Supporting Information for

Synthesis, Structure, and ^{19}F NMR Spectra of 1,3,7,10,14,17,23,28,31,40-$C_{60}(CF_3)_{10}$

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Table S-1. Crystal data and structure refinement for **$C_{60}(CF_3)_{10}$-3**

Empirical formula	$C_{70}F_{30}$	
Formula weight	1410.70	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 12.1433(7) Å	α = 82.2470(10)°
	b = 12.3153(7) Å	β = 86.6060(10)°
	c = 15.6682(9) Å	γ = 81.9760(10)°
Volume	2297.1(2) $Å^3$	
Z	2	
Density (calculated)	2.040 Mg m^{-3}	
Absorption coefficient	0.205 mm^{-1}	
F(000)	1380	
Crystal size	0.38 × 0.20 × 0.08 mm	
Theta range for data collection	1.68 to 28.28°	
Index ranges	$-15 \le h \le 16$, $-16 \le k \le 16$, $-20 \le l \le 19$	
Reflections collected	19398	
Independent reflections	10742 [R_{int} = 0.0434]	
Completeness to theta = 28.28°	94.2%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9838 and 0.9263	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	10742/0/902	
Goodness-of-fit on F^2	1.037	
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0529, wR_2 = 0.1292	
R indices (all data)	R_1 = 0.0802, wR_2 = 0.1447	
Extinction coefficient	0.0309(15)	
Largest diff. peak and hole	0.640 and –0.343 e $Å^{-3}$	

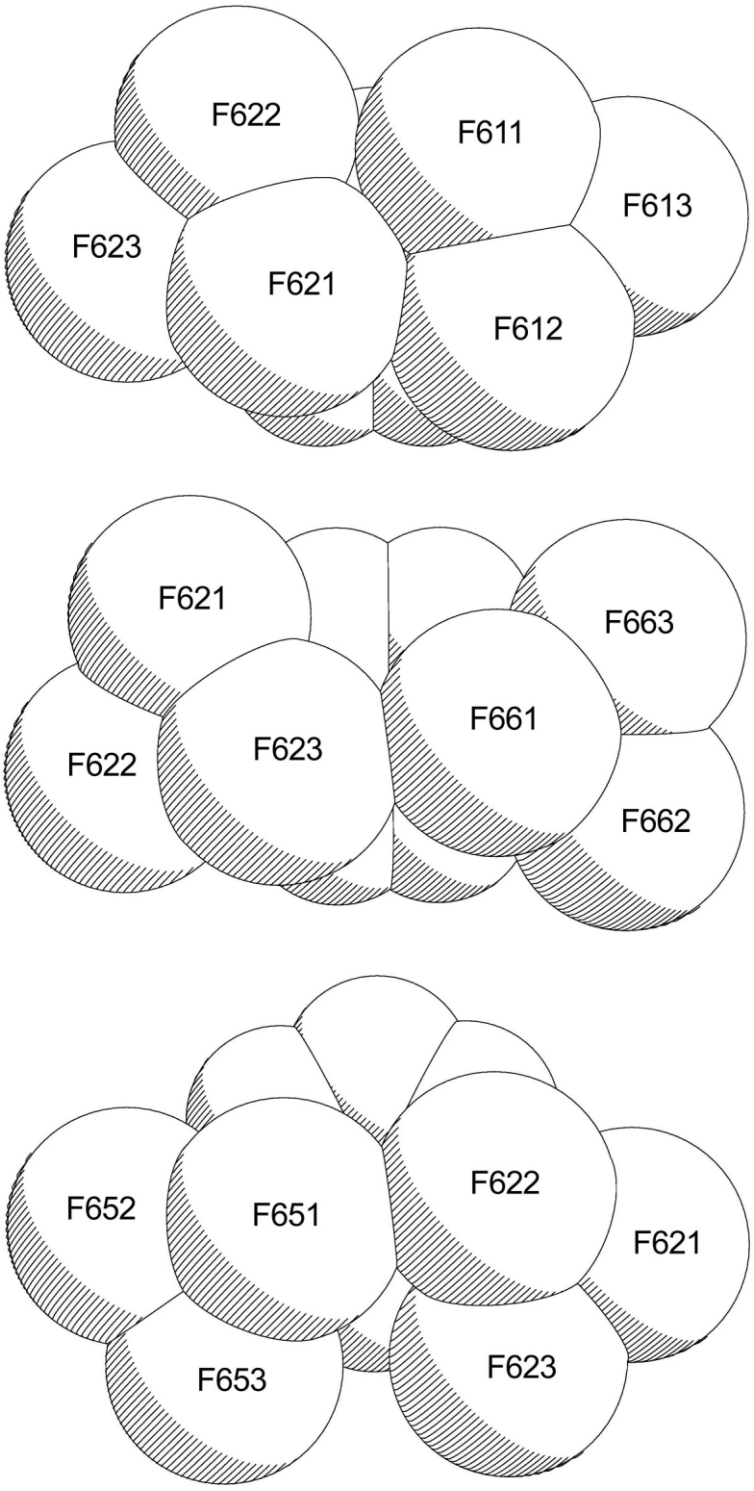


Figure S-1. Space-filling drawings of the three pairs of CF_3 groups involving the CF_3-1 group in 1,3,7,10,14,17,23,28,31,40-$C_{60}(CF_3)_{10}$ ($C_{60}(CF_3)_{10}$-3).

