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Electronic Supplementary Information

Highly Soluble C_{2v}-Symmetrical Fullerene Derivatives: Efficient Synthesis, Characterization, and Electrochemical Study

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Contents

General Remarks:

The starting octabromofullerene $C_{60}Br_8$ was prepared based on the improved synthetic method of $C_{60}Br_8$. All other reagents were commercially available and used as received without further purification. ^{1}H, ^{13}C, and ^{19}F NMR spectra were, respectively, recorded on a Brucker 600M system. The UV−visible spectrum was recorded on a UV-3600 spectrometer. High-resolution mass spectra were obtained by APCI using a TOF mass analyzer on a JEOL JMS-T100LC spectrometer. CV measurements were performed with a CHI660E voltammetric analyzer. CCDC 1885323 contains the supplementary crystallographic data for this paper.

Synthesis of compound 1: $C_{60}Br_8 \bullet Br_2$ (500 mg, 0.329 mmol), $(CH_3)_2CHOH$ (2.00 mL, 1.57 g, 26.2 mmol, 79.6 eq), and $AgCF_3SO_3$ (1.15 g, 4.48 mmol, 13.6 eq) were added to *o*-dichlorobenzene (50 mL). After stirring for 5 hours in dark, the solution was filtered to remove the silver salt. The filtrate was washed with saturated $NaHCO_3$ (aq.), then dried with Na_2SO_4, and the solvent was evaporated. Purification of the product was performed by preparative HPLC separation (Buckyprep column, eluent: chloroform/2-propanol = 1/1) to obtain the title compound (310 mg, 79.0% isolated yield, analytically pure) as orange crystals. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 1.12 (dd, *J* = 24.9, 6.1 Hz, 24H, OCH($C\underline{H}_3$)$_2$), 1.28 (dd, *J* = 16.6 Hz, 6.1 Hz, 24H, OCH($C\underline{H}_3$)$_2$), 4.34–4.41 (m, 4H, OC$\underline{H}$(CH_3)$_2$), 4.59–4.67 (m, 4H, OC$\underline{H}$(CH_3)$_2$). ^{13}C NMR (150 MHz, CD_2Cl_2) (all 4C (sp^2) unless indicated). δ 23.76 (4C, OCH($\underline{C}H_3$)$_2$), 23.91 (4C, OCH($\underline{C}H_3$)$_2$), 24.28 (4C, OCH($\underline{C}H_3$)$_2$), 24.47 (4C, OCH($\underline{C}H_3$)$_2$), 68.92 (4C, O$\underline{C}$H(CH_3)$_2$), 70.07 (4C, O$\underline{C}$H(CH_3)$_2$), 76.50 (4C, sp^3), 77.25 (4C, sp^3), 135.09, 142.82, 143.98, 144.14, 145.02 (2C), 145.09, 145.69, 145.73 (2C), 145.77, 146.46 (2C), 146.72, 148.50, 148.86, 149.95, 151.78 (2C). APCI–MS (–) for $C_{84}H_{56}O_8$ $[M]^-$; calcd. 1192.3975; found 1192.3960.

Synthesis of compound 2: $C_{60}Br_8 \bullet Br_2$ (500 mg, 0.329 mmol), CH_3CCl_3 (2.00 mL, 3.12g, 20.9 mmol, 63.5 eq), and $AgCF_3SO_3$ (1.15 g, 4.48 mmol, 13.6 eq) were added to *o*-dichlorobenzene (50 mL). After stirring for 5 hours in dark, the solution was filtered to remove the silver salt. The filtrate was washed with saturated $NaHCO_3$ (aq.), then dried with Na_2SO_4, and the solvent was evaporated. Purification of the product was performed by preparative HPLC separation (Buckyprep column, eluent: chloroform/2-propanol = 7/3) to obtain the title compound (415 mg, 66.2% isolated yield, analytically pure) as orange crystals. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 4.37 (d, J = 10.3 Hz, 4H, OC$\underline{H}_2$CCl$_3$), 4.61 (d, J = 10.3 Hz, 4H, OC$\underline{H}_2$CCl$_3$), 4.65 (d, J = 10.3 Hz, 4H, OC$\underline{H}_2$CCl$_3$), 4.79 (d, J = 10.3 Hz, 4H, OC$\underline{H}_2$CCl$_3$) ^{13}C NMR (150 MHz, CD_2Cl_2) (all 4C (sp^2) unless indicated). δ 76.50 (4C, O$\underline{C}$H$_2$CCl$_3$), 77.12 (4C, O$\underline{C}$H$_2$CCl$_3$), 78.36 (4C, sp^3), 79.14 (4C, sp^3), 95.26 (4C, OCH$_2\underline{C}$Cl$_3$), 95.34 (4C, OCH$_2\underline{C}$Cl$_3$), 133.39, 141.55, 142.40, 144.32, 144.76 (2C), 144.81, 144.88, 144.96 (2C), 145.98, 146.76 (2C), 147.52, 147.56, 148.50, 148.51, 152.88 (2C). APCI–MS (–) for $C_{76}H_{16}O_8Cl_{24}$ $[M]^-$; calcd. 1906.3256; found 1906* *High resolution mass spectrum could not be obtained due to the broadness of the signal.

Synthesis of compound 3: $C_{60}Br_8 \bullet Br_2$ (500 mg, 0.329 mmol), $(CH_2F)_2CHOH$ (2.00 mL, 2.48 g, 25.8 mmol, 78.4 eq), and $AgCF_3SO_3$ (1.15 g, 4.48 mmol, 13.6 eq) were added to *o*-dichlorobenzene (50 mL). After stirring for 5 hours in dark, the solution was filtered to remove the silver salt. The filtrate was washed with saturated $NaHCO_3$ (aq.), then dried with Na_2SO_4, and the solvent was evaporated. Purification of the product was performed by preparative HPLC separation (Buckyprep column, eluent: chloroform/2-propanol = 1/1) to obtain the title compound (209 mg, 42.9% isolated yield, analytically pure) as orange crystals. ^{1}H NMR (600 MHz, $CDCl_3$) δ 4.38–4.55 (m, 16H, OCH(C$\underline{H}_2$F)$_2$), 4.56–4.58 (m, 4H, OC$\underline{H}$(CH$_2$F)$_2$), 4.59–4.72 (m, 16H, OCH(C$\underline{H}_2$F)$_2$), 4.76–4.87 (m, 4H, OC$\underline{H}$(CH$_2$F)$_2$). ^{13}C NMR (150 MHz, CD_2Cl_2) (all 4C (sp^2) unless indicated). δ 73.57 (t, J = 19.9 Hz, 4C, O$\underline{C}$H(CH$_2$F)$_2$), 74.07 (t, J = 20.0 Hz, 4C, O$\underline{C}$H(CH$_2$F)$_2$), 76.57 (4C, sp^3), 77.35 (4C, sp^3), 81.26 (dd, J = 171.90 Hz, 7.8 Hz, 4C, OCH($\underline{C}$H$_2$F)$_2$), 81.34 (dd, J =

171.90 Hz, 6.5 Hz, 4C, OCH($\underline{C}H_2F)_2$), 81.34 (dd, *J* = 172.90 Hz, 6.8 Hz, 4C, OCH($\underline{C}H_2F)_2$), 82.15 (dd, *J* = 172.70 Hz, 6.6 Hz, 4C, OCH($\underline{C}H_2F)_2$), 133.81, 141.89, 141.97, 144.07 (2C), 144.39, 145.02, 145.12 (2C), 145.29, 145.81, 146.61 (2C), 147.27, 148.02, 148.33, 148.39, 152.31 (2C). APCI–MS (–) for $C_{84}H_{40}O_8F_{16}$ $[M]^-$; calcd. 1480.2468; found 1480.2489.

Synthesis of compound 4: $C_{60}Br_8$•Br_2 (500 mg, 0.329 mmol), CH_2FCH_2OH (2.00 mL, 2.18 g, 34.1 mmol, 104 eq), and $AgCF_3SO_3$ (1.15 g, 4.48 mmol, 13.6 eq) were added to *o*-dichlorobenzene (50 mL). After stirring for 5 hours in dark, the solution was filtered to remove the silver salt. The filtrate was washed with saturated $NaHCO_3$ (aq.), then dried with Na_2SO_4, and the solvent was evaporated. Purification of the product was performed by preparative HPLC separation (Buckyprep column, eluent: chloroform/2-propanol = 7/3) to obtain the title compound (254 mg, 63.1% isolated yield, analytically pure) as orange crystals. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 3.79–3.84 (m, 2H, $OCH_2C\underline{H}_2F$), 3.85–3.89 (m, 2H, 2H, $OCH_2C\underline{H}_2F$), 3.94–4.00 (m, 2H, 2H, $OCH_2C\underline{H}_2F$), 4.01–4.05 (m, 2H, 2H, $OCH_2C\underline{H}_2F$), 4.18–4.23 (m, 2H, 2H, $OCH_2C\underline{H}_2F$), 4.24–4.28 (m, 4H, 2H, $OCH_2C\underline{H}_2F$), 4.29–4.33 (m, 2H, 2H, $OCH_2C\underline{H}_2F$), 4.58 (s, 4H, 2H, $OC\underline{H}_2CH_2F$), 4.66 (s, 4H, $OC\underline{H}_2CH_2F$)), 4.72 (s, 4H, $OC\underline{H}_2CH_2F$)), 4.80 (s, 4H, $OC\underline{H}_2CH_2F$)).^{13}C NMR (150 MHz, CD_2Cl_2) (all 4C (sp^2) unless indicated). δ 66.78 (d, *J* = 19.7 Hz, 4C, $O\underline{C}H_2CH_2F$)), 67.42 (d, *J* = 19.6 Hz, 4C, $O\underline{C}H_2CH_2F$), 76.90 (4C, sp^3), 77.48 (4C, sp^3), 86.28 (d, *J* = 12.4 Hz, 4C, $OCH_2\underline{C}H_2F$), 83.40 (d, *J* = 11.9 Hz, 4C, $OCH_2\underline{C}H_2F$), 134.08, 142.84, 142.92, 144.45, 144.47, 144.82 (2C), 145.20 (2C), 145.29, 145.83, 146.63 (2C), 147.16, 148.45, 148.53, 148.81, 152.43 (2C). APCI–MS (–) for $C_{76}H_{32}O_8F_8$ $[M]^-$; calcd. 1224.1969; found 1224.1917.

Synthesis of compound 5: $C_{60}Br_8$•Br_2 (500 mg, 0.329 mmol), and $AgCF_3SO_3$ (1.15 g, 4.48 mmol, 13.6 eq) were added to 4-$CH_3OC_6H_5$ (20.0 mL, 19.9 g, 184 mmol, 560 eq). After stirring for 24 hours in dark, the solution was filtered to remove the silver salt. The filtrate was washed with saturated $NaHCO_3$ (aq.), then dried with Na_2SO_4, and

the solvent was evaporated. Purification of the product was performed by preparative HPLC separation (Buckyprep column, eluent: chloroform/2-propanol = 1/1) to obtain the title compound (104 mg, 20.0% isolated yield, analytically pure) as orange crystals. ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.62 (s, 12H, $C_6H_4OC\underline{H}_3$), 3.77 (s, 12H, $C_6H_4OC\underline{H}_3$), 6.21 (d, *J* = 8.8 Hz, 8H, $C_6\underline{H}_4OCH_3$), 6.40 (d, *J* = 8.8 Hz, 8H, $C_6\underline{H}_4OCH_3$), 6.67 (d, *J* = 8.8 Hz, 8H, $C_6\underline{H}_4OCH_3$), 7.30 (d, *J* = 8.6 Hz, 8H, $C_6\underline{H}_4OCH_3$). ^{13}C NMR (150 MHz, $CDCl_3$) (all 4C (sp^2) unless indicated). *δ* 55.21 (4C, $C_6H_4O\underline{C}H_3$), 55.42 (4C, $C_6H_4O\underline{C}H_3$), 56.99 (4C, sp^3), 57.14 (4C, sp^3), 112.53 (8C), 113.48 (8C), 130.14 (8C), 130.30 (8C), 130.65 (4C), 131.53 (4C), 134.71, 141.77, 142.35, 144.69, 144.85 (2C), 145.13, 145.50 (2C), 145.66, 146.29 (2C), 147.14, 148.76, 149.37, 150.11 (2C), 150.63, 152.34, 158.09 (4C), 158.90 (4C). APCI–MS (–) for $C_{116}H_{56}O_8$ $[M]^-$; calcd. 1577.4009; found 1577*

*High resolution mass spectrum could not be obtained due to the broadness of the signal.

