Supplementary Material (ESI) for Chemical Communications

Supporting information for Chemical Communications

Preparation, crystallographic characterization and theoretical study of $C_{70}(CF_3)_{16}$ and $C_{70}(CF_3)_{18}$

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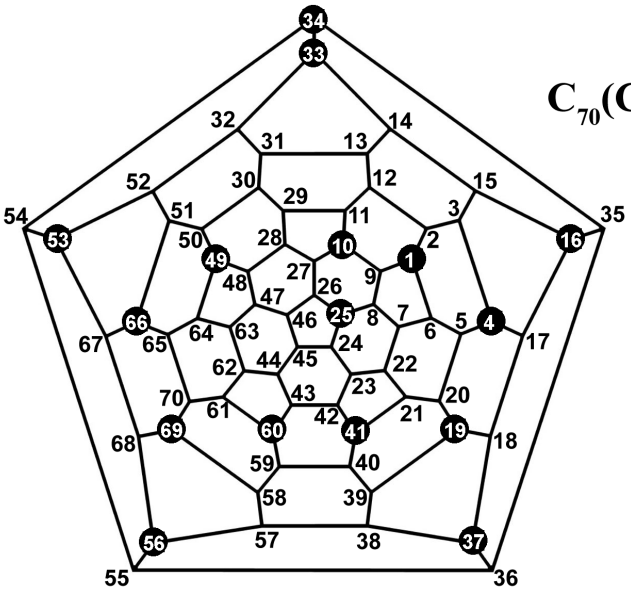
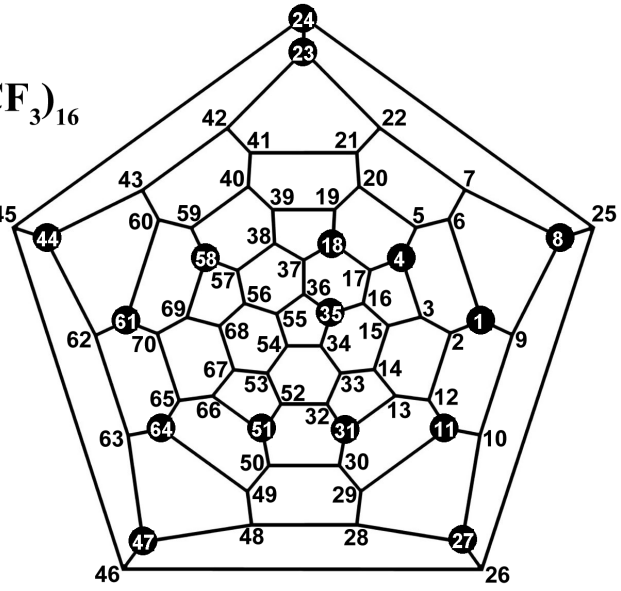
Carbon cage numeration of the experimental $C_{70}(CF_3)_{16}$ and $C_{70}(CF_3)_{18}$ isomers

