New insight on the metal cyanides and isocyanides abundances in the circumstellar gas

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Résumé

Metal cyanides/isocyanides are the most common metal-bearing molecules in the circumstellar gas. Heavy metals in the gas phase are important in controlling the ionization of a cold dark cloud and then the chemistry and the cloud evolution. In addition, observations of metal-bearing molecules can deliver important information on depletion into dust grains. Modelling of these molecules abundances relies on accurate determination of molecular stabilities, reaction probabilities as well as radiative and collisional excitations.
We present the computation of structural and spectroscopic properties of a series of metal cyanide / isocyanide species containing Mg, Al and Si atoms using highly correlated *ab initio* calculations [1]. Isomerization pathways and transitions states are detailed. We also present the calculations of new collisional rate coefficients for the rotational (de-)excitation of AlCN, AlNC, MgCN, MgNC, SiCN and SiNC molecules by collisions with He, as a model of H2 [2,3]. This is the first time that rotational excitation of metal cyanides and isocyanides has been studied using quantum approach. We have found that these isomers present significant differences in their excitation processes.

As an application, we simulate the excitation of these metal-bearing molecules in the circumstellar gas. We perform radiative transfer calculations for typical physical conditions encountered in the circumstellar gas and we obtain brightness and excitation temperatures of selected lines frequently observed. We find that local thermodynamic equilibrium (LTE) conditions are not fulfilled for these species and that radiative transfer calculations are needed in order to accurately determine their abundances. The calculations also show that the estimations of the cyanides/isocyanides abundance ratios deduced from line intensities ratios lead to large differences compared to exact radiative transfer calculations. As already noticed, we found that AlCN and MgCN are significantly less abundant than AlNC and MgNC respectively [4]. At the opposite of what was found previously, SiCN seems to be more abundant than SiNC, in agreement with the fact that SiCN is more stable than SiNC [3].

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