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Effect of the intersystem crossings in the S^++H2 reaction

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SH^+ is a widespread molecular ion in diffuse interstellar clouds, and has also been detected in emission toward the Orion Bar photodissociation region (PDR). In warm and dense PDRs, SH^+ is thought to form by exothermic reactions of S^+ with vibrationally excited H2 (v>1). The viability of this hypothesis have been confirmed by theoretical simulations reaction which demonstrate that for vibrational level v=2 or higher of H2, the reaction exhibit high rate constants[1].
From an experimental point of view, scarce data are available[2]. As the reaction of the ground state ion is endothermic by almost 1 eV, the SH^+ product is observed only at high collision energies where translational energy brings the needed energy to reach products, as predicted by the theoretical simulations. Interestingly, it appears from this experimental study that spin-orbit couplings between the quartet and first doublet state of the H2S+ system may play a significant role on the reaction, motivating a new theoretical study of the reaction, now including the spin-orbit interactions.

Exact quantum dynamics calculations show that spin-orbit interaction does indeed play an important role in this reaction, and that three electronic states are involve in the reaction mechanism.

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References
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