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.

ELECTRON-IMPACT EXCITATION OF INTERSTELLAR MOLECULES

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Abstract.

Electron-impact excitation of molecules plays a crucial role in astrophysical environments where the electron fraction is higher than about 10^{-5}, e.g. in the diffuse interstelar medium, in shocks and comets. We present here recent ab initio calculations of rate coefficients for the rotational excitation of HCN and HCO^+ by thermal electrons. Our calculations are based on the molecular $\mathbf{R}$-matrix method combined with the Adiabatic-Nuclei-Rotation (ANR) approximation corrected for threshold effects. Our major results are *i)* the prediction of collisional propensity rules less rigorous than previously assumed and *ii)* the prediction of significant excitation differences between ionic and neutral molecules.

1 Introduction

In low density astronomical environments, the intensity of molecular emission depends on a complex competition between radiative and collisional processes. A good knowledge of state-to-state collisional rates is thus necessary to interpret and model the nonthermal distributions of molecular energy levels. In regions where the fractional ionization ($n(\mathrm{e})/n(\mathrm{H})$) is above $\sim 10^{-5}$, electrons can dominate the molecular excitation because electron-impact excitation rates can exceed those for excitation by neutrals by typically 5 orders of magnitude.

2 Method

The reference methods for computing electron-impact excitation rates have been the Born and Coulomb-Born theories for neutral and ionic targets, respectively. Based on simple long-range approximations, these theories predict that transitions with $\Delta J = 1$ only are allowed for polar species. By employing the adiabatic-nuclei-rotation (ANR) approximation combined with R-matrix ab initio wavefunctions, we have shown that the inclusion of short-range interactions actually lead to significant rates for transitions with $\Delta J > 1$, in particular for molecular ions (Faure & Tennyson 2001). On the other hand, the collisional propensity rules were generally found to be consistent with the long-range theories. As a result, dipole-allowed transitions are always preferred for molecules with significant dipoles (e.g. HCO^+ and $\mathrm{H_2O}$) and the K quantum number is essentially conserved for symmetric-top molecules like H_3^+ (Faure & Tennyson 2003, Faure et al. 2004).

These R-matrix studies were, however, hampered by the use of the ANR approximation which is expected to become invalid close to a rotational threshold. Thus, the previous R-matrix calculations applied the "kinematic correction" factor k'/k, where k (k') is the initial (final) momentum of the electron, designed for neutral targets. We have shown recently in the case of H_3^+ that this correction is in fact incorrect for molecular ions (Faure et al. 2006). Thus, by comparison with rovibrational quantum defect theory (QDT) calculations based on the treatment described in (Kokoouline & Greene 2003), pure ANR excitation cross sections have been shown to be accurate for kinetic energies above the resonance regime caused by rotational closed-channels. These resonances were found to occur for transitions with $\Delta J = 1$ and $\Delta K = 0$ and for these, an analytical formula for averaging

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transition probabilities over the resonance structure was formulated. In the case of transitions with $\Delta J > 1$, the ANR theory was shown to be accurate down to threshold, provided a simple "Heaviside correction" is applied to the excitation cross sections. Full details can be found in Faure et al. (2006).

3 Results

As shown in Fig. 1, the highly accurate QDT rotational cross sections for H_3^+ are large and finite at threshold, in accord with the Wigner law for an attractive Coulomb field, with a significant but moderate contribution from closed channels. The range of validity of the ANR theory is therefore much wider than the usual classically derived condition that the impacting electron energy be large compared to the threshold energy. These results contrast with the case of neutral non-polar targets such as H_2 for which rotational cross sections fall steeply near threshold. This fondamental difference between ions and neutrals, which was actually predicted sometime ago (although the role of closed-channels was not considered), reflects the influence of the strong Coulomb field which ensures that the time scale for electron motion is always rapid compared to the nuclear motion. At the same time, the Coulomb potential provides the energy to access closed channels, thus creating substantial resonance effects. As such, H_3^+ is actually quite an unfavorable system for the ANR theory owing to its large rotational spacings that make threshold and closed-channel effects important up to large kinetic energies (> 10 meV).

