

**Synthesis, structure and theoretical study of mixed fluoro-
trifluoromethyl derivatives of C₆₀.
Molecular structures of C₆₀F₁₈(CF₃)₆ and C₆₀F₁₆(CF₃)₆**

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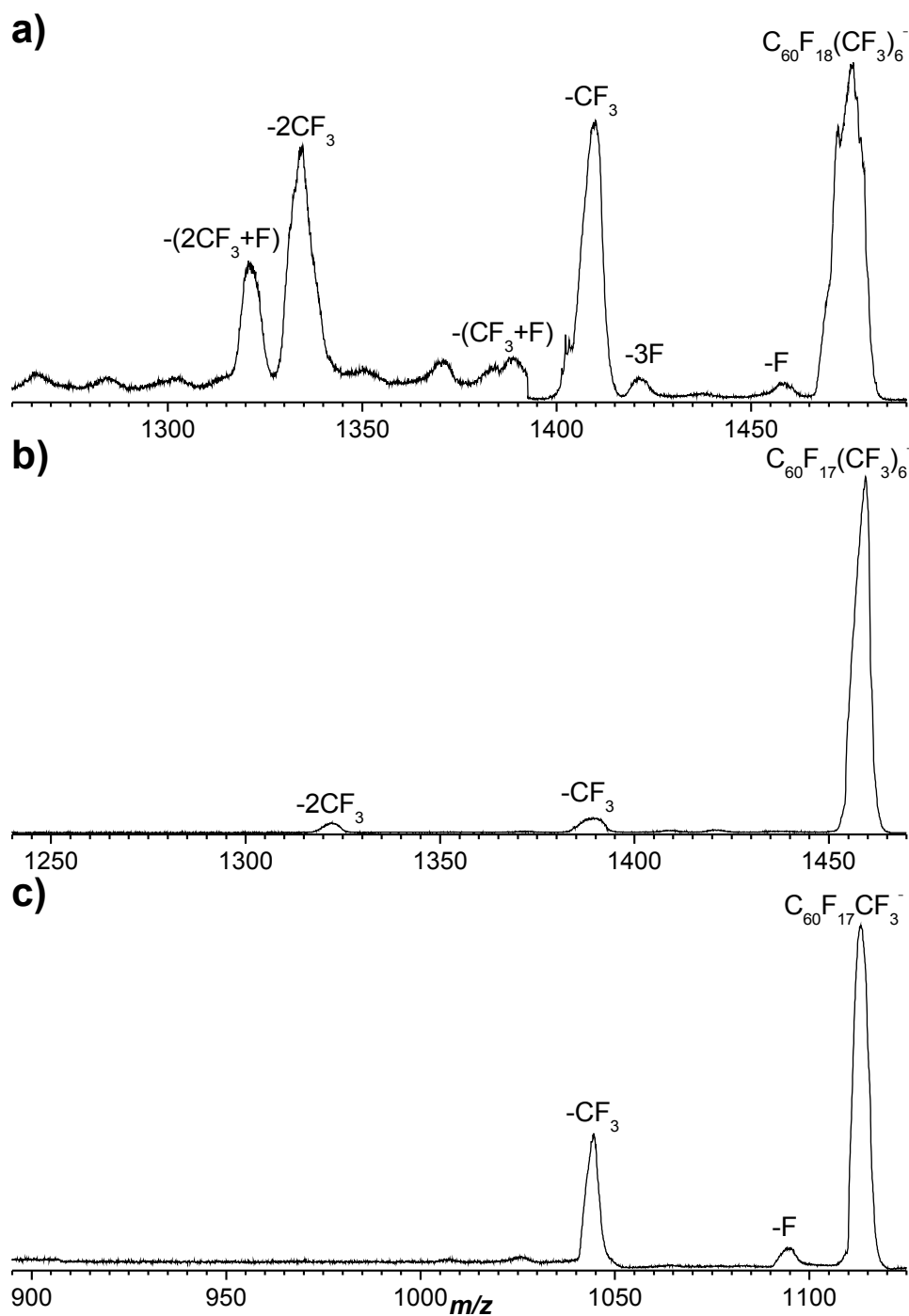
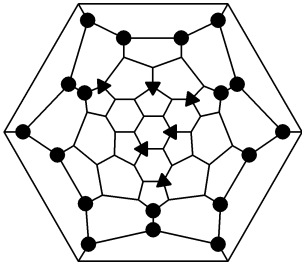
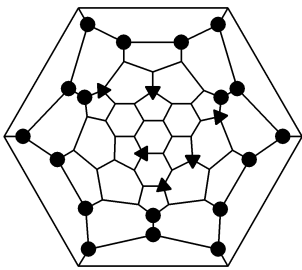
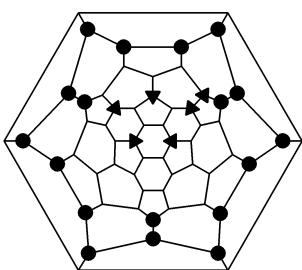
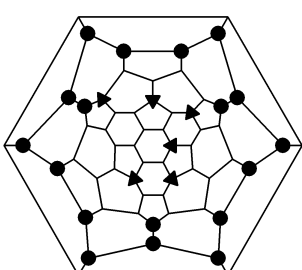
