Electronic supplementary materials

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Synthesis and molecular structure of 1,6,11,16,18,24,27,36-$C_{60}(CF_3)_8$

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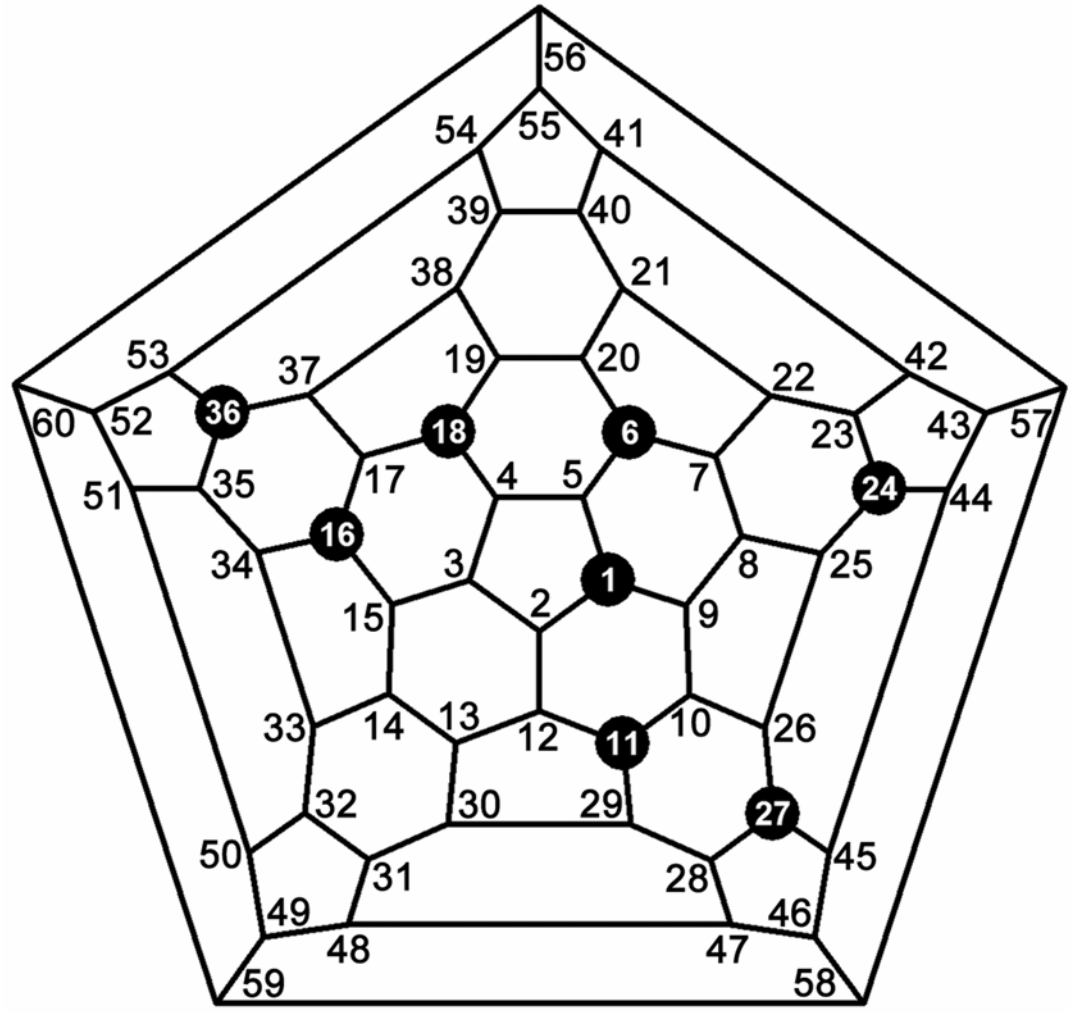
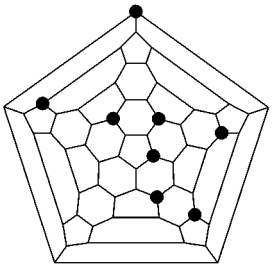
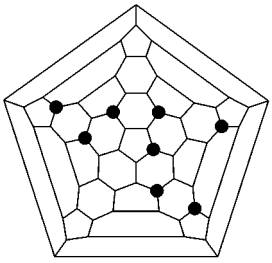
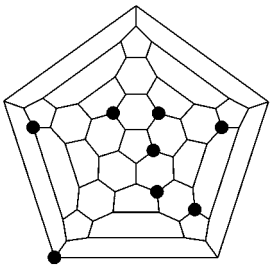
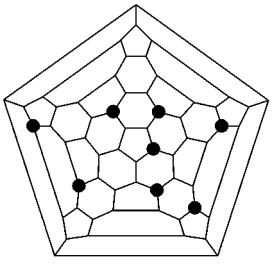
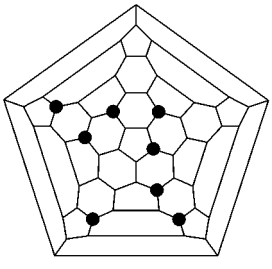