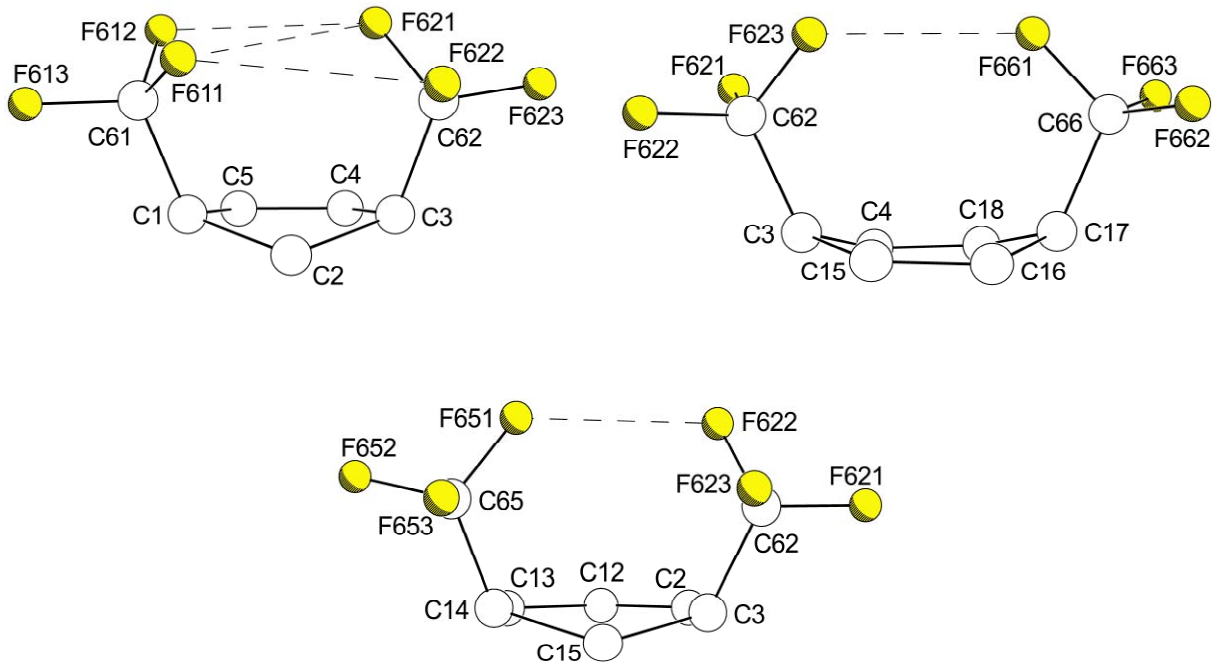
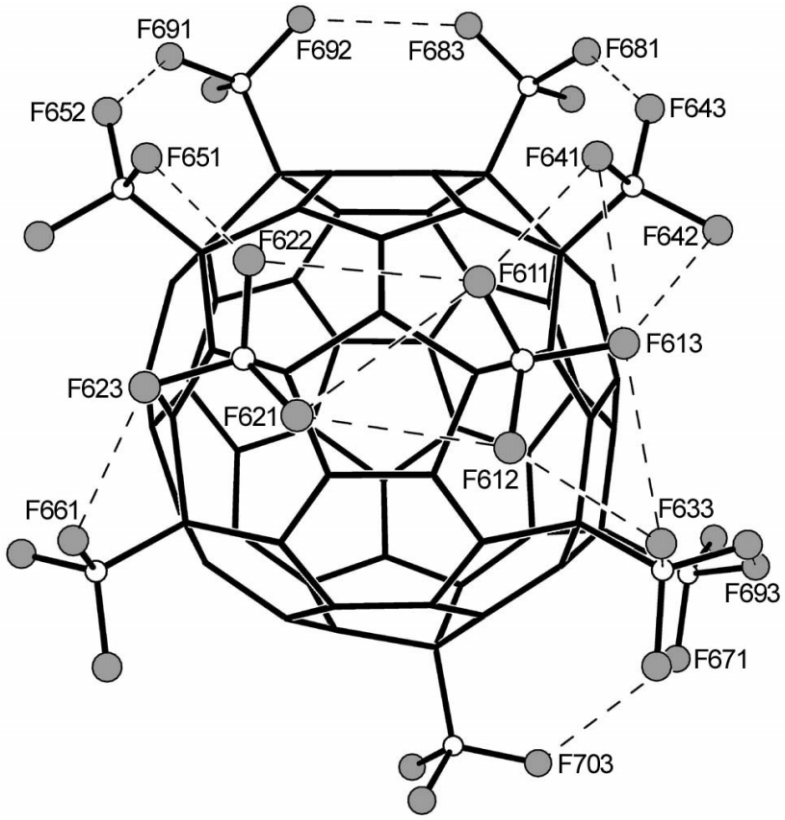


Figure S-2. The distortions of some of the substituted five- and six-membered rings from planarity. All three rings have C3 as a common atom. In the five-membered ring, atoms C1, C3, C4, and C5 are co-planar to within 0.002 Å, and C2 is 0.443 Å out of that plane. In the six-membered ring involving C17, atoms C4, C15, C16, and C18 are co-planar to within 0.02 Å, and C3 is 0.261 Å above that plane and C17 is 0.274 Å above that plane. For the six-membered ring involving C15, the other five atoms are co-planar to within 0.02 Å (the ave. deviation of those five atoms from the least-squares plane is 0.014 Å), and C15 is 0.384 out of that plane. In contrast, all six atoms of a benzenoid six-membered ring, such as the one formed by C33, C34, C35, C50, and C51, are co-planar to within 0.032 Å (ave. deviation 0.019 Å). More about this particular ring later. Another example is the C36, C37, C38, C39, C52, C53 ring, which is co-planar to within 0.018 Å (ave. deviation 0.009 Å).