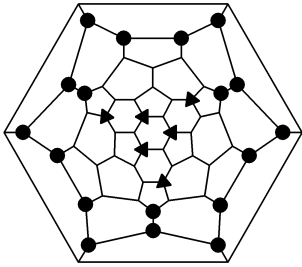
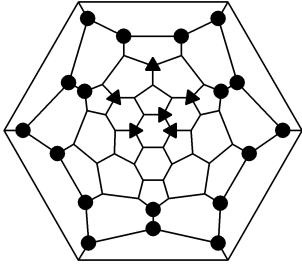
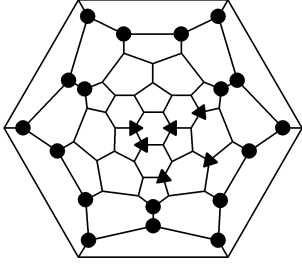
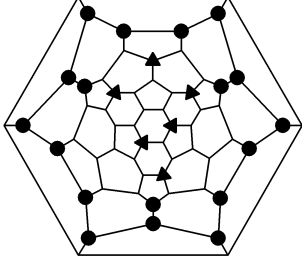
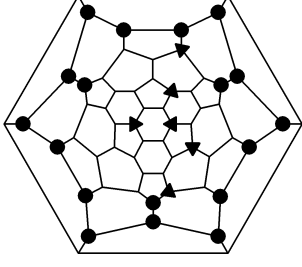
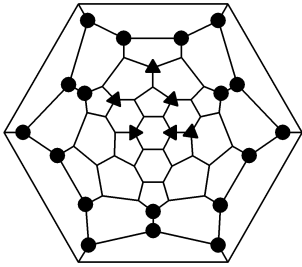
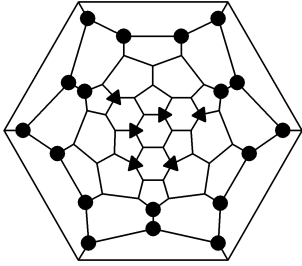
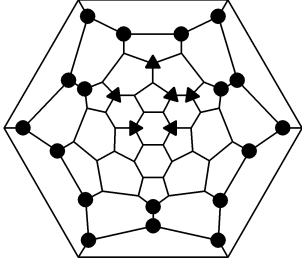
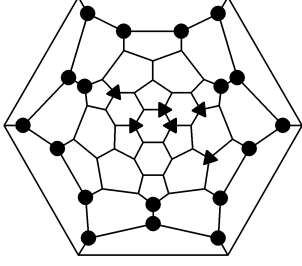
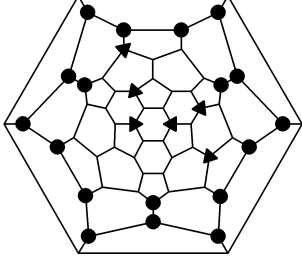


