Astrophysics > Galaxy Astrophysics

The rotational excitation of HCN and HNC by He: New insights on the HCN/HNC abundance ratio in molecular clouds

E. Sarrasin, D. Ben Abdallah, M. Wernli, A. Faure, J. Cernicharo, F. Lique

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Modeling of molecular emission from interstellar clouds requires the calculation of rates for excitation by collisions with the most abundant species. The present paper focuses on the calculation of rate coefficients for rotational excitation of the HCN and HNC molecules in their ground vibrational state in collision with He. The calculations are based on new two-dimensional potential energy surfaces obtained from highly correlated \textit{ab initio} calculations. Calculations of pure rotational (de)excitation cross sections of HCN and HNC by He were performed using the essentially exact close-coupling method. Cross sections for transitions among the 8 first rotational levels of HCN and HNC were calculated for kinetic energies up to 1000 cm^{-1}. These cross sections were used to determine collisional rate constants for temperatures ranging from 5 K to 100 K. A propensity for even Δj transitions is observed in the case of HCN--He collisions whereas a propensity for odd Δj transitions is observed in the case of HNC--He collisions. The consequences for astrophysical models are evaluated and it is shown that the use of HCN rate coefficients to interpret HNC observations can lead to significant inaccuracies in the determination of the HNC abundance, in particular in cold dark clouds for which the new HNC rates show that the $j=1-0$ line of this species will be more easily excited by collisions than HCN. An important result of the new HNC-He rates is that the HNC/HCN abundance ratio derived from observations in cold clouds has to be revised from $>$1 to $\simeq$1, in good agreement with detailed chemical models available in the literature.

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