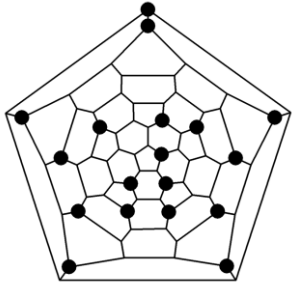
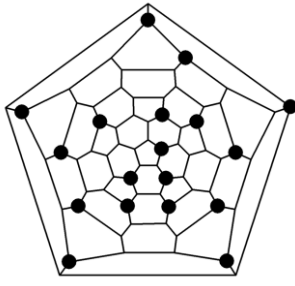
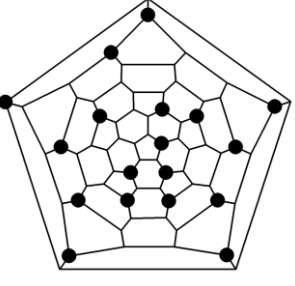


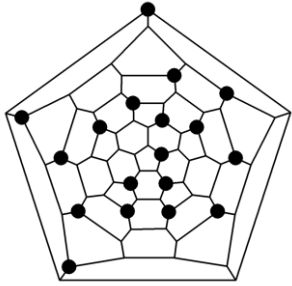
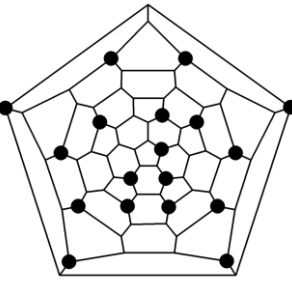
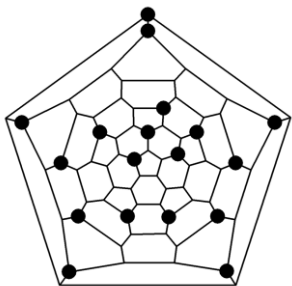
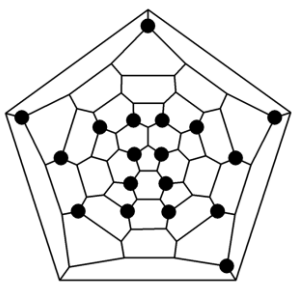
Supporting information for

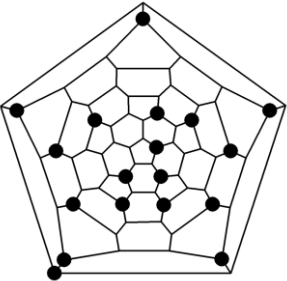
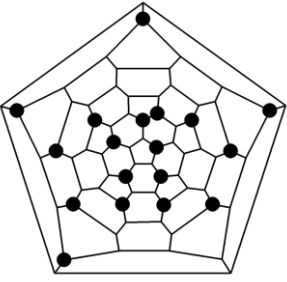
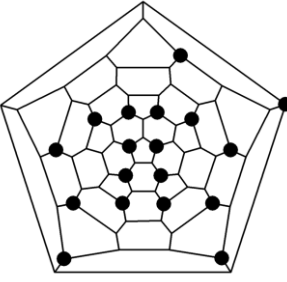
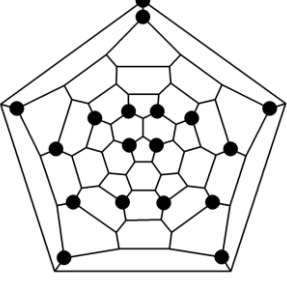
Isolation and structural characterization of the most highly trifluoromethylated fullerene, $C_{70}(CF_3)_{20}$