F611···F621 = 2.857 Å;

F612···F621 = 2.731 Å;

F611···F622 = 2.961 Å;

F611···F611 = 2.992 Å;

F612···F633 = 2.961 Å;

F613···F641 = 2.785 Å;

F613···F642 = 2.973 Å.

F613···F633 = 2.877 Å;

F622···F651 = 2.581 Å;

F623···F661 = 2.653 Å;

F632···F673 = 2.574 Å;

F643···F681 = 2.541 Å;

F652···F691 = 2.568 Å;

F671···F703 = 2.640 Å;

F683···F692 = 2.560 Å;

Figure S-3. The 15 intramolecular F···F interactions shorter than 3.0 Å.

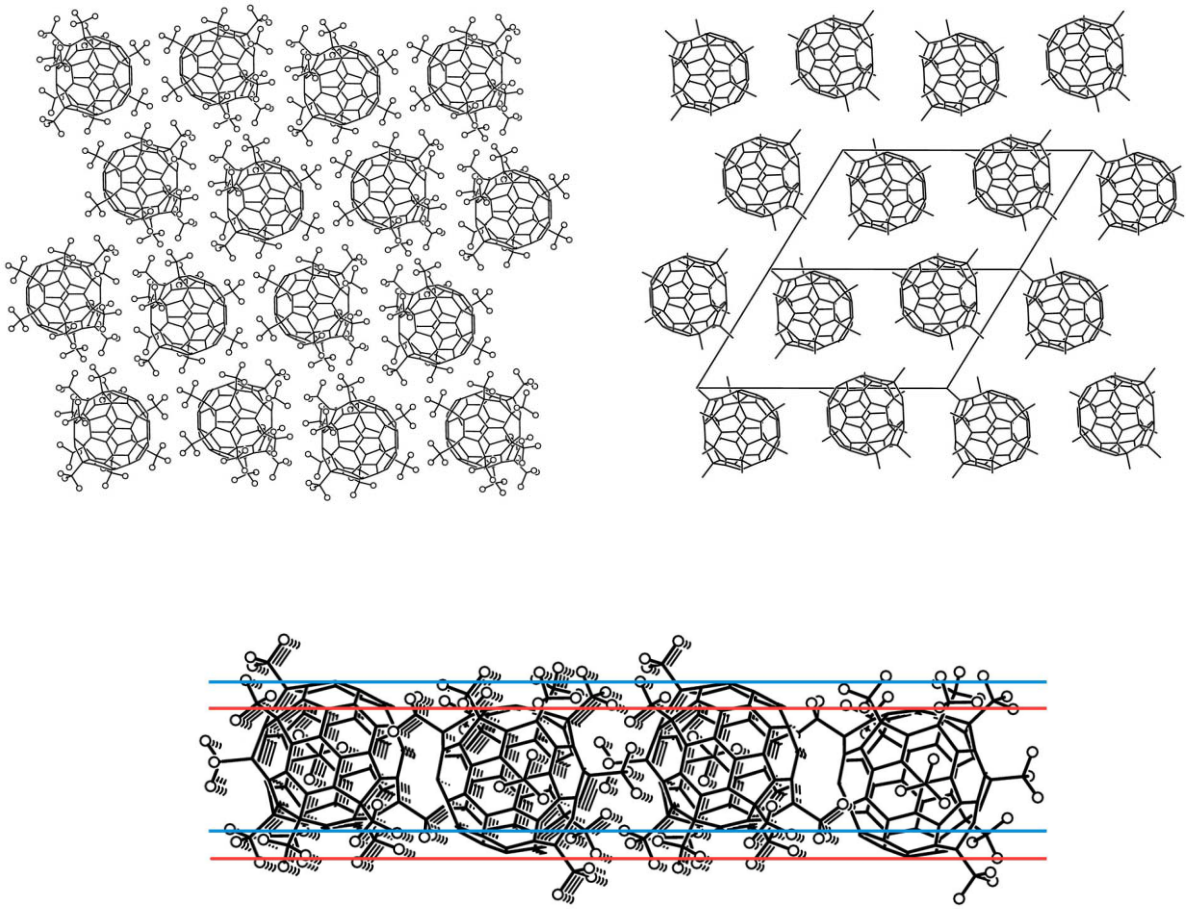
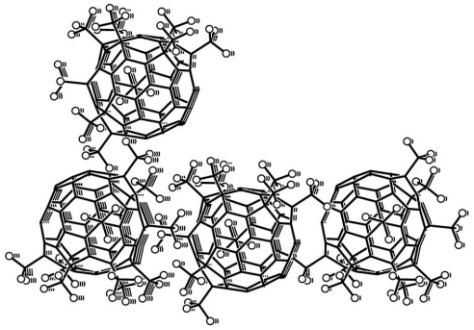


Figure S-4. Although the crystal system for $C_{60}(CF_3)_{10}$-3 is triclinic, the packing is approximately cubic closest packed. The diagram on the upper right is the same as the one on the upper left with fluorine atoms omitted for clarity. The lines connect co-planar C38 atoms in each molecule in the diagonal row and every other molecule in the horizontal row. Note that adjacent molecules in horizontal rows are not only not co-linear, they are not co-planar either, as shown in the bottom drawing, in which pairs of colored lines contain co-planar molecules.

