

Electronic Supporting Information:

Regioselective Synthesis of Fullerene Multiadducts via Tether-directed 1,3-Dipolar Cycloaddition

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General Information

PC₆₁BM (Solenne, 99%), *N*-phenylglycine and *o*-DCB were used in the reaction as received from suppliers. Dried toluene was obtained from glass contour solvent purification system. Flash chromatography purification was performed in standard methods on silica gel (Merck Silica Gel 60, 0.040-0.063 mm, 230-400 mesh ASTM).

¹H NMR and COSY spectroscopy were given out by using the Varian Inova-400 (400 MHz). ¹³C NMR, HSQC and HMBC spectroscopy were given out by using Oxford 500 (500 MHz). HPLC was carried out using a standard HPLC system with a UV-vis detector, a CosmosilR Buckyprep-D column (4.6 ID × 250 mm) and a silica gel column. FT-IR spectra were provided by a Perkin Elmer Spectrum One FT-IR spectrometer while UV-Vis spectra were recorded using a Cary UV-Vis spectrometer. All high resolution mass spectrometry (HRMS) experiments were conducted with use of a commercially available hybrid linear ion trap and Fourier-transform ion cyclotron resonance mass spectrometer, equipped with electrospray ionisation (ESI). Electrochemical measurements were recorded on a Solartron 1287A Potentiostat/Galvanostat.

Synthesis procedures

***N*-hexylglycine •KCl:** *N*-hexylamine (2.8 g, 28 mmol) and 2 e.q. glyoxylic acid monohydrate (5.0 g, 54 mmol) were dissolved in dichloromethane (200 mL) and stirred overnight at room temperature. The solvent then was removed with the residue being dissolved in HCl (1 M, 100mL) and refluxing overnight. The HCl was removed with the crude product being dissolved and precipitated by methanol and diethyl ether system. Followed, the crude product was dissolved in H₂O and neutralized by K₂CO₃ to pH=7.0. Water was removed to yield the *N*-hexylglycine•KCl white solid (4.09 g, 21.0 mmol, 75%). ¹H NMR (400 MHz, Deuterium Oxide) δ 3.75 (s, 2H), 3.01 – 2.86 (m, 2H), 1.64 – 1.45 (m, 2H), 1.29 – 1.07 (m, 6H), 0.80 – 0.65 (m, 3H). HRMS ESI+ (m/z): calcd. for C₈H₁₇NO₂, [M+H⁺] 160.1332; found 160.1332. Characterization data obtained is consistent with previous literature.¹

***N*-hexyl PC₆₁PF:** The intermediate (PC₆₁BM-aldehyde) was synthesized by adding DIBAL (1.2mL, 1.2 mmol) dropwisely to a stirred solution of PC₆₁BM (1.0 g, 1.1 mmol) at -78°C in toluene (100 mL) under nitrogen atmosphere for 1h before quenched with MeOH (1 mL). The crude aldehyde was treated with *N*-hexylglycine (750 mg, 3.2 mmol) at 180 °C in *o*-DCB (300 mL) for 1.5h to form the *N*-hexyl PC₆₁PF. The reaction was monitored by TLC (SiO₂, CS₂). The crude product was separated by flash chromatography (SiO₂, CS₂) to give the *N*-hexyl PC₆₁PF-1 (95.2 mg, 0.10 mmol) and *N*-hexyl PC₆₁PF-2 (151.9 mg, 0.16 mmol) with the yields of 9% and 14% respectively.

N-hexyl PC₆₁PF-1: ¹H NMR (400 MHz, CDCl₃) δ 7.50 – 7.26 (m, 5H), 5.09 (d, J = 10.6 Hz, 1H), 4.51 (d, J = 5.7 Hz, 1H), 4.44 (d, J = 10.6 Hz, 1H), 4.00 (ddd, J = 14.4, 12.7, 5.5 Hz, 1H), 3.26 (dt, J = 11.9, 7.9 Hz, 1H), 3.07 – 2.92 (m, 1H), 2.91 – 2.78 (m, 2H), 2.53 (dt, J = 15.5, 6.2 Hz, 1H), 2.44 – 2.30 (m, 1H), 2.04 (ddq, J = 18.2, 12.6, 6.2 Hz, 1H), 1.91 – 1.72 (m, 2H), 1.59 (ddt, J = 16.5, 13.5, 6.4 Hz, 2H), 1.45 – 1.29 (m, 4H), 1.02 – 0.90 (m, 3H). ¹³C NMR (126 MHz, cdcl₃) δ 155.45, 154.65, 153.18, 150.73, 149.08, 148.39, 148.30, 147.94, 147.90, 147.25, 147.18, 146.76, 146.45, 146.09, 145.90, 145.87, 145.86, 145.33, 145.32, 145.23, 145.12, 145.06, 144.77, 144.40, 144.29, 144.25, 144.18, 144.11, 144.02, 143.77, 143.69, 143.48, 143.36, 143.33, 143.25, 143.06, 142.97, 142.87, 142.75, 142.22, 142.19, 142.16, 141.94, 141.93, 141.73, 141.66, 140.40, 138.66, 138.54, 137.48, 136.81, 133.63, 131.79, 131.33, 127.20, 75.93, 70.08, 68.25, 67.22, 66.48, 66.41, 55.39, 53.35, 33.60, 31.94, 31.85, 31.81, 29.69, 29.34, 27.15, 27.03, 27.01, 26.91, 26.32, 22.77, 22.69, 22.04, 14.15, 14.11, 14.09; FT-IR (cm⁻¹, neat): 2923.0, 2853.7, 2330.1, 1678.7, 1600.2, 1512.6, 1461.8, 1189.6, 1075.8, 761.6, 697.6. HRMS ESI+ (m/z): calcd. for C₇₈H₂₇, [M+H⁺] 978.2216; found 978.2209.

N-hexyl PC₆₁PF-2: ¹H NMR (400 MHz, CDCl₃) δ 7.64 (dt, J = 6.9, 2.0 Hz, 1H), 7.34 – 7.28 (m, 1H), 7.24 – 7.19 (m, 1H), 7.20 – 7.10 (m, 2H), 5.62 (d, J = 1.6 Hz, 1H), 5.49 (d, J = 1.6 Hz, 1H), 4.73 (d, J = 8.4 Hz, 1H), 3.48 – 3.34 (m, 2H), 3.25 (d, J = 8.5 Hz, 1H), 3.12 – 2.90 (m, 2H), 2.84 (d, J = 15.9 Hz, 1H), 2.63 – 2.49 (m, 1H), 2.44 (dt, J = 11.7, 6.3 Hz, 1H), 2.27 (q, J = 12.7 Hz, 1H), 1.99 – 1.87 (m, 2H), 1.87 – 1.76 (m, 1H), 1.72 (dt, J = 14.3, 7.1 Hz, 1H), 1.65 – 1.42 (m, 5H), 1.07 – 0.92 (m, 3H). ¹³C NMR (126

MHz, cdcl₃) δ 152.78, 150.22, 149.98, 149.58, 149.45, 149.29, 149.18, 149.08, 148.90, 148.76, 148.66, 148.45, 147.77, 146.96, 146.92, 146.70, 146.58, 146.50, 146.25, 146.19, 146.10, 145.68, 145.60, 145.42, 145.21, 144.92, 144.72, 144.63, 144.58, 144.46, 144.25, 144.14, 144.09, 144.01, 143.32, 143.17, 142.92, 142.84, 142.77, 142.70, 142.27, 142.21, 141.78, 140.91, 140.67, 138.64, 135.42, 134.86, 134.56, 133.43, 130.93, 130.55, 128.49, 127.05, 79.86, 78.37, 69.19, 66.98, 64.30, 60.72, 56.90, 53.88, 53.37, 50.31, 41.28, 32.46, 30.58, 28.44, 28.04, 23.27, 20.16, 14.56. ; FT-IR (cm⁻¹, neat): 2922.0, 2855.7, 2788.0, 2333.3, 2160.3, 1600.9, 1509.5, 1459.8, 1445.2, 1148.3, 1076.4, 796.7, 757.5, 701.3. HRMS ESI+ (m/z): calcd. for C₇₈H₂₉N, [M+H⁺] 980.2373; found 980.2374.

