

Vibrations and Dynamics of Multi Atomic Encapsulates in Fullerene Cages

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Raman and infrared spectroscopy, supplemented by quantum-mechanical calculations, were used to clarify bonding and dynamical properties of four atomic encapsulates in novel endohedral fullerenes, as e.g. $\text{Sc}_3\text{N}@C_{80}$, and $\text{Sc}_2\text{C}_2@C_{84}$. Low frequency $\text{Sc}_3\text{N}-C_{80}$ and internal Sc_3N modes provided a clear evidence for the formation of a $\text{Sc}_3\text{N}-C_{80}$ bond and a strong scandium-nitrogen bond in $\text{Sc}_3\text{N}@C_{80}$, which are partly responsible for the unusual high stability and abundance of this material [1]. A distinct different behavior was found for endohedral discandium carbide, Sc_2C_2 , where the C_2 unit is only weakly bonded to the scandium atoms and the surrounding fullerene network.

[1] M. Krause, H. Kuzmany, P. Georgi, L. Dunsch, K. Vietze, G. Seifert, J. Chem. Phys. **115**, 6596 (2001)

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