Electron-Impact Study of *AlO*$^+$ using The *R*-Matrix Method

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The electron-impact of AlO^+ ion at low energy electron (less than 10eV) has been investigated by using the *R*-matrix method [1]. In the *R*-matrix theory the configuration space of the entire scattering system is divided into an inner and an outer region. Both the regions are treated differently in accordance with the different interactions in each region.

The calculation are carried out in two models namely Static Exchange (SE) and many state close-coupled (CC) approximation. In the SE calculation no correlation are included except exchange while in the CC calculation polarization and exchange correlation are added due to inclusion of excited states. In the CI calculation we include all single and double excitations.

We present excitation cross sections from the ground state X $^1\Sigma^+$ to the three low lying electronically excited states $^1\Pi$, $^3\Pi$ and $^3\Sigma^+$ of the AlO^+ ion by using the R-matrix theory. Configuration Interaction (CI) wavefunctions are used to represent the target states. The natural point group of the AlO^+ ion is $C_{\infty v}$, however the calculations are performed in the point group C_{2v}. We have also studied the potential energy curves for the valence states of the AlO^+ computed with our limited CI model in which we employed the 6311G* basis functions to represent the Al and O atoms.

All calculations are performed at the ground state minima of AlO^+ obtained at the bond length of 1.625 Å (3.07 au). In our CI model we keep the 12 core electrons frozen in doubly occupied molecular orbitals $1a_1$ ... $4a_1$, $1b_1$ and $1b_1$. The complete active space consists of 10 molecular orbitals : $5a_1$ ... $8a_1$, $2b_1$,... $4b_1$ and $2b_2$ ... $4b_2$ in which 8 valence electrons are allowed to move freely. The SE and CI ground state energies of the AlO+ ion are -316.370827 au and -316.45149 au respectively which compare well with the SCF energy of -316.38405 au at a bond length of 3.1 au [2]. Our calculated dipole moment of the ground state is 3.24 D and the rotational constant is 0.6357285 cm^{-1} .

Since the cross sections are dominated by resonances we present the effective collision strengths γ(T) for an electron temperature range 100-10 000 K assuming Maxwellian distribution of incident electrons.

References

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