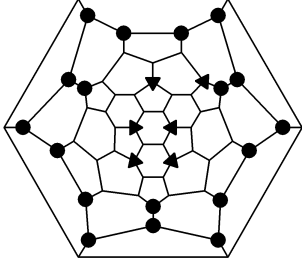
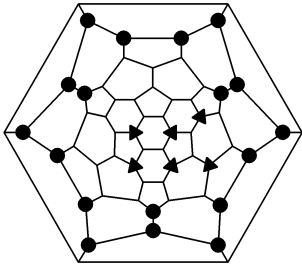
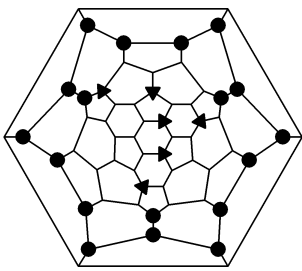
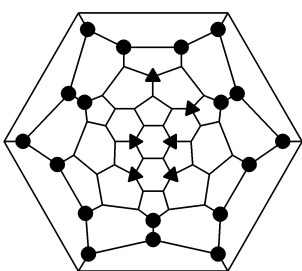
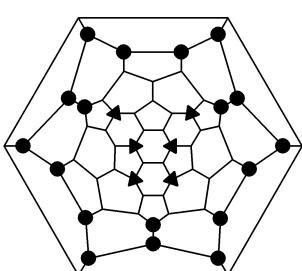
Figure S1. PSD mass spectra for (a) $C_{60}F_{18}(CF_3)_6^-$, (b) $C_{60}F_{17}(CF_3)_6^-$ and (c) $C_{60}F_{17}CF_3^-$ ions from MALDI mass spectra, 2-[(2E)-3-(4-*tert*-butylphenyl)-2-methylprop-2-enylidene]malononitrile (DCTB, $\geq 99\%$, Fluka) matrix, Bruker AutoFlex II time-of-flight reflectron device (N_2 laser, 337 nm, 1 ns pulse).

Table S1. Schlegel diagrams, relative energies (at the DFT and AM1 levels of theory), and IUPAC lowest-locant abbreviation for the isomers of $C_{60}F_{18}(CF_3)_6$ within DFT energy gap of 70 kJ mol^{-1} . Black circles denote attached fluorine atoms, black triangles denote positions of CF_3 groups. Field with the experimental isomer is marked gray.

<i>No.</i>	<i>Schlegel Diagrams of</i> $C_{60}F_{18}(CF_3)_6$	$\Delta \Delta_f H_0^\circ, \text{kJ mol}^{-1}$		<i>IUPAC lowest-locant abbreviation for</i> $C_{60}F_{18}(CF_3)_6$
		<i>DFT</i>	<i>AM1</i>	
1		0.0	2.6	11, 27, 44, 49, 52, 58- <i>hexakis</i> (trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C_{60} -I _h)[5,6]fullerene
2		11.4	34.8	11, 27, 32, 35, 44, 58- <i>hexakis</i> (trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C_{60} -I _h)[5,6]fullerene
3		14.9	31.9	2, 3, 14, 17, 32, 35- <i>hexakis</i> (trifluoromethyl)-1, 7, 8, 9, 10, 11, 22, 23, 28, 29, 41, 42, 43, 46, 47, 48, 57, 58-octadecafluoro-(C_{60} -I _h)[5,6]fullerene
4		29.3	26.1	11, 27, 44, 50, 58, 60- <i>hexakis</i> (trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C_{60} -I _h)[5,6]fullerene

