

Symmetry of Core-Excited States of the CHF₃ Molecule in the C 1s Excitation Region

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Angle-resolved ion yield spectroscopy is a powerful tool for investigating symmetry of core-excited states. This technique has been widely applied to diatomic and triatomic molecules in linear form. In the present study, we have applied this technique to a polyatomic molecule CHF₃ with C_{3v} symmetry. The experiments have been carried out on BL27SU at SPring-8. Angle-resolved ion yield spectra of CHF₃ in the C 1s excitation region were measured using two identical energetic ion detectors placed parallel and perpendicular to the electric vector of the incidence light. Asymmetry parameters of energetic fragment ions, without resolving the mass of the ions, were determined as a function of photon energy. There are some ambiguous cases in determining the symmetry of the excited states from the mass-unresolved ion yield spectra. In the present case, both H⁺ and F⁺ fragments may be energetic and thus included in the measured spectra. In this situation asymmetry parameters of H⁺ and F⁺ should be extracted separately in order to determine the symmetry of the excited states. For this purpose, we have measured angle-resolved TOF spectra in perpendicular, parallel and magic angle (54.7°) with respect to the electric vector of the incidence light. Asymmetry parameters and kinetic energy distributions of H⁺ and F⁺ were estimated by analyzing the shapes of the angle-resolved TOF spectra. Excitation-energy dependence of the asymmetry parameter of H⁺ turned out similar to that obtained from the mass-unresolved ion yield spectra. The symmetry of core-excited states were determined and all structures observed in the ion yield spectra were assigned.