As in the paper and the same as for $C_{70}(CF_3)_{10}$

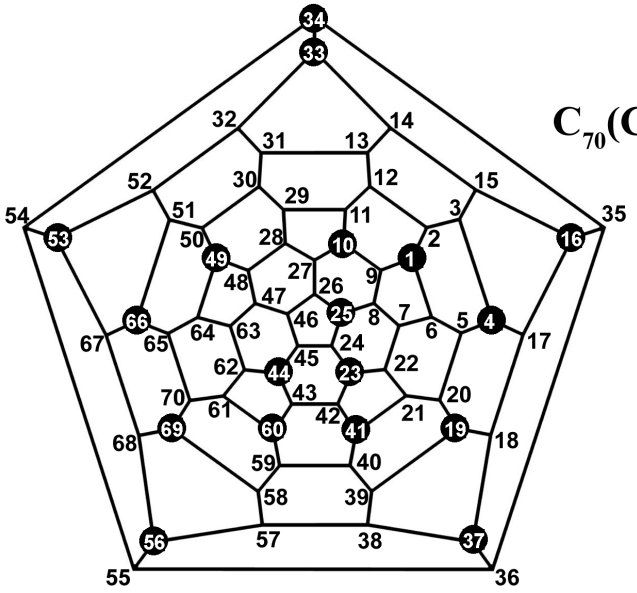
According to IUPAC recommendation

$C_{70}(CF_3)_{16}$





$C_{70}(CF_3)_{18}$



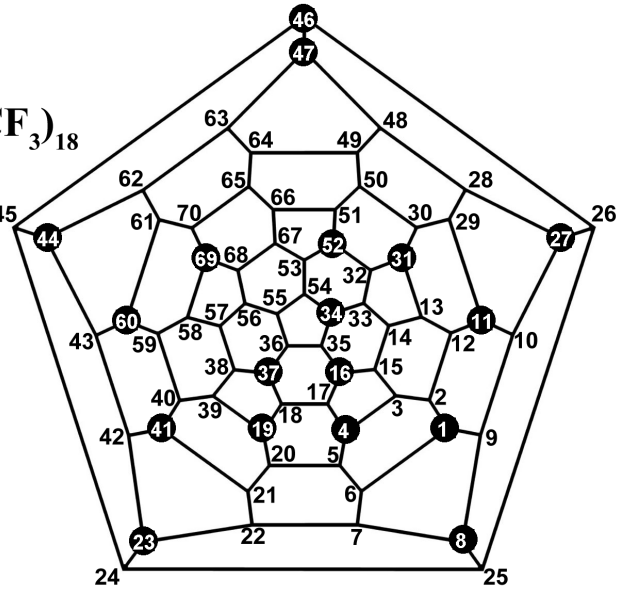
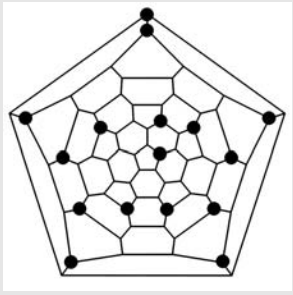
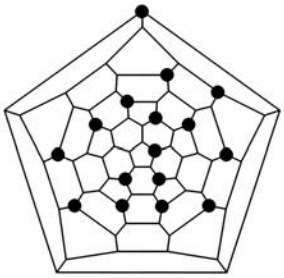
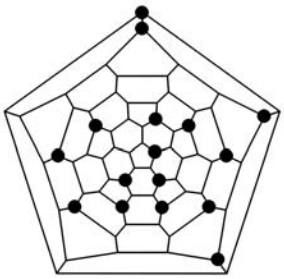
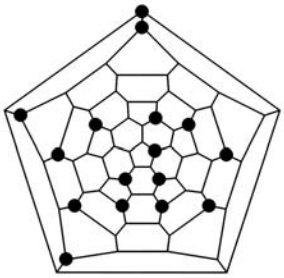
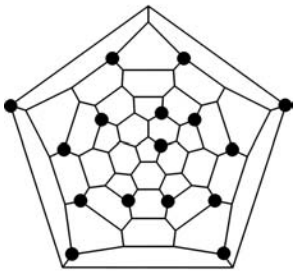
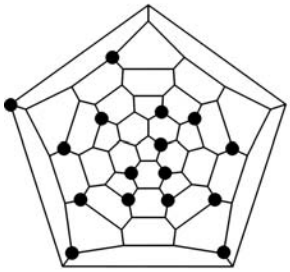
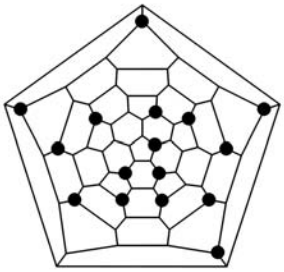
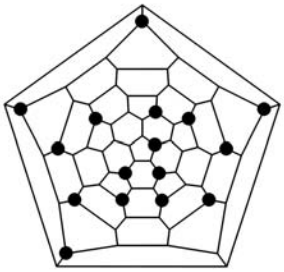
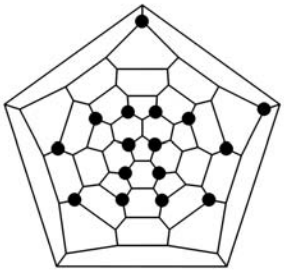
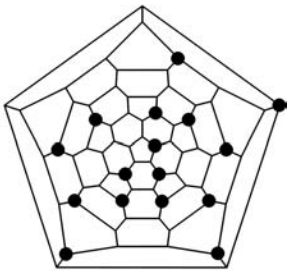
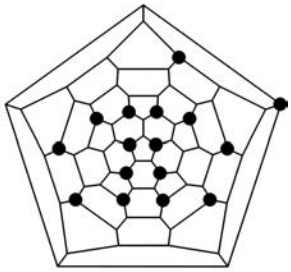
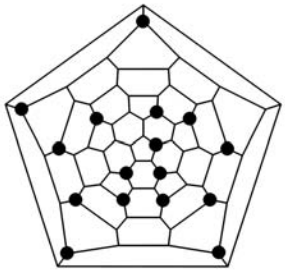
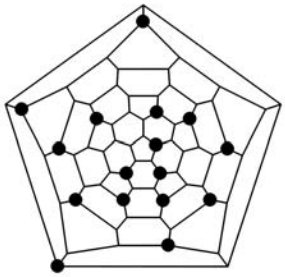
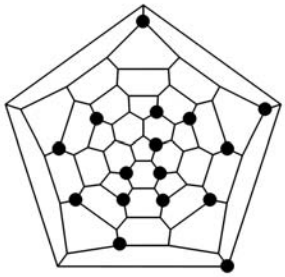
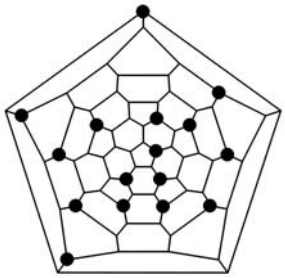
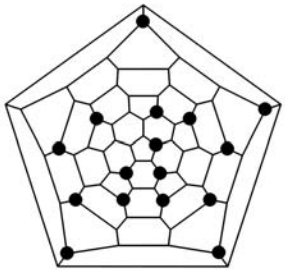
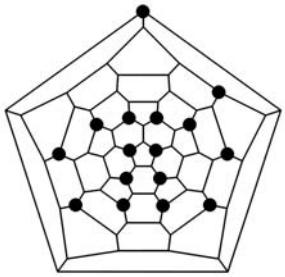
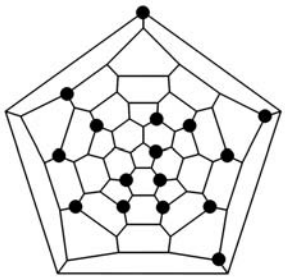
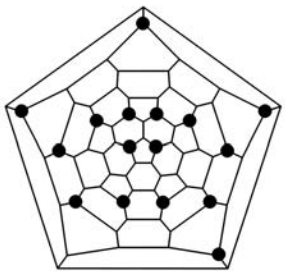
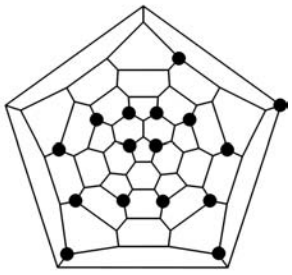