parallel view

of two layers



perpendicular view

of two layers

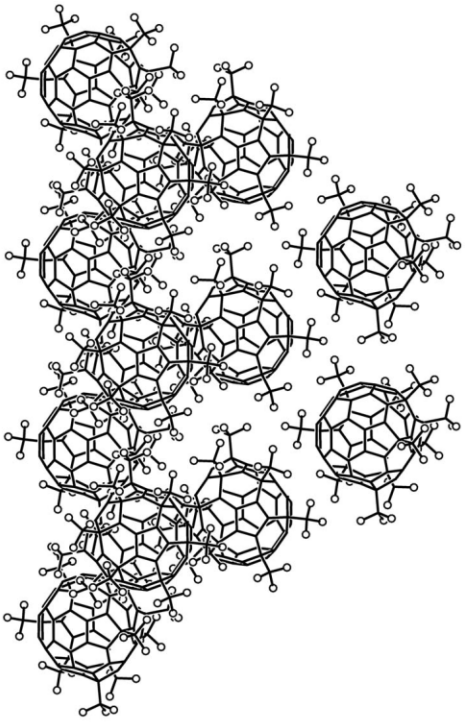


Figure S-5. The packing between molecules of $C_{60}(CF_3)_{10}$-3 in two adjacent layers.

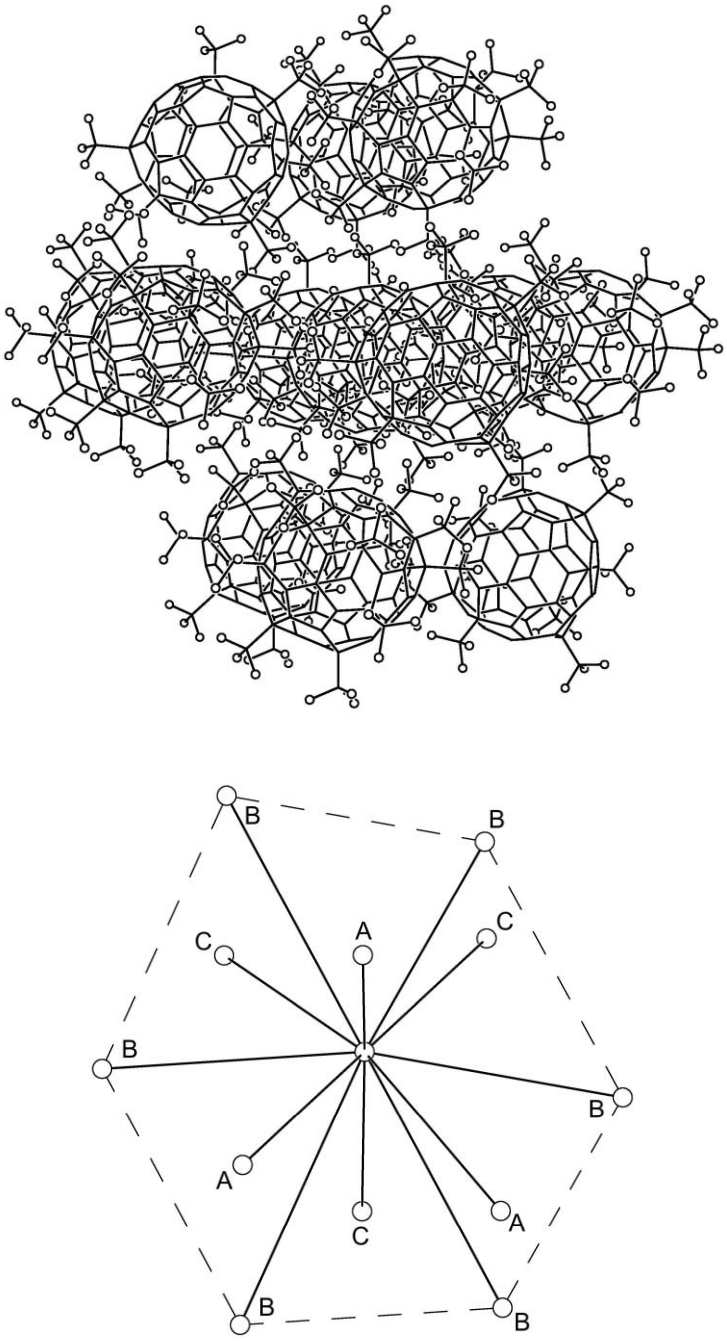
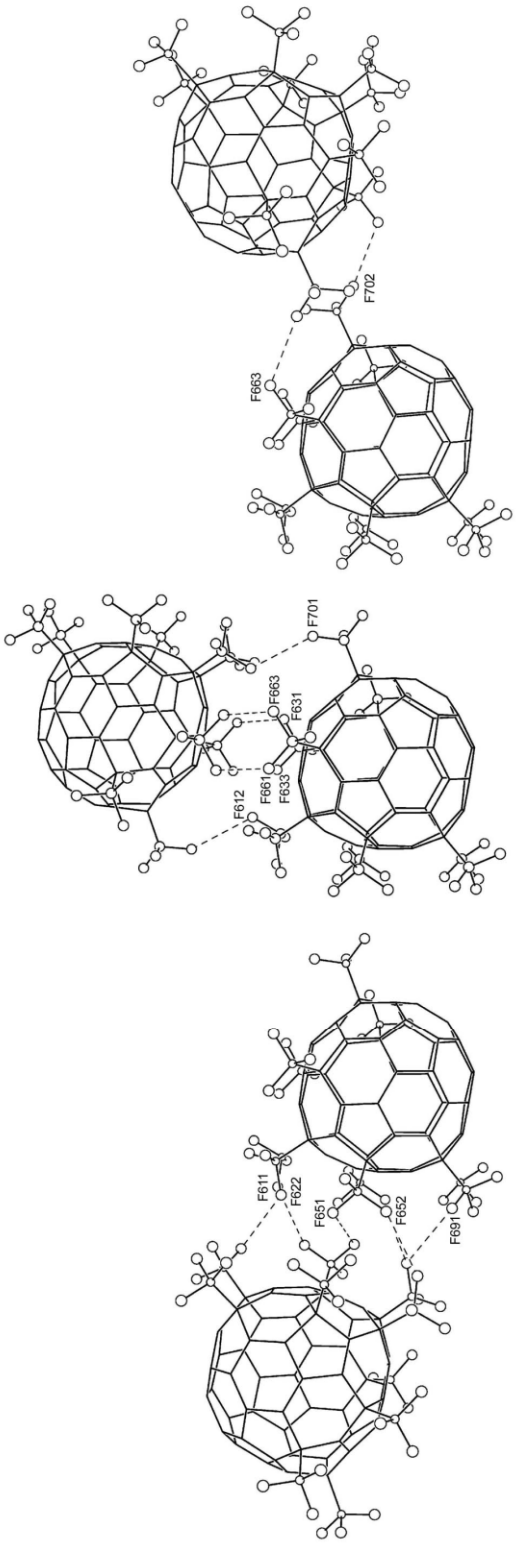