***N*-phenyl PC₆₁PF:** The intermediate (PC₆₁BM-aldehyde) was synthesized by adding DIBAL (0.12 mL, 0.12 mmol) dropwisely to a stirred solution of PC₆₁BM (100 mg, 0.11 mmol) at -78 °C in toluene (30 mL) under nitrogen atmosphere for 1h before quenched with MeOH (1 mL).Next, the crude product was treated with *N*-phenylglycine (70 mg, 0.55 mmol) at 180 °C in *o*-DCB (50 mL) for 1.5h to form the *N*-phenyl PC₆₁PF. The reaction was monitored by TLC (SiO₂, toluene:cyclohexane=1:4). The crude product was separated by flash chromatography (SiO₂, toluene:cyclohexane=1:4) to give the *N*-phenyl PC₆₁PF (15.5 mg, 0.016 mmol) with a 14% yields. ¹H NMR (400 MHz, CDCl₃) δ 7.66 (s, 2H), 7.54 – 7.28 (m, 5H), 7.12 – 7.00 (m, 2H), 6.94 – 6.83 (m, 1H), 5.82 (dd, J = 4.5, 2.5 Hz, 1H), 5.48 (d, J = 10.5 Hz, 1H), 5.34 (d, J = 10.6 Hz, 1H), 3.44 (ddd, J = 15.0, 12.9, 6.5 Hz, 1H), 3.16 – 2.97 (m, 3H), 2.15 – 1.86 (m, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 153.22, 152.85, 152.44,

149.86, 149.20, 148.24, 148.05, 147.94, 147.33, 147.28, 146.89, 146.74, 146.54, 146.47, 146.26, 146.01, 145.93, 145.72, 145.60, 145.45, 145.42, 145.41, 145.25, 145.17, 144.90, 144.72, 144.57, 144.38, 144.23, 144.06, 144.01, 143.90, 143.85, 143.81, 143.53, 143.38, 143.35, 143.32, 143.30, 143.22, 143.16, 143.04, 142.94, 142.40, 142.29, 142.16, 142.10, 142.02, 142.00, 141.67, 141.23, 140.36, 138.75, 137.83, 137.47, 137.40, 134.12, 132.46, 131.04, 129.57, 129.50, 127.60, 117.76, 113.91, 69.84, 68.36, 67.08, 67.05, 65.43, 61.35, 51.18, 34.38, 25.32, 20.27; FT-IR (cm⁻¹, neat): 2923.635, 2853.355, 1596.541, 1500.911, 1444.832, 1367.030, 1321.275, 1213.895, 749.791, 694.645. HRMS ESI⁺ (m/z): calcd. for C₇₈H₁₉N, [M+H⁺] 970.1590; found 970.1571.

***N*-hexyl PC₆₁PF-2D:** The synthesis process was the same as *N*-hexyl PC₆₁PF but in a smaller scale (PC₆₁BM, 200 mg). Also, D₂O (1 mL) was added to the 1,3-dipolar cycloaddition step. Two products were obtained, namely *N*-hexyl PC₆₁PF-1D (less than 10 mg) and *N*-hexyl PC₆₁PF-2D (13.8 mg, 6.3%). ¹H NMR (400 MHz, CDCl₃) δ 4.68 (d, *J* = 8.5 Hz, 1H), 3.39 – 3.31 (m, 2H), 3.21 (d, *J* = 8.6 Hz, 1H), 3.07 – 2.87 (m, 2H), 2.39 (dt, *J* = 10.9, 6.4 Hz, 1H), 2.21 (dd, *J* = 13.9, 10.8 Hz, 1H), 1.93 – 1.83 (m, 2H), 1.77 (dd, *J* = 13.9, 6.8 Hz, 1H), 1.67 (dp, *J* = 13.9, 6.6 Hz, 2H), 1.49 – 1.40 (m, 4H), 0.95 (td, *J* = 5.7, 4.6, 2.9 Hz, 3H). HRMS ESI⁺ (m/z): calcd. for C₇₈H₂D₄N, [M+H⁺] 984.2624; found 984.2624.

NMR spectra of PC₆₁PFs

N-hexyl PC₆₁PF-1

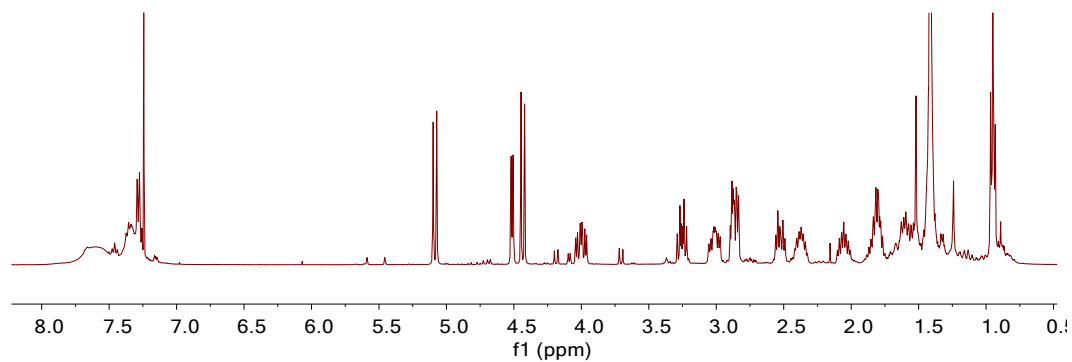


Figure S1. ¹H NMR spectrum of *N*-hexyl PC₆₁PF-1 in CDCl₃.

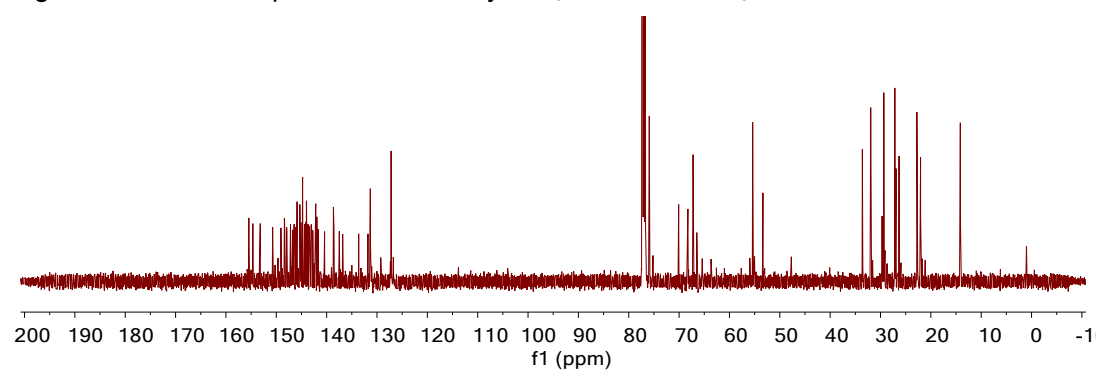


Figure S2. ¹³C NMR spectrum of *N*-hexyl PC₆₁PF-1 in CDCl₃.

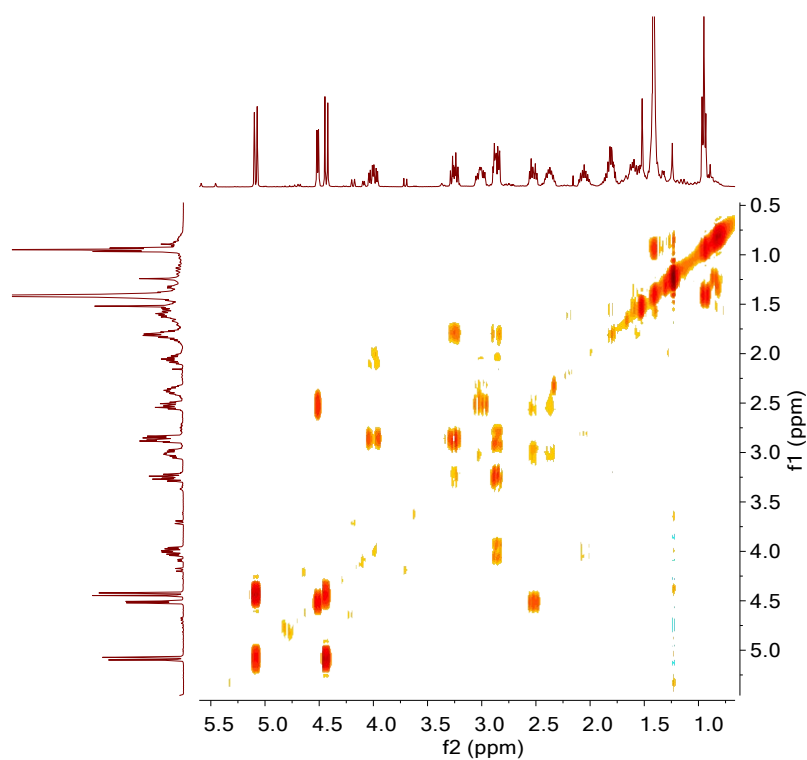


Figure S3. COSY spectrum of *N*-hexyl PC₆₁PF-1 in CDCl₃.

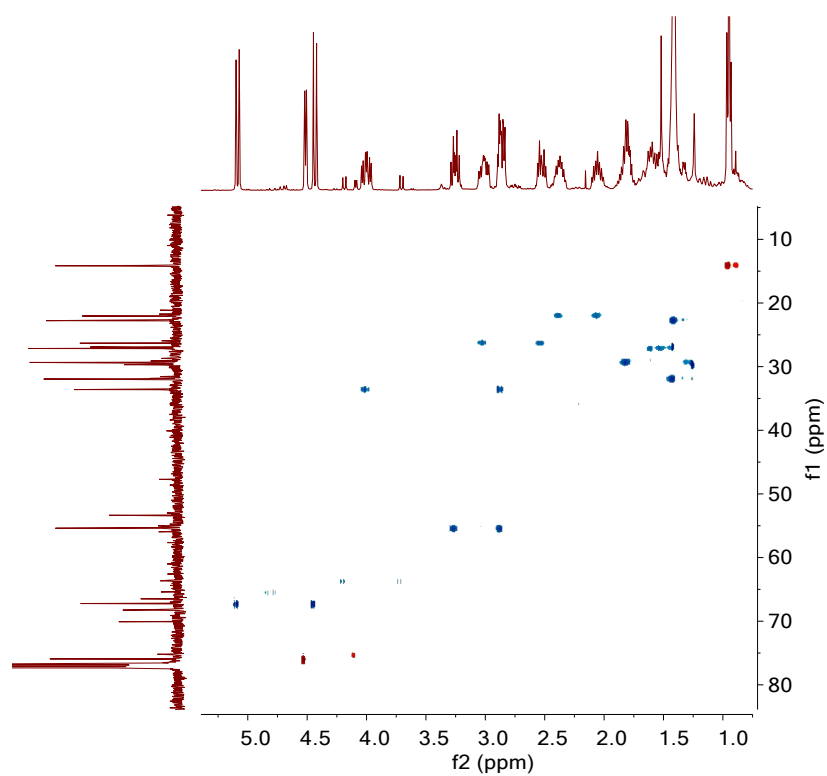


Figure S4. HSQC spectrum of *N*-hexyl PC₆₁PF-1 in CDCl₃.

