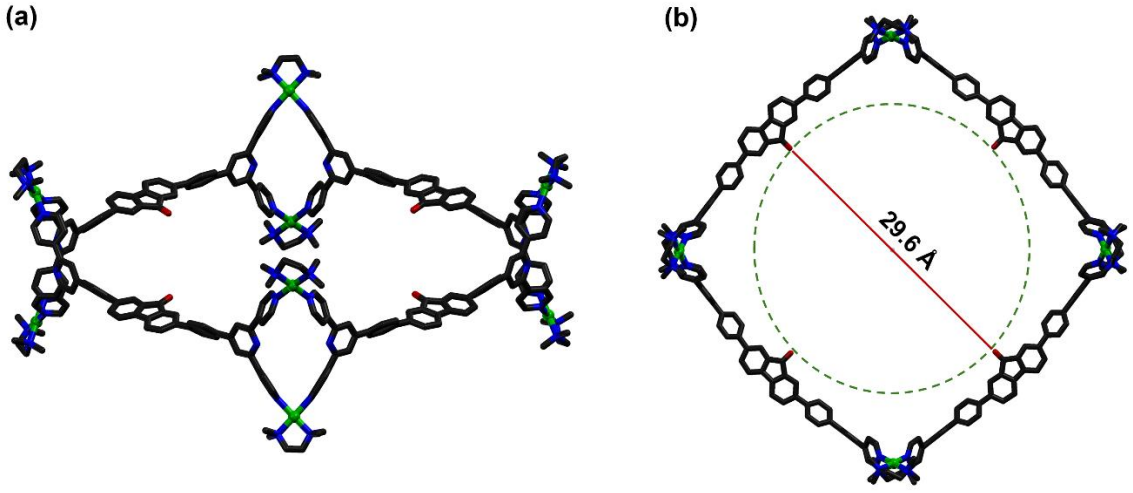


Fig. S38 PM6 optimized structure of tetrafacial barrel (**M2**, where the three ligands are oriented horizontally and clipped to eight "Pd" acceptors): (a) side view (b) top view. Color codes: carbon (black), nitrogen (blue), oxygen (red) and palladium (green). Hydrogen atoms are omitted for clarity.

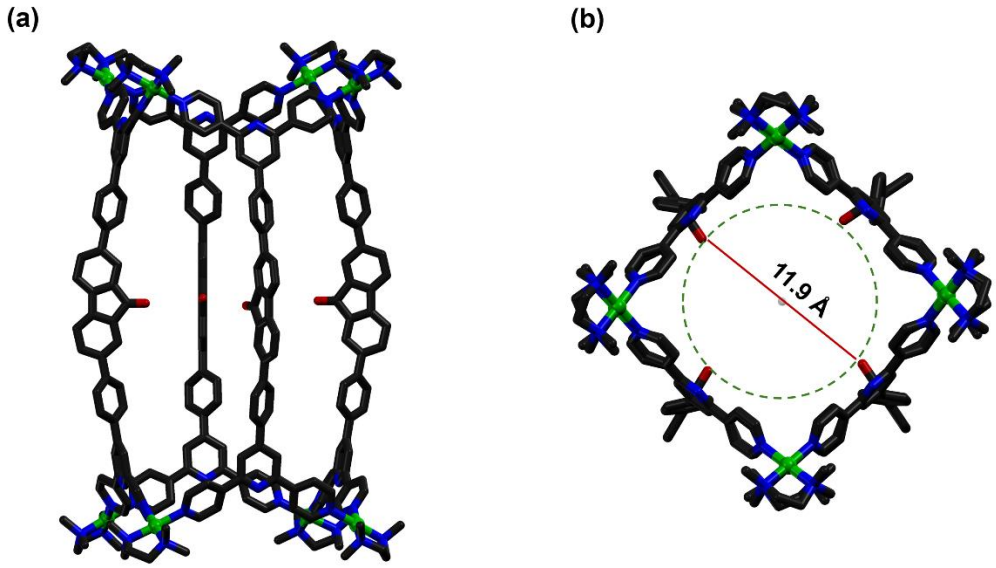


Fig. S39 PM6 optimized structure of tetrafacial tube (isomer of **M2**, where the three ligands are oriented vertically and clipped to eight "Pd" acceptors): (a) side view (b) top view. Color codes: carbon (black), nitrogen (blue), oxygen (red) and palladium (green). Hydrogen atoms are omitted for clarity.

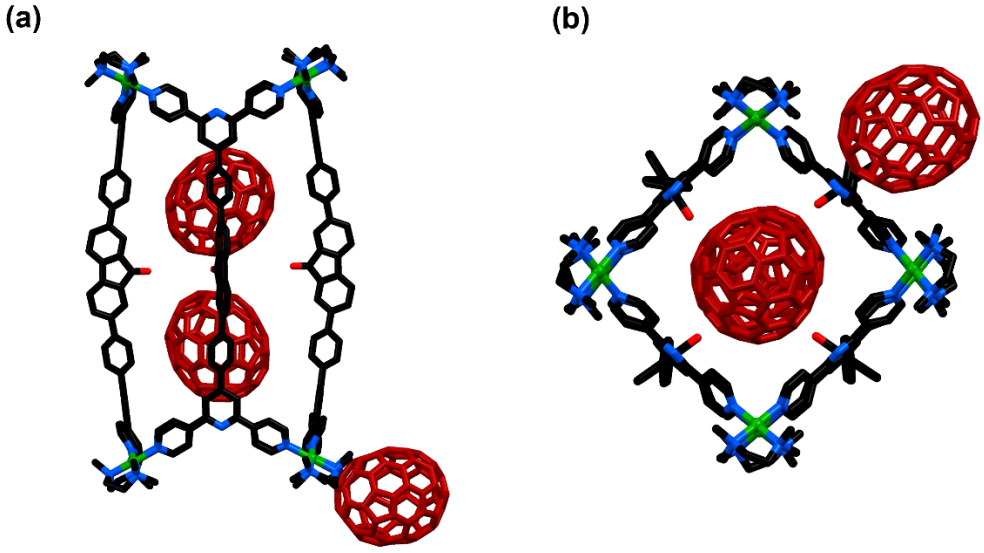


Fig. S40 PM6 optimized structure of tetrafacial tube (isomer of **M2**, where the three ligands are oriented vertically and clipped to eight "Pd" acceptors) with three C_{70} molecules. Structure optimization was carried out by putting three C_{70} molecules within the cavity of the tetrafacial tube which led to the expulsion of one C_{70} molecule due to lack of space within the cavity: (a) side view (b) top view. Color codes: carbons of host (black), nitrogen (blue), oxygen (red) and palladium (green), carbons of guest C_{70} (brown). Hydrogen atoms are omitted for clarity.

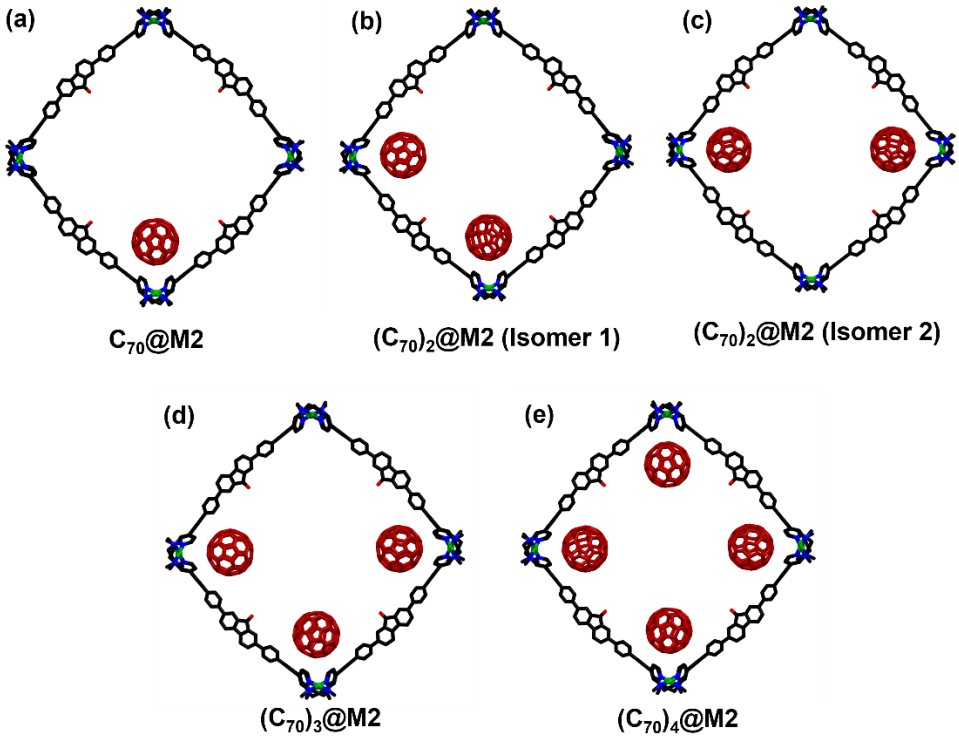


Fig. S41 PM6 optimized structures (top view) of tetrafacial barrel (isomer of **M2**, where the three ligands are oriented horizontally and clipped to eight "Pd" acceptors) with different number of C_{70} molecules: (a) **C_{70}@M2** (b) **$(C_{70})_2$@M2** (Isomer 1: adjacent placement) (c) **$(C_{70})_2$@M2** (Isomer 2: diagonal placement) (d) **$(C_{70})_3$@M2** (e) **$(C_{70})_4$@M2**. Structure optimization was carried out by putting C_{70} molecules at the corners. Color codes: carbons of host (black), nitrogen (blue), oxygen (red) and palladium (green), carbons of guest C_{70} (brown). Hydrogen atoms are omitted for clarity.

Calculation of host-guest stabilization energies due to incorporation of different number of fullerene molecules:

The structure of **M2**, **C_{70}@M2**, **$(C_{70})_2$@M2** (Isomer 1: adjacent placement), **$(C_{70})_2$@M2** (Isomer 2: diagonal placement), **$(C_{70})_3$@M2**, and **$(C_{70})_4$@M2** were optimized and energies calculated. Further, the energies of one, two, three and four fullerene in same position as within **M2** were optimized for normalizing the energies of the complexes with respect to **M2**.

Table S1 Optimized Energies

Species	Total energy (a.u.)	Total energy (kcal/mol)
M2	7.73798375	4855.6622
C_{70}@M2	9.12997976	5729.1536

$(C_{70})_2$@M2 (Isomer 1: adjacent)	10.52481105	6604.4242
$(C_{70})_2$@M2 (Isomer 2: diagonal)	10.52469618	6604.3521
$(C_{70})_3$@M2	11.91992457	7479.8719
$(C_{70})_4$@M2	13.31502690	8355.3125
Free C_{70}	1.40444517	881.3034
Free $(C_{70})_2$ (adjacent)	2.80887545	1762.5974
Free $(C_{70})_2$ (diagonal)	2.80889023	1762.6067
Free $(C_{70})_3$	4.21330824	2643.8931
Free $(C_{70})_4$	5.61774063	3525.1884

Host-guest stabilization energies:

The energies of the complexes were normalized (E_{norm}) with respect to **M2** by subtracting the optimized energy of that many number of C_{70} molecules in that particular arrangement from the optimized energies (E_{opt}). Then, the stabilization energy solely due host-guest non-covalent interactions (E_{stab}) were calculated by subtracting the normalized energies from the energy of free tetrafacial barrel, **M2** (E_{M2}).

E_{norm} = E_{opt} – Optimized Energy of that many number of free C_{70}

$E_{stab} = E_{M2} - E_{norm}$

Table S2 Host-Guest stabilization energy calculation

Species	**Optimized Energy (E_{opt}) (kcal/mol)**	**Normalized Energy (E_{norm}) (kcal/mol)**	**Host-Guest Stabilization Energy (E_{stab}) (kcal/mol)**

M2	4855.6622	4855.6622	0
C_{70}@M2	5729.1536	4847.8502	– 7.8120
$(C_{70})_2$@M2 (Isomer 1: adjacent)	6604.4242	4841.8268	– 13.8354
$(C_{70})_2$@M2 (Isomer 2: diagonal)	6604.3521	4841.7454	– 13.9168
$(C_{70})_3$@M2	7479.8719	4835.9788	– 19.6834
$(C_{70})_4$@M2	8355.3125	4830.1241	– 25.5381

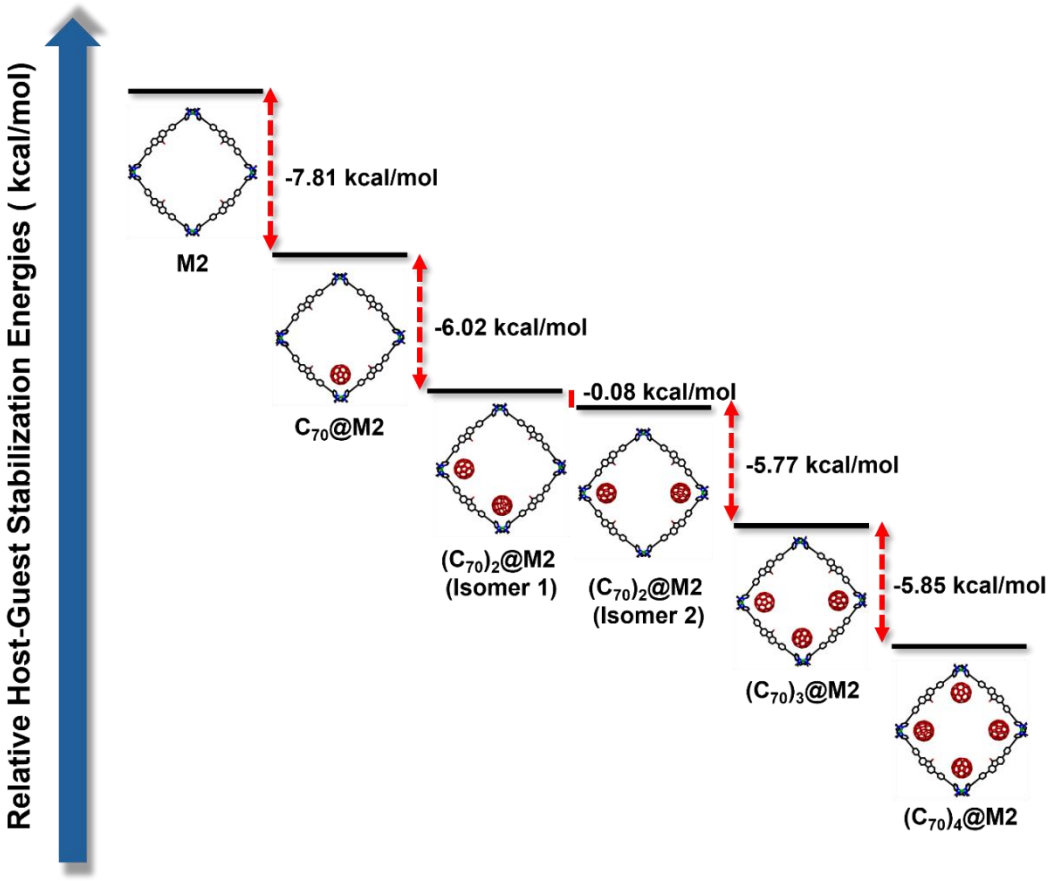


Fig. S42 The relative stabilization energies imparted solely due stepwise addition of C_{70} molecules into the cavity of **M2**. Clearly, the addition of more and more molecules into the corners of the cavity leads to enthalpic stabilization of the host guest complexes. However, these calculation do not consider the entropic effects of guest encapsulation. Although enthalpy favors the formation of **$(C_{70})_4$@M2**, it is entropically most disfavored. Again, only entropic consideration would favor **M2** (no encapsulation). Experimentally, unambiguously we observe only formation of **$(C_{70})_3$@M2**. So, the formation of **$(C_{70})_3$@M2** was achieved through a delicate balance between enthalpic and entropic effects.

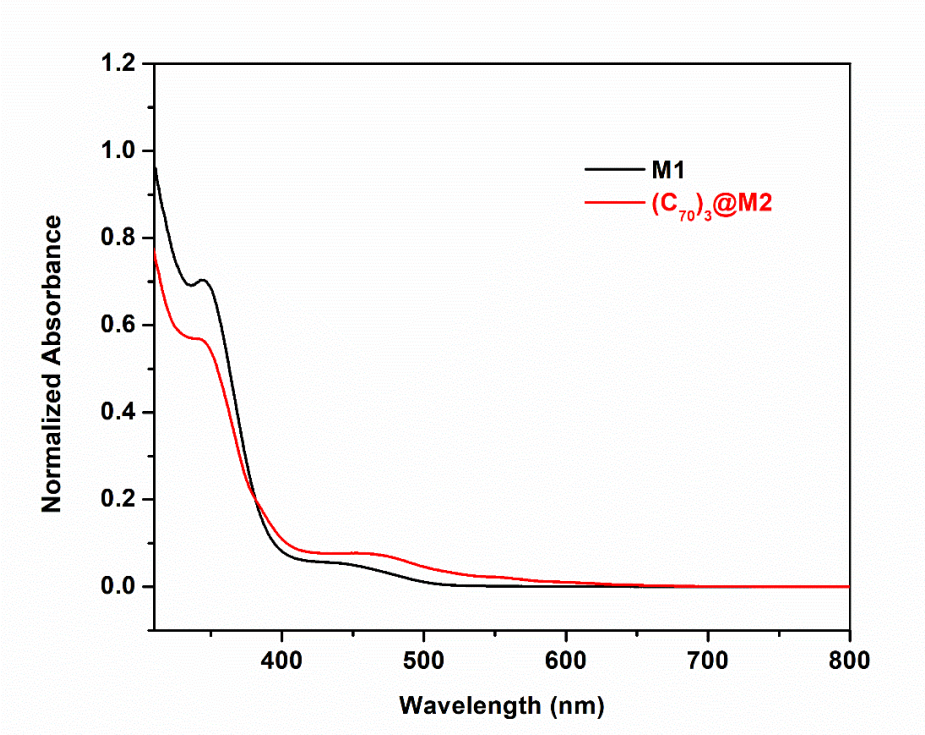


Fig. S43 Normalized absorption spectra of the PF_6^- analogues of **M1** and **$(C_{70})_3$@M2** in acetonitrile.

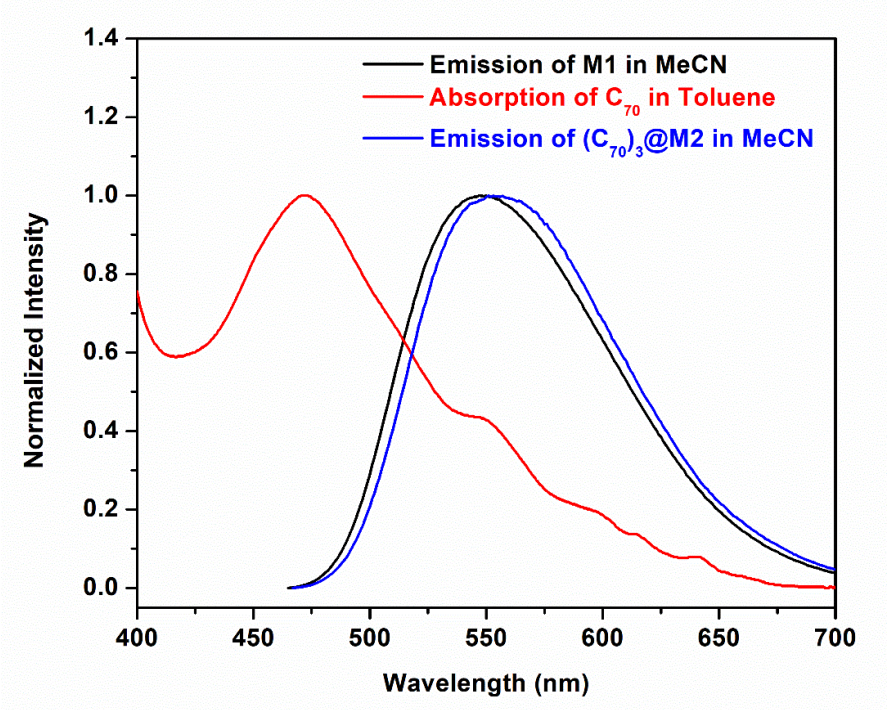


Fig. S44 Normalized emission spectra of the PF_6^- analogue of **M1**, PF_6^- analogue of **$(C_{70})_3$@M2** in acetonitrile and absorption spectrum of **C_{70}** in toluene. Free **M2** does not form. The emission of both **M1** and **$(C_{70})_3$@M2** show large overlap with absorption of **C_{70}** indicating possibility of FRET from **M2** to **C_{70}** when present in close proximity in **$(C_{70})_3$@M2** that facilitates sensitization of **C_{70}** encapsulated within **M2**.

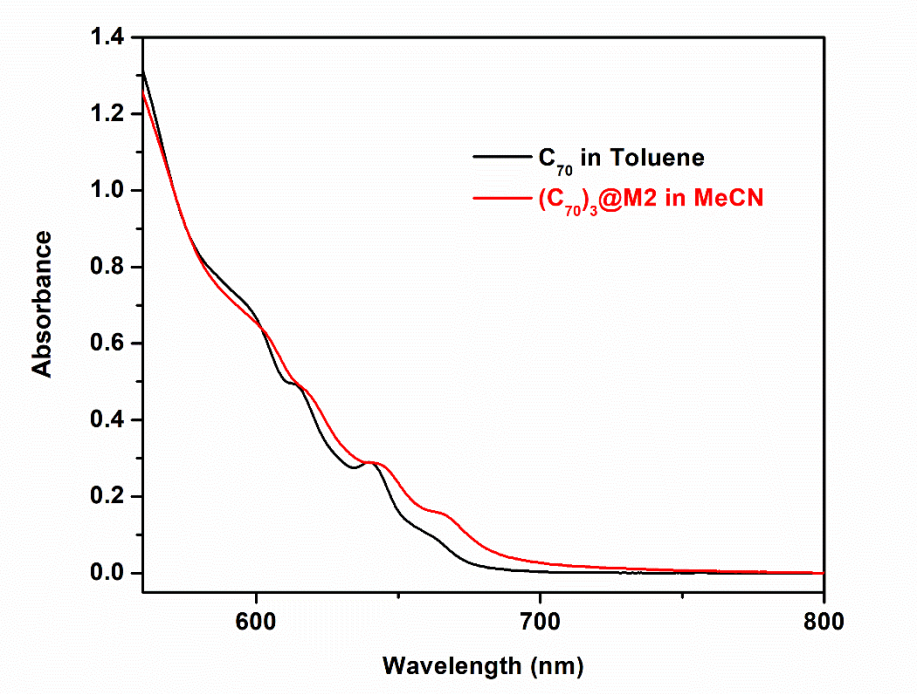


Fig. S45 Absorption spectra of PF_6^- analogue of **$(C_{70})_3$@M2** in acetonitrile (100 μM) and **C_{70}** in toluene (300 μM). Absorption in the red light region of visible light is shown here.

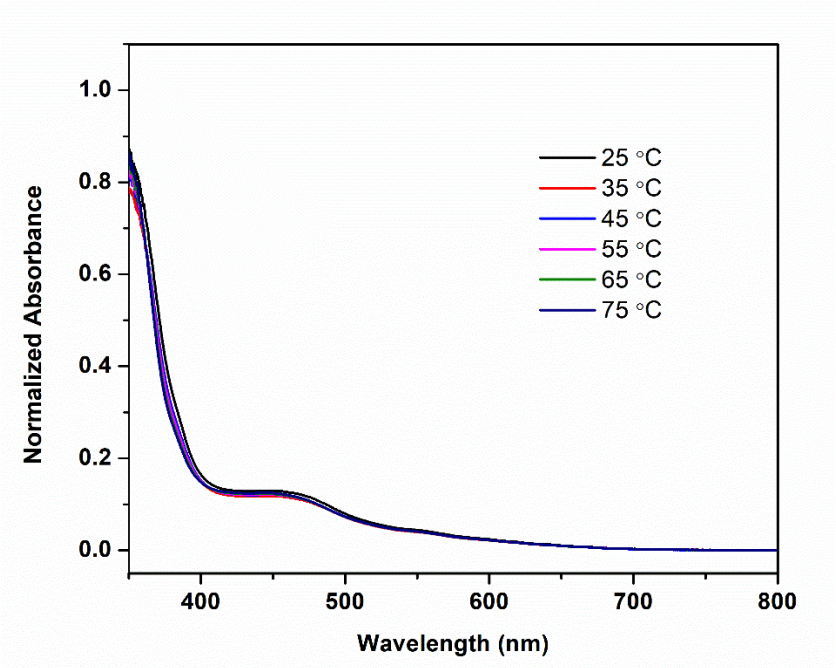


Fig. S46 Variable Temperature (VT) absorption spectra of the NO_3^- analogue of **$(C_{70})_3$@M2** in dimethyl sulfoxide. The absorption recorded at different temperatures in the range 25-75 ºC shows similar profiles with the broad absorption starting at *ca.* 450 nm and tailing up to *ca.* 700 nm characteristic of **C_{70}**. The similar absorption spectra further corroborates with the stability of the complex, **$(C_{70})_3$@M2** at higher temperatures.

6. Calculation of solvo-dynamic radii from DOSY and comparison with radii of optimized structures

The ^{1}H-DOSY NMR spectra for **M1** and **$(C_{70})_3$@M2** were recorded, and the corresponding solvo-dynamic 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 S3 Solvo-dynamic Radii of **M1** and **$(C_{70})_3$@M2**.

Compound	Diffusion Coefficient (m^2/s)	Solvo-dynamic radii (Å)	Non-solvated radii (from optimized structures) (Å)
M1	5.37×10^{-11}	20.4	21.6
Trifacial Tube	-	-	19.7
$(C_{70})_3$@M2	4.37×10^{-11}	25.1	25.8

The DOSY experiments were conducted at room temperature (T = 298 K) in DMSO. The coefficient of viscosity of DMSO at 298 K, η = 1.99 centipoise; Boltzmann constant (k_B) = 1.38 x 10^{-23} $m^2kgs^{-2}K^{-1}$.

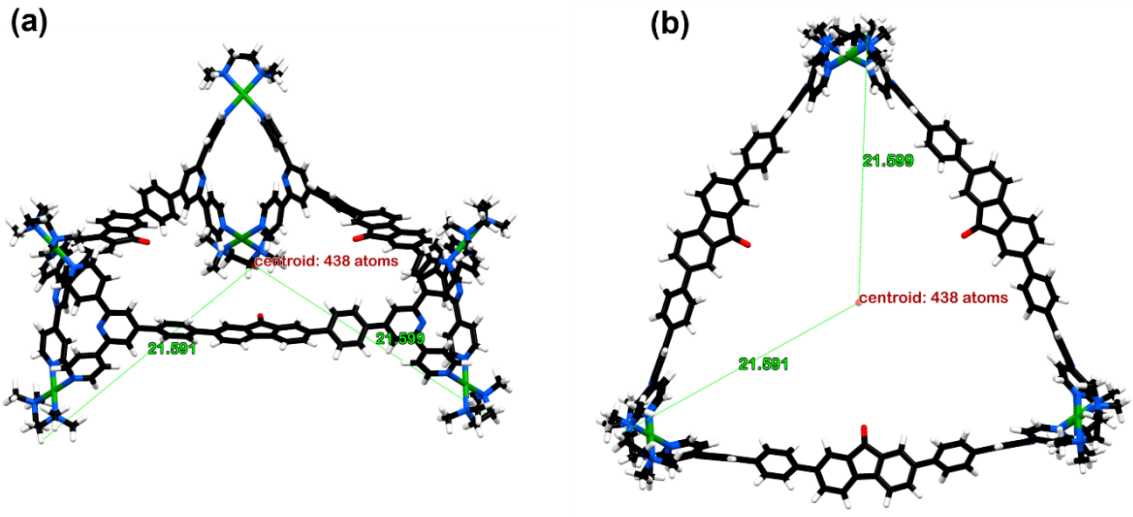


Fig. S47 Non-solvated radii of trifacial barrel **M1** obtained from DFT optimized structure.

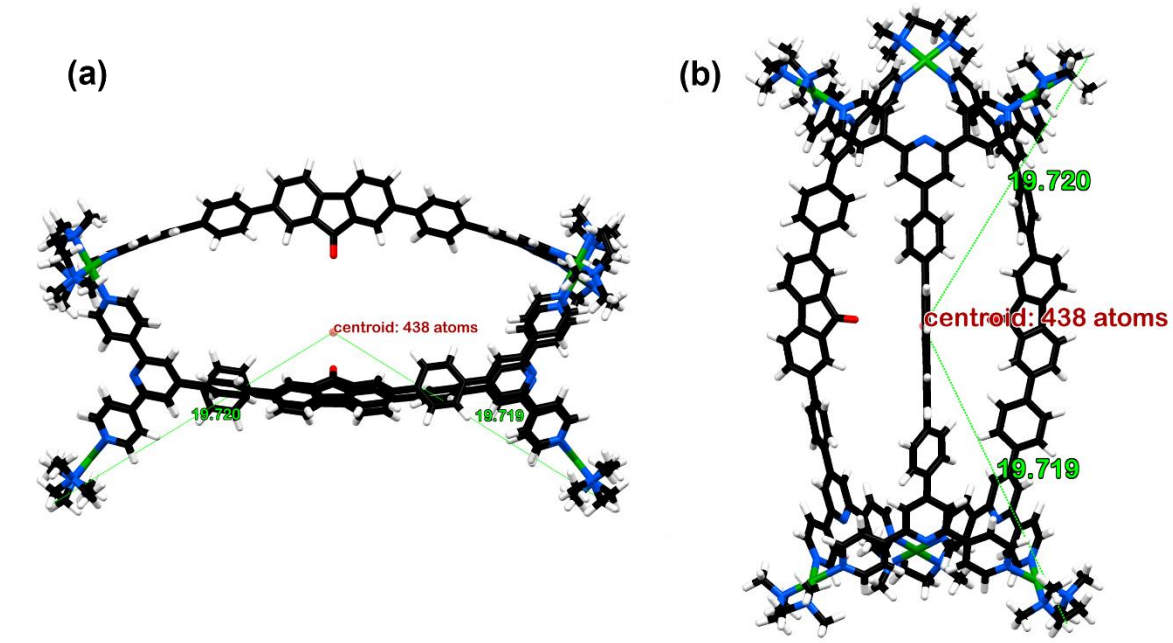


Fig. S48 Non-solvated radii of hypothetical trifacial tube obtained from DFT optimized structure.

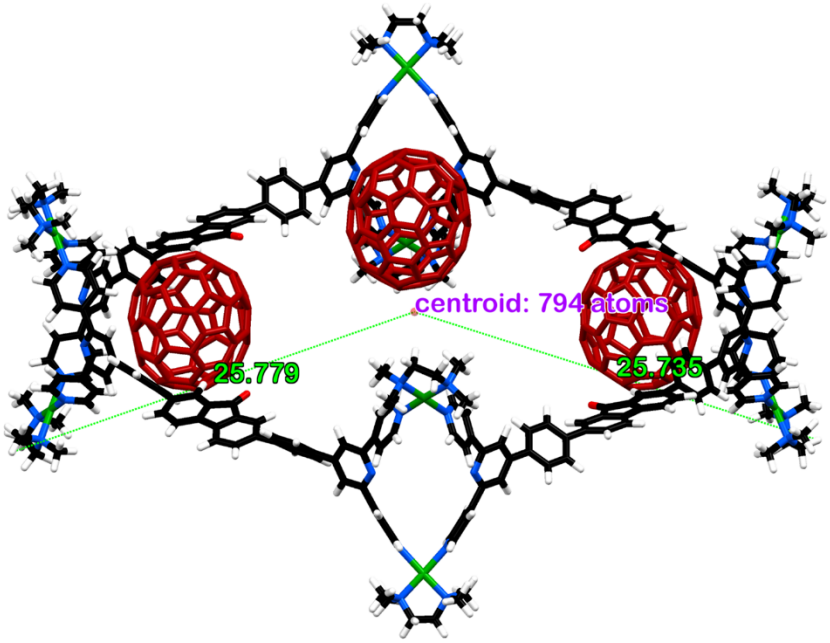


Fig. S49 Non-solvated radii of **$(C_{70})_3$@M2** obtained from optimized structure.

7. HOMO and LUMO calculations of $(C_{70})_3$@M2

HOMO and LUMO of **$(C_{70})_3$@M2** were analyzed. HOMO was composed of host cage (**M2**) orbitals while LUMO was distributed on **C_{70}** which indicates the tendency of photo-induced electron transfer (PET) from cage **M2** to **C_{70}**.

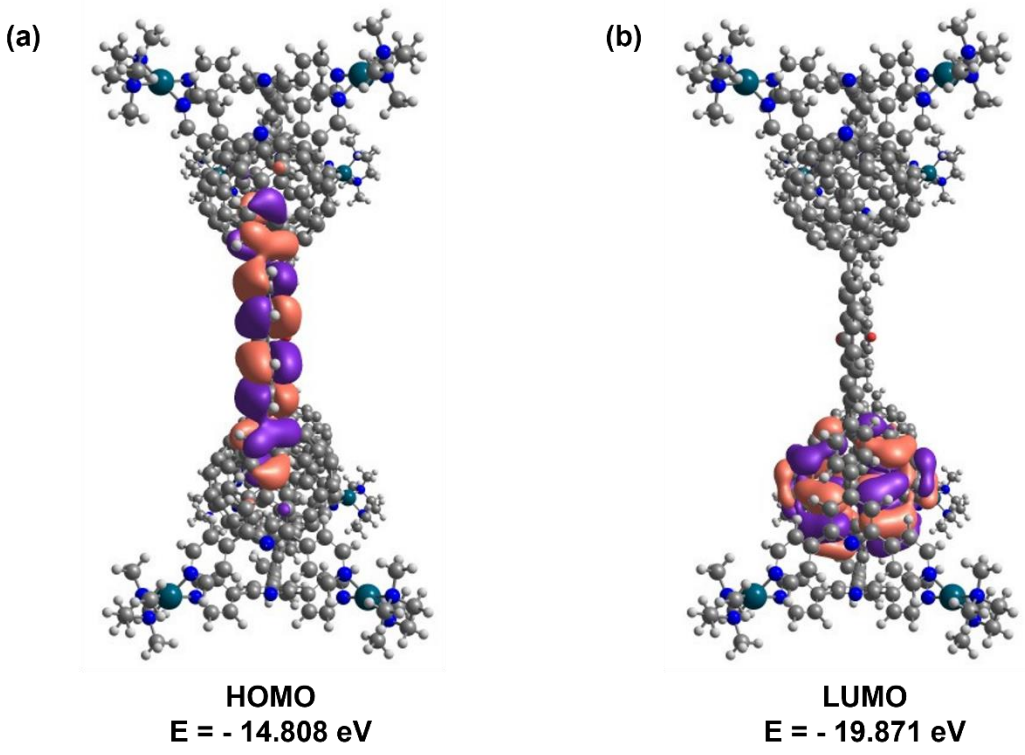


Fig. S50 HOMO and LUMO of **$(C_{70})_3$@M2**.

8. TD calculations for $(C_{70})_3$@M2 and simulated electronic spectra

The Time Dependent (TD)-PM6 calculations were performed using Gaussian 09 package.[S2] STO-3G basis set was used for carrying out the TD-PM6 calculations on the optimized geometry of **$(C_{70})_3$@M2**. The first six transitions and the simulated electronic spectra (Figure S51) due to those transitions are given below:

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.2181 eV 1017.88 nm f=0.0000 <S2>=0.000**

1155 ->1296 -0.10242

1158 ->1293 0.10314

1203 ->1244 -0.21192

1214 ->1235 -0.27826

1214 ->1241 0.12652

1219 ->1238 0.28084

1228 ->1235 -0.25353

1228 ->1241 -0.30688

Excited State 2: Singlet-A 1.2181 eV 1017.86 nm f=0.0000 <S2>=0.000**

1154 ->1295 -0.10256

1157 ->1292 -0.10307

1202 ->1243 -0.21141

1213 ->1234 0.27812

1213 ->1240 -0.12679

1218 ->1237 -0.28090

1227 ->1234 -0.25389

1227 ->1240 -0.30661

Excited State 3: Singlet-A 1.2183 eV 1017.64 nm f=0.0000 <S2>=0.000**

1156 ->1291 0.10130

1201 ->1242 0.21121

1212 ->1233 -0.27717

1212 ->1239 0.12765

1215 ->1236 0.28076

1226 ->1233 -0.25464

1226 ->1239 -0.30625

Excited State 4: Singlet-A 1.7704 eV 700.30 nm f=0.0414 <S2>=0.000**

1180 ->1236 0.10006

1201 ->1291 -0.10612

1215 ->1233 0.20151

1215 ->1239 0.14018

1218 ->1234 -0.18037

1218 ->1240 -0.12692

1219 ->1235 0.10494

1226 ->1236 -0.22228

1227 ->1237 -0.20009

1228 ->1238 -0.11695

Excited State 5: Singlet-A 1.7709 eV 700.12 nm f=0.0813 <S2>=0.000**

1182 ->1238 0.11588

1203 ->1293 0.12390

1218 ->1234 0.16802

1218 ->1240 0.11643

1219 ->1235 0.23552

1219 ->1241 0.16326

1227 ->1237 0.18507

1228 ->1238 -0.25908

Excited State 6: Singlet-A 1.7728 eV 699.38 nm f=0.0087 <S2>=0.000**

1180 ->1236 -0.10393

1201 ->1291 0.10918

1215 ->1233 -0.20247

1215 ->1239 -0.13989

1218 ->1234 -0.15693

1218 ->1240 -0.10710

1219 ->1235 0.13104

1226 ->1236 0.22167

1227 ->1237 -0.17205

1228 ->1238 -0.14195

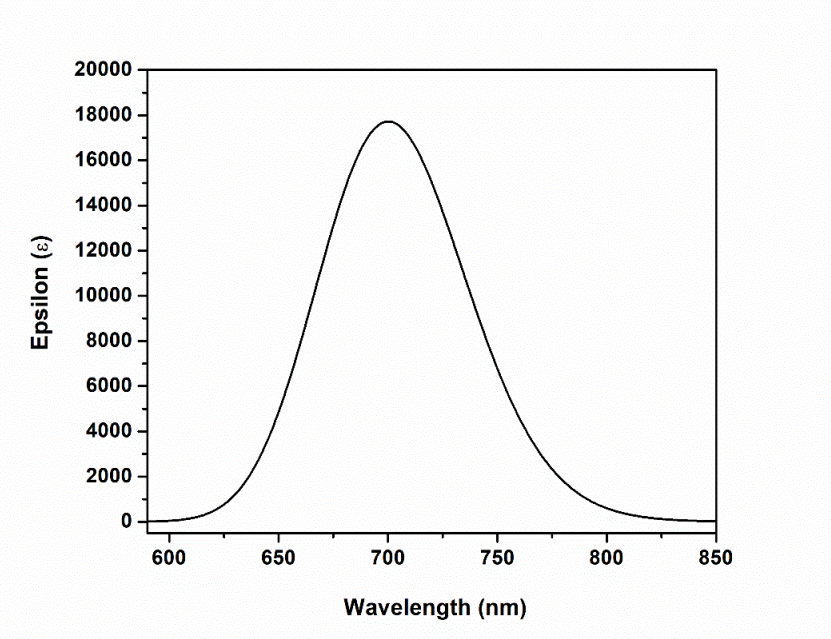


Fig. S51 Simulated electronic spectrum calculated from TD-PM6 calculations corresponding to the transitions in the red light region of visible light spectrum.

9. Optimization table for the oxidative cleavage of olefins

Table S4 Optimization conditions for the olefinic cleavage of S1 with O_2.

Entry	Catalyst (mol%)	Solvent	Light used [Wavelength](nm)	Time (h)	Yield (%)
1	$(C_{70})_3$@M2 (0.4)	MeCN	390	24	87
2	M1 (0.2)	MeCN	390	24	71
3	M1 (0.2)	MeCN	650	24	-
4	**$(C_{70})_3$@M2 (0.2)**	**MeCN**	**390**	**24**	**85**
5	**$(C_{70})_3$@M2 (0.2)**	**MeCN**	**650**	**24**	**74**
6	L (0.2)	MeCN	390	24	-
7	C_{70} (0.2)	MeCN	390	24	-
8	C_{70} (0.2)	MeCN	650	24	-
9	C_{70} (0.2)	Toluene	650	24	31
10	C_{70} (0.6)	Toluene	650	24	43
11	No catalyst	MeCN	390	24	-
12[a]	$(C_{70})_3$@M2 (0.2)	MeCN	390	24	-
13[b]	$(C_{70})_3$@M2 (0.2)	MeCN	390	28	69
14	L (0.2)	DMSO	390	24	51
15	L (0.2)	MeCN	390	24	-
16	No catalyst	MeCN	650	24	-
17	$(C_{70})_3$@M2 (0.2)	DMSO	650	24	65
18	$(C_{70})_3$@M2 (0.2)	MeCN	White light	24	80
19	L (0.6)	DMSO	390	24	63

[a]In the absence of light, [b]In normal air without any external oxygen balloon.

Measurement of solid catalyst using a weighing balance

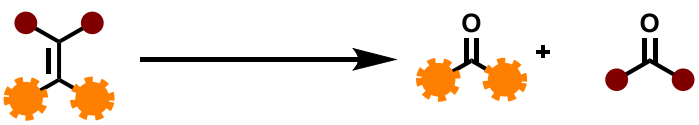
Catalyst Name	Molecular Weight	Catalyst (mol%)	Weight taken (for 0.2 mmol substrate)
$(C_{70})_3$@M2	9792.82	0.2	~3.9 mg
$(C_{70})_3$@M2	9792.82	0.4	~7.8 mg
M1	5454.61	0.2	~2.1 mg
L	794.28	0.2	~0.3 mg
L	794.28	0.6	~1.0 mg
C_{70}	840.77	0.2	~0.3 mg
C_{70}	840.77	0.6	~1.0 mg

10. General procedure

10.1 General procedure for oxidative cleavage of small alkene molecule

An oven-dried, screw-capped reaction tube (containing magnetic stir-bar) was charged with corresponding alkene (0.2 mmol) and catalyst (0.2 mol%) in 1.5 mL of acetonitrile (MeCN) solvent. The catalyst amount 3.9 mg [for **$(C_{70})_3$@M2**] was weighed in its solid form by a weighing balance. Alkenes, which are liquid in nature, are added after the addition of solvent. Finally, the reaction tube was placed inside the *EvoluChem* photoreactor (18 W, 390 nm or 650 nm HepatoChem lamp) and the reaction mixture was stirred for 24 h. The room temperature was maintained via the cooling system of the reactor. Upon completion, the mixture was diluted with ethyl acetate and evaporated under reduced pressure and the crude mixture was purified by column chromatography using silica (60-120 mesh size) and hexane/ethyl acetate as the eluent.

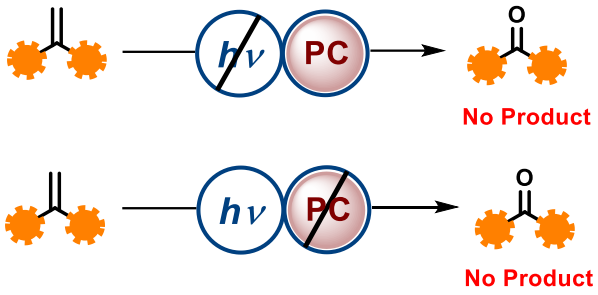
10.2 General procedure for the oxidative cleavage of bulky alkene molecule



An oven-dried, screw-capped reaction tube (containing magnetic stir-bar) was charged with corresponding alkene (0.2 mmol) and catalyst (0.2 mol%) in 1 mL of acetonitrile (MeCN) + 0.5 mL of dichloromethane (DCM) solvent. Alkenes, which are liquid in nature, are added after

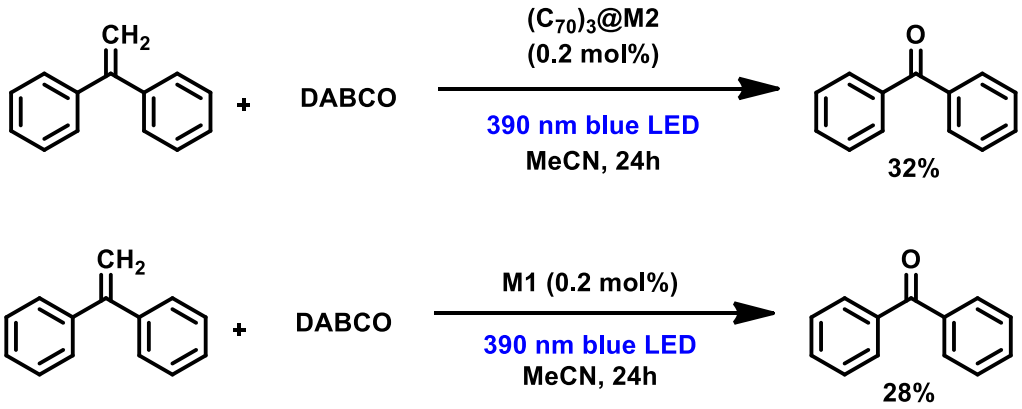
the addition of solvent. Finally, the reaction tube was placed inside the *EvoluChem* photoreactor (18 W, 390 nm or 650 nm HepatoChem lamp) while stirring for 24 h. The temperature was maintained via the cooling system of the reactor. Upon completion, the mixture was diluted with ethyl acetate and evaporated under reduced pressure and the crude mixture was purified by column chromatography using silica (60-120 mesh size) and hexane/ethyl acetate as the eluent.