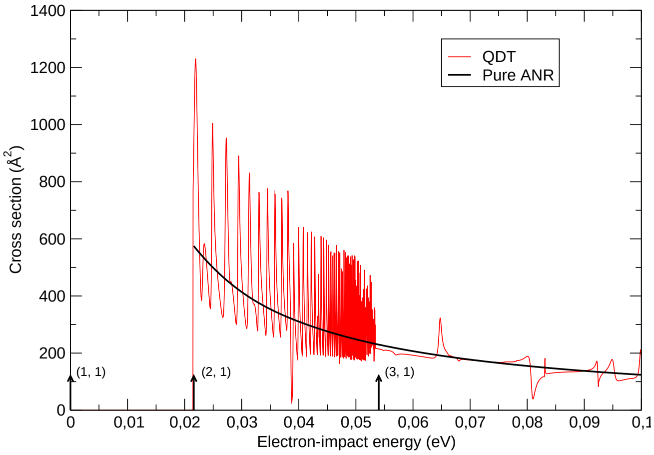

Fig. 1. Rotationally inelastic excitation cross sections for the transition (1, 1) → (2, 1) in H_3^+ as a function of electron-impact energy. The red line refers to the full rovibrational frame transformation calculation. The black line give the ANR cross section. Vertical arrows denote the (1, 1) → (2, 1) and (1, 1) → (3, 1) thresholds.

In the case of HCO^+, however, resonances due to the transitions $\Delta J > 1$ are not expected to contribute significantly to the dipolar rate coefficients ($\Delta J > 1$) owing to the large HCO^+ dipole (3.9 D) and its small rotational spacings. As a result, the Heaviside correction has been applied to the ANR excitation cross sections of HCO^+ but closed-channel effects were ignored. In the case of HCN, the kinematic correction factor k'/k was applied to the ANR cross sections. In Fig. 2 rate coefficients for the rotational excitation of HCO^+ and HCN are plotted as a function of temperature. As these two species have similar rotational constants and dipoles, their dipolar rates ($\Delta J = 1$) are very similar at high temperatures. Owing to different threshold laws, however, the HCO^+ rates are predicted to be significanlty larger than those of HCN at very low temperatures. Moreover, it can be noticed that rates for $\Delta J > 1$ are much larger for HCO^+ than for HCN, suggesting significant excitation differences between these two species in cold ionized media. We note in this context the recent suggestion by Jiménez et al. (2006) to use rotational emission of HCO^+, HCN and HNC to probe electron densities in interstellar C-type shocks.

4 Conclusion

Based on R-matrix ab initio wavefunctions combined with the adiabatic-nuclei-rotation (ANR) approximation corrected for threshold effects, we have computed rotational rate coefficients for HCN and HCO^+. These calculations have shown significant excitation differences between the ion and the neutral, a prediction that is

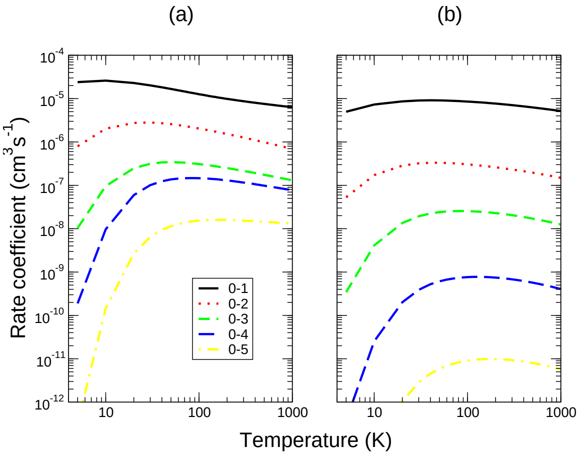

Fig. 2. Electron-impact rate coefficients for the rotational excitation of HCO$^+$ (a) and HCN (b) as a function of temperature.

beginning to be observed astrophysically (Jiménez et al. 2006). We note, however, that further studies are needed to quantitatively assess the near-threshold behaviour of rotational cross sections in the case of polar species.

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