

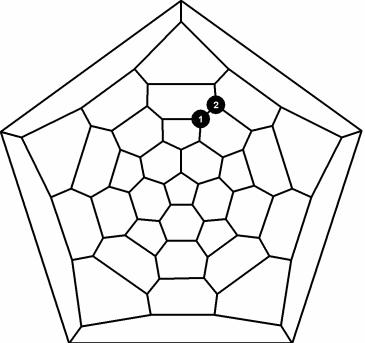
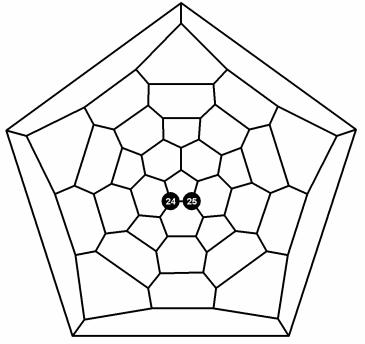
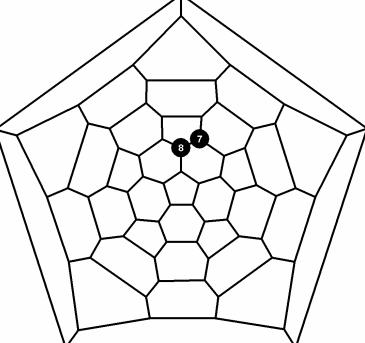
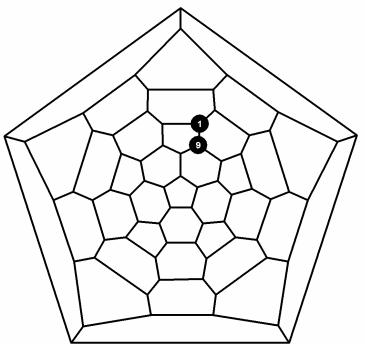
## Supporting information for

### Synthesis and structure of cycloperfluoroalkylated derivatives of C<sub>70</sub>, C<sub>70</sub>(C<sub>2</sub>F<sub>4</sub>) and C<sub>70</sub>(C<sub>4</sub>F<sub>8</sub>)<sub>n</sub>, n = 1 – 6

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Table S1. Schlegel diagrams, relative energies and IUPAC abbreviation for the most stable isomers of C<sub>70</sub>(C<sub>2</sub>F<sub>4</sub>) within the gap of 170 kJ mol<sup>-1</sup>.

Stability order	Schlegel diagram	$\Delta\Delta_fH_0^0$ , kJ mol <sup>-1</sup>	IUPAC abbreviation
1		0.0	8,25-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>
2		14.3	7,22-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>
3		40.6	1,6-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>

4	 A diagram of a C <sub>70</sub> molecule, which is a truncated icosahedron composed of 12 pentagonal and 20 hexagonal faces. Two small black circles labeled '1' and '2' are placed on the surface, representing the attachment points for the substituents.	58.5	1,2-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>
5	 A diagram of a C <sub>70</sub> molecule. Two small black circles labeled '24' and '25' are placed on the surface, representing the attachment points for the substituents.	69.6	24,25-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>
6	 A diagram of a C <sub>70</sub> molecule. Two small black circles labeled '7' and '8' are placed on the surface, representing the attachment points for the substituents.	72.3	7,8-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>
7	 A diagram of a C <sub>70</sub> molecule. Two small black circles labeled '1' and '9' are placed on the surface, representing the attachment points for the substituents.	80.7	1,9-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>