$N_2.N_2$	Schlegel Diagrams of $C_{60}F_{18}(CF_3)_6$	$\Delta\Delta_f H_0^o, kJ mol^{-1}$		IUPAC lowest-locant abbreviation for $C_{60}F_{18}(CF_3)_6$
		DFT	AMI	
5		29.6	0.0	29, 43, 46, 48, 51, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
6		31.1	25.1	26, 29, 44, 46, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
7		35.3	49.8	26, 29, 44, 46, 48, 49-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
8		39.1	29.8	26, 29, 44, 48, 51, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
9		39.1	52.5	10, 28, 32, 35, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene

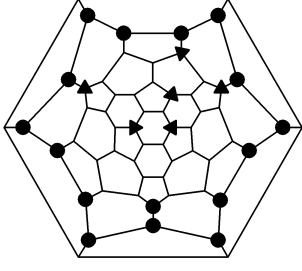
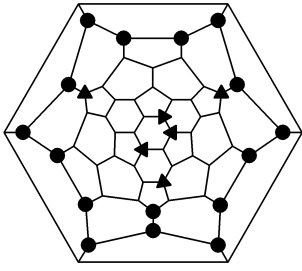
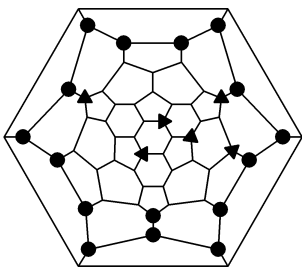
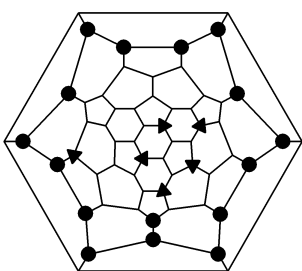
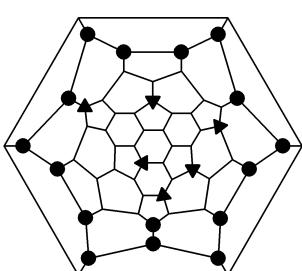
$N_2.N_2$	Schlegel Diagrams of $C_{60}F_{18}(CF_3)_6$	$\Delta\Delta_f H_0^o, kJ mol^{-1}$		IUPAC lowest-locant abbreviation for $C_{60}F_{18}(CF_3)_6$
		DFT	AMI	
10		41.7	34.5	26, 28, 31, 44, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
11		43.2	18.1	28, 31, 43, 46, 51, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
12		46.5	35.1	26, 28, 29, 44, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
13		47.3	46.8	26, 29, 47, 48, 51, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
14		48.8	49.7	10, 28, 43, 48, 55, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene

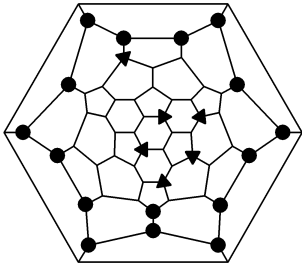
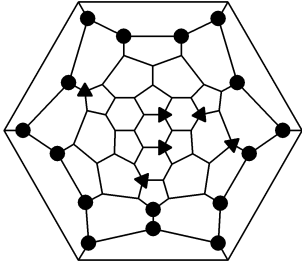
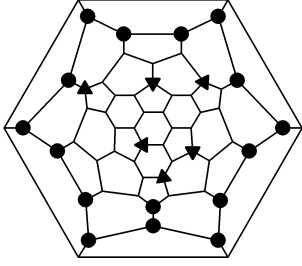
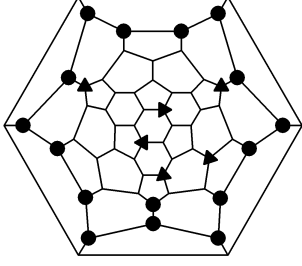
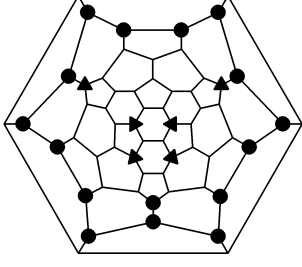
$N_2.N_2$	Schlegel Diagrams of $C_{60}F_{18}(CF_3)_6$	$\Delta\Delta_f H_0^o, kJ mol^{-1}$		IUPAC lowest-locant abbreviation for $C_{60}F_{18}(CF_3)_6$
		DFT	AMI	
15		48.8	47.1	11, 27, 48, 50, 58, 60-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
16		52.2	45.8	26, 28, 31, 44, 46, 49-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
17		56.9	52.5	11, 27, 43, 46, 51, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
18		65.1	47.0	26, 29, 48, 50, 58, 60-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
19		66.0	24.0	28, 31, 43, 46, 49, 52-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene

