

Cover Picture

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The cover picture shows a section of the electron charge density of the first metal carbide endohedral metallofullerene (Sc_2C_2)@ C_{84} obtained from a synchrotron X-ray powder diffraction study by the maximum entropy method (MEM). The several density maxima, which correspond to scandium and carbon atoms, are clearly seen inside the C_{84} carbon cage. The MEM charge density distribution also reveals that the C_{84} cage has D_{2d} symmetry (no. 23) and that the C_2 axis is parallel to the $\langle 100 \rangle$ face-centered cubic (fcc) direction of the unit cell. As a consequence of the site symmetry being $4mm$, the C_2 axis of (Sc_2C_2)@ C_{84} is oriented to six equivalent $\langle 100 \rangle$ directions and shows a merohedral disorder. The resultant $\text{Sc} \cdots \text{Sc}$ distances and $\text{C}-\text{C}$ bond lengths of the Sc_2C_2 cluster are 0.429(2) and 0.142(6) nm, respectively. The observed $\text{C}-\text{C}$ bond length is between that of a typical single and a double bond, and is very close to that of the $\text{C}-\text{C}$ bond (0.143 nm) combining two pentagons in a C_{60} molecule. More about this fascinating structure can be found in the contribution by Shinohara and co-workers on p. 397 ff.