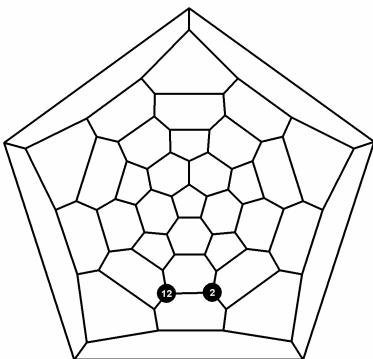
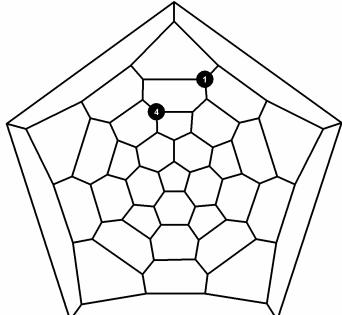
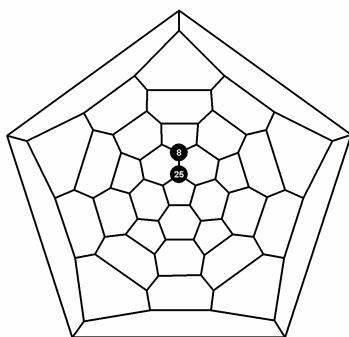
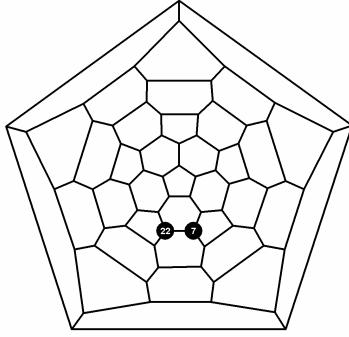
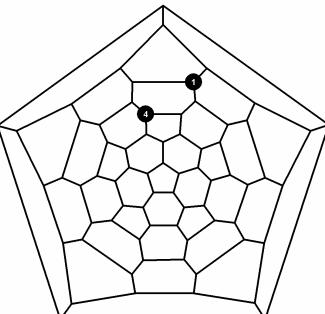
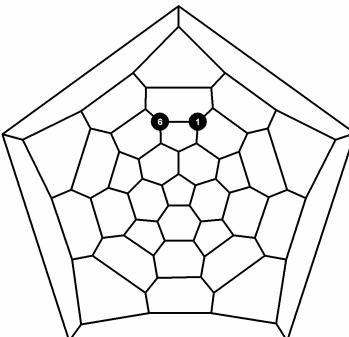
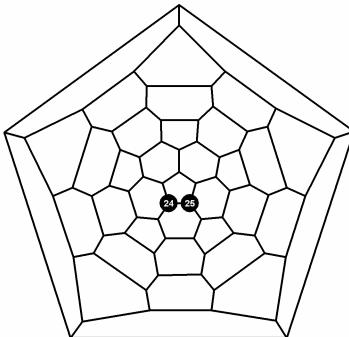
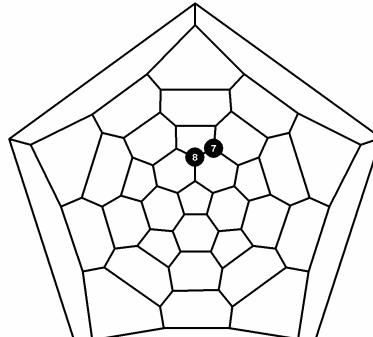
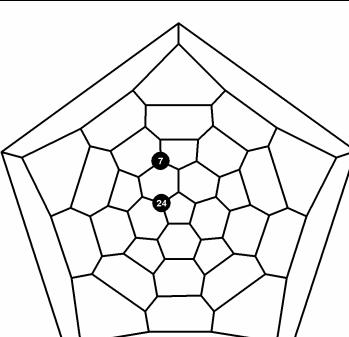
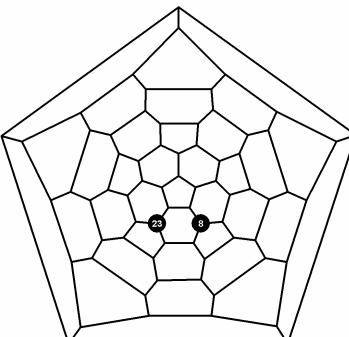
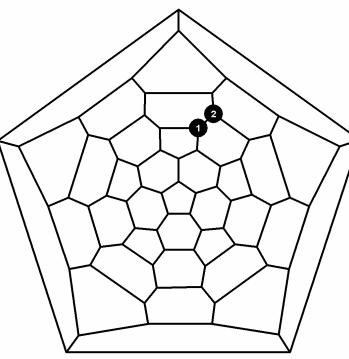
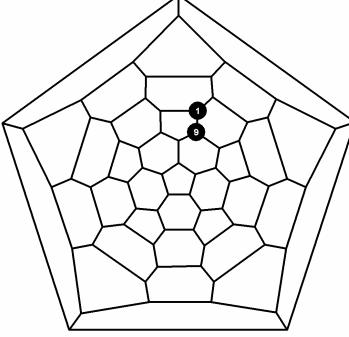
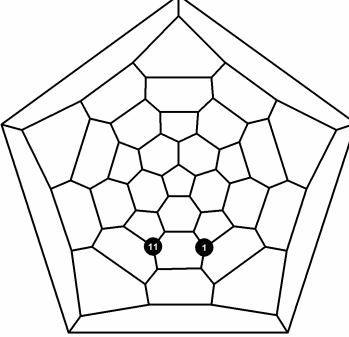
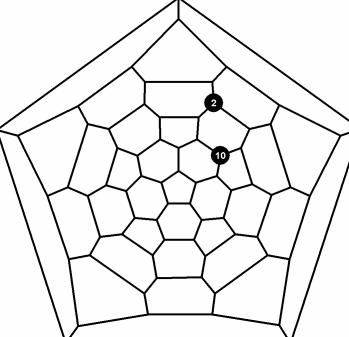
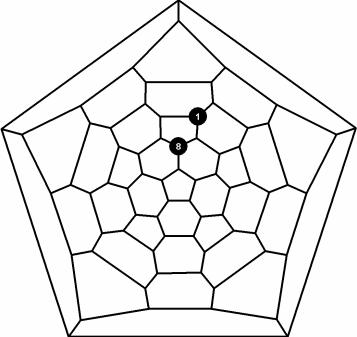
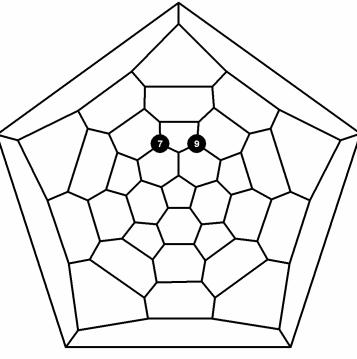
8		94.5	2,12-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>
9		167.9	1,4-C <sub>70</sub> C <sub>2</sub> F <sub>4</sub>

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	$\Delta\Delta_fH_0^0$ , 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-C70C4F8	chair
4		33.7	1,6-C70C4F8	boat
5		56.5	24,25-C70C4F8	boat
6		58.7	7,8-C70C4F8	boat
7		58.7	7,24-C70C4F8	chair_2

8		64.3	8,23-C70C4F8	chair
9		69.2	1,2-C70C4F8	boat
10		69.6	1,9-C70C4F8	boat
11		85.0	1,11-C70C4F8	chair
12		103.9	2,10-C70C4F8	chair_2

13		111.0	1,8-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	chair_1
14		111.6	7,9-C <sub>70</sub> C <sub>4</sub> F <sub>8</sub>	chair