Resonant vibrational-excitation electron-O₂ cross sections and rate constants

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A full set of resonant vibrational-excitation cross sections and the corresponding rate constants for electron scattering by molecular oxygen are presented [1]. The lowest four resonant states of O₂−, i.e. 2Πg, 2Πu, 4Σu− and 2Σu−, were taken into account, following the scheme:

\[ e^- + O_2(X^3\Sigma_g^-, v) \rightarrow O_2^- \rightarrow e^- + O_2(X^3\Sigma_g^-, v) \].

The calculations were performed by using the results of Noble at al. [2], which use a fixed-nuclei UK R-matrix [3] approach, for resonance positions and widths, and the boomerang model to study the nuclei motion [4]. The molecular potential energy curves of O₂(X^3Σ_g−) were obtained by using ab-initio program MOLPRO [5]. Figure 1 summarized the main results of the work. Results for CO, N₂ and NO molecules can be found in the Refs. [6,7].

The cross sections provide suitable input data for kinetic models, to describe non-equilibrium molecular plasma, in a state-to-state approach.

Figure 1. First column: Potential energy curves and widths for O₂ molecule and O₂− resonant states; Central and last column: Resonant cross sections and rate coefficients for vibration-excitation from ground state and for mono-quantic transitions.

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