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Structure determination of Sc_2C_2 cluster encaged fullerene

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Introduction

Endohedral metallofullerenes (EMFs) encapsulate one or more metal atoms inside a hollow fullerene cage.[1,2] These fullerenes have attracted special interest as new spherical molecules with unique properties that are not found in empty fullerenes. Especially, the Sc-containing EMFs are attractive not only because of the high production yield of some species but also because of the diversity of the metallic species that can be encapsulated. To date, one or two Sc atoms, scandium carbide (Sc_2C_2/Sc_3C_2/ Sc_4C_2), scandium nitride (Sc_3N), scandium oxide (Sc_2O/Sc_3O_2/ Sc_4O_3), scandium cyanide (Sc_3CN), and even scandium sulfide (Sc_2S) are all found for Sc-EMFs. However, structures of many isomers of Sc-EMFs remain undetermined. Because two carbon atoms, instead of constructing the fullerene cage, can be encapsulated with metals forming carbide clusters, structural identification of Sc-EMFs is fairly important and sometimes troublesome.

Result and discussion

Single crystallography is certainly the most reliable method for structural determination. However, the spherical shapes of fullerenes and EMFs have hindered direct X-ray diffraction (XRD) characterization because the molecules rotate rapidly in the crystal lattice. To solve this problem, Sc_2C_{82} was first functionalized with adamantylidene carbene (Ad) to obtain the cycloadducts. Then, single crystals of a monoadduct isomer suitable for synchrotron X-ray measurement were obtained by a diffusion method; its structure is firmly established, as shown in Figure 1.[3] The adduct results from the 6,6-addition of Ad and has an opened structure. Two C atoms and two Sc atoms are encaged inside the cage originating from $C_{2v}(5)$-C_{80}. At 90 K, the Sc_2C_2 moiety was observed to be no disordered, indicating localization of the Sc_2C_2 cluster in the C_{80} cage.

References

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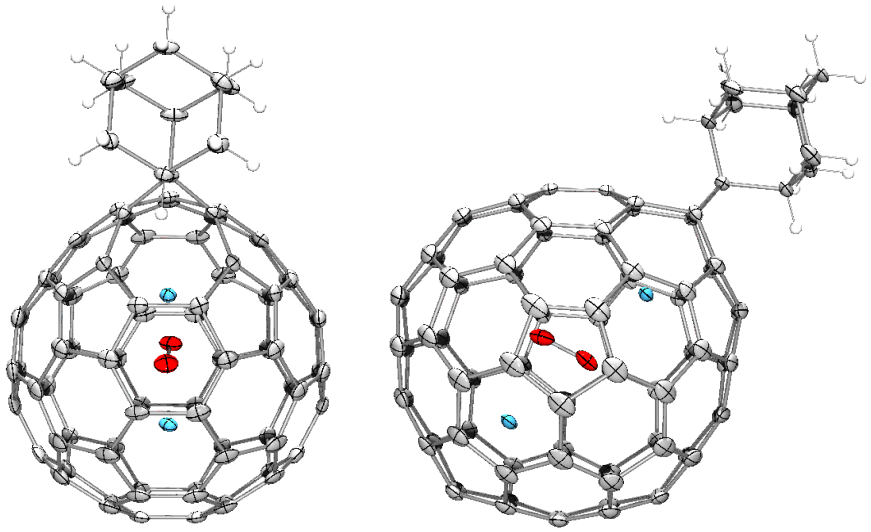

Figure 1
ORTEP drawing of a $Sc_2C_2@C_{80}$ derivative with 50% probability ellipsoids. Carbide, carbon, hydrogen and scandium atoms are colored red, gray, white and blue, respectively.