Figure S-6. Two representations of the pseudo cubic closest packing in $C_{60}(CF_3)_{10}$-3. The upper drawing is a view perpendicular to the ABC... packing direction (for clarity only the fluorine atoms are shown as circles). The lower drawing is a view looking down the ABC... packing direction and shows the C_{60} centroids of the 13 molecules in the upper drawing as spheres of arbitrary size. The centroid···centroid distances range from 10.17 Å to 14.17 Å, but 11 out of 12 span the narrower range 10.17–12.57 Å.



F621···F631' = 2.75 Å (× 2);

F622···F652' = 2.93 Å (× 2);

F622···F691' = 3.00 Å (× 2);

F611···F652' = 2.77 Å (× 2);

F612···F701' = 2.79 Å (× 2);

F661···F631' = 3.14 Å (× 2);

F662···F693' = 2.66 Å (× 2);

F663···F633' = 2.84 Å (× 2);

F663···F672' = 2.97 Å (× 2);

F663···F702' = 2.74 Å (× 2);

F651···F651' = 3.05 Å (× 1);

F653···F682' = 3.05 Å (× 2);

F642···F673' = 2.80 Å (× 2);

F653···F681' = 3.15 Å (× 2);

F632···F632' = 2.96 Å (× 2);

F632···F673' = 2.79 Å (× 2);

F672···F702' = 2.94 Å (× 2).

Figure S-7. Three of the six unique molecules that surround a given central molecule of $C_{60}(CF_3)_{10}$-3. The 31 intermolecular F···F distances shorter than 3.15 Å are listed.

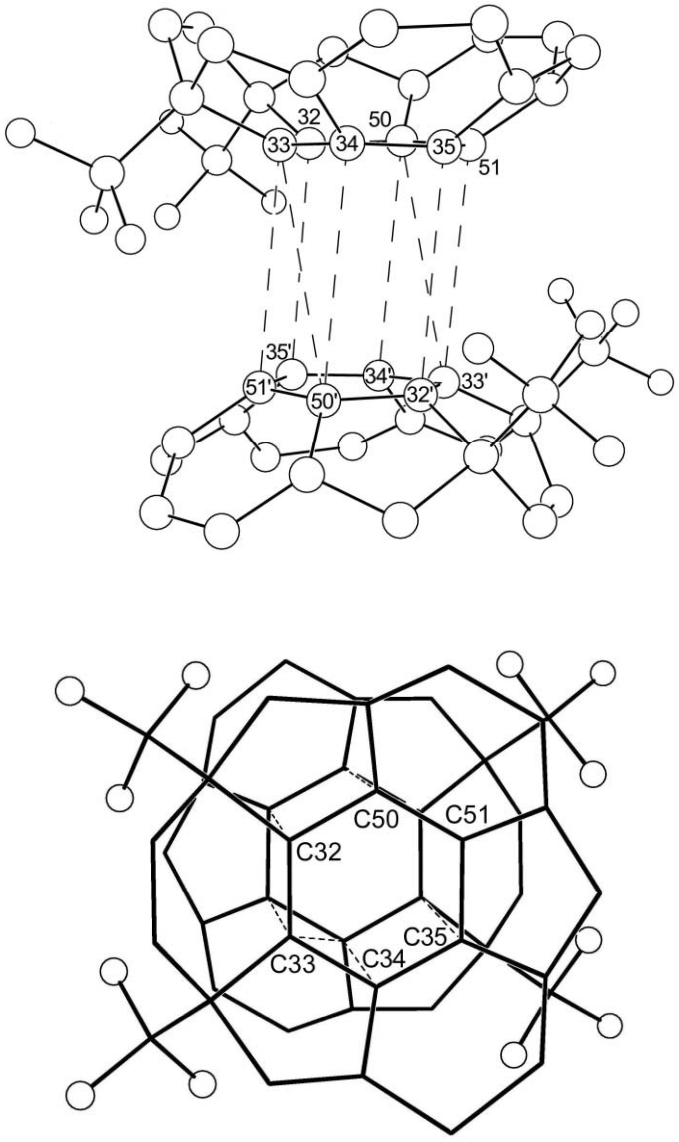


Figure S-8. Two views of the hex–hex π–π interaction between two nearest neighbor $C_{60}(CF_3)_{10}$-3 molecules. The separation between the least-squares plane formed by C32, C33, C34, and C51 and its inversion-center counterpart in the neighboring molecule is 3.59 Å.