11. Control experiments

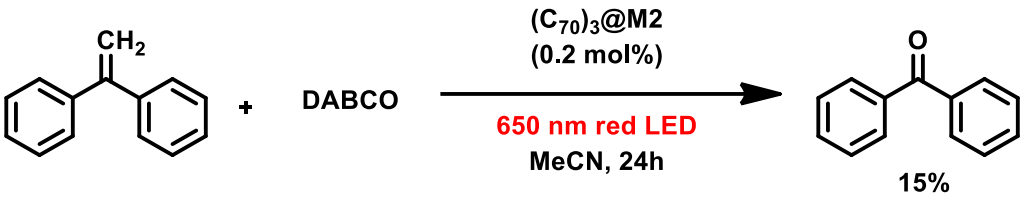


When the reaction was performed in the absence of photocatalyst **$(C_{70})_3$@M2,** keeping other optimized conditions identical, no product formation was observed. The same was true when LED light eliminated was from the optimized reaction condition. These experiments clearly indicate that both **$(C_{70})_3$@M2** and **LED light** source are indispensable for the reaction to take place.

Control reactions for singlet oxygen quenching

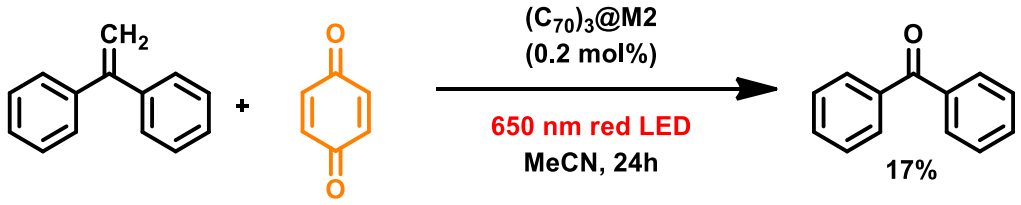


An oven-dried, screw-capped reaction tube (containing magnetic stir-bar) was charged with diphenylethylene (0.2 mmol), catalyst (0.2 mol%), and DABCO (2 eq.) in 1.5 mL of MeCN solvent. Finally, the reaction tube was placed inside the EvoluChem photoreactor (18 W, 390 nm HepatoChem lamp) and the reaction mixture was stirred for 24 h. The temperature was maintained via the cooling system of the reactor. Reduced amount of product formation was observed.



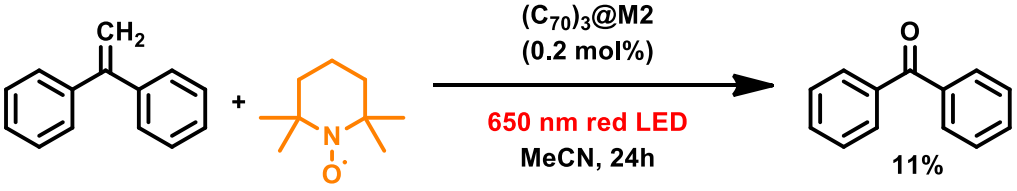
An oven-dried, screw-capped reaction tube (containing magnetic stir-bar) was charged with diphenylethylene (0.2 mmol), catalyst (0.2 mol%), and DABCO (2 eq.) in 1.5 mL of acetonitrile (MeCN) solvent. Finally, the reaction tube was placed inside the EvoluChem photoreactor (18 W, 650 nm HepatoChem lamp) and the reaction mixture was stirred for 24 h. The room temperature was maintained via the cooling system of the reactor. Non negligible product formation was observed.

Control reaction for superoxide radical quenching



An oven-dried, screw-capped reaction tube (containing magnetic stir-bar) was charged with diphenylethylene (0.2 mmol), catalyst (0.2 mol%), and *p*-benzoquinone (2 eq.) in 1.5 mL of acetonitrile solvent. Finally, the reaction tube was placed inside the EvoluChem photoreactor (18 W, 650 nm HepatoChem lamp) and the reaction mixture was stirred for 24 h. The room temperature was maintained via the cooling system of the reactor. Non negligible product formation was observed at the end of the reaction.

Control experiment to prove radical-based rection



An oven-dried, screw-capped reaction tube (containing magnetic stir-bar) was charged with diphenylethylene (0.2 mmol), catalyst (0.2 mol%), and TEMPO (2 eq.) in 1.5 mL of acetonitrile solvent. Finally, the reaction tube was placed inside the EvoluChem photoreactor (18 W, 650 nm HepatoChem lamp) and the reaction mixture was stirred for 24 h. The room temperature was maintained via the cooling system of the reactor. Low amount of product formation was observed at the end of the reaction.

Control reactions to find out the exact role of M2

An oven-dried, screw-capped reaction tube (containing magnetic stir-bar) was charged with diphenylethylene (0.2 mmol), C_{70} (0.2 mol%) + fluorenone (1 mol%), in 1.5 mL of toluene solvent. Finally, the reaction tube was placed inside the EvoluChem photoreactor (18 W, 650 nm HepatoChem lamp) and the reaction mixture was stirred for 24 h. The room temperature was maintained via the cooling system of the reactor. 26% product formation was observed at the end of the reaction.

Gram scale reaction

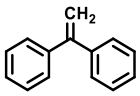
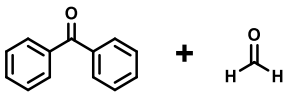
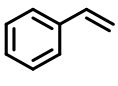
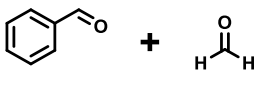
An oven-dried, screw-capped reaction tube (containing magnetic stir-bar) was charged with diphenylethylene (2.5 mmol), catalyst (0.2 mol%) in 5 mL of MeCN solvent. Finally, the reaction tube was placed inside the EvoluChem photoreactor (18 W, 650 nm HepatoChem lamp) and the reaction mixture was stirred for 24 h. The temperature was maintained via the cooling system of the reactor. From the crude NMR, we obtained a 45% NMR yield taking TMB as an internal standard.

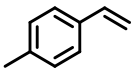
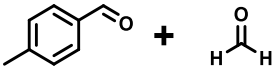
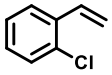
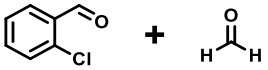
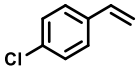
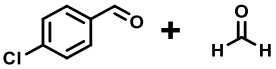
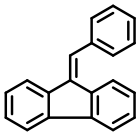
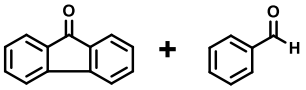
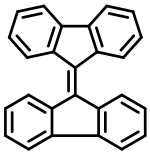
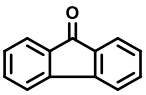
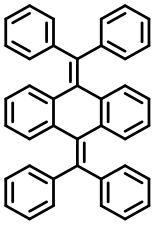
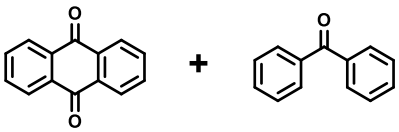
12. Substrate scope

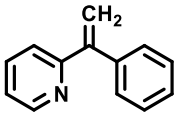
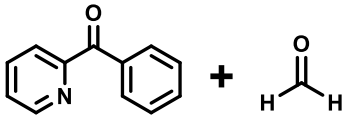
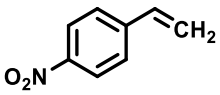
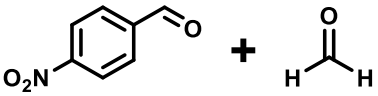
12.1 Substrate scope using 390 nm blue LED

An oven-dried, screw-capped reaction tube (containing magnetic stir-bar) was charged with corresponding alkene (0.2 mmol) and catalyst (0.2 mol%) in 1.5 mL of MeCN solvent. Alkenes, which are liquid in nature, are added after the addition of solvent. Finally, the reaction tube was placed inside the EvoluChem photoreactor (18 W, 390 nm HepatoChem lamp) with stirring for 24 h. The temperature was maintained via the cooling system of the reactor. Upon completion, the mixture was diluted with ethyl acetate and evaporated under reduced pressure and the crude mixture was purified by column chromatography using silica (60-120 mesh size) and Hexane/ethyl acetate as the eluent.

Table S5 Substrates scope for **$(C_{70})_3$@M2** at optimized reaction conditions[#] under 390 nm irradiation.

Entry No.	*Alkene Substrates*	*Product/(s)*	*Yields*
1.	 **S1**	 **P1a** **P1b**	**P1a (85 %)**
2.	 **S2**	 **P2a** **P2b**	**P2a (79 %)**

3.	 **S3**	 **P3a** **P3b**	**P3a (71%)**
4.	 **S4**	 **P4a** **P4b**	**P4a (76 %)**
5.	 **S5**	 **P5a** **P5b**	**P5a (73 %)**
6.	 **S6**	 **P6a** **P6b**	**P6a (88 %)**
7.	 **S7**	 **P7**	**P7 (91 %)**
8.	 **S8**	 **P8a** **P8b**	**P8a (89 %)**

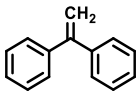
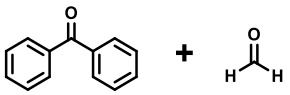
9.	 S9	 P9a P9b	P9a (45 %)
10.	 S10	 P10a P10b	P10a (74 %)*

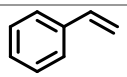
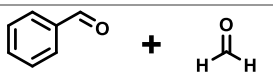
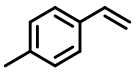
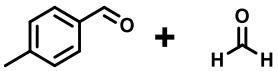
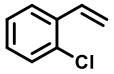
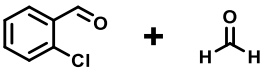
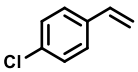
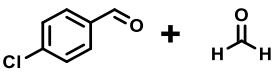
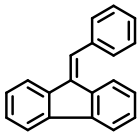
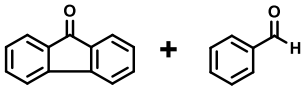
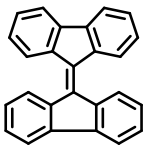
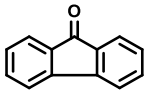
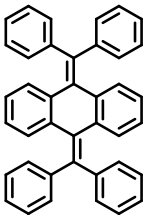
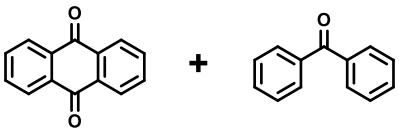
All reactions were carried out using 0.2 mol% of PF_6^- analogue of **$(C_{70})_3$@M2** as catalyst in acetonitrile (for substrates S7 and S8 acetonitrile-dichloromethane mixture was used) under oxygen balloon and irradiated with a light source of 390 nm for 24 h. *Control reaction carried out for substrate S10 in absence of the catalyst, keeping all other reaction conditions same, generated P10a in *ca.* 5% yield (crude NMR yield).

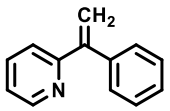
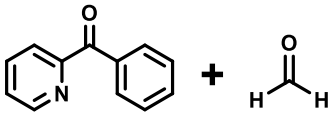
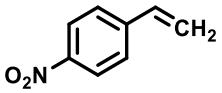
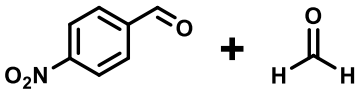
12.2 Substrates scope using 650 nm red LED

An oven-dried, screw-capped reaction tube (containing magnetic stir-bar) was charged with corresponding alkene (0.2 mmol) and catalyst (0.2 mol%) in 1.5 mL of MeCN solvent. Alkenes, which are liquid in nature, are added after the addition of solvent. Finally, the reaction tube was placed inside the EvoluChem photoreactor (18 W, 650 nm HepatoChem lamp) and the reaction mixture was stirred for 24 h. The temperature was maintained via the cooling system of the reactor. Upon completion, the mixture was diluted with ethyl acetate and evaporated under reduced pressure and the crude mixture was purified by column chromatography using silica (60-120 mesh size) and hexane/ethyl acetate as the eluent.

Table S6 Substrates scope for **$(C_{70})_3$@M2** at optimized reaction conditions[#] under 650 nm irradiation.

Entry No.	*Alkene Substrates*	*Product/(s)*	*Yields*
1.	 S1	 P1a P1b	P1a (74 %)

2.	 **S2**	 **P2a** **P2b**	**P2a (62 %)**
3.	 **S3**	 **P3a** **P3b**	**P3a (69%)**
4.	 **S4**	 **P4a** **P4b**	**P4a (63 %)**
5.	 **S5**	 **P5a** **P5b**	**P5a (61 %)**
6.	 **S6**	 **P6a** **P6b**	**P6a (58 %)**
7.	 **S7**	 **P7**	**P7 (32 %)**
8.	 **S8**	 **P8a** **P8b**	**Trace amount**

9.	 **S9**	 **P9a** **P9b**	**Trace amount**
10.	 **S10**	 **P10a** **P10b**	**P10a (21 %)**

All reactions were carried out using 0.2 mol% of PF_6^- analogue of **$(C_{70})_3$@M2** as catalyst in acetonitrile (for substrates S7 and S8 acetonitrile-dichloromethane mixture was used) under oxygen balloon and irradiation with a light source of 650 nm for 24 h.

13. Electron Paramagnetic Resonance (EPR) experiments in presence of ROS specific spin traps

The EPR experiments were conducted in presence of $^1O_2$ and $O_2^{\bullet-}$ specific spin traps, 2,2,6,6-tetramethylpiperidine (TEMP) and 5,5-dimethyl-1-pyrroline *N*-oxide (DMPO), respectively.

Two acetonitrile solutions of **$(C_{70})_3$@M2** were purged with oxygen and irradiated with a light source:

(i) One containing $^1O_2$ spin trap, 2,2,6,6-tetramethylpiperidine (TEMP) only.
(ii) Another containing $O_2^{\bullet-}$ spin trap, DMPO and olefin substrate, diphenylethylene (S1).

The EPR spectra of the solutions were recorded: Solution (i) gave a signal characteristic of TEMPO confirming $^1O_2$ generation. On the other hand, solution (ii) gave a signal characteristic of DMPO-OOH confirming $O_2^{\bullet-}$ generation.

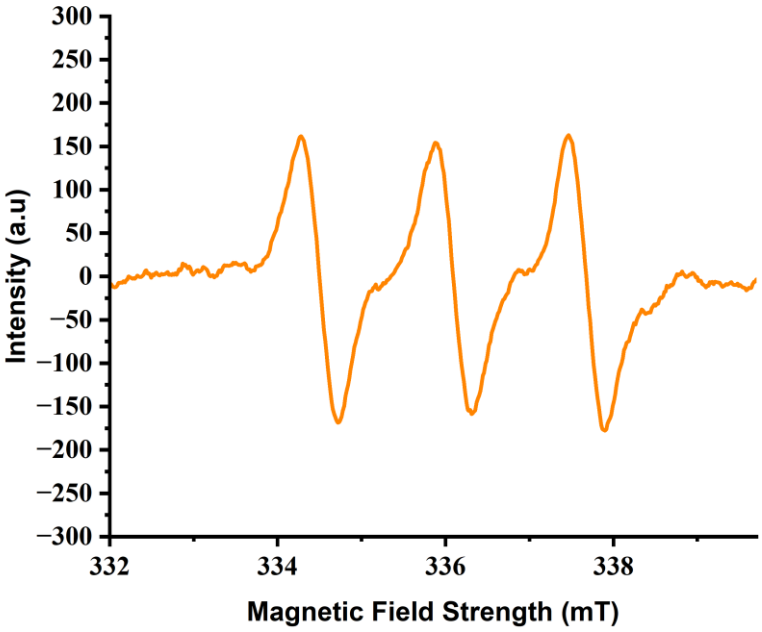


Fig. S52 EPR spectrum recorded after addition of TEMP to the light irradiated acetonitrile solution of **$(C_{70})_3$@M2** purged with oxygen. The generation of signal characteristic of TEMPO confirms $^1O_2$ generation.

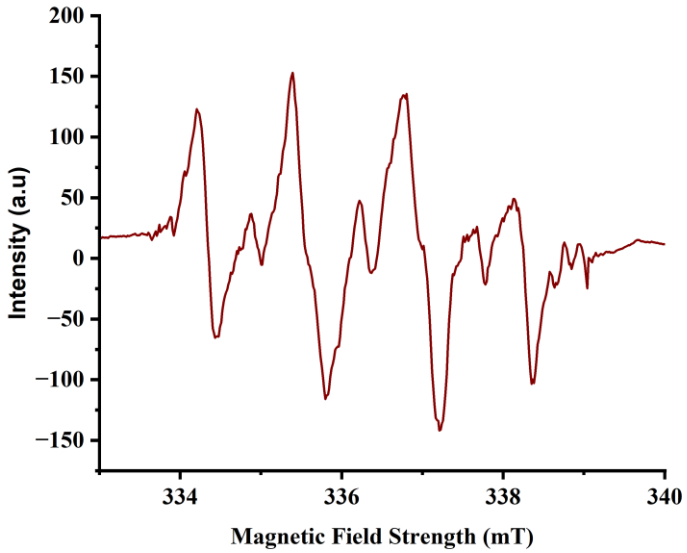


Fig. S53 EPR spectrum recorded after addition of DMPO to the light irradiated acetonitrile solution of **$(C_{70})_3$@M2** containing diphenylethylene purged with oxygen. The generation of signal characteristic of DMPO-OOH confirms $O_2^{\bullet-}$ generation.

14.1 Coordinates of DFT optimized structures

14.1.1. Trifacial barrel M1

Center Number	Atomic Number	Atomic Types	Coordinates (Å)		
			X	Y	Z
1	6	0	3.215263	13.07529	-0.04987
2	6	0	2.209371	12.09021	-0.03589
3	6	0	2.587553	10.72875	-0.00737
4	6	0	3.932843	10.40758	-0.00092
5	6	0	4.936301	11.40063	-0.00802
6	6	0	4.577364	12.74306	-0.03176
7	1	0	2.930049	14.12083	-0.04605
8	1	0	1.842445	9.940833	-0.01896
9	1	0	5.323064	13.52869	-0.03091
10	6	0	6.059793	9.332031	-0.00134
11	6	0	7.115827	8.438871	0.00492
12	6	0	8.436514	8.941206	0.034053
13	6	0	8.633711	10.33523	0.048873
14	6	0	7.558793	11.23539	0.030986
15	6	0	6.264842	10.72882	0.006597
16	1	0	6.922836	7.371746	0.015773
17	1	0	9.644856	10.72521	0.04538
18	1	0	7.749567	12.30163	0.030643
19	6	0	4.580666	9.047822	-0.00128
20	8	0	4.024579	7.948075	-0.00175
21	6	0	9.612209	8.02559	0.044674
22	6	0	10.70012	8.261028	0.906953
23	6	0	9.679319	6.914013	-0.81651
24	6	0	11.81022	7.421077	0.910172

25	1	0	10.66713	9.104603	1.585735
26	6	0	10.79635	6.082091	-0.8291
27	1	0	8.85883	6.720122	-1.49697
28	6	0	11.88052	6.320028	0.036194
29	1	0	12.64273	7.644387	1.568025
30	1	0	10.81611	5.229474	-1.49909
31	6	0	0.775109	12.49455	-0.0467
32	6	0	-0.16026	11.88935	0.813861
33	6	0	0.320288	13.51098	-0.90839
34	6	0	-1.49226	12.29631	0.826561
35	1	0	0.169542	11.11297	1.493792
36	6	0	-1.01407	13.90762	-0.9115
37	1	0	1.01948	13.98464	-1.58679
38	6	0	-1.94281	13.31134	-0.03801
39	1	0	-2.19092	11.80658	1.496088
40	1	0	-1.32734	14.71103	-1.56885
41	6	0	13.07661	5.442431	0.027044
42	6	0	13.64918	4.983526	-1.17691
43	6	0	13.69278	5.035211	1.227909
44	6	0	14.80804	4.199601	-1.1415
45	1	0	13.21418	5.2892	-2.11952
46	6	0	14.84276	4.240383	1.185651
47	1	0	13.26541	5.344115	2.17287
48	7	0	15.41135	3.865045	0.019839
49	6	0	-3.3583	13.75541	-0.02824
50	6	0	-4.06675	13.94413	1.176068
51	6	0	-4.05173	14.01186	-1.22865
52	6	0	-5.38461	14.41397	1.141498

53	1	0	-3.56259	13.77382	2.118407
54	6	0	-5.37308	14.46812	-1.18557
55	1	0	-3.55016	13.85102	-2.17395
56	7	0	-6.01182	14.70329	-0.01933
57	6	0	-6.20761	14.67592	-2.40277
58	6	0	-6.01173	13.97033	-3.60107
59	6	0	-7.31493	15.53949	-2.33762
60	6	0	-6.93437	14.09111	-4.6352
61	1	0	-5.17897	13.29036	-3.72308
62	6	0	-8.18589	15.63729	-3.40851
63	1	0	-7.49059	16.11017	-1.43803
64	7	0	-8.02703	14.89795	-4.54457
65	1	0	-6.81621	13.5239	-5.54872
66	1	0	-9.03917	16.30129	-3.37104
67	6	0	-6.21645	14.61707	2.361864
68	6	0	-7.31969	15.48654	2.298292
69	6	0	-6.01818	13.91839	3.563613
70	6	0	-8.1817	15.59992	3.374191
71	1	0	-7.49586	16.05119	1.39516
72	6	0	-6.9331	14.05376	4.603309
73	1	0	-5.18766	13.23619	3.687621
74	7	0	-8.01934	14.86954	4.515484
75	1	0	-9.02755	16.27313	3.339323
76	1	0	-6.81408	13.4897	5.518933
77	6	0	15.46558	3.649547	-2.36118
78	6	0	16.81869	3.27291	-2.29499
79	6	0	14.78735	3.397953	-3.5647
80	6	0	17.42177	2.64526	-3.37005

81	1	0	17.3763	3.463519	-1.39043
82	6	0	15.4394	2.74069	-4.60356
83	1	0	13.74663	3.66534	-3.69086
84	7	0	16.73909	2.345904	-4.51307
85	1	0	18.46455	2.360424	-3.33321
86	1	0	14.9162	2.504809	-5.5208
87	6	0	15.50331	3.690433	2.403167
88	6	0	16.85465	3.308367	2.338682
89	6	0	14.81788	3.430904	3.60104
90	6	0	17.44807	2.663708	3.409771
91	1	0	17.41925	3.504549	1.439501
92	6	0	15.46043	2.758289	4.63542
93	1	0	13.77701	3.700253	3.722577
94	7	0	16.75728	2.354404	4.545389
95	1	0	18.48819	2.368471	3.373008
96	1	0	14.93278	2.518234	5.548747
97	6	0	4.634373	-12.644	0.050462
98	6	0	3.525986	-11.7759	0.035017
99	6	0	3.751714	-10.381	0.005431
100	6	0	5.053372	-9.91347	-0.00058
101	6	0	6.160237	-10.7898	0.007933
102	6	0	5.951538	-12.1636	0.032717
103	1	0	4.466204	-13.7146	0.047504
104	1	0	2.924247	-9.6801	0.015919
105	1	0	6.779338	-12.8622	0.032962
106	6	0	7.048694	-8.60986	0.000122
107	6	0	7.999769	-7.60567	-0.0063
108	6	0	9.367825	-7.95929	-0.03441

109	6	0	9.717595	-9.32307	-0.04806
110	6	0	8.748518	-10.3363	-0.02995
111	6	0	7.406572	-9.97551	-0.00658
112	1	0	7.690268	-6.56635	-0.01811
113	1	0	10.76559	-9.59915	-0.04387
114	1	0	9.05573	-11.375	-0.02875
115	6	0	5.54724	-8.49055	-0.00082
116	8	0	4.873202	-7.45888	-0.00178
117	6	0	10.43539	-6.91962	-0.04513
118	6	0	11.54307	-7.0342	-0.90675
119	6	0	10.37906	-5.80686	0.815304
120	6	0	12.55382	-6.07702	-0.90999
121	1	0	11.60357	-7.87662	-1.58508
122	6	0	11.39761	-4.85692	0.827935
123	1	0	9.541744	-5.7041	1.495131
124	6	0	12.50191	-4.97444	-0.03665
125	1	0	13.40619	-6.20757	-1.56735
126	1	0	11.32285	-4.00686	1.497286
127	6	0	2.14504	-12.3359	0.045706
128	6	0	1.149184	-11.8385	-0.81608
129	6	0	1.804505	-13.395	0.90868
130	6	0	-0.12994	-12.3896	-0.82858
131	1	0	1.391877	-11.0315	-1.49702
132	6	0	0.521884	-13.9361	0.912001
133	1	0	2.551293	-13.7879	1.587961
134	6	0	-0.46645	-13.4468	0.037409
135	1	0	-0.87798	-11.9807	-1.49898
136	1	0	0.2986	-14.7681	1.570477

137	6	0	13.59418	-3.97058	-0.02729
138	6	0	14.11241	-3.45142	1.176805
139	6	0	14.16236	-3.49821	-1.22796
140	6	0	15.17821	-2.54502	1.141742
141	1	0	13.71329	-3.80296	2.119305
142	6	0	15.21806	-2.58187	-1.18538
143	1	0	13.77186	-3.85219	-2.17308
144	7	0	15.74166	-2.14632	-0.0194
145	6	0	-1.82465	-14.0435	0.028298
146	6	0	-2.50801	-14.3106	-1.17571
147	6	0	-2.48584	-14.3727	1.229149
148	6	0	-3.7665	-14.9219	-1.14036
149	1	0	-2.02541	-14.0874	-2.11829
150	6	0	-3.74923	-14.9711	1.186817
151	1	0	-2.00496	-14.1566	2.174171
152	7	0	-4.35832	-15.2764	0.020997
153	6	0	-4.55601	-15.2677	2.404307
154	6	0	-4.43911	-14.5431	3.601545
155	6	0	-5.56156	-16.248	2.340418
156	6	0	-5.34291	-14.7632	4.635927
157	1	0	-3.6862	-13.7755	3.722527
158	6	0	-6.41661	-16.4395	3.411476
159	1	0	-5.67315	-16.836	1.441763
160	7	0	-6.34009	-15.6856	4.546489
161	1	0	-5.28794	-14.1852	5.54869
162	1	0	-7.19163	-17.1934	3.37509
163	6	0	-4.57122	-15.2167	-2.36019
164	6	0	-5.57461	-16.1996	-2.29395

165	6	0	-4.44888	-14.5044	-3.56408
166	6	0	-6.41924	-16.4082	-3.36937
167	1	0	-5.68925	-16.7771	-1.38907
168	6	0	-5.34362	-14.7406	-4.60332
169	1	0	-3.69644	-13.7373	-3.6903
170	7	0	-6.33596	-15.6681	-4.51288
171	1	0	-7.18786	-17.1683	-3.33241
172	1	0	-5.28548	-14.1701	-5.52084
173	6	0	15.77089	-1.9263	2.361757
174	6	0	17.07507	-1.40473	2.296744
175	6	0	15.06814	-1.74966	3.564528
176	6	0	17.60524	-0.715	3.37221
177	1	0	17.65098	-1.53365	1.392753
178	6	0	15.64377	-1.0251	4.60379
179	1	0	14.06248	-2.12847	3.689736
180	7	0	16.8929	-0.49136	4.514505
181	1	0	18.61087	-0.31839	3.336161
182	1	0	15.09694	-0.84692	5.520272
183	6	0	15.81451	-1.96289	-2.40289
184	6	0	17.11625	-1.43604	-2.33875
185	6	0	15.1045	-1.7792	-3.60048
186	6	0	17.63562	-0.73041	-3.40989
187	1	0	17.69915	-1.56969	-1.43977
188	6	0	15.66965	-1.04036	-4.63488
189	1	0	14.09905	-2.16012	-3.72172
190	7	0	16.91488	-0.49781	-4.54524
191	1	0	18.63742	-0.32366	-3.37325
192	1	0	15.11855	-0.85858	-5.54782

193	6	0	-12.9366	-3.75397	-0.05109
194	6	0	-11.5806	-4.13288	-0.03659
195	6	0	-10.5904	-3.12489	-0.0085
196	6	0	-10.9845	-1.79915	-0.00292
197	6	0	-12.3462	-1.42629	-0.01046
198	6	0	-13.3295	-2.4081	-0.03383
199	1	0	-13.6996	-4.52355	-0.04708
200	1	0	-9.53553	-3.37651	-0.01972
201	1	0	-14.3827	-2.15483	-0.03334
202	6	0	-11.1159	0.580652	-0.00463
203	6	0	-10.87	1.941714	0.001181
204	6	0	-11.9651	2.834619	0.029969
205	6	0	-13.2711	2.308756	0.044867
206	6	0	-13.5136	0.927838	0.027392
207	6	0	-12.4282	0.060203	0.003383
208	1	0	-9.84925	2.307872	0.01205
209	1	0	-14.1143	2.989678	0.041301
210	1	0	-14.5325	0.560217	0.02723
211	6	0	-10.1305	-0.55849	-0.00405
212	8	0	-8.90002	-0.49059	-0.00404
213	6	0	-11.7596	4.31054	0.040535
214	6	0	-12.5073	5.135137	0.9028
215	6	0	-10.8303	4.924237	-0.82052
216	6	0	-12.3344	6.51642	0.906227
217	1	0	-13.2215	4.684912	1.581508
218	6	0	-10.6678	6.307521	-0.83291
219	1	0	-10.2522	4.310498	-1.50094
220	6	0	-11.4157	7.127628	0.03246

221	1	0	-12.9439	7.125832	1.564194
222	1	0	-9.93902	6.750797	-1.50269
223	6	0	-11.2139	-5.57723	-0.04661
224	6	0	-10.2225	-6.08441	0.814616
225	6	0	-11.8663	-6.47956	-0.90835
226	6	0	-9.90877	-7.4414	0.827742
227	1	0	-9.71541	-5.41036	1.49458
228	6	0	-11.5424	-7.83343	-0.91105
229	1	0	-12.6258	-6.11105	-1.58721
230	6	0	-10.562	-8.3393	-0.03706
231	1	0	-9.13556	-7.8014	1.497645
232	1	0	-12.0811	-8.50661	-1.5686
233	6	0	-11.2531	8.602189	0.023824
234	6	0	-11.1418	9.327968	-1.17985
235	6	0	-11.208	9.338906	1.224991
236	6	0	-11.0417	10.72348	-1.1438
237	1	0	-11.1896	8.798865	-2.12269
238	6	0	-11.094	10.73219	1.183369
239	1	0	-11.2618	8.813918	2.169728
240	7	0	-11.0531	11.41274	0.01782
241	6	0	-10.2381	-9.78704	-0.02751
242	6	0	-10.0481	-10.4954	1.176642
243	6	0	-10.1119	-10.5151	-1.22818
244	6	0	-9.79513	-11.8715	1.141627
245	1	0	-10.1539	-9.97409	2.119089
246	6	0	-9.84546	-11.8873	-1.18557
247	1	0	-10.2229	-9.99983	-2.1733
248	7	0	-9.73033	-12.5586	-0.01958

249	6	0	-9.60642	-12.7131	-2.40303
250	6	0	-9.09236	-12.1895	-3.60042
251	6	0	-9.80012	-14.104	-2.33912
252	6	0	-8.73426	-13.048	-4.63487
253	1	0	-8.9203	-11.1282	-3.7215
254	6	0	-9.44789	-14.9062	-3.41027
255	1	0	-10.2074	-14.5423	-1.44036
256	7	0	-8.88621	-14.3978	-4.54542
257	1	0	-8.30143	-12.6612	-5.54768
258	1	0	-9.59576	-15.9772	-3.37381
259	6	0	-9.55565	-12.6941	2.361715
260	6	0	-9.75331	-14.0847	2.29605
261	6	0	-9.05402	-12.1732	3.565371
262	6	0	-9.42095	-14.8884	3.371697
263	1	0	-10.1509	-14.5194	1.39141
264	6	0	-8.71413	-13.0337	4.604838
265	1	0	-8.88159	-11.1126	3.69123
266	7	0	-8.87371	-14.3826	4.514922
267	1	0	-9.57808	-15.9579	3.33512
268	1	0	-8.28859	-12.6486	5.522069
269	6	0	-10.8942	11.56847	-2.36312
270	6	0	-11.2448	12.92851	-2.29644
271	6	0	-10.337	11.10744	-3.56678
272	6	0	-11.0028	13.76507	-3.37116
273	1	0	-11.6889	13.31574	-1.39184
274	6	0	-10.0939	12.0012	-4.60529
275	1	0	-10.0481	10.07254	-3.69331
276	7	0	-10.402	13.32408	-4.51429

277	1	0	-11.2777	14.81049	-3.33397
278	1	0	-9.628	11.66643	-5.52266
279	6	0	-10.9475	11.57849	2.401333
280	6	0	-11.2905	12.94028	2.337299
281	6	0	-10.3814	11.11336	3.599409
282	6	0	-11.0287	13.77565	3.40901
283	1	0	-11.7414	13.33213	1.43791
284	6	0	-10.12	12.00529	4.634466
285	1	0	-10.0956	10.07687	3.720677
286	7	0	-10.417	13.33076	4.544933
287	1	0	-11.2917	14.8244	3.372509
288	1	0	-9.64927	11.66733	5.547937
289	6	0	19.32778	1.789052	-8.10557
290	6	0	18.80057	0.421106	-8.49488
291	1	0	20.26949	1.711344	-7.55803
292	1	0	19.4925	2.416557	-8.98898
293	1	0	17.8801	0.500525	-9.07727
294	1	0	19.53811	-0.13382	-9.08598
295	7	0	18.31714	2.473929	-7.18216
296	7	0	18.47217	-0.37065	-7.22698
297	6	0	17.56323	-1.52846	-7.60083
298	1	0	18.06345	-2.15146	-8.35094
299	1	0	17.36263	-2.12365	-6.71115
300	1	0	16.63342	-1.1355	-8.01656
301	6	0	19.747	-0.93783	-6.61835
302	1	0	19.48548	-1.50182	-5.72251
303	1	0	20.22467	-1.60771	-7.34231
304	1	0	20.43276	-0.12906	-6.36405

305	6	0	17.16888	3.04913	-7.99699
306	1	0	16.47065	3.540165	-7.31845
307	1	0	17.56367	3.786743	-8.70493
308	1	0	16.66179	2.253604	-8.54387
309	6	0	19.01663	3.616684	-6.46426
310	1	0	19.42518	4.311577	-7.20661
311	1	0	18.29526	4.137111	-5.83621
312	1	0	19.83025	3.215226	-5.85743
313	46	0	17.59571	0.987019	-5.88121
314	6	0	19.40528	0.346894	8.106915
315	6	0	18.73321	1.650357	8.494305
316	1	0	20.33302	0.525151	7.559033
317	1	0	19.63701	-0.25774	8.991236
318	1	0	17.82692	1.472646	9.077245
319	1	0	19.40651	2.282766	9.084256
320	7	0	18.47455	-0.44473	7.18477
321	7	0	18.32067	2.400017	7.225439
322	6	0	17.29241	3.453618	7.598494
323	1	0	17.72318	4.127874	8.347372
324	1	0	17.02817	4.022551	6.708267
325	1	0	16.41065	2.963368	8.01559
326	6	0	19.52636	3.100864	6.615074
327	1	0	19.20494	3.631125	5.718111
328	1	0	19.9285	3.820308	7.337368
329	1	0	20.29596	2.37094	6.362235
330	6	0	17.39536	-1.13957	8.000749
331	1	0	16.75458	-1.7046	7.323109
332	1	0	17.8677	-1.82876	8.710002

333	1	0	16.80496	-0.40268	8.546178
334	6	0	19.29363	-1.50608	6.468405
335	1	0	19.77499	-2.15157	7.211711
336	1	0	18.63284	-2.10253	5.841279
337	1	0	20.05903	-1.01982	5.860866
338	46	0	17.5957	0.953507	5.882269
339	6	0	-11.2131	15.84782	-8.10457
340	6	0	-9.76471	16.07639	-8.49279
341	1	0	-11.6173	16.7013	-7.55615
342	1	0	-11.8383	15.67756	-8.98852
343	1	0	-9.37258	15.24058	-9.07627
344	1	0	-9.65306	16.99349	-9.08251
345	7	0	-11.3008	14.62898	-7.18274
346	7	0	-8.91551	16.18656	-7.22434
347	6	0	-7.45801	15.98006	-7.59799
348	1	0	-7.16899	16.7263	-8.34671
349	1	0	-6.84261	16.1029	-6.70791
350	1	0	-7.33243	14.97918	-8.01544
351	6	0	-9.06279	17.57338	-6.61391
352	1	0	-8.44453	17.62785	-5.71738
353	1	0	-8.72085	18.323	-7.33652
354	1	0	-10.1064	17.76253	-6.36038
355	6	0	-11.2239	13.348	-7.9992
356	1	0	-11.3007	12.4969	-7.32187
357	1	0	-12.0594	13.32199	-8.70802
358	1	0	-10.2809	13.3074	-8.54521
359	6	0	-12.6406	14.66208	-6.46553
360	1	0	-13.4462	14.66921	-7.20833

361	1	0	-12.7308	13.77628	-5.8387
362	1	0	-12.7002	15.56662	-5.85755
363	46	0	-9.65298	14.74653	-5.88095
364	6	0	-9.99962	16.6228	8.110794
365	6	0	-10.793	15.38898	8.496766
366	1	0	-10.6177	17.33833	7.564321
367	1	0	-9.5911	17.12425	8.99564
368	1	0	-10.1863	14.69178	9.078635
369	1	0	-11.6771	15.65561	9.08727
370	7	0	-8.84932	16.21339	7.187523
371	7	0	-11.2367	14.65884	7.227035
372	6	0	-11.6353	13.24115	7.598093
373	1	0	-12.4337	13.27616	8.34792
374	1	0	-11.9971	12.7295	6.707398
375	1	0	-10.7696	12.7216	8.013323
376	6	0	-12.4463	15.354	6.617979
377	1	0	-12.7455	14.81177	5.720491
378	1	0	-13.2702	15.34222	7.340569
379	1	0	-12.1984	16.38562	6.366269
380	6	0	-7.70782	15.62457	8.002171
381	1	0	-6.89839	15.35295	7.323853
382	1	0	-7.34666	16.37705	8.712433
383	1	0	-8.05081	14.74412	8.546414
384	6	0	-8.33943	17.45437	6.472989
385	1	0	-8.02064	18.19267	7.217404
386	1	0	-7.49277	17.18108	5.845169
387	1	0	-9.14328	17.87536	5.866365
388	46	0	-9.62201	14.75543	5.88321

389	6	0	-9.03216	-16.4865	-8.49654
390	6	0	-8.11282	-17.6285	-8.10751
391	1	0	-8.50182	-15.7292	-9.07789
392	1	0	-9.8815	-16.8463	-9.08859
393	1	0	-8.6524	-18.405	-7.56103
394	1	0	-7.65164	-18.0848	-8.99092
395	7	0	-9.55382	-15.8067	-7.22849
396	7	0	-7.01435	-17.098	-7.18279
397	6	0	-6.37674	-18.2767	-6.46545
398	1	0	-5.97976	-18.9779	-7.20815
399	1	0	-5.56522	-17.914	-5.8365
400	1	0	-7.13244	-18.78	-5.85964
401	6	0	-5.94034	-16.3921	-7.99619
402	1	0	-5.16536	-16.0357	-7.31689
403	1	0	-5.5003	-17.1026	-8.70519
404	1	0	-6.37377	-15.5534	-8.5418
405	6	0	-10.684	-16.6263	-6.62134
406	1	0	-11.0417	-16.1179	-5.72545
407	1	0	-11.5025	-16.7034	-7.34602
408	1	0	-10.328	-17.6252	-6.36738
409	6	0	-10.1003	-14.4398	-7.60178
410	1	0	-10.8889	-14.5602	-8.35317
411	1	0	-10.5164	-13.9689	-6.71231
412	1	0	-9.29388	-13.8314	-8.01574
413	46	0	-7.94058	-15.7293	-5.88164
414	6	0	-9.40104	-16.9775	8.108159
415	6	0	-7.93626	-17.0431	8.496626
416	1	0	-9.7078	-17.8713	7.560836

417	1	0	-10.0414	-16.8767	8.991909
418	1	0	-7.63956	-16.1679	9.078785
419	1	0	-7.72333	-17.9412	9.087696
420	7	0	-9.62367	-15.7771	7.184778
421	7	0	-7.07985	-17.0598	7.228347
422	6	0	-5.65448	-16.6918	7.601672
423	1	0	-5.28418	-17.4004	8.351205
424	1	0	-5.02913	-16.7462	6.7117
425	1	0	-5.64126	-15.6827	8.018009
426	6	0	-7.07176	-18.4551	6.61951
427	1	0	-6.45133	-18.4412	5.722914
428	1	0	-6.64839	-19.1612	7.342814
429	1	0	-8.08775	-18.7595	6.366341
430	6	0	-9.69022	-14.4945	7.999587
431	1	0	-9.86071	-13.6581	7.321089
432	1	0	-10.5238	-14.5607	8.707964
433	1	0	-8.75791	-14.3486	8.546009
434	6	0	-10.9512	-15.9601	6.467326
435	1	0	-11.7512	-16.0564	7.209962
436	1	0	-11.1394	-15.0905	5.839637
437	1	0	-10.9093	-16.8662	5.860223
438	46	0	-7.97261	-15.7123	5.883229

14.1.2. Trifacial tube

Center Number	Atomic Number	Atomic Types	Coordinates (Å)		
			X	Y	Z
1	6	0	-3.04319	-8.20745	3.009436

2	6	0	-3.48687	-6.96553	2.517301
3	6	0	-2.52781	-5.99269	2.157022
4	6	0	-1.18685	-6.28855	2.300599
5	6	0	-0.74441	-7.53865	2.786472
6	6	0	-1.67803	-8.50519	3.143444
7	1	0	-3.77241	-8.96733	3.265451
8	1	0	-2.82977	-5.01479	1.798644
9	1	0	-1.37444	-9.47667	3.513896
10	6	0	1.188734	-6.26532	2.362935
11	6	0	2.529689	-5.94752	2.278312
12	6	0	3.48875	-6.91917	2.641754
13	6	0	3.04509	-8.18071	3.081196
14	6	0	1.679935	-8.49367	3.174338
15	6	0	0.746308	-7.52894	2.812505
16	1	0	2.831655	-4.97322	1.910248
17	1	0	3.774321	-8.92305	3.384301
18	1	0	1.376349	-9.47098	3.529129
19	6	0	0.00093	-5.41506	2.01096
20	8	0	0.000906	-4.25924	1.580923
21	6	0	4.941289	-6.60497	2.559237
22	6	0	5.862343	-7.52658	2.025646
23	6	0	5.430109	-5.3618	3.004232
24	6	0	7.214393	-7.20978	1.916923
25	1	0	5.510331	-8.49017	1.677581
26	6	0	6.782392	-5.04873	2.913452
27	1	0	4.741499	-4.64719	3.438623
28	6	0	7.69636	-5.96327	2.357446
29	1	0	7.901995	-7.94731	1.517891

30	1	0	7.127179	-4.07598	3.246914
31	6	0	-4.93942	-6.67378	2.37457
32	6	0	-5.42836	-6.02354	1.225416
33	6	0	-5.86037	-7.02268	3.380825
34	6	0	-6.78065	-5.72716	1.089734
35	1	0	-4.73984	-5.76647	0.429549
36	6	0	-7.21242	-6.7118	3.256264
37	1	0	-5.50827	-7.52463	4.273933
38	6	0	-7.69451	-6.05607	2.108334
39	1	0	-7.12549	-5.20867	0.201711
40	1	0	-7.89992	-7.00932	4.040361
41	6	0	9.124372	-5.59332	2.213485
42	6	0	9.817125	-4.91526	3.231728
43	6	0	9.836784	-5.86376	1.032508
44	6	0	11.14767	-4.52294	3.039497
45	1	0	9.303634	-4.71793	4.161831
46	6	0	11.16041	-5.42869	0.891106
47	1	0	9.326616	-6.37646	0.229722
48	7	0	11.80108	-4.76258	1.879351
49	6	0	-9.12252	-5.68188	1.975773
50	6	0	-9.81531	-5.83344	0.761856
51	6	0	-9.8349	-5.11538	3.04674
52	6	0	-11.1459	-5.41091	0.651258
53	1	0	-9.30182	-6.29145	-0.07137
54	6	0	-11.1585	-4.69354	2.86968
55	1	0	-9.32477	-4.97946	3.989549
56	7	0	-11.7993	-4.83471	1.686342
57	6	0	-11.9149	-4.01561	3.964853

