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The effect of H₂O and electron collisions on rotational populations of cometary CO

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Abstract. We present a simple model of CO excitation in comets, including solar pumping, ro-vibrational (de)excitation by H₂O and electron collisions, and fluorescence. Collisional data for H₂O–CO are taken from quantum statistical calculations while Born dipole cross-sections are calculated for electron-CO collisions. In the non-LTE regime, i.e. at H₂O densities in the range $10^3 - 10^8$ cm⁻³, CO excitation is found to be largely dominated by H₂O collisions, with electron collisions becoming significant only for density profiles with scaling factors $x_{n_e} > 3$.

Keywords: Comets: molecules, molecular data, molecular processes

1 Introduction

In cometary comas, collisional excitation is dominated by H₂O and/or electrons and, for comets at large heliocentric distances, by the more volatile CO. In a significant fraction of the coma, however, the density is too low for collisions to maintain a local thermodynamical equilibrium (LTE) (see e.g. Refs. [1, 2]). As for the interstellar medium [3], the knowledge of accurate collisional data is therefore crucial to properly model the cometary molecular populations. In coma models, molecular excitation due to H₂O collisions is usually based on simple prescriptions with energy-independent cross sections (see e.g. [4, 1]). Recently, however, Dubernet & Quintas-Sánchez [5] and Faure et al. [6] have computed quantum cross sections and rate coefficients for the rotational excitation of HCN and CO by H₂O, respectively. Rate coefficients for self-collisions of H₂O and CO, i.e. H₂O–H₂O and CO–CO collisions, were also determined [7, 8]. Faure et al. [6], in particular, have compared different sets of H₂O–CO rate coefficients and they have also investigated their impact on the CO rotational populations using a simple cometary excitation model.

Here, we extend the work of Ref. [6] by investigating the effect of electron collisions on CO excitation. The next Section describes the CO spectroscopic and collisional data employed in our excitation model. In Section 3 non-LTE calculations are presented and discussed. Conclusions are given in Section 4.

2 CO spectroscopic and collisional data

2.1 CO spectroscopy

CO energy levels (v_2, j_2) (v_2 and j_2 are the vibrational and rotational quantum numbers), frequencies and spontaneous emission Einstein coefficients were taken from the HITRAN database (<https://hitran.org>). Only the first excited vibrational level $v_2 = 1$ was taken into account because the solar excitation rate of $v_2 = 1$ is at least two orders of magnitude larger than those of $v_2 > 1$. The lowest 80 ro-vibrational levels were thus included, i.e. up to level (1, 32) which lies 0.51 eV above the ground state (0, 0).

2.2 CO excitation by H₂O

Quantum calculations for the CO excitation by H₂O were performed in Ref. [6] using the statistical adiabatic channel model (SACM). Cross sections were obtained for rotational transitions among the first 11 energy levels of CO (up to $j_2 = 10$) and the first 8 energy levels of both p-H₂O and o-H₂O (up to $j_1 = 3$) and for collision energies up to 0.062 eV. Rate coefficients for thermal distributions of each nuclear-spin isomer of H₂O were then deduced for kinetic temperatures in the range 5–100 K. Faure et al. [6] have provided detailed comparisons with literature data and significant differences (by up to a factor of 3) were observed. Full details about the SACM calculations can be found in Refs. [9, 6]. For CO rotational levels above $j_2 = 10$ and for ro-vibrational transitions, *total* de-excitation rate coefficients were fixed at 10^{-10} cm³s⁻¹ and 10^{-13} cm³s⁻¹, respectively, with an equal distribution among final levels and no temperature dependence. We note that, in practice, collisional transitions among levels above $j_2 = 10$ play a negligible role at the investigated kinetic temperature.

2.3 CO excitation by electrons

For the electron-impact excitation of CO, cross sections were computed using the Born approximation. As shown by Itikawa [10], Born dipole calculations for rotational cross sections are in good agreement with more elaborate methods at electron energies below 1 eV (11,160 K). They are also consistent (to within a factor of two) with experimental backward-scattering cross sections in the very low-energy range 2–160 meV [11]. In the case of vibrational excitation, it has been shown that the Born dipole approximation is also adequate at low energies, i.e. below the ²Π shape resonance centred at about 2 eV (Sohn et al. [12]). The CO dipole being small (0.11 D), however, we expect dipole forbidden transitions to also play a role and more studies are needed. In the present work, Born cross sections were obtained for all dipolar transitions ($\Delta j_2 = \pm 1$) among the lowest 80 ro-vibrational levels of CO and for electron energies up to 9 eV. They were then integrated over Maxwell-Boltzmann energy distributions to yield thermally averaged rate coefficients in the range 10–10,000 K.

