Deexcitation rate coefficients of C_3 by collision with H_2 at low temperatures

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Abstract

Context. An accurate analysis of the physical-chemical conditions in the regions of the interstellar medium in which C3 is observed requires knowing the collisional rate coefficients of this molecule with He, H2, electrons, and H. Aims. The main goals of this study are to present the first potential energy surface for the C3 +H2 complex, to study the dynamics of the system, and to report a set of rate coefficients at low temperature for the lower rotational states of C3 with para- and ortho-H2. Methods. A large grid of ab initio energies was computed at the explicitly correlated coupled-cluster with single-, double-, and perturbative triple-excitation level of theory, together with the augmented correlation-consistent quadruple zeta basis set (CCSD(T)-F12a/aug-cc-pVQZ). This grid of energies was fit to an analytical function. The potential energy surface was employed in close-coupling calculations at low collisional energies. Results. We present a high-level four-dimensional potential energy surface (PES) for studying the collision of C3 with H2. The global minimum of the surface is found in the linear HH-CCC configuration. Rotational deexcitation state-to-state cross sections of C3 by collision with para- and ortho-H2 are computed. Furthermore, a reduced two-dimensional surface is developed by averaging the surface over the orientation of H2. The cross sections for the collision with para-H2 using this approximation and those from the four-dimensional PES agree excellently. Finally, a set of rotational rate coefficients for the collision of C3 with para- and ortho-H2 at low temperatures are reported. © ESO 2022.

Author keywords

Astrochemistry; ISM: molecules; Molecular data; Molecular processes; Scattering