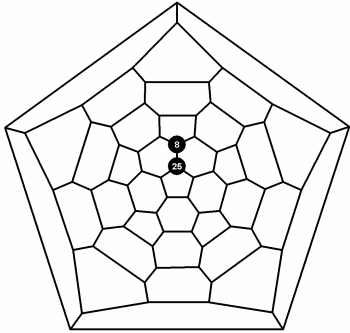
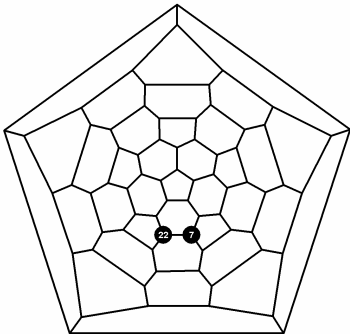
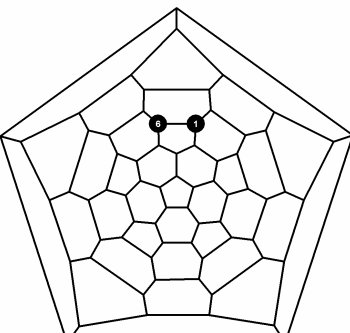


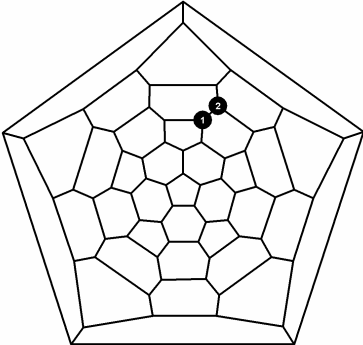
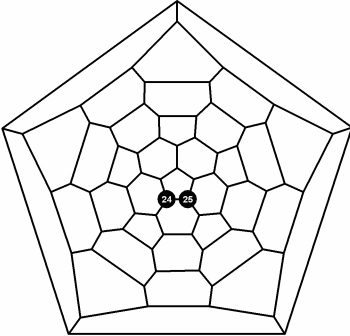
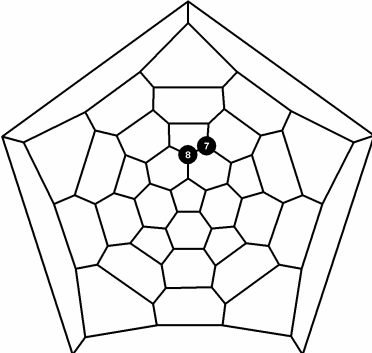
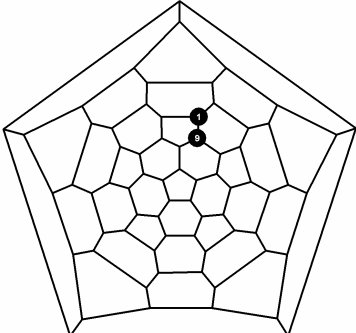
## Supporting information for

### Synthesis and structure of cycloperfluoroalkylated derivatives of $C_{70}$ , $C_{70}(C_2F_4)$ and $C_{70}(C_4F_8)_n$ , $n = 1 - 6$

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Table S1. Schlegel diagrams, relative energies and IUPAC abbreviation for the most stable isomers of  $C_{70}(C_2F_4)$  within the gap of  $170 \text{ kJ mol}^{-1}$ .

