Symmetry Breaking of BF_3 by Core Excitation Probed by Quadruple-Ion Coincidence

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The inner-shell excited states decay via Auger emission with the lifetime of the order of femto-seconds. The nuclear motion of free molecules may however proceed in the core-excited state within this lifetime and thus the molecular symmetry breaking may occur. We focus here to the symmetry breaking of the D_{3h} plane molecule BF_3 due to core excitation.

The B $1s^{-1}2a_2''$ core-excited state of BF_3 is expected to have a pyramidal stable geometry in C_{3v} where the central B atom is out of the plane formed by the three F atoms and thus the out-of-plane vibration (a_2'') is expected to proceed after the B 1s $\rightarrow 2a_2''$ excitation. The F 1s ionization, on the other hand, is expected to cause in-plane asymmetric vibration (e'). We have carried out quadruple-ion coincidence momentum imaging experiment, in order to probe these nuclear motions responsible for the symmetry breaking.

The experiment was carried out on the beamline 27SU at SPring-8 in Japan. Using the time-of-flight method combined with a position-sensitive detector, we extracted complete information on the linear momenta of the four ions produced from the BF_3^{4+} parent ion via core excitation. The production of quadruply charged BF_3^{4+} parent ion proceeds via simultaneous four electron emission in the resonant Auger decay after core excitation or simultaneous three electron emission in the normal Auger decay after core ionization.

The momentum imaging clearly indicates that the B^+ ion is ejected in the direction perpendicular to the molecular plane defined by the three F atom after the B 1s $\rightarrow 2a_2''$ excitation and that the three F^+ ions are ejected aymmetrically within the molecular plane after the F 1s ionization, confirming the symmetry breaking due to core excitation.