State-to-state rate constants calculations for the reaction C^+ +H2 and S^+ +H2

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Résumé

H2 is the most abundant molecule in the universe. Reactions between atoms or ions with H2 are thus of particular interest to understand the chemistry of the interstellar medium (ISM). In general, reaction between cations and H2 are endothermic. For a long time, they were thus assumed to be slow at low temperature and not relevant from an astrochemical point of view. However, the use of thermal rate constants is not always a good approximation to describe the chemistry kinetics in the ISM. The reason is that the very low density in this medium does not always allow a fast thermalisation of the present species. As a consequence, the rotational, vibrational and translational temperatures are not always identical. As we will see with the study of the title reactions, this can have two important consequences for the understanding of ISM. The rovibrational excitation of the reactant molecule (in our case, H2) can provide sufficient energy to overcome the energy barrier of reaction and greatly enhance reaction rate constants, even at low translational energy. The second consequence is that the rovibrational excitation of the product molecule can be warmer than the temperature of the region where it is observed and can thus lead to bad estimations of the physical conditions of the medium. To take in account these effects in astrochemical models, it is thus useful to use, when they are available, state-to-state rate constants.

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