Electron–impact study of O_2 molecule: *R*-matrix method

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Molecular oxygen plays a fundamental role in the physics and chemistry of earth's atmosphere [1]. A detailed information about collisions between low-energy electrons and oxygen molecules is required in studies of the physics of planetary atmosphere, gaseous discharges, and both astrophysical and laboratory plasmas [2]. It is the electronic transition from the $X\ ^3\Sigma_g^-$ state of oxygen to the $a\ ^1\Delta_g$ and $b\ ^1\Sigma_g^+$ states which give rise to the infrared and red bands in the atmospheric spectrum. The long life time of the metastable state ($a\ ^1\Delta_g$) of oxygen, which make scattering from an excited molecular target state possible [3].

We have computed elastic differential, momentum-transfer, excitation, and ionization cross sections for electron-impact on O_2 molecule, which are computed using the *R*-matrix method [4–5]. The results of the static exchange, correlated one-state, 22-state close-coupling approximation are presented. We have detected a stable anionic bound state $^2\Pi_g$ of $O_2{}^-$, with a vertical electron affinity value of 0.389 eV for O_2 which is in good agreement, with theoretical value 0.390 eV [6],and experimental value of 0.451 ± 0.007 eV [7]. We detected two shape resonances of $^2\Pi_u$ symmetry in the excitation cross sections of the $^1\Delta_g$ and $^1\Sigma_g^+$ excited states and compared our results with [8]. The dissociative nature of these resonances is explored by performing scattering calculations in which O-O bond is stretched. The variation of position and width of these resonances as a function of internuclear distance is in good agreement with previous results of [9]. These resonances support dissociative attachment yielding O, O^- in dissociation of O_2. We have reasonable agreement with the previous calculations [2] for vertical excitation energies. The ionization cross sections are calculated in the binary-encounter Bethe model and compared with previous results [10]. The results of DCSs, at 3, 5, 7 and 9 eV, are comparable to the results of [11]. We have included up to *g*-partial wave ($l = 4$) in the scattering calculations. The Born-correction for dipole-allowed transition ($X\ ^3\Sigma_g^-$ to $B\ ^3\Sigma_u^-$) [12] has been carried out to account for the contribution of partial waves higher than *g* wave ($l = 4$). The scattering length of O_2 molecule is calculated which is 1.989 a_0.

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