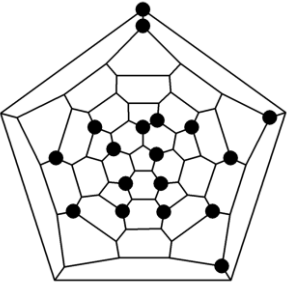
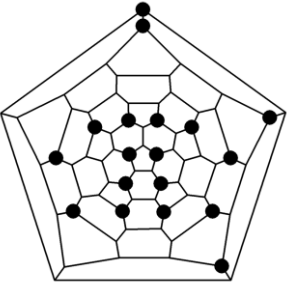
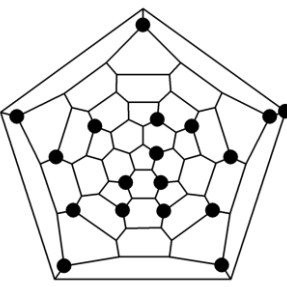
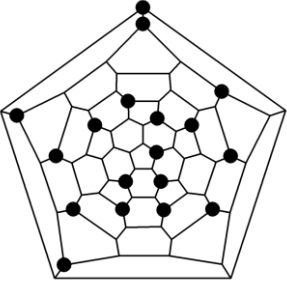
Daria V. Ignat'eva, Alexey A. Goryunkov, Nadezhda B. Tamm, Ilya N. Ioffe, Lev N. Sidorov and Sergey I. Troyanov*

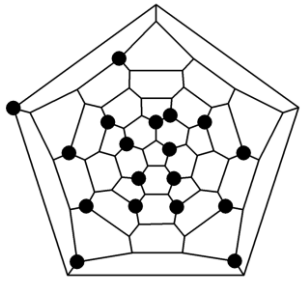
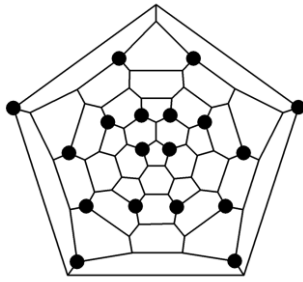
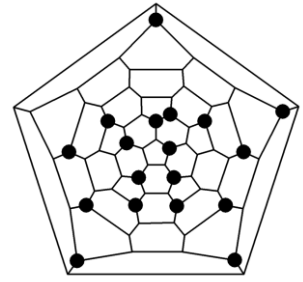
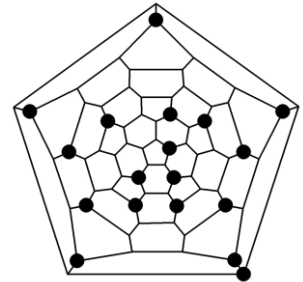
Table 1. The Schlegel diagrams, relative energies (at the DFT and AM1 levels of theory), and IUPAC lowest-locant abbreviations for the most stable isomers of $C_{70}(CF_3)_{18}$ within the gap of 40 kJ mol^{-1} (the fields with experimentally observed isomers are shadowed).

<i>N</i>	Schlegel Diagram of $C_{70}(CF_3)_{18}$	$\Delta_f H_0^\circ$ kJ mol^{-1}		IUPAC lowest-locant abbreviation for octadeca(trifluoromethyl)(C_{70} - $D_{5h(6)}$)[5,6]fullerene
		DFT	AM1	
1		0.0	0.0	1, 4, 8, 11, 16, 19, 23, 27, 31, 34, 37, 41, 44, 46, 47, 52, 60, 69
2		3.4	22.9	1, 4, 8, 11, 16, 19, 23, 26, 31, 34, 37, 41, 44, 47, 48, 52, 60, 69
3		7.9	20.2	1, 4, 8, 11, 16, 19, 23, 26, 31, 37, 41, 44, 47, 48, 55, 60, 67, 69

<i>N₀</i>	Schlegel Diagram of <i>C</i> ₇₀ (<i>CF</i> ₃) ₁₈	$\Delta_f H_0^\circ$ kJ mol ⁻¹		IUPAC lowest-locant abbreviation for octadeca(trifluoromethyl)(<i>C</i> ₇₀ - <i>D</i> _{5h(6)})[5,6]fullerene
		DFT	AMI	
4		9.8	10.0	1, 4, 7, 11, 18, 21, 24, 31, 33, 35, 39, 44, 47, 51, 53, 58, 61, 64
5		11.1	17.6	1, 4, 8, 11, 16, 19, 23, 26, 31, 34, 37, 41, 45, 48, 52, 60, 63, 69
6		23.0	35.5	1, 4, 8, 11, 16, 19, 23, 24, 27, 31, 37, 44, 47, 51, 55, 58, 61, 64
7		27.0	6.9	1, 4, 8, 11, 16, 19, 24, 27, 31, 37, 41, 43, 46, 51, 53, 56, 62, 64