3 Non-LTE model of CO in comets

We have selected physical conditions corresponding to an *average* comet located at $R_h = 1$ AU from the Sun with a total production rate from the nucleus $Q_{\text{H}_2\text{O}} = 10^{29} \text{ s}^{-1}$, an expansion velocity $v_{\text{exp}} = 0.8 \text{ km s}^{-1}$ and a neutral gas temperature $T_k = 30 \text{ K}$. The background radiation field includes the 2.73 K cosmic microwave background and the Sun radiation. Water is the dominant neutral collider and the H₂O density is described by a standard isotropic Haser model. For the electron density and temperature radial profiles, we used the model described in Zakharov et al. [13] where full details can be found (see also [14]). The scaling factor x_{n_e} for the electron density is used as a free parameter below. We note that the ‘default’ value $x_{n_e} = 1$ was derived from *Giotto* measurements in comet 1P/Halley [13]. Temperature and density profiles are shown in Fig. 1 where R_{cs} is the distance of the ‘contact’ surface (separating the purely cometary plasma from the region containing solar wind charged particles) and where R_{rec} is the distance of the ‘recombination’ surface (outside which the recombination rate of electrons with ions is negligible). We note that the bump in the electron density can be partly attributed to the decrease of the recombination rate of electrons with ions caused by the strong increase of the electron temperature.

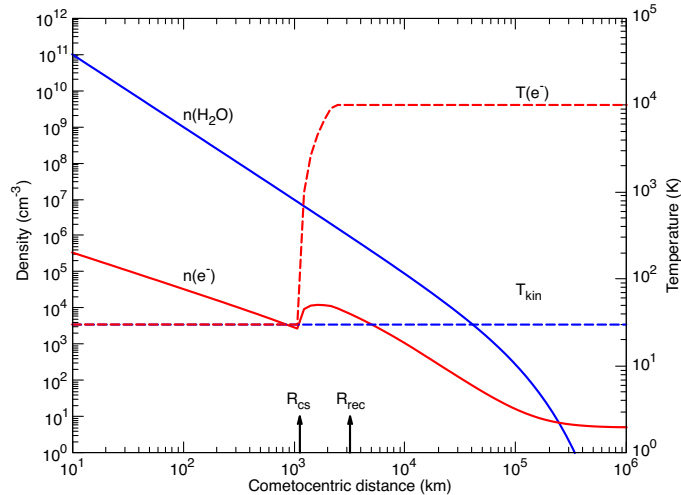


Fig. 1. Evolution of H₂O and electron density and temperature as a function of the nucleocentric distance for $Q_{\text{H}_2\text{O}} = 10^{29} \text{ s}^{-1}$. The scaling factor x_{n_e} is fixed at 1. See text for details.

The coupled radiative transfer and statistical equilibrium equations were solved at steady-state within the large velocity gradient (LVG) approximation using the public version of the RADEX code where we have implemented different

kinetic temperatures for the neutrals (H_2O) and the electrons. The CO column density was set to 10^{14} cm^{-2} and the ortho-to-para ratio of H_2O was fixed at 3, as in Ref. [6] where other details can be found. Results are presented in Fig. 2 where we can observe three distinct density regimes: the fluorescence equilibrium ($n_{\text{H}_2\text{O}} < 10^3 \text{ cm}^{-3}$), the non-LTE regime ($10^3 \leq n_{\text{H}_2\text{O}} \leq 10^8 \text{ cm}^{-3}$) and the LTE equilibrium ($n_{\text{H}_2\text{O}} > 10^8 \text{ cm}^{-3}$). The impact of the colliders can be seen in the non-LTE regime, where electrons do not significantly modify the CO populations except if the scaling factor x_{n_e} is larger than 3. Thus, for $x_{n_e} = 10$, CO populations are modified by up to 15% in the region of the bump in electron density. We note that this weak sensitivity of CO populations to electron collisions was already observed by Biver et al. [1] (see their Fig. 6). As noted by these authors, this is specific to weakly polar species: the Born dipole cross sections indeed scale with the square of the dipole moment. Thus, in the case of H_2O where the dipole is 1.85 D, the contribution of electron collisions was found to be important [4].

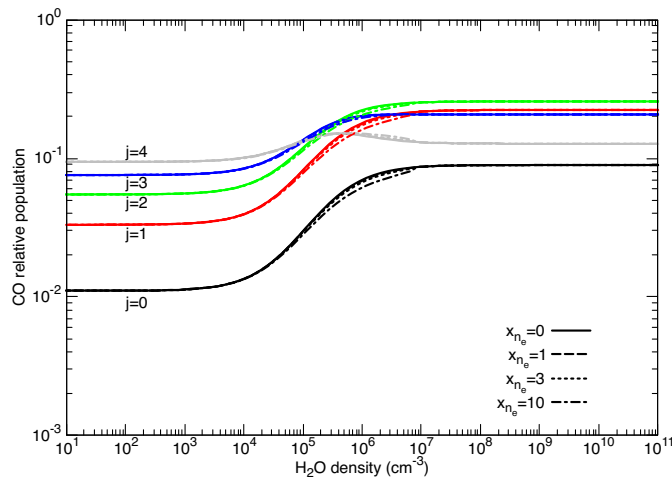


Fig. 2. Level populations of CO ($j = 0 - 4$) as a function of H_2O density for a kinetic temperature of 30 K, with $x_{n_e} = 0, 1, 3, 10$.

4 Conclusions

We have investigated the effect of H_2O and electron collisions on rotational populations of CO in comets. Using a simple cometary excitation model including solar pumping, ro-vibrational (de)excitation by H_2O and electrons, and fluorescence, we have found that the contribution of electron collisions is insignificant except for electron density profiles with a scaling factor $x_{n_e} > 3$. This result

confirms the conclusions of previous studies and reflects the small CO dipole moment. Future works will explore the additional contribution of CO–CO collisions.

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