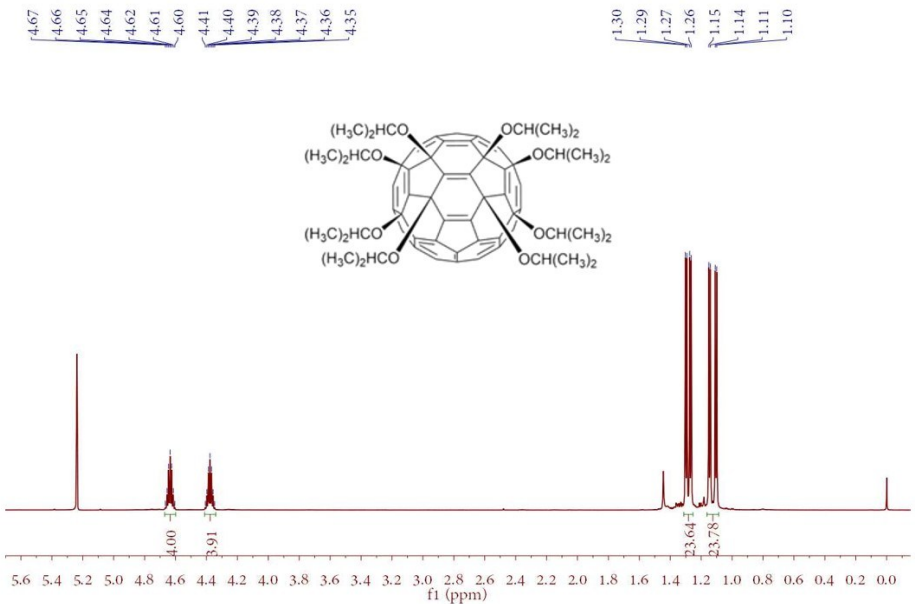


Figure S1. ^{1}H NMR spectrum of **1** in CD_2Cl_2

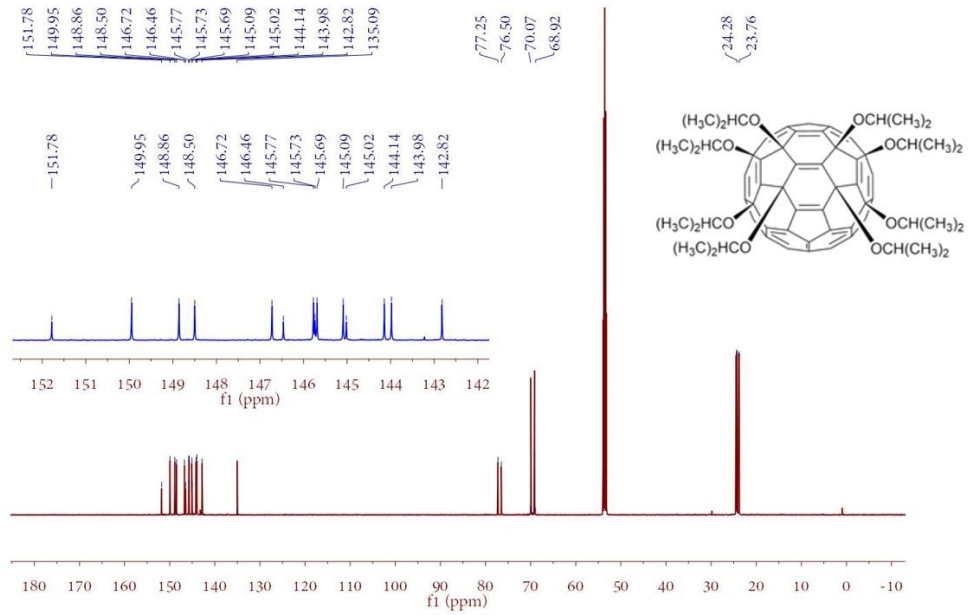


Figure S2. ^{13}C NMR spectrum of **1** in CD_2Cl_2

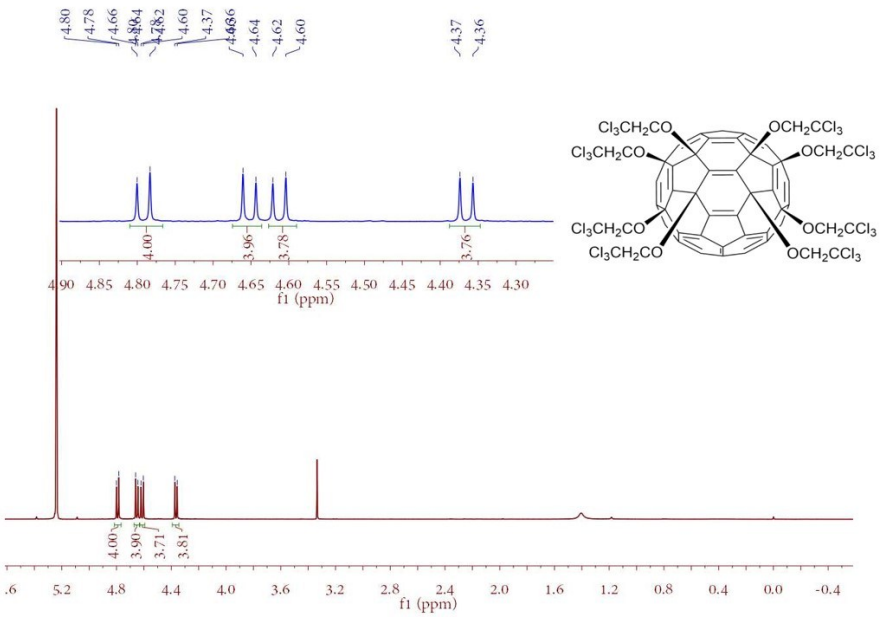


Figure S3. ^{1}H NMR spectrum of **2** in CD_2Cl_2

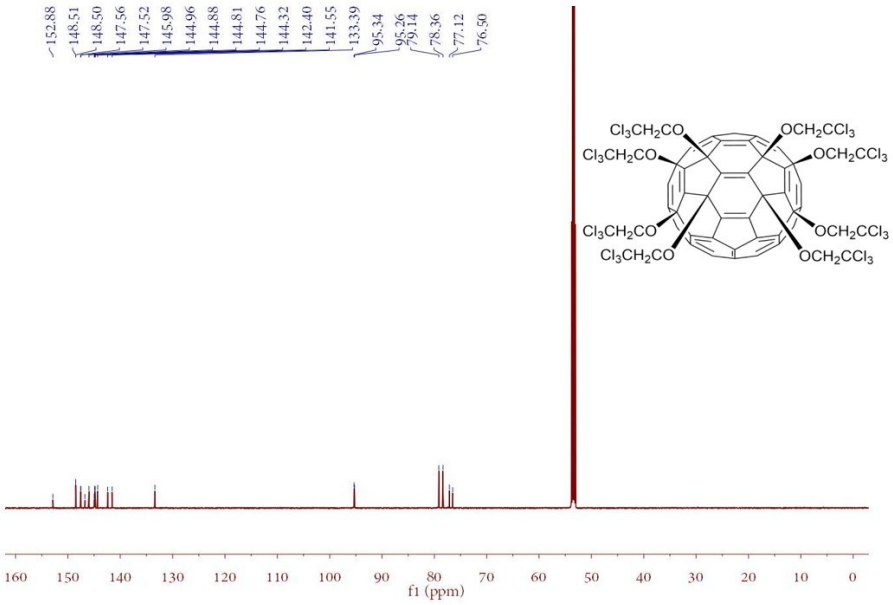


Figure S4. ^{13}C NMR spectrum of **2** in CD_2Cl_2

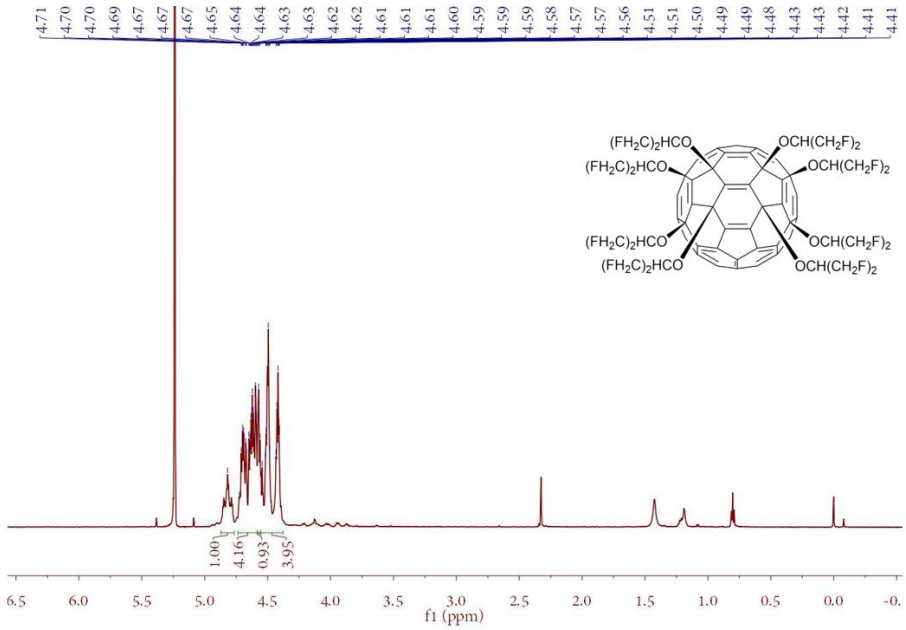


Figure S5. ^{1}H NMR spectrum of **3** in CD_2Cl_2

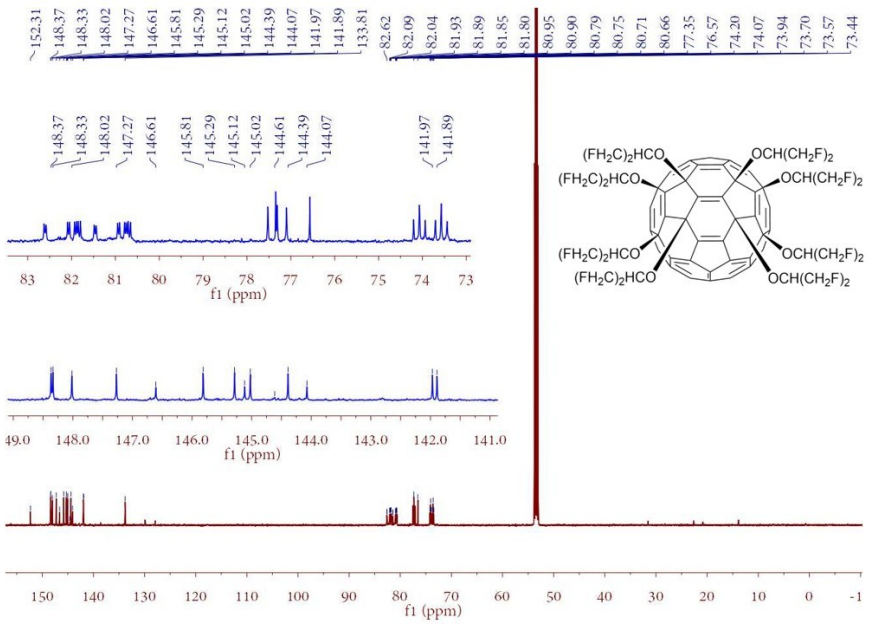


Figure S6. ^{13}C NMR spectrum of **3** in CD_2Cl_2

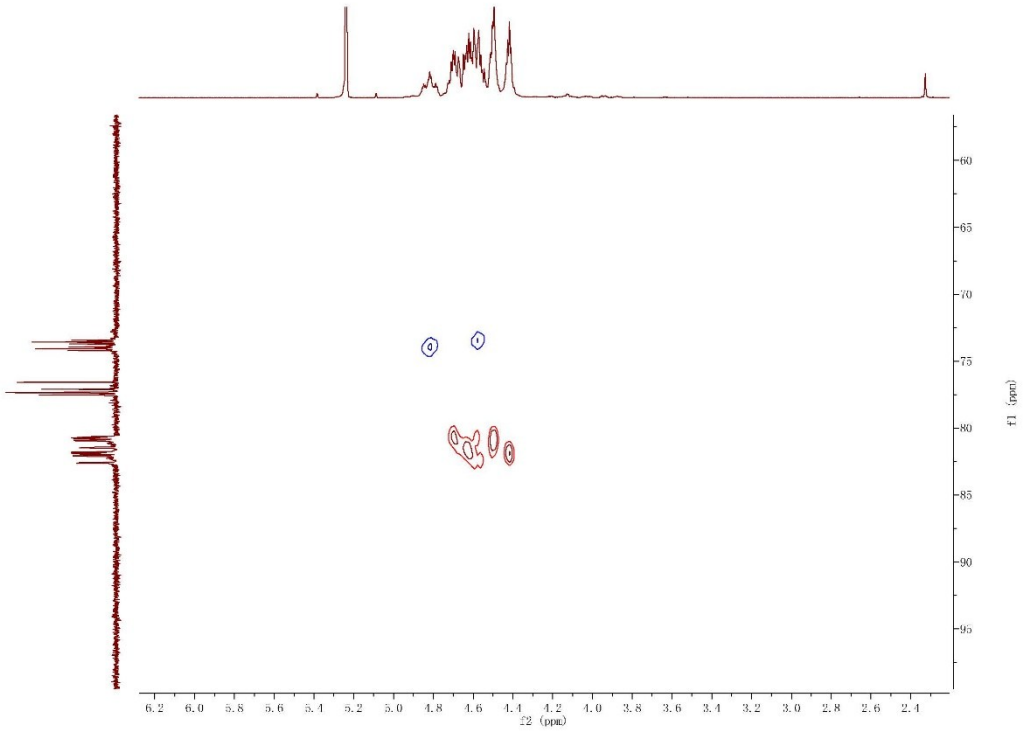


Figure S7. HSQC spectrum of **3** in CD_2Cl_2

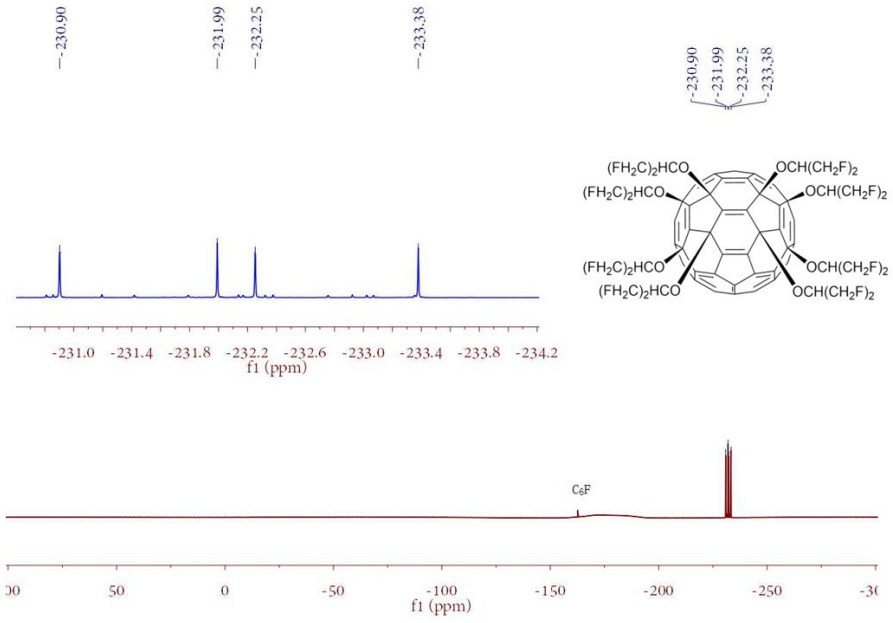


Figure S8. ^{19}F NMR spectrum of 3 in CD_2Cl_2

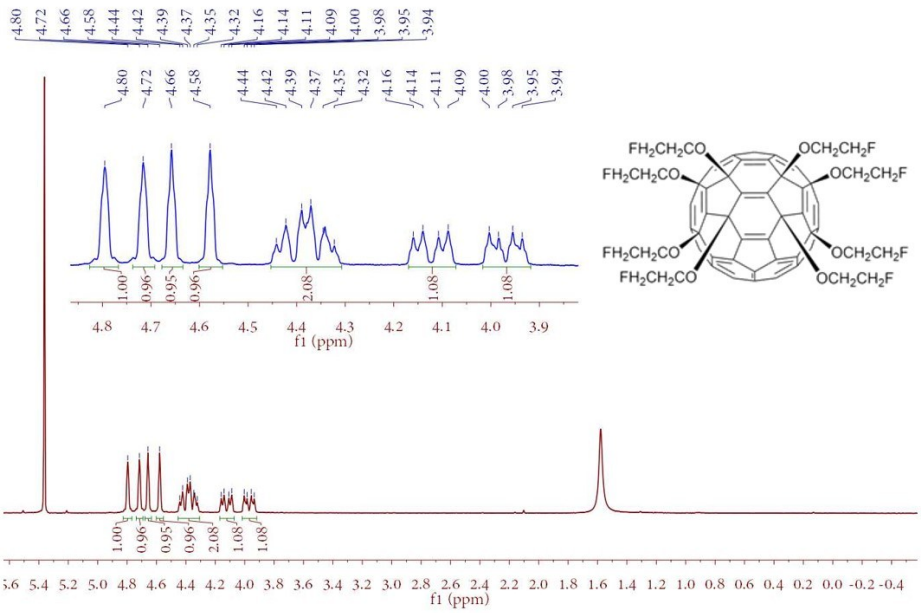


Figure S9. ^{1}H NMR spectrum of **4** in CD_2Cl_2

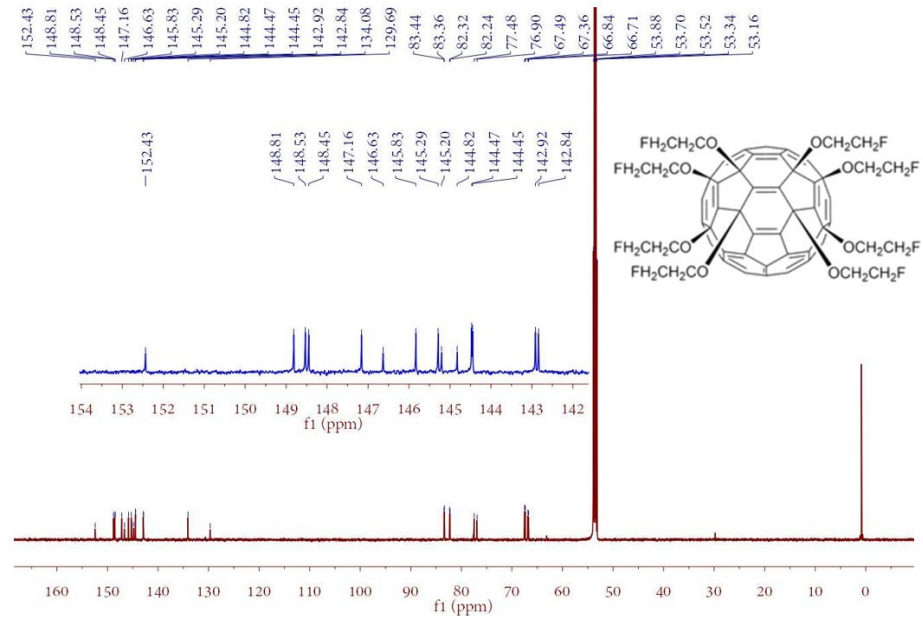


Figure S10. ^{13}C NMR spectrum of **4** in CD_2Cl_2

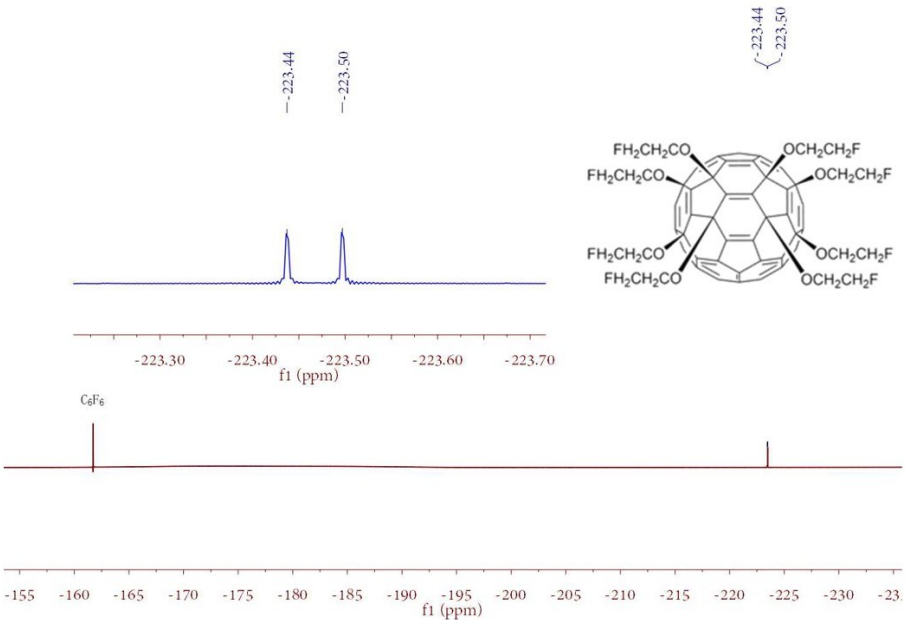