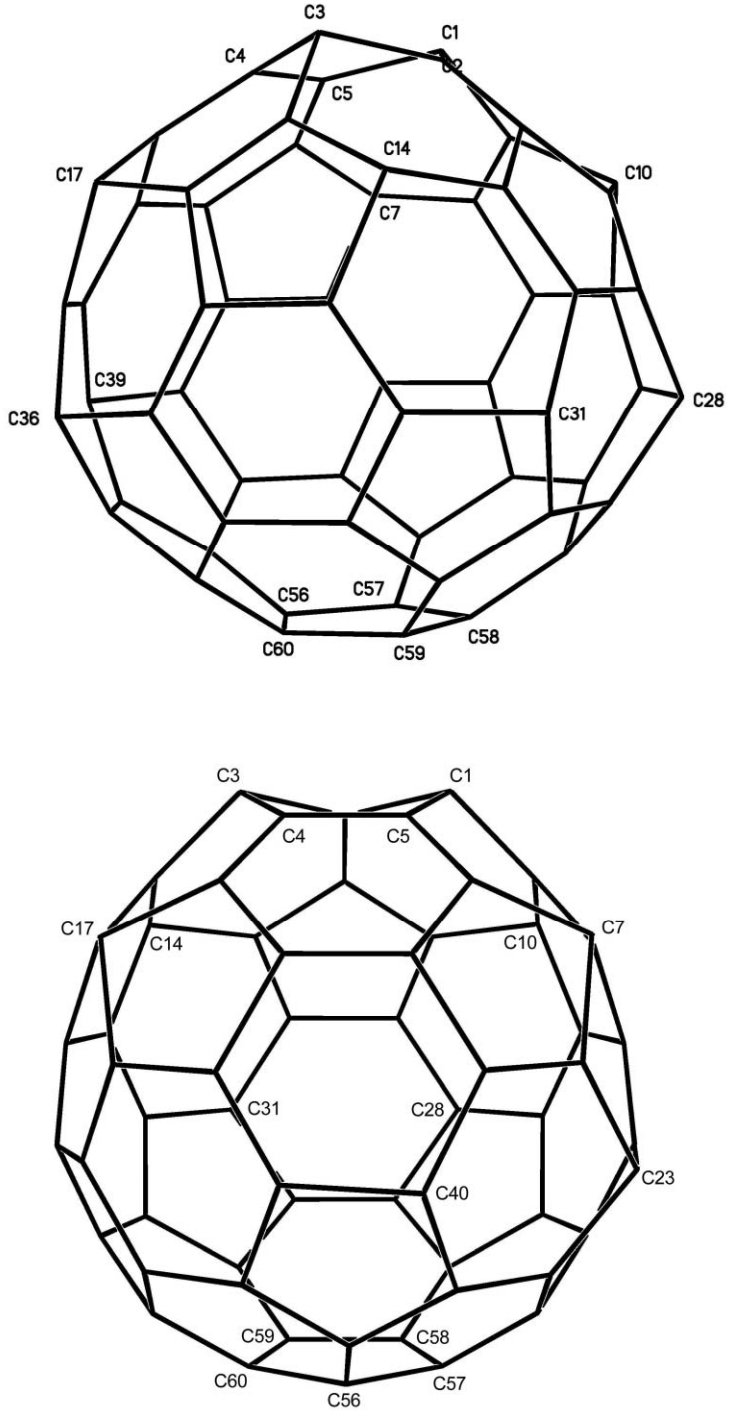


Figure S-9. Two views of the distortions of the C_{60} core in $C_{60}(CF_3)_{10}$-3. The CF_3 groups have been omitted for clarity.