Table 1. Schlegel diagrams, relative energies (at the DFT and AM1 levels of theory), and IUPAC lowest-locant abbreviation for the most stable isomers of $C_{70}(CF_3)_{16}$ within the gap of 40 kJ/mol (the field with experimentally observed isomer is shadowed).

№№	*Schlegel Diagrams of* $C_{70}(CF_3)_{16}$	$\Delta_f H^o_0$ kJ/mol		*IUPAC lowes-locant abbreviation for hexadeca(trifluoromethyl)(C_{70}-$D_{5h(6)}$)[5,6]fullerene*
		DFT	**AM1**	
1		0.0	0.0	1, 4, 8, 11, 18, 23, 24, 27, 31, 35, 44, 47, 51, 58, 61, 64
2		0.8	11.1	1, 4, 7, 11, 18, 21, 24, 31, 33, 35, 39, 51, 53, 58, 61, 64
3		3.5	17.8	1, 4, 8, 11, 16, 19, 24, 27, 31, 37, 41, 43, 51, 55, 56, 64
4		3.5	19.4	1, 4, 8, 11, 16, 19, 27, 31, 37, 41, 46, 47, 55, 60, 67, 69
5		4.3	15.0	1, 4, 8, 11, 19, 23, 26, 31, 34, 41, 45, 48, 52, 60, 63, 69

№№	*Schlegel Diagrams of* $C_{70}(CF_3)_{16}$	$\Delta_f H_0^o$ kJ/mol		*IUPAC lowes-locant abbreviation for hexadeca(trifluoromethyl)*(C_{70}-$D_{5h(6)}$)*[5,6]fullerene*
		DFT	**AM1**	
6		4.8	8.6	1, 4, 8, 11, 16, 19, 23, 26, 31, 37, 41, 48, 55, 60, 67, 69
7		8.0	5.6	1, 4, 8, 11, 16, 19, 24, 27, 31, 37, 41, 43, 51, 53, 56, 64
8		8.3	5.3	1, 4, 8, 11, 16, 19, 27, 31, 37, 41, 44, 47, 55, 60, 67, 69
9		15.4	15.2	1, 4, 8, 11, 18, 23, 31, 33, 35, 38, 51, 53, 55, 58, 61, 64
10		15.4	10.4	1, 4, 8, 11, 16, 19, 23, 26, 31, 34, 37, 41, 48, 52, 60, 69