58	6	0	-11.3727	-3.77315	5.239901
59	6	0	-13.2261	-3.56195	3.737931
60	6	0	-12.1115	-3.08885	6.195577
61	1	0	-10.3807	-4.10662	5.509026
62	6	0	-13.9169	-2.88339	4.731015
63	1	0	-13.6854	-3.74867	2.778529
64	7	0	-13.3714	-2.63188	5.955952
65	1	0	-11.6977	-2.90085	7.177176
66	1	0	-14.925	-2.52826	4.562601
67	6	0	-11.906	-5.55337	-0.62659
68	6	0	-13.1897	-4.99268	-0.7479
69	6	0	-11.3989	-6.22501	-1.75342
70	6	0	-13.8867	-5.08377	-1.94332
71	1	0	-13.6239	-4.49172	0.104604
72	6	0	-12.1421	-6.28337	-2.92516
73	1	0	-10.4361	-6.71589	-1.73731
74	7	0	-13.3743	-5.71508	-3.03878
75	1	0	-14.8751	-4.65595	-2.04408
76	1	0	-11.7537	-6.79645	-3.79502
77	6	0	11.90763	-3.79623	4.100295
78	6	0	13.19078	-3.2912	3.825782
79	6	0	11.40085	-3.57017	5.392607
80	6	0	13.88763	-2.57947	4.790717
81	1	0	13.6248	-3.46768	2.852771
82	6	0	12.14384	-2.84919	6.318253
83	1	0	10.43856	-3.95348	5.70115
84	7	0	13.37552	-2.34342	6.03298
85	1	0	14.87563	-2.18872	4.587467

86	1	0	11.75574	-2.67077	7.312381
87	6	0	11.91672	-5.63061	-0.38103
88	6	0	13.2275	-5.1378	-0.50612
89	6	0	11.3748	-6.28085	-1.50443
90	6	0	13.91791	-5.2723	-1.70155
91	1	0	13.68669	-4.65193	0.34202
92	6	0	12.11319	-6.38641	-2.67532
93	1	0	10.38331	-6.71027	-1.48986
94	7	0	13.37248	-5.88254	-2.79306
95	1	0	14.92564	-4.8925	-1.80644
96	1	0	11.6995	-6.8859	-3.54107
97	6	0	3.043142	6.757402	5.545753
98	6	0	3.486778	5.747223	4.671596
99	6	0	2.527701	4.94744	4.010899
100	6	0	1.18676	5.179208	4.244295
101	6	0	0.744358	6.19919	5.115218
102	6	0	1.677997	6.99415	5.770687
103	1	0	3.772384	7.390447	6.037873
104	1	0	2.829645	4.14238	3.350126
105	1	0	1.37443	7.789155	6.440756
106	6	0	-1.18881	5.136519	4.295878
107	6	0	-2.52978	4.864357	4.111312
108	6	0	-3.48879	5.661861	4.774834
109	6	0	-3.0451	6.708034	5.605542
110	6	0	-1.67994	6.972827	5.796541
111	6	0	-0.74635	6.18132	5.136833
112	1	0	-2.83178	4.06585	3.44266
113	1	0	-3.77432	7.308992	6.136415

114	1	0	-1.37632	7.778593	6.453606
115	6	0	-0.00105	4.449818	3.68322
116	8	0	-0.00109	3.500679	2.895838
117	6	0	-4.94133	5.392417	4.59341
118	6	0	-5.86238	6.438391	4.393366
119	6	0	-5.43014	4.072041	4.603784
120	6	0	-7.2144	6.175112	4.186204
121	1	0	-5.51036	7.462858	4.382358
122	6	0	-6.7824	3.806366	4.414779
123	1	0	-4.74151	3.254201	4.778365
124	6	0	-7.69636	4.853059	4.191198
125	1	0	-7.90199	7.002953	4.052473
126	1	0	-7.12716	2.778045	4.408898
127	6	0	4.939306	5.518875	4.440534
128	6	0	5.428168	5.283824	3.141221
129	6	0	5.860305	5.516489	5.505505
130	6	0	6.78042	5.048633	2.915349
131	1	0	4.739593	5.303535	2.305143
132	6	0	7.21232	5.263935	5.285351
133	1	0	5.50826	5.69595	6.51418
134	6	0	7.694328	5.023232	3.985403
135	1	0	7.125193	4.851808	1.906028
136	1	0	7.899859	5.286225	6.123664
137	6	0	-9.12432	4.551266	3.933047
138	6	0	-9.81727	3.575436	4.670653
139	6	0	-9.83649	5.195969	2.907123
140	6	0	-11.1478	3.268649	4.359666
141	1	0	-9.30395	3.082385	5.483734

142	6	0	-11.16	4.831829	2.629816
143	1	0	-9.32619	5.944763	2.318481
144	7	0	-11.801	3.877359	3.343213
145	6	0	9.122259	4.713344	3.736923
146	6	0	9.815254	5.256409	2.64086
147	6	0	9.834407	3.825381	4.561381
148	6	0	11.14579	4.893666	2.397295
149	1	0	9.301973	5.963565	2.005117
150	6	0	11.15802	3.485312	4.255394
151	1	0	9.324097	3.386379	5.406637
152	7	0	11.79898	4.00847	3.184753
153	6	0	11.91417	2.484379	5.066255
154	6	0	11.37147	1.835229	6.189907
155	6	0	13.22561	2.130953	4.703162
156	6	0	12.10999	0.874285	6.867047
157	1	0	10.37928	2.061269	6.553394
158	6	0	13.9161	1.163117	5.417544
159	1	0	13.68529	2.62344	3.859109
160	7	0	13.37011	0.521945	6.490909
161	1	0	11.69574	0.373277	7.731645
162	1	0	14.92436	0.883395	5.141991
163	6	0	11.90604	5.449164	1.237818
164	6	0	13.18941	4.959172	0.938238
165	6	0	11.39934	6.455112	0.395588
166	6	0	13.88659	5.439023	-0.16036
167	1	0	13.62332	4.204884	1.57781
168	6	0	12.14264	6.89625	-0.69142
169	1	0	10.43687	6.913741	0.572829

170	7	0	13.37457	6.396575	-0.98625
171	1	0	14.87475	5.067811	-0.39675
172	1	0	11.75456	7.667705	-1.34333
173	6	0	-11.9081	2.233019	5.121489
174	6	0	-13.1912	1.846799	4.695443
175	6	0	-11.4018	1.593651	6.267277
176	6	0	-13.8883	0.856921	5.371701
177	1	0	-13.6248	2.334135	3.834797
178	6	0	-12.145	0.607917	6.903311
179	1	0	-10.4396	1.853774	6.685231
180	7	0	-13.3766	0.224574	6.466899
181	1	0	-14.8763	0.555065	5.050705
182	1	0	-11.7573	0.111681	7.783151
183	6	0	-11.916	5.44172	1.495045
184	6	0	-13.2275	5.019287	1.215459
185	6	0	-11.3729	6.424189	0.647489
186	6	0	-13.9176	5.54032	0.130987
187	1	0	-13.6874	4.282219	1.856896
188	6	0	-12.1111	6.909944	-0.42324
189	1	0	-10.3806	6.823269	0.801799
190	7	0	-13.3712	6.474759	-0.69942
191	1	0	-14.9259	5.217597	-0.09251
192	1	0	-11.6965	7.665604	-1.07692
193	6	0	3.044311	1.422255	-8.62565
194	6	0	3.487945	1.171444	-7.31351
195	6	0	2.528887	0.999958	-6.29039
196	6	0	1.187953	1.085788	-6.6079
197	6	0	0.74552	1.328908	-7.92689

198	6	0	1.679156	1.498311	-8.94321
199	1	0	3.773552	1.531293	-9.42003
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201	1	0	1.375589	1.680236	-9.9669
202	6	0	-1.18758	1.151626	-6.5967
203	6	0	-2.5285	1.128092	-6.2686
204	6	0	-3.48761	1.303113	-7.29107
205	6	0	-3.04402	1.498414	-8.61262
206	6	0	-1.67888	1.531204	-8.93758
207	6	0	-0.7452	1.356469	-7.9222
208	1	0	-2.8304	0.949013	-5.24258
209	1	0	-3.77328	1.657092	-9.39857
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211	6	0	0.000198	0.965019	-5.6956
212	8	0	0.000222	0.759227	-4.47967
213	6	0	-4.94009	1.280868	-6.96681
214	6	0	-5.86128	0.584268	-7.77214
215	6	0	-5.42867	1.950521	-5.82871
216	6	0	-7.21322	0.536592	-7.44022
217	1	0	-5.50945	0.062143	-8.65371
218	6	0	-6.78085	1.919752	-5.50379
219	1	0	-4.73994	2.510949	-5.20813
220	6	0	-7.69494	1.202396	-6.29795
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222	1	0	-7.12542	2.429179	-4.61044
223	6	0	4.940438	1.085674	-7.00007
224	6	0	5.429111	0.078354	-6.1463
225	6	0	5.861528	2.008885	-7.53079

226	6	0	6.781295	0.000454	-5.8294
227	1	0	4.74044	-0.65535	-5.7451
228	6	0	7.213487	1.944625	-7.20172
229	1	0	5.509594	2.792367	-8.19099
230	6	0	7.695297	0.939579	-6.34272
231	1	0	7.125948	-0.77492	-5.15387
232	1	0	7.901134	2.659237	-7.64041
233	6	0	-9.1228	1.129867	-5.90718
234	6	0	-9.81565	2.256765	-5.43121
235	6	0	-9.835	-0.08096	-5.95202
236	6	0	-11.1461	2.141029	-5.00973
237	1	0	-9.30234	3.207456	-5.41134
238	6	0	-11.1585	-0.13879	-5.49796
239	1	0	-9.32477	-0.96531	-6.30583
240	7	0	-11.7994	0.956434	-5.02826
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242	6	0	9.815992	-0.34142	-5.87164
243	6	0	9.835332	2.037375	-5.59328
244	6	0	11.14645	-0.371	-5.43549
245	1	0	9.302658	-1.24557	-6.16608
246	6	0	11.15886	1.942409	-5.14551
247	1	0	9.32511	2.988916	-5.63607
248	7	0	11.79971	0.753594	-5.06285
249	6	0	11.91491	3.145162	-4.68412
250	6	0	11.37217	4.442838	-4.68406
251	6	0	13.22623	3.00752	-4.19614
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253	1	0	10.38008	4.644545	-5.06188

254	6	0	13.91653	4.110181	-3.71503
255	1	0	13.68595	2.030323	-4.20037
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257	1	0	11.69624	6.509051	-4.18895
258	1	0	14.92469	4.011526	-3.33472
259	6	0	11.90656	-1.65295	-5.33658
260	6	0	13.19053	-1.66726	-4.76376
261	6	0	11.39916	-2.88553	-5.78526
262	6	0	13.88768	-2.85863	-4.63013
263	1	0	13.62494	-0.7361	-4.43132
264	6	0	12.14248	-4.04748	-5.624
265	1	0	10.4361	-2.96155	-6.26986
266	7	0	13.37506	-4.0528	-5.0453
267	1	0	14.87637	-2.87764	-4.19162
268	1	0	11.75391	-4.99791	-5.96524
269	6	0	-11.9062	3.318892	-4.49417
270	6	0	-13.1897	3.143599	-3.94738
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274	6	0	-12.1425	5.674702	-3.97811
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276	7	0	-13.3745	5.48897	-3.42864
277	1	0	-14.8749	4.097942	-3.00739
278	1	0	-11.7544	6.684643	-3.98825
279	6	0	-11.9145	-1.42642	-5.45863
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282	6	0	-13.9158	-2.65714	-4.86087
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285	1	0	-10.3803	-2.71721	-6.31091
286	7	0	-13.3699	-3.84331	-5.25626
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288	1	0	-11.6962	-4.76536	-6.10096
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295	7	0	15.34759	8.607125	-1.86433
296	7	0	15.30773	7.616795	-4.53508
297	6	0	14.37963	7.696271	-5.73634
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305	6	0	14.36293	9.739514	-1.60686
306	1	0	13.6201	9.400436	-0.88438
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309	6	0	16.02545	8.254576	-0.55098

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311	1	0	15.26673	7.975339	0.178478
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313	46	0	14.35261	6.983245	-2.76633
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318	1	0	-15.0356	-2.48536	10.36789
319	1	0	-16.6292	-3.18683	10.02746
320	7	0	-15.3511	-0.22486	8.801203
321	7	0	-15.3113	-3.03362	8.327341
322	6	0	-14.3837	-4.19898	8.631083
323	1	0	-14.9368	-4.96111	9.191618
324	1	0	-14.027	-4.62567	7.694944
325	1	0	-13.5458	-3.84411	9.234012
326	6	0	-16.4519	-3.54242	7.457998
327	1	0	-16.0359	-3.92858	6.526961
328	1	0	-16.9727	-4.35043	7.984228
329	1	0	-17.1531	-2.73392	7.248941
330	6	0	-14.3676	0.239254	9.866725
331	1	0	-13.6239	0.885238	9.399382
332	1	0	-14.9082	0.806874	10.63259
333	1	0	-13.8804	-0.62014	10.32824
334	6	0	-16.0279	0.999716	8.208735
335	1	0	-16.5817	1.52095	8.997755
336	1	0	-15.2685	1.664211	7.799495
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341	1	0	-17.2755	-7.01369	-5.35554
342	1	0	-16.7513	-8.65912	-5.76466
343	1	0	-15.0318	-7.73797	-7.33696
344	1	0	-16.6254	-7.09254	-7.77464
345	7	0	-15.3483	-7.51193	-4.59608
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351	6	0	-16.4488	-4.68971	-6.79702
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354	1	0	-17.1497	-4.91292	-5.99209
355	6	0	-14.3643	-8.66635	-4.72714
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358	1	0	-13.877	-8.63587	-5.70211
359	6	0	-16.0253	-7.61188	-3.23952
360	1	0	-16.5784	-8.55628	-3.18291
361	1	0	-15.2661	-7.58921	-2.45927
362	1	0	-16.7197	-6.77771	-3.12283
363	46	0	-14.3522	-5.68212	-4.91282
364	6	0	-15.8564	9.613114	-2.66504
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369	1	0	-16.7482	9.323419	-4.61935
370	7	0	-15.3082	8.731008	-1.53912
371	7	0	-15.3469	7.736706	-4.20838
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373	1	0	-16.5767	7.035617	-5.81986
374	1	0	-15.2654	5.924551	-5.34346
375	1	0	-16.7193	6.094601	-4.30958
376	6	0	-14.3616	8.426197	-5.14215
377	1	0	-13.6182	7.697689	-5.46679
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383	1	0	-17.1512	7.64894	-1.26119
384	6	0	-14.3804	9.57581	-0.68101
385	1	0	-14.9328	10.44311	-0.30208
386	1	0	-14.0253	8.978275	0.157123
387	1	0	-13.5415	9.919277	-1.28908
388	46	0	-14.3528	7.096006	-2.46426
389	6	0	16.4244	-7.00199	-6.42405
390	6	0	15.8592	-8.19672	-5.6827
391	1	0	17.27633	-6.57015	-5.89449
392	1	0	16.74918	-7.27943	-7.43346
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394	1	0	16.62716	-8.96131	-5.51859
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415	6	0	16.42545	-2.05812	9.275687
416	1	0	15.03216	-1.06915	10.60951
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420	7	0	15.30846	0.120681	8.863563
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423	1	0	16.58133	-4.39977	7.996674
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426	6	0	14.36586	-3.47708	9.23819
427	1	0	13.62273	-3.93326	8.583666
428	1	0	14.90649	-4.26518	9.774512
429	1	0	13.87801	-2.81796	9.956853
430	6	0	16.44928	0.887752	8.210975
431	1	0	16.03354	1.559088	7.45899
432	1	0	16.96962	1.47731	8.974313
433	1	0	17.15081	0.193424	7.747494
434	6	0	14.3801	1.120649	9.533612
435	1	0	14.93258	1.656022	10.31406
436	1	0	14.02342	1.831548	8.789971
437	1	0	13.54228	0.586621	9.985724
438	46	0	14.35319	-1.09479	7.431065

14.2. Coordinates of PM6 optimized structures

14.2.1. Tetrafacial barrel M2

Center Number	Atomic Number	Atomic Types	Coordinates (Å)		
			X	Y	Z
1	6	0	-18.9025	2.96365	-0.44827
2	6	0	-17.8162	2.133287	-0.14913
3	6	0	-16.5365	2.702014	0.081068
4	6	0	-16.3998	4.07416	0.005687
5	6	0	-17.5135	4.917012	-0.2986

6	6	0	-18.761	4.36451	-0.52727
7	1	0	-19.8879	2.527727	-0.63372
8	1	0	-15.6812	2.068966	0.321223
9	1	0	-19.6251	4.987309	-0.76289
10	6	0	-15.6583	6.351723	0.001372
11	6	0	-14.961	7.541645	0.071856
12	6	0	-15.6604	8.754026	-0.16325
13	6	0	-17.0275	8.720982	-0.46192
14	6	0	-17.7381	7.505107	-0.53505
15	6	0	-17.055	6.324929	-0.3017
16	1	0	-13.8969	7.550481	0.311892
17	1	0	-17.5674	9.652556	-0.65189
18	1	0	-18.8034	7.509568	-0.77008
19	6	0	-15.1748	4.935235	0.204074
20	8	0	-14.0575	4.57202	0.458524
21	6	0	-14.9594	10.05924	-0.10085
22	6	0	-15.4733	11.10587	0.68712
23	6	0	-13.7894	10.29012	-0.84665
24	6	0	-14.8462	12.35262	0.716414
25	1	0	-16.3749	10.94137	1.283734
26	6	0	-13.1654	11.53907	-0.82507
27	1	0	-13.3745	9.487691	-1.46022
28	6	0	-13.6886	12.58748	-0.04705
29	1	0	-15.2754	13.15113	1.323308
30	1	0	-12.2619	11.69353	-1.41351
31	6	0	-18.0183	0.665807	-0.08005
32	6	0	-17.2213	-0.21204	-0.83671
33	6	0	-19.0374	0.125597	0.726008

34	6	0	-17.4525	-1.58888	-0.80732
35	1	0	-16.4235	0.190279	-1.46454
36	6	0	-19.2641	-1.25126	0.763756
37	1	0	-19.6596	0.791823	1.330129
38	6	0	-18.4794	-2.1251	-0.00985
39	1	0	-16.8238	-2.24787	-1.40463
40	1	0	-20.0708	-1.64207	1.385575
41	6	0	-13.0441	13.91814	-0.03964
42	6	0	-12.7115	14.56654	-1.24763
43	6	0	-12.7473	14.5735	1.173966
44	6	0	-12.1153	15.83636	-1.20173
45	1	0	-12.9472	14.08952	-2.20129
46	6	0	-12.1454	15.84117	1.139416
47	1	0	-12.9952	14.09374	2.122965
48	7	0	-11.8378	16.47587	-0.02903
49	6	0	-18.7405	-3.58043	0.009476
50	6	0	-18.8897	-4.30461	-1.19219
51	6	0	-18.8481	-4.28019	1.229447
52	6	0	-19.1508	-5.68253	-1.13424
53	1	0	-18.8302	-3.78218	-2.14934
54	6	0	-19.1085	-5.65931	1.206842
55	1	0	-18.7364	-3.74378	2.173926
56	7	0	-19.2673	-6.35806	0.046127
57	6	0	-19.2209	-6.49929	2.432279
58	6	0	-20.2839	-7.41172	2.570628
59	6	0	-18.2477	-6.45803	3.443187
60	6	0	-20.3123	-8.2763	3.671151
61	1	0	-21.0747	-7.45478	1.81264

62	6	0	-18.3378	-7.35089	4.52193
63	1	0	-17.4161	-5.74795	3.388814
64	7	0	-19.3436	-8.26684	4.635826
65	1	0	-21.1225	-9.01156	3.796119
66	1	0	-17.5838	-7.34794	5.323012
67	6	0	-19.3159	-6.5454	-2.33745
68	6	0	-20.3464	-7.50437	-2.383
69	6	0	-18.4268	-6.47946	-3.4217
70	6	0	-20.4229	-8.38518	-3.46751
71	1	0	-21.0738	-7.56942	-1.56524
72	6	0	-18.5627	-7.39047	-4.48096
73	1	0	-17.6244	-5.73547	-3.44169
74	7	0	-19.534	-8.34868	-4.50619
75	1	0	-21.2085	-9.15455	-3.52138
76	1	0	-17.8733	-7.36725	-5.33816
77	6	0	-11.7192	16.60658	-2.41415
78	6	0	-12.0522	17.96977	-2.52693
79	6	0	-10.9572	16.02432	-3.43932
80	6	0	-11.5813	18.70723	-3.61954
81	1	0	-12.6638	18.45267	-1.75582
82	6	0	-10.52	16.82029	-4.50907
83	1	0	-10.6921	14.96313	-3.4037
84	7	0	-10.811	18.15077	-4.60255
85	1	0	-11.8134	19.77849	-3.72513
86	1	0	-9.91452	16.39245	-5.32182
87	6	0	-11.7688	16.61107	2.357941
88	6	0	-12.0333	17.99235	2.431494
89	6	0	-11.09	16.01034	3.429806

90	6	0	-11.574	18.72582	3.531081
91	1	0	-12.5814	18.49131	1.623619
92	6	0	-10.6606	16.8038	4.5051
93	1	0	-10.882	14.93544	3.427309
94	7	0	-10.878	18.15006	4.557842
95	1	0	-11.7531	19.80941	3.607112
96	1	0	-10.1174	16.36028	5.352981
97	6	0	8.720485	17.01591	0.445079
98	6	0	8.752387	15.64874	0.146889
99	6	0	7.539346	14.94867	-0.08229
100	6	0	6.349539	15.64573	-0.007
101	6	0	6.323698	17.04242	0.296205
102	6	0	7.504673	17.726	0.523982
103	1	0	9.652917	17.55615	0.629807
104	1	0	7.547648	13.88439	-0.32165
105	1	0	7.509812	18.79134	0.758817
106	6	0	4.071835	16.38682	-0.00249
107	6	0	2.699398	16.52339	-0.07259
108	6	0	2.131004	17.80259	0.1616
109	6	0	2.962469	18.88864	0.459009
110	6	0	4.36368	18.74751	0.531801
111	6	0	4.915651	17.50045	0.299362
112	1	0	2.06583	15.6681	-0.31166
113	1	0	2.527194	19.87361	0.648211
114	1	0	4.987175	19.61157	0.765877
115	6	0	4.932363	15.16206	-0.20452
116	8	0	4.568302	14.04478	-0.45792
117	6	0	0.663215	18.00414	0.099653

118	6	0	0.119166	19.03435	-0.68968
119	6	0	-0.21171	17.19547	0.847353
120	6	0	-1.25786	19.26134	-0.71843
121	1	0	0.782547	19.66534	-1.28776
122	6	0	-1.58868	17.4263	0.82635
123	1	0	0.193084	16.38868	1.46195
124	6	0	-2.12865	18.46522	0.047011
125	1	0	-1.65104	20.0774	-1.32643
126	1	0	-2.24504	16.7879	1.416313
127	6	0	10.05781	14.9486	0.077644
128	6	0	10.29928	13.78821	0.83487
129	6	0	11.09382	15.45452	-0.72917
130	6	0	11.54882	13.16542	0.805525
131	1	0	9.504874	13.37995	1.463151
132	6	0	12.34071	14.82811	-0.76684
133	1	0	10.92072	16.3491	-1.33389
134	6	0	12.58622	13.68009	0.007556
135	1	0	11.71218	12.26972	1.403332
136	1	0	13.13103	15.25032	-1.3892
137	6	0	-3.58371	18.72765	0.040405
138	6	0	-4.30228	18.84325	1.248989
139	6	0	-4.28942	18.87065	-1.17287
140	6	0	-5.67977	19.1084	1.203862
141	1	0	-3.77689	18.75518	2.202297
142	6	0	-5.66846	19.13035	-1.13751
143	1	0	-3.75659	18.78635	-2.12217
144	7	0	-6.36119	19.25795	0.031453
145	6	0	13.91717	13.03608	-0.01136

146	6	0	14.59093	12.73203	1.190359
147	6	0	14.54722	12.71207	-1.23098
148	6	0	15.86003	12.13494	1.132797
149	1	0	14.13296	12.99077	2.147403
150	6	0	15.81685	12.11371	-1.20803
151	1	0	14.04757	12.93618	-2.17566
152	7	0	16.47575	11.83241	-0.04725
153	6	0	16.56238	11.71503	-2.43487
154	6	0	17.9243	12.04249	-2.5744
155	6	0	15.95678	10.95516	-3.44814
156	6	0	18.63807	11.56875	-3.68147
157	1	0	18.42495	12.65157	-1.81272
158	6	0	16.72974	10.5145	-4.53314
159	1	0	14.89507	10.69412	-3.39111
160	7	0	18.05926	10.80047	-4.65304
161	1	0	19.7079	11.79674	-3.80834
162	1	0	16.28357	9.910026	-5.33681
163	6	0	16.65475	11.76615	2.337766
164	6	0	18.03526	12.0407	2.385177
165	6	0	16.07853	11.08878	3.423871
166	6	0	18.79078	11.59715	3.476214
167	1	0	18.51625	12.5855	1.564255
168	6	0	16.89339	10.67528	4.489375
169	1	0	15.00623	10.87061	3.440816
170	7	0	18.2375	10.9096	4.52098
171	1	0	19.87398	11.78585	3.532415
172	1	0	16.46881	10.13504	5.348778
173	6	0	-6.5364	19.24259	2.415545

174	6	0	-7.4431	20.31386	2.526012
175	6	0	-6.51663	18.28359	3.440508
176	6	0	-8.32334	20.36364	3.613225
177	1	0	-7.46907	21.09467	1.756921
178	6	0	-7.42412	18.3952	4.505
179	1	0	-5.812	17.44683	3.408426
180	7	0	-8.33463	19.40856	4.591406
181	1	0	-9.05461	21.18049	3.716169
182	1	0	-7.43774	17.65294	5.316843
183	6	0	-6.51473	19.2763	-2.35486
184	6	0	-7.47747	20.30164	-2.42761
185	6	0	-6.42956	18.37291	-3.42588
186	6	0	-8.34268	20.35997	-3.52573
187	1	0	-7.55803	21.03886	-1.62012
188	6	0	-7.32576	18.49072	-4.4998
189	1	0	-5.6822	17.57283	-3.42382
190	7	0	-8.28723	19.4578	-4.55201
191	1	0	-9.11463	21.14127	-3.60103
192	1	0	-7.28761	17.78961	-5.34696
193	6	0	17.01968	-8.71267	0.460337
194	6	0	15.6527	-8.74666	0.161271
195	6	0	14.9522	-7.53479	-0.07302
196	6	0	15.64844	-6.34429	-0.00152
197	6	0	17.04499	-6.31647	0.302108
198	6	0	17.72909	-7.49619	0.534766
199	1	0	17.56039	-9.64396	0.649473
200	1	0	13.88812	-7.54449	-0.31327
201	1	0	18.79431	-7.49984	0.770162

202	6	0	16.38796	-4.06607	-0.00434
203	6	0	16.52363	-2.69377	-0.07901
204	6	0	17.80267	-2.124	0.152431
205	6	0	18.88943	-2.95366	0.452013
206	6	0	18.74907	-4.35468	0.530051
207	6	0	17.50219	-4.90815	0.300168
208	1	0	15.66788	-2.0614	-0.31956
209	1	0	19.87429	-2.51705	0.638639
210	1	0	19.61357	-4.97687	0.76593
211	6	0	15.16382	-4.92809	-0.20372
212	8	0	14.04632	-4.56565	-0.45844
213	6	0	18.00358	-0.65633	0.084511
214	6	0	19.02611	-0.1149	-0.71647
215	6	0	17.20226	0.220704	0.837501
216	6	0	19.25221	1.262103	-0.75228
217	1	0	19.65156	-0.78032	-1.3181
218	6	0	17.43264	1.597703	0.809869
219	1	0	16.40164	-0.18238	1.461241
220	6	0	18.46325	2.135113	0.018014
221	1	0	20.06186	1.653637	-1.36982
222	1	0	16.80038	2.255937	1.404309
223	6	0	14.95316	-10.0526	0.097191
224	6	0	13.78605	-10.2874	0.846272
225	6	0	15.46579	-11.0959	-0.69594
226	6	0	13.16353	-11.5371	0.822699
227	1	0	13.37222	-9.4875	1.46383
228	6	0	14.84003	-12.3433	-0.72742
229	1	0	16.36528	-10.9282	-1.29489

230	6	0	13.68537	-12.5821	0.039199
231	1	0	12.26233	-11.6948	1.413751
232	1	0	15.26801	-13.1392	-1.33863
233	6	0	18.72436	3.590433	0.001958
234	6	0	18.86233	4.313596	1.205388
235	6	0	18.84379	4.291324	-1.21657
236	6	0	19.12618	5.691035	1.149916
237	1	0	18.79227	3.791711	2.162099
238	6	0	19.10317	5.670614	-1.19143
239	1	0	18.74186	3.754643	-2.16199
240	7	0	19.25287	6.367869	-0.02788
241	6	0	13.0422	-13.9134	0.028527
242	6	0	12.71895	-14.5697	1.23503
243	6	0	12.73769	-14.5615	-1.18679
244	6	0	12.12254	-15.8394	1.186601
245	1	0	12.9625	-14.0979	2.189333
246	6	0	12.13896	-15.8307	-1.15473
247	1	0	12.97672	-14.0758	-2.13505
248	7	0	11.839	-16.4724	0.011129
249	6	0	11.75731	-16.5952	-2.37533
250	6	0	12.08176	-17.9606	-2.48634
251	6	0	11.01375	-16.0051	-3.40961
252	6	0	11.61592	-18.6935	-3.58418
253	1	0	12.68165	-18.4488	-1.70949
254	6	0	10.58082	-16.7969	-4.48415
255	1	0	10.75894	-14.9409	-3.37685
256	7	0	10.85631	-18.1311	-4.57195
257	1	0	11.84016	-19.7666	-3.68818

258	1	0	9.988238	-16.3634	-5.30337
259	6	0	11.73346	-16.6161	2.396869
260	6	0	12.00913	-17.9953	2.470293
261	6	0	11.03551	-16.0245	3.46144
262	6	0	11.5469	-18.7348	3.564495
263	1	0	12.56942	-18.4878	1.666786
264	6	0	10.60388	-16.8237	4.531603
265	1	0	10.81523	-14.9525	3.45781
266	7	0	10.83967	-18.1668	4.588007
267	1	0	11.73605	-19.8167	3.640639
268	1	0	10.04729	-16.3871	5.374363
269	6	0	19.28404	6.552821	2.355092
270	6	0	20.35477	7.46316	2.43831
271	6	0	18.34806	6.53453	3.401121
272	6	0	20.42621	8.347653	3.52083
273	1	0	21.11815	7.488539	1.651885
274	6	0	18.48083	7.446332	4.45953
275	1	0	17.51277	5.827523	3.390348
276	7	0	19.4933	8.359887	4.52017
277	1	0	21.24297	9.081703	3.602789
278	1	0	17.75686	7.460811	5.287688
279	6	0	19.22513	6.512043	-2.41471
280	6	0	20.25093	7.471985	-2.51286
281	6	0	18.29879	6.42493	-3.46575
282	6	0	20.28777	8.33289	-3.61526
283	1	0	21.00536	7.553787	-1.72157
284	6	0	18.39565	7.316818	-4.54532
285	1	0	17.49715	5.679541	-3.44362

286	7	0	19.36368	8.275684	-4.62175
287	1	0	21.06907	9.102668	-3.7102
288	1	0	17.67639	7.277319	-5.37708
289	6	0	-2.95828	-18.9006	-0.45522
290	6	0	-2.12772	-17.8137	-0.15847
291	6	0	-2.69698	-16.5346	0.074149
292	6	0	-4.06947	-16.399	0.003281
293	6	0	-4.91241	-17.5135	-0.2981
294	6	0	-4.35954	-18.7604	-0.52904
295	1	0	-2.52223	-19.8855	-0.64301
296	1	0	-2.06402	-15.6787	0.312638
297	1	0	-4.98236	-19.6251	-0.76267
298	6	0	-6.34763	-15.6594	0.006124
299	6	0	-7.53788	-14.963	0.080201
300	6	0	-8.7504	-15.6638	-0.14968
301	6	0	-8.71743	-17.0312	-0.44711
302	6	0	-7.50117	-17.7406	-0.5245
303	6	0	-6.32074	-17.0563	-0.2962
304	1	0	-7.5469	-13.8987	0.319106
305	1	0	-9.64936	-17.572	-0.63256
306	1	0	-7.50555	-18.8061	-0.75871
307	6	0	-4.93088	-15.1747	0.204055
308	8	0	-4.56769	-14.057	0.456904
309	6	0	-10.0561	-14.9641	-0.08243
310	6	0	-11.095	-15.4725	0.719112
311	6	0	-10.2949	-13.8011	-0.83659
312	6	0	-12.342	-14.8461	0.754465
313	1	0	-10.9241	-16.369	1.321561

314	6	0	-11.5444	-13.1782	-0.80938
315	1	0	-9.49837	-13.3909	-1.46091
316	6	0	-12.5847	-13.6954	-0.01683
317	1	0	-13.1345	-15.2706	1.372454
318	1	0	-11.7055	-12.2804	-1.40471
319	6	0	-0.65984	-18.0143	-0.09516
320	6	0	0.214923	-17.2088	-0.84644
321	6	0	-0.1157	-19.0404	0.699438
322	6	0	1.592053	-17.4387	-0.82353
323	1	0	-0.19011	-16.4053	-1.46519
324	6	0	1.26148	-19.2662	0.730285
325	1	0	-0.77911	-19.669	1.300031
326	6	0	2.132134	-18.4731	-0.03849
327	1	0	2.24839	-16.8029	-1.41631
328	1	0	1.654946	-20.0788	1.342702
329	6	0	-13.9155	-13.0511	-0.00104
330	6	0	-14.5815	-12.7377	-1.20457
331	6	0	-14.5526	-12.7349	1.217328
332	6	0	-15.8505	-12.1406	-1.14937
333	1	0	-14.1183	-12.9886	-2.1612
334	6	0	-15.8205	-12.1332	1.191945
335	1	0	-14.0588	-12.9679	2.162874
336	7	0	-16.4724	-11.8444	0.028295
337	6	0	3.587495	-18.734	-0.02855
338	6	0	4.307236	-18.8602	-1.23558
339	6	0	4.292109	-18.8649	1.186446
340	6	0	5.685329	-19.1221	-1.18785
341	1	0	3.781324	-18.7828	-2.18953

342	6	0	5.671097	-19.125	1.153629
343	1	0	3.759464	-18.771	2.134967
344	7	0	6.3654	-19.2614	-0.01265
345	6	0	6.51617	-19.2617	2.373109
346	6	0	7.43193	-20.3251	2.484383
347	6	0	6.476706	-18.3112	3.405436
348	6	0	8.300807	-20.3758	3.580688
349	1	0	7.474118	-21.0988	1.708808
350	6	0	7.373876	-18.4231	4.478591
351	1	0	5.764518	-17.4804	3.372242
352	7	0	8.292588	-19.429	4.566861
353	1	0	9.038635	-21.1866	3.684772
354	1	0	7.372024	-17.6872	5.296279
355	6	0	6.54342	-19.2637	-2.39741
356	6	0	7.499587	-20.2953	-2.46835
357	6	0	6.475675	-18.3514	-3.4621
358	6	0	8.376247	-20.3507	-3.55747
359	1	0	7.565762	-21.0401	-1.6665
360	6	0	7.382524	-18.4668	-4.52732
361	1	0	5.73372	-17.5469	-3.46205
362	7	0	8.338146	-19.4397	-4.57673
363	1	0	9.143474	-21.1368	-3.63093
364	1	0	7.358089	-17.759	-5.36942
365	6	0	-16.6396	-11.7612	-2.35501
366	6	0	-18.0055	-12.0914	-2.43945
367	6	0	-16.0732	-11.0149	-3.40048
368	6	0	-18.762	-11.6282	-3.52233
369	1	0	-18.4758	-12.6942	-1.65373

370	6	0	-16.8878	-10.5852	-4.45924
371	1	0	-15.01	-10.7558	-3.38895
372	7	0	-18.2222	-10.866	-4.52081
373	1	0	-19.836	-11.8567	-3.6052
374	1	0	-16.4729	-9.99105	-5.2869
375	6	0	-16.5722	-11.7361	2.415326
376	6	0	-17.9516	-12.0018	2.515124
377	6	0	-15.9563	-11.0364	3.464933
378	6	0	-18.6689	-11.5238	3.617383
379	1	0	-18.4618	-12.5655	1.725241
380	6	0	-16.7339	-10.5888	4.544372
381	1	0	-14.8821	-10.8263	3.441703
382	7	0	-18.0787	-10.808	4.622113
383	1	0	-19.7507	-11.7035	3.713518
384	1	0	-16.2785	-10.0288	5.374927
385	6	0	-20.344	-11.1259	8.399162
386	6	0	-20.3626	-9.62476	8.701344
387	1	0	-21.3413	-11.4666	8.024408
388	1	0	-20.1921	-11.6989	9.350919
389	1	0	-21.1929	-9.39865	9.420696
390	1	0	-19.4314	-9.31668	9.237283
391	7	0	-20.4878	-8.84908	7.410702
392	7	0	-19.2808	-11.4231	7.367589
393	6	0	-19.5908	-12.7217	6.688426
394	1	0	-18.7713	-13.0272	6.015265
395	1	0	-19.7422	-13.5684	7.391748
396	1	0	-20.5152	-12.6294	6.08913
397	6	0	-17.9224	-11.4752	7.997271

398	1	0	-17.1513	-11.6966	7.238566
399	1	0	-17.6719	-10.5027	8.459759
400	6	0	-21.9022	-8.85538	6.917683
401	1	0	-22.6333	-8.43986	7.642869
402	1	0	-21.999	-8.25544	5.996154
403	1	0	-22.2282	-9.88645	6.686105
404	6	0	-20.0141	-7.44355	7.620562
405	1	0	-20.2039	-6.8217	6.728327
406	1	0	-20.5133	-6.92703	8.467391
407	1	0	-18.9276	-7.43306	7.822593
408	46	0	-19.3071	-9.84185	6.049265
409	1	0	-17.8238	-12.2479	8.787814
410	6	0	-10.8249	19.9496	-8.62326
411	6	0	-9.92576	21.1433	-8.2891
412	1	0	-10.2534	19.16608	-9.17903
413	1	0	-11.6281	20.27457	-9.33549
414	1	0	-9.46435	21.54132	-9.23039
415	1	0	-10.5313	21.99625	-7.8928
416	7	0	-8.89267	20.73075	-7.26663
417	7	0	-11.3847	19.3637	-7.348
418	6	0	-11.8277	17.95399	-7.59362
419	1	0	-12.3487	17.5408	-6.71221
420	1	0	-12.534	17.85093	-8.4444
421	1	0	-10.9549	17.31157	-7.81003
422	6	0	-12.5254	20.1882	-6.83567
423	1	0	-12.9583	19.73655	-5.92614
424	1	0	-12.1829	21.20749	-6.5776
425	6	0	-7.76423	19.98788	-7.91429

426	1	0	-7.22923	20.57316	-8.69082
427	1	0	-7.01091	19.69411	-7.16248
428	1	0	-8.13488	19.06614	-8.39943
429	6	0	-8.37801	21.94501	-6.55654
430	1	0	-7.53627	21.69214	-5.88909
431	1	0	-8.0009	22.73559	-7.24013
432	1	0	-9.17951	22.40015	-5.94614
433	46	0	-9.84859	19.43622	-5.982
434	1	0	-13.3599	20.30053	-7.55959
435	6	0	-9.75246	20.49574	8.61884
436	6	0	-11.2488	20.47668	8.293816
437	1	0	-9.45548	19.57206	9.173757
438	1	0	-9.5349	21.3364	9.328774
439	1	0	-11.8369	20.34101	9.238822
440	1	0	-11.5808	21.46913	7.898699
441	7	0	-11.5332	19.39863	7.274181
442	7	0	-8.95662	20.59886	7.338554
443	6	0	-7.55582	20.12483	7.577297
444	1	0	-6.91985	20.29899	6.691796
445	1	0	-7.05079	20.63617	8.423882
446	1	0	-7.55146	19.04166	7.796668
447	6	0	-8.9513	22.00549	6.823657
448	1	0	-8.33588	22.08673	5.910859
449	1	0	-9.97758	22.33016	6.570168
450	6	0	-11.6003	18.05031	7.923954
451	1	0	-12.3862	17.96665	8.703154
452	1	0	-11.812	17.26825	7.173839
453	1	0	-10.6365	17.80401	8.406306

454	6	0	-12.8194	19.70224	6.569146
455	1	0	-13.1167	18.87348	5.903695
456	1	0	-13.677	19.86708	7.256107
457	1	0	-12.7142	20.617	5.957355
458	46	0	-9.93147	19.39936	5.980921
459	1	0	-8.54582	22.74672	7.54422
460	6	0	9.643943	-20.546	8.607805
461	6	0	11.14569	-20.5225	8.309183
462	1	0	9.33605	-19.6269	9.164332
463	1	0	9.415288	-21.3923	9.30747
464	1	0	11.71701	-20.393	9.265336
465	1	0	11.48612	-21.5115	7.912748
466	7	0	11.44636	-19.4366	7.302711
467	7	0	8.870472	-20.6404	7.313162
468	6	0	7.464677	-20.1716	7.532094
469	1	0	6.843903	-20.3407	6.635002
470	1	0	6.947086	-20.6903	8.366504
471	1	0	7.454023	-19.0901	7.759414
472	6	0	8.877308	-22.0428	6.786844
473	1	0	8.278879	-22.1176	5.862326
474	1	0	9.908723	-22.3634	6.549338
475	6	0	11.50042	-18.0929	7.963346
476	1	0	12.27385	-18.0135	8.755392
477	1	0	11.72248	-17.3051	7.222269
478	1	0	10.52864	-17.8519	8.432135
479	6	0	12.74489	-19.7334	6.617731
480	1	0	13.05297	-18.899	5.964144
481	1	0	13.59066	-19.9026	7.318169

482	1	0	12.65143	-20.6434	5.997029
483	46	0	9.8674	-19.4284	5.982366
484	1	0	8.460554	-22.7907	7.493923
485	6	0	20.65285	11.26777	8.200541
486	6	0	20.67669	9.770702	8.521733
487	1	0	21.6369	11.59926	7.784579
488	1	0	20.53893	11.85402	9.149643
489	1	0	21.5326	9.550241	9.212289
490	1	0	19.76504	9.473995	9.096388
491	7	0	20.74986	8.977273	7.237828
492	7	0	19.55297	11.55611	7.205659
493	6	0	19.84399	12.84204	6.494906
494	1	0	19.00104	13.14226	5.84873
495	1	0	20.02645	13.69867	7.178657
496	1	0	20.74433	12.73504	5.862441
497	6	0	18.21969	11.62608	7.885434
498	1	0	17.42156	11.83979	7.15295
499	1	0	17.982	10.66284	8.373203
500	6	0	22.14411	8.972709	6.690311
501	1	0	22.90185	8.565902	7.392732
502	1	0	22.20399	8.358995	5.774755
503	1	0	22.46296	9.999435	6.431234
504	6	0	20.28143	7.576091	7.485266
505	1	0	20.43553	6.941277	6.595284
506	1	0	20.81187	7.069966	8.319383
507	1	0	19.20356	7.571395	7.729313
508	46	0	19.51956	9.956559	5.911067
509	1	0	18.15523	12.41224	8.666269

510	6	0	20.97386	9.899095	-8.39776
511	6	0	19.77529	10.79956	-8.7102
512	1	0	21.83575	10.50416	-8.02049
513	1	0	21.35184	9.434331	-9.34562
514	1	0	20.08726	11.60028	-9.431
515	1	0	18.97968	10.22807	-9.24844
516	7	0	19.21631	11.36383	-7.42486
517	7	0	20.58032	8.869633	-7.36421
518	6	0	21.80799	8.353929	-6.67835
519	1	0	21.56716	7.514594	-6.00345
520	1	0	22.58316	7.973083	-7.37732
521	1	0	22.27774	9.155928	-6.0798
522	6	0	19.82149	7.741245	-7.99321
523	1	0	19.54153	6.990778	-7.2333
524	1	0	18.89073	8.112805	-8.4601
525	6	0	20.05287	12.50473	-6.9327
526	1	0	20.15093	13.33745	-7.66069
527	1	0	19.62117	12.93998	-6.01466
528	1	0	21.07699	12.16145	-6.69547
529	6	0	17.80269	11.80871	-7.64324
530	1	0	17.40816	12.3325	-6.75502
531	1	0	17.68363	12.51276	-8.49369
532	1	0	17.15459	10.93633	-7.84428
533	46	0	19.31447	9.831858	-6.0558
534	1	0	20.38924	7.202669	-8.78017
535	6	0	-20.0674	-10.9675	-8.52096
536	6	0	-21.2594	-10.0643	-8.19221
537	1	0	-19.2907	-10.4055	-9.09576

538	1	0	-20.3979	-11.7852	-9.21396
539	1	0	-21.6678	-9.62184	-9.13819
540	1	0	-22.1073	-10.6636	-7.7759
541	7	0	-20.8385	-9.01096	-7.19417
542	7	0	-19.4671	-11.5011	-7.24105
543	6	0	-18.0601	-11.9488	-7.49356
544	1	0	-17.6366	-12.4515	-6.60654
545	1	0	-17.9664	-12.6722	-8.33088
546	1	0	-17.4207	-11.0804	-7.73537
547	6	0	-20.2852	-12.6318	-6.69702
548	1	0	-19.8233	-13.0463	-5.78415
549	1	0	-21.3018	-12.2845	-6.43451
550	6	0	-20.1065	-7.89279	-7.87133
551	1	0	-20.7024	-7.37402	-8.65088
552	1	0	-19.8067	-7.12455	-7.13718
553	1	0	-19.1893	-8.26979	-8.36013
554	6	0	-22.046	-8.48637	-6.4798
555	1	0	-21.7879	-7.63147	-5.83122
556	1	0	-22.8454	-8.12403	-7.16112
557	1	0	-22.4919	-9.27744	-5.84934
558	46	0	-19.527	-9.93727	-5.90582
559	1	0	-20.4052	-13.4805	-7.40298
560	6	0	10.94416	-19.8952	-8.60933
561	6	0	10.03965	-21.092	-8.30183
562	1	0	10.38214	-19.1066	-9.16751
563	1	0	11.75962	-20.2135	-9.31056
564	1	0	9.594154	-21.4809	-9.25453
565	1	0	10.63847	-21.9488	-7.90369