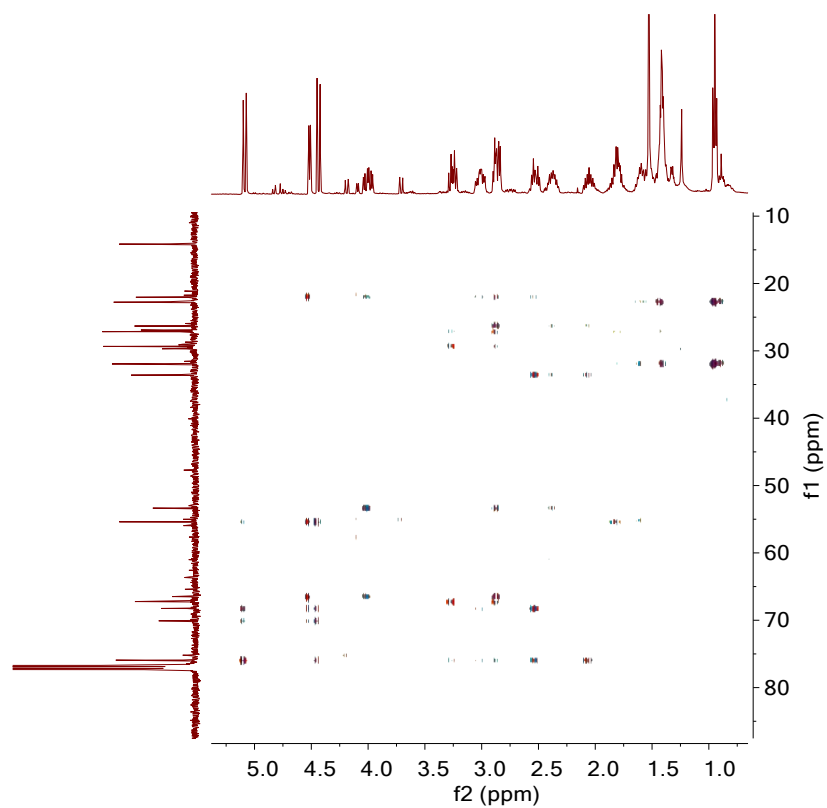


Figure S5. HMBC spectrum of *N*-hexyl PC₆₁PF-1 in CDCl₃.

***N*-hexyl PC₆₁PF-2**

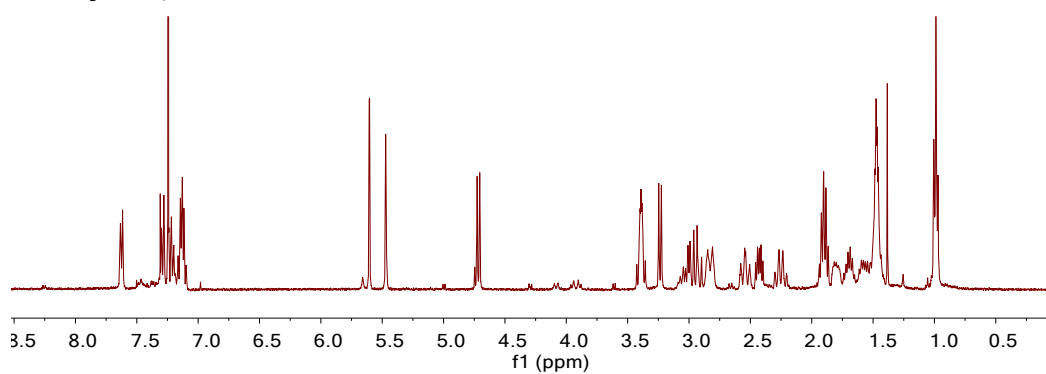


Figure S6. ¹H NMR spectrum of *N*-hexyl PC₆₁PF-2 in CDCl₃.

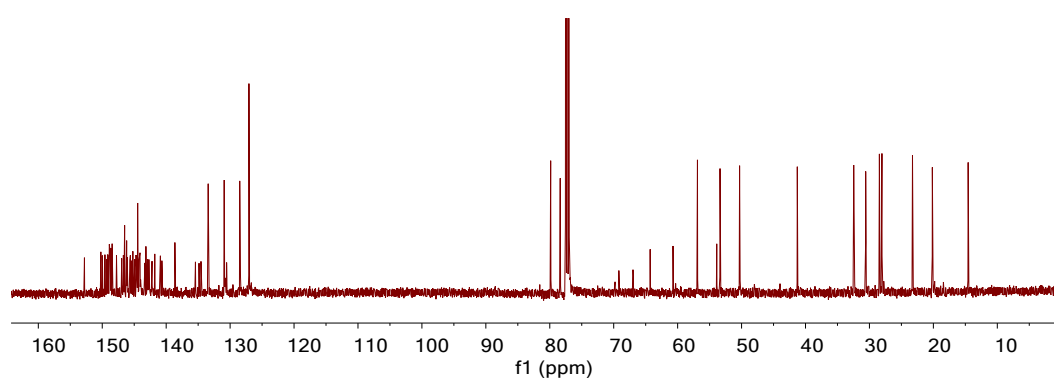


Figure S7. ¹³C NMR spectrum of *N*-hexyl PC₆₁PF-2 in CDCl₃.

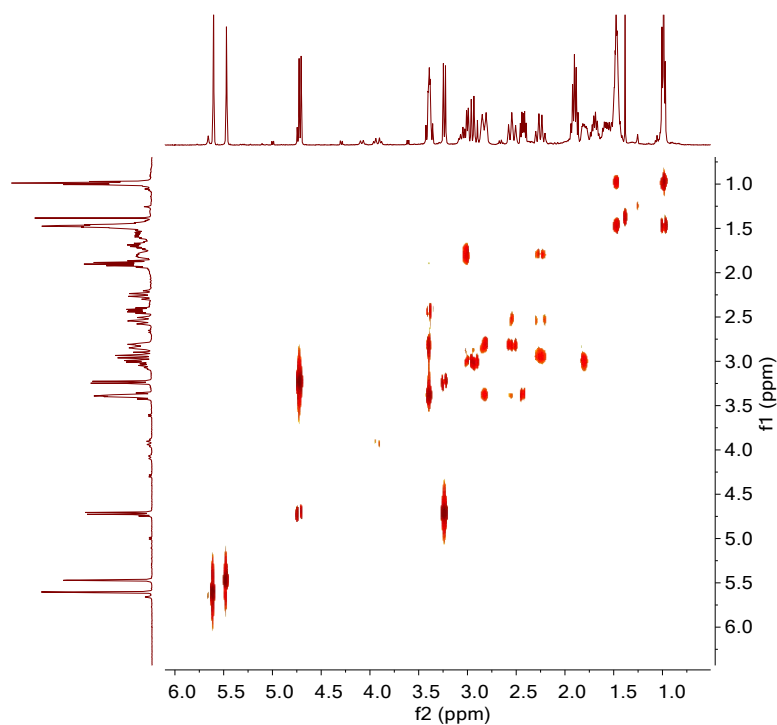


Figure S8. COSY spectrum of *N*-hexyl PC₆₁PF-2 in CDCl₃.

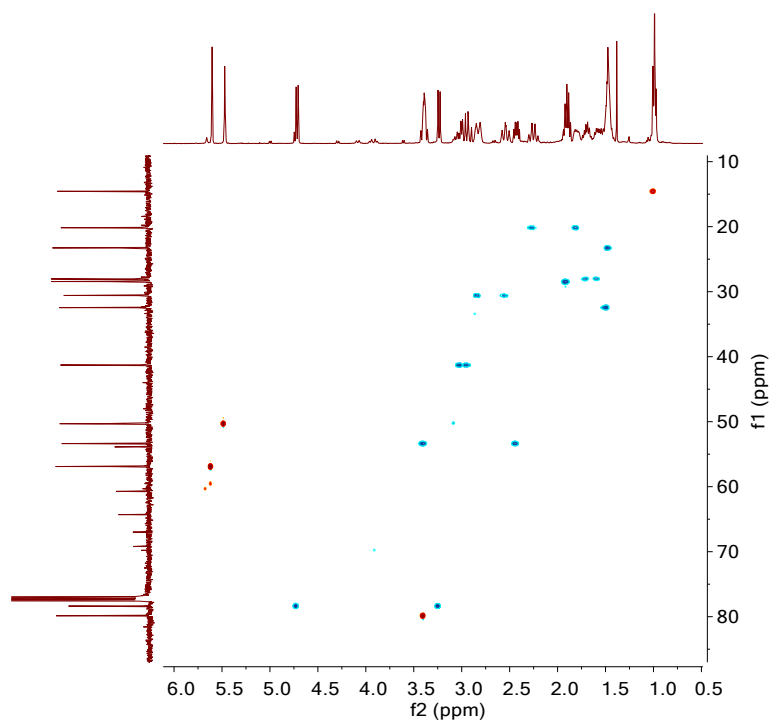


Figure S9. HSQC spectrum of *N*-hexyl PC₆₁PF-2 in CDCl₃.

