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ORIGINAL ARTICLE

Rotational excitation of protonated hydrogen cyanide ($HCNH^+$) by He atom at low temperature

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Abstract We report on ab initio coupled-cluster calculations of the interaction potential energy surface for the $HCNH^+$–He complex. The aug-cc-pVTZ Gaussian basis, to which is added a set of bond functions placed at mid-distance between $HCNH^+$ center of mass and He atom is used. The $HCNH^+$ bonds length are set to their values at the equilibrium geometry, i.e., $r_e[\text{HC}] = 1.0780$ Å, $r_e[\text{CN}] = 1.1339$ Å and $r_e[\text{NH}] = 1.0126$ Å. The interaction energy presents a global minimum located 266.9 cm^{-1} below the $HCNH^+$–He dissociation limit. Using the interaction potential obtained, we have computed rotational excitation cross sections in the close-coupling approach and downward rate coefficients at low temperature ($T \leq 120$ K). It is expected that the data worked out in this study may be beneficial for further astrophysical investigations as well as laboratory experiments.

Keywords CCSD(T) · PES · Collision · Cross sections · Rate coefficients

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1 Introduction

The linear hydrogen cyanide molecular ion, $HCNH^+$, is one of the key species in the ion–molecule scheme of interstellar cloud chemistry (Herbst and Klemperer 1973, Herbst 1978, Watson 1974; Brown 1977; Brown and Rice 1981; Huntress and Mitchell 1978; Prasad and Huntress 1980; Capone et al. 1981). Its was reported for the first time as regards Sgr B2 by Ziurys and Turner (1986) who observed three rotational transitions: the $J = 1 \rightarrow 0$ line at 74 GHz by using the National Radio Astronomy Observatory (NRAO) 12 meter antenna, the $J = 2 \rightarrow 1$ and $J = 3 \rightarrow 2$ transitions at 148 GHz and 222 GHz, measured with the Millimeter wave observatory (MWO) 4.9 meter dish. Later, i.e., in 1992, Ziurys et al. (1992) succeeded to detect $HCNH^+$ toward TCM-1. The hyperfine structure of the $J = 1 \rightarrow 0$ transition was then solved and the quadrupole coupling constant of the nitrogen nucleus determined. Indeed, $HCNH^+$ is expected to be the main precursor of HCN, HNC, and CN via dissociative recombination with an electron (Herbst and Klemperer 1973, Watson 1973; Herbst 1978). The latter species have been observed in many interstellar clouds (Herbst and Klemperer 1973, Watson 1973). All the above clearly illustrate the importance of $HCNH^+$ in the interstellar medium (ISM) and hence the effort devoted to conduct investigations on it.

$HCNH^+$ has been the subject of numerous studies of both theoretical and experimental interest (Lee and Schaefer 1984; DeFrees et al. 1982; DeFrees and McLean 1985; Pearson and Schaefer 1974; Summers and Tyrrell 1976; Saebq 1977; Allen et al. 1980, Dardi and Dykstra 1980; Del Bene et al. 1982; Hirao et al. 1982; Pople 1983; Ha and Nguyen 1983). On the experimental side, most of the efforts have been devoted to the observation of the infrared vibration–rotation spectrum of the ν_1 (NH stretch), (Altman et al. 1984a), ν_2 (CH stretch) (Altman et al. 1984b) and ν_5