<i>N</i> ₀	Schlegel Diagram of <i>C</i> ₇₀ (<i>CF</i> ₃) ₁₈	$\Delta_f H_0^\circ$ kJ mol ⁻¹		IUPAC lowest-locant abbreviation for octadeca(trifluoromethyl)(<i>C</i> ₇₀ - <i>D</i> _{5h(6)})[5,6]fullerene
		DFT	AMI	
8		27.4	20.5	1, 4, 8, 11, 16, 19, 23, 24, 27, 31, 34, 37, 41, 44, 47, 52, 60, 69
9		27.6	31.1	1, 4, 8, 11, 16, 19, 23, 27, 31, 37, 41, 44, 46, 51, 53, 56, 62, 64
10		27.6	15.0	1, 4, 8, 11, 16, 19, 23, 26, 31, 34, 37, 41, 48, 52, 55, 60, 67, 69
11		27.7	5.8	1, 4, 8, 11, 18, 23, 24, 27, 31, 35, 38, 44, 47, 51, 55, 58, 61, 64

<i>N₀</i>	Schlegel Diagram of <i>C</i> ₇₀ (<i>CF</i> ₃) ₁₈	$\Delta_f H_0^\circ$ kJ mol ⁻¹		IUPAC lowest-locant abbreviation for octadeca(trifluoromethyl)(<i>C</i> ₇₀ - <i>D</i> _{5h(6)})[5,6]fullerene
		DFT	AMI	
12		27.8	42.6	1, 4, 8, 11, 16, 19, 24, 27, 31, 37, 41, 43, 44, 47, 51, 55, 56, 64
13		28.0	21.1	1, 4, 8, 11, 16, 19, 24, 27, 31, 37, 41, 43, 46, 51, 55, 56, 62, 64
14		28.8	22.9	1, 4, 8, 11, 16, 19, 23, 26, 27, 31, 34, 37, 41, 44, 47, 52, 60, 69
15		29.4	46.5	1, 4, 7, 11, 18, 23, 24, 31, 33, 35, 39, 44, 47, 51, 53, 58, 61, 64

<i>N</i> ₀	Schlegel Diagram of <i>C</i> ₇₀ (CF ₃) ₁₈	$\Delta_f H_0^\circ$ kJ mol ⁻¹		IUPAC lowest-locant abbreviation for octadeca(trifluoromethyl)(<i>C</i> ₇₀ - <i>D</i> _{5h(6)})[5,6]fullerene
		DFT	AMI	
16		31.6	31.7	1, 4, 8, 11, 16, 19, 23, 26, 31, 33, 37, 41, 48, 53, 55, 60, 67, 69
17		32.0	27.7	1, 4, 8, 11, 19, 23, 26, 31, 34, 41, 45, 48, 52, 55, 60, 63, 67, 69
18		33.7	34.2	1, 4, 8, 11, 16, 19, 23, 27, 31, 33, 41, 44, 46, 51, 53, 56, 62, 64
19		33.7	20.0	1, 4, 8, 11, 16, 19, 23, 24, 27, 31, 37, 41, 44, 47, 55, 60, 67, 69

