Charge-induced Restructuring and Decomposition of Bucky-diamonds †

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1 Supplementary Information



Fig. 1 Average C–C bond distance ($\langle d \rangle$) for the anionic (top) and cationic (bottom) C₇₀₅ (left) and C₈₃₇ (right) bucky-diamonds, as a function of electrons (i.e. charge state).



Fig. 2 Average C–C–C bond angle ($\langle \theta \rangle$) and average C–C–C–C dihedral angle ($\langle \phi \rangle$) of anionic C₇₀₅ (left) and C₈₃₇ (right) bucky-diamonds, as a function of electrons (i.e. charge state).



Fig. 3 C–C–C bond angle ($\langle \theta \rangle$) and average C–C–C–C dihedral angle ($\langle \phi \rangle$) of cationic C₇₀₅ (left) and C₈₃₇ (right) bucky-diamonds, as a function of cations (i.e. charge state).

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