Rotational relaxation of H2S by collision with He

Denis-Alpizar O.

Stoecklin T.

Context. The H2S molecule has been detected in several regions of the interstellar medium (ISM). The use of non-LTE models requires knowledge of accurate collisional rate coefficients of the molecules detected with the most common collider in the ISM. Aims. The main goal of this work is to study the collision of H2S with He. Methods. A grid of ab initio energies was computed at the coupled cluster level of theory including single, double, and perturbative triple excitations (CCSD(T)) and using the augmented correlation consistent polarized quadruple zeta (aug-cc-pVQZ) basis set supplemented by a set of mid-bond functions. These energies were fitted to an analytical function, which was employed to study the dynamics of the system. Close coupling calculations were performed to study the collision of H2S with He. Results. The rate coefficients determined from the close coupling calculation were compared with those of the collision with H2O+He, and large differences were found. Finally, the rate coefficients for the lower rotational de-excitation of H2S by collision with He are reported. © 2020 ESO.

Astrochemistry

ISM: molecules

Molecular data

Molecular processes

Scattering

Molecules

Numerical methods

Analytical functions

Close coupling calculation

Collisional rates

Coupled clusters

Interstellar mediums

Perturbative triple excitations

Rate coefficients

Rotational relaxations

Calculations