

## X-RAY MOLECULAR SPECTROSCOPIC DYNAMICS

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Ultrafast X-ray spectroscopic investigations and molecular dynamics are now approachable with short pulses of laboratory, laser-produced high-order harmonics. Those X-rays probe transitions from localized inner shells of specific atomic sites in the molecules to valence orbitals, conveying new information about photochemical transformations. The interpretations of these spectra involve a new regime of core-to-valence X-ray probing that depends on energy shifts due to the surrounding electronic densities, spin coupling effects, energy shifts due to bond elongation with vibrational excitation, and even Jahn-Teller distortions. Coherent vibrational superpositions reveal different slopes of inner shell potentials with bond extension and Fermi resonance coupling, for the first time, in the X-ray. Open shell radicals have characteristic features of singly occupied orbitals and energetic shifts upon bond cleavage, which can be viewed from the localized atomic perspective. Corresponding theory work by collaborators provides a powerful assessment of the X-ray spectroscopic dynamics. Progress for revealing the full potential of time-resolved X-ray spectroscopy for the investigation of numerous novel features in molecular photochemistry is discussed.