№№	*Schlegel Diagrams of* $C_{70}(CF_3)_{16}$	$\Delta_f H_0^o$ kJ/mol		*IUPAC lowes-locant abbreviation for hexadeca(trifluoromethyl)(C_{70}-$D_{5h(6)}$)[5,6]fullerene*
		DFT	**AM1**	
11		18.0	9.5	1, 4, 8, 11, 19, 24, 27, 31, 36, 41, 43, 46, 51, 57, 62, 64
12		23.4	11.4	1, 4, 8, 11, 16, 19, 23, 27, 31, 37, 41, 47, 55, 60, 67, 69
13		24.0	20.9	1, 4, 7, 11, 16, 19, 24, 31, 34, 37, 41, 44, 47, 52, 60, 69
14		24.1	20.3	1, 4, 7, 11, 16, 19, 24, 31, 37, 41, 44, 47, 55, 60, 67, 69
15		24.8	24.0	1, 4, 7, 11, 18, 24, 31, 33, 35, 44, 47, 51, 53, 58, 61, 64

№№	*Schlegel Diagrams of* $C_{70}(CF_3)_{16}$	$\Delta_f H_0^o$ kJ/mol		*IUPAC lowes-locant abbreviation for hexadeca(trifluoromethyl)(C_{70}-$D_{5h(6)}$)[5,6]fullerene*
		DFT	**AM1**	
16		26.3	10.6	1, 4, 8, 11, 16, 19, 23, 27, 31, 34, 37, 41, 47, 52, 60, 69
17		27.8	24.0	1, 4, 7, 11, 18, 24, 31, 33, 35, 38, 51, 53, 55, 58, 61, 64
18		28.2	24.1	1, 4, 7, 11, 24, 31, 33, 38, 44, 47, 51, 53, 55, 58, 61, 64
19		29.4	10.5	1, 4, 8, 11, 18, 23, 27, 31, 35, 38, 44, 51, 55, 58, 61, 64
20		34.5	16.1	1, 4, 8, 11, 19, 23, 26, 31, 34, 41, 48, 52, 55, 60, 67, 69

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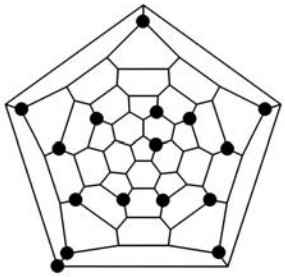
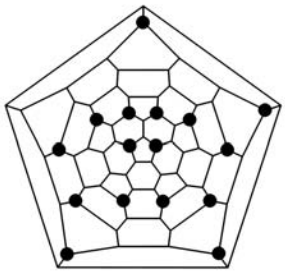
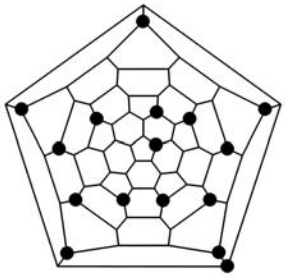
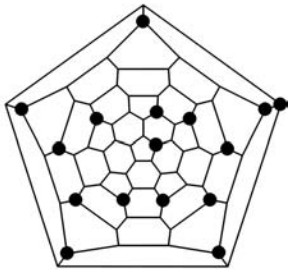
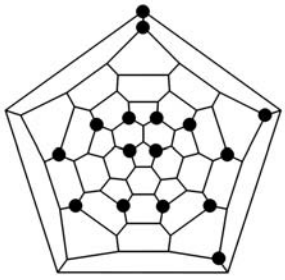
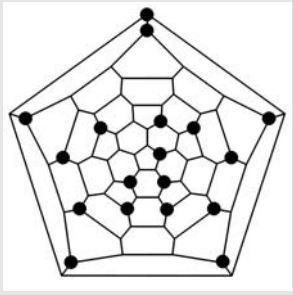
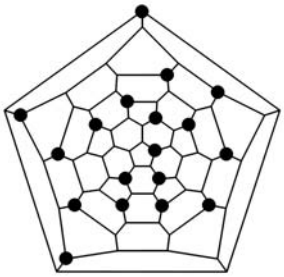
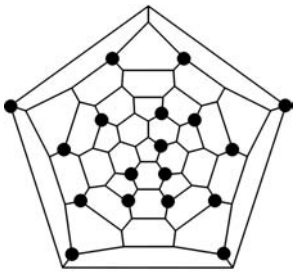
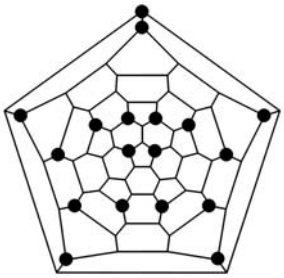
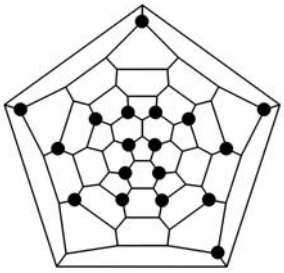
		DFT	**AM1**	
21		37.3	20.4	1, 4, 8, 11, 18, 23, 27, 31, 35, 44, 46, 47, 51, 58, 61, 64
22		42.5	15.4	1, 4, 8, 11, 18, 23, 27, 31, 35, 38, 47, 51, 55, 58, 61, 64
23		> 30	19.9	1, 4, 8, 11, 18, 23, 26, 27, 31, 35, 44, 47, 51, 58, 61, 64
24		> 30	22.7	1, 4, 8, 11, 18, 23, 25, 27, 31, 35, 44, 47, 51, 58, 61, 64
25		> 30	23.9	1, 4, 8, 11, 18, 23, 24, 27, 31, 35, 38, 51, 55, 58, 61, 64