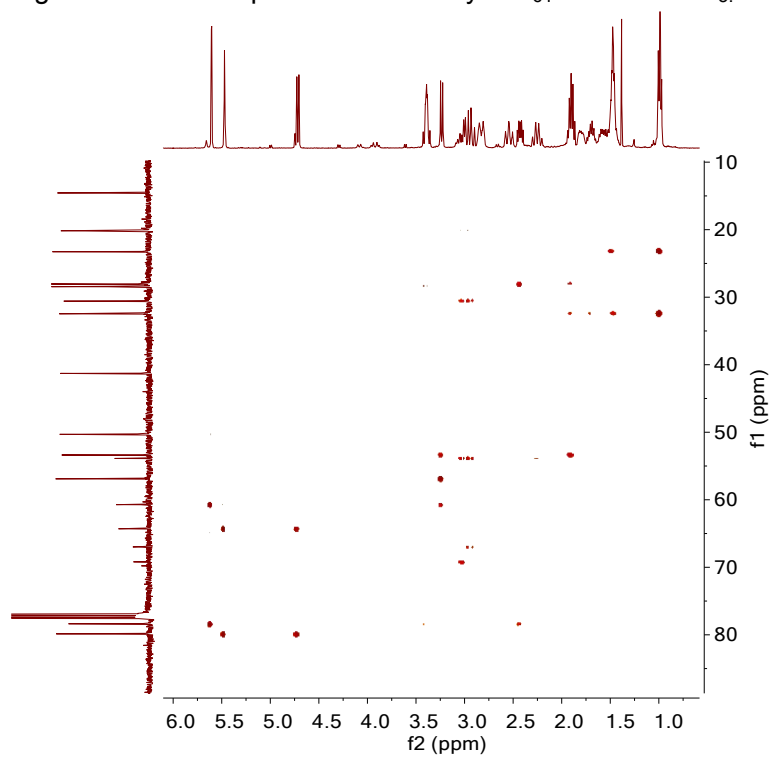


Figure S10. HMBC spectrum of *N*-hexyl PC₆₁PF-2 in CDCl₃.

***N*-phenyl PC₆₁PF**

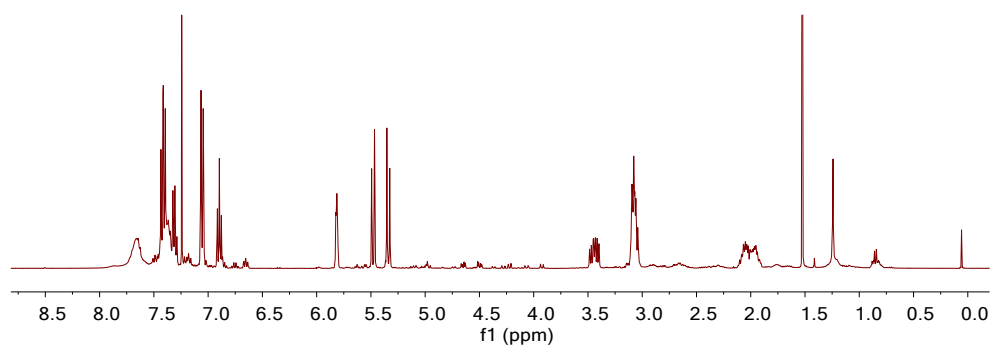


Figure S11. ¹H NMR spectrum of *N*-phenyl PC₆₁PF in CDCl₃.

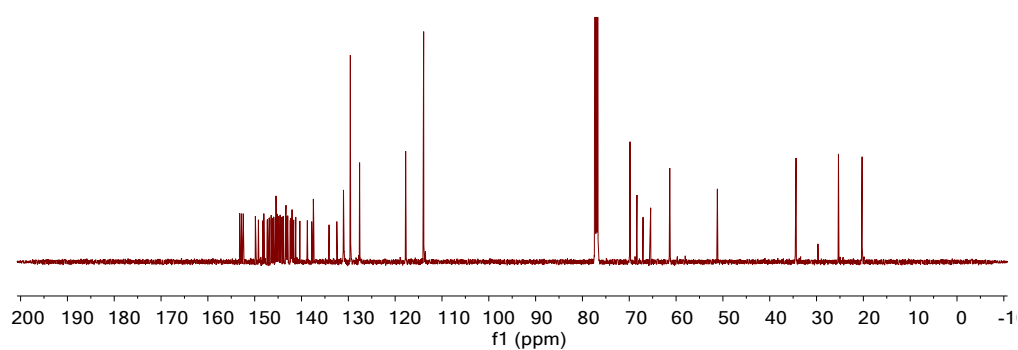


Figure S12. ¹³C NMR spectrum of *N*-phenyl PC₆₁PF in CDCl₃.

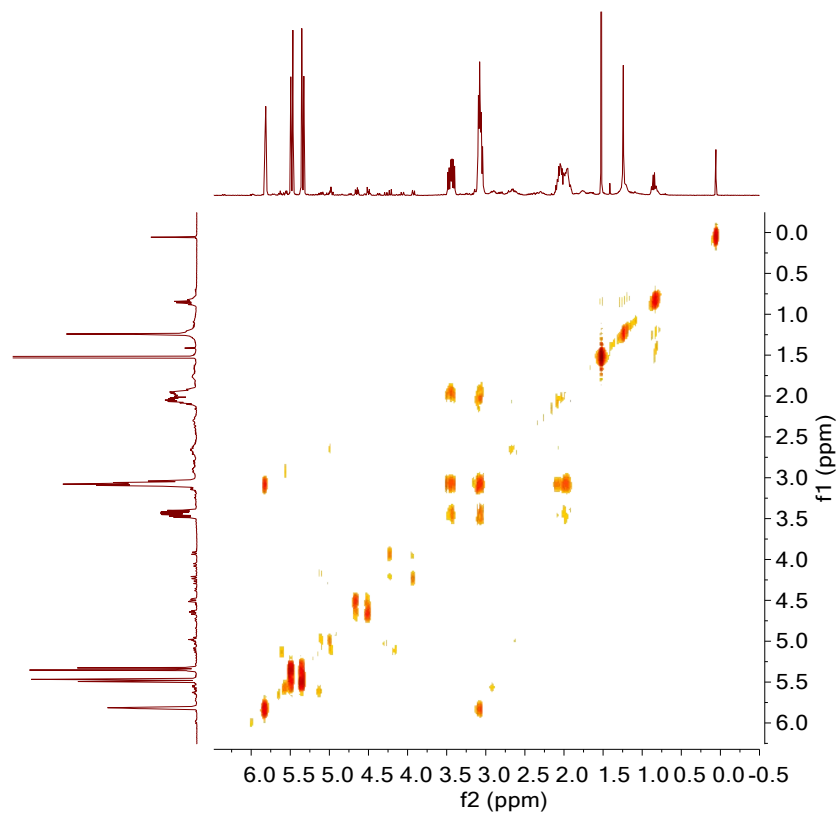


Figure S13. COSY spectrum of *N*-phenyl PC₆₁PF in CDCl₃.

