RESONANCE SURFACES FOR H_2O^-

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Electron collisions with water are very important for the understanding of radiation damage in biological system, atmospheric processes, masers, etc.. These collisions can result in the rotational, vibrational and/or electronic excitation of the molecule but they can also induce fragmentation. Specifically, low-energy electrons can produce fragmentation via dissociative electron attachment (DEA) and electronic excitation into dissociative states.

Experimental work on water break-up has focused on dissociative attachment. More recently measurements of ground state OH production via electron impact have been performed [1] showing the different contributions of DEA and dissociative excitation. Few theoretical studies on the resonance curves for DEA of water are available [2]. Among them, one has been carried out taking into account a single dissociative coordinate [3], the assumption being that dissociation proceeds into the formation of H and OH. The discrepancy between the theoretical results and the experimental measurements of [1] suggest that full three-dimensional studies are needed.

The R-matrix method and the R-matrix polyatomic code [4] is used to treat the electronic part of the process. We have performed fixed-nuclei calculations for 840 geometries of H_2O. These were obtained by varying the internal nuclear coordinates of the molecule, using 8 different angles and 14 different OH internuclear distances. Following [3], we have incorporated nine target states in the close-coupling expansion and calculated cross sections for electronic excitation into the first 4 excited states as a function of geometry. In accordance with previous calculations and experiments [5] we found three Feshbach resonances below the ionisation threshold. In C_{2v} symmetry these resonances are labelled $^2B_1$, $^2A_1$ and $^2B_2$. The DEA process is likely to proceed via these resonances. Since the first four excited states of H_2O are dissociative, excitation into any of these will produce fragmentation.

We will present resonance positions and widths as a function of geometry and for the resonances. These results are the starting point for a full-dimensional study of the DEA and dissociative excitation processes.

References

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