

Novel Monometallic Cyanide Clusterfullerenes Based on Popular Fullerene Cages

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Since the first proposal that fullerenes are capable of hosting atoms, ions, or clusters by the late Smalley in 1985, tremendous examples of endohedral metallofullerenes (EMFs) have been reported. It has been commonly believed that monometallofullerenes (mono-EMFs) always exist as a simple form of $M@C_{2n}$ and clusterfullerenes always require multiple (two to four) metal cations to stabilize a cluster that is unstable as a single moiety.¹⁻⁶ We present here the first isolation of an unprecedented monometallic cyanide endohedral clusterfullerene based on the popular fullerene cages, for which the cage symmetry and the endohedral cyanide structure have been determined unambiguously by X-ray crystallography and ¹³C NMR spectroscopy.

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