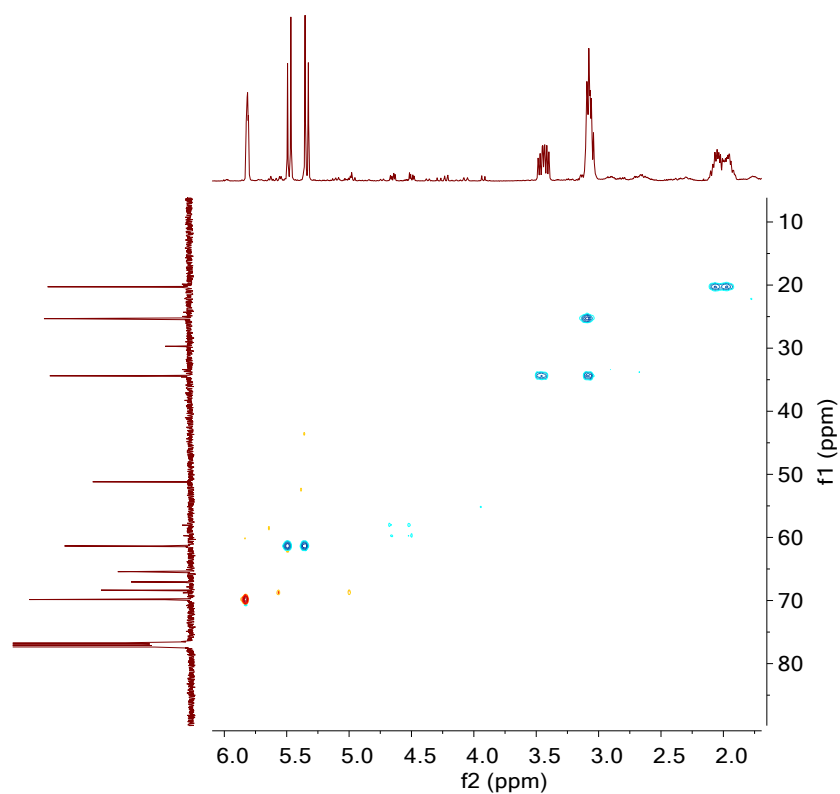


Figure S14. HSQC spectrum of *N*-phenyl PC₆₁PF in CDCl₃

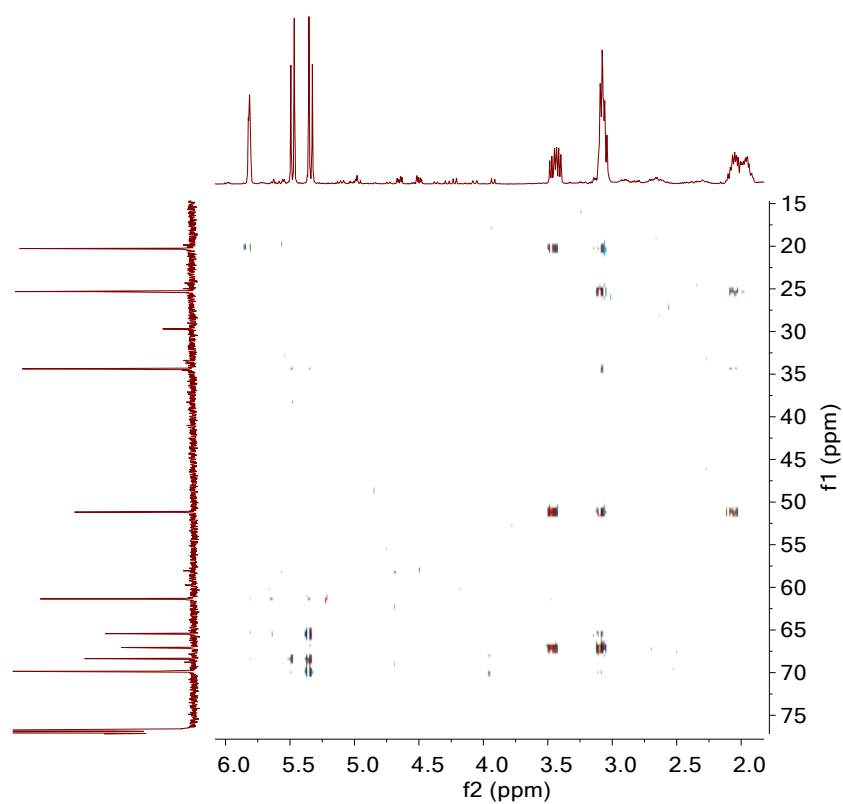


Figure S15. HMBC spectrum of *N*-phenyl PC₆₁PF in CDCl₃

Deuterium Exchange Experiments

N-hexyl PC₆₁PF-1

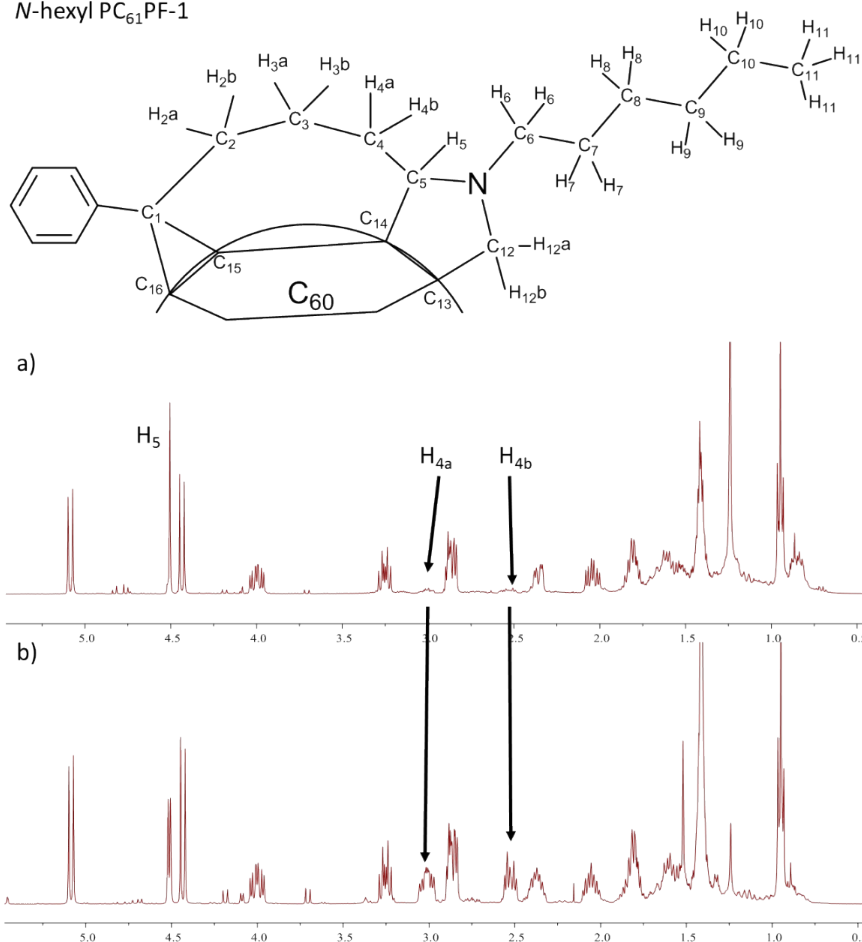


Figure S16. Comparison between ¹H NMR spectrum of *N*-hexyl PC₆₁PF-2 synthesized a) with and b) without D₂O. Note that the resonance for the H_{4a} and H_{4b} protons are reduced significantly indicating the deuteration at that position.

N-hexyl PC₆₁PF-2

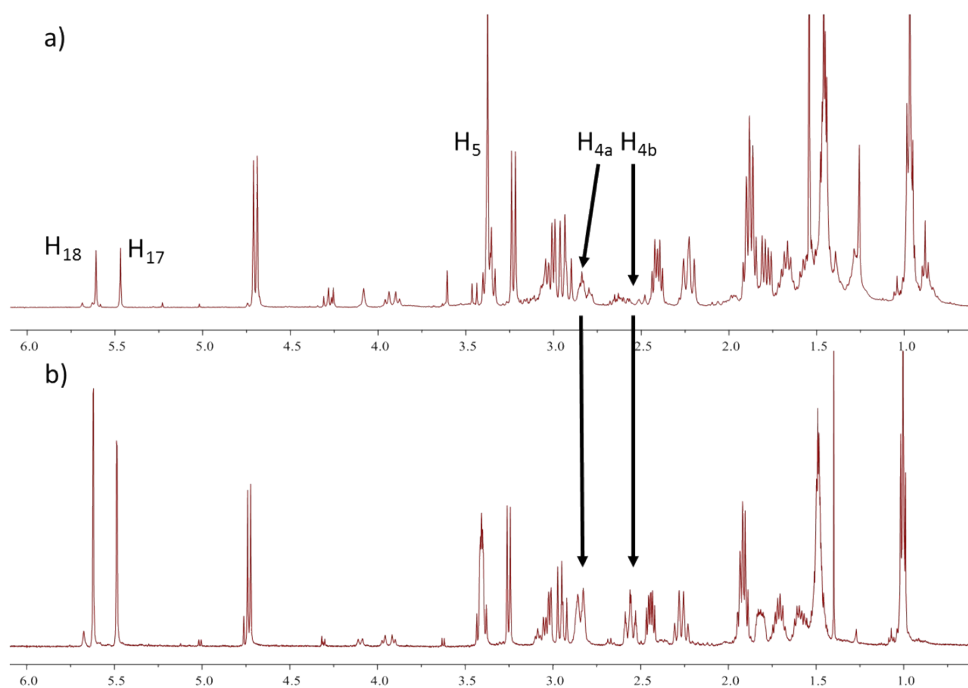
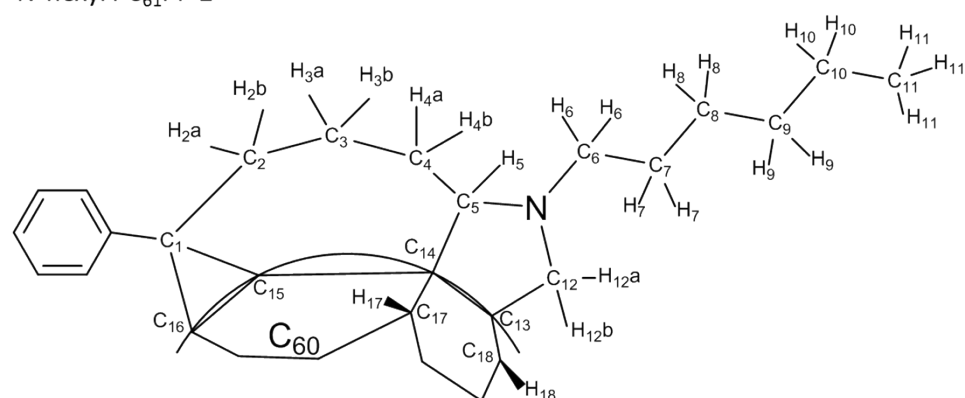


Figure S17. Comparison between ¹H NMR spectrum of *N*- hexyl PC₆₁PF-2 synthesized a) with and b) without D₂O. Note that the resonance for the H₁₇, H₁₈, H_{4a} and H_{4b} protons are reduced significantly indicating the deuteration at that position.

