Charge-induced Restructuring and Decomposition of Bucky-diamonds †

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1 Supplementary Information

Fig. 1 Average C–C bond distance (\(d\)) for the anionic (top) and cationic (bottom) \(C_{705}\) (left) and \(C_{837}\) (right) bucky-diamonds, as a function of electrons (i.e. charge state).

Fig. 2 Average C–C bond angle (\(\theta\)) and average C–C–C–C dihedral angle (\(\phi\)) of anionic \(C_{705}\) (left) and \(C_{837}\) (right) bucky-diamonds, as a function of electrons (i.e. charge state).

Fig. 3 C–C bond angle (\(\theta\)) and average C–C–C–C dihedral angle (\(\phi\)) of cationic \(C_{705}\) (left) and \(C_{837}\) (right) bucky-diamonds, as a function of cations (i.e. charge state).

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