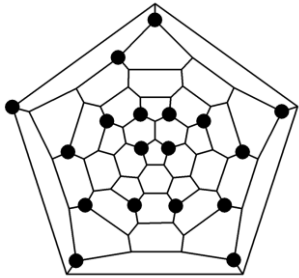
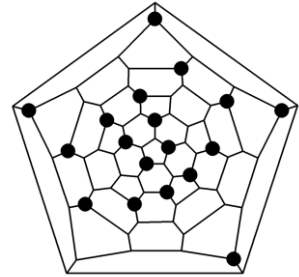
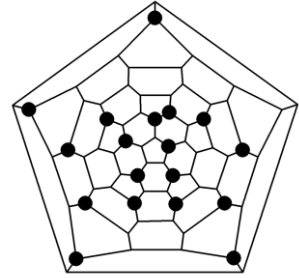
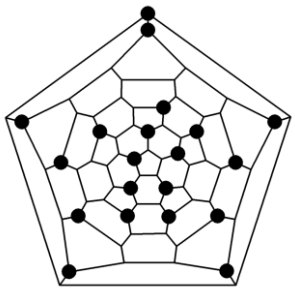
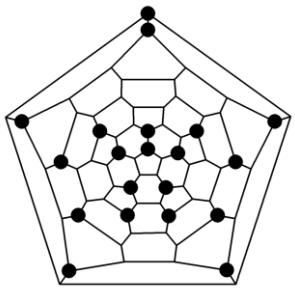
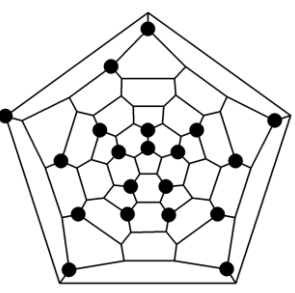
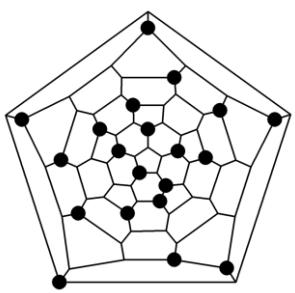
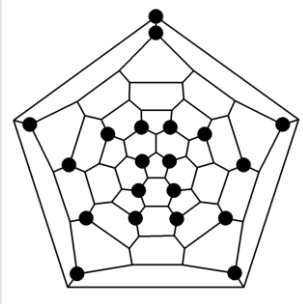
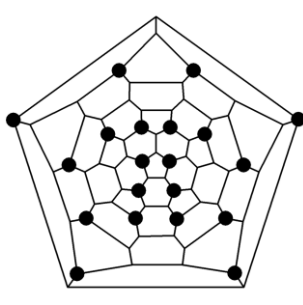
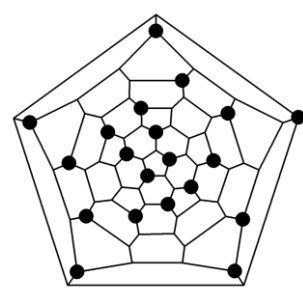
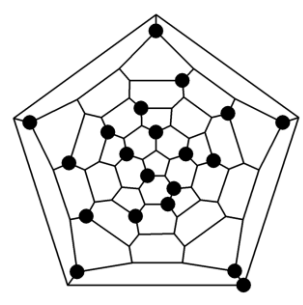
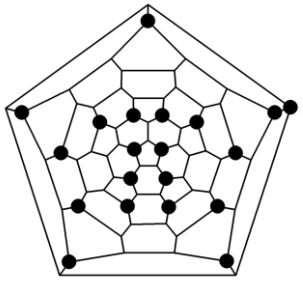
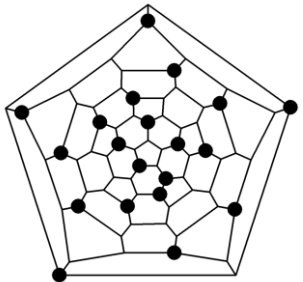
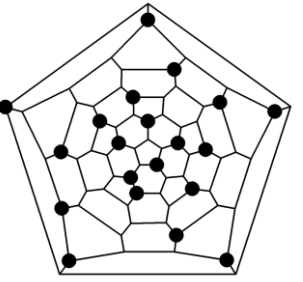
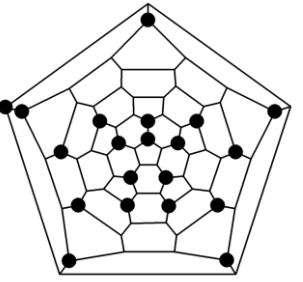
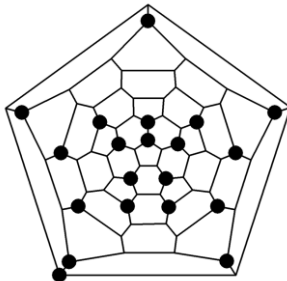
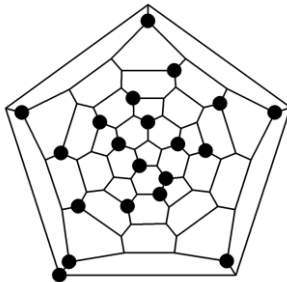
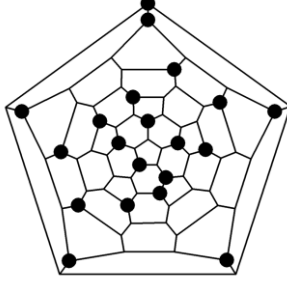
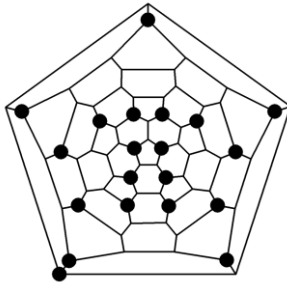
<i>N</i> ₀	Schlegel Diagram of <i>C</i> ₇₀ (<i>CF</i> ₃) ₁₈	$\Delta_f H_0^0$ kJ mol ⁻¹		IUPAC lowest-locant abbreviation for octadeca(trifluoromethyl)(<i>C</i> ₇₀ - <i>D</i> _{5h(6)})[5,6]fullerene
		DFT	AMI	
20		36.7	29.1	1, 4, 8, 11, 18, 23, 27, 31, 35, 38, 42, 45, 47, 51, 55, 58, 61, 64
21		36.7	13.9	1, 4, 8, 11, 16, 19, 23, 27, 31, 34, 37, 41, 47, 52, 55, 60, 67, 69
22		36.9	32.7	1, 4, 8, 11, 16, 19, 23, 27, 31, 33, 37, 41, 44, 46, 51, 56, 62, 64