Figure S11. ^{19}F NMR spectrum of **4** in CD_2Cl_2

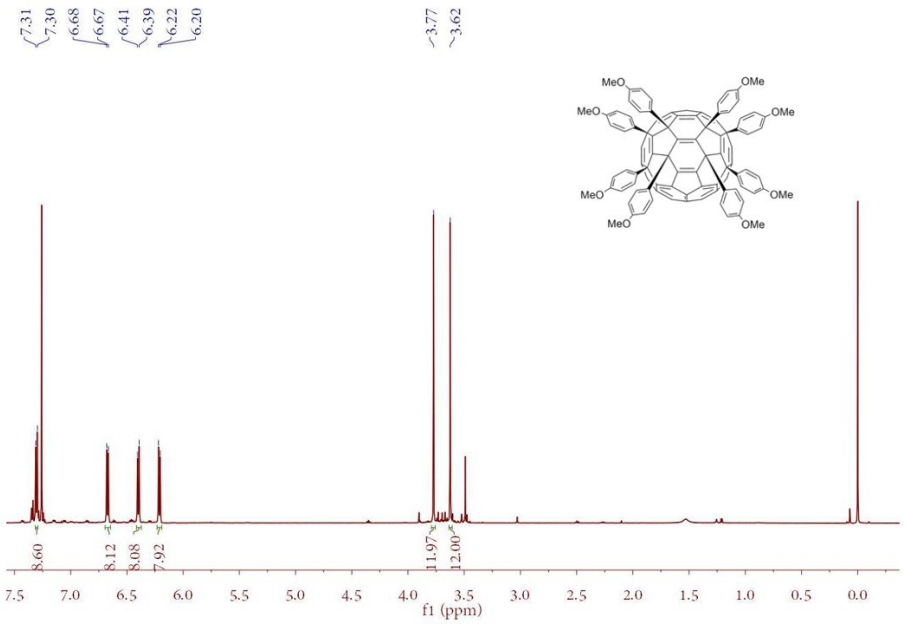


Figure S12. ^{1}H NMR spectrum of **5** in CD_2Cl_2

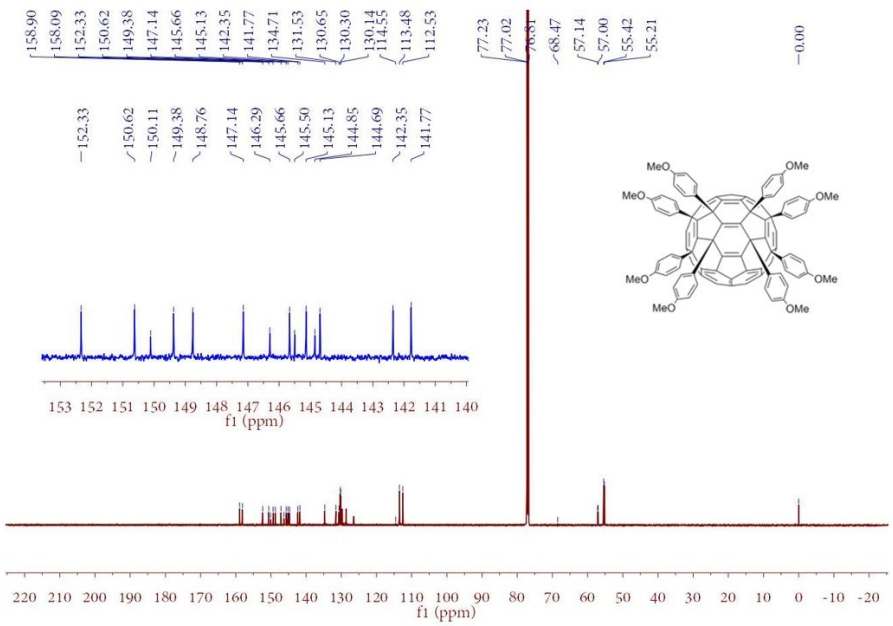


Figure S13. ^{13}C NMR spectrum of **5** in CD_2Cl_2

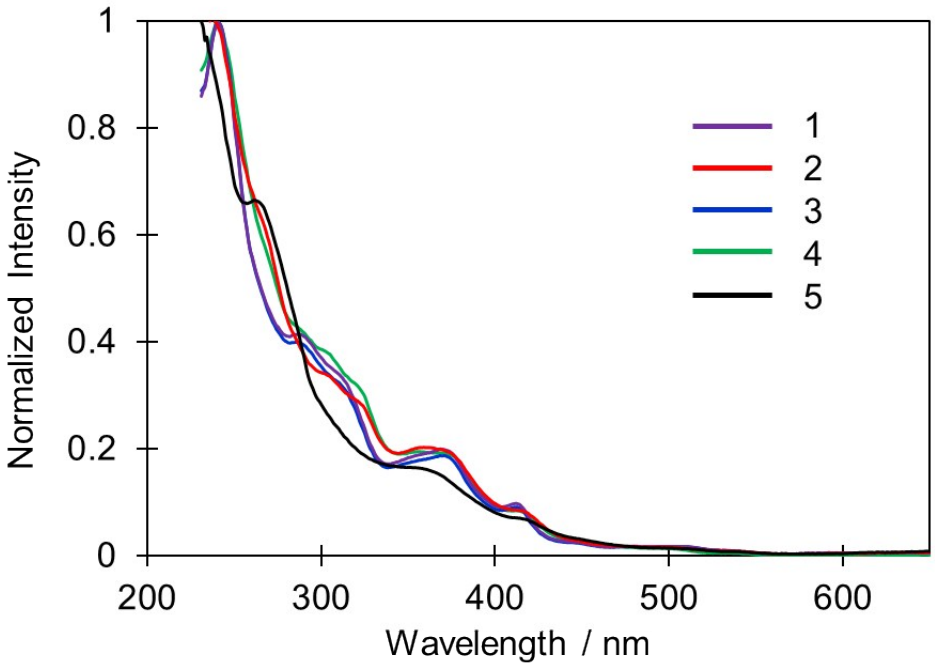
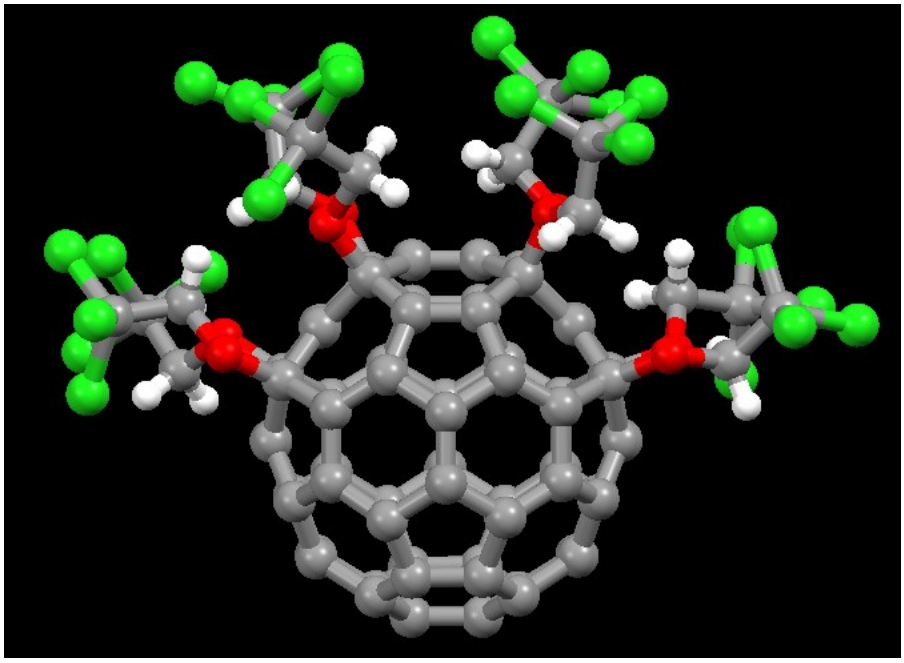


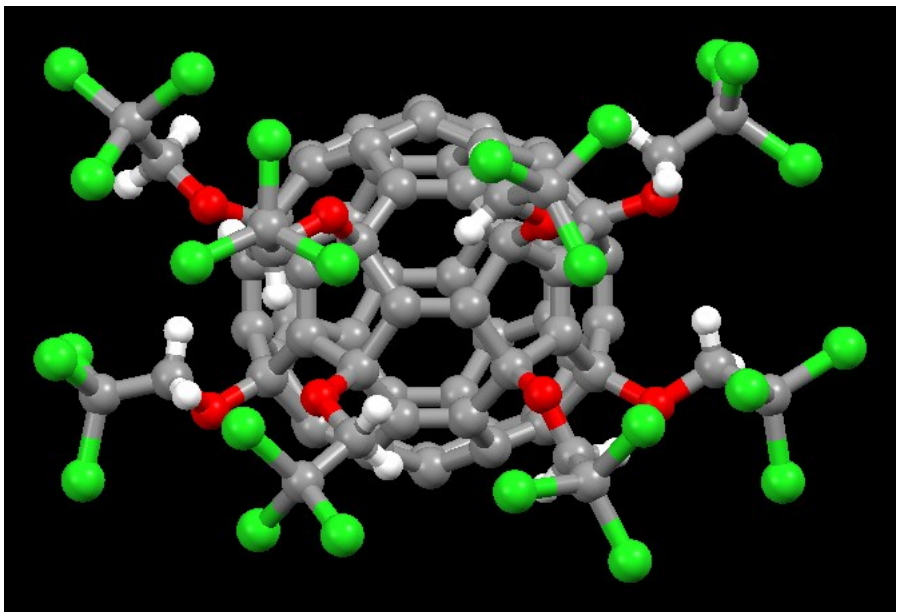
Figure S14. UV-vis absorption spectra of **1–5** measured in CH_2Cl_2.

X-ray structure analyses

Structural characterization of $C_{60}(OCH_2CCl_3)_8$ (**2**) and $C_{60}(OCH_2CH_2F)_8$ (**4**) were performed by means of single crystal X-ray diffraction measurements. The X-ray diffraction patterns were collected using the RIGAKU Saturn724+ at 93 K. The crystal structure analysis was performed by using *SHELX*. The results are summarized in Tables S1 and S2, and the CIF files (CCDC 1885323 and 1885661).

(a)





(b)

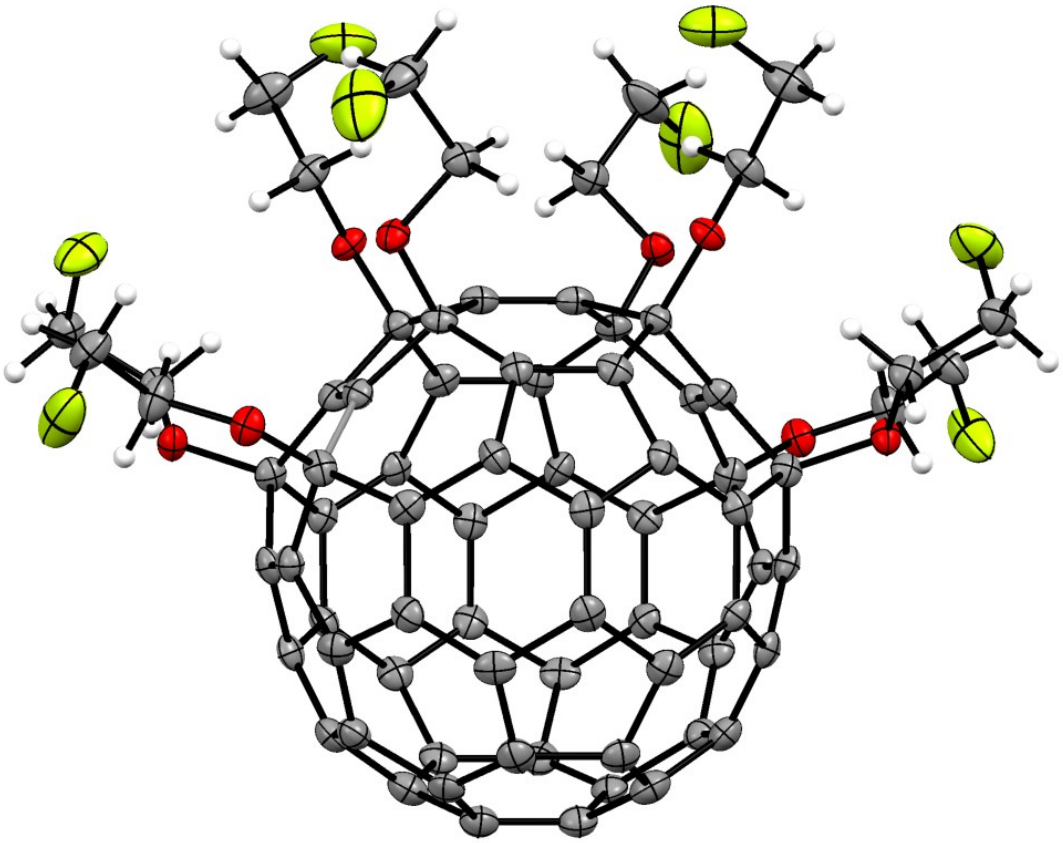