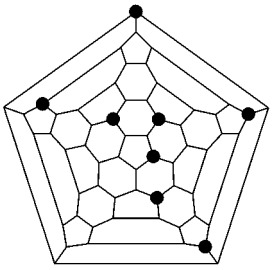
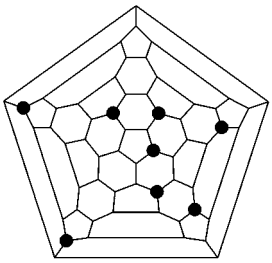
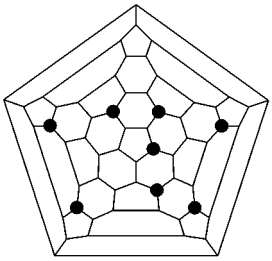
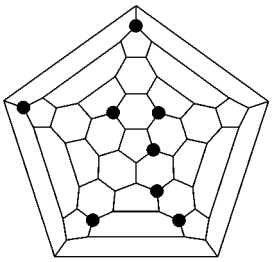
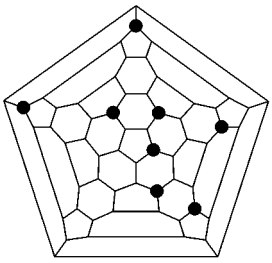
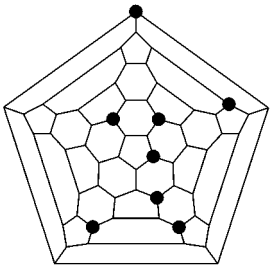
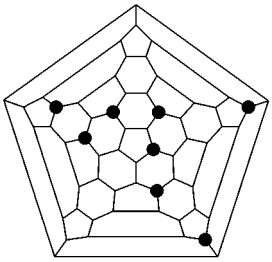
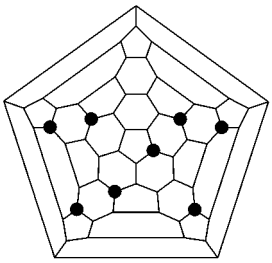
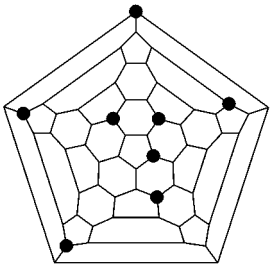
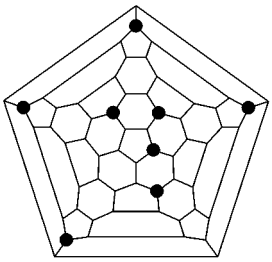
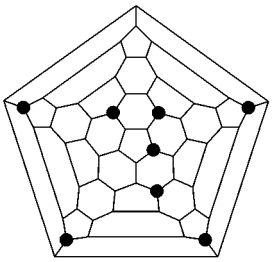
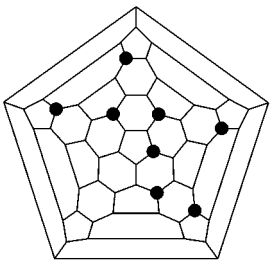