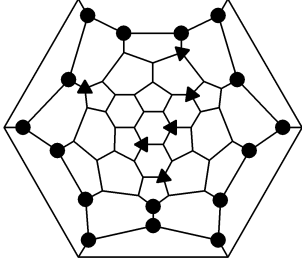
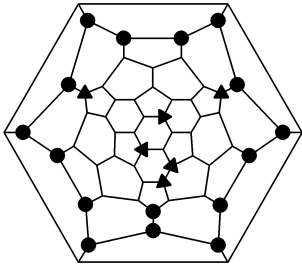
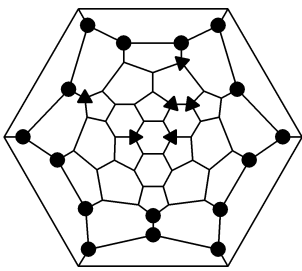
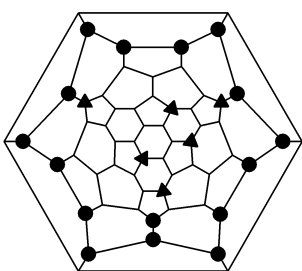
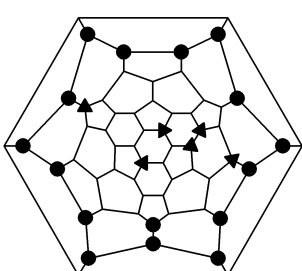
$N_2.N_2$	<i>Schlegel Diagrams of</i> $C_{60}F_{18}(CF_3)_6$	$\Delta\Delta_f H_0^o, kJ mol^{-1}$		<i>IUPAC lowest-locant abbreviation for</i> $C_{60}F_{18}(CF_3)_6$
		<i>DFT</i>	<i>AMI</i>	
20		67.7	48.7	26, 27, 29, 44, 48, 58- <i>hexakis</i> (trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
21		69.4	47.4	11, 27, 43, 46, 49, 52- <i>hexakis</i> (trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 23, 36, 37, 38, 39, 40-octadecafluoro-(C ₆₀ -I _h)[5,6]fullerene

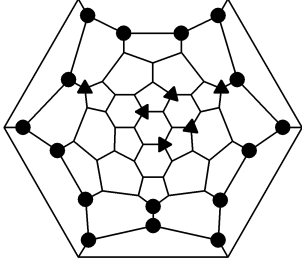
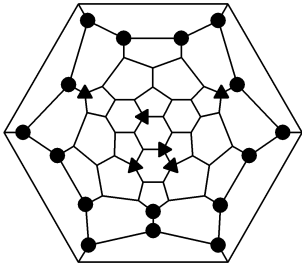
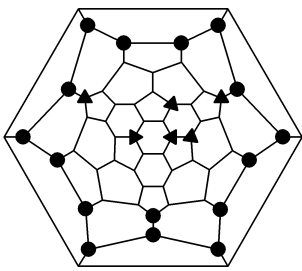
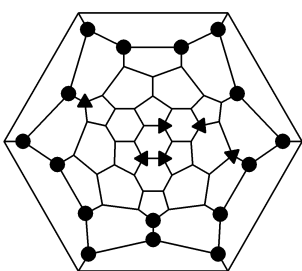
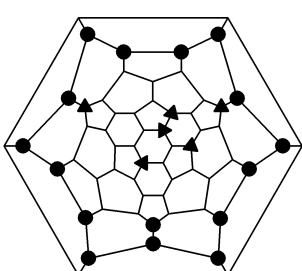
Table S2. Schlegel diagrams, relative energies (at the DFT and AM1 levels of theory), and IUPAC lowest-locant abbreviation for the isomers of $C_{60}F_{16}(CF_3)_6$ within 40 $\text{kJ}\cdot\text{mol}^{-1}$ DFT energy gap. Black circles denote attached fluorine atoms, black triangles denote positions of CF_3 groups. Field with the experimental isomer is marked gray.

