

Theoretical study of the HCS^+-H_2 van der Waals complex: potential energy surface, rovibrational bound states, and rotationally inelastic collisional cross sections

- Quintas-Sánchez E.^a,
- Dawes R.^a
- Denis-Alpizar O.^b

Abstract

An accurate ground-state intermolecular potential energy surface (PES) was calculated for the HCS (Formula presented.) $-\text{H}$ (Formula presented.) complex. The surface was constructed from 3023 ab initio energies, computed with explicitly correlated coupled-cluster theory, CCSD(T)-F12b, with extrapolation to the complete basis set limit (VTZ-F12/VQZ-F12). The new 4D PES was used to compute rovibrational energies, rotational constants, and close-coupling quantum scattering calculations at low collision energies. A symmetry-adapted Lanczos algorithm was used to variationally compute the low-lying rovibrational bound states. Rotational constants for states of two isomers were determined from the energy levels and reported in hopes of motivating experiments. The rotationally inelastic state-to-state cross sections of HCS (Formula presented.) by collision with para- and ortho- H (Formula presented.) were computed and compared, and trends and propensities are discussed. © 2021 Informa UK Limited, trading as Taylor & Francis Group.

Author keywords

inelastic scattering; ISM; PES; rovibrational