566	7	0	8.989512	-20.6891	-7.29303
567	7	0	11.48171	-19.321	-7.3192
568	6	0	11.93024	-17.9097	-7.54496
569	1	0	12.43543	-17.5043	-6.65093
570	1	0	12.65159	-17.8001	-8.38212
571	1	0	11.06187	-17.2648	-7.7718
572	6	0	12.6129	-20.1509	-6.79438
573	1	0	13.02901	-19.7085	-5.87263
574	1	0	12.26546	-21.1726	-6.55256
575	6	0	7.871525	-19.9408	-7.95249
576	1	0	7.348693	-20.5198	-8.74191
577	1	0	7.106479	-19.653	-7.21019
578	1	0	8.249724	-19.0153	-8.42438
579	6	0	8.46366	-21.9098	-6.60239
580	1	0	7.610802	-21.663	-5.94674
581	1	0	8.09793	-22.6942	-7.29912
582	1	0	9.255046	-22.3703	-5.98298
583	46	0	9.921769	-19.4058	-5.98067
584	1	0	13.46029	-20.2566	-7.50412

14.2.2 Tetrafacial tube

Center Number	Atomic Number	Atomic Types	Coordinates (Å)		
			X	Y	Z
1	6	0	3.027222	7.196958	-7.02379
2	6	0	3.477108	6.09407	-6.28943
3	6	0	2.539854	5.207216	-5.69884

4	6	0	1.194584	5.463414	-5.86598
5	6	0	0.739216	6.592218	-6.61662
6	6	0	1.651271	7.457034	-7.19398
7	1	0	3.747612	7.885259	-7.47533
8	1	0	2.875235	4.337731	-5.13278
9	1	0	1.327998	8.324765	-7.77259
10	6	0	-1.19532	5.464799	-5.86184
11	6	0	-2.54031	5.210207	-5.68995
12	6	0	-3.4786	6.09836	-6.27692
13	6	0	-3.02991	7.200825	-7.01271
14	6	0	-1.65428	7.45915	-7.18793
15	6	0	-0.74123	6.593111	-6.61399
16	1	0	-2.87468	4.341004	-5.12286
17	1	0	-3.75101	7.890265	-7.46137
18	1	0	-1.332	8.326561	-7.76758
19	6	0	0.000079	4.700126	-5.35116
20	8	0	0.000661	3.706797	-4.67233
21	6	0	-4.93103	5.864606	-6.10615
22	6	0	-5.79317	5.874881	-7.21747
23	6	0	-5.47629	5.646284	-4.82737
24	6	0	-7.16606	5.681587	-7.0552
25	1	0	-5.38489	6.037417	-8.2195
26	6	0	-6.84913	5.459723	-4.66237
27	1	0	-4.81871	5.638697	-3.95619
28	6	0	-7.70878	5.477156	-5.77478
29	1	0	-7.81684	5.712652	-7.93035
30	1	0	-7.251	5.294654	-3.66417
31	6	0	4.929803	5.857823	-6.12425

32	6	0	5.479966	5.641289	-4.84731
33	6	0	5.787077	5.863158	-7.23937
34	6	0	6.852868	5.450175	-4.68792
35	1	0	4.826222	5.638396	-3.97323
36	6	0	7.159932	5.665116	-7.08274
37	1	0	5.374963	6.025222	-8.23992
38	6	0	7.707394	5.460925	-5.80429
39	1	0	7.258719	5.286606	-3.69109
40	1	0	7.80704	5.691996	-7.96086
41	6	0	-9.16573	5.303118	-5.59988
42	6	0	-9.88047	6.093762	-4.68205
43	6	0	-9.88159	4.351585	-6.34713
44	6	0	-11.2705	5.920073	-4.54183
45	1	0	-9.34279	6.846477	-4.10095
46	6	0	-11.2715	4.22163	-6.16019
47	1	0	-9.34496	3.720818	-7.05855
48	7	0	-11.9615	4.98303	-5.25967
49	6	0	9.163998	5.277809	-5.63575
50	6	0	9.890147	6.066154	-4.72592
51	6	0	9.867881	4.316373	-6.38277
52	6	0	11.28001	5.879879	-4.59791
53	1	0	9.364193	6.82309	-4.14047
54	6	0	11.25663	4.168591	-6.20272
55	1	0	9.320235	3.692836	-7.09304
56	7	0	11.95846	4.932329	-5.31062
57	6	0	12.01461	3.150474	-6.98895
58	6	0	13.28925	2.697421	-6.60071
59	6	0	11.46414	2.589515	-8.15778

60	6	0	13.9464	1.718233	-7.36062
61	1	0	13.77371	3.122956	-5.71431
62	6	0	12.16862	1.60711	-8.86736
63	1	0	10.48794	2.920249	-8.53263
64	7	0	13.40231	1.163953	-8.48502
65	1	0	14.94605	1.358515	-7.07505
66	1	0	11.74467	1.155036	-9.77854
67	6	0	12.05957	6.733446	-3.65349
68	6	0	13.21628	6.269995	-3.00153
69	6	0	11.63593	8.044579	-3.36323
70	6	0	13.88306	7.100739	-2.08806
71	1	0	13.60234	5.268951	-3.21954
72	6	0	12.338	8.816659	-2.42724
73	1	0	10.7663	8.479212	-3.87183
74	7	0	13.4545	8.362258	-1.78508
75	1	0	14.79549	6.761218	-1.5771
76	1	0	12.00581	9.837019	-2.174
77	6	0	-12.0401	6.769096	-3.585
78	6	0	-13.2957	6.384515	-3.07963
79	6	0	-11.5172	7.99807	-3.13768
80	6	0	-13.9612	7.207031	-2.15818
81	1	0	-13.7593	5.451831	-3.42016
82	6	0	-12.227	8.767313	-2.20537
83	1	0	-10.5603	8.373642	-3.52104
84	7	0	-13.4418	8.388719	-1.70962
85	1	0	-14.9475	6.926319	-1.76024
86	1	0	-11.8231	9.724855	-1.83858
87	6	0	-12.04	3.217675	-6.95403

88	6	0	-13.2082	2.607642	-6.46229
89	6	0	-11.5966	2.825643	-8.23167
90	6	0	-13.8669	1.637088	-7.23228
91	1	0	-13.6094	2.902593	-5.48705
92	6	0	-12.2923	1.837866	-8.94285
93	1	0	-10.7159	3.29302	-8.68821
94	7	0	-13.4203	1.237863	-8.46038
95	1	0	-14.7875	1.157237	-6.86993
96	1	0	-11.9453	1.506712	-9.93551
97	6	0	-3.01796	-7.63063	-6.57541
98	6	0	-3.46864	-6.49403	-5.89478
99	6	0	-2.53141	-5.58125	-5.34487
100	6	0	-1.18601	-5.84598	-5.49717
101	6	0	-0.73	-7.0083	-6.19444
102	6	0	-1.64185	-7.89883	-6.73162
103	1	0	-3.73788	-8.33954	-6.99483
104	1	0	-2.86691	-4.68555	-4.82135
105	1	0	-1.31837	-8.79281	-7.26877
106	6	0	1.203964	-5.84591	-5.49284
107	6	0	2.548792	-5.58116	-5.33552
108	6	0	3.488089	-6.49411	-5.88159
109	6	0	3.039868	-7.63074	-6.56386
110	6	0	1.664384	-7.89885	-6.72539
111	6	0	0.750523	-7.00827	-6.1917
112	1	0	2.882271	-4.68534	-4.81092
113	1	0	3.761298	-8.33987	-6.98031
114	1	0	1.342897	-8.79284	-7.26373
115	6	0	0.008076	-5.06099	-5.01532

116	8	0	0.006904	-4.04137	-4.37649
117	6	0	4.940353	-6.24958	-5.72461
118	6	0	5.802863	-6.32217	-6.83336
119	6	0	5.485634	-5.9576	-4.46053
120	6	0	7.17553	-6.1179	-6.68247
121	1	0	5.395192	-6.5422	-7.82464
122	6	0	6.858099	-5.75924	-4.30668
123	1	0	4.828302	-5.90133	-3.59114
124	6	0	7.718127	-5.83899	-5.41614
125	1	0	7.826295	-6.1985	-7.55455
126	1	0	7.259573	-5.53598	-3.31978
127	6	0	-4.92141	-6.24846	-5.74411
128	6	0	-5.47243	-5.95875	-4.48206
129	6	0	-5.77843	-6.31685	-6.8574
130	6	0	-6.84512	-5.75659	-4.33484
131	1	0	-4.81948	-5.90691	-3.60911
132	6	0	-7.15118	-6.10858	-6.7132
133	1	0	-5.3663	-6.53634	-7.84697
134	6	0	-7.69931	-5.82994	-5.44916
135	1	0	-7.25121	-5.53516	-3.34941
136	1	0	-7.79776	-6.18552	-7.58882
137	6	0	9.174664	-5.65148	-5.25117
138	6	0	9.889644	-6.38	-4.28336
139	6	0	9.889772	-4.74814	-6.05675
140	6	0	11.27877	-6.19338	-4.1514
141	1	0	9.35313	-7.09615	-3.65692
142	6	0	11.27909	-4.60305	-5.87634
143	1	0	9.353158	-4.16545	-6.80811

144	7	0	11.96889	-5.30284	-4.92696
145	6	0	-9.15551	-5.63312	-5.29222
146	6	0	-9.8833	-6.35916	-4.33307
147	6	0	-9.85722	-4.71947	-6.09893
148	6	0	-11.2723	-6.15977	-4.21535
149	1	0	-9.35953	-7.07952	-3.70146
150	6	0	-11.2453	-4.55577	-5.9277
151	1	0	-9.30852	-4.14459	-6.84843
152	7	0	-11.9483	-5.25787	-4.98718
153	6	0	-12.0016	-3.58845	-6.77737
154	6	0	-13.2782	-3.1144	-6.42205
155	6	0	-11.4479	-3.09942	-7.9766
156	6	0	-13.9344	-2.18523	-7.24319
157	1	0	-13.765	-3.485	-5.51258
158	6	0	-12.1518	-2.16421	-8.74803
159	1	0	-10.4697	-3.45038	-8.32689
160	7	0	-13.3875	-1.7007	-8.39806
161	1	0	-14.9355	-1.81019	-6.98353
162	1	0	-11.7255	-1.76859	-9.68404
163	6	0	-12.0542	-6.94602	-3.21597
164	6	0	-13.2117	-6.43726	-2.59986
165	6	0	-11.6335	-8.23469	-2.83529
166	6	0	-13.882	-7.20243	-1.63341
167	1	0	-13.5957	-5.45294	-2.887
168	6	0	-12.3392	-8.93988	-1.85024
169	1	0	-10.7636	-8.7047	-3.31081
170	7	0	-13.4564	-8.441	-1.24354
171	1	0	-14.7954	-6.82753	-1.14953

172	1	0	-12.0093	-9.94103	-1.52699
173	6	0	12.04888	-6.97523	-3.13923
174	6	0	13.30271	-6.55432	-2.65881
175	6	0	11.52879	-8.17311	-2.61173
176	6	0	13.96896	-7.31166	-1.68366
177	1	0	13.76439	-5.64518	-3.06023
178	6	0	12.23918	-8.87647	-1.62909
179	1	0	10.57377	-8.57637	-2.97087
180	7	0	13.45206	-8.46225	-1.15787
181	1	0	14.95404	-7.00243	-1.30417
182	1	0	11.83728	-9.80863	-1.1999
183	6	0	12.04767	-3.65122	-6.73199
184	6	0	13.21599	-3.0117	-6.27945
185	6	0	11.60516	-3.3409	-8.03214
186	6	0	13.87586	-2.09271	-7.10939
187	1	0	13.61651	-3.24397	-5.28714
188	6	0	12.30205	-2.40098	-8.80452
189	1	0	10.72422	-3.83554	-8.4585
190	7	0	13.43032	-1.77238	-8.36078
191	1	0	14.79657	-1.59131	-6.77782
192	1	0	11.95571	-2.13352	-9.81645
193	6	0	3.022042	7.042793	7.156474
194	6	0	3.472199	6.315794	6.048804
195	6	0	2.534989	5.733904	5.156183
196	6	0	1.189571	5.901288	5.411901
197	6	0	0.734056	6.643343	6.54634
198	6	0	1.646037	7.212992	7.416325
199	1	0	3.742316	7.488257	7.848908

200	1	0	2.870617	5.173927	4.282939
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202	6	0	-1.20056	5.897665	5.412799
203	6	0	-2.54566	5.726046	5.15818
204	6	0	-3.48399	6.304628	6.05177
205	6	0	-3.03514	7.033039	7.159084
206	6	0	-1.65948	7.207768	7.417687
207	6	0	-0.74642	6.641056	6.546913
208	1	0	-2.88018	5.165181	4.285082
209	1	0	-3.75619	7.475961	7.852344
210	1	0	-1.33722	7.781354	8.28917
211	6	0	-0.00502	5.39492	4.643213
212	8	0	-0.00439	4.727747	3.641828
213	6	0	-4.93663	6.132218	5.819755
214	6	0	-5.80139	7.241345	5.838134
215	6	0	-5.47959	4.85334	5.596311
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217	1	0	-5.39509	8.243596	6.004418
218	6	0	-6.85268	4.685991	5.413664
219	1	0	-4.82004	3.983769	5.582115
220	6	0	-7.7151	5.796115	5.440065
221	1	0	-7.82739	7.950266	5.68629
222	1	0	-7.25275	3.687647	5.245105
223	6	0	4.925141	6.148977	5.814512
224	6	0	5.473257	4.872012	5.593039
225	6	0	5.784842	7.262127	5.827805
226	6	0	6.846473	4.710568	5.405602
227	1	0	4.817721	3.999353	5.583813

228	6	0	7.158061	7.103481	5.633353
229	1	0	5.374511	8.262818	5.993665
230	6	0	7.703499	5.824902	5.424868
231	1	0	7.250718	3.713635	5.238663
232	1	0	7.806967	7.980118	5.66661
233	6	0	-9.1725	5.617677	5.27187
234	6	0	-9.88056	4.695701	6.063767
235	6	0	-9.89495	6.364544	4.325069
236	6	0	-11.2707	4.55078	5.89561
237	1	0	-9.33771	4.11507	6.813084
238	6	0	-11.2847	6.172321	4.199965
239	1	0	-9.36386	7.080023	3.694271
240	7	0	-11.968	5.267707	4.962527
241	6	0	9.160593	5.653676	5.246676
242	6	0	9.881636	4.740637	6.036073
243	6	0	9.869654	6.400813	4.289208
244	6	0	11.27183	4.609462	5.854554
245	1	0	9.35157	4.155217	6.79015
246	6	0	11.25849	6.217248	4.145748
247	1	0	9.326281	7.114091	3.665484
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249	6	0	12.02242	7.002355	3.131131
250	6	0	13.29573	6.608069	2.679456
251	6	0	11.47949	8.175502	2.572051
252	6	0	13.95859	7.366294	1.70285
253	1	0	13.77474	5.718318	3.104081
254	6	0	12.18941	8.883007	1.591883
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257	1	0	14.95744	7.076242	1.344423
258	1	0	11.77118	9.797427	1.140909
259	6	0	12.04687	3.662108	6.709057
260	6	0	13.20517	3.010633	6.248775
261	6	0	11.61799	3.369042	8.017836
262	6	0	13.86869	2.095519	7.080315
263	1	0	13.59516	3.23048	5.249628
264	6	0	12.31713	2.431591	8.790883
265	1	0	10.74664	3.8767	8.450075
266	7	0	13.4355	1.7904	8.339748
267	1	0	14.78233	1.585065	6.743249
268	1	0	11.981	2.176503	9.809486
269	6	0	-12.034	3.5899	6.745832
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271	6	0	-11.5058	3.142576	7.972453
272	6	0	-13.9493	2.156425	7.188151
273	1	0	-13.7569	3.42099	5.433783
274	6	0	-12.2103	2.207209	8.742913
275	1	0	-10.5488	3.52837	8.34539
276	7	0	-13.4249	1.708264	8.367789
277	1	0	-14.9352	1.755671	6.910041
278	1	0	-11.8021	1.840587	9.698727
279	6	0	-12.061	6.963539	3.199926
280	6	0	-13.2306	6.466665	2.596413
281	6	0	-11.6253	8.242803	2.805118
282	6	0	-13.8977	7.233448	1.629243
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285	1	0	-10.7442	8.703521	3.267648
286	7	0	-13.4583	8.463262	1.226859
287	1	0	-14.8196	6.867322	1.15479
288	1	0	-11.9884	9.944856	1.487495
289	6	0	3.028421	-7.18579	7.020188
290	6	0	3.478923	-6.08109	6.288842
291	6	0	2.54162	-5.19184	5.701864
292	6	0	1.196113	-5.44748	5.869012
293	6	0	0.74035	-6.57832	6.616451
294	6	0	1.652339	-7.44535	7.190569
295	1	0	3.748534	-7.87611	7.469327
296	1	0	2.877288	-4.32089	5.138408
297	1	0	1.328982	-8.3146	7.767029
298	6	0	-1.19414	-5.44773	5.865663
299	6	0	-2.53923	-5.19249	5.694566
300	6	0	-3.47801	-6.08223	6.278406
301	6	0	-3.02924	-7.18676	7.01115
302	6	0	-1.65361	-7.44578	7.185783
303	6	0	-0.7402	-6.57848	6.614345
304	1	0	-2.87344	-4.32149	5.130313
305	1	0	-3.7504	-7.87751	7.457948
306	1	0	-1.33168	-8.31491	7.763233
307	6	0	0.001627	-4.68206	5.357698
308	8	0	0.002454	-3.68602	4.682387
309	6	0	-4.93069	-5.84886	6.107451
310	6	0	-5.79422	-5.86484	7.217599
311	6	0	-5.47522	-5.62602	4.829113

312	6	0	-7.16743	-5.6732	7.054628
313	1	0	-5.38709	-6.03088	8.21958
314	6	0	-6.84825	-5.441	4.663421
315	1	0	-4.81696	-5.61398	3.95868
316	6	0	-7.70931	-5.46449	5.774627
317	1	0	-7.81905	-5.70899	7.929104
318	1	0	-7.24941	-5.27275	3.66552
319	6	0	4.931969	-5.84592	6.123393
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321	6	0	5.790371	-5.85669	7.237601
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327	1	0	7.260258	-5.26919	3.690695
328	1	0	7.811247	-5.69119	7.958241
329	6	0	-9.16661	-5.29211	5.597982
330	6	0	-9.87871	-6.0827	4.678041
331	6	0	-9.88457	-4.34155	6.344476
332	6	0	-11.2684	-5.90911	4.534101
333	1	0	-9.33966	-6.83535	4.098267
334	6	0	-11.274	-4.21136	6.153779
335	1	0	-9.35027	-3.71188	7.058548
336	7	0	-11.9611	-4.97241	5.250675
337	6	0	9.167217	-5.26769	5.63347
338	6	0	9.89341	-6.05514	4.722862
339	6	0	9.870407	-4.30542	6.380045

340	6	0	11.28281	-5.8664	4.592704
341	1	0	9.368202	-6.81343	4.138563
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345	6	0	12.01694	-3.13548	6.98229
346	6	0	13.2903	-2.68149	6.590754
347	6	0	11.46871	-2.57408	8.151849
348	6	0	13.94823	-1.70099	7.34825
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355	6	0	12.06428	-6.71688	3.646883
356	6	0	13.22253	-6.25018	2.999679
357	6	0	11.64302	-8.02738	3.351039
358	6	0	13.89325	-7.07748	2.086128
359	1	0	13.60689	-5.24938	3.221853
360	6	0	12.3493	-8.79613	2.415104
361	1	0	10.77231	-8.46472	3.855355
362	7	0	13.46738	-8.33881	1.778104
363	1	0	14.80717	-6.73556	1.57939
364	1	0	12.01912	-9.81617	2.157975
365	6	0	-12.0365	-6.7565	3.574428
366	6	0	-13.2908	-6.36978	3.067309
367	6	0	-11.5144	-7.98538	3.126312

368	6	0	-13.9558	-7.19033	2.143793
369	1	0	-13.754	-5.43702	3.408207
370	6	0	-12.2237	-8.75266	2.191759
371	1	0	-10.5588	-8.36286	3.510902
372	7	0	-13.4372	-8.37215	1.694512
373	1	0	-14.9413	-6.90804	1.744746
374	1	0	-11.8203	-9.71024	1.824429
375	6	0	-12.0464	-3.20773	6.944478
376	6	0	-13.2172	-2.60478	6.449821
377	6	0	-11.6061	-2.80929	8.22104
378	6	0	-13.8814	-1.63527	7.216189
379	1	0	-13.6163	-2.90478	5.475221
380	6	0	-12.3075	-1.8227	8.928735
381	1	0	-10.7236	-3.27074	8.680069
382	7	0	-13.4379	-1.22989	8.443571
383	1	0	-14.8043	-1.16142	6.851778
384	1	0	-11.963	-1.48689	9.920714
385	6	0	16.48773	1.09539	11.43624
386	6	0	15.92284	-0.21253	11.99158
387	1	0	17.36243	0.902039	10.76727
388	1	0	16.90863	1.709104	12.27779
389	1	0	16.73548	-0.78033	12.51933
390	1	0	15.16572	-0.01339	12.79104
391	7	0	15.29481	-1.006	10.86888
392	7	0	15.40806	1.824748	10.66991
393	6	0	16.03945	2.829865	9.755796
394	1	0	15.28107	3.4761	9.282793
395	1	0	16.74583	3.515997	10.27266

396	1	0	16.60775	2.317231	8.958799
397	6	0	14.45544	2.498428	11.6096
398	1	0	13.72563	3.118264	11.06283
399	1	0	13.89515	1.748131	12.19826
400	6	0	16.34309	-1.74246	10.09159
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403	1	0	17.05063	-1.03177	9.625672
404	6	0	14.29544	-1.96606	11.43764
405	1	0	13.93047	-2.67188	10.67332
406	1	0	14.70149	-2.59457	12.26124
407	1	0	13.42964	-1.4169	11.85147
408	46	0	14.41024	0.367509	9.613282
409	1	0	14.95015	3.174603	12.34095
410	6	0	-15.9947	-11.9178	0.997637
411	6	0	-16.5419	-11.4513	-0.35184
412	1	0	-15.248	-12.7403	0.863335
413	1	0	-16.8191	-12.3913	1.595525
414	1	0	-16.9689	-12.3298	-0.90682
415	1	0	-17.4091	-10.7591	-0.21496
416	7	0	-15.4468	-10.7532	-1.12533
417	7	0	-15.3558	-10.7496	1.712897
418	6	0	-14.3725	-11.262	2.720084
419	1	0	-14.0038	-10.455	3.37459
420	1	0	-14.795	-12.0343	3.400931
421	1	0	-13.5077	-11.7248	2.209837
422	6	0	-16.3975	-9.90572	2.382555
423	1	0	-15.9328	-9.06552	2.924885

424	1	0	-17.0968	-9.48749	1.635018
425	6	0	-14.4988	-11.7504	-1.718
426	1	0	-14.9952	-12.5233	-2.34499
427	1	0	-13.7555	-11.2584	-2.3671
428	1	0	-13.9537	-12.2895	-0.92061
429	6	0	-16.0586	-9.90978	-2.20178
430	1	0	-15.2892	-9.4952	-2.87459
431	1	0	-16.7652	-10.4686	-2.85398
432	1	0	-16.6216	-9.07034	-1.75555
433	46	0	-14.4477	-9.60508	0.259756
434	1	0	-17.0132	-10.4608	3.122979
435	6	0	-16.4537	0.334612	-11.522
436	6	0	-15.8836	-1.00693	-11.984
437	1	0	-17.3341	0.185414	-10.8492
438	1	0	-16.8676	0.89042	-12.4061
439	1	0	-16.6916	-1.60944	-12.4793
440	1	0	-15.1198	-0.86086	-12.7885
441	7	0	-15.2645	-1.7232	-10.8058
442	7	0	-15.3809	1.114497	-10.7968
443	6	0	-16.0207	2.176063	-9.95525
444	1	0	-15.2669	2.853457	-9.52003
445	1	0	-16.7243	2.825387	-10.5211
446	1	0	-16.5942	1.715534	-9.13062
447	6	0	-14.422	1.727164	-11.7713
448	1	0	-13.6952	2.379842	-11.2598
449	1	0	-13.8586	0.940973	-12.3078
450	6	0	-16.3191	-2.40453	-9.98777
451	1	0	-16.9218	-3.1418	-10.5611

452	1	0	-15.8684	-2.95362	-9.14439
453	1	0	-17.0286	-1.66334	-9.57557
454	6	0	-14.2626	-2.72046	-11.3014
455	1	0	-13.9035	-3.37294	-10.4885
456	1	0	-14.6641	-3.40317	-12.083
457	1	0	-13.3935	-2.20139	-11.7459
458	46	0	-14.3875	-0.26804	-9.64001
459	1	0	-14.9117	2.355821	-12.547
460	6	0	-16.531	11.48748	0.331357
461	6	0	-15.9834	11.94515	-1.021
462	1	0	-17.4037	10.80136	0.198711
463	1	0	-16.9502	12.37098	0.8842
464	1	0	-16.8059	12.42193	-1.6189
465	1	0	-15.2309	12.76309	-0.89127
466	7	0	-15.3537	10.77031	-1.73349
467	7	0	-15.4394	10.78392	1.104835
468	6	0	-16.0552	9.946706	2.183873
469	1	0	-15.2877	9.528624	2.856535
470	1	0	-16.7575	10.51139	2.835739
471	1	0	-16.6243	9.110036	1.74007
472	6	0	-14.484	11.77601	1.694249
473	1	0	-13.7401	11.27926	2.338961
474	1	0	-13.94	12.31327	0.894922
475	6	0	-16.4024	9.928648	-2.39498
476	1	0	-17.0178	10.48313	-3.13609
477	1	0	-15.944	9.083114	-2.93449
478	1	0	-17.1012	9.517903	-1.64283
479	6	0	-14.3722	11.27319	-2.74722

480	1	0	-14.0098	10.46116	-3.3991
481	1	0	-14.794	12.04378	-3.43031
482	1	0	-13.5033	11.73462	-2.24297
483	46	0	-14.4471	9.627333	-0.27842
484	1	0	-14.9738	12.55053	2.324211
485	6	0	16.01112	-11.9523	-0.23017
486	6	0	16.55606	-11.3996	1.087245
487	1	0	15.26464	-12.7649	-0.04423
488	1	0	16.83663	-12.463	-0.79505
489	1	0	16.98248	-12.2402	1.698405
490	1	0	17.42331	-10.7173	0.907278
491	7	0	15.45954	-10.6534	1.812328
492	7	0	15.3728	-10.8331	-1.02031
493	6	0	14.39179	-11.4102	-1.9942
494	1	0	14.02366	-10.6473	-2.69998
495	1	0	14.81618	-12.2242	-2.62325
496	1	0	13.5264	-11.84	-1.45688
497	6	0	16.41514	-10.0333	-1.74107
498	1	0	15.95082	-9.23016	-2.33727
499	1	0	17.11282	-9.56718	-1.02083
500	6	0	14.51105	-11.6106	2.466956
501	1	0	15.00672	-12.3405	3.143955
502	1	0	13.76614	-11.0779	3.080995
503	1	0	13.96792	-12.201	1.705333
504	6	0	16.06936	-9.7417	2.832774
505	1	0	15.29876	-9.28467	3.47601
506	1	0	16.77514	-10.2567	3.520916
507	1	0	16.63289	-8.93276	2.333871

508	46	0	14.46164	-9.598	0.354416
509	1	0	17.03257	-10.6344	-2.44315
510	6	0	-16.5039	-0.33578	11.47477
511	6	0	-15.9565	1.017231	11.93065
512	1	0	-17.3785	-0.20423	10.79088
513	1	0	-16.9203	-0.88881	12.35951
514	1	0	-16.7784	1.614416	12.40944
515	1	0	-15.2018	0.888525	12.74665
516	7	0	-15.3307	1.730056	10.75395
517	7	0	-15.4133	-1.10837	10.76863
518	6	0	-16.0303	-2.1883	9.93343
519	1	0	-15.2634	-2.86086	9.514121
520	1	0	-16.731	-2.84022	10.50007
521	1	0	-16.6016	-1.74536	9.09776
522	6	0	-14.4548	-1.69651	11.75846
523	1	0	-13.7116	-2.34066	11.26005
524	1	0	-13.9102	-0.89647	12.29412
525	6	0	-16.3823	2.389923	9.914738
526	1	0	-16.9976	3.130128	10.47067
527	1	0	-15.9268	2.930136	9.068108
528	1	0	-17.081	1.636707	9.50572
529	6	0	-14.3492	2.745197	11.25404
530	1	0	-13.99	3.397603	10.44102
531	1	0	-14.7699	3.42773	12.02577
532	1	0	-13.4783	2.242194	11.71309
533	46	0	-14.4252	0.275577	9.609232
534	1	0	-14.9421	-2.32671	12.53443
535	6	0	16.46973	-1.06854	-11.4692

536	6	0	15.9032	0.242592	-12.0152
537	1	0	17.3494	-0.87926	-10.8056
538	1	0	16.88386	-1.67942	-12.3161
539	1	0	16.71332	0.811399	-12.5458
540	1	0	15.14053	0.047974	-12.8105
541	7	0	15.28352	1.032393	-10.8853
542	7	0	15.39424	-1.79934	-10.6984
543	6	0	16.03052	-2.80751	-9.79108
544	1	0	15.27464	-3.45477	-9.31557
545	1	0	16.73358	-3.49237	-10.3141
546	1	0	16.60377	-2.29744	-8.99599
547	6	0	14.4354	-2.46977	-11.6341
548	1	0	13.70602	-3.08697	-11.0839
549	1	0	13.87496	-1.7175	-12.2201
550	6	0	16.338	1.76135	-10.1094
551	1	0	16.94303	2.460493	-10.7263
552	1	0	15.88692	2.362623	-9.30255
553	1	0	17.04547	1.045995	-9.65056
554	6	0	14.28483	1.998835	-11.4444
555	1	0	13.92569	2.701803	-10.6747
556	1	0	14.68932	2.630411	-12.2664
557	1	0	13.41529	1.454924	-11.8573
558	46	0	14.40172	-0.34507	-9.63219
559	1	0	14.92474	-3.14726	-12.3678
560	6	0	15.94832	12.00744	0.221988
561	6	0	16.51347	11.45108	-1.08541
562	1	0	15.19378	12.80917	0.022132
563	1	0	16.76165	12.5326	0.79117

564	1	0	16.93754	12.29173	-1.69817
565	1	0	17.386	10.77957	-0.8911
566	7	0	15.4327	10.68806	-1.81661
567	7	0	15.31594	10.88619	1.01403
568	6	0	14.31631	11.45723	1.972468
569	1	0	13.94791	10.69353	2.677201
570	1	0	14.72338	12.27942	2.602139
571	1	0	13.45266	11.87364	1.421873
572	6	0	16.36083	10.10589	1.75212
573	1	0	15.90073	9.305155	2.35464
574	1	0	17.06874	9.638811	1.042575
575	6	0	14.48338	11.63061	-2.49093
576	1	0	14.98083	12.36118	-3.16592
577	1	0	13.75305	11.08609	-3.11215
578	1	0	13.9235	12.22011	-1.74099
579	6	0	16.06287	9.772801	-2.82145
580	1	0	15.30389	9.30175	-3.46843
581	1	0	16.77103	10.28822	-3.50681
582	1	0	16.6288	8.974278	-2.30858
583	46	0	14.43053	9.633115	-0.36121
584	1	0	16.96662	10.72169	2.451648

14.2.3 $(C_{70})_3$@M2

Center Number	Atomic Number	Atomic Types	Coordinates (Å)		
			X	Y	Z
1	6	0	15.42625	-9.55881	-0.44203

2	6	0	14.83523	-8.32688	-0.1377
3	6	0	13.43667	-8.25383	0.091229
4	6	0	12.69174	-9.4144	0.011925
5	6	0	13.30272	-10.6698	-0.29453
6	6	0	14.66489	-10.7427	-0.52441
7	1	0	16.50226	-9.61659	-0.62798
8	1	0	12.96228	-7.30237	0.33399
9	1	0	15.15244	-11.6891	-0.76281
10	6	0	10.99971	-11.111	0.009295
11	6	0	9.84099	-11.8591	0.08546
12	6	0	9.918068	-13.2571	-0.14572
13	6	0	11.1521	-13.8444	-0.44873
14	6	0	12.33415	-13.0798	-0.52786
15	6	0	12.25726	-11.7181	-0.2961
16	1	0	8.88791	-11.3876	0.327461
17	1	0	11.21305	-14.92	-0.63631
18	1	0	13.28226	-13.5645	-0.76535
19	6	0	11.20988	-9.62885	0.208808
20	8	0	10.37661	-8.79828	0.458945
21	6	0	8.707347	-14.1108	-0.07303
22	6	0	8.701944	-15.2648	0.732188
23	6	0	7.55899	-13.8102	-0.82697
24	6	0	7.58873	-16.1064	0.767067
25	1	0	9.580416	-15.5071	1.336555
26	6	0	6.447239	-14.6553	-0.79927
27	1	0	7.544804	-12.9165	-1.45341
28	6	0	6.451182	-15.8171	-0.00725
29	1	0	7.617758	-17.0039	1.386725

30	1	0	5.570586	-14.4047	-1.3963
31	6	0	15.68594	-7.11432	-0.06052
32	6	0	15.38541	-5.96524	-0.81332
33	6	0	16.83731	-7.10806	0.748459
34	6	0	16.22795	-4.85163	-0.7807
35	1	0	14.49367	-5.9518	-1.44264
36	6	0	17.67632	-5.99309	0.788282
37	1	0	17.07953	-7.98717	1.351934
38	6	0	17.38704	-4.85469	0.015227
39	1	0	15.97749	-3.97428	-1.3767
40	1	0	18.57176	-6.02122	1.410983
41	6	0	5.288814	-16.7324	0.001182
42	6	0	4.721826	-17.1868	-1.20747
43	6	0	4.72207	-17.1739	1.214689
44	6	0	3.630518	-18.0687	-1.16205
45	1	0	5.15021	-16.8713	-2.16092
46	6	0	3.630424	-18.0561	1.179008
47	1	0	5.138713	-16.8336	2.164493
48	7	0	3.092296	-18.5108	0.010817
49	6	0	18.29973	-3.6903	0.030277
50	6	0	18.76296	-3.12242	-1.17469
51	6	0	18.73017	-3.12296	1.247286
52	6	0	19.6426	-2.0295	-1.12255
53	1	0	18.45581	-3.55192	-2.13034
54	6	0	19.61106	-2.03007	1.218386
55	1	0	18.38266	-3.53957	2.194498
56	7	0	20.07444	-1.49103	0.054426
57	6	0	20.11735	-1.34274	2.4394

58	6	0	21.48836	-1.05017	2.568197
59	6	0	19.24895	-0.90916	3.453287
60	6	0	21.93407	-0.30099	3.663267
61	1	0	22.19811	-1.39122	1.805826
62	6	0	19.76258	-0.16679	4.527454
63	1	0	18.17548	-1.12593	3.400999
64	7	0	21.0851	0.155565	4.632708
65	1	0	22.9973	-0.03991	3.778751
66	1	0	19.10355	0.194761	5.330509
67	6	0	20.18397	-1.34572	-2.33012
68	6	0	21.54904	-1.00653	-2.39678
69	6	0	19.35446	-0.96455	-3.39626
70	6	0	22.0244	-0.26785	-3.48595
71	1	0	22.22994	-1.30416	-1.59098
72	6	0	19.89775	-0.23212	-4.46311
73	1	0	18.28743	-1.21495	-3.39177
74	7	0	21.21217	0.132992	-4.5104
75	1	0	23.08238	0.028009	-3.55412
76	1	0	19.26886	0.085984	-5.30776
77	6	0	2.945697	-18.5997	-2.37371
78	6	0	2.640511	-19.9705	-2.47095
79	6	0	2.527075	-17.7523	-3.41146
80	6	0	1.893117	-20.4355	-3.55931
81	1	0	2.970771	-20.6649	-1.68983
82	6	0	1.785568	-18.2845	-4.47693
83	1	0	2.755268	-16.6805	-3.38446
84	7	0	1.450203	-19.6059	-4.55143
85	1	0	1.622708	-21.4987	-3.65081

86	1	0	1.435485	-17.6421	-5.29831
87	6	0	2.946119	-18.576	2.395902
88	6	0	2.628734	-19.9444	2.49464
89	6	0	2.542776	-17.7261	3.437332
90	6	0	1.890121	-20.4043	3.590342
91	1	0	2.942849	-20.6403	1.708139
92	6	0	1.811937	-18.2546	4.512906
93	1	0	2.774651	-16.655	3.406836
94	7	0	1.468933	-19.5734	4.591592
95	1	0	1.610691	-21.465	3.682827
96	1	0	1.476973	-17.6097	5.338714
97	6	0	-15.3906	-9.64932	0.431452
98	6	0	-14.805	-8.41118	0.141985
99	6	0	-13.4048	-8.32723	-0.07288
100	6	0	-12.6529	-9.4834	0.004861
101	6	0	-13.2584	-10.7452	0.295517
102	6	0	-14.6222	-10.8289	0.511847
103	1	0	-16.4678	-9.71568	0.607158
104	1	0	-12.9344	-7.37086	-0.3038
105	1	0	-15.1057	-11.7802	0.738408
106	6	0	-10.9495	-11.1684	0.012054
107	6	0	-9.78477	-11.9079	-0.0571
108	6	0	-9.85486	-13.3081	0.161885
109	6	0	-11.088	-13.9065	0.445958
110	6	0	-12.2761	-13.1506	0.518674
111	6	0	-12.206	-11.7865	0.299203
112	1	0	-8.83225	-11.4279	-0.28433
113	1	0	-11.1435	-14.9841	0.623519

114	1	0	-13.2233	-13.6436	0.74192
115	6	0	-11.1678	-9.68626	-0.17862
116	8	0	-10.3378	-8.84826	-0.41466
117	6	0	-8.63732	-14.1527	0.096677
118	6	0	-8.60991	-15.2941	-0.72589
119	6	0	-7.50458	-13.8567	0.87549
120	6	0	-7.49027	-16.1273	-0.7544
121	1	0	-9.47639	-15.5331	-1.34858
122	6	0	-6.38688	-14.6939	0.854401
123	1	0	-7.50786	-12.973	1.516273
124	6	0	-6.36774	-15.8428	0.043775
125	1	0	-7.50306	-17.0154	-1.38791
126	1	0	-5.52374	-14.4476	1.472609
127	6	0	-15.6628	-7.20361	0.065609
128	6	0	-15.3727	-6.05536	0.823792
129	6	0	-16.8105	-7.2012	-0.74865
130	6	0	-16.2214	-4.9465	0.790849
131	1	0	-14.4841	-6.03887	1.457542
132	6	0	-17.6559	-6.0911	-0.78847
133	1	0	-17.0448	-8.0795	-1.35641
134	6	0	-17.3768	-4.95351	-0.01045
135	1	0	-15.9787	-4.06968	1.390834
136	1	0	-18.5484	-6.12249	-1.41521
137	6	0	-5.20031	-16.7516	0.041079
138	6	0	-4.63529	-17.2025	1.252202
139	6	0	-4.62998	-17.1962	-1.16978
140	6	0	-3.54433	-18.0851	1.211876
141	1	0	-5.06627	-16.8851	2.203791

142	6	0	-3.54096	-18.0817	-1.12969
143	1	0	-5.0436	-16.8577	-2.12149
144	7	0	-3.00567	-18.5328	0.041204
145	6	0	-18.2959	-3.79421	-0.02628
146	6	0	-18.7643	-3.22938	1.178166
147	6	0	-18.7273	-3.22849	-1.24372
148	6	0	-19.6493	-2.14089	1.125086
149	1	0	-18.4567	-3.65784	2.13415
150	6	0	-19.6141	-2.14038	-1.21577
151	1	0	-18.3759	-3.6426	-2.19059
152	7	0	-20.0821	-1.60419	-0.05237
153	6	0	-20.1222	-1.45554	-2.43742
154	6	0	-21.4948	-1.17181	-2.56896
155	6	0	-19.2545	-1.01582	-3.44924
156	6	0	-21.9431	-0.42519	-3.66474
157	1	0	-22.2039	-1.51771	-1.80818
158	6	0	-19.7707	-0.27657	-4.52431
159	1	0	-18.1797	-1.22547	-3.39462
160	7	0	-21.0951	0.037102	-4.63231
161	1	0	-23.0078	-0.17094	-3.78233
162	1	0	-19.1124	0.089495	-5.32589
163	6	0	-20.1956	-1.4599	2.331998
164	6	0	-21.562	-1.12558	2.39615
165	6	0	-19.3696	-1.07623	3.399936
166	6	0	-22.042	-0.38877	3.484545
167	1	0	-22.2403	-1.42545	1.589003
168	6	0	-19.9174	-0.3458	4.465814
169	1	0	-18.3017	-1.32309	3.397583

170	7	0	-21.2331	0.014827	4.510554
171	1	0	-23.1012	-0.0967	3.550781
172	1	0	-19.2912	-0.02564	5.311726
173	6	0	-2.86011	-18.6113	2.42597
174	6	0	-2.52479	-19.9758	2.515145
175	6	0	-2.47081	-17.7642	3.475415
176	6	0	-1.77604	-20.433	3.605886
177	1	0	-2.83293	-20.6711	1.725743
178	6	0	-1.72515	-18.288	4.542065
179	1	0	-2.72652	-16.6987	3.457356
180	7	0	-1.35946	-19.6017	4.60796
181	1	0	-1.48302	-21.4906	3.69145
182	1	0	-1.39646	-17.6449	5.371721
183	6	0	-2.85767	-18.6097	-2.34365
184	6	0	-2.51406	-19.9733	-2.42174
185	6	0	-2.48139	-17.7715	-3.40449
186	6	0	-1.77546	-20.4379	-3.51547
187	1	0	-2.80805	-20.6615	-1.62078
188	6	0	-1.74805	-18.304	-4.47634
189	1	0	-2.73631	-16.7056	-3.39228
190	7	0	-1.37834	-19.6166	-4.53419
191	1	0	-1.47634	-21.4944	-3.59224
192	1	0	-1.43291	-17.6672	-5.31625
193	6	0	-11.2557	16.89425	0.436741
194	6	0	-10.0179	16.30666	0.149984
195	6	0	-9.93698	14.90724	-0.072
196	6	0	-11.0953	14.15824	-0.00194
197	6	0	-12.3566	14.76521	0.288075

198	6	0	-12.4374	16.12841	0.50959
199	1	0	-11.3202	17.97076	0.617075
200	1	0	-8.98111	14.43481	-0.30211
201	1	0	-13.3883	16.61332	0.734969
202	6	0	-12.7832	12.45815	-0.00468
203	6	0	-13.5236	11.29451	-0.07812
204	6	0	-14.924	11.36517	0.140613
205	6	0	-15.5212	12.59799	0.427958
206	6	0	-14.764	13.7852	0.504688
207	6	0	-13.3999	13.71453	0.28615
208	1	0	-13.0443	10.3423	-0.3083
209	1	0	-16.5988	12.6541	0.605213
210	1	0	-15.2565	14.73216	0.730521
211	6	0	-11.3005	12.67413	-0.19314
212	8	0	-10.4641	11.84411	-0.43306
213	6	0	-15.7678	10.14734	0.071359
214	6	0	-16.9111	10.12237	-0.74842
215	6	0	-15.4669	9.01046	0.842304
216	6	0	-17.7406	9.000108	-0.78325
217	1	0	-17.1545	10.99243	-1.3644
218	6	0	-16.3004	7.890041	0.814753
219	1	0	-14.5821	9.012144	1.481588
220	6	0	-17.4503	7.872612	0.00567
221	1	0	-18.6302	9.014336	-1.41481
222	1	0	-16.0497	7.023173	1.425624
223	6	0	-8.80573	17.15858	0.085881
224	6	0	-7.66052	16.84976	0.841894
225	6	0	-8.79211	18.31642	-0.71399

226	6	0	-6.54375	17.68781	0.818794
227	1	0	-7.65214	15.95304	1.464916
228	6	0	-7.67361	19.151	-0.74472
229	1	0	-9.66839	18.56643	-1.31869
230	6	0	-6.53789	18.85164	0.029027
231	1	0	-5.6704	17.42818	1.415589
232	1	0	-7.69692	20.05101	-1.36093
233	6	0	-18.3529	6.700461	-0.00642
234	6	0	-18.8049	6.125353	1.1993
235	6	0	-18.7896	6.135239	-1.22262
236	6	0	-19.6836	5.031547	1.148415
237	1	0	-18.4927	6.550954	2.154998
238	6	0	-19.6669	5.039414	-1.19296
239	1	0	-18.4501	6.557471	-2.17022
240	7	0	-20.1218	4.496101	-0.02694
241	6	0	-5.36648	19.75395	0.019211
242	6	0	-4.78552	20.19752	1.226214
243	6	0	-4.80181	20.19539	-1.19584
244	6	0	-3.68294	21.06478	1.178543
245	1	0	-5.21672	19.88684	2.180204
246	6	0	-3.69797	21.06189	-1.16319
247	1	0	-5.23164	19.86729	-2.14442
248	7	0	-3.14397	21.50187	0.003165
249	6	0	-3.01111	21.57436	-2.38213
250	6	0	-2.68592	22.93987	-2.48992
251	6	0	-2.60969	20.7147	-3.41679
252	6	0	-1.93591	23.38652	-3.58418
253	1	0	-3.00468	23.64471	-1.71312