Table 2. Schlegel diagrams, relative energies (at the DFT and AM1 levels of theory), and IUPAC lowest-locant abbreviation for the most stable isomers of $C_{70}(CF_3)_{18}$ within the gap of 40 kJ/mol (the field with experimentally observed isomer is shadowed).

№№	*Schlegel Diagrams of $C_{70}(CF_3)_{18}$*	$\Delta_f H^o_0$ kJ/mol		*IUPAC lowes-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		6.4	10.0	1, 4, 7, 11, 18, 21, 24, 31, 33, 35, 39, 44, 47, 51, 53, 58, 61, 64
3		8.6	17.6	1, 4, 8, 11, 16, 19, 23, 26, 31, 34, 37, 41, 45, 48, 52, 60, 63, 69
4		24.3	5.8	1, 4, 8, 11, 18, 23, 24, 27, 31, 35, 38, 44, 47, 51, 55, 58, 61, 64
5		24.9	6.9	1, 4, 8, 11, 16, 19, 24, 27, 31, 37, 41, 43, 46, 51, 53, 56, 62, 64

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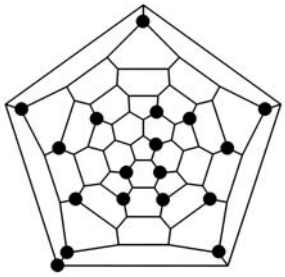
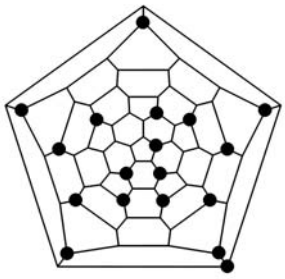
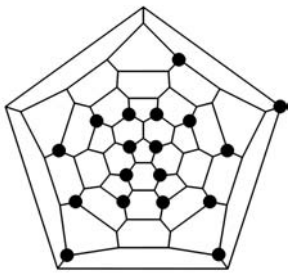
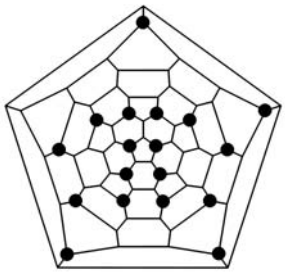
		DFT	**AM1**	
6		29.7	20.5	1, 4, 8, 11, 16, 19, 23, 24, 27, 31, 34, 37, 41, 44, 47, 52, 60, 69
7		30.3	20.0	1, 4, 8, 11, 16, 19, 23, 24, 27, 31, 37, 41, 44, 47, 55, 60, 67, 69
8		34.7	15.0	1, 4, 8, 11, 16, 19, 23, 26, 31, 34, 37, 41, 48, 52, 55, 60, 67, 69
9		43.8	13.9	1, 4, 8, 11, 16, 19, 23, 27, 31, 34, 37, 41, 47, 52, 55, 60, 67, 69