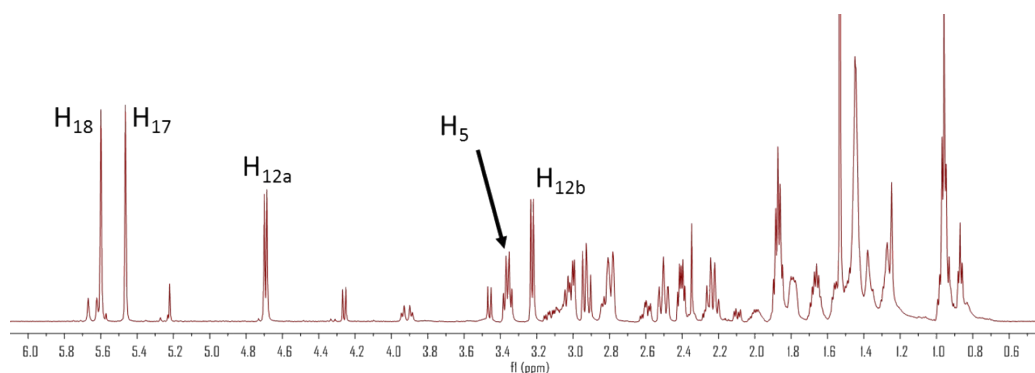


Figure S18. ^1H NMR spectrum of *N*-hexyl $\text{PC}_{61}\text{PF-2}$ synthesized by deuterated DIBAL. Note that the resonance for the H_5 proton is missing indicating a deuterium at that position. The resonances for H_{17} and H_{18} did not diminish compared to the H_{12} protons.

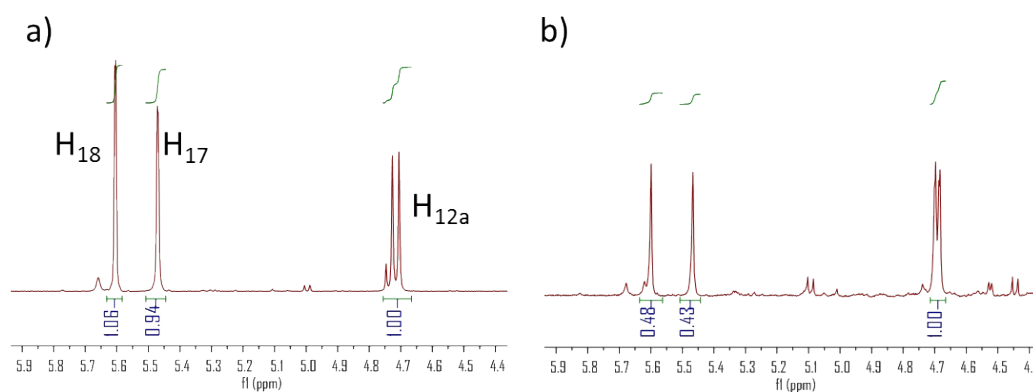


Figure S19. Comparison of the integration for H_{17} , H_{18} and H_{12} resonances for ^1H NMR spectrum of *N*-hexyl $\text{PC}_{61}\text{PF-2}$ a) before (400 MHz) and b) after (600 MHz) reaction with D_2O and *N*-hexylglycine $\cdot\text{KCl}$. This data shows the H_{17} and H_{18} protons are labile under reaction conditions and readily exchanges with deuterium from D_2O .

Mass Spectrum of PC₆₁PFs

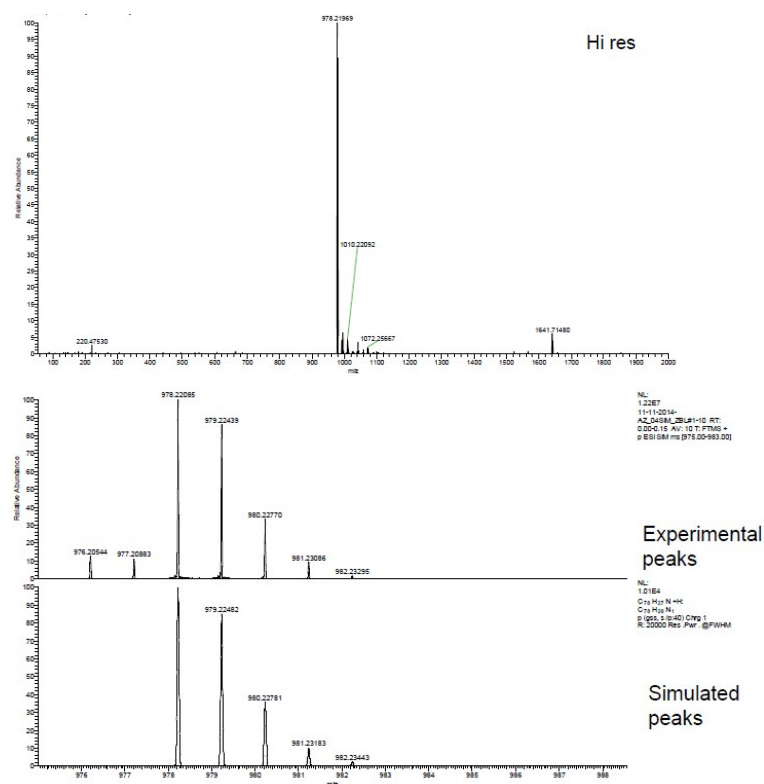


Figure S20. High resolution ESI+ mass spectrum of *N*-hexyl PC₆₁PF-1.

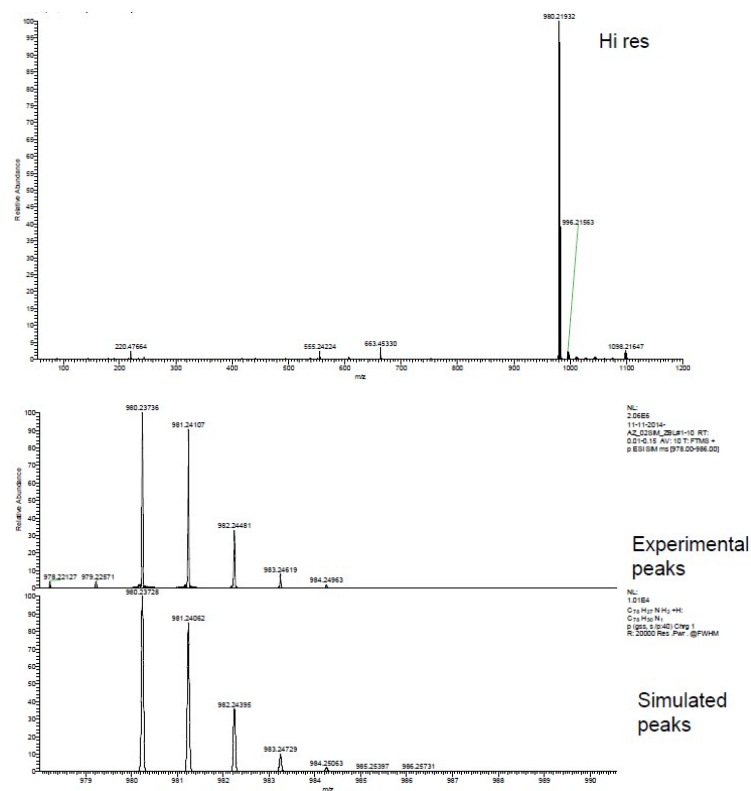
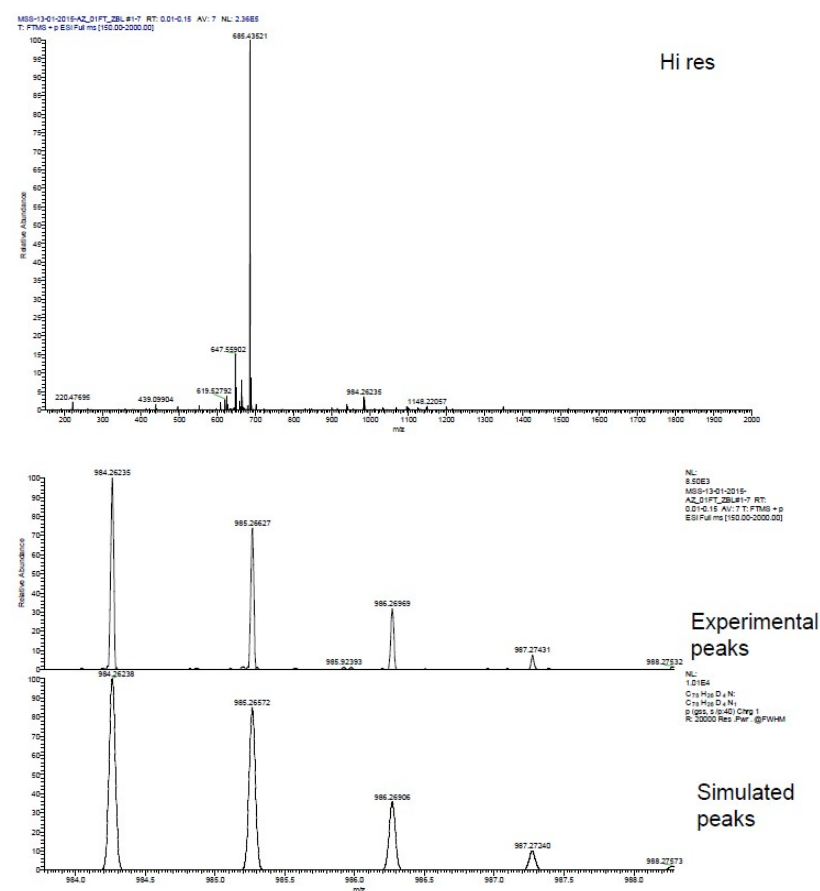
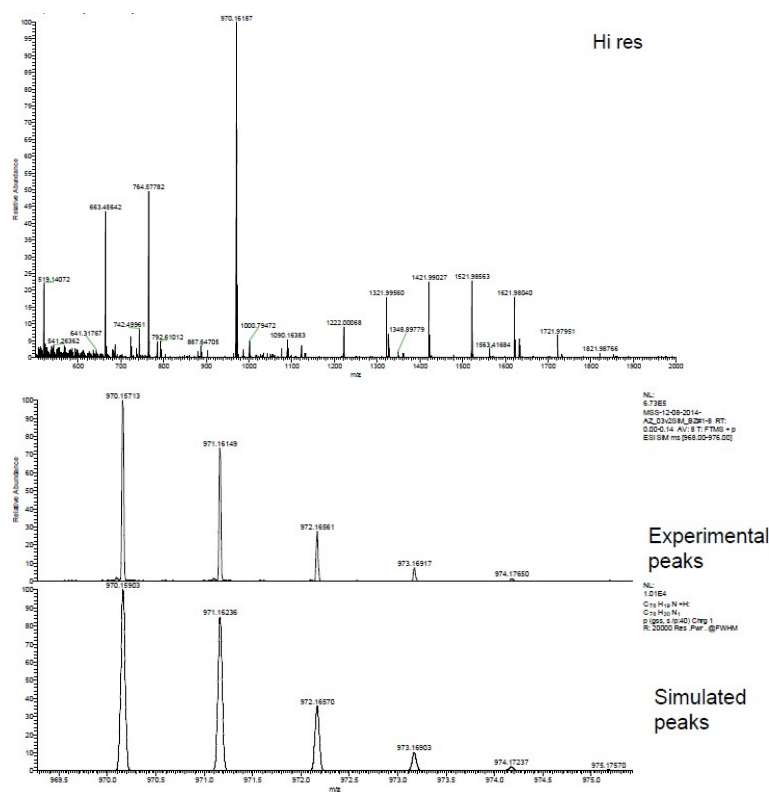