Stability order	Schlegel diagram	$\Delta\Delta_f H_0^0$ , $\text{kJ mol}^{-1}$	IUPAC abbreviation
1		0.0	8,25- $C_{70}C_2F_4$
2		14.3	7,22- $C_{70}C_2F_4$
3		40.6	1,6- $C_{70}C_2F_4$

4		58.5	1,2-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>
5		69.6	24,25-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>
6		72.3	7,8-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>
7		80.7	1,9-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>

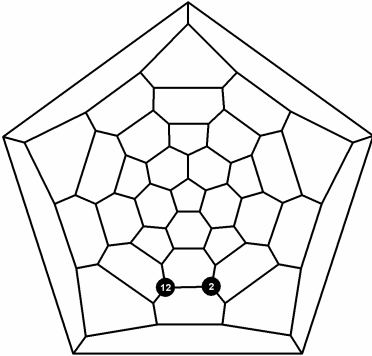
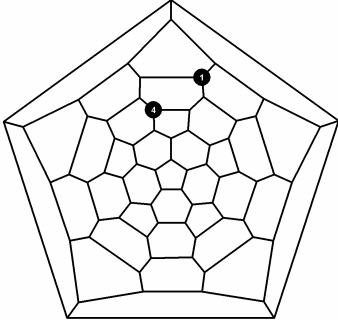
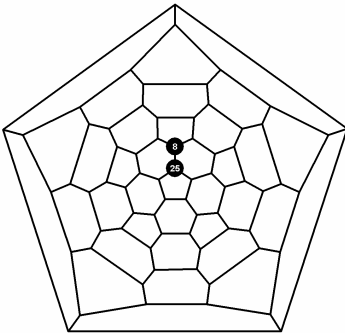
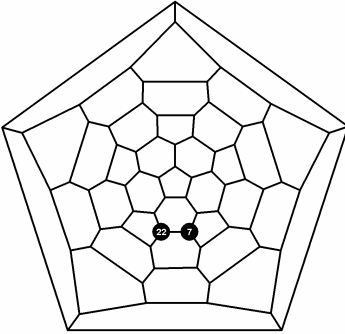
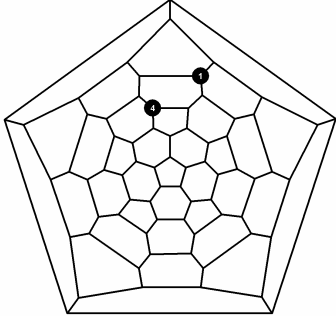
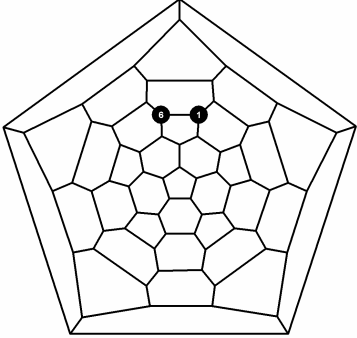
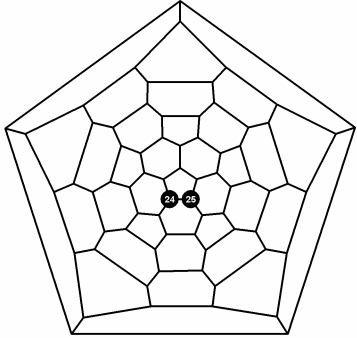
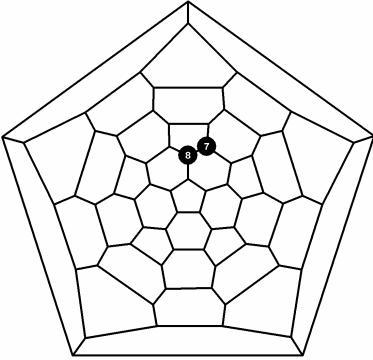
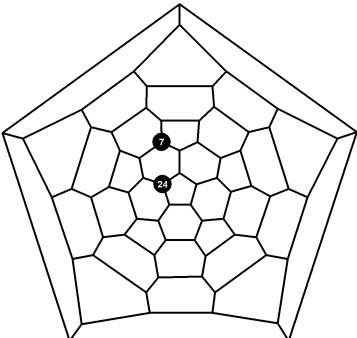
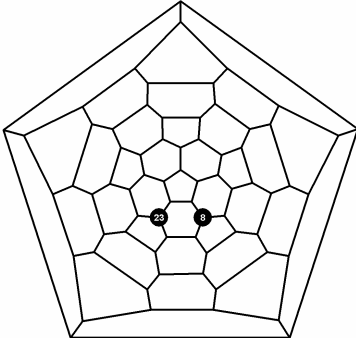
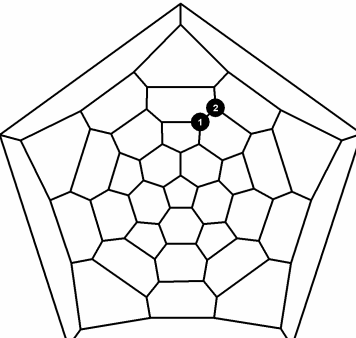
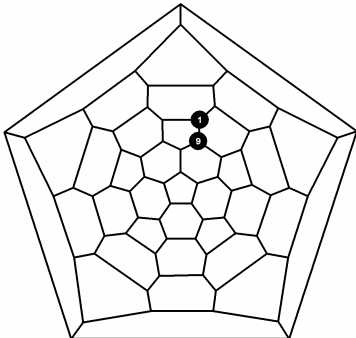
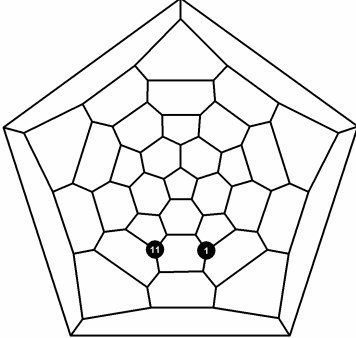
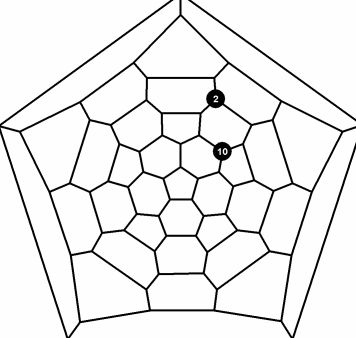
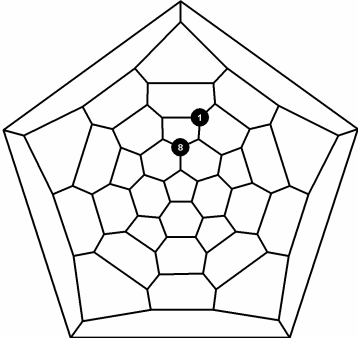
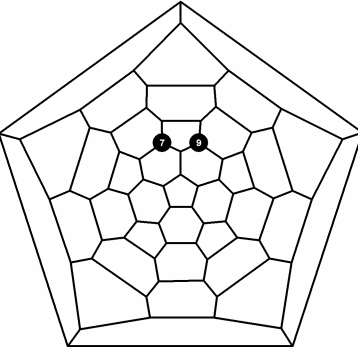
8		94.5	2,12-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>
9		167.9	1,4-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>

Table S2. Schlegel diagrams, relative energies and IUPAC abbreviation for the most stable isomers of C<sub>70</sub>(C<sub>4</sub>F<sub>8</sub>) within the gap of 120 kJ mol<sup>-1</sup>.

Stability order	Schlegel diagram	$\Delta\Delta_f H_0^0$ , kJ mol <sup>-1</sup>	IUPAC abbreviation	Conformation
1		0.0	8,25-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	boat
2		13.7	7,22-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	boat

3		24.9	1,4-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	chair
4		33.7	1,6-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	boat
5		56.5	24,25-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	boat
6		58.7	7,8-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	boat
7		58.7	7,24-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	chair_2

8		64.3	8,23-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	chair
9		69.2	1,2-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	boat
10		69.6	1,9-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	boat
11		85.0	1,11-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	chair
12		103.9	2,10-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	chair_2

13		111.0	1,8-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	chair <sub>1</sub>
14		111.6	7,9-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	chair