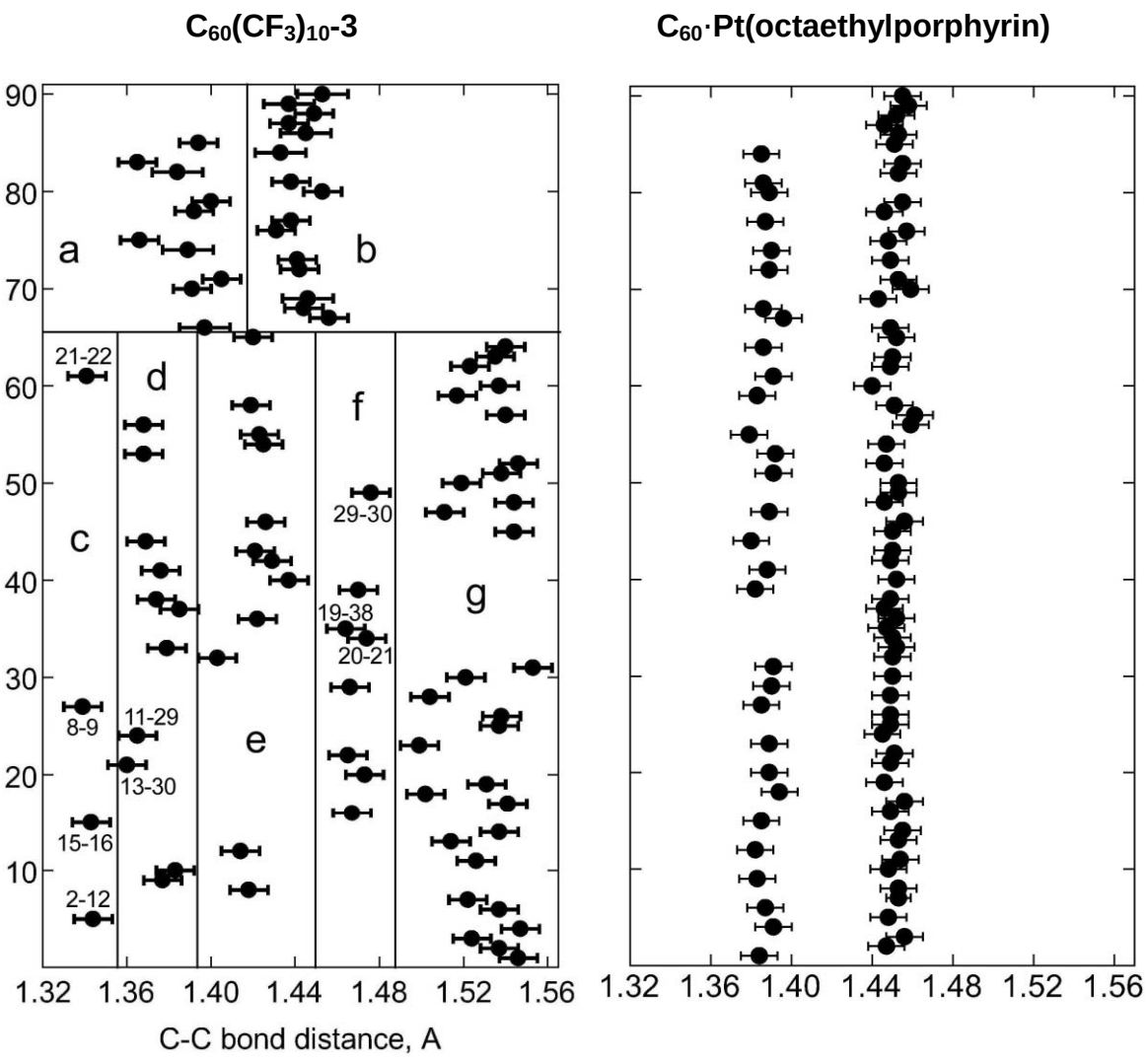


Figure S-10. The 90 fullerene-cage C–C bond distances in $C_{60}(CF_3)_{10}$-3 (left). The four shortest C=C double-bond distances are in region **c**, and are indicated by their carbon atom numbers (e.g., 2-12 is C2–C12). Three of these double bonds, C8–C9, C15–C16, and C21–C22, are 5,6 junctions. The fourth, C2–C12, is the 6,6 junction of the fulvenoid fragment described in the text. The five distances within the fulvenoid pentagon defined by C11, C12, C13, C29, and C30 are also specifically indicated. The graph on the right inset shows the 90 fullerene-cage C-C distances in C_{60}·Pt(OEP)·$2C_6H_6$ (Olmstead, M. M.; de Bettencourt-Dias, A.; Lee, H. M.; Pham, D.; Balch, A. L. *Dalton Trans.* **2003**, 3227–3232).

