Cyanide/isocyanide abundances in the interstellar medium. Inelastic rate coefficients of Al and Mg compounds.

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Modelling molecular abundances in the interstellar medium requires accurate molecular data. Hence, accurate determination of collisional rate coefficients is an essential step in order to estimate molecular abundances in interstellar clouds. Cyanide/isocyanide species are the most common metal-containing molecules in circumstellar gas [1,2]. It is crucial to provide collisional data for the cyanide/isocyanide molecules .

In this work, we have carried out calculations of rate coefficients for the rotational excitation of aluminum cyanide (AlCN) , aluminum isocyanide (AlNC) , magnesium cyanide (MgCN) and magnesium isocyanide (MgNC) 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 *ab initio* calculations. Coupled states quantum approximation was used to obtain pure rotational (de-)excitation cross-sections of AlCN, AlNC, MgCN and MgNC by He. Rates coefficients for transitions among the 26 first rotational levels of AlCN and AlNC and among the first 41 fine structure levels of MgCN and MgNC were calculated for the temperature range between 5 and 100 K . Significant differences between the rate coefficients of both isomers were observed. These differences confirm that specific calculations have to be performed for each isomer in order to obtain the necessary level of detail. The new rate coefficients should induce important consequences on the determination of metal abundance in the ISM. In particular, our work confirms [3] that the AlCN molecule is significantly less abundant than AlNC in the ISM.

Références

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