Figure S15. X-ray crystal structures. (a) Ball-and-stick model of $C_{60}(OCH_2Cl_3)_8$ (**2**). (b) ORTEP figure of $C_{60}(OCH_2CH_2F)_8$ (**4**). The thermal ellipsoids are shown at the 50% probability level.

Table S1. Crystallographic data for $C_{60}(OCH_2Cl_3)_8$ (**2**).

Compound	$C_{60}(OCH_2Cl_3)_8$
Formula	$C_{76}H_{16}Cl_{24}O_8$
M	1907.69
Crystal system	monoclinic
Space group	$P2_1/n$
a / Å	21.782
b / Å	13.957
c / Å	24.511
α / º	90
β / º	110.66
γ / º	90
Volume / Å^3	6972.5
Z	4
R	0.1397

Table S2. Crystallographic data for $C_{60}(OCH_2CH_2F)_8$ (**4**).

Compound	$C_{60}(OCH_2CH_2F)_8$
Formula	$C_{76}H_{32}F_8O_8$
M	1225.02
Crystal system	monoclinic
Space group	*C*2/*c*
a / Å	22.035(12)
b / Å	15.426(7)
c / Å	17.593(10)
α / º	90
β / º	121.518(7)
γ / º	90
Volume / Å^3	5098(5)
Z	4
R	0.0915

Particle size distribution

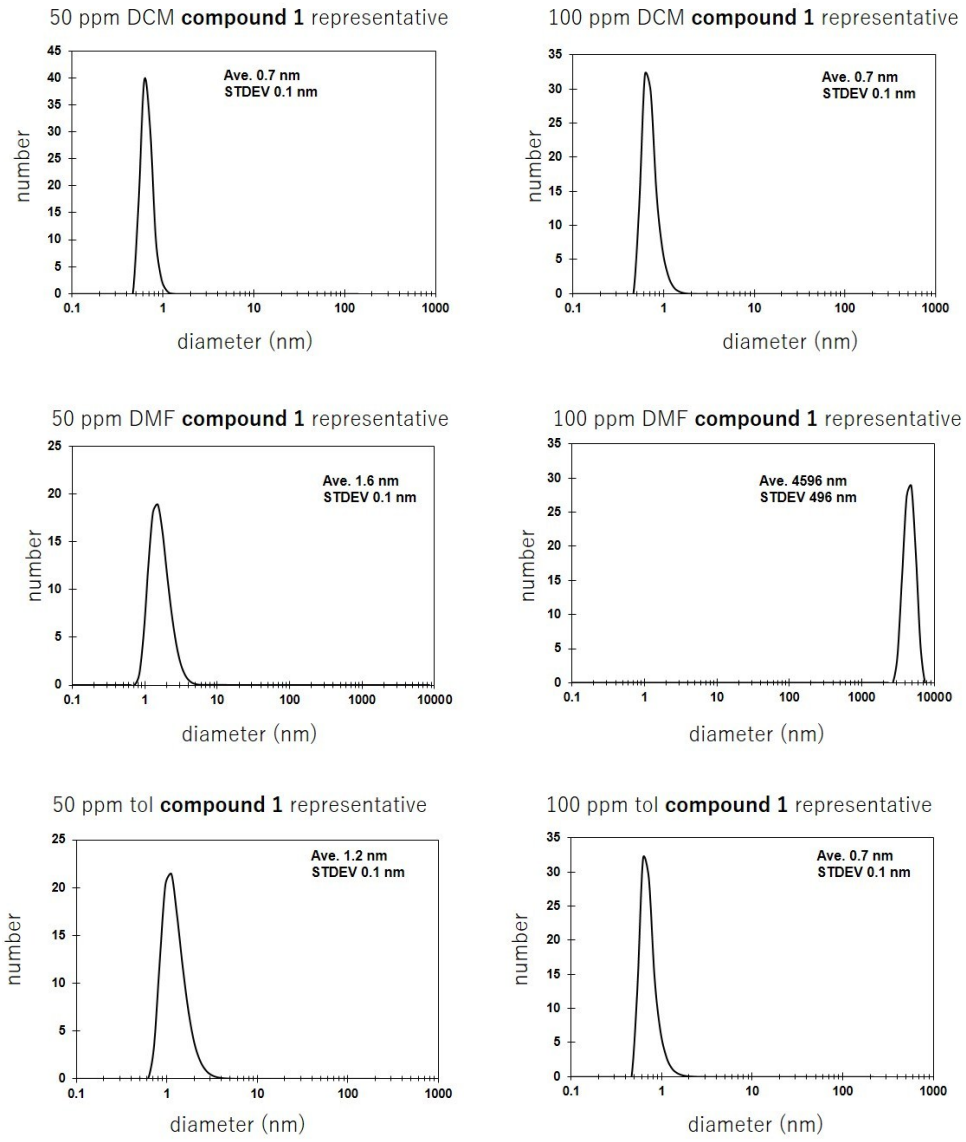


Figure S16. Particle size distribution of compound **1** in CH_2Cl_2, DMF, and toluene measured by DLS.