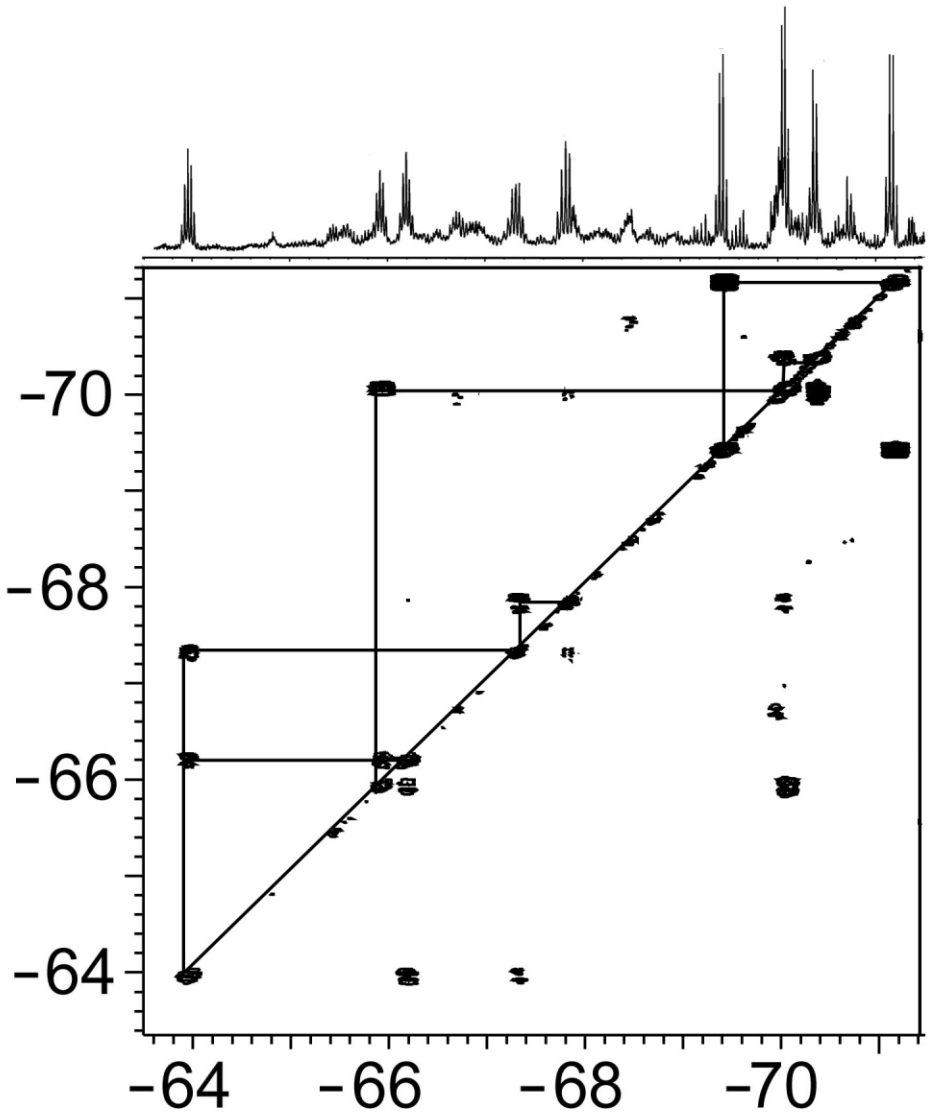


Figure S-11. 1D and 2D-COSY ^{19}F NMR spectra of $C_{60}(CF_3)_{10}$-1 (376.5 MHz, benzene-d_6, 25 °C, C_6F_6 int. std. (δ −164.9)).

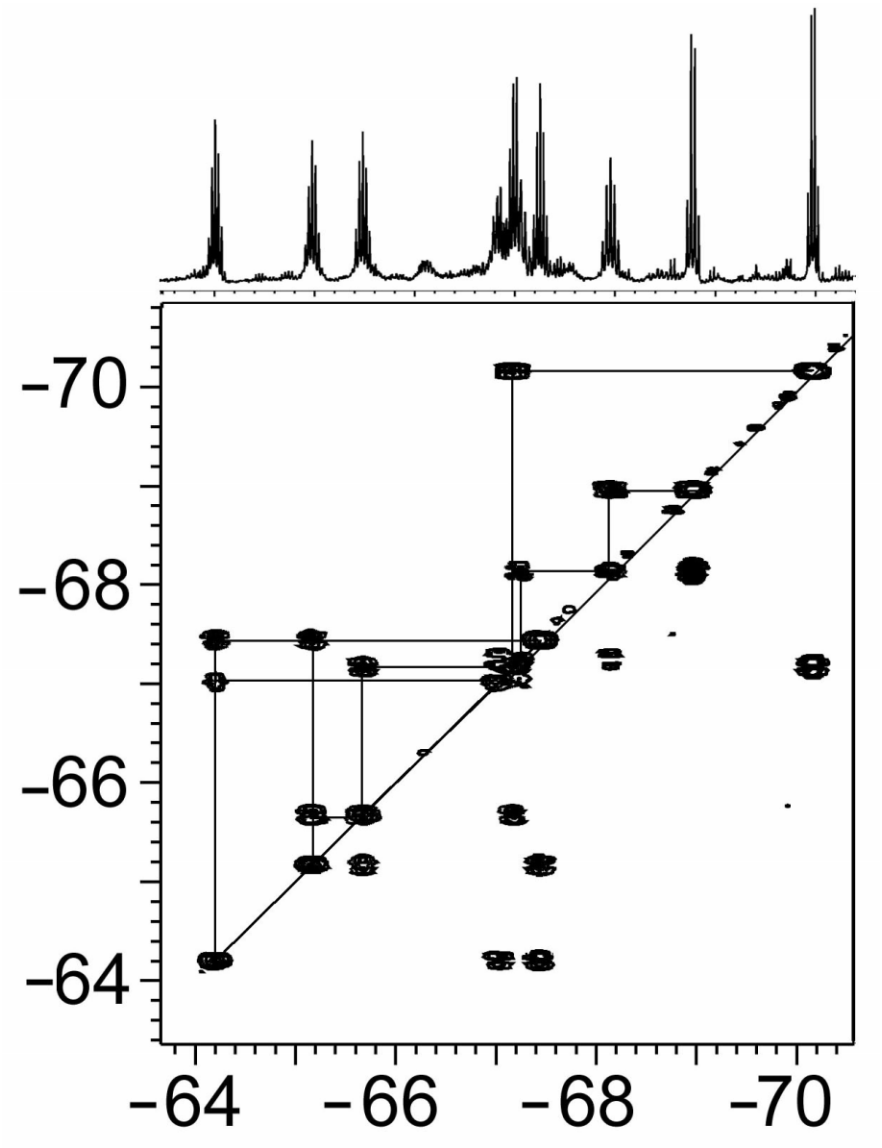


Figure S-12. 1D and 2D-COSY ^{19}F NMR spectra of $C_{60}(CF_3)_{10}$-2 (376.5 MHz, benzene-d_6, 25 °C, C_6F_6 int. std. (δ −164.9)).

Complete reference 80

80. Mallory, F. B.; Mallory, C. W.; Butler, K. E.; Lewis, M. B.; Xia, A. Q.; Luzik, J., E. D.; Fredenburgh, L. E.; Ramanjulu, M. M.; Van, Q. N.; Franci, M. M.; Freed, D. A.; Wray, C. C.; Hann, C.; Nerz-Stormes, M.; Carroll, P. J.; Chirlian, L. E. *J. Am. Chem. Soc.* **2000**, *122*, 4108-4116.