Coriolis Coupled Dynamics of the H(2S) + CH*(X^1Σ^+) Reaction: A Full-Dimensional Quantum Wavepacket Study

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Introduction

1. Reactions between the atoms and molecular ions are known to play a significant role in the chemistry of diffuse interstellar and circumstellar regions, planetary atmospheres, and single star environments.

2. The reaction CH + H and H + CH* species are extensively studied in the past few decades. CH* is typical millimeter ion, and most important in the interstellar medium (ISM).

3. It was the first molecular ion identified in the ISM.

Initial state

At Coriolis (CS) of accurate results, the initial state (2) is preferred.

Minimum Energy Path (MEP)

Effective potential of the H + CH* (v = 0, J = 3) system along the Jacobi coordinate R for different J and Q values.

Initial state and channel specific rate constants of the title reaction over the temperature range of 100–1000 K, obtained from the CC (solid line - CC) and CS (dashed line) methods, are compared for different J = 1–3 levels of the CH* reagent.

References


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Thank you.