

Detuning Effect on Molecular Deformation of Core-Excited States in Linear Molecules CO₂ and N₂O

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Core-excited Π states of linear molecules, such as CO₂ and N₂O, are split into in-plane bent and out-of-plane linear states due to the Renner-Teller effects. The lifetime of the core-excited states is of the order of femtoseconds. Within this short time, molecular deformation can proceed from linear to bent geometry. Because the bending force depends on the position on the potential surface of the bent state, one may be able to control the molecular deformation by detuning the excitation photon energy.

We have investigated the detuning effect on the molecular deformation in Π core-excited states in CO₂ and N₂O. The experiments were performed on the c-branch of BL27SU at SPring-8 and beamline SA22 at Super-ACO. We have measured linear momenta of three fragment ions detected in coincidence. Based on the momentum analysis we have selected separately the events of excitation to the bent and linear states of the Renner-Teller pair.

It is found that the probability for excitation to the bent state increases when the excitation energy becomes lower, whereas the probability for excitation to the linear state follows the opposite trend. Fragmentation with smaller angles between the two linear momenta of the two terminal ions (two O⁺ for CO₂ and N_t⁺ and O⁺ for N₂O) from the bent state increases when the photon energy becomes lower, illustrating that the molecule experiences stronger bending force at the lower side of the resonance.

Comparison between the distribution of the measured angles between the two linear momenta and the classical trajectory calculations based on the Coulomb explosion model will be presented.