Figure S21. High resolution ESI+ mass spectrum of *N*-hexyl PC₆₁PF-2.



HPLC analysis of PC₆₁PFs

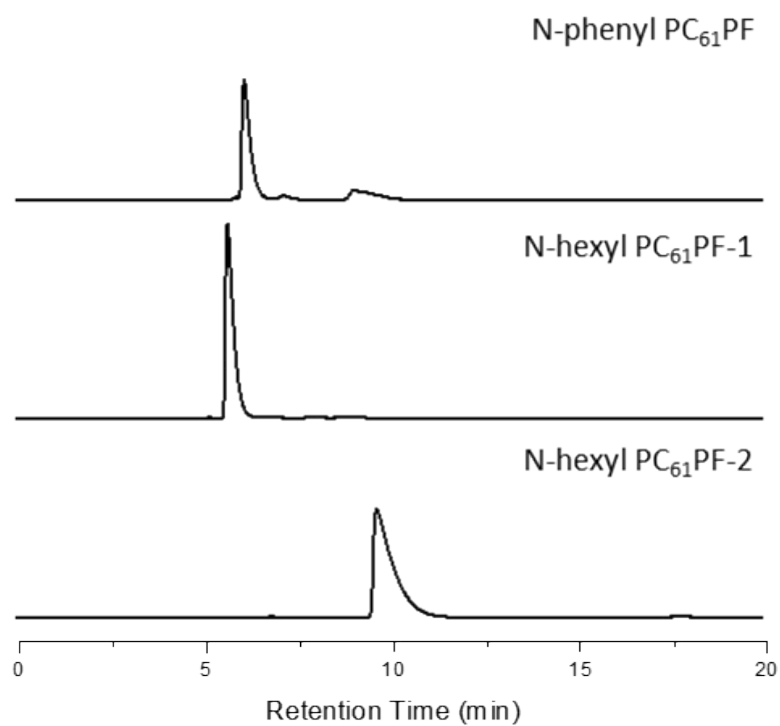


Figure S24. HPLC chromatography of a) *N*-hexyl PC₆₁PF-1; b) *N*-hexyl PC₆₁PF-2 and c) *N*-phenyl PC₆₁PF.

Electrochemical properties

All cyclic voltammograms (CV) were carried out in $\text{CH}_2\text{Cl}_2/\text{MeCN}$ 9:1 with 0.1 M TBA PF_6 . The reference electrode was a silver wire Ag/Ag^+ pseudo reference, the counter electrode was platinum and the working electrode was glassy carbon. The CVs were measured at a scan rate of 50 mV/s and ferrocene was added in the system as the internal reference. The experiments were performed at 22 °C and the first reduction observed in the fullerene derivatives was reversible as was expected.

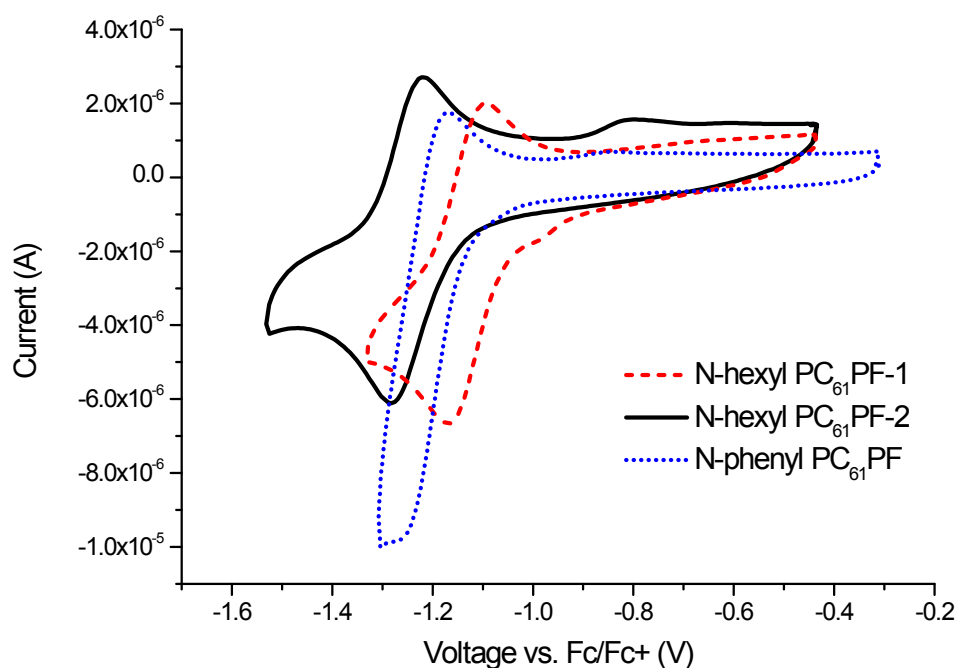


Figure S25. HPLC chromatography of *N*-hexyl PC_{61}PF -1, *N*-hexyl PC_{61}PF -2 and *N*-phenyl PC_{61}PF .

X-ray crystal experimental procedures and data of *N*-hexyl PC₆₁PF-2

Intensity data for *N*-hexyl PC₆₁PF-2 was collected at 100 K on the MX1 beamline² at the Australian Synchrotron. The structures were solved by direct methods and difference Fourier synthesis.³ Thermal ellipsoid plots were generated using the program ORTEP-3⁴ integrated within the WINGX⁵ suite of programs.

Crystal data for *N*-hexyl PC₆₁PF-2 dimer C₁₅₆H₅₈N₂ (CHCl₃), $M = 2079.41$, $T = 100(2)$ K, $\lambda = 0.71073$ Å, Monoclinic, space group P_n, $a = 17.530(3)$ b = 9.800(2), $c = 26.749(5)$ Å, $\beta = 92.39(3)^\circ$. $V = 4591.3(15)$ Å³, $Z = 2$, $D_c = 1.504$ Mg/m³, $\mu(\text{Mo-K}\alpha) 0.171$ mm⁻¹, $F(000) = 2132$, crystal size 0.05 x 0.05 x 0.01 mm³. 45637 reflections measured to a maximum $\theta = 23.544^\circ$, 12986 independent reflections ($R_{\text{int}} = 0.1188$), the final R was 0.1435 [$I > 2\sigma(I)$] and $wR(F^2)$ was 0.4076 (all data).

Theoretical calculations

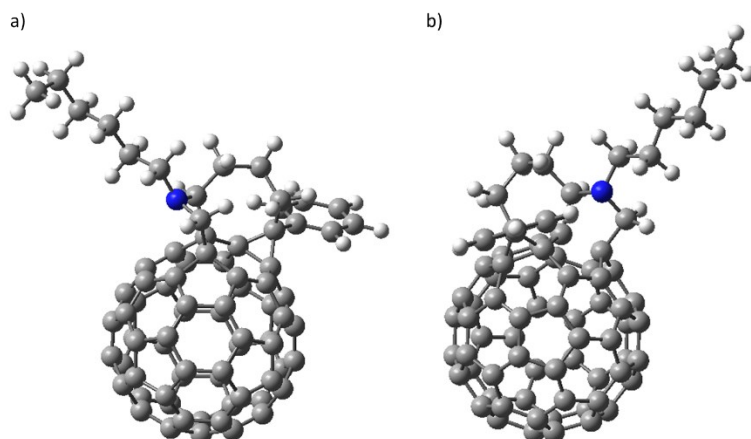


Figure S26. The DFT optimized configurations for a) *cis*-1 and b) *cis*-1,2-IM of *N*-hexyl PC₆₁PF.

