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THE SPIN TEMPERATURE OF METHANOL IN COMET HALE-BOPP

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Abstract. Measurements of the ortho-to-para ratio (OPR) of small hydrogenated molecules (H_2O, NH_2 which leads to NH_3, and CH_4) in the coma of comets give spin temperatures clustered around 30 K, which is most of the time lower than the associated rotational temperatures. We investigate here the spin temperature of methanol from the observations of the 241 and 145 GHz sets of rotational lines, obtained on C/1995 O1 (Hale-Bopp) on two different dates with the 15-m and 30-m antennas of IRAM.

1 Introduction

Molecules such as H_2O, H_2CO, NH_3, CH_4, CH_3OH... exist in several nuclear spin isomer species. Nuclear spin conversion between such isomers is thought to be radiatively and collisionally forbidden, so spin temperatures could remain unchanged for a long time, provided no conversion occurs in the solid phase. The spin temperatures measured for H_2O and NH_3 (traced from NH_2) are found to cluster near 30 K for different comets, whatever their dynamical origin, their distance to the Sun or their activity level (e.g., Kawakita et al. 2004; Bonev et al. 2007). The interpretation of this temperature is subject to debates. It might be of pristine origin, reflecting how the molecules were formed in the early Solar System (but the preservation of the spin temperature over cosmological times seems unlikely). Or it could result from recent re-equilibration (but why all spin temperatures are similar is still to be understood).

We investigate here the case for cometary methanol. CH_3OH is organized in two independent manifolds (Fig. 1): E-type ($I = 1/2$) and A-type ($I = 3/2$). As mentioned earlier (Crovisier 1998) the A/E ratio of this molecule is less sensitive to temperature than the ortho-to-para ratio of water. Despite this difficulty, we tried to constrain the spin temperature by applying the rotational diagram method to two sets of spectroscopic data secured on comet Hale-Bopp.

2 Observational data

We analysed two sets of data containing pure rotational lines of methanol coming from comet C/1995 O1 (Hale-Bopp). The first set was recorded on 12 March 1997, 19 days before perihelion, at 241 GHz, with the 15-m antennas of the IRAM interferometer used in single-dish mode (heliocentric distance $r_h = 0.98$ AU, geocentric distance $\Delta = 1.36$ AU). The second set was recorded on 29 May 1997, in the 145 GHz frequency band with the 30-m single-dish antenna of IRAM ($r_h = 1.36$ AU, $\Delta = 2.24$ AU). Figure 1 shows the pattern of the CH_3OH rotational levels with the transitions observed for this study. Corresponding spectra are presented in Fig. 2.

3 Data analysis

3.1 Excitation model

As shown previously in Bockelée-Morvan et al. (1994), cometary methanol is out of equilibrium. A direct estimation of the spin temperature of methanol in comet Hale-Bopp from the observational data is thus not

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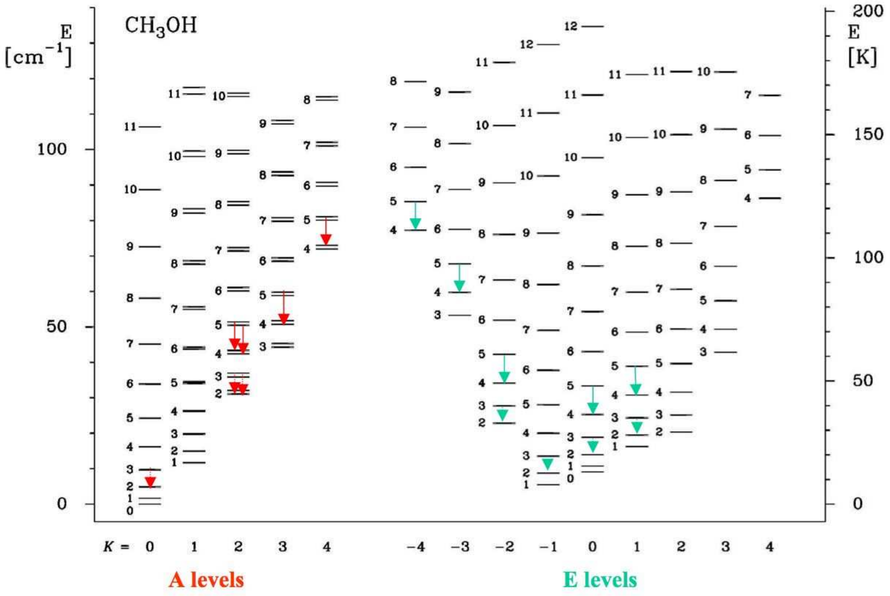

Fig. 1. Rotational levels of methanol. The rotational transitions analysed in the present study are indicated by arrows.