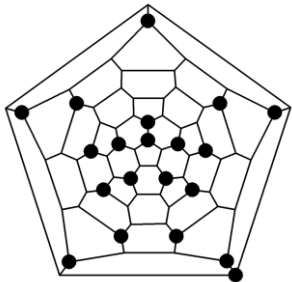
Table 2. The Schlegel diagrams, relative energies (at the DFT and AM1 levels of theory), and IUPAC lowest-locant abbreviations for the most stable isomers of $C_{70}(CF_3)_{20}$ within the gap of 40 kJ mol^{-1} (the fields with experimentally observed isomers are shadowed).

$N\bar{2}$	Schlegel Diagram of $C_{70}(CF_3)_{20}$	$\Delta_f H_0^o$ kJ mol^{-1}		IUPAC lowest-locant abbreviation for <i>icosa(trifluoromethyl)(C_{70}-$D_{5h(6)}$)[5,6]fullerene</i>
		DFT	AMI	
1		0.0	14.9	1, 4, 8, 11, 16, 19, 23, 24, 27, 31, 33, 37, 44, 47, 51, 53, 55, 58, 61, 64
2		8.4	33.4	1, 4, 8, 11, 16, 19, 23, 27, 31, 33, 37, 41, 44, 45, 47, 51, 53, 55, 56, 64
3		8.6	50.5	1, 4, 8, 11, 16, 19, 23, 26, 31, 33, 37, 41, 44, 47, 48, 53, 54, 56, 60, 69
4		9.5	42.4	1, 4, 8, 11, 16, 19, 23, 26, 31, 34, 37, 41, 44, 47, 48, 52, 53, 56, 60, 69