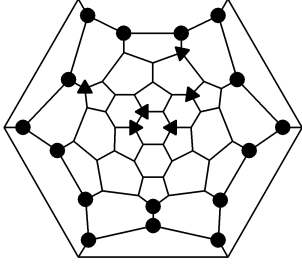
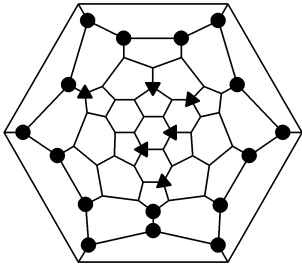
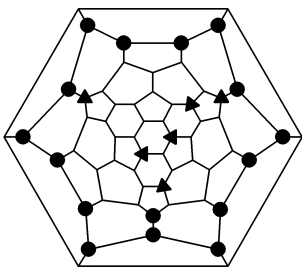
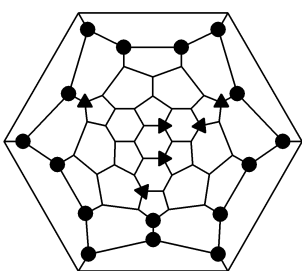
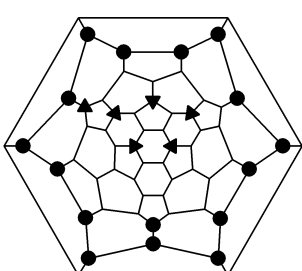
<i>No.</i>	<i>Schlegel Diagrams of</i> $C_{60}F_{16}(CF_3)_6$	$\Delta \Delta_f H_0^\circ, \text{kJ mol}^{-1}$		<i>IUPAC lowest-locant abbreviation for</i> $C_{60}F_{16}(CF_3)_6$
		<i>DFT</i>	<i>AM1</i>	
1		0.0	0.0	23, 30, 32, 47, 51, 59- <i>hexakis</i> (trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 37, 38, 39, 40-hexadecafluoro-(C_{60} -I _h)[5,6]fullerene
2		0.5	35.8	10, 13, 23, 32, 51, 59- <i>hexakis</i> (trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 36, 37, 38, 39, 40-hexadecafluoro-(C_{60} -I _h)[5,6]fullerene
3		2.3	39.3	11, 23, 27, 36, 48, 58- <i>hexakis</i> (trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 37, 38, 39, 40-hexadecafluoro-(C_{60} -I _h)[5,6]fullerene
4		8.2	27.1	10, 23, 28, 36, 48, 58- <i>hexakis</i> (trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 37, 38, 39, 40-hexadecafluoro-(C_{60} -I _h)[5,6]fullerene