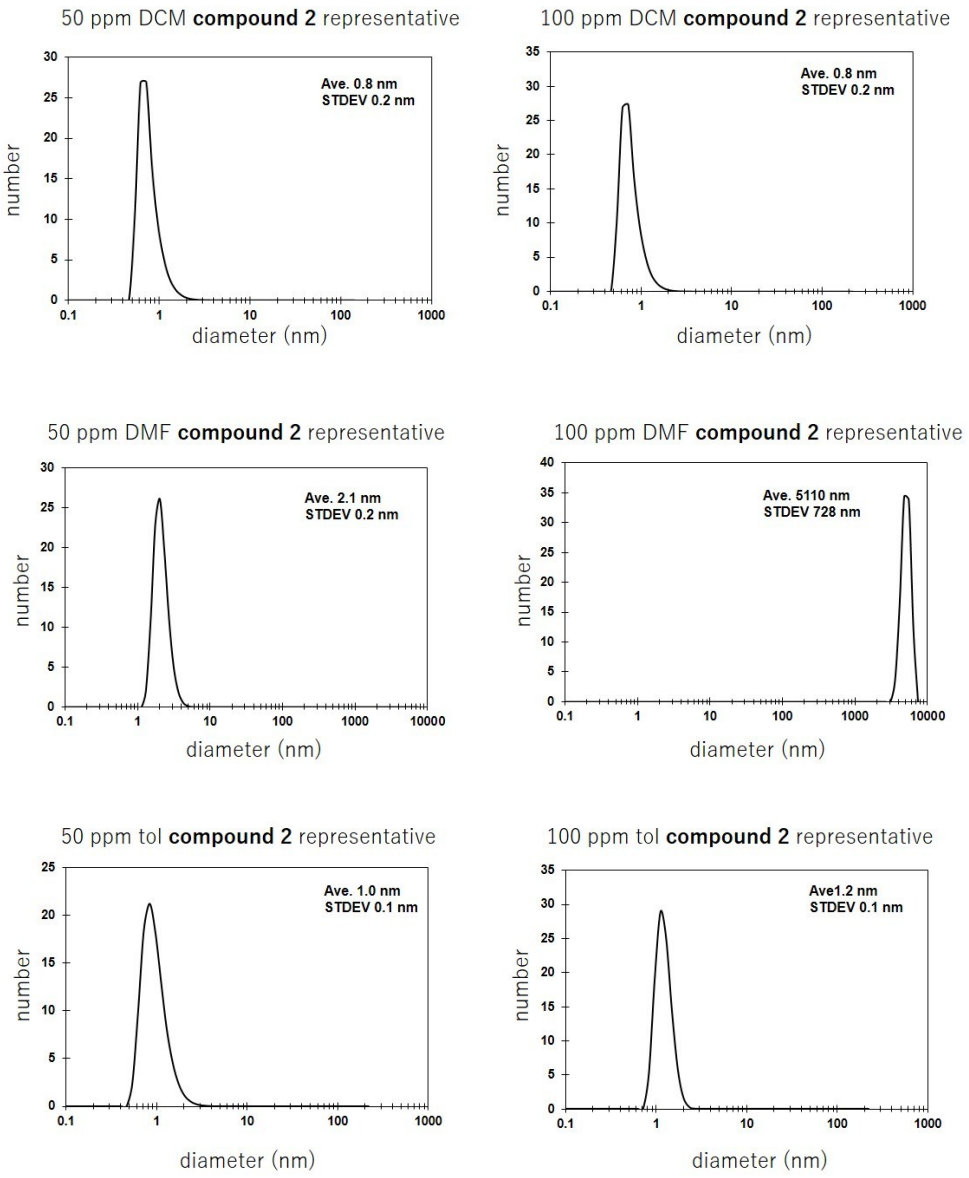


Figure S17. Particle size distribution of compound **2** in CH_2Cl_2, DMF, and toluene measured by DLS.

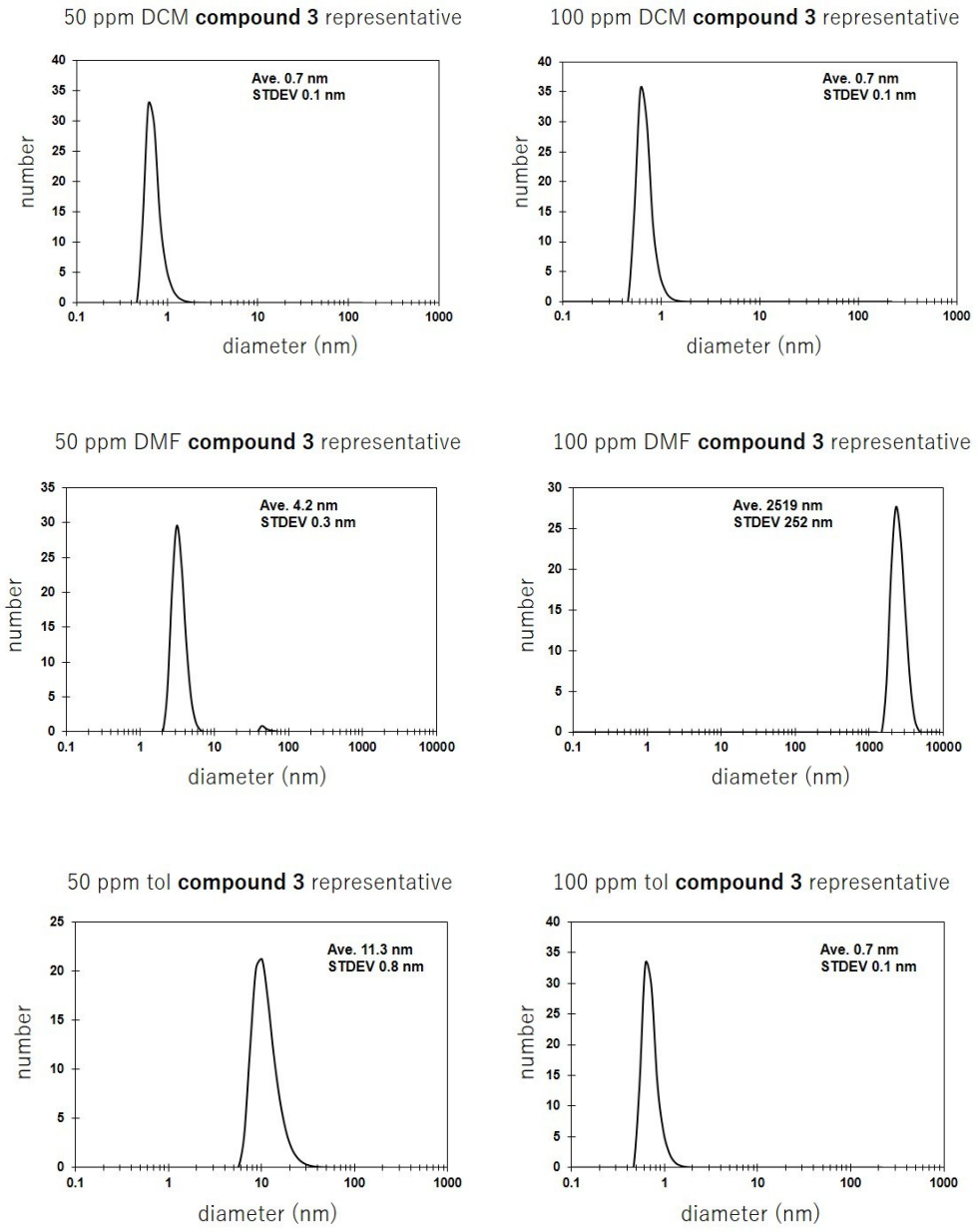


Figure S18. Particle size distribution of compound **3** in CH_2Cl_2, DMF, and toluene measured by DLS.

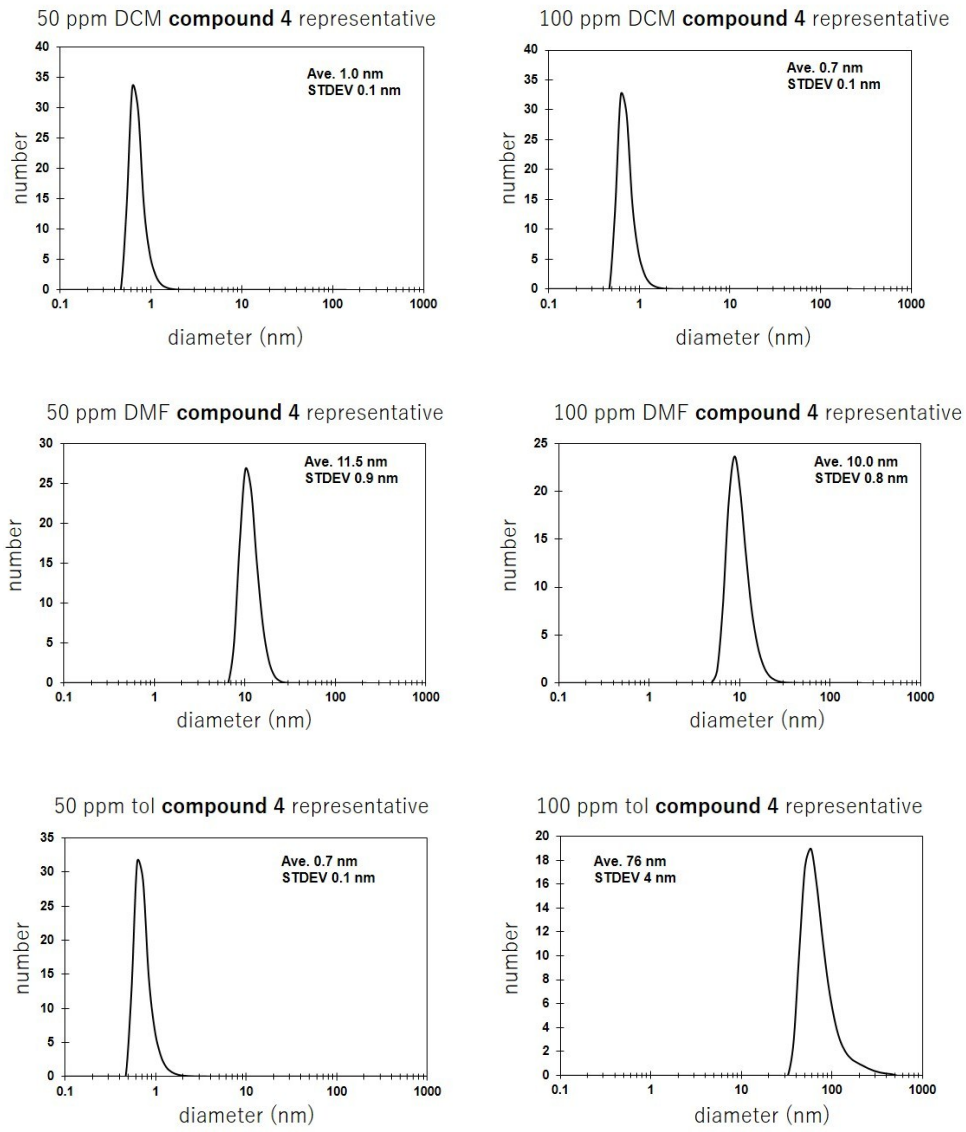


Figure S19. Particle size distribution of compound **4** in CH_2Cl_2, DMF, and toluene measured by DLS.

