Photoionization and photofragmentation of $Lu_3N@C_{80}^{q+}$ ions (q = 1, 2, 3)

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Synopsis Cross sections for photoionization and photofragmentation of singly, doubly and triply charged $Lu_3N@C_{80}$ ions have been measured using the photon-ion merged-beams technique at the PETRA III synchrotron light source. The measured spectra exhibit prominent resonance features at energies around the carbon K edge. In contrast to that, no signatures of the nitogen K and lutetium M edges have been found in the experimentally investigated reaction channels.

We have measured cross sections for photoionization and photofragmentation of endohedral fullerene ions $Lu_3N@C_{80}^{q+}$ (q=1,2,3) [1] employing the photon-ion merged-beams technique [2] at the PIPE end-station [3] of beamline P04 [4] of the PETRA III synchrotron at DESY in Hamburg, Germany. Photo-reaction channels $Lu_3N@C_{80}^{q+} \rightarrow Lu_3N@C_{80-2r}^{p+}$ [q=1,2,3; p=2,3,4,5,6; r=0,1,3,4] were investigated in the photon energy ranges 280–330 eV around the carbon K-shell threshold, 380–435 eV around the nitrogen K-Shell threshold, and 1500–1700 eV around the lutetium M-shell threshold. The present work substantially extends previous studies on (endohedral) fullerenes [5, 6, 7, 8].

In the energy range 280 – 330 eV we could identify a group of resonances present in all investigated reaction channels. Since this group of resonances seems to make up for the most prominent structures in all spectra, we attempted to model each spectrum (see Fig. 1) as a sum of seven Fano resonances (full lines), a threshold feature (dashed line), and a constant background (dash-dotted line). In the multiple ionization channels, a threshold can be observed at about 294 eV. We observe a shift of the ionization threshold towards higher photon energies when comparing double ionization of $Lu_3N@C_{80}^{2+}$ with double ionization of $Lu_3N@C_{80}^{+}$. On the basis of this threshold shift the radius of the endohedral fullerene molecule has been determined to be 0.50 ± 0.04 nm. The cross sections measured at higher photon energies of 380–435 eV and of 1500–1700 eV are monotonically decreasing with increasing photon energy and do not exhibit any structures associated with the nitrogen K edge or the lutetium M edge, respectively. Most probably, the absorption of an energetic 1600-eV photon by one of the Lu atoms leads to a much more violent fragmentation event, such that large fragments cannot be observed. This is interesting, for example, from a radiobiological point of view, and will be more closely investigated in future follow-up experiments.

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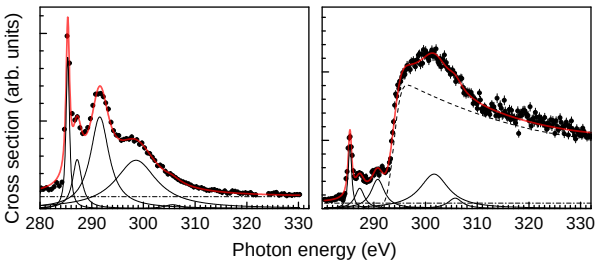

Figure 1. Measured (symbols) and fitted (lines) cross sections for single (left) and double (right) photoionization of $Lu_3N@C_{80}^{+}$ at energies around the C K edge [1].

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