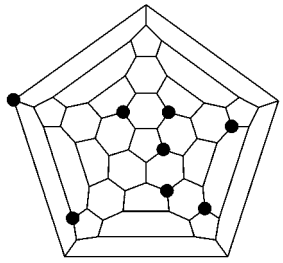
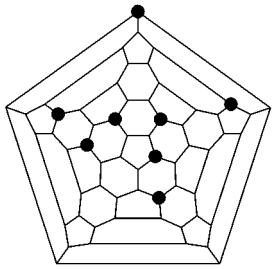
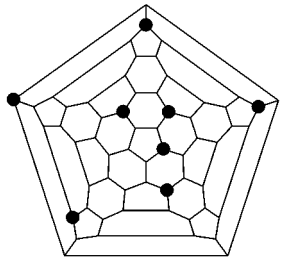
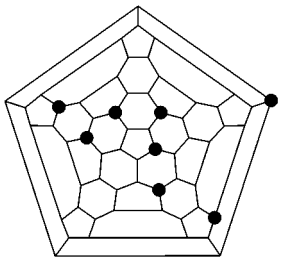
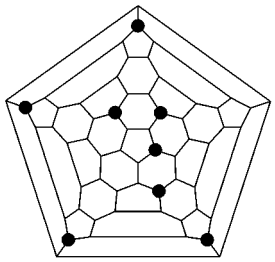
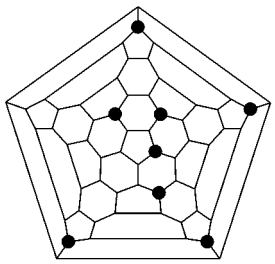
Figure 1. Carbon cage numeration of the experimental $p^3(mp)^2$-$C_{60}(CF_3)_8$ isomer

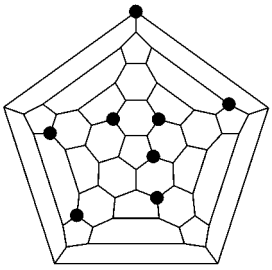
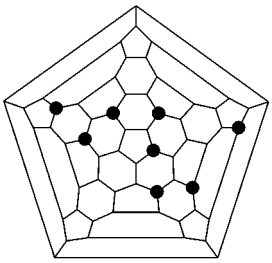
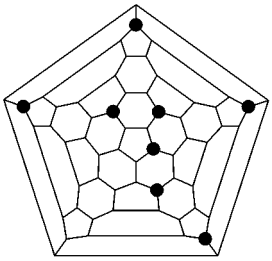
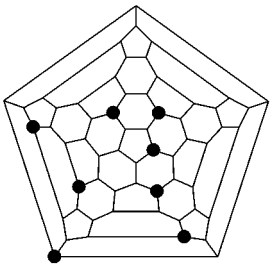
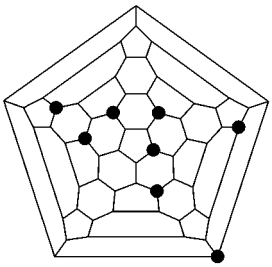
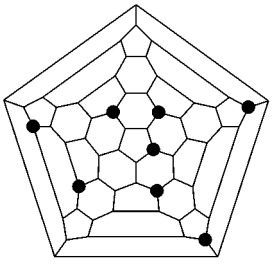
Table 1. The Schlegel diagrams, relative energies (at the DFT and AM1 levels of theory), and IUPAC lowest-locant abbreviation for the most stable isomers of $C_{60}(CF_3)_8$ within the gap of 20 kJ mol^{-1} and for the C_{2v} structure with the addition pattern of $C_{60}Br_8$ (the fields with experimentally observed isomer are shadowed).