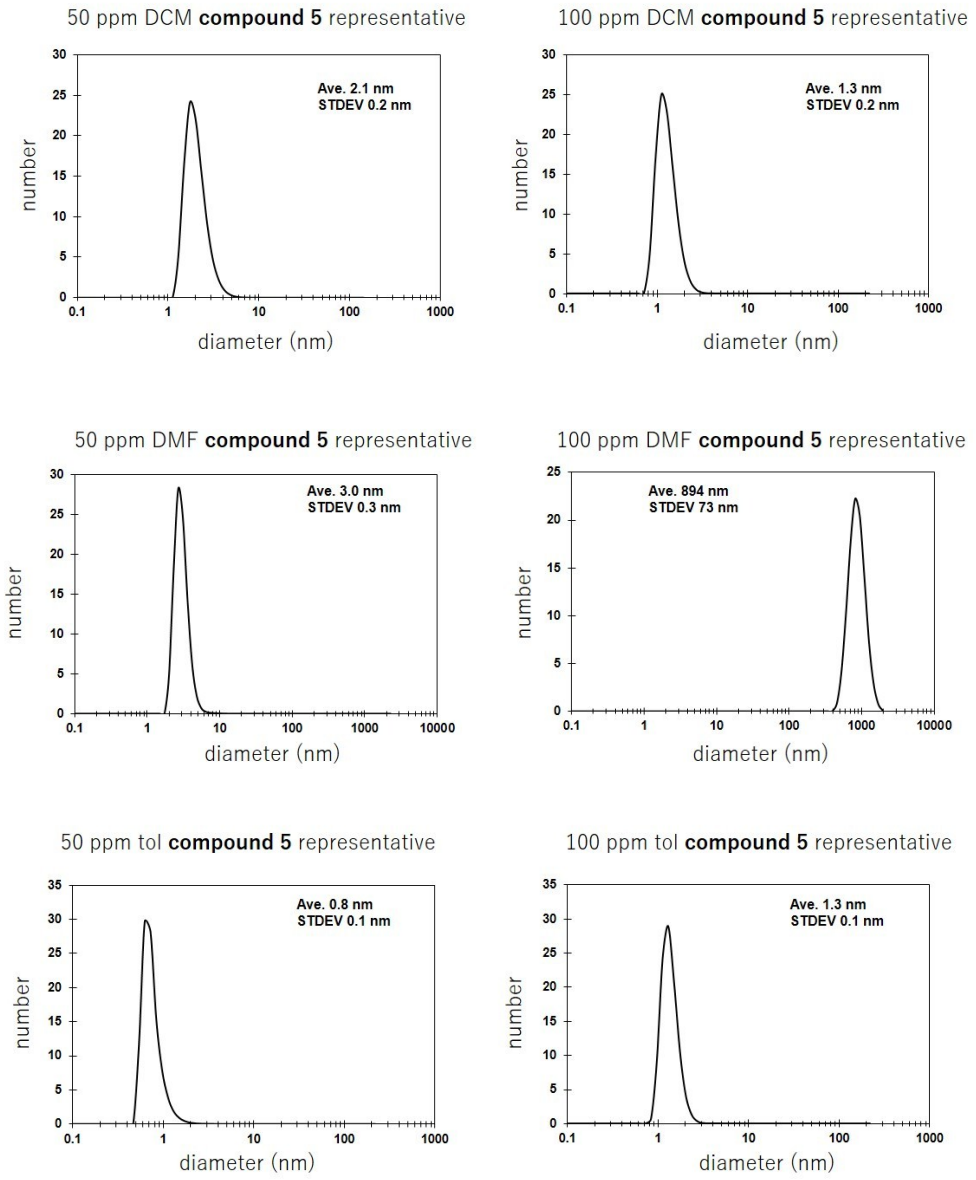


Figure S20. Particle size distribution of compound **5** in CH_2Cl_2, DMF, and toluene measured by DLS.

Details of theoretical calculation

All calculations were carried out using Gaussian09[1] package at the B3LYP/6-31G(d) level.

Table S3. HOMO and LUMO energy levels, total free energies, and number of imaginary frequencies, for optimized structures of compounds **1–5**.

Compounds	free energy[a] (a.u.)	HOMO (a.u.)	LUMO (a.u.)	HOMO (eV)	LUMO (eV)	number of imaginary frequencies
$C_{60}(OCH(CH_3)_2)_8$ (**1**)	-3835.05178	-0.2072	-0.1105	-5.637	-3.007	0
$C_{60}(OCH2CCl_3)_8$ (**2**)	-14551.13369	-0.2407	-0.1444	-6.550	-3.930	0
$C_{60}(OCH(CH_2F)_2)_8$ (**3**)	-5422.802187	-0.2180	-0.1214	-5.931	-3.304	0
$C_{60}(OCH_2CH_2F)_8$ (**4**)	-4314.634359	-0.2159	-0.1190	-5.874	-3.239	0
$C_{60}(4\text{-}MeOC_6H_4)_8$ (**5**)	-5054.271543	-0.1908	-0.0969	-5.193	-2.637	0

1 Hartree = 27.2114 eV, 1 eV = 96.49 kJ / mol

[a] in standard conditions

[1] Gaussian 09, Revision E.01, 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, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Table S4. Cartesian coordinates for optimized structures of compounds **1–5**.

$C_{60}(OCH(CH_3)_2)_8$ (**1**)

Symbol	X	Y	Z				
O	0.013396	-0.008611	0.003919	O	2.783520	-3.849818	6.685191
O	0.014076	0.002846	8.958234	C	-1.665449	-2.725020	7.964116
O	2.712021	-0.001243	6.464031	C	0.880013	-4.388621	3.806897
O	2.727526	-0.476954	2.065400	C	-4.739165	-3.265084	5.956275
C	-1.761260	-1.511087	0.972277	C	-2.452324	-4.743703	2.253575
C	0.890671	0.161822	5.053540	C	-2.394124	-4.636989	6.812441
C	-4.782190	-0.982248	3.056087	C	-3.159351	-5.172883	3.383767
C	-2.402540	0.498346	6.693491	C	-4.337820	-4.442180	3.828191
C	-2.462649	0.398751	2.138907	C	-1.028849	-5.547771	4.533098
C	-3.139968	0.928028	5.583968	C	1.637365	-3.336181	5.978883
C	-4.328362	0.195930	5.171847	C	-4.319294	-4.410250	5.276247
C	-1.041849	1.310652	4.378012	C	0.643839	-2.720340	6.989287
C	1.596591	-0.884593	2.859965	C	-5.205280	-2.109007	5.212019
C	-4.348233	0.164695	3.723944	C	-0.957680	-4.639750	6.796629
C	0.566932	-1.510643	1.893971	C	-0.320510	-5.105799	3.356774
C	-5.223874	-2.139845	3.812705	C	-1.011414	-4.753911	2.221964
C	-1.024656	0.409072	2.114216	C	-2.831633	-3.452079	7.520770
C	-0.302477	0.868421	5.533467	C	-3.129449	-5.120022	5.722002
C	-0.962553	0.511113	6.684604	C	1.615050	-3.404438	2.936290
C	-2.916760	-0.787271	1.443151	C	0.896358	-4.359852	5.162794
C	-3.172592	0.879034	3.246611	C	0.600599	-2.854835	1.900109
C	1.648356	-0.807299	5.929882	C	-3.989166	-2.785641	7.105280
C	0.891131	0.152929	3.694240	C	-3.991518	-1.343911	7.071083
C	0.657141	-1.375820	6.974376	C	3.416774	-5.078276	6.245803
C	-4.060340	-1.458992	1.888277	C	-2.424122	-5.586554	4.553440
C	-4.056580	-2.900860	1.922746	C	-2.908701	-3.586680	1.512793
C	3.341836	0.837287	2.063974	C	1.906199	-2.116178	3.753952
C	-2.437266	1.345105	4.395605	C	-0.483351	-3.713426	1.217726
C	-2.835435	-0.655366	7.452205	C	-0.392220	-3.568649	7.737130
C	1.936355	-2.091226	5.099383	C	0.457997	-3.475181	10.047822
C	-0.403045	-0.514437	7.683945	C	-0.294573	-5.054500	5.669681
C	-0.485203	-0.668584	1.166168	C	-4.777473	-3.328592	3.109341
C	0.339993	-0.828326	-1.147697	C	3.812006	-3.447589	1.719907
C	-0.331651	0.826552	3.222575	C	0.754465	-5.346146	-0.201325
C	-4.744279	-0.918975	5.903035	C	-1.668409	-1.358443	7.921896
C	3.862739	-0.453700	7.227605	C	1.774382	-4.032758	10.580920
C	0.675289	1.289633	9.053241	C	-0.677426	-3.591279	11.065121
C	-1.757922	-2.876212	1.019913	H	0.591464	-2.424135	9.765985
O	0.134425	-4.253010	8.870194	H	2.558254	-3.950570	9.823127
O	-0.135071	-4.211840	-0.076871	H	1.658407	-5.090648	10.843582
O	2.732510	-4.133529	2.403108	H	-0.839437	-4.641468	11.333010

H	-1.612518	-3.189402	10.664170	H	4.911423	0.328030	3.465309
H	2.090207	-3.488291	11.478153	H	3.533452	1.152579	4.221253
H	-0.433177	-3.034237	11.977355	H	1.815980	2.341767	2.548390
C	1.428710	1.262056	10.382377	H	1.720211	1.695988	0.895404
C	-0.328499	2.447288	9.047939	H	4.680821	2.069178	3.225789
H	1.382939	1.390138	8.220569	H	3.008346	2.835900	1.345519
H	2.159569	0.451478	10.419955	C	4.416990	-4.470037	0.761447
H	0.722830	1.123985	11.209077	C	4.863560	-2.951739	2.712787
H	-1.069253	2.302856	9.842507	H	3.404441	-2.597770	1.163236
H	-0.857007	2.542834	8.097694	H	3.693701	-4.799166	0.012918
H	1.956209	2.209720	10.536553	H	4.761784	-5.349554	1.31722
H	0.195262	3.392514	9.233389	H	5.268122	-3.794231	3.286189
C	4.922219	-1.096578	6.336244	H	4.450456	-2.220032	3.407408
C	3.548168	-1.301351	8.459264	H	5.277629	-4.035877	0.240317
H	4.250323	0.512202	7.573539	H	5.691130	-2.475832	2.173110
H	5.203214	-0.427271	5.519957	C	1.489270	-5.134197	-1.522984
H	4.561499	-2.038238	5.918764	C	-0.034405	-6.657376	-0.208924
H	3.333623	-2.335875	8.192289	H	1.468032	-5.337496	0.630955
H	2.698294	-0.896404	9.010909	H	2.046836	-4.192749	-1.515223
H	5.820120	-1.312288	6.928108	H	0.770384	-5.097829	-2.349337
H	4.422606	-1.292011	9.121985	H	-0.775729	-6.646423	-1.015866
C	2.832463	-6.273420	7.000951	H	-0.557031	-6.824349	0.736327
C	4.912269	-4.929669	6.514210	H	2.189485	-5.955055	-1.713716
H	3.257378	-5.196968	5.168186	H	0.642548	-7.504289	-0.372537
H	1.757669	-6.375252	6.834308	C	1.760143	-0.469112	-1.575090
H	2.994209	-6.153541	8.077701	C	-0.696008	-0.562991	-2.238133
H	5.094278	-4.722829	7.574876	H	0.306476	-1.885464	-0.864060
H	5.345914	-4.117558	5.924816	H	2.460559	-0.655433	-0.755542
H	3.318336	-7.201727	6.677389	H	1.821772	0.590729	-1.848647
H	5.432474	-5.858609	6.254553	H	-0.701287	0.499103	-2.508070
C	4.158689	1.109545	3.325372	H	-1.699630	-0.836368	-1.897475
C	2.403664	1.990579	1.696061	H	2.063608	-1.064619	-2.444178
H	4.042840	0.716107	1.229671	H	-0.468979	-1.148255	-3.136950

$C_{60}(OCH2CCl_3)_8$ (**2**)

Symbol	X	Y	Z				
Cl	1.429637	-0.222876	0.174009	Cl	-4.192949	5.197742	-1.190436
Cl	0.225162	-1.906899	11.483210	Cl	-8.505939	3.499637	3.263399
Cl	0.422415	-0.259093	13.911390	Cl	-6.786194	1.177811	2.710609
Cl	-6.448679	3.651647	1.168012	Cl	2.658212	-3.688327	7.647677
Cl	2.752455	-0.568844	12.144936	Cl	-2.883226	-3.544054	3.952859
Cl	6.969136	1.723450	8.286903	Cl	-0.257027	-3.719521	8.018627
Cl	5.383366	1.513214	3.945267	Cl	4.744555	-0.843761	2.306896
Cl	-3.981016	-1.592588	2.053189	Cl	-2.872316	7.292681	0.395827

