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Intrinsically Polyatomic Phenomena in Electron-Molecule Scattering[1]

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Resonant collisions of electrons with molecules are one of the most efficient pathways for the transfer of energy from electronic to nuclear motion. As the field of electron-molecule scattering developed, both experimentally and theoretically, the phenomena of vibrational excitation and dissociative attachment were first understood for diatomics, and it seemed natural to extend that understanding to polyatomic molecules using one-dimensional or single-mode models of the nuclear motion. However a series of recent experimental measurements of these phenomena in small polyatomic molecules have proven to be uninterpretable in terms of atomic motion with a single degree of freedom. Why do resonant collisions of electrons with CO_2 preferentially excite particular members of nearly degenerate groups (Fermi polyads) of vibrational levels? Why does dissociative attachment of electrons to H_2O at 6.5 eV produce primarily H^- + OH while attachment at 11.5 eV produces mostly O^- + H_2? How does a π shape resonance in electron scattering from formic acid produce dissociative attachment products of an obviously different symmetry? The answers to these questions involve multidimensional nuclear motion, multiple potential surfaces for the metastable anions, and conical intersections. Using *ab initio* methods of electron scattering and bound state quantum chemistry we can generate those multidimensional potential surfaces for small molecules. With wave packet propagation on those coupled surfaces we can elucidate the mechanisms and reveal how they are probed in the experiments. It appears that these complexities are a general feature of electronic collisions with polyatomic molecules, and that they may hold the key to understanding how collisions of low-energy electrons produced by ionizing radiation damage biological molecules.

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