254	6	0	-1.86288	21.22876	-4.4879
255	1	0	-2.86169	19.64978	-3.38705
256	7	0	-1.50728	22.54406	-4.57193
257	1	0	-1.65244	24.44581	-3.68518
258	1	0	-1.52655	20.57637	-5.30733
259	6	0	-2.98548	21.58595	2.387501
260	6	0	-2.60571	22.94058	2.454598
261	6	0	-2.63002	20.74698	3.45525
262	6	0	-1.85162	23.39357	3.542686
263	1	0	-2.88641	23.63103	1.650478
264	6	0	-1.87668	21.2671	4.519447
265	1	0	-2.9229	19.69254	3.458582
266	7	0	-1.47041	22.56905	4.565017
267	1	0	-1.52776	24.44345	3.612827
268	1	0	-1.57625	20.62901	5.363957
269	6	0	-20.2183	4.342993	2.356475
270	6	0	-21.5893	4.035794	2.446572
271	6	0	-19.3757	3.923742	3.397823
272	6	0	-22.0587	3.286108	3.531411
273	1	0	-22.2803	4.366545	1.662682
274	6	0	-19.9125	3.180549	4.45992
275	1	0	-18.3043	4.153322	3.376511
276	7	0	-21.2337	2.843233	4.527371
277	1	0	-23.122	3.013762	3.616904
278	1	0	-19.274	2.830865	5.284474
279	6	0	-20.1782	4.354712	-2.41308
280	6	0	-21.5337	3.981791	-2.49764
281	6	0	-19.329	4.004399	-3.4742

282	6	0	-21.9786	3.2398	-3.59726
283	1	0	-22.2306	4.25554	-1.69695
284	6	0	-19.8414	3.264679	-4.55127
285	1	0	-18.2695	4.284916	-3.45837
286	7	0	-21.1452	2.865991	-4.61497
287	1	0	-23.0282	2.918791	-3.67979
288	1	0	-19.1952	2.967792	-5.39063
289	6	0	11.1486	16.95646	-0.43782
290	6	0	9.914019	16.362	-0.15135
291	6	0	9.840889	14.96217	0.070732
292	6	0	11.00339	14.21963	0.001063
293	6	0	12.26139	14.8336	-0.28864
294	6	0	12.33459	16.19721	-0.51027
295	1	0	11.20719	18.03329	-0.61826
296	1	0	8.887597	14.48443	0.300614
297	1	0	13.28291	16.68739	-0.73542
298	6	0	12.70074	12.52898	0.004388
299	6	0	13.44762	11.36948	0.078086
300	6	0	14.84763	11.44795	-0.14026
301	6	0	15.43808	12.68407	-0.42747
302	6	0	14.67428	13.86704	-0.50448
303	6	0	13.31049	13.78876	-0.28634
304	1	0	12.97357	10.41462	0.308159
305	1	0	16.51536	12.74618	-0.60441
306	1	0	15.16148	14.81671	-0.73021
307	6	0	11.2168	12.7367	0.192423
308	8	0	10.38501	11.90204	0.432175
309	6	0	15.69825	10.23487	-0.07081

310	6	0	16.84134	10.21622	0.749445
311	6	0	15.40414	9.096461	-0.84213
312	6	0	17.67727	9.098735	0.784267
313	1	0	17.0794	11.08748	1.365787
314	6	0	16.244	7.980858	-0.8146
315	1	0	14.51954	9.093236	-1.48171
316	6	0	17.39374	7.969848	-0.00514
317	1	0	18.56648	9.117904	1.416174
318	1	0	15.99858	7.112746	-1.42584
319	6	0	8.697154	17.20717	-0.08765
320	6	0	7.553777	16.89177	-0.84371
321	6	0	8.676973	18.36514	0.711915
322	6	0	6.432347	17.7236	-0.82098
323	1	0	7.550457	15.99485	-1.46649
324	6	0	7.553846	19.19348	0.742266
325	1	0	9.55176	18.62018	1.316673
326	6	0	6.419902	18.88759	-0.03154
327	1	0	5.560526	17.45893	-1.4178
328	1	0	7.572059	20.09378	1.35824
329	6	0	18.30326	6.803039	0.006603
330	6	0	18.75835	6.230906	-1.19938
331	6	0	18.7436	6.240031	1.222535
332	6	0	19.64309	5.141993	-1.14901
333	1	0	18.44354	6.655026	-2.15489
334	6	0	19.62735	5.149418	1.192357
335	1	0	18.40181	6.659991	2.170341
336	7	0	20.08491	4.608891	0.026092
337	6	0	5.243478	19.78336	-0.02209

338	6	0	4.660069	20.22322	-1.22927
339	6	0	4.676336	20.22213	1.192777
340	6	0	3.552675	21.08435	-1.18195
341	1	0	5.09301	19.91459	-2.18314
342	6	0	3.567693	21.08246	1.159781
343	1	0	5.107963	19.89678	2.141492
344	7	0	3.011269	21.5189	-0.00675
345	6	0	2.878005	21.59161	2.378509
346	6	0	2.545251	22.95534	2.485739
347	6	0	2.481356	20.73017	3.413534
348	6	0	1.79277	23.39828	3.579821
349	1	0	2.860084	23.66162	1.70865
350	6	0	1.731715	21.24053	4.484433
351	1	0	2.73926	19.66665	3.38423
352	7	0	1.368829	22.55386	4.567921
353	1	0	1.503424	24.45602	3.680378
354	1	0	1.399013	20.58662	5.304134
355	6	0	2.852348	21.60117	-2.39112
356	6	0	2.465067	22.95365	-2.45875
357	6	0	2.501543	20.75982	-3.45854
358	6	0	1.708473	23.40201	-3.54701
359	1	0	2.741933	23.64596	-1.6549
360	6	0	1.745328	21.27534	-4.52294
361	1	0	2.800259	19.70702	-3.46145
362	7	0	1.33184	22.575	-4.56902
363	1	0	1.378789	24.45006	-3.61756
364	1	0	1.448432	20.63525	-5.36719
365	6	0	20.18062	4.45625	-2.35742

366	6	0	21.55284	4.155104	-2.44813
367	6	0	19.33938	4.033539	-3.39853
368	6	0	22.02512	3.407545	-3.53324
369	1	0	22.24273	4.488822	-1.66452
370	6	0	19.87894	3.292901	-4.46096
371	1	0	18.26704	4.258396	-3.37664
372	7	0	21.20163	2.961229	-4.5289
373	1	0	23.0895	3.139771	-3.61915
374	1	0	19.24171	2.940701	-5.28542
375	6	0	20.14331	4.467655	2.412181
376	6	0	21.5012	4.103536	2.496358
377	6	0	19.29655	4.111464	3.473343
378	6	0	21.95114	3.364113	3.595684
379	1	0	22.19612	4.382053	1.695633
380	6	0	19.81403	3.374878	4.550144
381	1	0	18.23522	4.384871	3.457652
382	7	0	21.12043	2.984677	4.613493
383	1	0	23.00278	3.049831	3.677819
384	1	0	19.16989	3.073597	5.389578
385	6	0	23.36633	2.243238	8.345601
386	6	0	22.70189	0.899845	8.661312
387	1	0	24.40254	2.089365	7.953562
388	1	0	23.50897	2.823898	9.293913
389	1	0	23.34868	0.320909	9.371231
390	1	0	21.7414	1.052858	9.211934
391	7	0	22.43756	0.150147	7.376381
392	7	0	22.53959	2.991627	7.326318
393	6	0	23.3978	4.000961	6.627644

394	1	0	22.7968	4.644626	5.962218
395	1	0	23.93283	4.687036	7.318274
396	1	0	24.16561	3.492513	6.016031
397	6	0	21.36774	3.663264	7.974805
398	1	0	20.76783	4.205738	7.222907
399	1	0	20.71009	2.915776	8.455397
400	6	0	23.69073	-0.48944	6.862483
401	1	0	24.16666	-1.18856	7.581652
402	1	0	23.48648	-1.07168	5.947105
403	1	0	24.44456	0.280036	6.61254
404	6	0	21.37898	-0.8847	7.605649
405	1	0	21.24757	-1.52334	6.714558
406	1	0	21.60281	-1.57227	8.447974
407	1	0	20.411	-0.398	7.824152
408	46	0	21.80991	1.570668	6.025952
409	1	0	21.64855	4.401533	8.754043
410	6	0	0.702396	-21.2782	-8.55526
411	6	0	-0.65096	-21.9204	-8.23604
412	1	0	0.564465	-20.3244	-9.1212
413	1	0	1.276128	-21.9432	-9.25252
414	1	0	-1.22954	-22.0685	-9.18479
415	1	0	-0.51236	-22.9529	-7.829
416	7	0	-1.39267	-21.0699	-7.23148
417	7	0	1.449779	-21.004	-7.27108
418	6	0	2.500169	-19.9635	-7.51223
419	1	0	3.137361	-19.8274	-6.62075
420	1	0	3.188052	-20.2101	-8.34802
421	1	0	2.028104	-18.9924	-7.74794

422	6	0	2.06994	-22.2574	-6.73432
423	1	0	2.648558	-22.0467	-5.81804
424	1	0	1.289444	-22.9977	-6.47839
425	6	0	-2.04474	-19.8973	-7.89837
426	1	0	-2.78544	-20.1778	-8.67538
427	1	0	-2.57929	-19.2784	-7.15617
428	1	0	-1.2862	-19.258	-8.38646
429	6	0	-2.41747	-21.9049	-6.52721
430	1	0	-3.05613	-21.2864	-5.8731
431	1	0	-3.1074	-22.4391	-7.21463
432	1	0	-1.92304	-22.6719	-5.90336
433	46	0	0.032221	-20.3393	-5.93576
434	1	0	2.767833	-22.7527	-7.44153
435	6	0	-0.59496	-21.2467	8.619315
436	6	0	0.771548	-21.8642	8.30781
437	1	0	-0.47734	-20.2885	9.182563
438	1	0	-1.15882	-21.9201	9.316587
439	1	0	1.349445	-21.9966	9.259289
440	1	0	0.654096	-22.9011	7.905269
441	7	0	1.500717	-21.0049	7.301594
442	7	0	-1.34239	-20.9908	7.331393
443	6	0	-2.41368	-19.9703	7.565609
444	1	0	-3.05087	-19.8499	6.671874
445	1	0	-3.09927	-20.2275	8.400143
446	1	0	-1.96158	-18.9894	7.79965
447	6	0	-1.93632	-22.2574	6.79586
448	1	0	-2.51108	-22.0608	5.873986
449	1	0	-1.14112	-22.9852	6.549291

450	6	0	2.125179	-19.8147	7.963973
451	1	0	2.869694	-20.0748	8.744381
452	1	0	2.647753	-19.1883	7.21953
453	1	0	1.351566	-19.1895	8.446591
454	6	0	2.546336	-21.8232	6.608575
455	1	0	3.176278	-21.1961	5.954289
456	1	0	3.242937	-22.3389	7.303436
457	1	0	2.071361	-22.6043	5.987115
458	46	0	0.067063	-20.3076	5.996852
459	1	0	-2.63091	-22.7617	7.499965
460	6	0	0.630514	24.18148	8.596182
461	6	0	-0.71949	24.83259	8.282497
462	1	0	0.488746	23.22551	9.157725
463	1	0	1.209068	24.83952	9.296464
464	1	0	-1.296	24.97913	9.23309
465	1	0	-0.57651	25.86681	7.880902
466	7	0	-1.46738	23.99107	7.274872
467	7	0	1.374297	23.91084	7.309065
468	6	0	2.417118	22.86093	7.541818
469	1	0	3.054096	22.72739	6.650069
470	1	0	3.106694	23.09627	8.379898
471	1	0	1.938429	21.89161	7.771368
472	6	0	2.00321	25.16355	6.780934
473	1	0	2.578845	24.95623	5.862173
474	1	0	1.228272	25.91262	6.533245
475	6	0	-2.12315	22.81804	7.937234
476	1	0	-2.85503	23.09834	8.723167
477	1	0	-2.67043	22.20989	7.195812

478	1	0	-1.36601	22.16898	8.414422
479	6	0	-2.48995	24.83487	6.577848
480	1	0	-3.13494	24.2238	5.923131
481	1	0	-3.17491	25.3694	7.270515
482	1	0	-1.99385	25.60299	5.956601
483	46	0	-0.04878	23.26827	5.969751
484	1	0	2.70622	25.64786	7.491088
485	6	0	-23.5705	0.730707	8.192485
486	6	0	-22.9355	2.085898	8.518044
487	1	0	-24.6003	0.866189	7.777523
488	1	0	-23.7241	0.150665	9.139474
489	1	0	-23.6077	2.656585	9.210829
490	1	0	-21.9855	1.950615	9.091039
491	7	0	-22.654	2.83553	7.236723
492	7	0	-22.7097	-0.00718	7.193949
493	6	0	-23.5357	-1.03363	6.481654
494	1	0	-22.91	-1.67043	5.832616
495	1	0	-24.0741	-1.72556	7.163876
496	1	0	-24.2986	-0.54081	5.851435
497	6	0	-21.5406	-0.65658	7.869603
498	1	0	-20.9144	-1.18893	7.131944
499	1	0	-20.9074	0.103221	8.363541
500	6	0	-23.9055	3.451697	6.690972
501	1	0	-24.4094	4.1462	7.395463
502	1	0	-23.6898	4.032956	5.777571
503	1	0	-24.6406	2.668661	6.427601
504	6	0	-21.6192	3.88937	7.486751
505	1	0	-21.4781	4.527467	6.596706

506	1	0	-21.8747	4.575877	8.320962
507	1	0	-20.6484	3.420497	7.729904
508	46	0	-21.9734	1.421353	5.905734
509	1	0	-21.8253	-1.39889	8.643573
510	6	0	-23.3835	2.110483	-8.34876
511	6	0	-22.7113	0.770656	-8.6631
512	1	0	-24.4193	1.951046	-7.95783
513	1	0	-23.5283	2.689911	-9.2975
514	1	0	-23.354	0.187876	-9.3736
515	1	0	-21.7509	0.928748	-9.21254
516	7	0	-22.4445	0.022947	-7.37751
517	7	0	-22.5621	2.863888	-7.32891
518	6	0	-23.4267	3.868455	-6.63127
519	1	0	-22.83	4.515562	-5.96528
520	1	0	-23.9649	4.551405	-7.32255
521	1	0	-24.1923	3.355764	-6.02037
522	6	0	-21.3935	3.542045	-7.9765
523	1	0	-20.7977	4.088643	-7.22433
524	1	0	-20.7309	2.798134	-8.45581
525	6	0	-23.6948	-0.62327	-6.86496
526	1	0	-24.1664	-1.32472	-7.58473
527	1	0	-23.4884	-1.20465	-5.94951
528	1	0	-24.4528	0.142241	-6.61562
529	6	0	-21.3799	-1.00617	-7.60498
530	1	0	-21.2461	-1.64361	-6.7134
531	1	0	-21.599	-1.69538	-8.44723
532	1	0	-20.4144	-0.51425	-7.82255
533	46	0	-21.8259	1.447549	-6.02721

534	1	0	-21.6778	4.278093	-8.75658
535	6	0	22.90259	2.208866	-8.52081
536	6	0	23.54281	0.856075	-8.19543
537	1	0	21.9526	2.069985	-9.09296
538	1	0	23.57217	2.781786	-9.21434
539	1	0	23.69754	0.27625	-9.14237
540	1	0	24.57258	0.995414	-7.78159
541	7	0	22.68573	0.115447	-7.19571
542	7	0	22.61957	2.957855	-7.23947
543	6	0	21.58071	4.007878	-7.48891
544	1	0	21.43812	4.645731	-6.59893
545	1	0	21.83306	4.695065	-8.32353
546	1	0	20.61138	3.535456	-7.73109
547	6	0	23.86927	3.578719	-6.69497
548	1	0	23.65227	4.158894	-5.78118
549	1	0	24.60769	2.798499	-6.43264
550	6	0	21.5181	-0.53816	-7.86982
551	1	0	21.80446	-1.27991	-8.64371
552	1	0	20.89444	-1.07215	-7.1312
553	1	0	20.8819	0.219289	-8.36349
554	6	0	23.5162	-0.90798	-6.48418
555	1	0	22.89338	-1.54682	-5.8343
556	1	0	24.05619	-1.59814	-7.16689
557	1	0	24.27806	-0.41237	-5.85493
558	46	0	21.94561	1.54175	-5.90721
559	1	0	24.36965	4.275346	-7.39986
560	6	0	-0.77804	24.17428	-8.60076
561	6	0	0.568338	24.83298	-8.28731

562	1	0	-0.63097	23.21891	-9.16197
563	1	0	-1.36024	24.82885	-9.30127
564	1	0	1.144011	24.9824	-9.23796
565	1	0	0.41961	25.86653	-7.88607
566	7	0	1.320896	23.99598	-7.27941
567	7	0	-1.5203	23.89996	-7.31354
568	6	0	-2.55729	22.84421	-7.54592
569	1	0	-3.19351	22.70746	-6.65413
570	1	0	-3.24817	23.07545	-8.38408
571	1	0	-2.07324	21.87748	-7.77515
572	6	0	-2.15613	25.14935	-6.78583
573	1	0	-2.73067	24.93914	-5.86704
574	1	0	-1.38534	25.90274	-6.53832
575	6	0	1.98319	22.8264	-7.94138
576	1	0	2.713522	23.11051	-8.72739
577	1	0	2.533817	22.22153	-7.19975
578	1	0	1.229682	22.17298	-8.41839
579	6	0	2.33875	24.8457	-6.58268
580	1	0	2.987164	24.23845	-5.92778
581	1	0	3.02071	25.38382	-7.27553
582	1	0	1.838378	25.61124	-5.96167
583	46	0	-0.09366	23.26574	-5.97404
584	1	0	-2.86176	25.62956	-7.49617
585	6	0	-15.683	4.138213	1.372204
586	6	0	-15.0652	4.684032	0.218
587	6	0	-13.6212	4.989687	0.26317
588	6	0	-12.9068	4.727111	1.459191
589	6	0	-13.5971	4.26473	2.676613

590	6	0	-14.9429	3.982547	2.636729
591	6	0	-15.4658	2.808025	3.33564
592	6	0	-14.6093	1.973175	4.041011
593	6	0	-13.1732	2.277123	4.087843
594	6	0	-12.6856	3.393568	3.424395
595	6	0	-14.7623	0.517468	3.935146
596	6	0	-15.7632	-0.01301	3.131791
597	6	0	-16.657	0.875151	2.387155
598	6	0	-16.5134	2.240079	2.48564
599	6	0	-16.6435	3.079069	1.281863
600	6	0	-17.0181	2.522203	0.033093
601	6	0	-17.1722	1.057276	-0.07301
602	6	0	-16.9384	0.262562	1.077481
603	6	0	-16.2205	-0.9747	1.001599
604	6	0	-15.7113	-1.46528	-0.22779
605	6	0	-16.1812	-0.80555	-1.39154
606	6	0	-16.8995	0.432129	-1.31557
607	6	0	-16.577	1.222146	-2.51613
608	6	0	-16.4332	2.587098	-2.41678
609	6	0	-16.6044	3.248316	-1.11169
610	6	0	-15.6437	4.3079	-1.02094
611	6	0	-14.8627	4.330037	-2.27018
612	6	0	-15.3601	3.266726	-3.14409
613	6	0	-14.4792	2.537462	-3.93161
614	6	0	-14.6323	1.08177	-4.03685
615	6	0	-15.6573	0.445848	-3.34879
616	6	0	-15.404	-0.81087	-2.64303
617	6	0	-14.1462	-1.36816	-2.65956

618	6	0	-13.0595	-0.70871	-3.38958
619	6	0	-13.291	0.483987	-4.05924
620	6	0	-12.3078	1.572026	-3.96727
621	6	0	-11.1591	1.39634	-3.21047
622	6	0	-10.9258	0.134087	-2.50229
623	6	0	-11.8449	-0.88431	-2.59034
624	6	0	-12.1885	-1.66596	-1.38727
625	6	0	-13.5895	-1.9627	-1.43133
626	6	0	-14.3632	-2.06722	-0.24845
627	6	0	-13.6284	-2.13227	0.962215
628	6	0	-12.2279	-1.83527	1.005789
629	6	0	-11.5086	-1.46449	-0.15913
630	6	0	-10.5206	-0.37057	-0.06553
631	6	0	-10.3272	0.268126	1.185539
632	6	0	-11.006	-0.21314	2.403455
633	6	0	-11.9251	-1.23171	2.317376
634	6	0	-13.1654	-1.16754	3.093452
635	6	0	-14.2261	-1.71498	2.242969
636	6	0	-15.4841	-1.15817	2.264428
637	6	0	-13.4212	-0.08055	3.916748
638	6	0	-12.4381	1.007208	4.010835
639	6	0	-11.265	0.937307	3.274469
640	6	0	-10.7603	2.121301	2.572941
641	6	0	-11.4473	3.30953	2.646493
642	6	0	-11.5988	4.143868	1.439131
643	6	0	-10.9547	3.802144	0.222695
644	6	0	-10.2161	2.525454	0.144421
645	6	0	-10.1779	1.688613	1.288497

646	6	0	-10.2882	0.43747	-1.20729
647	6	0	-10.1389	1.857997	-1.10427
648	6	0	-10.6802	2.46856	-2.33324
649	6	0	-11.5597	4.313256	-0.95376
650	6	0	-11.3673	3.656906	-2.26102
651	6	0	-12.5798	3.852675	-3.05923
652	6	0	-13.5171	4.612502	-2.22654
653	6	0	-12.8679	4.896682	-0.93406
654	6	0	-13.0429	2.841798	-3.88863
655	6	0	1.127515	-8.77714	1.31539
656	6	0	1.96187	-8.98993	0.188879
657	6	0	3.024623	-10.012	0.275484
658	6	0	3.171039	-10.743	1.481833
659	6	0	2.364327	-10.4222	2.674602
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661	6	0	0.08646	-9.69445	3.25582
662	6	0	-0.14316	-10.8652	3.962885
663	6	0	0.913839	-11.8822	4.047804
664	6	0	2.131612	-11.6604	3.421429
665	6	0	-1.42995	-11.5598	3.820128
666	6	0	-2.4028	-11.0369	2.980809
667	6	0	-2.15021	-9.80148	2.235514
668	6	0	-0.94585	-9.15226	2.367574
669	6	0	-0.2847	-8.58316	1.178014
670	6	0	-0.91719	-8.59425	-0.09102
671	6	0	-2.2111	-9.29216	-0.23363
672	6	0	-2.77313	-9.92578	0.903859
673	6	0	-3.39188	-11.2147	0.817503

674	6	0	-3.47098	-11.9197	-0.40989
675	6	0	-3.15361	-11.169	-1.56973
676	6	0	-2.53485	-9.88	-1.483
677	6	0	-1.6615	-9.70768	-2.65961
678	6	0	-0.4573	-9.05848	-2.52628
679	6	0	-0.04642	-8.5375	-1.20873
680	6	0	1.365729	-8.7315	-1.07145
681	6	0	1.863376	-9.37776	-2.3004
682	6	0	0.732212	-9.57049	-3.21282
683	6	0	0.651227	-10.7127	-3.99522
684	6	0	-0.63591	-11.4073	-4.13634
685	6	0	-1.75735	-10.913	-3.48659
686	6	0	-2.6756	-11.8262	-2.79953
687	6	0	-2.43187	-13.1801	-2.80287
688	6	0	-1.25218	-13.7101	-3.48772
689	6	0	-0.37354	-12.8525	-4.13598
690	6	0	1.073647	-13.0513	-3.99477
691	6	0	1.552088	-14.0964	-3.21536
692	6	0	0.617976	-14.9914	-2.53105
693	6	0	-0.73892	-14.8049	-2.66266
694	6	0	-1.61631	-14.9562	-1.48899
695	6	0	-2.64532	-13.9624	-1.57256
696	6	0	-3.20685	-13.3727	-0.41144
697	6	0	-2.88296	-14.0078	0.814521
698	6	0	-1.85364	-15.001	0.898577
699	6	0	-1.10643	-15.3929	-0.24041
700	6	0	0.349817	-15.5932	-0.09849
701	6	0	0.94596	-15.3857	1.170837

702	6	0	0.130377	-15.0854	2.359904
703	6	0	-1.22653	-14.8984	2.227292
704	6	0	-1.89715	-13.834	2.975551
705	6	0	-2.92023	-13.2739	2.091765
706	6	0	-3.16316	-11.9199	2.091422
707	6	0	-1.16709	-13.0048	3.816703
708	6	0	0.279986	-13.2039	3.957197
709	6	0	0.907184	-14.2205	3.248929
710	6	0	2.190777	-13.9776	2.58927
711	6	0	2.781554	-12.7376	2.669205
712	6	0	3.427199	-12.1526	1.480601
713	6	0	3.544656	-12.8842	0.272443
714	6	0	2.90644	-14.2128	0.183364
715	6	0	2.20043	-14.7072	1.309287
716	6	0	1.183904	-15.3392	-1.21625
717	6	0	2.438006	-14.6608	-1.07799
718	6	0	2.67866	-13.8832	-2.30598
719	6	0	3.665576	-12.1067	-0.90687
720	6	0	3.269617	-12.6436	-2.22092
721	6	0	2.777153	-11.5365	-3.04527
722	6	0	2.85305	-10.3285	-2.22081
723	6	0	3.409143	-10.6975	-0.90523
724	6	0	1.708025	-11.7297	-3.90813
725	6	0	10.31896	0.348884	-1.19769
726	6	0	10.50748	-0.30247	0.047573
727	6	0	11.5005	-1.39229	0.135737
728	6	0	12.22922	-1.74665	-1.0284
729	6	0	11.93188	-1.13034	-2.33529

730	6	0	11.00809	-0.11557	-2.41629
731	6	0	11.26683	1.045634	-3.273
732	6	0	12.4443	1.129553	-4.00084
733	6	0	13.43241	0.045858	-3.91215
734	6	0	13.17687	-1.05136	-3.10245
735	6	0	13.17336	2.40395	-4.05915
736	6	0	12.67575	3.510579	-3.38678
737	6	0	11.43285	3.411747	-2.618
738	6	0	10.75146	2.219304	-2.56193
739	6	0	10.16302	1.769631	-1.28613
740	6	0	10.18943	2.594096	-0.13278
741	6	0	10.92195	3.87531	-0.19227
742	6	0	11.57214	4.233599	-1.40065
743	6	0	12.87725	4.823682	-1.40576
744	6	0	13.58247	5.076801	-0.20227
745	6	0	12.82184	4.966858	0.988894
746	6	0	11.51662	4.376589	0.99364
747	6	0	11.31908	3.705006	2.292375
748	6	0	10.63769	2.512461	2.347118
749	6	0	10.10757	1.912637	1.108026
750	6	0	10.26347	0.491843	1.196531
751	6	0	10.89419	0.177565	2.49231
752	6	0	11.11631	1.433161	3.215728
753	6	0	12.25922	1.606393	3.981922
754	6	0	12.98823	2.880688	3.921972
755	6	0	12.52533	3.898206	3.100623
756	6	0	13.46409	4.671867	2.282445
757	6	0	14.81077	4.395789	2.331826

758	6	0	15.30796	3.325498	3.197318
759	6	0	14.42578	2.583209	3.971097
760	6	0	14.58569	1.127252	4.061455
761	6	0	15.61844	0.504124	3.373212
762	6	0	16.53948	1.294154	2.555127
763	6	0	16.3893	2.659357	2.469744
764	6	0	16.56557	3.335707	1.173079
765	6	0	15.60002	4.391308	1.087586
766	6	0	15.02771	4.777975	-0.15095
767	6	0	15.65582	4.247972	-1.30695
768	6	0	16.62106	3.192736	-1.22184
769	6	0	16.99048	2.624219	0.023199
770	6	0	17.15144	1.159025	0.114309
771	6	0	16.9293	0.375739	-1.0463
772	6	0	16.65324	1.001177	-2.351
773	6	0	16.50317	2.36635	-2.43552
774	6	0	15.45823	2.938267	-3.28617
775	6	0	14.92481	4.102403	-2.57794
776	6	0	13.57781	4.378126	-2.62357
777	6	0	14.61067	2.106823	-4.00618
778	6	0	14.77052	0.650841	-3.9152
779	6	0	15.76893	0.116677	-3.11117
780	6	0	15.49003	-1.03932	-2.2582
781	6	0	14.23485	-1.60265	-2.25102
782	6	0	13.63094	-2.03698	-0.97887
783	6	0	14.35746	-1.98142	0.237242
784	6	0	15.70264	-1.37248	0.231962
785	6	0	16.21727	-0.86593	-0.98863

786	6	0	16.87384	0.518954	1.348159
787	6	0	16.16148	-0.72312	1.405915
788	6	0	15.37618	-0.74607	2.652129
789	6	0	13.57557	-1.8938	1.416076
790	6	0	14.1212	-1.30995	2.654383
791	6	0	13.02642	-0.66403	3.384365
792	6	0	11.81794	-0.83704	2.575286
793	6	0	12.17339	-1.60371	1.36605
794	6	0	13.24739	0.522425	4.068503

14.2.4. $(C_{60})_3$@M2

Center Number	Atomic Number	Atomic Types	Coordinates (Å)		
			X	Y	Z
1	6	0	-11.073	16.8976	0.408778
2	6	0	-9.84117	16.29473	0.128559
3	6	0	-9.77479	14.89304	-0.08358
4	6	0	-10.9412	14.15708	-0.01066
5	6	0	-12.1965	14.7794	0.273086
6	6	0	-12.263	16.1449	0.484928
7	1	0	-11.1263	17.97601	0.581219
8	1	0	-8.82355	14.40884	-0.30843
9	1	0	-13.2091	16.64152	0.705295
10	6	0	-12.6468	12.47497	-0.00413
11	6	0	-13.399	11.31848	-0.06964
12	6	0	-14.7987	11.40483	0.148027
13	6	0	-15.3835	12.64583	0.425528
14	6	0	-14.6143	13.82584	0.493812

15	6	0	-13.2507	13.73971	0.277105
16	1	0	-12.9291	10.35985	-0.29272
17	1	0	-16.4605	12.71433	0.601958
18	1	0	-15.0972	14.77941	0.712196
19	6	0	-11.1617	12.67401	-0.19242
20	8	0	-10.334	11.83373	-0.42631
21	6	0	-15.6535	10.19424	0.089432
22	6	0	-16.8028	10.17436	-0.72217
23	6	0	-15.356	9.058124	0.863013
24	6	0	-17.6407	9.058072	-0.74691
25	1	0	-17.044	11.0437	-1.34002
26	6	0	-16.1977	7.943906	0.84544
27	1	0	-14.4667	9.055577	1.496212
28	6	0	-17.3532	7.931236	0.044082
29	1	0	-18.5345	9.076693	-1.37225
30	1	0	-15.9486	7.077753	1.457915
31	6	0	-8.61962	17.1328	0.060314
32	6	0	-7.48149	16.82061	0.825507
33	6	0	-8.58966	18.2804	-0.75368
34	6	0	-6.35501	17.64545	0.796745
35	1	0	-7.4862	15.93183	1.459878
36	6	0	-7.46135	19.1014	-0.79035
37	1	0	-9.46072	18.53292	-1.36482
38	6	0	-6.33232	18.79849	-0.00826
39	1	0	-5.48735	17.38375	1.400886
40	1	0	-7.47147	19.99367	-1.41806
41	6	0	-18.2629	6.76481	0.042554
42	6	0	-18.7011	6.189303	1.253443

43	6	0	-18.7188	6.202495	-1.16803
44	6	0	-19.5855	5.100106	1.212575
45	1	0	-18.3728	6.610456	2.205737
46	6	0	-19.6023	5.11214	-1.12749
47	1	0	-18.3892	6.622819	-2.11998
48	7	0	-20.0462	4.570215	0.043291
49	6	0	-5.14965	19.68593	-0.02675
50	6	0	-4.57065	20.14531	1.175217
51	6	0	-4.57208	20.09668	-1.24643
52	6	0	-3.45711	20.99793	1.117904
53	1	0	-5.01147	19.85812	2.132182
54	6	0	-3.45763	20.94975	-1.22336
55	1	0	-5.00019	19.75558	-2.19121
56	7	0	-2.90547	21.40549	-0.06226
57	6	0	-2.75729	21.4294	-2.44791
58	6	0	-2.41791	22.78902	-2.58261
59	6	0	-2.35779	20.54377	-3.46119
60	6	0	-1.65708	23.20482	-3.68155
61	1	0	-2.73426	23.51333	-1.82292
62	6	0	-1.59952	21.02744	-4.53835
63	1	0	-2.62011	19.48213	-3.40999
64	7	0	-1.231	22.33723	-4.64843
65	1	0	-1.36261	24.25888	-3.80341
66	1	0	-1.26426	20.35429	-5.34129
67	6	0	-2.76039	21.534	2.320789
68	6	0	-2.36403	22.88488	2.363675
69	6	0	-2.42151	20.71183	3.406838
70	6	0	-1.61016	23.34964	3.446946

71	1	0	-2.63171	23.56293	1.544714
72	6	0	-1.66738	21.24326	4.464886
73	1	0	-2.72797	19.6615	3.42928
74	7	0	-1.24473	22.5406	4.487246
75	1	0	-1.27355	24.3966	3.498466
76	1	0	-1.3798	20.61819	5.323475
77	6	0	-20.1001	4.407309	2.427
78	6	0	-21.4768	4.149775	2.565338
79	6	0	-19.2326	3.933697	3.423856
80	6	0	-21.9313	3.396365	3.654173
81	1	0	-22.1849	4.521557	1.815701
82	6	0	-19.7556	3.192175	4.493885
83	1	0	-18.1547	4.12037	3.360498
84	7	0	-21.0855	2.904596	4.608787
85	1	0	-22.9999	3.160943	3.776114
86	1	0	-19.0994	2.803222	5.286274
87	6	0	-20.1308	4.430594	-2.34207
88	6	0	-21.4969	4.101021	-2.42953
89	6	0	-19.2869	4.040612	-3.39383
90	6	0	-21.9602	3.363712	-3.52497
91	1	0	-22.1882	4.404352	-1.63467
92	6	0	-19.8186	3.310954	-4.46821
93	1	0	-18.2184	4.282965	-3.37177
94	7	0	-21.135	2.955641	-4.53594
95	1	0	-23.0191	3.074886	-3.60903
96	1	0	-19.179	2.987175	-5.30258
97	6	0	-11.2822	-13.9832	-0.43651
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103	1	0	-11.3478	-15.0601	-0.61427
104	1	0	-9.00428	-11.5272	0.301566
105	1	0	-13.414	-13.6989	-0.73866
106	6	0	-12.8039	-9.54455	0.001274
107	6	0	-13.5435	-8.3804	0.075729
108	6	0	-14.9434	-8.44879	-0.14694
109	6	0	-15.5407	-9.68058	-0.43964
110	6	0	-14.7848	-10.8685	-0.51589
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112	1	0	-13.0636	-7.42946	0.309846
113	1	0	-16.6175	-9.73542	-0.6217
114	1	0	-15.2775	-11.8145	-0.74499
115	6	0	-11.3216	-9.76269	0.191048
116	8	0	-10.4843	-8.9336	0.431799
117	6	0	-15.7869	-7.23099	-0.07658
118	6	0	-16.9489	-7.21833	0.717067
119	6	0	-15.4674	-6.08098	-0.82052
120	6	0	-17.7795	-6.09683	0.750329
121	1	0	-17.2063	-8.09757	1.314122
122	6	0	-16.3006	-4.96047	-0.79364
123	1	0	-14.5676	-6.07223	-1.43846
124	6	0	-17.4705	-4.95737	-0.0134
125	1	0	-18.6837	-6.12067	1.360495
126	1	0	-16.0345	-4.08266	-1.3818

127	6	0	-8.83382	-14.2516	-0.08216
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130	6	0	-6.58706	-14.8099	-0.83797
131	1	0	-7.69912	-13.0871	-1.5103
132	6	0	-7.69753	-16.2274	0.779991
133	1	0	-9.68123	-15.62	1.369457
134	6	0	-6.5731	-15.9528	-0.01893
135	1	0	-5.72263	-14.5715	-1.4574
136	1	0	-7.71474	-17.1117	1.418778
137	6	0	-18.3722	-3.78466	-0.00573
138	6	0	-18.8079	-3.20328	-1.21445
139	6	0	-18.8174	-3.2201	1.207622
140	6	0	-19.6748	-2.10001	-1.16883
141	1	0	-18.4901	-3.62961	-2.16799
142	6	0	-19.6825	-2.11478	1.171876
143	1	0	-18.4922	-3.64917	2.157146
144	7	0	-20.1203	-1.56335	0.003096
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146	6	0	-4.83998	-17.3274	-1.21135
147	6	0	-4.83515	-17.2901	1.210331
148	6	0	-3.74711	-18.2068	-1.16005
149	1	0	-5.27223	-17.023	-2.16661
150	6	0	-3.74304	-18.172	1.180399
151	1	0	-5.24833	-16.9403	2.158164
152	7	0	-3.20679	-18.6381	0.016532
153	6	0	-3.05415	-18.6773	2.401027
154	6	0	-2.78055	-20.0509	2.541206

155	6	0	-2.60144	-17.8053	3.403417
156	6	0	-2.03255	-20.497	3.637149
157	1	0	-3.13562	-20.763	1.787354
158	6	0	-1.8629	-18.3196	4.479761
159	1	0	-2.80234	-16.7296	3.340006
160	7	0	-1.5601	-19.6458	4.596863
161	1	0	-1.78582	-21.5628	3.761162
162	1	0	-1.48892	-17.6589	5.275612
163	6	0	-3.06353	-18.7499	-2.36696
164	6	0	-2.71952	-20.1139	-2.42978
165	6	0	-2.68556	-17.9223	-3.43587
166	6	0	-1.97865	-20.5898	-3.51729
167	1	0	-3.01518	-20.7937	-1.62212
168	6	0	-1.95062	-18.4659	-4.50075
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173	6	0	-20.1818	-1.39725	-2.38051
174	6	0	-21.5507	-1.0933	-2.50252
175	6	0	-19.3122	-0.96034	-3.3923
176	6	0	-21.9937	-0.3314	-3.59007
177	1	0	-22.2609	-1.43634	-1.74133
178	6	0	-19.8236	-0.20704	-4.45968
179	1	0	-18.2415	-1.18667	-3.34476
180	7	0	-21.1441	0.125693	-4.55858
181	1	0	-23.0552	-0.06067	-3.7
182	1	0	-19.1651	0.154524	-5.26315

183	6	0	-20.1941	-1.42448	2.388652
184	6	0	-21.5472	-1.04305	2.469236
185	6	0	-19.3443	-1.07612	3.450325
186	6	0	-21.9898	-0.29583	3.566461
187	1	0	-22.244	-1.31428	1.667525
188	6	0	-19.8549	-0.33255	4.525375
189	1	0	-18.2871	-1.36332	3.435985
190	7	0	-21.1566	0.07413	4.585539
191	1	0	-23.0375	0.032442	3.645681
192	1	0	-19.2096	-0.03946	5.36671
193	6	0	15.37581	-9.91237	-0.41725
194	6	0	14.7901	-8.6696	-0.14942
195	6	0	13.3888	-8.58079	0.056531
196	6	0	12.63586	-9.73681	-0.00977
197	6	0	13.24086	-11.0034	-0.28061
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199	1	0	16.45406	-9.98266	-0.58491
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201	1	0	15.08946	-12.0468	-0.69718
202	6	0	10.92914	-11.418	-0.00763
203	6	0	9.76197	-12.1533	0.061144
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205	6	0	11.06261	-14.1607	-0.41241
206	6	0	12.25348	-13.4088	-0.48408
207	6	0	12.18602	-12.0424	-0.27941
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209	1	0	11.11638	-15.24	-0.57918
210	1	0	13.2008	-13.907	-0.69551

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212	8	0	10.31999	-9.09219	0.390597
213	6	0	8.607223	-14.3939	-0.07897
214	6	0	8.571415	-15.5352	0.74333
215	6	0	7.476034	-14.089	-0.85689
216	6	0	7.444276	-16.3582	0.774637
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218	6	0	6.350776	-14.9158	-0.83263
219	1	0	7.485953	-13.2061	-1.49871
220	6	0	6.322062	-16.0633	-0.02018
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223	6	0	15.64666	-7.4604	-0.08804
224	6	0	15.36051	-6.32759	-0.87062
225	6	0	16.78725	-7.43928	0.73574
226	6	0	16.20497	-5.21545	-0.84977
227	1	0	14.47822	-6.32613	-1.51346
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229	1	0	17.01955	-8.30614	1.360452
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232	1	0	18.51489	-6.34296	1.398565
233	6	0	5.143014	-16.9565	-0.00988
234	6	0	4.561552	-17.3991	-1.21609
235	6	0	4.57395	-17.3911	1.205685
236	6	0	3.458124	-18.2657	-1.16627
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239	1	0	5.000471	-17.0586	2.153912
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242	6	0	18.71443	-3.46573	-1.23859
243	6	0	18.71364	-3.47515	1.18298
244	6	0	19.60193	-2.37912	-1.19372
245	1	0	18.39248	-3.88889	-2.19215
246	6	0	19.60268	-2.38911	1.14654
247	1	0	18.37467	-3.89099	2.133602
248	7	0	20.05633	-1.84978	-0.021
249	6	0	20.12726	-1.70921	2.363987
250	6	0	21.50267	-1.43602	2.485385
251	6	0	19.27022	-1.26398	3.38268
252	6	0	21.96491	-0.69515	3.579577
253	1	0	22.20343	-1.78553	1.718445
254	6	0	19.80032	-0.5326	4.45608
255	1	0	18.19376	-1.46504	3.334254
256	7	0	21.12808	-0.22957	4.554998
257	1	0	23.03231	-0.44877	3.689229
258	1	0	19.15163	-0.16468	5.26454
259	6	0	20.1285	-1.69064	-2.40519
260	6	0	21.49764	-1.376	-2.49968
261	6	0	19.28104	-1.2793	-3.44584
262	6	0	21.96098	-0.63175	-3.59033
263	1	0	22.19155	-1.69695	-1.71403
264	6	0	19.81301	-0.54412	-4.51644
265	1	0	18.21057	-1.50997	-3.41829
266	7	0	21.13272	-0.20311	-4.59036

267	1	0	23.02243	-0.3541	-3.67942
268	1	0	19.17109	-0.20423	-5.34257
269	6	0	2.760676	-18.7864	-2.37547
270	6	0	2.468276	-20.1586	-2.48822
271	6	0	2.318401	-17.9282	-3.39443
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273	1	0	2.815406	-20.8606	-1.72125
274	6	0	1.572276	-18.4536	-4.46001
275	1	0	2.533394	-16.8546	-3.35223
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279	6	0	2.776138	-18.7596	2.393181
280	6	0	2.399426	-20.1135	2.483263
281	6	0	2.420215	-17.9025	3.446228
282	6	0	1.648605	-20.5497	3.580499
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284	6	0	1.672916	-18.4068	4.521789
285	1	0	2.7035	-16.8442	3.425106
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287	1	0	1.323925	-21.5979	3.667004
288	1	0	1.373136	-17.7553	5.35603
289	6	0	15.59884	12.41426	0.434991
290	6	0	14.99944	11.18451	0.138863
291	6	0	13.60031	11.11967	-0.08975
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293	6	0	13.48239	13.53875	0.282694
294	6	0	14.84527	13.60383	0.510723

295	1	0	16.67525	12.46611	0.620243
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299	6	0	10.02562	14.74399	-0.09207
300	6	0	10.10991	16.14239	0.134827
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305	1	0	11.41479	17.80099	0.613763
306	1	0	13.47785	16.43628	0.740036
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308	8	0	10.54506	11.68065	-0.4616
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310	6	0	8.892261	18.15347	-0.73728
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314	6	0	6.639772	17.53743	0.79484
315	1	0	7.74176	15.80116	1.448185
316	6	0	6.638748	18.69815	0.000612
317	1	0	7.803135	19.88901	-1.39213
318	1	0	5.764935	17.2831	1.391753
319	6	0	15.83901	9.963769	0.071189
320	6	0	15.52079	8.820885	0.826443
321	6	0	16.99472	9.940877	-0.73113
322	6	0	16.34894	7.696621	0.800838

