Electron-impact study of O_2^+ ion: *R*-matrix method

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Molecular oxygen and its positive ions plays a fundamental role in the physics and chemistry of earth's atmosphere. A detailed information about collisions between low-energy electrons and positive ions of oxygen molecule is required in studies of the physics of planetary atmosphere, gaseous discharges, and both astrophysical and laboratory plasmas.

The ion O_2^+ is an open-shell system that has ground state ($X\ ^2\Pi_g$) configuration $1\sigma_g^2$-$3\sigma_g^2\ 1\sigma_u^2$-$2\sigma_u^2\ 1\pi_u^4\ 1\pi_g^1$ in the $D_{\infty h}$ point group which is reduced to the D_{2h} point group when the symmetry is lowered. The Multi-state close-coupling calculations are performed, using the UK molecular R-matrix method [1, 2], to compute the excitation cross sections. The target states are represented by including correlation via a configuration interaction technique, and results are compared with previous work [3, 4]. The CI calculations yields the ground state energy of -149.20544 Hartree and rotational constant 1.6901 cm^{-1} (Expt. Value B_e = 1.6913 cm^{-1} [5]) at the equilibrium bond length of 2.1 a_0. We obtain the effective collision strength for electron temperature range 100 - 10000 K assuming Maxwellian distribution of incident electron. Detailed results will be presented in the conference.

References:

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