Charge exchange in ion collisions with atoms and molecules

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The evaluation of charge exchange rate coefficients for modeling photoionized plasmas requires the calculation of the corresponding total cross sections at low energies ($E < 10$ eV/u), which in turn involves the use of a quantal description of both nuclear and electronic degrees of freedom. In particular, the ab initio methods require high-precission calculations of electronic energies of a number of electronic states of the collisional system, and the non-adiabatic couplings between them, in a set of nuclear geometries. At the lowest energies (meV), isotope effects can be important and, depending on the collisional system [1], this effect can go from a factor of two in the cross sections to several orders of magnitude, which has a significant impact on the reaction rates.

When describing ion-molecule collisions at low energies, the main difficulty is the treatment of the vibro-rotational degrees of freedom. Besides, competition between reactive and non-reactive charge exchange reactions must be considered [2]; this will be illustrated for collisions of protons with hydrogen molecules.

X-ray emission by comets is attributed to charge exchange between solar wind ions, with energies above 1 keV, with cometary atoms and molecules. At these energies, a classical trajectory Monte Carlo (CTMC) method can be applied (see [3]). We shall present results of CTMC calculations for collisions between multicharged ions and small molecules.

References

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