

Direct, Nonadiabatic, Molecular Reaction Dynamics

The basis and computational implementation of Electron Nuclear Dynamics (END) theory [1] will be discussed. This approach to the study of molecular processes employs approximate quantum mechanical Lagrangians and uses the principle of least action to derive dynamical equations that approximate the time-dependent Schrödinger equation. The system wavefunction parameters, such as molecular orbital coefficients, average nuclear positions and momenta, carry the time-dependence and constitute the dynamical variables. This approach to the simultaneous dynamics of all electrons and atomic nuclei admits a hierarchy of treatments. Minimal END treats the nuclei as classical particles and the electrons are described by a complex spin unrestricted single determinantal wavefunction in terms of nonorthogonal spin orbitals.

This approach is well suited for molecular collision energies from a few electron volts to several keV [2, 3, 4, 5]. Absolute differential and integral cross sections for a great variety of reactive collisions involving atomic and molecular ions [6, 7, 8, 9, 10], and neutrals have been calculated with standard semi-classical corrections yielding good agreements with the best experiments. Rovibrational resolution can be obtained via *a posteriori* analysis using coherent states [11].

References

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