

# The Role of Nuclear Motion in the Relaxation of Core-Excited Polyatomic Molecules

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The resonant excitation of a core electron into an empty molecular orbital results in a radical rearrangement of the whole electronic cloud which may induce strong conformational changes in a polyatomic molecule. The bonding/anti-bonding character of the resonant state, the core-hole lifetime of the inner shell vacancy and the mass of the involved atoms, may be directly be reflected in the fragmentation pattern of the excited molecule. In order to investigate such processes and their influence on the final fragmentation pattern of polyatomic molecules, high resolution electron spectroscopy and electron/ion coincidence spectroscopy are necessary. High resolution PES is ideally suited to give a picture of the system evolution at a very short time scale, whereas coincident measurements are absolutely necessary to disentangle the role of the final state internal energy in the dissociation.

Several examples will be given from experiments performed both at LURE (SA22 beamline) and MAX II (I411 beamline) storage rings. Specific fragmentation channels are shown to be induced via a bending mode excitation in the case of CO<sub>2</sub> (C1s→π\*) and BF<sub>3</sub> (B1s-2a''<sub>2</sub>). In H<sub>2</sub>S, the ultra fast dissociation following the S2p→6a<sub>1</sub> transition results in a specific three-step fragmentation process.

In the case of much more complex systems, internal energy is rapidly redistributed among the numerous vibrational modes. However, it is still possible to observe some selective effects, as illustrated in the case of the Si(CH<sub>3</sub>)<sub>3</sub>OSi(CH<sub>3</sub>)<sub>3</sub> molecule, for which the localization of the inner shell can be successfully used to enhance the production of a particular ion.