Charge-induced Restructuring and Decomposition of Bucky-diamonds [†]

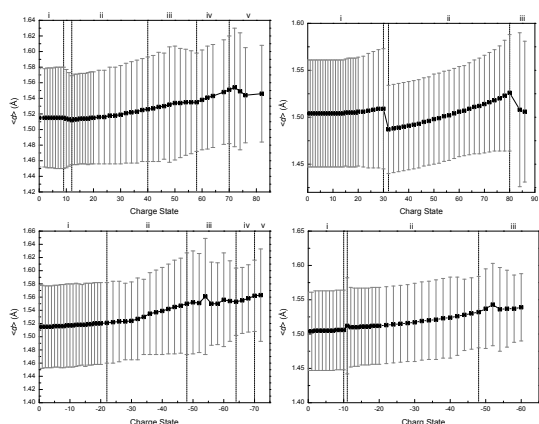**Lin Lai,**[*a] **Amanda S. Barnard**[a]

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).
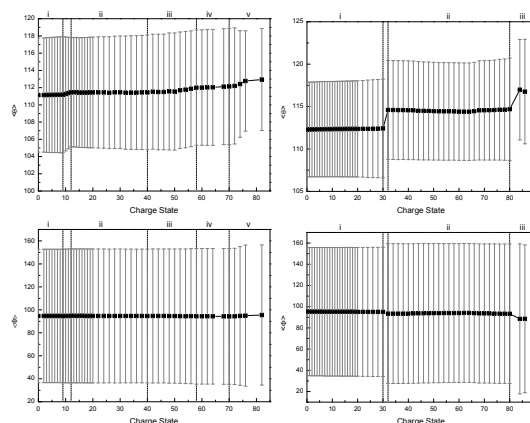

Fig. 2 Average C–C–C bond angle ($<\theta>$) and average C–C–C–C dihedral angle ($<\phi>$) of anionic C_{705} (left) and C_{837} (right) bucky-diamonds, as a function of electrons (i.e. charge state).
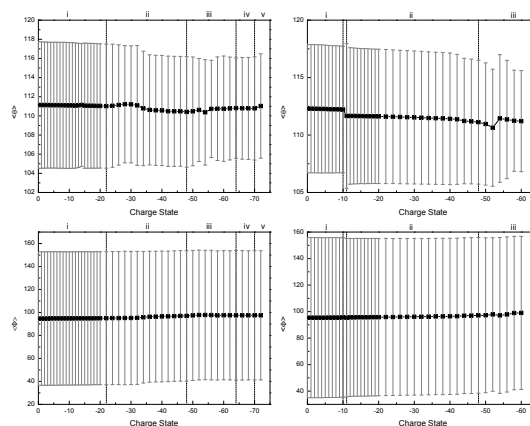
Fig. 3 C–C–C bond angle ($<\theta>$) and average C–C–C–C dihedral angle ($<\phi>$) of cationic C_{705} (left) and C_{837} (right) bucky-diamonds, as a function of cations (i.e. charge state).

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