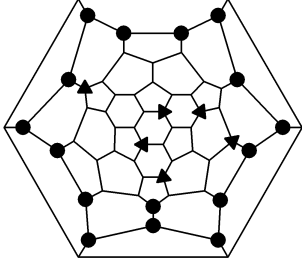
$N_2.N_2$	Schlegel Diagrams of $C_{60}F_{16}(CF_3)_6$	$\Delta\Delta_f H_0^o, kJ mol^{-1}$		IUPAC lowest-locant abbreviation for $C_{60}F_{16}(CF_3)_6$
		DFT	AMI	
5		12.0	30.3	10, 12, 23, 28, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 36, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
6		12.3	27.3	23, 29, 36, 46, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
7		13.6	30.3	10, 12, 28, 36, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
8		14.8	31.4	10, 43, 46, 49, 52, 56-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
9		18.3	31.1	11, 27, 32, 36, 44, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene

$N_2.N_2$	Schlegel Diagrams of $C_{60}F_{16}(CF_3)_6$	$\Delta\Delta_f H_0^o, kJ mol^{-1}$		IUPAC lowest-locant abbreviation for $C_{60}F_{16}(CF_3)_6$
		DFT	AMI	
10		19.0	32.2	10, 43, 46, 49, 52, 56-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 36, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
11		20.0	26.9	10, 29, 36, 43, 46, 48-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
12		20.2	32.9	11, 23, 27, 32, 51, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 36, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
13		21.6	28.8	23, 26, 29, 36, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
14		24.0	34.5	23, 28, 31, 36, 46, 49-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene

$N_2.N_2$	Schlegel Diagrams of $C_{60}F_{16}(CF_3)_6$	$\Delta\Delta_f H_0^o, kJ mol^{-1}$		IUPAC lowest-locant abbreviation for $C_{60}F_{16}(CF_3)_6$
		DFT	AMI	
15		24.2	28.8	10, 23, 29, 48, 51, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 36, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
16		24.6	35.0	23, 28, 29, 36, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
17		25.0	34.0	10, 23, 28, 29, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 36, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
18		25.5	33.5	12, 28, 31, 36, 44, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
19		25.9	34.0	10, 28, 29, 36, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene

$N_2.N_2$	Schlegel Diagrams of $C_{60}F_{16}(CF_3)_6$	$\Delta\Delta_f H_0^o, kJ mol^{-1}$		IUPAC lowest-locant abbreviation for $C_{60}F_{16}(CF_3)_6$
		DFT	AMI	
20		26.2	34.1	12, 28, 31, 36, 46, 49-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
21		27.5	39.9	23, 28, 31, 36, 47, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
22		28.4	39.5	12, 28, 31, 36, 47, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
23		28.9	37.6	10, 29, 36, 46, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
24		28.9	39.5	12, 23, 28, 31, 47, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 36, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene

$N_2.N_2$	Schlegel Diagrams of $C_{60}F_{16}(CF_3)_6$	$\Delta\Delta_f H_0^o, kJ mol^{-1}$		IUPAC lowest-locant abbreviation for $C_{60}F_{16}(CF_3)_6$
		DFT	AMI	
25		29.3	38.0	10, 23, 29, 46, 48, 58-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 36, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
26		36.2	26.9	23, 30, 47, 49, 52, 56-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
27		36.5	37.1	23, 29, 36, 43, 46, 48-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 12, 15, 16, 17, 21, 22, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
28		36.6	36.4	12, 29, 36, 43, 46, 48-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene
29		37.6	19.1	12, 30, 32, 47, 51, 59-hexakis(trifluoromethyl)-1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C ₆₀ -I _h)[5,6]fullerene

$N_2.N_2$	<i>Schlegel Diagrams of</i> $C_{60}F_{16}(CF_3)_6$	$\Delta\Delta_f H_0^o, kJ mol^{-1}$		<i>IUPAC lowest-locant abbreviation for</i> $C_{60}F_{16}(CF_3)_6$
		<i>DFT</i>	<i>AM1</i>	
30		39.4	28.2	10, 29, 36, 44, 48, 58- <i>hexakis</i> (trifluoromethyl)- 1, 2, 3, 7, 8, 9, 15, 16, 17, 21, 22, 23, 37, 38, 39, 40-hexadecafluoro-(C_{60} -I _h)[5,6]fullerene

