MUTUAL STABILISATION OF TRIMETAL NITRIDE CLUSTERS AND *I_h*-C_{80} FULLERENE

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Infrared and Raman spectroscopy, supported by quantum-mechanical calculations, were used to study stability and structure of endohedral trimetal nitride fullerenes. The variation of the carbon cage size and of the encaged metal pointed to a particularly high stability of $M_3N@C_{80}$ structures, which is due to a mutual stabilisation of trimetal nitride cluster and I_h-C_{80} fullerene. Compared to classical dimetallofullerenes as I_h-$La_2@C_{80}$ and I_h-$Ce_2@C_{80}$ the endohedral $M_3N@C_{80}$ structures are further stabilized by the formation of a M_3N-C_{80} bond and the presence of three strong metal-nitrogen bonds [1].

For $Sc_3N@C_{80}$ the vibrational spectra reveal a Sc_3N cluster structure with a threefold symmetry axis. A reduction of the carbon cage size on the one hand and an increasing size of the trimetal nitride cluster on the other hand induce structural deformations of the cluster. As a consequence, the antisymmetric metal-nitrogen vibration splits into two components for $Sc_3N@C_{78}$, and as shown in Fig. 1, for $M_3N@C_{80}$ fullerenes with larger metal atoms than scandium.

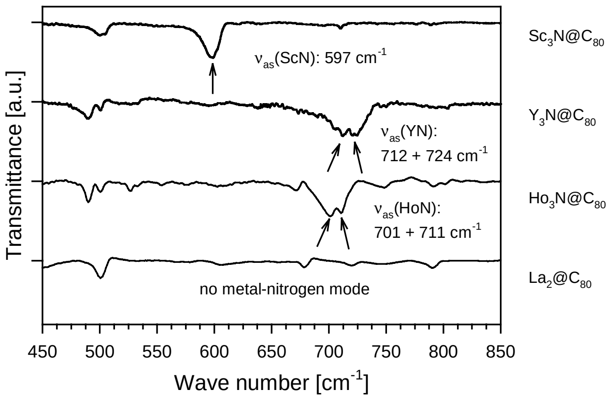

Fig.1: Selected parts of the FTIR spectra of I_h-C_{80} based endohedral fullerenes at 293 K

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