Quantum calculation of the radiative association rate of MG^+ with HCN

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The major carriers of positive charge within dense interstellar clouds and circumstellar envelopes are considered to be Metal ions[1] Na^+, Mg^+, Fe^+, . . . while the circumstellar metal-containing molecules detected so far in cold outer parts of carbon-rich star are magnesium-containing radicals such as MgCN and MgNC. The formation of these radicals is assumed to be resulting from reaction sequences initiated by the radiative association (RA) of Mg^+ and the cyanopolyynes $HC_{2n+1}N$, (n=0,1.,,) which are highly abundant in these environments. Notoriously difficult to measure in the laboratory and difficult to obtain using exact quantum approaches, the evaluation of the RA rates has long been based on variational transition state theory. The recent development of exact quantum approaches for calculating the RA rates of atomic ions with linear molecules[2] have revealed discrepancies when compared with the reaction rates obtained using statistical methods, sometimes differing by up to several orders of magnitude. The present work which is part of a combined theoretical and experimental study is dedicated to quantum calculations of the Mg^++ HCN rate. To this aim a potential energy surface of the system is developed and used to solve the driven equations of the system. The results are discussed and compared to those available given by transition state theory.

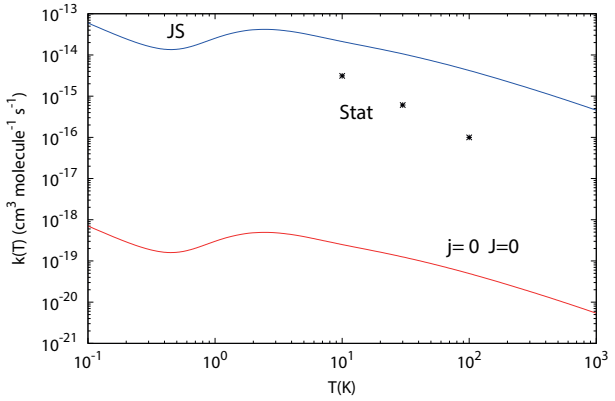

Figure 1: *REA rate coefficient of Mg^+ with HCN*

Index Terms: radiative association, driven equations, interstellar chemistry

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[2] Stoecklin, T., Halvick, P., Lara-Moreno, M., Trabelsi, T., Hochlaf, M., "On the gas-phase formation of the HCO- anion: Accurate quantum study of the H-+CO radiative association and HCO radiative electron attachment', Faraday Discussions, 212 : 101–116, 2018.