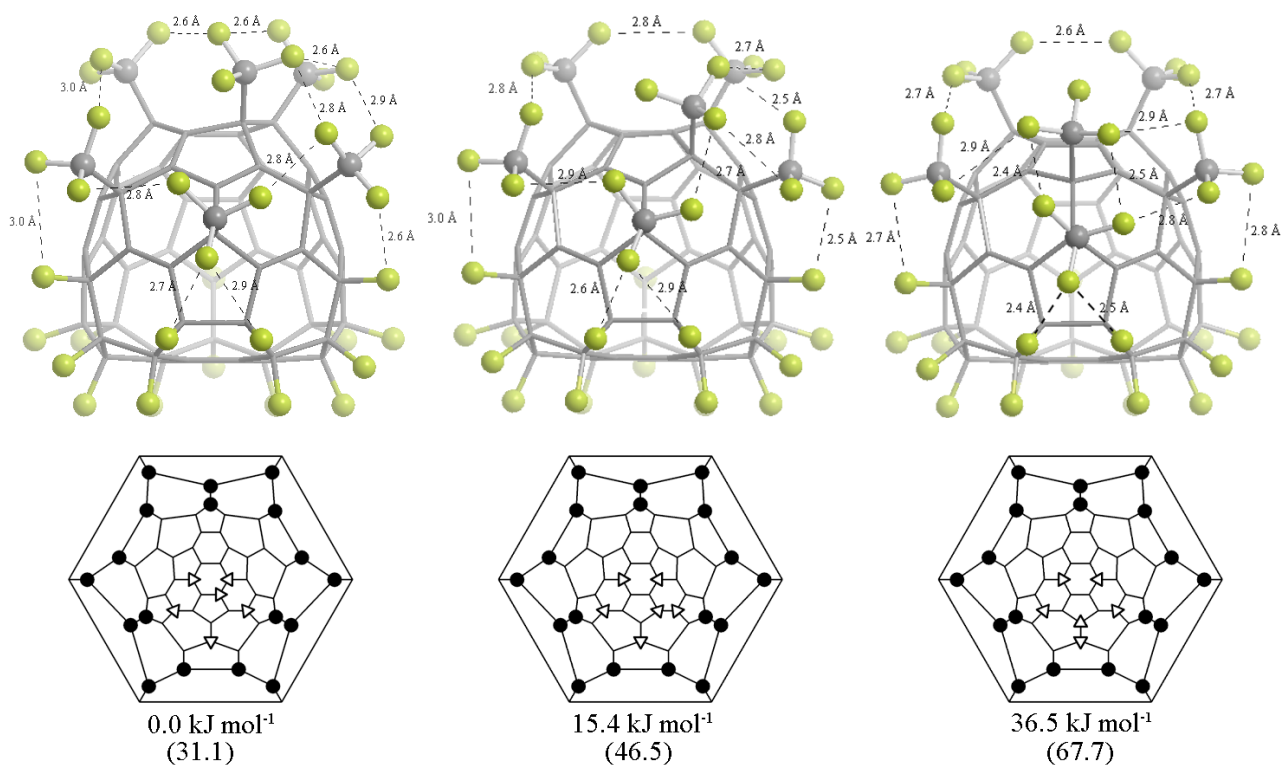


Figure S2. DFT-optimized structures with some non-bonding $F \cdots F$ distances (\AA), corresponding Schlegel diagrams and DFT energies ($\text{kJ}\cdot\text{mol}^{-1}$) for three possible isomers of $C_{60}F_{18}(CF_3)_6$ with skew pentagonal pyramid addition pattern of attached CF_3 groups. The DFT energies are given relative to the most stable of three isomers; the DFT energies relative to the most stable isomer $C_{60}F_{18}(CF_3)_6$ (see *Table S1*) are given in the parentheses.