323	1	0	14.62601	8.820699	1.45179
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325	1	0	17.25149	10.8153	-1.33543
326	6	0	17.51141	7.681915	0.009768
327	1	0	16.08414	6.824903	1.398635
328	1	0	18.71866	8.830523	-1.38164
329	6	0	5.46986	19.60375	-0.01481
330	6	0	4.893207	20.06092	1.188875
331	6	0	4.90355	20.03451	-1.2331
332	6	0	3.794305	20.93241	1.133976
333	1	0	5.323973	19.75757	2.145428
334	6	0	3.801152	20.90311	-1.20757
335	1	0	5.331887	19.69616	-2.17875
336	7	0	3.252604	21.35801	-0.04368
337	6	0	18.40615	6.503899	0.000305
338	6	0	18.8459	5.922771	1.207935
339	6	0	18.84187	5.934647	-1.21411
340	6	0	19.70726	4.815221	1.160872
341	1	0	18.53568	6.353771	2.161917
342	6	0	19.70397	4.826982	-1.17991
343	1	0	18.51255	6.361358	-2.16327
344	7	0	20.14497	4.275258	-0.01322
345	6	0	20.2097	4.134672	-2.3982
346	6	0	21.57352	3.805004	-2.51119
347	6	0	19.34333	3.732783	-3.42712
348	6	0	22.01307	3.052048	-3.60643
349	1	0	22.28229	4.120519	-1.7368
350	6	0	19.85068	2.985668	-4.50065

351	1	0	18.27678	3.980873	-3.38666
352	7	0	21.16515	2.627186	-4.5908
353	1	0	23.07022	2.7624	-3.7099
354	1	0	19.19387	2.650339	-5.3167
355	6	0	20.21887	4.113618	2.371108
356	6	0	21.57626	3.748594	2.455251
357	6	0	19.36645	3.739776	3.421772
358	6	0	22.02145	2.992906	3.545499
359	1	0	22.27459	4.03993	1.662011
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361	1	0	18.30554	4.012301	3.404594
362	7	0	21.18664	2.599719	4.554656
363	1	0	23.07269	2.676713	3.627093
364	1	0	19.23323	2.677567	5.324247
365	6	0	3.103147	21.47128	2.339049
366	6	0	2.789045	22.84126	2.420756
367	6	0	2.687699	20.63367	3.386136
368	6	0	2.036134	23.31364	3.502121
369	1	0	3.119233	23.52963	1.63398
370	6	0	1.938989	21.17305	4.443423
371	1	0	2.930508	19.56665	3.377115
372	7	0	1.594318	22.49257	4.50202
373	1	0	1.761201	24.37693	3.582569
374	1	0	1.592262	20.53833	5.272323
375	6	0	3.111209	21.40161	-2.43026
376	6	0	2.733371	22.75493	-2.52634
377	6	0	2.760224	20.54142	-3.48253
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381	1	0	3.051809	19.48635	-3.46256
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383	1	0	1.6631	24.23521	-3.72025
384	1	0	1.715165	20.38571	-5.39324
385	6	0	0.87965	24.52654	-8.40292
386	6	0	-0.47138	23.87325	-8.70764
387	1	0	0.7386	25.56969	-8.02441
388	1	0	1.460272	24.65044	-9.35419
389	1	0	-1.04485	24.51765	-9.42454
390	1	0	-0.33067	22.90463	-9.24735
391	7	0	-1.22119	23.63352	-7.4179
392	7	0	1.620737	23.70462	-7.37433
393	6	0	2.643249	24.56003	-6.6915
394	1	0	3.283128	23.96121	-6.0207
395	1	0	3.332905	25.07707	-7.39267
396	1	0	2.147064	25.3431	-6.08923
397	6	0	2.275206	22.51542	-8.00853
398	1	0	2.817572	21.9217	-7.25196
399	1	0	1.5177	21.85851	-8.4743
400	6	0	-1.84757	24.89976	-6.91987
401	1	0	-2.54566	25.37115	-7.6434
402	1	0	-2.42792	24.71461	-5.99933
403	1	0	-1.07081	25.65108	-6.68505
404	6	0	-2.26695	22.58253	-7.63188
405	1	0	-2.90805	22.47095	-6.74007
406	1	0	-2.95219	22.80183	-8.4778

407	1	0	-1.79088	21.60665	-7.83794
408	46	0	0.194555	23.01518	-6.05923
409	1	0	3.010892	22.77618	-8.79756
410	6	0	-22.7051	2.172565	8.637676
411	6	0	-23.3901	0.839805	8.321147
412	1	0	-21.7444	2.004417	9.183582
413	1	0	-23.3404	2.758754	9.352037
414	1	0	-23.5379	0.258861	9.26854
415	1	0	-24.4254	1.009536	7.933368
416	7	0	-22.5775	0.082198	7.297239
417	7	0	-22.4357	2.921933	7.353552
418	6	0	-21.3637	3.943083	7.581674
419	1	0	-21.2269	4.581933	6.69153
420	1	0	-21.5766	4.631811	8.425946
421	1	0	-20.4012	3.4441	7.79654
422	6	0	-23.6827	3.578151	6.845612
423	1	0	-23.4738	4.165695	5.934737
424	1	0	-24.4446	2.818274	6.590745
425	6	0	-21.4159	-0.61115	7.941163
426	1	0	-21.7077	-1.34724	8.718542
427	1	0	-20.8266	-1.16144	7.186607
428	1	0	-20.745	0.123528	8.423242
429	6	0	-23.4533	-0.91001	6.59587
430	1	0	-22.8641	-1.5617	5.927776
431	1	0	-23.9994	-1.5893	7.284673
432	1	0	-24.2131	-0.38648	5.9868
433	46	0	-21.8285	1.495735	5.999961
434	1	0	-24.1508	4.276714	7.570553

435	6	0	-22.7597	0.89715	-8.58112
436	6	0	-23.3999	2.252358	-8.26612
437	1	0	-21.7968	1.032418	-9.13206
438	1	0	-23.417	0.329428	-9.29054
439	1	0	-23.532	2.835094	-9.21473
440	1	0	-24.4389	2.117337	-7.87435
441	7	0	-22.56	2.986261	-7.24705
442	7	0	-22.5086	0.143556	-7.29581
443	6	0	-21.4715	-0.91267	-7.52595
444	1	0	-21.3518	-1.5536	-6.63485
445	1	0	-21.7108	-1.59628	-8.36738
446	1	0	-20.4943	-0.44609	-7.74669
447	6	0	-23.7735	-0.47032	-6.77944
448	1	0	-23.5795	-1.05824	-5.8655
449	1	0	-24.5105	0.31439	-6.52656
450	6	0	-21.377	3.637654	-7.89593
451	1	0	-21.6454	4.382682	-8.67313
452	1	0	-20.766	4.167224	-7.14371
453	1	0	-20.7339	2.879366	-8.37941
454	6	0	-23.4006	4.010282	-6.54832
455	1	0	-22.7883	4.645062	-5.88468
456	1	0	-23.9253	4.70422	-7.23908
457	1	0	-24.176	3.515177	-5.93532
458	46	0	-21.8521	1.553233	-5.94793
459	1	0	-24.2659	-1.15845	-7.49829
460	6	0	22.77495	1.874687	-8.62029
461	6	0	23.39881	0.509249	-8.31705
462	1	0	21.81187	1.755756	-9.17479

463	1	0	23.4404	2.441622	-9.32273
464	1	0	23.52518	-0.06619	-9.27091
465	1	0	24.43881	0.628503	-7.92288
466	7	0	22.54953	-0.22446	-7.30563
467	7	0	22.52939	2.618785	-7.32841
468	6	0	21.50413	3.688122	-7.55062
469	1	0	21.38989	4.322286	-6.65403
470	1	0	21.75218	4.376594	-8.38557
471	1	0	20.52237	3.234091	-7.77731
472	6	0	23.79972	3.21433	-6.8037
473	1	0	23.61047	3.790275	-5.88114
474	1	0	24.53009	2.419859	-6.56221
475	6	0	21.35756	-0.85302	-7.96073
476	1	0	21.61563	-1.59373	-8.74555
477	1	0	20.73976	-1.38191	-7.21359
478	1	0	20.72471	-0.08124	-8.43617
479	6	0	23.37685	-1.26737	-6.61917
480	1	0	22.75667	-1.90204	-5.96278
481	1	0	23.8921	-1.96019	-7.31824
482	1	0	24.15909	-0.78975	-6.0011
483	46	0	21.85897	1.20438	-5.99254
484	1	0	24.2979	3.908328	-7.51276
485	6	0	-0.8487	-22.0893	-8.23937
486	6	0	0.504009	-21.4453	-8.55742
487	1	0	-0.70934	-23.1222	-7.83357
488	1	0	-1.42694	-22.2371	-9.18844
489	1	0	1.078128	-22.1081	-9.25649
490	1	0	0.365369	-20.4901	-9.1209

491	7	0	1.251237	-21.1739	-7.27249
492	7	0	-1.59139	-21.2402	-7.2343
493	6	0	-2.6125	-22.0775	-6.52738
494	1	0	-3.25311	-21.4603	-5.87395
495	1	0	-3.30127	-22.6156	-7.21311
496	1	0	-2.11475	-22.8416	-5.90244
497	6	0	-2.24792	-20.0704	-7.90159
498	1	0	-2.7867	-19.4541	-7.16036
499	1	0	-1.49178	-19.4279	-8.38911
500	6	0	1.870935	-22.4287	-6.73871
501	1	0	2.563363	-22.9263	-7.44982
502	1	0	2.45587	-22.2199	-5.82614
503	1	0	1.089681	-23.1668	-6.47834
504	6	0	2.301788	-20.133	-7.51103
505	1	0	2.937972	-19.998	-6.61872
506	1	0	2.990505	-20.3782	-8.34656
507	1	0	1.82988	-19.1616	-7.74583
508	46	0	-0.16749	-20.5082	-5.9389
509	1	0	-2.98666	-20.3543	-8.67941
510	6	0	0.490885	-21.9223	8.334371
511	6	0	-0.84679	-21.2417	8.639569
512	1	0	0.328044	-22.96	7.949974
513	1	0	1.066455	-22.0634	9.286056
514	1	0	-1.43493	-21.8768	9.352525
515	1	0	-0.68619	-20.2783	9.182963
516	7	0	-1.5889	-20.9804	7.349606
517	7	0	1.251564	-21.1111	7.311672
518	6	0	2.253681	-21.9853	6.622556

519	1	0	2.907069	-21.3963	5.955949
520	1	0	2.930877	-22.5237	7.319427
521	1	0	1.738874	-22.7514	6.014032
522	6	0	1.93391	-19.9421	7.954195
523	1	0	2.486263	-19.3539	7.200295
524	1	0	1.192145	-19.2727	8.427284
525	6	0	-2.23783	-22.2316	6.842792
526	1	0	-2.94183	-22.6973	7.563992
527	1	0	-2.8172	-22.0289	5.925312
528	1	0	-1.47403	-22.9933	6.599051
529	6	0	-2.61496	-19.9107	7.566752
530	1	0	-3.24881	-19.7801	6.672189
531	1	0	-3.30797	-20.1221	8.407895
532	1	0	-2.1204	-18.9457	7.780364
533	46	0	-0.15673	-20.3757	6.000973
534	1	0	2.666006	-20.2256	8.738367
535	6	0	0.86	24.20286	8.49631
536	6	0	-0.48099	24.86407	8.165554
537	1	0	0.704812	23.25888	9.074367
538	1	0	1.443655	24.86653	9.186999
539	1	0	-1.05931	25.03457	9.111047
540	1	0	-0.32424	25.88911	7.745974
541	7	0	-1.23494	24.01326	7.170336
542	7	0	1.605438	23.90034	7.217264
543	6	0	2.635279	22.84303	7.473159
544	1	0	3.274189	22.68612	6.586577
545	1	0	3.324413	23.08578	8.309528
546	1	0	2.144723	21.88357	7.718409

547	6	0	2.250712	25.13597	6.668996
548	1	0	2.828619	24.90524	5.757256
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550	6	0	-1.90781	22.86079	7.851372
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553	1	0	-1.16068	22.21145	8.343742
554	6	0	-2.24412	24.85635	6.453228
555	1	0	-2.89365	24.24112	5.806933
556	1	0	-2.92553	25.41182	7.132811
557	1	0	-1.736	25.60679	5.820197
558	46	0	0.179854	23.24965	5.884663
559	1	0	2.9557	25.62566	7.373519
560	6	0	22.76574	0.473922	8.582643
561	6	0	23.4371	1.815935	8.276168
562	1	0	21.80738	0.627872	9.136715
563	1	0	23.41085	-0.11435	9.286455
564	1	0	23.58468	2.388445	9.228732
565	1	0	24.47184	1.659401	7.881244
566	7	0	22.61286	2.576952	7.264203
567	7	0	22.49427	-0.264	7.292383
568	6	0	21.43182	-1.296	7.516467
569	1	0	21.29464	-1.92666	6.620618
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571	1	0	20.4668	-0.80701	7.742608
572	6	0	23.74302	-0.90494	6.769458
573	1	0	23.53344	-1.47941	5.850419
574	1	0	24.49933	-0.13677	6.52281

575	6	0	21.44601	3.250266	7.920003
576	1	0	21.73259	3.982061	8.703328
577	1	0	20.84714	3.800843	7.173166
578	1	0	20.78574	2.503168	8.397557
579	6	0	23.4758	3.586962	6.572388
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584	1	0	24.21844	-1.61144	7.481778
585	6	0	-11.3862	3.385664	-1.7404
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587	6	0	-10.7097	1.007322	-1.72869
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589	6	0	-12.458	1.788263	-3.29354
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593	6	0	-10.4142	2.483312	0.23299
594	6	0	-10.4164	1.390814	1.084936
595	6	0	-10.7121	-0.15128	-0.82513
596	6	0	-12.2891	-0.56601	-2.5555
597	6	0	-13.6332	-0.77166	-2.82249
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608	6	0	-15.3029	4.494282	-1.02203
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615	6	0	-14.6204	-2.0073	0.538586
616	6	0	-13.6459	-1.75245	1.608212
617	6	0	-13.982	-0.92537	2.667999
618	6	0	-15.3121	-0.30428	2.720127
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620	6	0	-17.2015	0.356605	-0.25918
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622	6	0	-15.7868	-0.92453	-1.83014
623	6	0	-14.4571	-1.54566	-1.88534
624	6	0	-13.8905	-2.07142	-0.73509
625	6	0	-12.3141	-1.65795	0.995541
626	6	0	-11.3945	-0.74052	1.477346
627	6	0	-11.751	0.13667	2.601381
628	6	0	-13.0069	0.046402	3.179721
629	6	0	-13.7341	1.268006	3.548703
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635	6	0	-16.9045	2.989756	0.798412
636	6	0	-15.9303	3.961753	1.310101
637	6	0	-15.331	3.405352	2.529471
638	6	0	-13.9858	3.608916	2.793816
639	6	0	-13.1641	2.51009	3.319731
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641	6	0	-11.1463	1.454021	2.358694
642	6	0	-12.4654	-1.85503	-0.45246
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644	6	0	-16.2325	-0.54716	1.713018
645	6	0	0.501089	-8.87043	-0.57649
646	6	0	-0.01512	-9.31666	-1.87784
647	6	0	-1.3433	-9.68958	-2.00548
648	6	0	-2.23575	-9.63907	-0.83949
649	6	0	-1.74908	-9.21841	0.387524
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653	6	0	1.035788	-10.1042	-2.53733
654	6	0	0.69855	-11.2194	-3.28715
655	6	0	-1.70057	-10.8729	-2.79991
656	6	0	-3.14481	-10.791	-0.91296
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661	6	0	0.136879	-9.28351	1.834005
662	6	0	1.428531	-9.7655	1.970824
663	6	0	2.321004	-9.8163	0.804757
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665	6	0	3.440623	-11.7587	-0.2389
666	6	0	3.128723	-11.0397	0.903732
667	6	0	2.734952	-11.7456	2.131025
668	6	0	1.684295	-10.9576	2.790665
669	6	0	0.634183	-11.5992	3.427351
670	6	0	-0.73534	-11.0878	3.28295
671	6	0	-1.64447	-12.2391	3.2079
672	6	0	-2.74355	-12.2012	2.365102
673	6	0	-2.81375	-11.5541	-2.12445
674	6	0	-2.00811	-15.2997	0.45338
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676	6	0	-1.56645	-14.9165	-1.94911
677	6	0	-0.27415	-15.3986	-1.81246
678	6	0	0.202446	-15.8588	-0.50216
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680	6	0	-1.17496	-14.58	2.558324
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682	6	0	-3.0995	-13.3847	1.57014
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686	6	0	-0.77277	-13.0824	-3.40444

687	6	0	0.596775	-13.5938	-3.2582
688	6	0	0.839211	-14.7202	-2.48796
689	6	0	2.003812	-14.76	-1.5946
690	6	0	1.609701	-15.463	-0.36726
691	6	0	2.096429	-15.0421	0.86019
692	6	0	1.204623	-14.9919	2.025871
693	6	0	-0.83664	-13.4624	3.3047
694	6	0	0.571758	-13.0667	3.441116
695	6	0	1.563056	-13.8097	2.820169
696	6	0	2.676634	-13.1301	2.14651
697	6	0	3.005844	-13.8914	0.934984
698	6	0	3.376734	-13.226	-0.22256
699	6	0	2.85945	-13.6722	-1.52328
700	6	0	2.60502	-12.4801	-2.34347
701	6	0	1.506012	-12.4421	-3.1865
702	6	0	-2.87388	-12.9385	-2.11029
703	6	0	-0.70969	-11.6152	-3.42194
704	6	0	-0.63952	-15.8109	0.597715
705	6	0	12.93241	2.619741	-3.12847
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707	6	0	12.89446	0.148027	-3.18435
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716	6	0	11.54831	-0.94746	-1.55996
717	6	0	10.92958	-0.79451	-0.32985
718	6	0	10.31702	0.49178	0.029733
719	6	0	10.35842	1.55179	-0.86136
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721	6	0	11.47441	3.586215	-1.38001
722	6	0	12.48469	4.444877	-0.97804
723	6	0	13.78644	4.414757	-1.65788
724	6	0	16.26543	3.009142	-1.84398
725	6	0	16.0348	3.947109	-0.73833
726	6	0	14.83142	4.628328	-0.64733
727	6	0	14.17495	4.791328	0.657023
728	6	0	12.72487	4.677587	0.452479
729	6	0	11.9406	4.038989	1.399494
730	6	0	10.86841	3.129005	0.973365
731	6	0	10.8244	2.004891	1.918451
732	6	0	10.55688	0.725003	1.460519
733	6	0	12.82351	-1.67088	-1.65509
734	6	0	13.57722	-0.93811	2.841887
735	6	0	13.79444	-1.82378	1.798778
736	6	0	15.09668	-1.85085	1.118837
737	6	0	16.10895	-0.99464	1.522051
738	6	0	15.87925	-0.0562	2.627837
739	6	0	14.03676	1.258329	3.626922
740	6	0	12.58651	1.142767	3.424089
741	6	0	12.30258	-0.21449	2.938822
742	6	0	11.31781	-0.41723	1.985602

743	6	0	11.54839	-1.35647	0.878922
744	6	0	12.75027	-2.03984	0.788667
745	6	0	14.85676	-2.0842	-0.31173
746	6	0	15.64198	-1.4468	-1.25924
747	6	0	16.71254	-0.53721	-0.83233
748	6	0	16.93805	-0.31714	0.51738
749	6	0	17.22254	1.038893	1.00259
750	6	0	16.56683	1.200563	2.306496
751	6	0	15.98861	2.413956	2.644885
752	6	0	14.68739	2.444077	3.324984
753	6	0	11.86932	2.219825	2.928915
754	6	0	12.5595	3.477017	2.608043
755	6	0	13.92737	3.586174	2.801375
756	6	0	14.75849	4.261853	1.797105
757	6	0	16.0326	3.537957	1.700419
758	6	0	16.65084	3.384529	0.469692
759	6	0	17.26323	2.099045	0.110919
760	6	0	17.02424	1.866537	-1.31888
761	6	0	16.75671	0.586133	-1.77678
762	6	0	13.40668	-2.20086	-0.51549
763	6	0	15.02447	-0.88614	-2.46748
764	6	0	14.64945	-0.0274	3.266259

14.2.5 $(C_{70})_3$@Tetrafacial tube

Center Number	Atomic Number	Atomic Types	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	7.324309	9.671293	-0.2658
2	6	0	7.476189	8.286775	-0.40558

3	6	0	6.331175	7.454566	-0.50382
4	6	0	5.082582	8.043095	-0.46805
5	6	0	4.935591	9.459346	-0.3356
6	6	0	6.049543	10.27192	-0.22928
7	1	0	8.206145	10.31299	-0.17678
8	1	0	6.43669	6.375264	-0.61488
9	1	0	5.958831	11.35491	-0.12229
10	6	0	2.749004	8.57498	-0.48658
11	6	0	1.369331	8.585302	-0.54169
12	6	0	0.697131	9.832097	-0.46004
13	6	0	1.431788	11.01513	-0.31847
14	6	0	2.840198	11.0041	-0.2603
15	6	0	3.493222	9.78826	-0.34847
16	1	0	0.807498	7.658027	-0.65426
17	1	0	0.913819	11.97615	-0.2445
18	1	0	3.389784	11.94141	-0.15095
19	6	0	3.713126	7.417252	-0.55398
20	8	0	3.446613	6.245188	-0.64385
21	6	0	-0.78152	9.899834	-0.52038
22	6	0	-1.41441	10.78275	-1.4144
23	6	0	-1.57639	9.112147	0.330795
24	6	0	-2.80542	10.89149	-1.44227
25	1	0	-0.81104	11.395	-2.09105
26	6	0	-2.96778	9.221422	0.305827
27	1	0	-1.09857	8.42373	1.030295
28	6	0	-3.59699	10.11777	-0.57537
29	1	0	-3.27164	11.60139	-2.12717
30	1	0	-3.56509	8.602867	0.974757
31	6	0	8.838685	7.70694	-0.45094
32	6	0	9.200906	6.640434	0.390293

33	6	0	9.80473	8.239044	-1.3249
34	6	0	10.49998	6.128967	0.371365
35	1	0	8.463214	6.220355	1.076816
36	6	0	11.10317	7.729062	-1.34569
37	1	0	9.53759	9.063722	-1.99218
38	6	0	11.46649	6.671648	-0.49267
39	1	0	10.7578	5.300142	1.02948
40	1	0	11.8409	8.1748	-2.01464
41	6	0	-5.06704	10.27212	-0.57167
42	6	0	-5.76377	10.4648	0.635096
43	6	0	-5.80933	10.24945	-1.76547
44	6	0	-7.16101	10.63424	0.616099
45	1	0	-5.20462	10.49488	1.572592
46	6	0	-7.20587	10.42555	-1.71849
47	1	0	-5.29323	10.08779	-2.71338
48	7	0	-7.88216	10.60094	-0.54489
49	6	0	12.85337	6.160785	-0.49519
50	6	0	13.57214	6.013514	0.704357
51	6	0	13.50099	5.824101	-1.6977
52	6	0	14.90131	5.550378	0.666501
53	1	0	13.09165	6.274024	1.649472
54	6	0	14.83152	5.364598	-1.67027
55	1	0	12.95654	5.920612	-2.63917
56	7	0	15.52474	5.213709	-0.50129
57	6	0	15.53702	5.017781	-2.9391
58	6	0	16.64244	4.147387	-2.96751
59	6	0	15.10418	5.547902	-4.16966
60	6	0	17.25108	3.829458	-4.19062
61	1	0	17.03593	3.732983	-2.03238
62	6	0	15.74892	5.180245	-5.35901

63	1	0	14.27148	6.259749	-4.21244
64	7	0	16.81531	4.327974	-5.38608
65	1	0	18.12142	3.157863	-4.23104
66	1	0	15.4133	5.578585	-6.33009
67	6	0	15.6797	5.40911	1.932001
68	6	0	16.66914	4.42263	2.094204
69	6	0	15.4253	6.257018	3.026363
70	6	0	17.33901	4.302198	3.320792
71	1	0	16.92442	3.761874	1.259307
72	6	0	16.11951	6.072513	4.230645
73	1	0	14.69731	7.073722	2.946809
74	7	0	17.06975	5.105505	4.393025
75	1	0	18.1238	3.545584	3.464848
76	1	0	15.91713	6.715133	5.103218
77	6	0	-7.90758	10.85491	1.889207
78	6	0	-9.26669	10.51931	2.028262
79	6	0	-7.25799	11.39586	3.015207
80	6	0	-9.90944	10.70655	3.261043
81	1	0	-9.82393	10.12763	1.170016
82	6	0	-7.95421	11.54349	4.222884
83	1	0	-6.21131	11.71861	2.958732
84	7	0	-9.26938	11.20336	4.361347
85	1	0	-10.9738	10.45884	3.386834
86	1	0	-7.45475	11.95052	5.116977
87	6	0	-8.00456	10.4191	-2.97926
88	6	0	-9.32209	9.92873	-3.02503
89	6	0	-7.44654	10.89024	-4.18239
90	6	0	-10.0152	9.905526	-4.24435
91	1	0	-9.80824	9.580462	-2.10769
92	6	0	-8.18872	10.82494	-5.37043

93	1	0	-6.43931	11.32246	-4.20269
94	7	0	-9.46334	10.33761	-5.41747
95	1	0	-11.0496	9.536191	-4.30016
96	1	0	-7.75936	11.17224	-6.32442
97	6	0	-0.94104	0.416089	-9.50931
98	6	0	-1.32089	0.871624	-8.24181
99	6	0	-0.36781	0.927333	-7.19228
100	6	0	0.927755	0.529398	-7.45622
101	6	0	1.309831	0.06821	-8.75467
102	6	0	0.381347	0.007589	-9.77779
103	1	0	-1.67784	0.365863	-10.3167
104	1	0	-0.65183	1.285884	-6.20258
105	1	0	0.652544	-0.34316	-10.7757
106	6	0	3.25982	-0.01027	-7.42039
107	6	0	4.591265	-0.21741	-7.11718
108	6	0	5.452282	-0.69763	-8.13733
109	6	0	4.942354	-0.96186	-9.41454
110	6	0	3.584196	-0.74888	-9.72434
111	6	0	2.750163	-0.26871	-8.73112
112	1	0	4.97558	-0.00711	-6.11915
113	1	0	5.601285	-1.34698	-10.1986
114	1	0	3.21345	-0.95864	-10.7298
115	6	0	2.132931	0.488207	-6.55011
116	8	0	2.18123	0.776417	-5.38102
117	6	0	6.893012	-0.92335	-7.87601
118	6	0	7.85637	-0.40837	-8.76397
119	6	0	7.326069	-1.67618	-6.77046
120	6	0	9.213733	-0.66262	-8.5682
121	1	0	7.538326	0.193841	-9.62019
122	6	0	8.684607	-1.93611	-6.57589

123	1	0	6.592038	-2.07742	-6.06985
124	6	0	9.641484	-1.43965	-7.47689
125	1	0	9.939015	-0.27252	-9.2839
126	1	0	8.999296	-2.52543	-5.71508
127	6	0	-2.72357	1.289351	-8.01068
128	6	0	-3.47929	0.727494	-6.967
129	6	0	-3.33135	2.236	-8.85509
130	6	0	-4.81432	1.090801	-6.78144
131	1	0	-3.02121	-0.01284	-6.30901
132	6	0	-4.66528	2.602233	-8.66913
133	1	0	-2.75542	2.685902	-9.66905
134	6	0	-5.42313	2.029183	-7.63265
135	1	0	-5.38244	0.643458	-5.96636
136	1	0	-5.12135	3.320743	-9.35194
137	6	0	11.07831	-1.74419	-7.30752
138	6	0	11.52168	-3.06911	-7.14491
139	6	0	12.04422	-0.72275	-7.32996
140	6	0	12.89913	-3.33464	-7.02447
141	1	0	10.78719	-3.87696	-7.13028
142	6	0	13.40723	-1.05216	-7.20101
143	1	0	11.72217	0.314301	-7.44042
144	7	0	13.83577	-2.33838	-7.03599
145	6	0	-6.84669	2.388977	-7.46041
146	6	0	-7.82606	1.392277	-7.3085
147	6	0	-7.26641	3.731872	-7.45716
148	6	0	-9.17802	1.760535	-7.16519
149	1	0	-7.52698	0.342452	-7.31579
150	6	0	-8.6335	4.035229	-7.3125
151	1	0	-6.52152	4.522657	-7.56196
152	7	0	-9.58286	3.063728	-7.1515

153	6	0	-9.10016	5.452736	-7.32745
154	6	0	-10.3057	5.848861	-6.71893
155	6	0	-8.33306	6.455731	-7.95005
156	6	0	-10.687	7.198429	-6.73646
157	1	0	-10.9524	5.099386	-6.2479
158	6	0	-8.76491	7.789304	-7.92146
159	1	0	-7.40242	6.207206	-8.47308
160	7	0	-9.9304	8.173738	-7.32313
161	1	0	-11.6301	7.525269	-6.27382
162	1	0	-8.16927	8.586322	-8.39482
163	6	0	-10.2201	0.70255	-7.01824
164	6	0	-11.3475	0.867163	-6.1964
165	6	0	-10.0766	-0.52816	-7.68772
166	6	0	-12.2612	-0.18926	-6.04773
167	1	0	-11.5183	1.818794	-5.68347
168	6	0	-11.0164	-1.54613	-7.4822
169	1	0	-9.24302	-0.69645	-8.38011
170	7	0	-12.1039	-1.39488	-6.66842
171	1	0	-13.1541	-0.08234	-5.41265
172	1	0	-10.9081	-2.52332	-7.98112
173	6	0	13.38789	-4.73754	-6.87965
174	6	0	14.61915	-5.04159	-6.27004
175	6	0	12.6147	-5.81873	-7.34359
176	6	0	15.01841	-6.37897	-6.13026
177	1	0	15.27107	-4.23287	-5.92156
178	6	0	13.06522	-7.1339	-7.16022
179	1	0	11.66436	-5.6474	-7.86347
180	7	0	14.25526	-7.42844	-6.55921
181	1	0	15.98198	-6.63552	-5.66564
182	1	0	12.46407	-7.9902	-7.50645

183	6	0	14.44249	0.022277	-7.23814
184	6	0	15.63837	-0.06664	-6.5031
185	6	0	14.23808	1.185706	-8.00363
186	6	0	16.55803	0.992153	-6.53714
187	1	0	15.85525	-0.96686	-5.91872
188	6	0	15.1911	2.214059	-7.98192
189	1	0	13.34552	1.295433	-8.6307
190	7	0	16.34583	2.133819	-7.25757
191	1	0	17.50354	0.938298	-5.97828
192	1	0	15.03681	3.139483	-8.56068
193	6	0	5.29401	0.534335	9.544073
194	6	0	5.797319	0.633581	8.241635
195	6	0	4.935684	0.996656	7.174638
196	6	0	3.608184	1.25092	7.45638
197	6	0	3.102395	1.154998	8.790351
198	6	0	3.938616	0.794453	9.831235
199	1	0	5.955262	0.244447	10.36621
200	1	0	5.317035	1.082739	6.156821
201	1	0	3.572045	0.712657	10.8566
202	6	0	1.280639	1.807825	7.433181
203	6	0	-0.01321	2.179924	7.126046
204	6	0	-0.96593	2.249548	8.175002
205	6	0	-0.58556	1.938726	9.485989
206	6	0	0.735507	1.559814	9.799445
207	6	0	1.663508	1.499109	8.775916
208	1	0	-0.29535	2.424427	6.102184
209	1	0	-1.32151	1.981567	10.29458
210	1	0	1.006387	1.32552	10.83101
211	6	0	2.482706	1.652052	6.535868
212	8	0	2.531721	1.799786	5.341011

213	6	0	-2.36761	2.645033	7.902962
214	6	0	-2.98392	3.642611	8.68079
215	6	0	-3.11707	2.012313	6.895414
216	6	0	-4.32233	3.980104	8.475877
217	1	0	-2.41088	4.155899	9.458612
218	6	0	-4.45815	2.344318	6.693563
219	1	0	-2.65157	1.240334	6.280676
220	6	0	-5.07717	3.325328	7.486948
221	1	0	-4.78435	4.740197	9.107829
222	1	0	-5.0239	1.836494	5.913041
223	6	0	7.231276	0.355959	7.994082
224	6	0	7.631108	-0.55613	7.0017
225	6	0	8.218564	0.9844	8.775312
226	6	0	8.982416	-0.85025	6.809567
227	1	0	6.876019	-1.05254	6.389829
228	6	0	9.569676	0.695245	8.581604
229	1	0	7.924943	1.703862	9.545396
230	6	0	9.965022	-0.23145	7.600697
231	1	0	9.27107	-1.5617	6.036312
232	1	0	10.31552	1.178281	9.214845
233	6	0	-6.50972	3.64697	7.311855
234	6	0	-7.47772	2.626886	7.302612
235	6	0	-6.94799	4.975729	7.170502
236	6	0	-8.83894	2.959147	7.165284
237	1	0	-7.15918	1.588726	7.41617
238	6	0	-8.32362	5.242611	7.032365
239	1	0	-6.21304	5.782413	7.163006
240	7	0	-9.26208	4.249673	7.015328
241	6	0	11.39545	-0.56082	7.42598
242	6	0	11.83591	-1.89599	7.429957

243	6	0	12.35855	0.451708	7.268154
244	6	0	13.20885	-2.17534	7.289289
245	1	0	11.10599	-2.69822	7.55479
246	6	0	13.71674	0.108071	7.127189
247	1	0	12.03525	1.494386	7.252319
248	7	0	14.14179	-1.1915	7.123083
249	6	0	14.74952	1.173981	6.968859
250	6	0	15.98858	0.93059	6.348129
251	6	0	14.50526	2.482798	7.427129
252	6	0	16.90875	1.977549	6.189943
253	1	0	16.23873	-0.07939	6.004453
254	6	0	15.46211	3.487502	7.226075
255	1	0	13.57614	2.728855	7.954441
256	7	0	16.65887	3.253068	6.611968
257	1	0	17.88574	1.804163	5.71504
258	1	0	15.27865	4.519144	7.567524
259	6	0	13.68851	-3.58839	7.317336
260	6	0	14.8003	-4.01617	6.569812
261	6	0	13.01478	-4.55538	8.08714
262	6	0	15.18047	-5.36642	6.5964
263	1	0	15.37476	-3.2931	5.981681
264	6	0	13.43714	-5.89206	8.056976
265	1	0	12.16744	-4.27477	8.724758
266	7	0	14.50861	-6.31035	7.320873
267	1	0	16.05301	-5.71952	6.027962
268	1	0	12.90792	-6.66476	8.63849
269	6	0	-9.87896	1.889172	7.177757
270	6	0	-11.0965	2.023822	6.48647
271	6	0	-9.66055	0.687018	7.876551
272	6	0	-12.0241	0.971526	6.497181

273	1	0	-11.3242	2.953729	5.954838
274	6	0	-10.623	-0.3318	7.834166
275	1	0	-8.74975	0.538793	8.46888
276	7	0	-11.7996	-0.20588	7.153162
277	1	0	-12.9858	1.059052	5.96987
278	1	0	-10.4598	-1.28514	8.362118
279	6	0	-8.80954	6.646448	6.890233
280	6	0	-9.97403	6.960632	6.165596
281	6	0	-8.09901	7.715262	7.467544
282	6	0	-10.3688	8.298952	6.026061
283	1	0	-10.5774	6.158947	5.726257
284	6	0	-8.54018	9.033022	7.277602
285	1	0	-7.20769	7.532024	8.07875
286	7	0	-9.66249	9.338623	6.563047
287	1	0	-11.2818	8.565024	5.47366
288	1	0	-7.98465	9.882057	7.708219
289	6	0	3.14216	-9.34389	0.258605
290	6	0	3.882157	-8.16767	0.424873
291	6	0	3.216017	-6.92047	0.540311
292	6	0	1.83664	-6.90318	0.489219
293	6	0	1.085733	-8.10867	0.322498
294	6	0	1.733486	-9.32499	0.204405
295	1	0	3.655866	-10.3051	0.161524
296	1	0	3.781837	-5.99863	0.676062
297	1	0	1.179379	-10.2571	0.074882
298	6	0	-0.49261	-6.35708	0.487235
299	6	0	-1.73678	-5.76071	0.536533
300	6	0	-2.88823	-6.58024	0.408782
301	6	0	-2.74521	-7.96158	0.233255
302	6	0	-1.47458	-8.57108	0.187424

303	6	0	-0.35473	-7.77045	0.317844
304	1	0	-1.83412	-4.6848	0.679832
305	1	0	-3.63111	-8.59427	0.122016
306	1	0	-1.39213	-9.65169	0.053734
307	6	0	0.879893	-5.74157	0.58798
308	8	0	1.156265	-4.57451	0.70522
309	6	0	-4.24565	-5.9883	0.454358
310	6	0	-5.2386	-6.55411	1.274786
311	6	0	-4.5753	-4.8748	-0.33887
312	6	0	-6.53432	-6.0348	1.286393
313	1	0	-4.99658	-7.41254	1.908019
314	6	0	-5.87155	-4.3563	-0.33123
315	1	0	-3.81603	-4.42524	-0.97995
316	6	0	-6.86496	-4.93576	0.476233
317	1	0	-7.29408	-6.50399	1.91379
318	1	0	-6.10891	-3.49561	-0.95505
319	6	0	5.360815	-8.23652	0.476961
320	6	0	6.148773	-7.43861	-0.37134
321	6	0	6.00013	-9.12331	1.362334
322	6	0	7.540765	-7.53669	-0.34657
323	1	0	5.664856	-6.7508	-1.06672
324	6	0	7.392118	-9.21774	1.392703
325	1	0	5.400875	-9.74815	2.031199
326	6	0	8.177378	-8.42743	0.535011
327	1	0	8.133534	-6.91135	-1.01336
328	1	0	7.864342	-9.92832	2.072856
329	6	0	-8.24638	-4.40587	0.461016
330	6	0	-8.95478	-4.28597	-0.74702
331	6	0	-8.88499	-4.01133	1.649365
332	6	0	-10.257	-3.74936	-0.7407

333	1	0	-8.49314	-4.63602	-1.67279
334	6	0	-10.1996	-3.50979	1.593333
335	1	0	-8.35182	-4.09631	2.597171
336	7	0	-10.8707	-3.35508	0.414585
337	6	0	9.650126	-8.54841	0.546387
338	6	0	10.36785	-8.71595	-0.65095
339	6	0	10.3764	-8.5085	1.75026
340	6	0	11.76955	-8.84199	-0.61031
341	1	0	9.824503	-8.75803	-1.59697
342	6	0	11.77822	-8.63936	1.725853
343	1	0	9.838946	-8.37009	2.690506
344	7	0	12.47443	-8.78989	0.558279
345	6	0	12.56136	-8.61023	2.996382
346	6	0	13.93129	-8.28933	3.024959
347	6	0	11.94222	-8.89385	4.228889
348	6	0	14.61459	-8.24652	4.249259
349	1	0	14.46551	-8.08999	2.088954
350	6	0	12.67935	-8.82198	5.419248
351	1	0	10.88612	-9.1849	4.272632
352	7	0	14.00641	-8.50186	5.446147
353	1	0	15.6873	-8.00597	4.289424
354	1	0	12.20435	-9.03073	6.391439
355	6	0	12.53406	-9.0318	-1.87777
356	6	0	13.8372	-8.53117	-2.0481
357	6	0	11.94988	-9.70236	-2.96907
358	6	0	14.48817	-8.68775	-3.28093
359	1	0	14.34498	-8.03381	-1.21529
360	6	0	12.64862	-9.80941	-4.17975
361	1	0	10.95499	-10.1564	-2.88201
362	7	0	13.90704	-9.30768	-4.35108

363	1	0	15.5111	-8.31387	-3.43173
364	1	0	12.19618	-10.3117	-5.05068
365	6	0	-11.0275	-3.58736	-2.00734
366	6	0	-12.4266	-3.44626	-2.01384
367	6	0	-10.3723	-3.58413	-3.25361
368	6	0	-13.1053	-3.29324	-3.23167
369	1	0	-12.9937	-3.4733	-1.06923
370	6	0	-11.1138	-3.44828	-4.43479
371	1	0	-9.2866	-3.70186	-3.31486
372	7	0	-12.4706	-3.28992	-4.44141
373	1	0	-14.2087	-3.19262	-3.25088
374	1	0	-10.6181	-3.47944	-5.41588
375	6	0	-10.921	-3.11679	2.838028
376	6	0	-11.937	-2.14302	2.829657
377	6	0	-10.6018	-3.71073	4.073055
378	6	0	-12.5742	-1.791	4.027497
379	1	0	-12.2426	-1.67913	1.884116
380	6	0	-11.2693	-3.30447	5.237298
381	1	0	-9.84782	-4.50345	4.136624
382	7	0	-12.2485	-2.35348	5.229896
383	1	0	-13.3809	-1.0439	4.040784
384	1	0	-11.0243	-3.75088	6.214449
385	6	0	16.90937	-9.50643	9.171574
386	6	0	16.07785	-10.6943	8.685675
387	1	0	17.8386	-9.39157	8.560563
388	1	0	17.28109	-9.70986	10.21188
389	1	0	16.70689	-11.6245	8.697204
390	1	0	15.24591	-10.9181	9.399627
391	7	0	15.51671	-10.3898	7.315734
392	7	0	16.08199	-8.24425	9.087682

393	6	0	16.98934	-7.05223	9.102828
394	1	0	16.41741	-6.11234	9.180785
395	1	0	17.7013	-7.0486	9.957104
396	1	0	17.59139	-7.01881	8.176886
397	6	0	15.1068	-8.17332	10.22272
398	1	0	14.56399	-7.2135	10.22274
399	1	0	14.36214	-8.98765	10.14622
400	6	0	16.54971	-10.6254	6.256076
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402	1	0	16.13598	-10.4253	5.253586
403	1	0	17.41955	-9.95974	6.407728
404	6	0	14.31258	-11.2464	7.070445
405	1	0	13.96679	-11.1701	6.026242
406	1	0	14.49299	-12.3293	7.251514
407	1	0	13.48505	-10.9439	7.73826
408	46	0	15.04818	-8.3837	7.314011
409	1	0	15.5786	-8.26409	11.22555
410	6	0	-15.2124	-5.00933	-7.39285
411	6	0	-15.5811	-3.72918	-8.14539
412	1	0	-14.4374	-5.59367	-7.94844
413	1	0	-16.1037	-5.69004	-7.34843
414	1	0	-15.9372	-3.98738	-9.1778
415	1	0	-16.4589	-3.22542	-7.66986
416	7	0	-14.3879	-2.80104	-8.15581
417	7	0	-14.6896	-4.6512	-6.02087
418	6	0	-13.9662	-5.82608	-5.43878
419	1	0	-13.7626	-5.68961	-4.36092
420	1	0	-14.5362	-6.77825	-5.50838
421	1	0	-13.0037	-5.97885	-5.95969
422	6	0	-15.8098	-4.22498	-5.12347

423	1	0	-15.4271	-3.93685	-4.12292
424	1	0	-16.3436	-3.3534	-5.54252
425	6	0	-13.457	-3.1722	-9.2698
426	1	0	-13.9549	-3.25222	-10.2606
427	1	0	-12.6566	-2.42486	-9.39232
428	1	0	-12.9899	-4.15404	-9.06657
429	6	0	-14.8502	-1.384	-8.30593
430	1	0	-13.9972	-0.69694	-8.43418
431	1	0	-15.5138	-1.22269	-9.18241
432	1	0	-15.4126	-1.07096	-7.40669
433	46	0	-13.4429	-3.05275	-6.33418
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435	6	0	-12.1562	12.35359	-8.26282
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437	1	0	-13.1327	12.00293	-7.84634
438	1	0	-12.3412	13.424	-8.54854
439	1	0	-12.6001	11.61323	-10.2646
440	1	0	-10.8945	12.01402	-10.0248
441	7	0	-11.4512	10.12946	-9.11237
442	7	0	-11.0731	12.21089	-7.2182
443	6	0	-11.6262	12.57508	-5.87437
444	1	0	-10.8321	12.61367	-5.1098
445	1	0	-12.1194	13.57148	-5.8537
446	1	0	-12.3799	11.83179	-5.5575
447	6	0	-9.89724	13.0772	-7.55165
448	1	0	-9.14025	13.0467	-6.75046
449	1	0	-9.41771	12.73692	-8.48854
450	6	0	-12.7075	9.332639	-8.93257
451	1	0	-13.3452	9.292885	-9.84192
452	1	0	-12.4745	8.288581	-8.66408

453	1	0	-13.3281	9.763987	-8.12541
454	6	0	-10.5836	9.505963	-10.1623
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460	6	0	-12.0223	12.76767	8.01193
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529	6	0	-13.1053	-1.13814	9.942347
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536	6	0	19.6235	5.442206	-8.62204
537	1	0	20.66957	3.517602	-8.50155
538	1	0	20.29555	4.043732	-10.1514
539	1	0	20.58691	6.01922	-8.63324
540	1	0	18.9638	5.997897	-9.33474
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552	1	0	19.56265	5.164102	-5.19061
553	1	0	20.53019	4.20479	-6.34809
554	6	0	18.25966	6.687416	-7.00354
555	1	0	17.91376	6.762189	-5.95925
556	1	0	18.88244	7.592096	-7.18201
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559	1	0	18.13999	3.445343	-11.1628
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562	1	0	19.24	6.696775	8.74146
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581	1	0	20.83969	6.970555	4.418875
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584	1	0	20.31256	3.203904	9.040158
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594	6	0	10.8698	-1.90251	0.303853
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605	6	0	3.68208	-1.02082	1.084881
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631	6	0	8.459008	-0.62419	-3.28616
632	6	0	8.511163	-2.07924	-3.0537

