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A nonperturbative quantum mechanical approach to ion-molecule collisions TOM KIRCHNER, Department of Physics and Astronomy, York University, Toronto, Ontario M3J 1P3, TOBIAS SPRANGER, Institut fuer Theoretische Physik, TU Clausthal, D-38678 Clausthal-Zellerfeld, Germany, HANS JÜRGEN LÜDDE, Institut fuer Theoretische Physik, Goethe-Universitaet, D-60438 Frankfurt, Germany — A nonperturbative quantum mechanical approach to ion-molecule collisions is presented. Its key ingredients are an expansion of the initially populated molecular orbitals in terms of a single-center basis and a spectral representation of the molecular Hamiltonian. Effectively, the approach amounts to a separation of molecular geometry and collision dynamics and offers the possibility to use well-established ion-atom methods with relatively minor modifications. We apply this rather general approach to ion-water-molecule collisions and calculate cross sections for electron transfer and ionization at impact energies from the few-keV to the few-MeV regime. Different geometries are considered, and the variation of the results with respect to the orientation of the molecule is studied. To compare results with experimental data and other calculations we average the orientation-dependent parts of the Hamiltonian over the three standard Euler angles. This short cut is, of course, an approximation, but first results indicate that it yields reliable total cross sections.

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