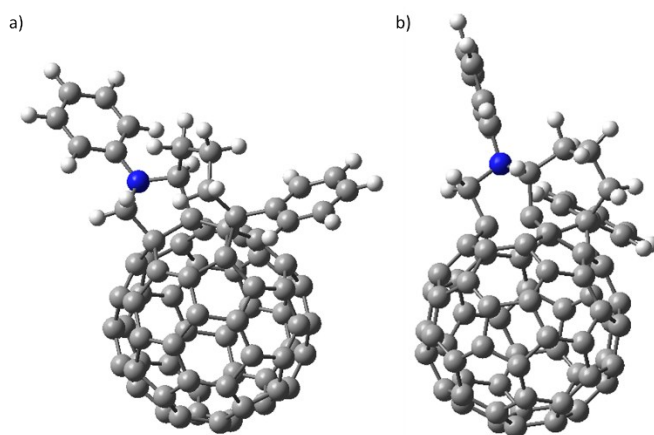


Figure S27. The DFT optimized configurations for a) *cis*-1 and b) *cis*-1,2-IM of *N*-phenyl PC₆₁PF.

Table S1. Gas-phase and solution^a (1,2-dichlorobenzene) Gibbs free energy difference ΔG in kcal.mol⁻¹ relative to the start point for the extreme located along the pathway of the [3+2] cycloaddition of PC₆₁PFs.

N-methyl PC61PF	Start point	TS-1	cis-1	TS-2	cis-1,2-IM	cis-1,2
Gas phase ΔG	0.00	4.72	-35.15	10.63	-17.79	-785.10
Solution ΔG	0.00	4.30	-32.59	8.15	-15.20	-783.57
N-hexyl PC61PF	Start point	TS-1	cis-1	TS-2	cis-1,2-IM	cis-1,2
Gas phase ΔG	0.00	6.26	-21.57	11.17	-15.99	-782.84
Solution ΔG	0.00	3.60	-19.61	9.03	-13.29	-781.32
N-phenyl PC61PF	Start point	TS-1	cis-1	TS-2	cis-1,2-IM	cis-1,2
Gas phase ΔG	0.00	8.50	-30.29	9.78	-19.99	-787.03
Solution ΔG	0.00	5.89	-31.08	7.76	-18.91	-787.21

^a SMD is the used solvation model.

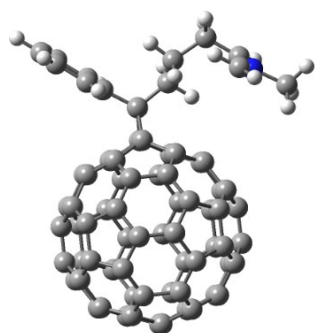
Cartesian coordinates (Å) and energies (Hartree) data of PC₆₁PFs

Computational details

Quantum-chemical calculations were performed with the Gaussian09⁶ suite employing the B3LYP-D3^{7, 8} density functional in combination with the 6-311G(d,p) basis set. Geometry optimizations were performed with tight SCF and convergence criteria and an ultrafine integration grid, applying the GEDIIS optimization algorithm. The nature of each stationary point was confirmed by a frequency analysis. SMD is the used solvation model and the SMD energy is obtained by single point calculation of the optimized structure employing the B3LYP-D3 density functional in combination with the 6-311G(d,p) basis set. Solution Gibbs free energy is the sum of the SMD energy and the thermal correction to Gibbs free energy acquired from frequency calculations.

N-methyl PC₆₁PF

start point:

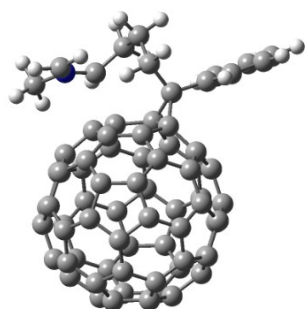


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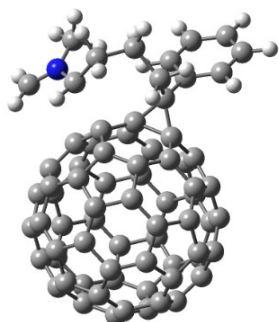


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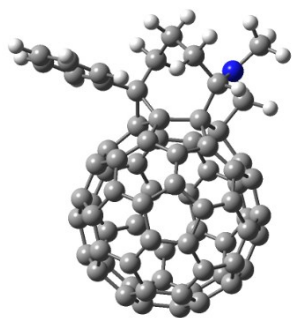


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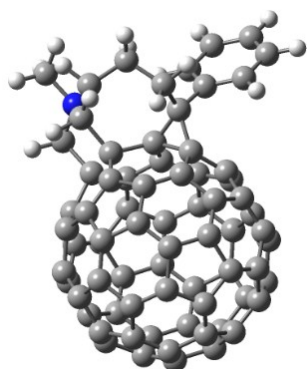


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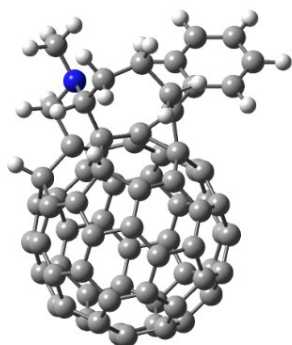


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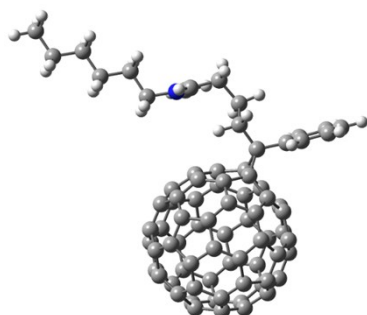
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N-hexyl PC61PF

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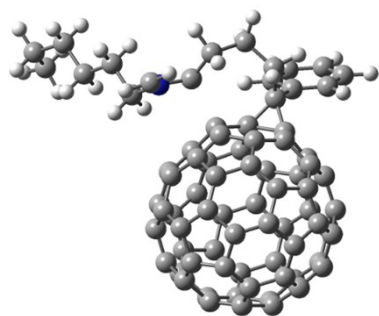


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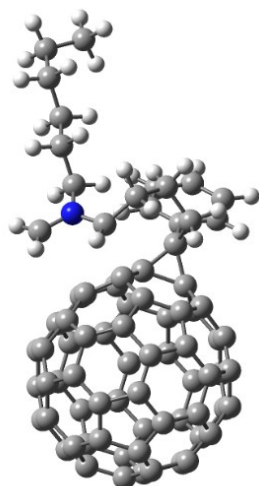


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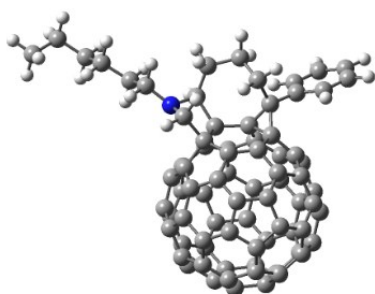
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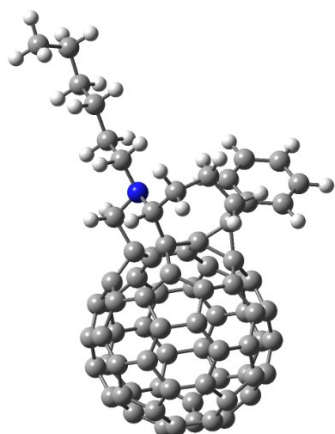


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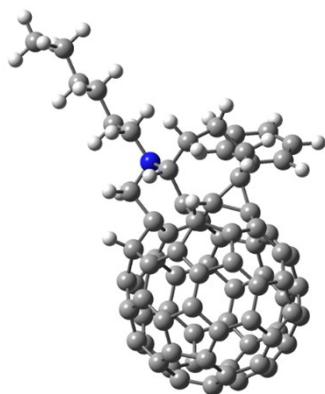


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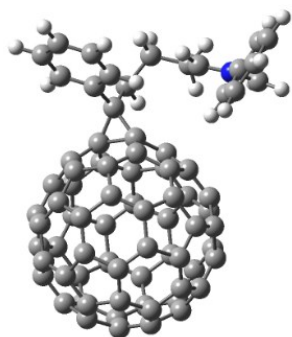
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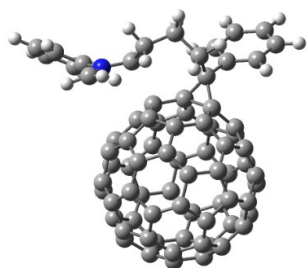


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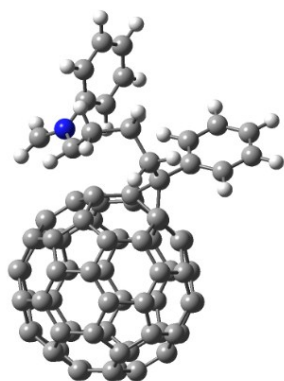


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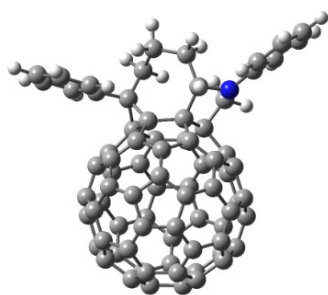


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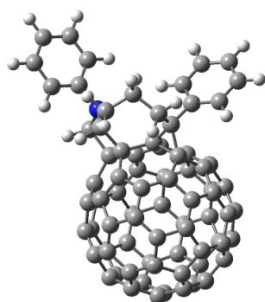


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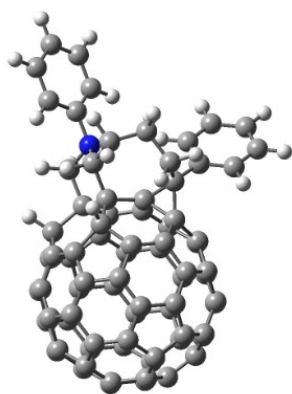


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