633	6	0	7.344301	-2.77974	-2.85591
634	6	0	7.28159	-3.82613	-1.83213
635	6	0	5.952645	-3.74107	-1.22141
636	6	0	5.802053	-3.94681	0.12962
637	6	0	8.394329	-4.11121	-1.05399
638	6	0	9.638804	-3.36121	-1.26287
639	6	0	9.69052	-2.37519	-2.2385
640	6	0	10.34467	-1.09475	-1.95983
641	6	0	10.91635	-0.86673	-0.72969
642	6	0	10.7549	0.446461	-0.0806
643	6	0	10.11302	1.521941	-0.74507
644	6	0	9.500503	1.276785	-2.06618
645	6	0	9.577353	-0.02527	-2.62189
646	6	0	7.246048	1.438099	-3.10738
647	6	0	8.36477	2.037358	-2.44186
648	6	0	7.860817	3.132226	-1.59346
649	6	0	9.541469	2.508682	0.097853
650	6	0	8.431215	3.360877	-0.36299
651	6	0	7.587296	3.684115	0.78872
652	6	0	8.174781	3.01033	1.94754
653	6	0	9.385077	2.294751	1.506039
654	6	0	6.208202	3.757807	0.64666
655	6	0	-15.0595	-7.53582	2.896694
656	6	0	-15.7321	-8.76565	3.114535
657	6	0	-17.0897	-8.74262	3.694365
658	6	0	-17.6713	-7.48936	4.013905
659	6	0	-16.9093	-6.23957	3.875528
660	6	0	-15.6404	-6.257	3.342248
661	6	0	-15.224	-5.20971	2.408937
662	6	0	-16.1022	-4.19178	2.058703

663	6	0	-17.4518	-4.16647	2.636213
664	6	0	-17.84	-5.16256	3.520953
665	6	0	-16.1988	-3.76277	0.660261
666	6	0	-15.4108	-4.37937	-0.30505
667	6	0	-14.492	-5.45432	0.070441
668	6	0	-14.4051	-5.85985	1.383738
669	6	0	-14.3013	-7.29158	1.706963
670	6	0	-14.191	-8.26969	0.685262
671	6	0	-14.2887	-7.83811	-0.72299
672	6	0	-14.4905	-6.46092	-1.00422
673	6	0	-15.3954	-6.02692	-2.02371
674	6	0	-16.1395	-6.95509	-2.79967
675	6	0	-15.7331	-8.30834	-2.69585
676	6	0	-14.8215	-8.7432	-1.674
677	6	0	-15.168	-10.1271	-1.31165
678	6	0	-15.0784	-10.5289	0.002057
679	6	0	-14.6334	-9.57107	1.029383
680	6	0	-15.3923	-9.81566	2.222637
681	6	0	-16.3186	-10.9308	1.959253
682	6	0	-16.1171	-11.3828	0.581426
683	6	0	-17.1993	-11.7871	-0.18837
684	6	0	-17.2963	-11.3572	-1.58971
685	6	0	-16.3035	-10.5508	-2.13159
686	6	0	-16.6589	-9.41569	-2.98367
687	6	0	-17.9814	-9.14414	-3.25317
688	6	0	-19.0355	-9.99138	-2.6915
689	6	0	-18.7071	-11.0683	-1.88007
690	6	0	-19.4845	-11.3196	-0.6568
691	6	0	-20.5361	-10.4783	-0.3261
692	6	0	-20.8724	-9.34054	-1.18852

693	6	0	-20.1459	-9.1063	-2.33267
694	6	0	-19.7748	-7.72629	-2.692
695	6	0	-18.4539	-7.7491	-3.25606
696	6	0	-17.5579	-6.6661	-3.08946
697	6	0	-18.1263	-5.46839	-2.58305
698	6	0	-19.4426	-5.44683	-2.01888
699	6	0	-20.2437	-6.61544	-1.94432
700	6	0	-21.0252	-6.86632	-0.71644
701	6	0	-20.9463	-5.92899	0.343755
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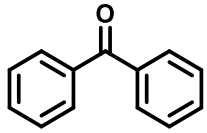
703	6	0	-19.469	-4.4325	-0.94871
704	6	0	-18.1421	-3.82082	-0.86094
705	6	0	-17.3054	-4.4809	-1.86599
706	6	0	-15.9777	-4.7397	-1.60413
707	6	0	-17.6072	-3.47309	0.371633
708	6	0	-18.3837	-3.72112	1.59345
709	6	0	-19.64	-4.30184	1.502797
710	6	0	-20.0403	-5.35593	2.440414
711	6	0	-19.1675	-5.77095	3.418963
712	6	0	-19.0476	-7.20746	3.731119
713	6	0	-19.8943	-8.16551	3.119556
714	6	0	-20.8325	-7.71915	2.069198
715	6	0	-20.8518	-6.3479	1.710398
716	6	0	-21.2752	-8.20887	-0.33086
717	6	0	-21.181	-8.62742	1.035548
718	6	0	-20.7174	-10.0293	1.057876
719	6	0	-19.3774	-9.48645	3.055776
720	6	0	-19.8449	-10.4447	2.035369
721	6	0	-18.733	-11.3371	1.69628
722	6	0	-17.5836	-10.9073	2.499183

723	6	0	-18.0008	-9.76883	3.33836
724	6	0	-18.5513	-11.7642	0.389341
725	6	0	-2.3892	5.667623	1.104517
726	6	0	-3.77957	5.767633	0.845005
727	6	0	-4.23241	5.887379	-0.55541
728	6	0	-3.25944	5.897565	-1.58695
729	6	0	-1.81717	5.906304	-1.28172
730	6	0	-1.3956	5.794981	0.022662
731	6	0	-0.2423	4.955045	0.352121
732	6	0	0.426508	4.263723	-0.64848
733	6	0	-0.02331	4.382437	-2.04219
734	6	0	-1.11445	5.185171	-2.34468
735	6	0	0.833173	2.870992	-0.42066
736	6	0	0.545584	2.26044	0.791378
737	6	0	-0.16381	2.996702	1.840148
738	6	0	-0.54491	4.300553	1.626701
739	6	0	-1.87133	4.756591	2.081271
740	6	0	-2.72444	3.911042	2.835968
741	6	0	-2.31359	2.511193	3.06573
742	6	0	-1.08165	2.065869	2.522884
743	6	0	-0.95533	0.779616	1.90477
744	6	0	-2.05522	-0.1104	1.806404
745	6	0	-3.19108	0.233633	2.582083
746	6	0	-3.31769	1.519269	3.200154
747	6	0	-4.74723	1.877629	3.22579
748	6	0	-5.13026	3.181179	3.012975
749	6	0	-4.10772	4.212099	2.758501
750	6	0	-4.62556	5.123325	1.782456
751	6	0	-5.97934	4.676115	1.409428
752	6	0	-6.30084	3.47538	2.184062

753	6	0	-7.02742	2.443443	1.606587
754	6	0	-6.61961	1.051617	1.834455
755	6	0	-5.51083	0.781679	2.623885
756	6	0	-4.53941	-0.23459	2.212693
757	6	0	-4.7249	-0.92921	1.040535
758	6	0	-5.89417	-0.65327	0.20227
759	6	0	-6.81754	0.310141	0.582805
760	6	0	-7.3476	1.244228	-0.41822
761	6	0	-6.92063	1.153979	-1.73577
762	6	0	-5.94295	0.136586	-2.1275
763	6	0	-5.44567	-0.73808	-1.18996
764	6	0	-4.01325	-1.08585	-1.19799
765	6	0	-3.57394	-1.20157	0.160133
766	6	0	-2.25428	-0.85641	0.547152
767	6	0	-1.33796	-0.65442	-0.51651
768	6	0	-1.77686	-0.53871	-1.87516
769	6	0	-3.14951	-0.61964	-2.22105
770	6	0	-3.68302	0.320582	-3.22698
771	6	0	-2.80237	1.267937	-3.80865
772	6	0	-1.35754	1.254507	-3.51622
773	6	0	-0.86156	0.380101	-2.57805
774	6	0	0.164162	0.824709	-1.63171
775	6	0	-0.14107	0.190295	-0.34683
776	6	0	0.043604	0.884399	0.825186
777	6	0	0.635798	2.128774	-1.67362
778	6	0	0.106763	3.06327	-2.67597
779	6	0	-0.86217	2.631812	-3.57091
780	6	0	-2.01232	3.48464	-3.87937
781	6	0	-2.13419	4.719649	-3.28675
782	6	0	-3.45268	5.174403	-2.80873

783	6	0	-4.62589	4.413572	-3.04393
784	6	0	-4.49508	3.087621	-3.68016
785	6	0	-3.20105	2.626202	-4.0306
786	6	0	-5.03961	0.722094	-3.13429
787	6	0	-5.43804	2.079596	-3.35657
788	6	0	-6.5964	2.365676	-2.49158
789	6	0	-5.68993	4.630203	-2.13219
790	6	0	-6.71865	3.600883	-1.89898
791	6	0	-7.17222	3.705815	-0.51076
792	6	0	-6.4019	4.787874	0.105422
793	6	0	-5.49663	5.353011	-0.91122
794	6	0	-7.47762	2.562279	0.214513

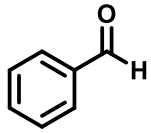
15. Analytical data for synthesized products



Benzophenone:

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 – 7.75 (m, 4H), 7.59 (dd, *J* = 8.4, 6.5 Hz, 2H), 7.49 (t, *J* = 7.6 Hz, 4H).

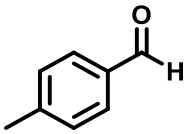
^{13}C NMR (101 MHz, $CDCl_3$): δ 197.25, 138.07, 132.88, 130.53, 128.74.



Benzaldehyde:

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.98 (s, 1H), 7.83 (d, *J* = 8.6 Hz, 2H), 7.52 (d, *J* = 8.6 Hz, 2H).

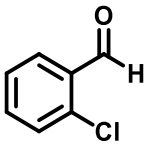
^{13}C NMR (101 MHz, $CDCl_3$): δ 191.33, 141.43, 135.17, 131.37, 129.93.



4-methylbenzaldehyde

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.96 (s, 1H), 7.77 (d, *J* = 7.8 Hz, 2H), 7.32 (d, *J* = 7.8 Hz, 2H), 2.43 (s, 3H).

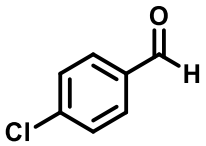
^{13}C NMR (101 MHz, $CDCl_3$): δ 192.46, 145.99, 134.63, 130.29, 130.15, 22.31.



2-chlorobenzaldehyde:

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.49 (s, 1H), 7.93 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.53 (td, *J* = 7.6, 1.8 Hz, 1H), 7.47 (d, *J* = 1.3 Hz, 1H), 7.40 (d, *J* = 7.6 Hz, 1H).

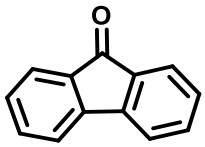
^{13}C NMR (101 MHz, $CDCl_3$): δ 190.31, 135.59, 131.08, 129.85, 127.76.



4-chlorobenzaldehyde:

^{1}H NMR (400 MHz, $CDCl_3$):δ 9.99 (s, 1H), 7.85 – 7.81 (m, 2H), 7.55 – 7.50 (m, 2H).

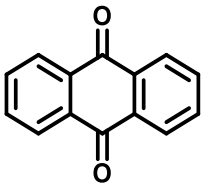
^{13}C NMR (101 MHz, $CDCl_3$): δ 190.69, 140.80, 134.55, 130.74, 129.30.



9H-fluoren-9-one:

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 7.3 Hz, 2H), 7.55 – 7.45 (m, 4H), 7.29 (td, *J* = 7.3, 1.4 Hz, 2H).

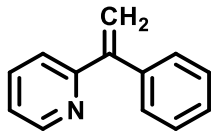
^{13}C NMR (101 MHz, $CDCl_3$): δ 194.42, 144.91, 135.15, 134.62, 129.55, 124.80, 120.77.



anthracene-9,10-dione:

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.33 (dd, *J* = 5.8, 3.3 Hz, 4H), 7.81 (dd, *J* = 5.8, 3.3 Hz, 4H).

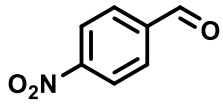
^{13}C NMR (101 MHz, $CDCl_3$): δ 183.02, 133.97, 133.36, 127.08.



2-(1-phenylvinyl)pyridine:

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 – 8.69 (m, 1H), 8.06 (tt, *J* = 8.9, 1.4 Hz, 3H), 7.90 (td, *J* = 7.7, 1.8 Hz, 1H), 7.64 – 7.56 (m, 1H), 7.54 – 7.45 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 194.04, 155.25, 148.69, 137.19, 136.40, 133.06, 131.12, 128.30, 126.29, 124.76.



4-nitrobenzaldehyde:

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.16 (s, 1H), 8.40 (d, *J* = 8.7 Hz, 2H), 8.08 (d, *J* = 8.7 Hz, 2H).

16. ^{1}H NMR spectra for the crude reaction mixture after oxidative cleavage of olefin.

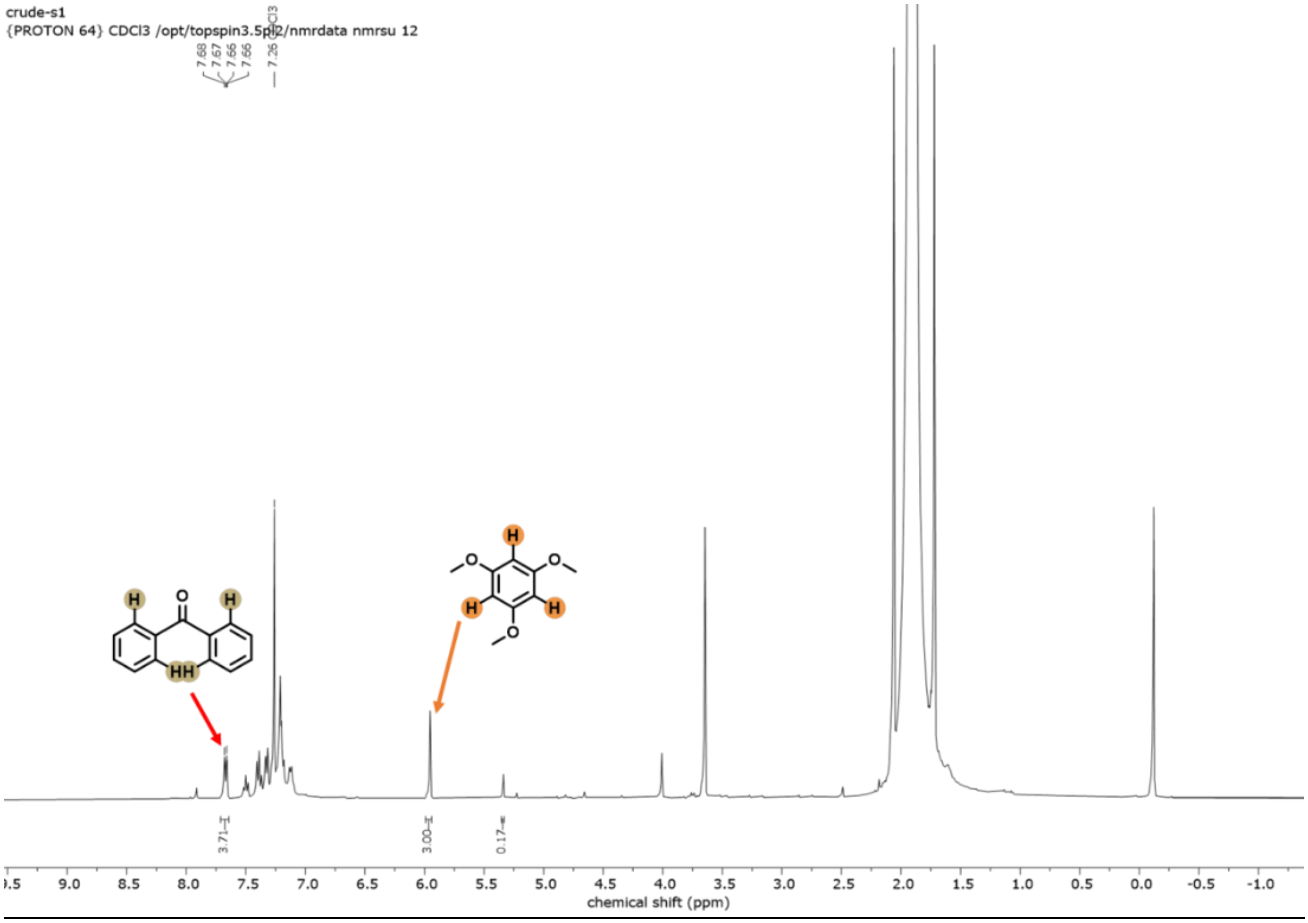


Fig. S54 Crude ^{1}H NMR after reaction with substrate S1. 1,3,5-trimethoxybenzene was added (as 1:1 ratio to reactant) as standard and appropriate peak area was integrated to calculate yield. The reaction was performed under 0.2 mol% of the **$(C_{70})_3$@M2** loading under 390 nm irradiation. From the crude NMR, we obtained a 93% NMR yield, while our isolated yield was 85%.

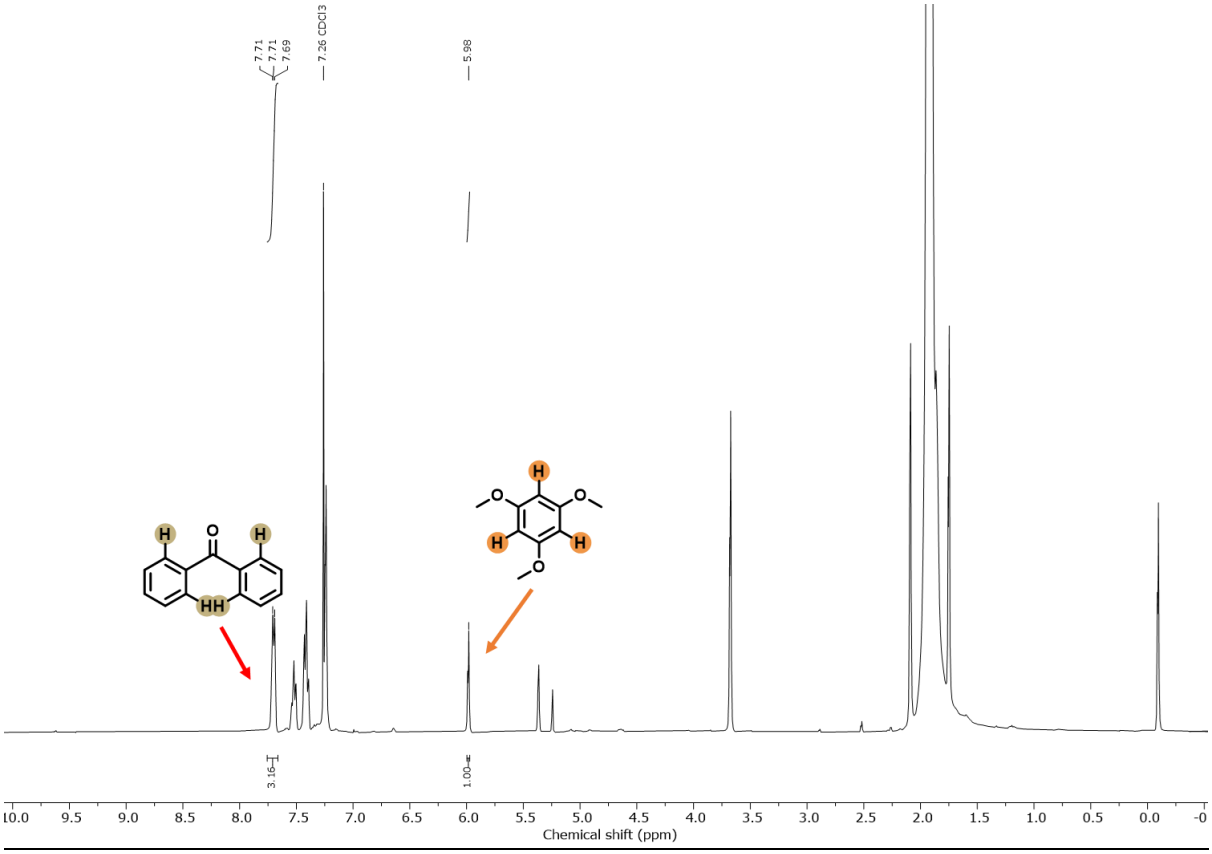


Fig. S55 Crude ^{1}H NMR after reaction with substrate S1. 1,3,5-trimethoxybenzene was added (as 1:3 ratio to reactant) as standard and appropriate peak area was integrated to calculate yield. The reaction was performed under 0.2 mol% of the **$(C_{70})_3$@M2** loading under 650 nm irradiation. From the crude NMR, we obtained a 79% NMR yield, while our isolated yield was 74%.

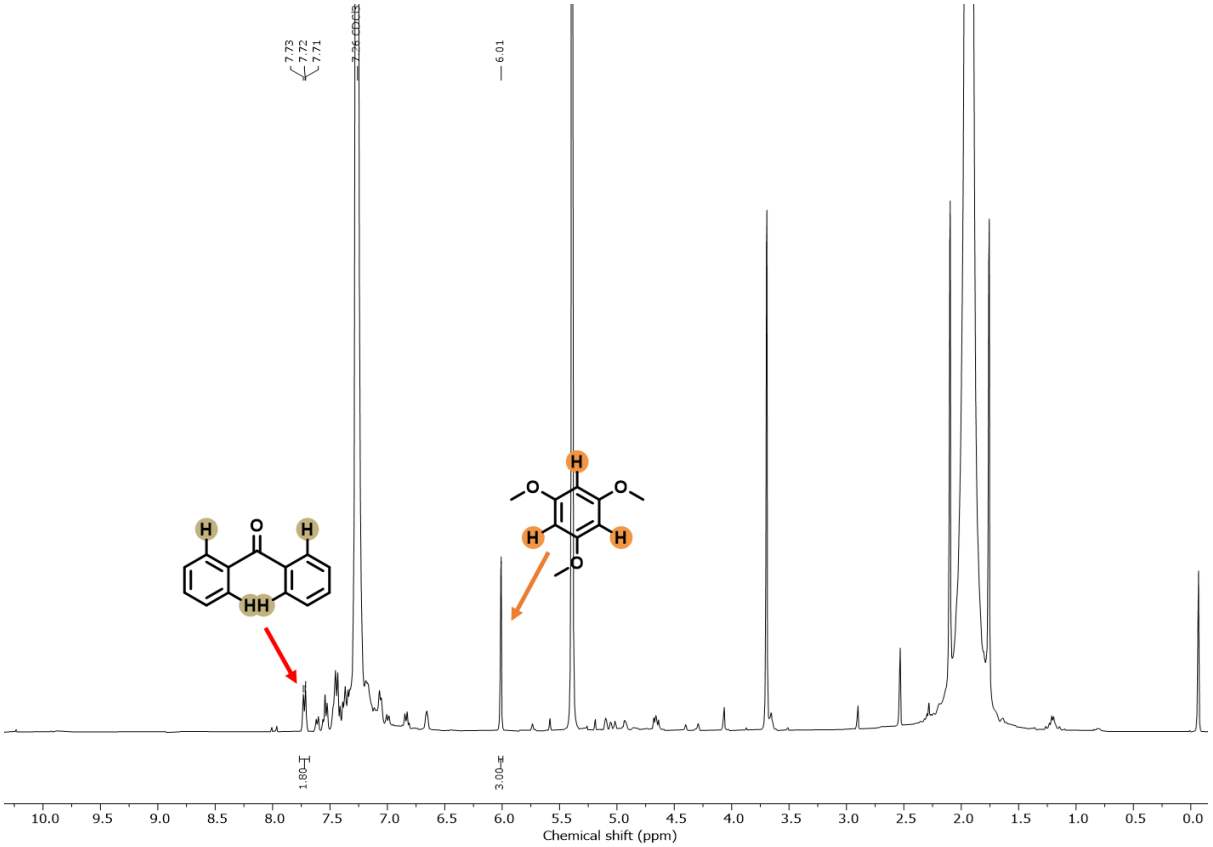
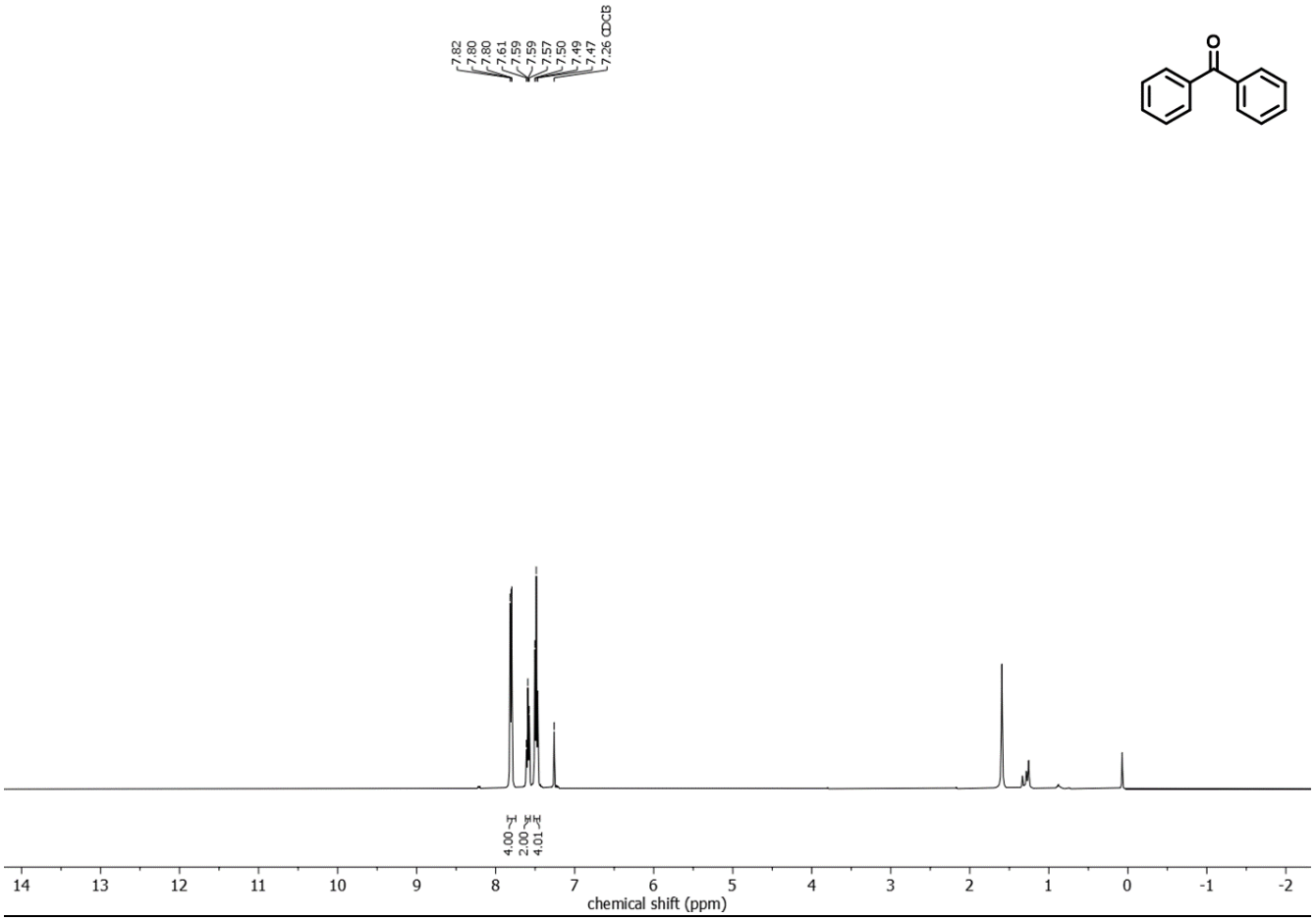
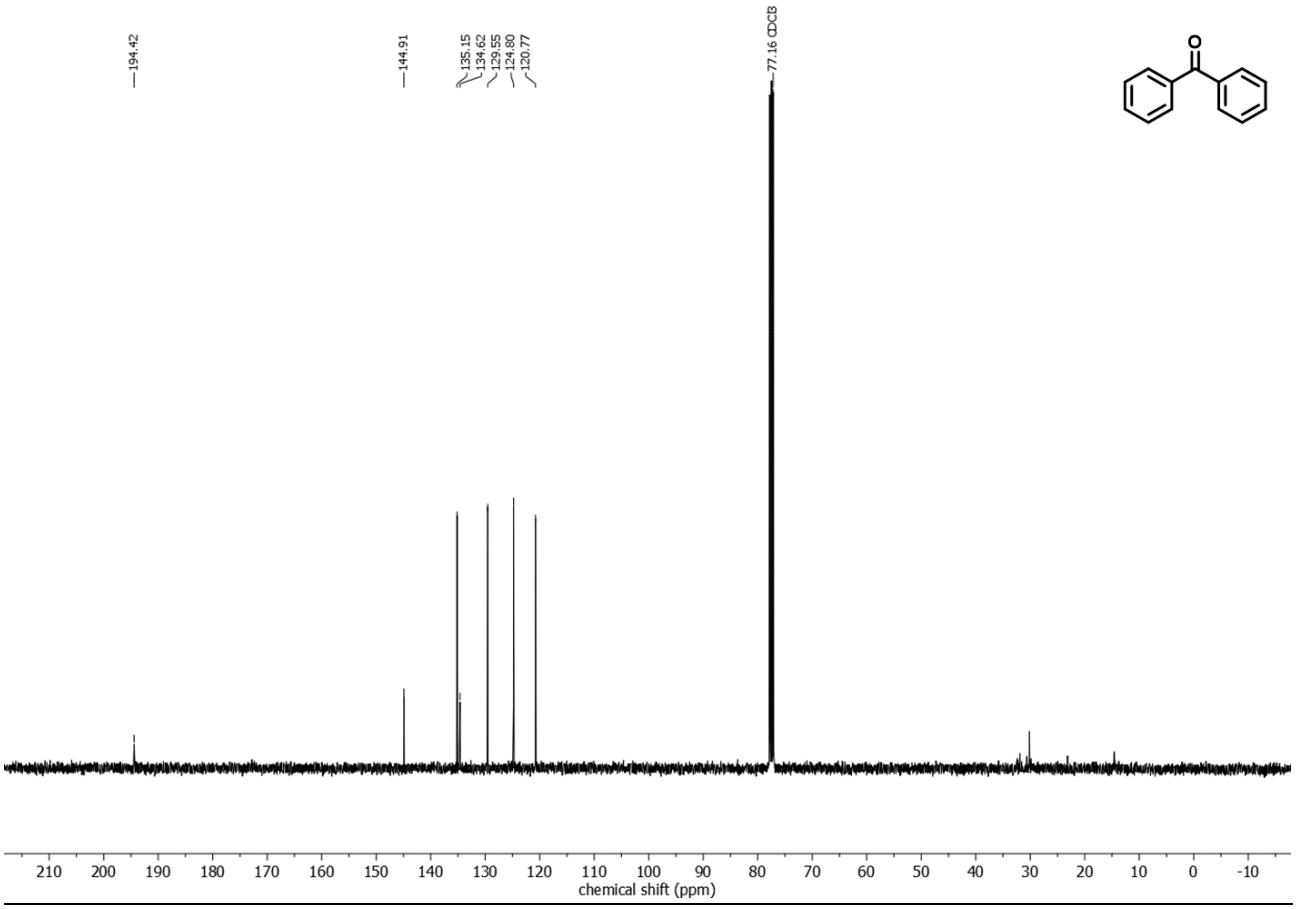
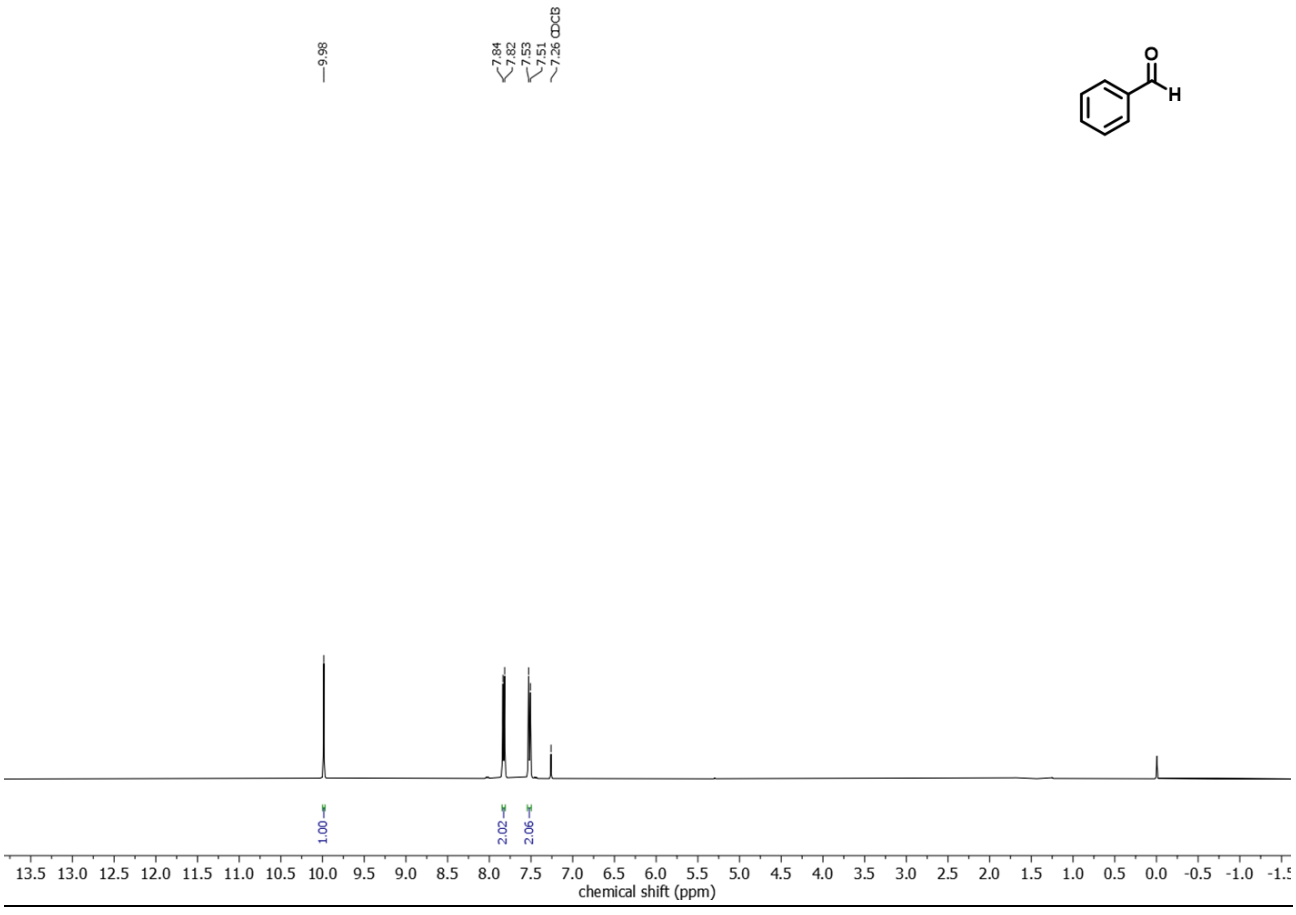


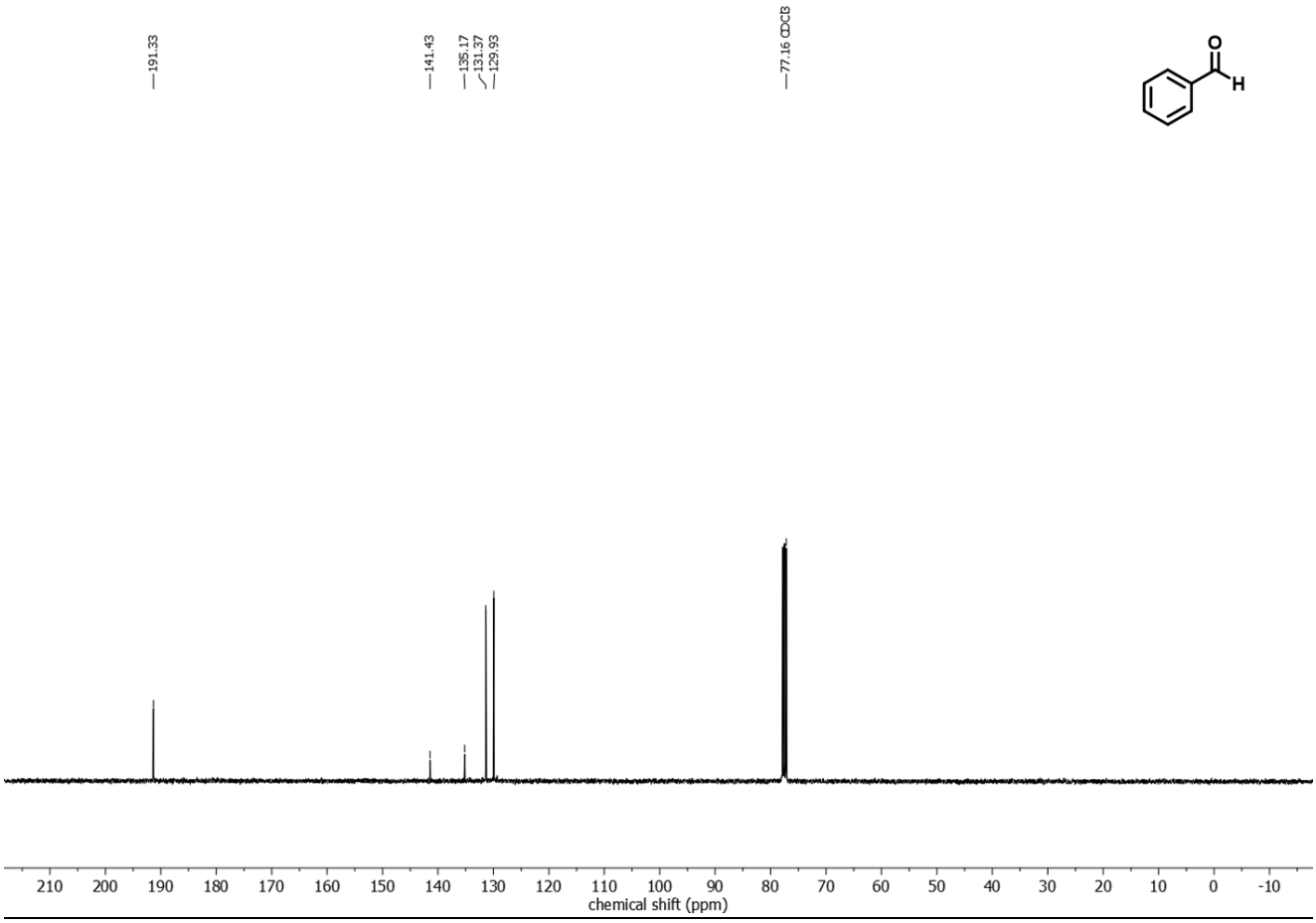
Fig. S56 Crude ^{1}H NMR after reaction with substrate S1. 1,3,5-trimethoxybenzene was added (as 1:1 ratio to reactant) as standard and appropriate peak area was integrated to calculate yield. The reaction was performed under 0.2 mol% of the **$(C_{70})_3$@M2** loading and reactant was taken in 2.5 mmol under 650 nm irradiation. From the crude NMR, we obtained a 45% NMR yield.