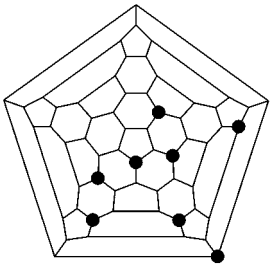
№№	***Schlegel Diagrams of $C_{60}(CF_3)_8$***	$\Delta_f H_0^o$ **kJ mol^{-1}**		***IUPAC lowest-locant abbreviation for octa(trifluoromethyl)(C_{60}-I_h)[5,6]fullerene***
		DFT	***AM1***	
1		0.0	8.5	1, 6, 11, 18, 24, 27, 53, 56
2		2.6	0.0	1, 6, 11, 16, 18, 24, 27, 36
3		3.8	8.3	1, 6, 11, 18, 24, 27, 51, 59
4		6.5	7.2	1, 6, 11, 18, 24, 27, 33, 51
5		10.3	8.8	1, 6, 11, 16, 18, 28, 31, 36

		$\Delta_f H_0^o$ **kJ mol^{-1}**		
6		10.8	20.4	1, 6, 11, 18, 43, 46, 53, 56
7		11.0	11.1	1, 6, 11, 18, 24, 27, 49, 52
8		11.1	14.2	1, 6, 11, 18, 24, 27, 32, 35
9		11.4	22.2	1, 6, 11, 18, 28, 31, 52, 55
10		11.4	11.7	1, 6, 11, 18, 24, 27, 52, 55
11		12.3	21.7	1, 6, 11, 18, 28, 31, 42, 56

		$\Delta_f H_0^o$ **kJ mol^{-1}**		
12		12.4	21.5	1, 6, 11, 16, 18, 36, 43, 46
13		12.9	8.8	1, 7, 11, 24, 33, 47, 51, 59
14		13.0	21.2	1, 6, 11, 18, 42, 49, 52, 56
15		15.2	9.8	1, 6, 11, 18, 43, 49, 52, 55
16		16.3	11.4	1, 6, 11, 18, 43, 46, 49, 52
17		16.3	20.9	1, 6, 11, 18, 24, 27, 36, 39

		$\Delta_f H_0^o$ **kJ mol^{-1}**		
18		16.6	13.5	1, 6, 11, 18, 24, 27, 50, 60
19		17.0	26.5	1, 6, 11, 16, 18, 36, 42, 56
20		17.1	24.1	1, 6, 11, 18, 43, 50, 55, 60
21		17.6	26.8	1, 6, 11, 16, 18, 36, 45, 57
22		18.0	11.9	1, 6, 11, 18, 46, 49, 52, 55
23		18.8	11.2	1, 6, 11, 18, 43, 46, 49, 55

		$\Delta_f H_0^o$ **kJ mol^{-1}**		
24		19.1	35.7	1, 6, 11, 18, 32, 35, 42, 56
25		19.1	12.4	1, 6, 11, 16, 18, 26, 36, 44
26		19.2	11.3	1, 6, 11, 18, 43, 46, 52, 55
27		19.8	19.1	1, 6, 11, 18, 33, 47, 51, 59
28		20.3	25.2	1, 6, 11, 16, 18, 36, 44, 58
29		21.2	30.6	1, 6, 11, 18, 33, 43, 46, 51

		$\Delta_f H_0^o$ **kJ mol^{-1}**		
30		21.3	24.9	1, 6, 11, 18, 24, 27, 41, 57
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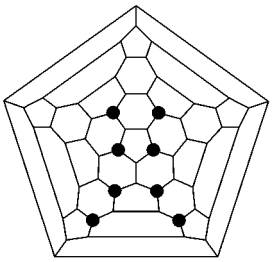
75		46.2	57.1	1, 3, 6, 11, 13, 18, 28, 31