Cl	0.873554	-3.187146	5.366263	C	-0.082986	0.573353	6.923766
Cl	5.332265	-1.155127	5.168015	C	0.415082	1.052906	5.541094
Cl	-4.788865	-1.505376	4.875665	C	-3.429062	-1.838883	3.743045
Cl	-1.216473	0.913679	-0.384460	C	-1.127367	6.212600	9.679564
Cl	-1.295947	5.594154	-1.406930	C	-1.062586	2.107900	9.322740
Cl	1.190321	2.151041	-1.539887	C	-3.250048	5.955035	8.455930
Cl	5.643008	2.869424	10.642099	C	0.679964	7.152059	8.514755
Cl	5.906160	-0.049268	10.367575	C	0.445631	1.804106	9.257053
O	0.175992	1.580353	2.247738	C	2.665000	5.440755	7.402043
O	-4.568617	3.097296	3.520026	C	2.213367	6.550868	6.678577
O	4.117361	2.572777	7.990665	C	1.852636	1.972231	7.166673
O	-1.285834	4.895239	1.500678	C	2.143979	5.168039	8.727324
O	-2.612235	0.415565	3.852845	C	-3.130244	6.814710	6.147244
O	0.889667	0.727616	10.097977	C	1.025298	3.193240	9.599202
O	-0.056628	-0.840733	7.151957	C	-5.884588	3.501296	3.841705
O	2.890228	0.603703	5.512356	C	-1.951188	1.389531	4.662690
C	-1.948607	1.653874	8.372259	C	-3.272863	5.046064	4.426322
C	-2.222243	5.596274	3.739524	C	2.024847	2.835430	4.849583
C	-4.095750	4.588538	6.576884	C	-2.511468	4.609604	0.846225
C	0.964244	-0.437351	12.198576	C	1.186870	-1.445524	7.466234
C	1.173531	6.014442	9.273304	C	-1.565175	6.768172	4.264050
C	-2.283782	2.771152	4.080454	C	-3.880353	3.321602	5.927992
C	-2.350022	1.360504	6.117964	C	0.102739	5.396979	3.367568
C	1.217442	4.659703	3.692380	C	-0.414216	1.420948	4.557442
C	-2.021323	7.392527	5.429540	C	-3.137597	2.411756	8.068508
C	-0.015240	2.377047	3.423665	C	-1.256976	3.302831	3.399816
C	2.083422	3.739439	8.919162	C	-3.883799	4.746040	7.950770
C	-2.357931	5.570604	9.529344	C	2.789554	3.028747	7.742152
C	0.666617	2.244452	1.097651	C	-2.444192	4.125883	9.682583
C	3.069318	0.063076	4.214289	C	-1.217607	4.754081	2.927539
C	-1.510262	1.008442	7.126410	C	0.495654	0.817949	11.453970
C	0.774112	7.170257	4.947147	C	-1.291456	3.380442	9.953808
C	-3.556037	3.529080	4.435860	C	-1.074772	7.909001	6.403972
C	2.911557	4.188014	6.749081	C	5.646111	1.497319	9.475317
C	1.851920	1.588369	5.679669	C	2.165876	5.172506	4.649817
C	-2.233336	-0.930677	4.063459	C	-1.606690	7.645198	7.728504
C	-0.140967	6.651138	4.023762	C	2.647512	4.045653	5.407673
C	-3.380208	2.265463	6.653177	C	1.954920	6.407909	5.267612
C	1.184595	3.195980	3.839015	C	-6.848101	2.962184	2.777820
C	0.515359	1.300343	-0.101291	C	1.099214	-2.940816	7.139277
C	-2.698745	5.634548	-0.285661	C	-0.014128	4.047750	10.116601
C	1.189081	7.417437	7.242404	C	-3.718854	5.644541	5.658025
C	-2.881106	6.969073	7.569973	C	-3.385762	3.626392	8.710985
C	0.822997	1.426856	7.832370	C	-0.744352	7.273244	8.765749

C	0.062385	5.438046	9.988729	H	2.011304	-1.027002	6.881417
C	0.296758	7.802065	6.168832	H	1.404562	-1.343668	8.535116
C	4.572714	-0.090824	3.934570	H	0.109149	3.162158	0.881305
C	4.286820	1.402102	8.765509	H	1.731817	2.488439	1.200020
H	0.945473	1.689417	11.945882	H	-1.407988	-1.207615	3.396942
H	-0.595036	0.873053	11.549800	H	-1.937588	-1.126146	5.100086
H	3.513391	1.287675	9.532950	H	-6.200924	3.096988	4.810646
H	4.298073	0.513098	8.124264	H	-5.983168	4.594407	3.859473
H	2.608904	-0.928876	4.147993	H	-2.488561	3.608777	0.400903
H	2.642827	0.705090	3.438415	H	-3.370814	4.678397	1.519109

$C_{60}(OCH(CH_2F)_2)_8$ (**3**)

Symbol	X	Y	Z				
O	-0.003249	0.002781	-0.000048	C	-0.535158	-0.679940	1.133532
O	0.001938	-0.003105	8.820702	C	0.457169	-0.765744	-1.119328
O	2.505582	0.000942	6.481362	C	-0.437175	0.825929	3.186937
O	2.567004	-0.397982	2.085933	C	-4.914021	-0.916127	5.758153
C	-1.807616	-1.521249	0.899009	C	3.617785	-0.416863	7.282350
C	0.723210	0.147382	5.050925	C	-0.588852	1.121637	9.483657
C	-4.879287	-0.984452	2.911987	C	-1.811067	-2.886871	0.956165
C	-2.593486	0.499328	6.608369	O	-0.138614	-4.261639	8.875936
C	-2.538916	0.391440	2.050367	O	-0.183454	-4.227346	-0.106569
C	-3.301506	0.928313	5.478297	O	2.616782	-4.139722	2.409303
C	-4.480061	0.197554	5.036708	O	2.609806	-3.830029	6.720145
C	-1.173341	1.315777	4.325724	C	-1.897172	-2.723897	7.903468
C	1.482546	-0.904296	2.881241	C	0.747584	-4.402947	3.815099
C	-4.462937	0.163701	3.588767	C	-4.916363	-3.261709	5.816463
C	0.490986	-1.528664	1.885965	C	-2.538049	-4.752535	2.176001
C	-5.343373	-2.139782	3.658881	C	-2.598086	-4.638229	6.735865
C	-1.101433	0.399037	2.065892	C	-3.274014	-5.177098	3.289560
C	-0.467008	0.873212	5.502337	C	-4.461752	-4.443077	3.701798
C	-1.154892	0.517013	6.638896	C	-1.175889	-5.553286	4.494004
C	-2.974360	-0.794961	1.343508	C	1.455895	-3.350211	5.994874
C	-3.274769	0.874328	3.140335	C	-4.481250	-4.408646	5.149686
C	1.456980	-0.820529	5.938249	C	0.441370	-2.738488	6.986236
C	0.752973	0.127882	3.695834	C	-5.360426	-2.106306	5.058007
C	0.444018	-1.395664	6.951775	C	-1.160930	-4.648675	6.759423
C	-4.128770	-1.464453	1.763751	C	-0.440069	-5.116675	3.335599
C	-4.129978	-2.906381	1.801336	C	-1.099051	-4.764906	2.182738
C	3.555090	0.469161	2.671419	C	-3.050386	-3.450604	7.430243
C	-2.569023	1.343544	4.308062	C	-3.305364	-5.121073	5.627728
C	-3.046629	-0.654375	7.357242	C	1.498312	-3.422046	2.959137
C	1.774566	-2.105789	5.122332	C	0.739589	-4.379356	5.171156
C	-0.617987	-0.530850	7.630902	C	0.517651	-2.872087	1.897761

C	-4.194446	-2.781795	6.982940	H	3.215103	-5.314326	5.367423
C	-4.191969	-1.340407	6.945816	F	1.652460	-6.994769	6.159674
C	3.161484	-5.129327	6.445909	H	1.674834	-5.858882	7.844407
C	-2.570878	-5.590840	4.478826	H	4.560649	-4.878435	8.077046
C	-2.974136	-3.595216	1.422462	F	5.361957	-4.163474	6.362662
C	1.787742	-2.134394	3.776713	H	3.040157	-6.980257	7.610465
C	-0.546030	-3.730421	1.188194	H	5.040435	-6.092769	6.849918
C	-0.624408	-3.569836	7.706696	C	3.136689	1.938683	2.703329
C	0.309441	-3.514777	10.009759	C	4.784469	0.338874	1.781092
C	-0.468730	-5.062585	5.649562	H	3.798910	0.146511	3.690481
C	-4.881838	-3.330539	2.969506	H	2.135777	2.069116	3.117375
C	3.849188	-3.447601	2.163578	F	3.154446	2.473877	1.419789
C	0.802892	-5.263384	-0.267397	H	4.485327	0.443123	0.735425
C	-1.896521	-1.357369	7.863802	F	5.390879	-0.910739	1.948293
C	1.538924	-4.234970	10.555266	H	3.850184	2.499009	3.321861
C	-0.761076	-3.455454	11.099758	H	5.526054	1.102376	2.037681
H	0.580541	-2.491136	9.726038	C	4.442132	-4.012985	0.889273
F	2.546562	-4.263379	9.596661	C	4.806922	-3.624264	3.334096
H	1.291173	-5.271017	10.814312	H	3.677234	-2.381325	2.013166
H	-1.275598	-4.420222	11.167453	F	3.610578	-3.699692	-0.191654
F	-1.700942	-2.472353	10.819784	H	4.535204	-5.101224	0.948527
H	1.928226	-3.720380	11.440738	F	5.011543	-4.987179	3.569160
H	-0.310016	-3.216544	12.071744	H	4.399676	-3.178372	4.240115
C	0.591290	2.002476	9.895780	H	5.421293	-3.561747	0.700167
C	-1.428813	0.708514	10.681404	H	5.772755	-3.156244	3.118715
H	-1.222619	1.690677	8.794246	C	1.507705	-4.998426	-1.593982
H	1.162084	2.290527	9.007593	C	0.156286	-6.644258	-0.325242
H	1.252978	1.469537	10.589828	H	1.542804	-5.217895	0.538806
H	-0.908946	-0.054201	11.269587	H	1.763422	-3.942803	-1.688214
F	-2.641979	0.178777	10.257452	F	0.672526	-5.349926	-2.654214
F	0.114076	3.146076	10.526224	H	-0.694318	-6.624119	-1.010825
H	-1.631894	1.587441	11.302281	F	-0.291409	-7.052160	0.927648
C	4.642441	-1.239386	6.527765	H	2.422306	-5.597150	-1.664096
C	3.246593	-1.070187	8.616748	H	0.886546	-7.383358	-0.676604
H	4.082140	0.543679	7.534428	C	1.973836	-0.896415	-1.137117
F	5.103912	-0.525269	5.415951	C	-0.059940	-0.007766	-2.341008
H	4.231132	-2.185932	6.187793	H	0.028843	-1.776531	-1.114018
H	3.003267	-2.129881	8.524367	H	2.340197	-1.436708	-0.264634
H	2.408882	-0.531537	9.067904	F	2.563976	0.366641	-1.149292
H	5.494602	-1.441132	7.184186	H	0.343971	1.009116	-2.344897
F	4.364178	-0.959657	9.452905	H	-1.154031	0.029755	-2.331056
C	2.368671	-6.270957	7.109079	H	2.272573	-1.425667	-2.049288
C	4.576933	-5.112699	7.006762	F	0.359550	-0.665544	-3.493597

$C_{60}(OCH_2CH_2F)_8$ (**4**)