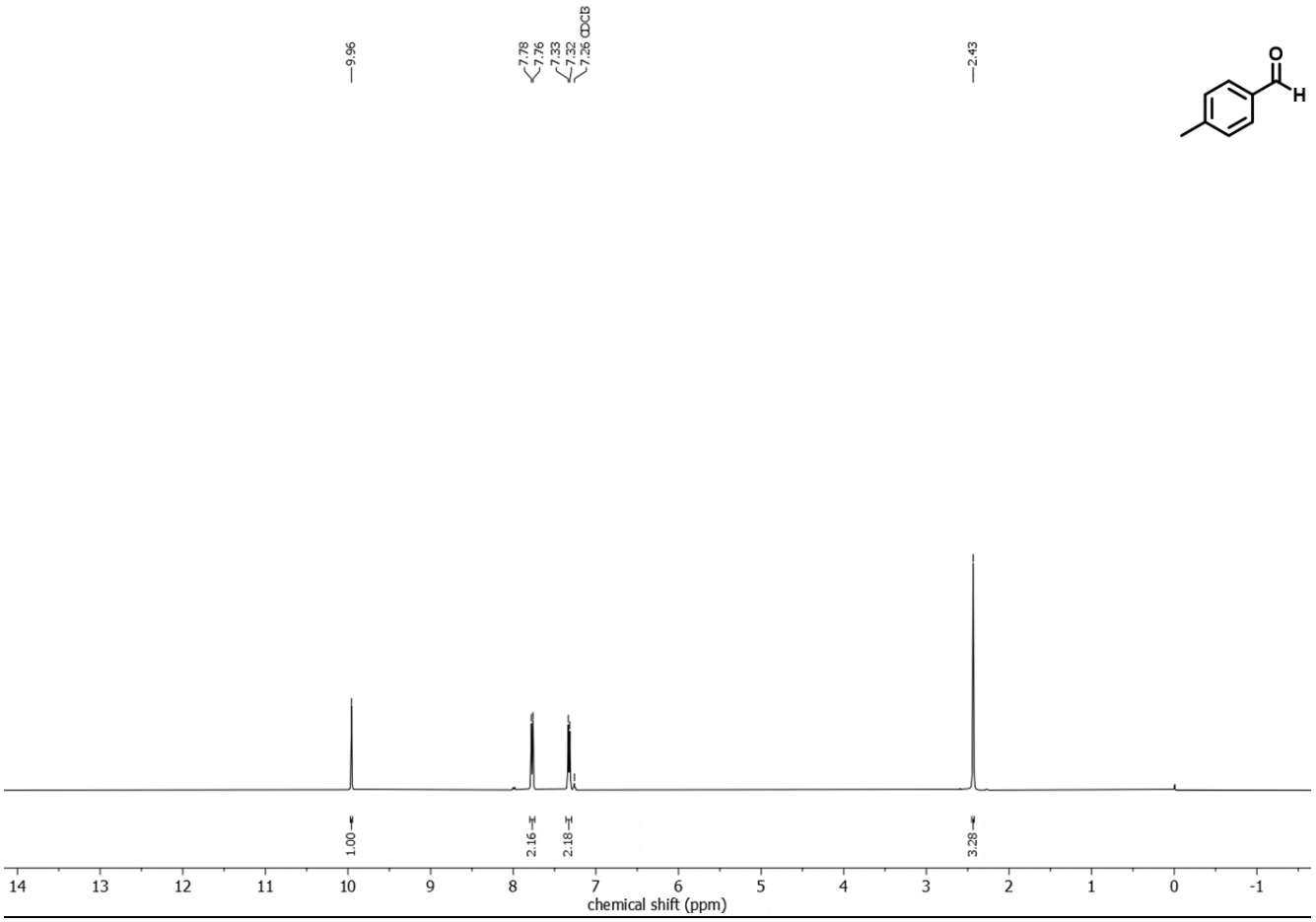
17. ^{1}H &^{13}C NMR spectra of the synthesized compounds

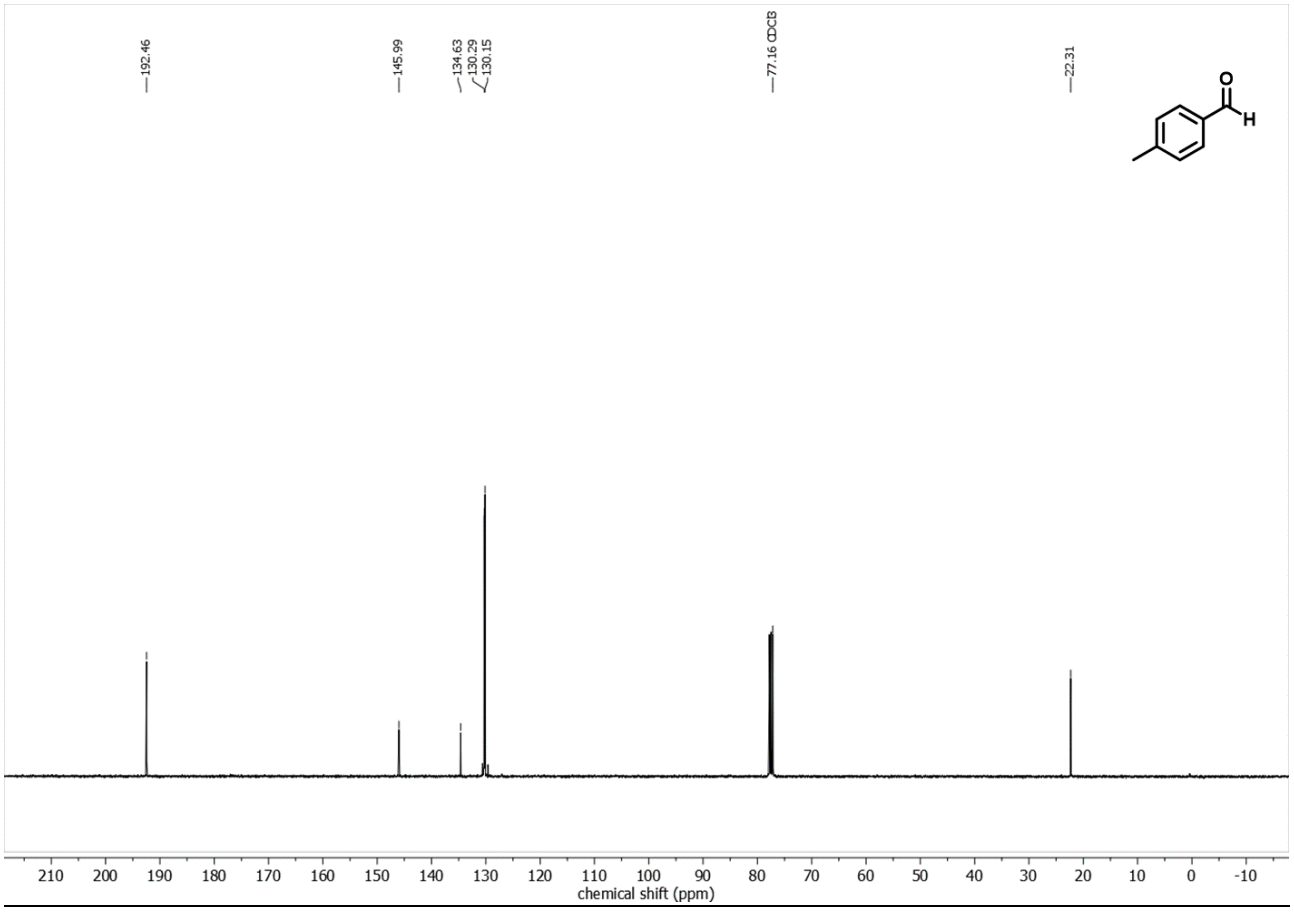


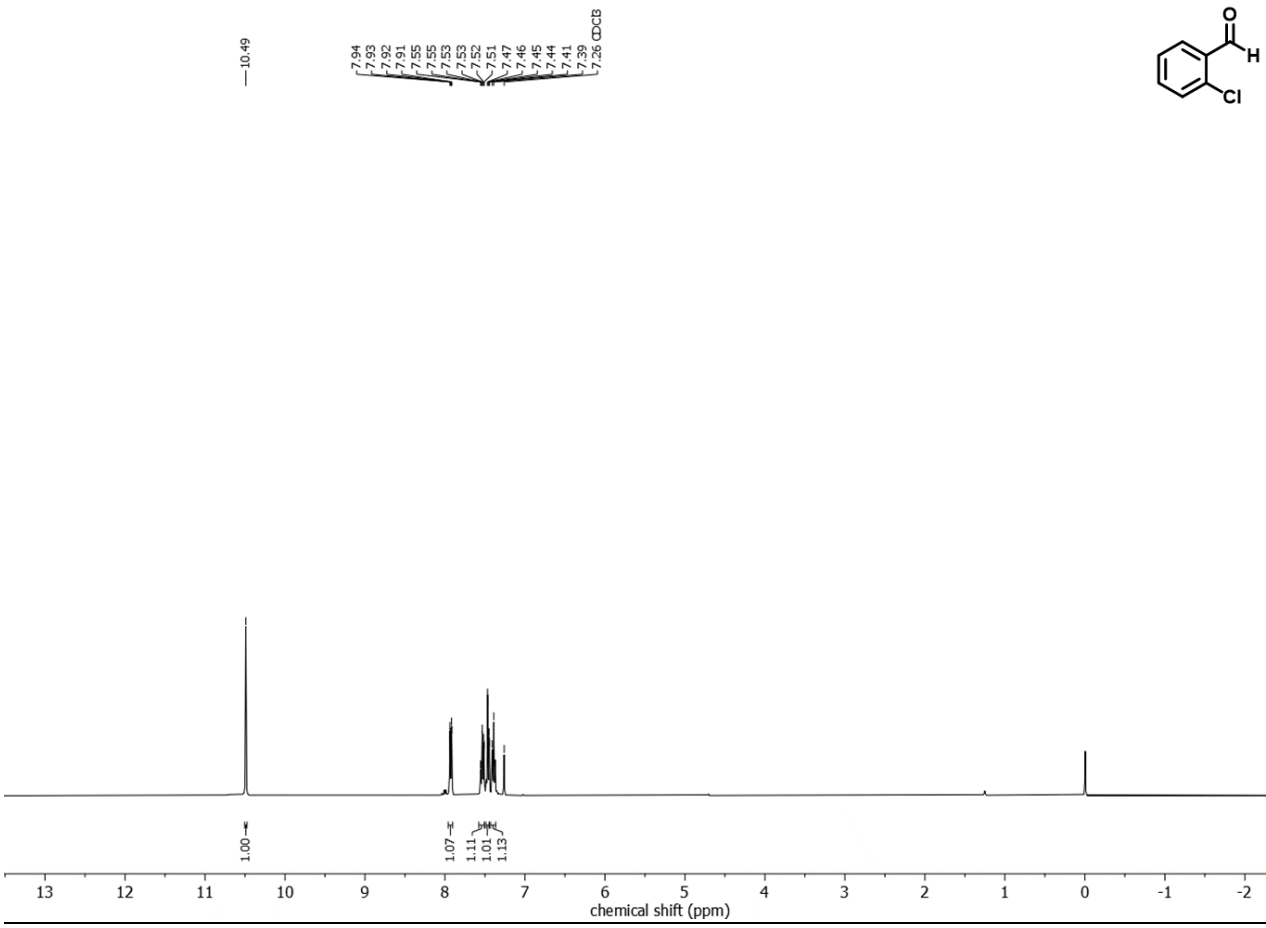

194.42
144.91
135.15
134.62
129.55
124.80
120.77
77.16 CDCl3
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
chemical shift (ppm)

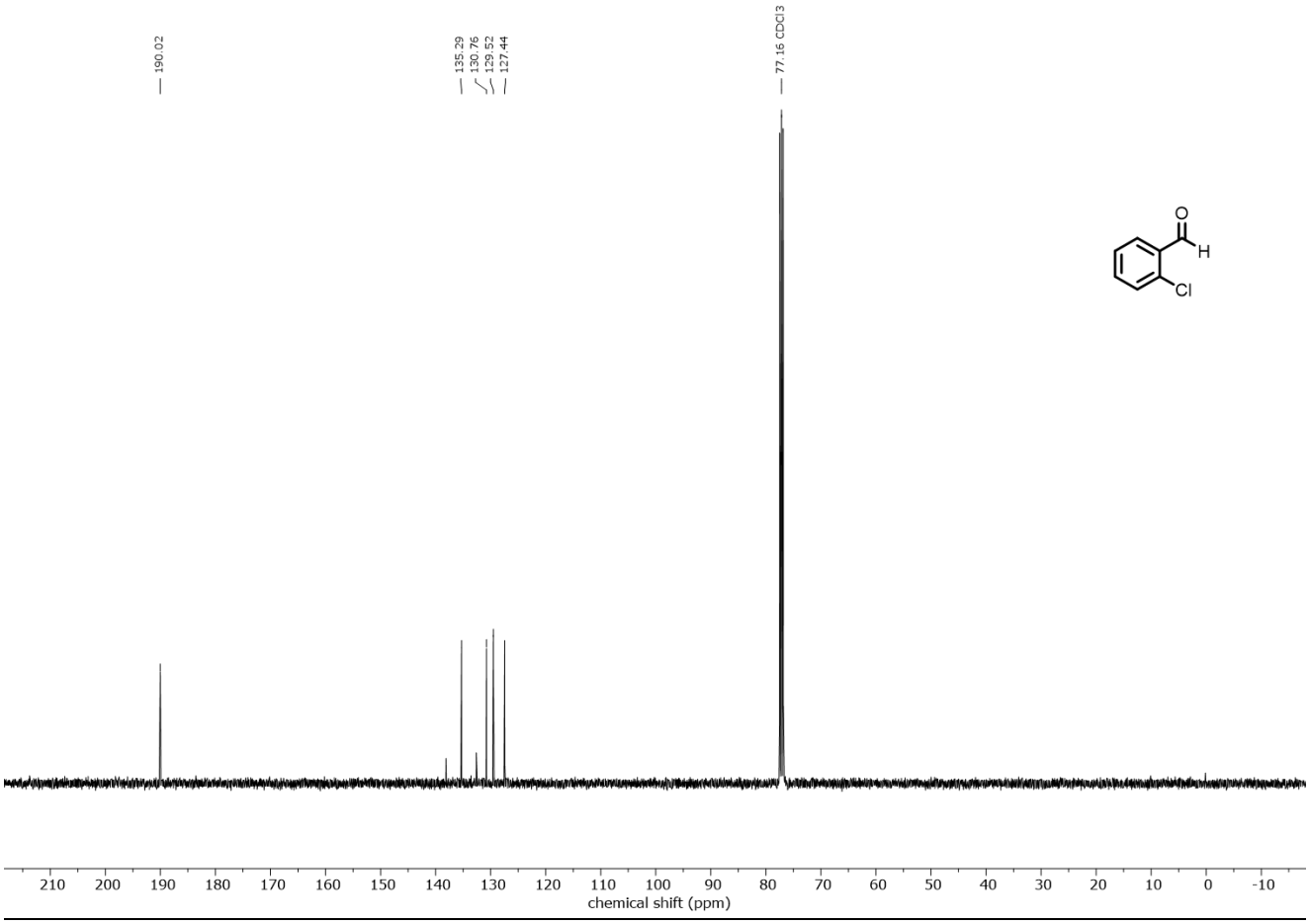

9.98
7.84
7.82
7.53
7.51
7.26 CDCl3
O
H
1.00
2.02
2.06
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
chemical shift (ppm)

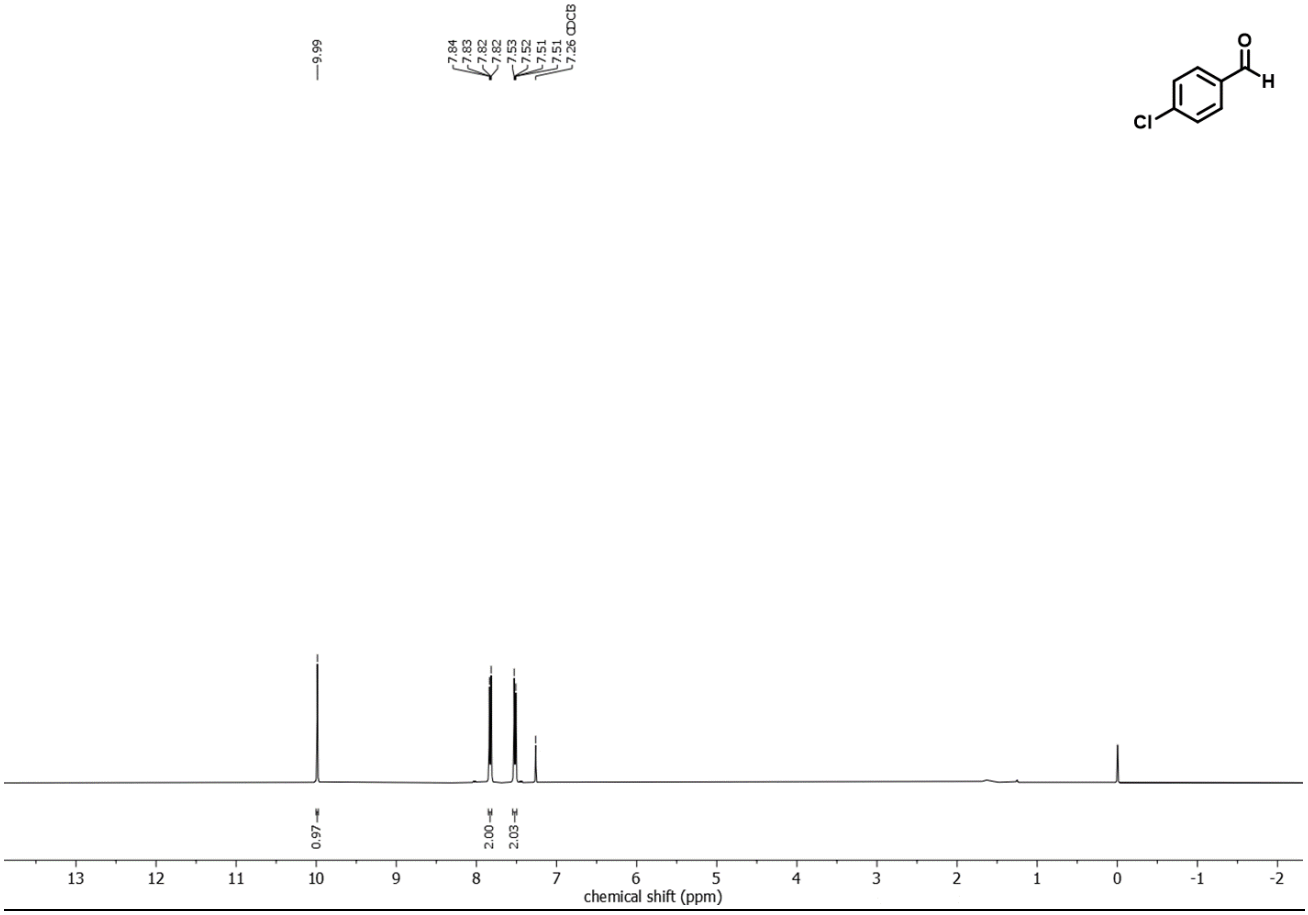

191.33
141.43
135.17
131.37
129.93
77.16 CDCl3
O
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
chemical shift (ppm)

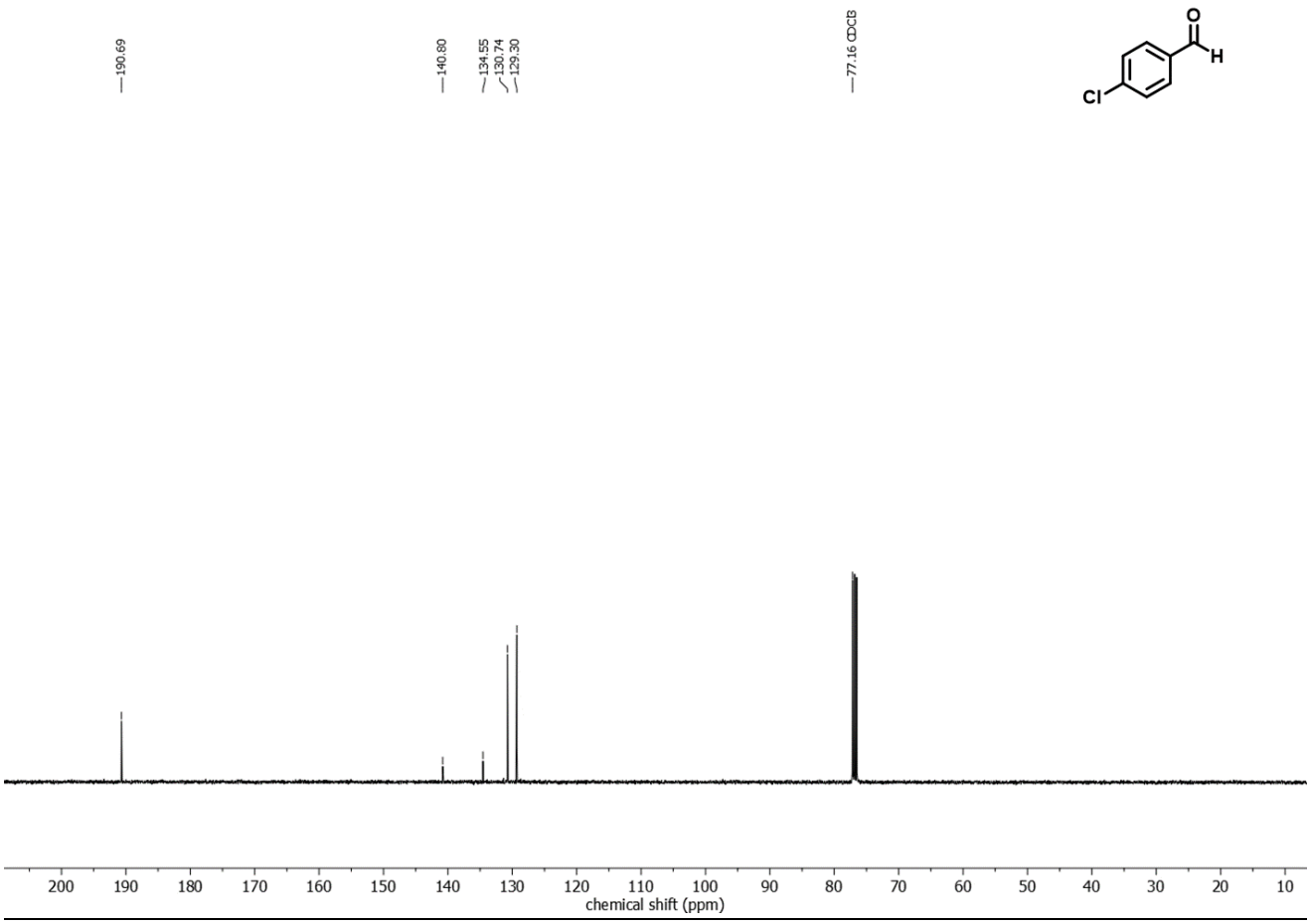

9.96
7.78
7.76
7.33
7.32
7.26 CDCl3
2.43
1.00
2.16
2.18
3.28
chemical shift (ppm)

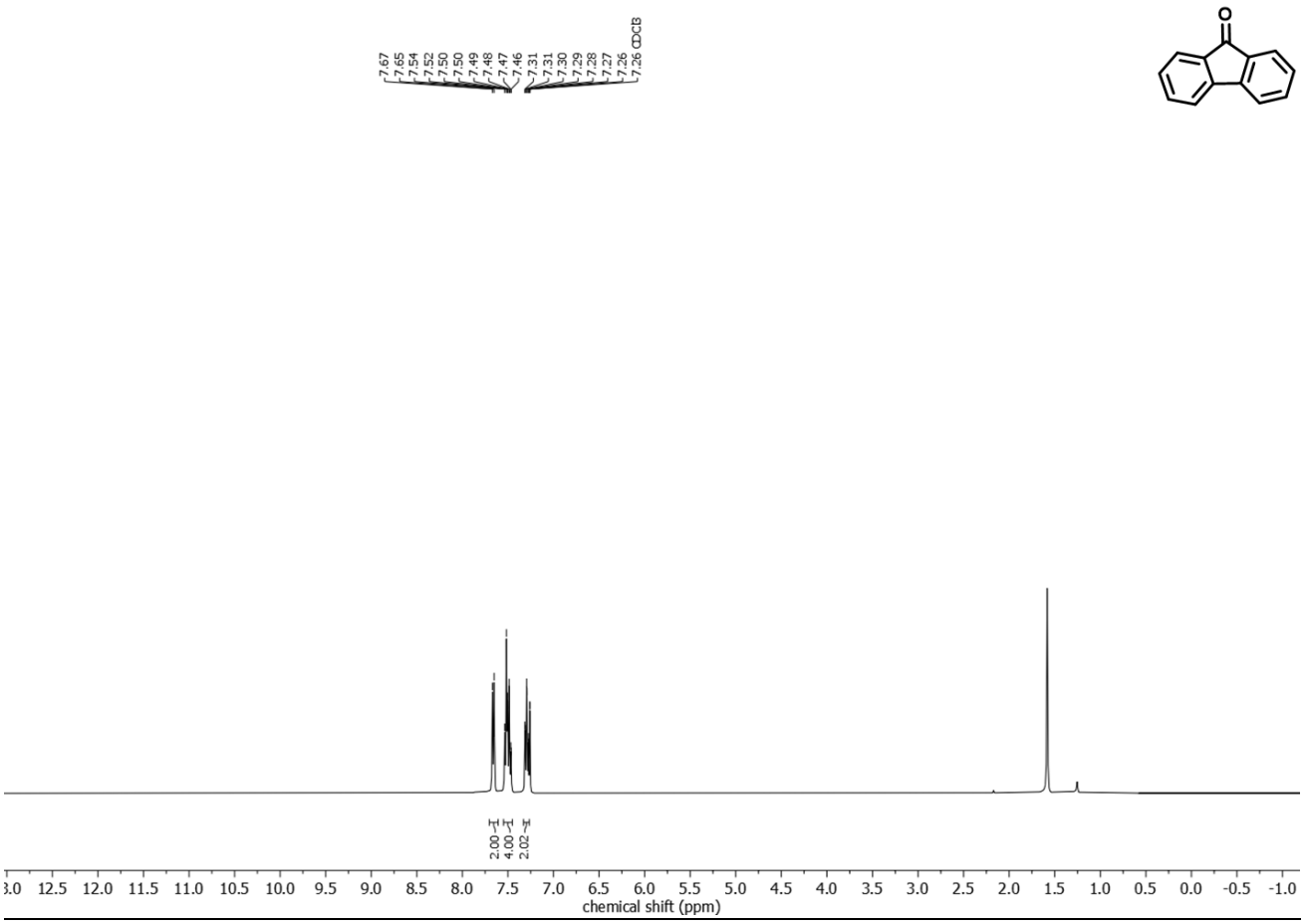

192.46
145.99
134.63
130.29
130.15
77.16 CDCl3
22.31
chemical shift (ppm)

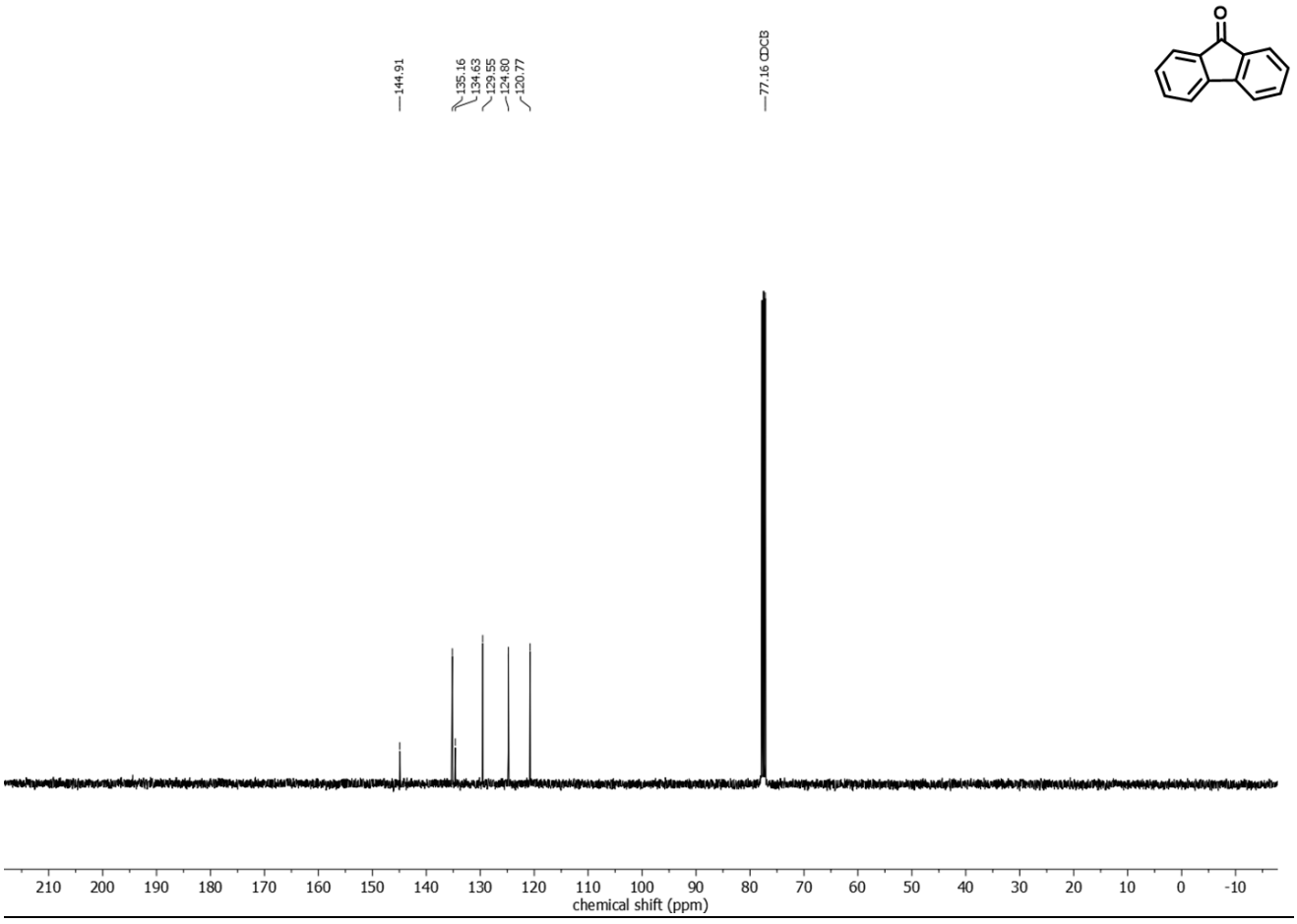

10.49
7.94
7.93
7.92
7.91
7.55
7.53
7.53
7.52
7.51
7.47
7.46
7.45
7.44
7.41
7.39
7.26 CDCl3
O
H
Cl
1.00
1.07
1.11
1.01
1.13
chemical shift (ppm)

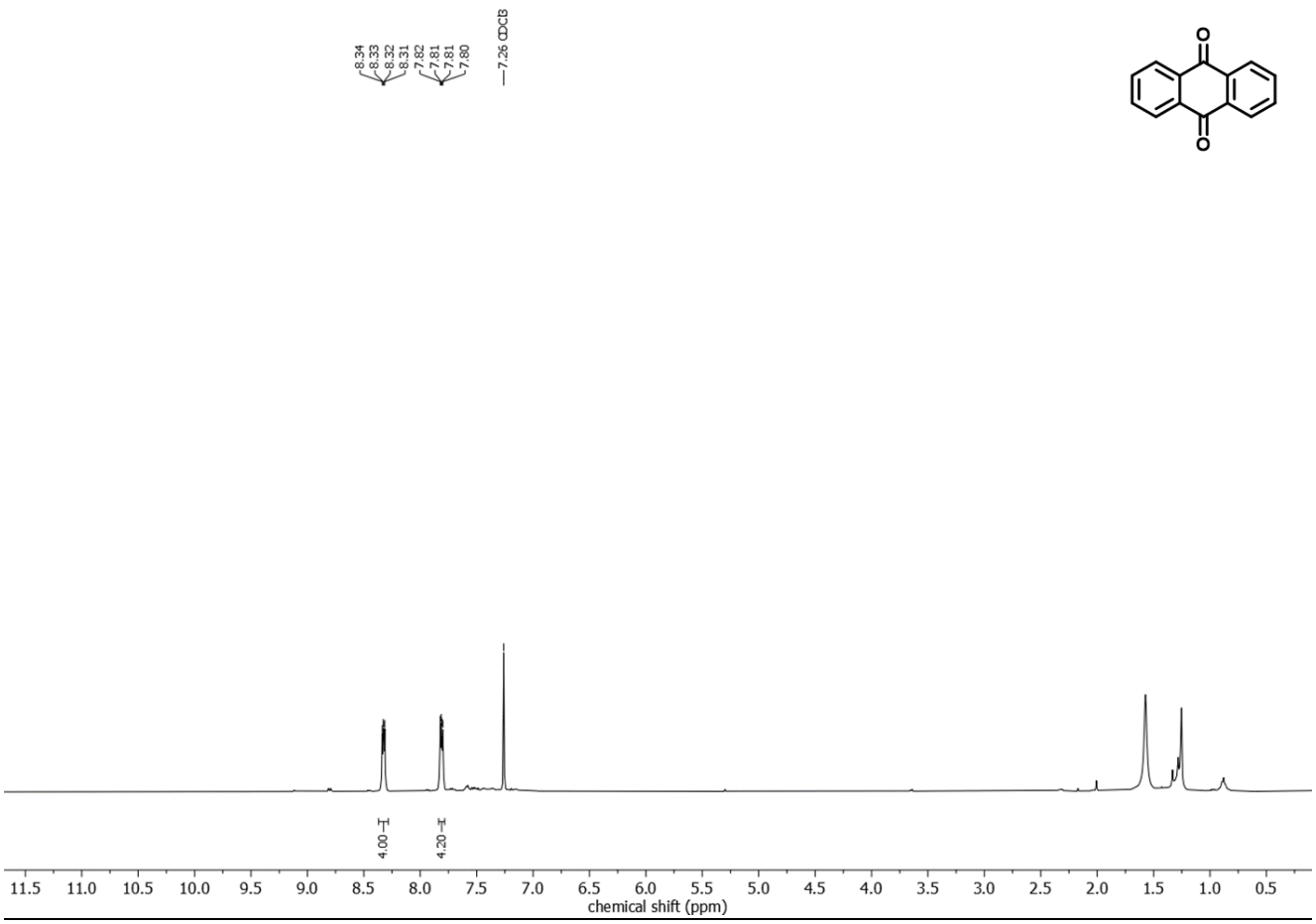

190.02
135.29
130.76
129.52
127.44
77.16 CDCl3
O
H
Cl
chemical shift (ppm)

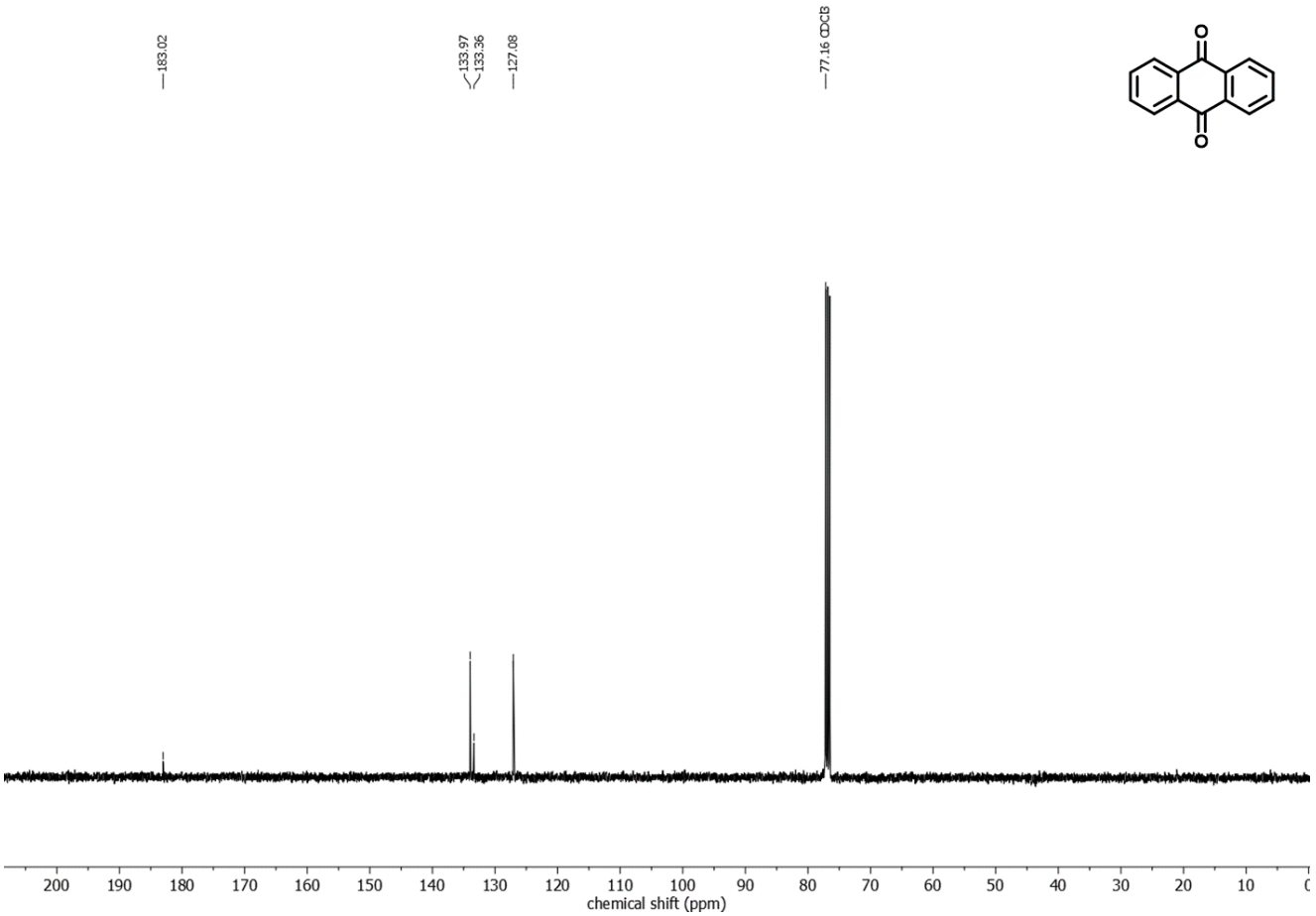

9.99
7.84
7.83
7.82
7.82
7.53
7.52
7.51
7.51
7.26 CDCl3
O
H
Cl
0.97
2.00
2.03
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
chemical shift (ppm)

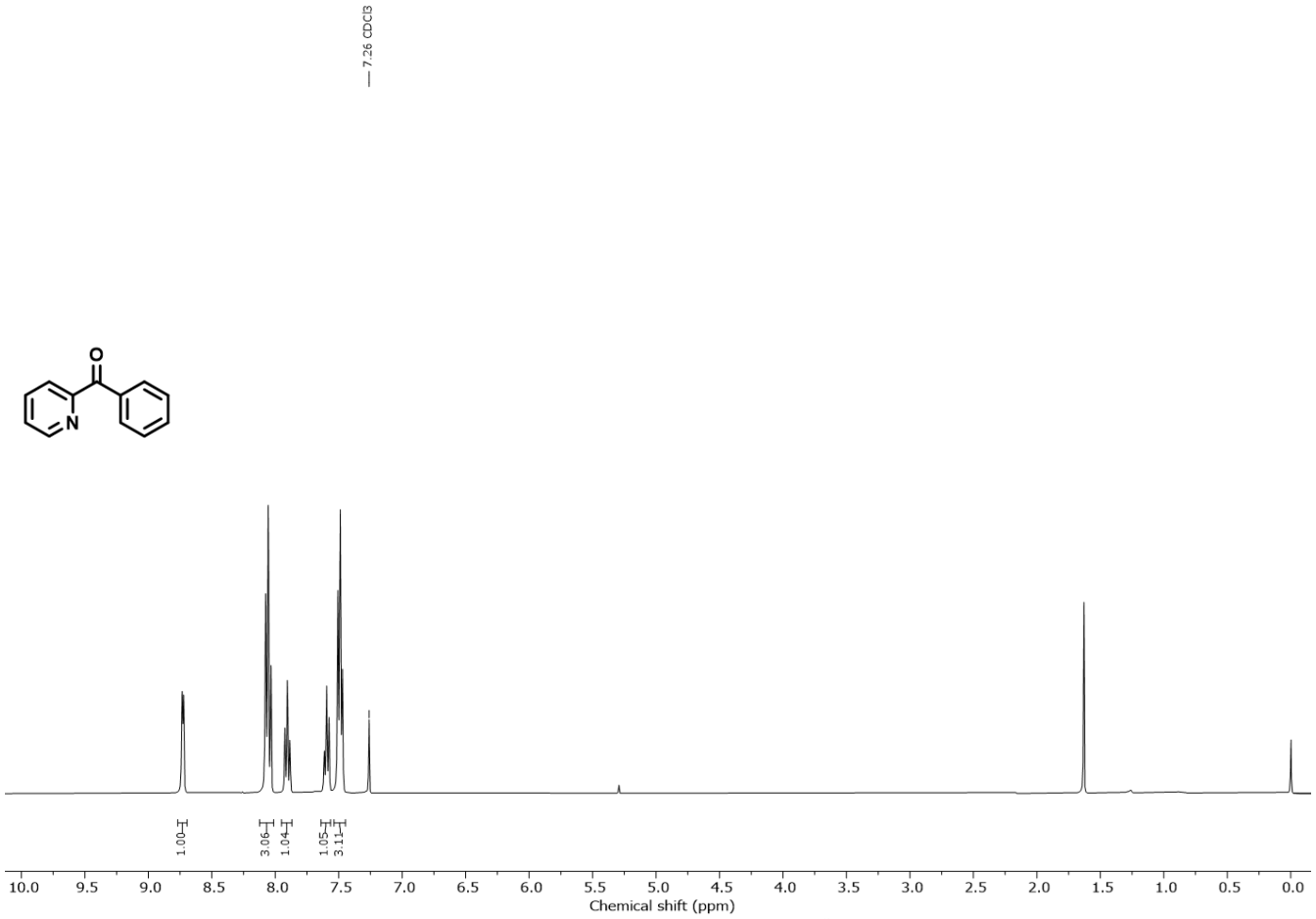

190.69
140.80
134.55
130.74
129.30
77.16 CDCl3
O
H
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
chemical shift (ppm)

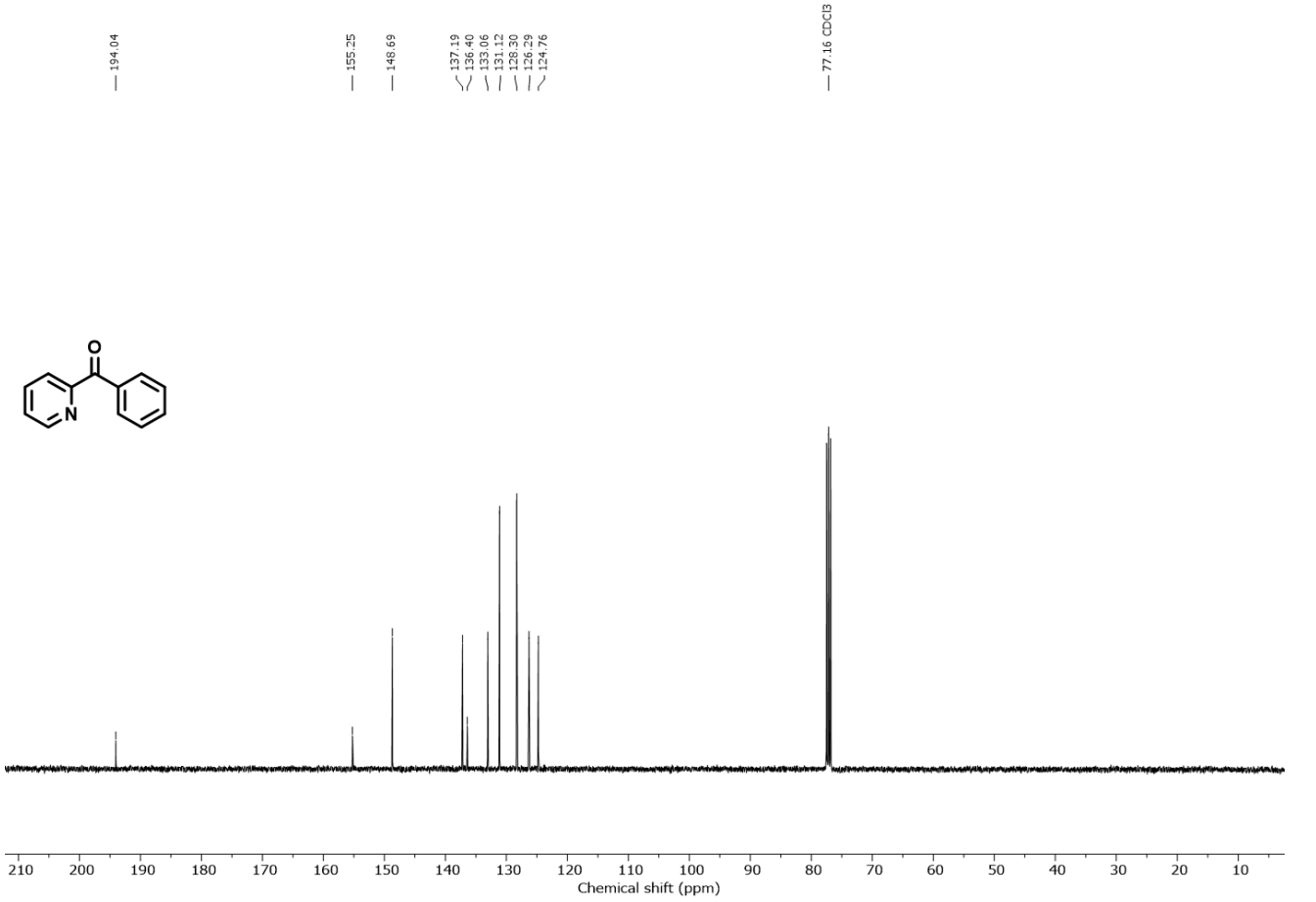

7.67
7.65
7.54
7.52
7.50
7.50
7.49
7.48
7.47
7.46
7.31
7.31
7.30
7.29
7.28
7.27
7.26
7.26 CDCl3
2.00
4.00
2.02
chemical shift (ppm)

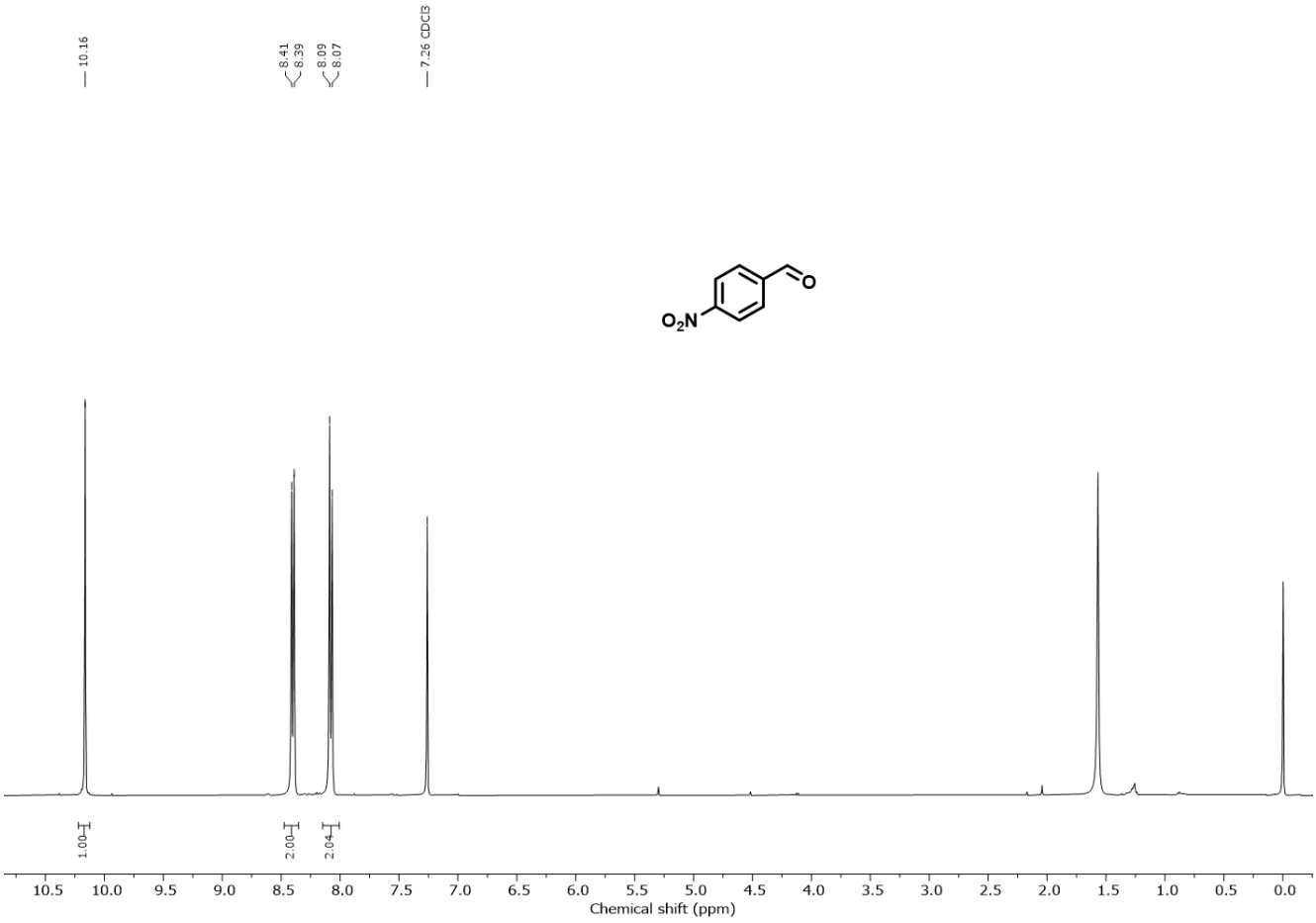

144.91
135.16
134.63
129.55
124.80
120.77
77.16 CDCl3
chemical shift (ppm)


8.34
8.33
8.32
8.31
7.82
7.81
7.81
7.80
7.26 CDCl3
4.00
4.20
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
chemical shift (ppm)


183.02
133.97
133.36
127.08
77.16 CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
chemical shift (ppm)


7.26 CDCl3
1.00
3.06
1.04
1.05
3.11
Chemical shift (ppm)


194.04
155.25
148.69
137.19
136.40
133.06
131.12
128.30
126.29
124.76
77.16 CDCl3
Chemical shift (ppm)



18. References

S1 F. Salami, Y. Zhao, *New J. Chem.*, 2020, **44**, 9179-9189.

S2 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, K. A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Wallingford CT*, 2009, **201**.