<i>N₀</i>	Schlegel Diagram of <i>C₇₀(CF₃)₂₀</i>	$\Delta_f H_0^0$ kJ mol ⁻¹		IUPAC lowest-locant abbreviation for <i>icosa(trifluoromethyl)(C₇₀-D_{5h(6)})[5,6]fullerene</i>
		DFT	AMI	
5		10.2	0.0	1, 4, 8, 11, 16, 19, 23, 27, 31, 34, 37, 41, 44, 46, 47, 52, 55, 60, 67, 69
6		10.4	30.4	1, 4, 8, 11, 16, 19, 23, 26, 31, 34, 37, 41, 45, 48, 52, 55, 60, 63, 67, 69
7		18.0	24.4	1, 4, 8, 11, 16, 19, 23, 26, 31, 34, 37, 41, 44, 47, 48, 52, 55, 60, 67, 69
8		18.8	23.5	1, 4, 8, 11, 16, 19, 23, 27, 31, 33, 37, 41, 44, 46, 47, 53, 55, 60, 67, 69

<i>N</i> ₀	Schlegel Diagram of <i>C</i> ₇₀ (<i>CF</i> ₃) ₂₀	$\Delta_f H_0^{\circ}$ kJ mol ⁻¹		IUPAC lowest-locant abbreviation for icosa(trifluoromethyl)(<i>C</i> ₇₀ - <i>D</i> _{5h(6)})[5,6]fullerene
		DFT	AMI	
9		24.7	23.7	1, 4, 8, 11, 16, 19, 23, 26, 27, 31, 34, 37, 41, 44, 47, 52, 55, 60, 67, 69
10		25.1	41.6	1, 4, 8, 11, 16, 19, 23, 26, 31, 33, 37, 41, 45, 48, 53, 55, 60, 63, 67, 69
11		27.1	48.6	1, 4, 8, 11, 16, 19, 23, 26, 31, 33, 37, 41, 44, 47, 48, 53, 55, 60, 67, 69
12		31.6	50.4	1, 4, 8, 11, 16, 19, 23, 26, 27, 31, 33, 37, 41, 44, 47, 53, 54, 56, 60, 69

<i>N₀</i>	<i>Schlegel Diagram of C₇₀(CF₃)₂₀</i>	$\Delta_f H_0^0$ kJ mol ⁻¹		<i>IUPAC lowest-locant abbreviation for icos(trifluoromethyl)(C₇₀-D_{5h(6)})[5,6]fullerene</i>
		<i>DFT</i>	<i>AMI</i>	
13		32.0	49.4	1, 4, 8, 11, 16, 19, 23, 24, 27, 31, 33, 37, 41, 44, 47, 53, 54, 56, 60, 69
14		32.2	48.5	1, 4, 8, 11, 16, 19, 23, 26, 27, 31, 34, 37, 41, 44, 47, 52, 53, 56, 60, 69
15		33.2	48.5	1, 4, 8, 11, 16, 19, 23, 24, 27, 31, 34, 37, 41, 44, 47, 52, 53, 56, 60, 69
16		37.3	28.0	1, 4, 8, 11, 16, 19, 23, 24, 27, 31, 34, 37, 41, 44, 47, 52, 55, 60, 67, 69

<i>N₀</i>	<i>Schlegel Diagram of C₇₀(CF₃)₂₀</i>	$\Delta_f H_0^0$ kJ mol ⁻¹		<i>IUPAC lowest-locant abbreviation for icoso(trifluoromethyl)(C₇₀-D_{5h(6)})[5,6]fullerene</i>
		<i>DFT</i>	<i>AMI</i>	
17		40.6	48.0	1, 4, 8, 11, 16, 19, 23, 25, 27, 31, 33, 37, 41, 44, 47, 51, 53, 55, 56, 64