Symbol	X	Y	Z				
F	0.008718	0.040696	-0.009880	C	1.104110	0.610269	-0.664555
F	-0.016727	-0.022894	5.602315	H	0.943847	1.693147	-0.728222
F	9.354740	0.001820	9.500545	H	1.148333	0.186954	-1.673694
F	4.345576	2.821820	7.716761	C	8.009598	-0.289565	9.686628
O	7.553726	-0.796460	7.412770	H	7.428836	0.626885	9.531756
O	2.614699	-1.089271	-0.021676	H	7.867012	-0.641607	10.716507
O	1.907111	0.149081	3.381405	C	7.549140	-3.959138	0.458766
O	4.264964	0.037791	7.013621	C	0.494734	-0.087532	3.270960
C	7.824131	-2.959542	6.157964	H	0.260962	-1.152899	3.318662
C	4.186001	-0.385741	3.559170	H	0.153735	0.295790	2.302819
C	9.127620	-3.934214	2.827833	C	2.374894	0.311115	0.096540
C	5.870839	-1.654663	0.522064	H	3.205222	0.883972	-0.344202
C	8.396269	-1.616502	4.320700	H	2.266264	0.615205	1.143899
C	7.192624	-1.572152	0.977291	C	-0.225323	0.634768	4.384846
C	8.044781	-2.752350	0.956890	H	0.139508	1.662610	4.488909
C	6.426980	-0.225736	2.879712	H	-1.304648	0.650631	4.188425
C	4.487995	-0.955890	6.004836	C	3.213934	2.023527	7.805054
C	8.847535	-2.739305	2.162185	H	2.325521	2.658295	7.691674
C	5.567750	-1.929904	6.504912	H	3.194372	1.560676	8.799372
C	8.622653	-5.191760	2.307101	C	7.306109	-4.177407	6.500704
C	7.336900	-0.947788	5.028315	F	5.156155	-3.324861	10.910015
C	5.073303	-0.317832	2.388481	F	0.769148	-1.184090	8.073672
C	4.802708	-0.980431	1.212169	F	-1.612772	-5.212004	0.285671
C	8.691132	-2.855618	5.010903	F	-2.248302	-3.834844	4.390427
C	8.488153	-1.552231	2.924453	O	1.031580	-4.771822	1.284240
C	2.801331	-0.970367	3.481145	O	6.159854	-4.564914	8.559167
C	4.937942	-0.373338	4.689302	O	2.749044	-3.276160	7.860751
C	2.768239	-1.954746	2.295969	O	0.435406	-3.169255	4.160830
C	9.058747	-3.989517	4.278115	C	3.442637	-4.240616	0.716526
C	8.516845	-5.273042	4.650975	C	3.220924	-4.435768	5.874362
C	3.215262	0.968990	6.723799	C	6.665670	-6.045924	1.068452
H	2.241645	0.461899	6.704009	C	6.464123	-6.198817	5.657589
H	3.379733	1.441833	5.747847	C	3.935946	-6.231391	1.862774
C	7.473086	-0.839390	2.188024	C	6.213068	-6.939410	4.495865
C	5.357283	-2.909350	0.008677	C	7.116150	-6.838813	3.357792
C	2.577380	-1.953374	4.657207	C	3.837618	-6.353857	4.668649
C	3.464960	-1.696858	0.956281	C	1.864923	-3.214401	4.122071
C	7.062428	-1.634236	6.373965	C	6.312514	-6.851132	2.153156
C	7.559409	-1.362538	8.723049	C	2.286036	-3.157066	2.647736
H	8.245132	-2.219378	8.771087	C	7.845883	-5.203983	1.143060
H	6.561369	-1.715872	9.016393	C	2.863703	-5.585559	2.567588
C	6.358516	-0.294024	4.319483	C	4.118199	-5.600677	5.867550

C	5.395706	-5.556654	6.378942	C	5.318958	-4.706178	10.763026
C	4.300272	-5.400941	0.732262	H	4.600719	-5.209504	11.421095
C	4.916557	-6.957754	2.550342	H	6.338558	-4.956886	11.074466
C	3.532536	-3.190358	6.660701	C	-1.159571	-3.987514	0.764132
C	2.464228	-4.449325	4.746451	H	-1.348099	-3.940369	1.842579
C	5.059506	-3.119767	6.867121	H	-1.716926	-3.188682	0.256419
C	5.640714	-5.317971	0.339098	C	8.246286	-6.022477	3.436075
C	6.184474	-4.035635	-0.034762	C	2.802139	-2.196465	8.805553
C	-0.161529	-3.354225	5.446545	H	3.339095	-1.335528	8.400592
H	0.293923	-2.696923	6.197654	H	3.330490	-2.532838	9.705677
H	-0.042536	-4.396892	5.768253	C	5.085640	-5.105707	9.324327
C	4.864119	-7.015042	3.990735	H	5.073395	-6.204123	9.250392
C	7.636023	-5.349690	5.733868	H	4.115288	-4.728369	8.982380
C	3.321488	-1.941108	5.771885	C	1.389099	-1.801771	9.163857
C	5.932619	-4.345501	7.163828	H	0.793546	-2.680087	9.436874
C	2.315895	-4.399758	1.762896	H	1.393675	-1.092785	10.001368
C	0.318179	-3.826922	0.480500	C	-1.626777	-3.009028	5.322209
H	0.523474	-4.016697	-0.581769	H	-2.119814	-3.143482	6.293176
H	0.610760	-2.793818	0.701772	H	-1.749139	-1.969045	5.003932
C	2.829408	-5.624128	3.940298	C	3.968447	-3.024802	0.372179

$C_{60}(4\text{-}MeOC_6H_4)_8$ (**5**)

Symbol	X	Y	Z				
C	-0.001932	-0.001254	-0.001983	C	1.667520	-0.765531	6.104210
C	0.001908	0.002445	9.184129	C	0.834290	0.152455	3.886800
C	2.873865	0.004254	6.687897	C	0.719822	-1.438937	7.148424
C	2.870819	-0.075995	2.390132	C	-3.915175	-1.862692	1.998269
C	-1.608527	-1.685071	1.107307	C	-3.777703	-3.296828	2.009012
C	0.833155	0.158404	5.245895	C	-2.584822	1.039857	4.568432
C	-4.690011	-1.473398	3.163662	C	-2.822539	-1.046838	7.584179
C	-2.490328	0.154580	6.850097	C	2.031053	-2.003979	5.256805
C	-2.499707	0.129090	2.296339	C	-0.410742	-0.679881	7.859992
C	-3.256117	0.537184	5.740618	C	-0.423917	-0.719419	1.299246
C	-4.367387	-0.294597	5.303878	C	-0.427734	0.732894	3.410013
C	-1.192806	1.132077	4.566140	C	-4.686206	-1.455360	6.011540
C	1.659146	-0.787069	3.037816	C	-1.479097	-3.046651	1.120820
C	-4.370383	-0.302713	3.854890	C	0.425305	-4.355800	9.180677
C	0.710283	-1.477423	2.020884	C	0.401791	-4.368866	-0.005445
C	-5.030553	-2.680091	3.896716	C	3.229151	-3.831566	2.481716
C	-1.068126	0.270730	2.287142	C	3.223939	-3.752884	6.777958
C	-0.425070	0.743468	5.723471	C	-1.473804	-3.007907	8.075533
C	-1.058576	0.299008	6.859174	C	1.257492	-4.363324	3.929294
C	-2.831004	-1.082642	1.580374	C	-4.467102	-3.792820	6.027962
C	-3.261728	0.524504	3.403396	C	-2.012440	-4.981582	2.334592

C	-2.013116	-4.957358	6.888836	H	1.522166	2.867530	-1.039501
C	-2.689929	-5.500364	3.446255	O	1.072963	1.904388	-3.572627
C	-3.935719	-4.890946	3.886524	C	4.450419	-3.198369	2.720167
C	-0.548494	-5.698633	4.614816	C	3.252761	-5.030432	1.745581
C	1.898786	-3.279711	6.134776	C	4.439373	-5.554975	1.253237
C	-3.935959	-4.883096	5.335459	C	5.656403	-3.714365	2.233669
C	0.840369	-2.778542	7.154325	C	5.655321	-4.898434	1.492538
C	-5.029407	-2.671330	5.296076	H	2.330868	-5.568657	1.553052
C	-0.580101	-4.829052	6.894277	H	4.448883	-6.477836	0.681739
C	0.129452	-5.173357	3.455460	H	4.477325	-2.281419	3.297732
C	-0.579036	-4.855553	2.321605	H	6.578157	-3.184558	2.445354
C	-2.563127	-3.828567	7.605719	O	6.768011	-5.495160	0.969307
C	-2.691017	-5.488443	5.783738	C	3.403061	-0.490466	1.167013
C	1.902121	-3.300057	3.068772	C	3.495372	1.004330	3.036786
C	1.261563	-4.357153	5.288293	C	4.600240	1.638801	2.482597
C	0.842381	-2.816006	2.027240	C	4.511598	0.137155	0.593463
C	-3.775294	-3.265073	7.191141	C	5.117317	1.211226	1.252256
C	-3.908732	-1.830607	7.180260	H	3.111575	1.358184	3.987609
C	-1.933145	-5.868333	4.616510	H	5.076797	2.473480	2.987484
C	-2.565225	-3.863636	1.601700	H	2.955958	-1.325934	0.641028
C	2.030052	-2.015286	3.915186	H	4.883505	-0.219675	-0.360158
C	-0.128118	-3.773784	1.319005	O	6.201041	1.902548	0.786057
C	-0.129692	-3.734501	7.879760	C	3.674239	-3.247154	7.999507
C	0.131698	-5.162936	5.768820	C	4.036272	-4.698175	6.128310
C	-4.468018	-3.810588	3.179870	C	5.241629	-5.116515	6.678216
C	-1.601561	-1.646178	8.061396	C	4.882072	-3.658089	8.568886
C	0.013933	-5.643803	-0.428119	C	5.674449	-4.600811	7.907234
C	1.241278	-3.630096	-0.853531	H	3.721920	-5.116930	5.178377
C	1.674810	-4.143451	-2.068479	H	5.863371	-5.847694	6.170762
C	0.443594	-6.177608	-1.646489	H	3.081014	-2.509534	8.527252
C	1.280364	-5.425150	-2.476705	H	5.184844	-3.238561	9.521461
H	1.559521	-2.635444	-0.563261	O	6.869317	-5.079260	8.369335
H	2.326365	-3.567617	-2.718250	C	4.191123	-0.386552	6.439983
H	-0.634309	-6.248652	0.198249	C	2.675546	1.183108	7.430056
H	0.119992	-7.172753	-1.929636	C	3.745064	1.919198	7.920131
O	1.762872	-5.841935	-3.683476	C	5.281248	0.344835	6.923838
C	0.642752	1.238631	0.041368	C	5.061428	1.503762	7.672034
C	-0.274562	-0.552178	-1.263735	H	1.670083	1.538308	7.628714
C	0.097173	0.101767	-2.432504	H	3.583548	2.825688	8.495134
C	1.022770	1.909125	-1.122832	H	4.386844	-1.278648	5.856060
C	0.750840	1.339521	-2.371555	H	6.285015	-0.000846	6.704474
H	-0.790651	-1.503684	-1.337484	O	6.045248	2.295797	8.195001
H	-0.118138	-0.327035	-3.406297	C	0.983810	-0.545553	10.011792
H	0.858736	1.703268	0.997799	C	-0.642221	1.171389	9.624058

C	-0.311411	1.767020	10.834376	C	1.713404	3.169696	-3.566724
C	1.326693	0.038227	11.233991	H	1.737016	-7.919164	-3.461056
C	0.678806	1.204798	11.652034	H	0.304836	-7.217560	-4.272364
H	-1.411593	1.630451	9.011225	H	1.880023	-7.255397	-5.112426
H	-0.808468	2.673005	11.167025	H	1.089071	3.936942	-3.089936
H	1.498203	-1.450504	9.709550	H	2.684683	3.129769	-3.055487
H	2.098465	-0.422951	11.839484	H	1.868716	3.431919	-4.614998
O	0.934542	1.865039	12.818807	H	7.122126	0.477817	-0.433774
C	1.281086	-5.460544	9.138750	H	6.028466	1.613702	-1.275978
C	0.071951	-3.850347	10.441433	H	7.594934	2.187683	-0.638509
C	0.567035	-4.416448	11.610343	H	8.066120	-3.871112	0.765451
C	1.787412	-6.041277	10.303237	H	8.257255	-4.819956	2.269299
C	1.431204	-5.517670	11.550769	H	8.763462	-5.513908	0.703534
H	-0.605168	-3.005742	10.514175	H	7.635154	0.951093	8.366565
H	0.287041	-4.025298	12.583612	H	7.618799	1.930775	6.870668
H	1.566747	-5.887608	8.183044	H	8.003121	2.697125	8.437351
H	2.449344	-6.895654	10.220946	H	7.514346	-3.508249	9.586391
O	1.862521	-6.003895	12.752402	H	6.653830	-4.827545	10.432027
C	1.933248	1.341260	13.679345	H	8.297257	-5.100508	9.788389
C	7.393496	1.936546	7.945542	H	1.679593	0.330187	14.024792
C	7.346478	-4.593475	9.612248	H	2.916173	1.318304	13.190261
C	2.713283	-7.138594	12.748161	H	1.972990	2.015344	14.537006
C	6.755569	1.512932	-0.458932	H	2.226932	-8.007033	12.284509
C	8.024461	-4.880104	1.197634	H	3.657395	-6.935272	12.224986
C	1.392038	-7.131338	-4.143925	H	2.922877	-7.360173	13.796387