THE STUDY OF THE INTERACTIONS OF LOW ENERGY ELECTRONS WITH OH

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Abstract:

The hydroxyl radical OH is an important component in a diverse array of physical environments. It is one of the most extensively studied diatomic hydrides as it is an important constituent of combustion gases, of both clean and polluted terrestrial atmospheres, of cometary gases and of diffuse, dense, and shocked regions of the interstellar gas. It is also an important species in biology being readily formed by the dissociation of water by radiation. Ionising radiation may form OH radicals in the body which can subsequently induced DNA damage which can lead to cell death or mutation. Within cells the major secondary species of any ionising irradiation are secondary electrons, therefore the interaction of electrons with OH is important in may areas of radiation chemistry. To date it has not been possible to prepare targets of OH radicals for electron bema experiments such it is necessary to develop theoretical models of such interactions.

We have used the UK R-matrix code for the low energy electron impact study on the OH molecule. The R-matrix method is now established as the most versatile and efficient method for the modelling of low energy scattering by electrons (and positrons) by atomic and molecular targets [1].The R-matrix method is used to treat electron collisions with the diatomic OH molecule as a function of inter-nuclear separation R. These calculations concentrate on obtaining low-energy (< 10 eV) elastic excitation cross sections of the seven lowest-lying electronically excited states of symmetries $^2\Pi$, $^2\Sigma^+$, $^2\Sigma^-$, $^2\Delta$, $^4\Sigma^+$, $^4\Sigma^-$ and $^4\Pi$. We used an equilibrium value for the O-H bond length R_e = 1.8342 a_o. The basis set of slater type functions consisted of $24\,\Sigma$, $10\,\Pi$ and 2Δ orbitals and a complete active space configuration interaction model [2].The range of scattering energies is restricted to 12 eV. Resonance positions and widths are found using the RESON program. In order to study the dissociative behaviour of resonances we performed calculations in which the O-H bond was stretched for R = 1.3 a_o to 3.5 a_o. We have calculated the total elastic cross sections for 6 geometries R = 1.3, 1.5, 1.6, 1.75, 1.8342 and 1.9 a_o. Detailed results will be presented during the conference.

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References:

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