Photoionization and photofragmentation of $Sc_3N@C_{80}^+$ at energies from the carbon K edge to the scandium L and nitrogen K edges

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Synopsis Photoionization of endohedral $Sc_3N@C_{80}^+$ fullerene ions is investigated using synchrotron radiation in the energy range 280 to 420 eV. In the product channels $Sc_3N@C_{80}^{2+}$ and $Sc_3N@C_{78}^{2+}$ clear signatures of the cross section contributions arising from L-shell photoabsorption by the encapsulated Sc atoms have been detected.

Photon-induced reactions of $Sc_3N@C_{80}^+$ ions have been investigated in the energy range 280 – 420 eV employing the **P**hoton-**I**on Spectrometer at **PE**TRA III (PIPE) [1]. The measurements cover photoabsorption near the K edge of carbon, the L edge of scandium and the K edge of nitrogen. Several reaction channels were studied. As an example, Fig. 1 shows the preliminary cross section for single ionization of $Sc_3N@C_{80}^+$ ions. Very clear signatures mainly arising from photoabsorption by Sc atoms near the L edge are visible on top of the contribution of the C_{80} cage. Similar results were obtained for the $Sc_3N@C_{78}^{2+}$ product channel which shows a slightly different spectral shape.

Only the single-ionization channels with and without fragmentation showed significant contributions arising from photoabsorption by one of the encapsulated Sc atoms. This is quite surprising considering that about 400 eV are deposited in the $Sc_3N@C_{80}^+$ molecule when a photon is absorbed by an encapsulated scandium atom with promotion of an L-shell electron. Previous studies on Xe 4d photoabsorption by $Xe@C_{60}^+$ at much lower photon energies of 60 to 150 eV showed strong contributions of double ionization associated with multiple fragmentation [2]. A recent experiment with $Lu_3N@C_{80}^{q+}$, $q = 1,2,3$, exploring photoabsorption near the Lu 3d edge [3] suggested that the whole fullerene molecule explodes when a 1500 to 1700 eV photon is absorbed by one of the Lu atoms. In contrast to that, the present findings for $Sc_3N@C_{80}^+$ indicate that an initial vacancy in the L shell of one of the Sc atoms predominantly results in net single ionization of the atom and subsequently also the whole molecule. Redistribution of 2p and 2s absorption oscillator strengths [4] may then be the reason for different spectral shapes of the measured excess cross sections.

We thank G. Hartmann, F. Scholz, J. Seltmann, and J. Viefhaus for their assistance in using beamline P04. SK acknowledges support from the European Cluster of Advanced Laser Light Sources (EUCALL) project which has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 654220. Funding by BMBF (contracts 05K10RG1, 05K10GUB, 05K16RG1, and 05K16GUC) and DFG (grant Mu-1068/22) is gratefully acknowledged.

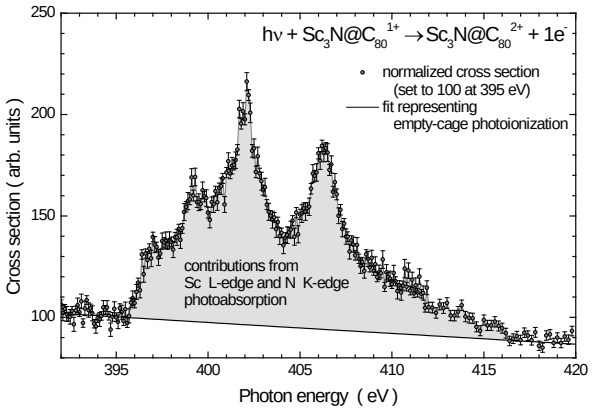

Figure 1. Cross section for single photoionization of $Sc_3N@C_{80}^+$ in the vicinity of the scandium L edge. The data are normalized to 100 Mb at 392 eV.

References

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