

Supplementary Information

Table I: TURBOMOLE V6.1 RI-MP2/def2-TZVP, NATURAL POPULATION ANALYSIS atomic charge distribution of iodo derivatives of parent anion **1**.

Cluster position	CB ₇ H ₈ ⁻	CB ₇ H ₇ -I ⁻	CB ₇ H ₆ -I ₂ ⁻	CB ₇ H ₅ -I ₃ ⁻	CB ₇ H ₂ -I ₆ ⁻
C1	-0,67	-0,67	-0,66	-0,68	-0,75
B2	0,05	0,06	0,06	0,05	0,02
B3	-0,01	-0,01	-0,01	0,00	-0,04
B4	-0,01	-0,01	-0,01	0,00	-0,04
B5	0,10	0,11	0,11	0,10	0,10
B6	-0,12	-0,11	-0,11	-0,13	-0,15
B7	-0,23	-0,22	-0,24	-0,25	-0,28
B8	-0,23	-0,22	-0,24	-0,25	-0,28

Table II: Calculated proton affinities of the parent anion **1** and iodo-derivatives

Compound	E/Hartree	deprotonised E/Hartree	proton affinity [kJ/mol]
CB ₇ H ₈ ⁻	-216.3739	-215.6091	2007.81
7-I-CB ₇ H ₇ ⁻	-512.9993	-512.2548	1954.73
7,8-I ₂ -CB ₇ H ₆ ⁻	-809.6230	-808.8946	1912.20
6,7,8-I ₃ -CB ₇ H ₅ ⁻	-1106.2443	-1105.5318	1870.53
2,6,7,8-I ₄ -CB ₇ H ₄ ⁻	-1402.8635	-1402.1704	1819.72
3,6,7,8-I ₄ -CB ₇ H ₄ ⁻	-1402.8636	-1402.1659	1831.60
5,6,7,8-I ₄ -CB ₇ H ₄ ⁻	-1402.8637	-1402.1698	1821.94
3,4,6,7,8-I ₅ -CB ₇ H ₃ ⁻	-1699.4820	-1698.7978	1796.15
2,5,6,7,8-I ₅ -CB ₇ H ₃ ⁻	-1699.4820	-1698.8049	1777.63
2,3,6,7,8-I ₅ -CB ₇ H ₃ ⁻	-1699.4826	-1698.8018	1787.45
3,5,6,7,8-I ₅ -CB ₇ H ₃ ⁻	-1699.4828	-1698.8014	1789.22
2,3,4,6,7,8-I ₆ -CB ₇ H ₂ ⁻	-1996.1010	-1995.4315	1757.89
2,3,4,5,6,7,8-I ₇ -CB ₇ H ⁻	-2292.7201	-2292.0631	1725.06