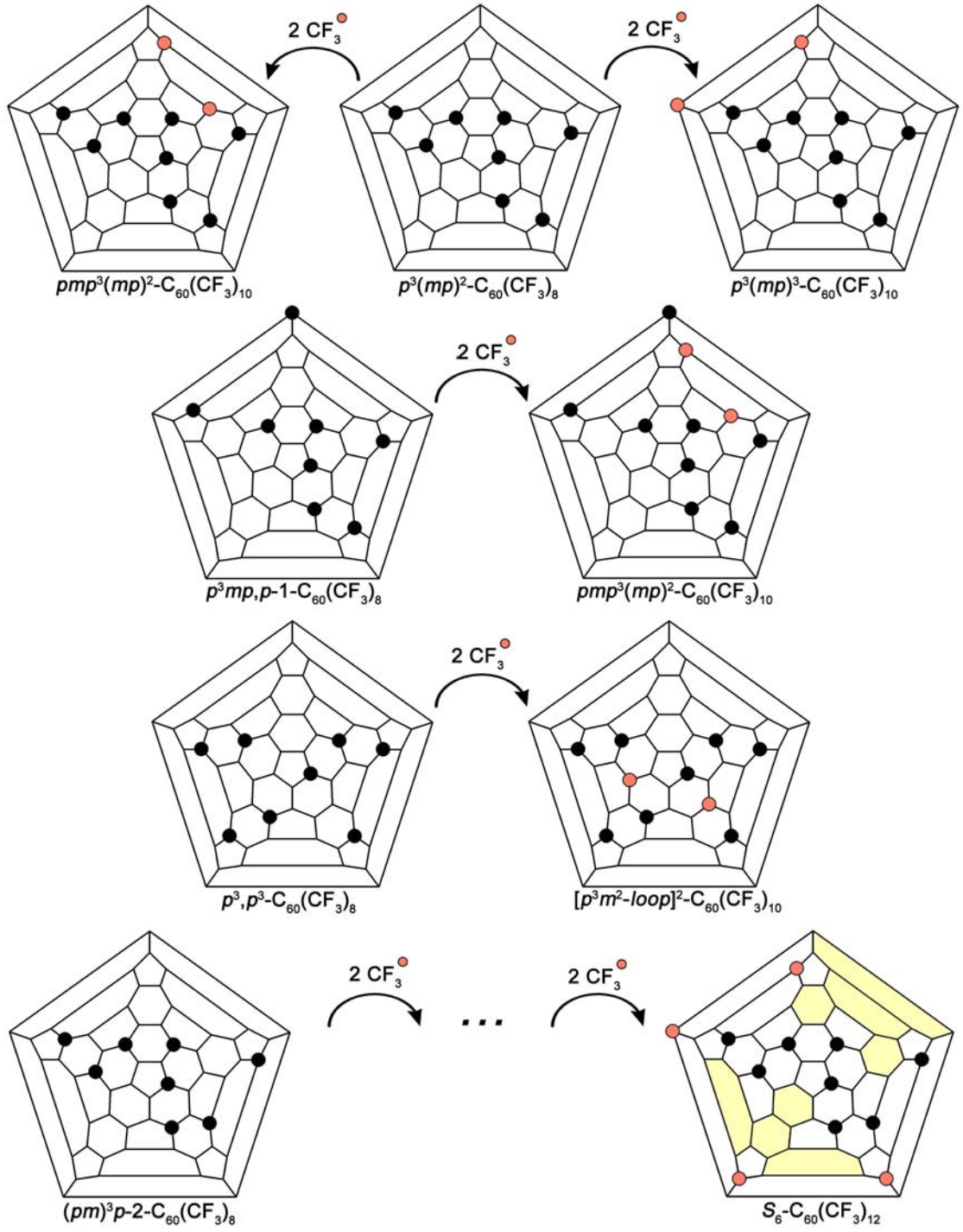


Figure 2. Relations between experimental and theoretically considered $C_{60}(CF_3)_8$ isomers and experimentally found isomers of $C_{60}(CF_3)_{10}$[2-4] and S_6-$C_{60}(CF_3)_{12}$[5]

References

1 P. R. Birkett, P. B. Hitchcock, H. W. Kroto, R. Taylor, and D. R. M. Walton. *Nature*, 1992, **357**, 479.

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5 S. I. Troyanov, Dimitrov A., and E. Kemnitz. *Angew. Chem. Int. Ed.*, 2006, **45**, 1971.