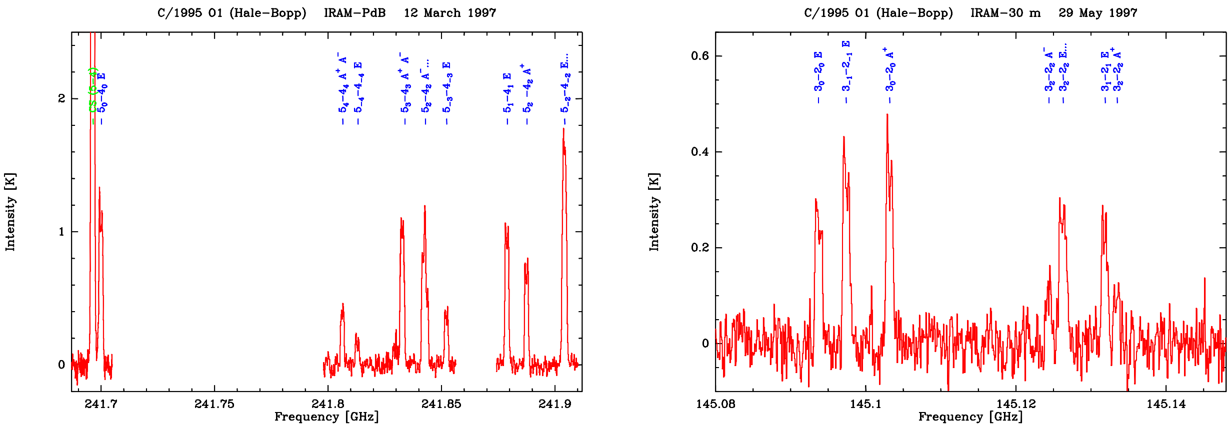

Fig. 2. IRAM spectra of methanol observed in comet Hale-Bopp. Left: 241 GHz group observed on 12 March 1997 with the Plateau-de-Bure interferometer. Right: 145 GHz group observed on 29 May 1997 with the 30-m telescope.

possible. The excitation of methanol is governed by collisions with water molecules and electrons, spontaneous relaxation and excitation of the fundamental vibrational bands by solar radiation. In the present analysis, radiative excitation follows the model of Bockelée-Morvan et al. (1994) whereas collisions with electrons are modelled following the formalism of Xie & Mumma (1992) and Biver (1997).

For collisions, the model parameters are the collisional cross section with water molecules ($\sigma_{\rm coll} = 5 \times 10^{-14}$ cm^2), the water production rate ($Q_{\rm H_2O} = 6 \times 10^{30}$ s^{-1} and 4×10^{30} s^{-1} for the two sets of data, respectively, as determined from other observations; Biver et al. 2002), the neutral gas kinetic temperature ($T_{\rm kin} = 110$ K and 72 K for the two sets of data, respectively, also determined from other observations) and x_{ne} which is a scaling factor accounting for electronic collisions (as discussed by Xie & Mumma 1992, Biver 1997 and Biver et al. 1999).

3.2 Rotational diagrams

When studying intensities linked with pure rotational transitions, it is of interest to use the rotational diagram method, currently employed in interstellar molecule studies (Goldsmith et al. 1999). In this method, $\mathrm{Ln}(\gamma_u W/g_u)$ is plotted as a function of E_u for $u \rightarrow l$ transitions, where W is the line intensity, g_u is the statistical weight of the u level, $\gamma_u = (8\pi\nu_{ul}^2)/(hc^3 A_{ul})$ with ν_{ul} and A_{ul} being the frequency and Einstein coefficient of the transition. E_u is the energy of the u level (in K units).

In such a diagram, all points should be aligned if the rotational distribution of the molecule is thermal and if the lines are optically thin (which is the case here for cometary methanol). The inverse of the slope is then the rotational temperature T_{rot}. If the excitation processes of methanol are governed by collisions, all the observational points relevant from a spin isomer are expected to be aligned, with $T_{\mathrm{rot}} = T_{\mathrm{kin}}$.

The rotational diagrams resulting from our observations are plotted in Fig. 3, together with those simulated with the excitation model.

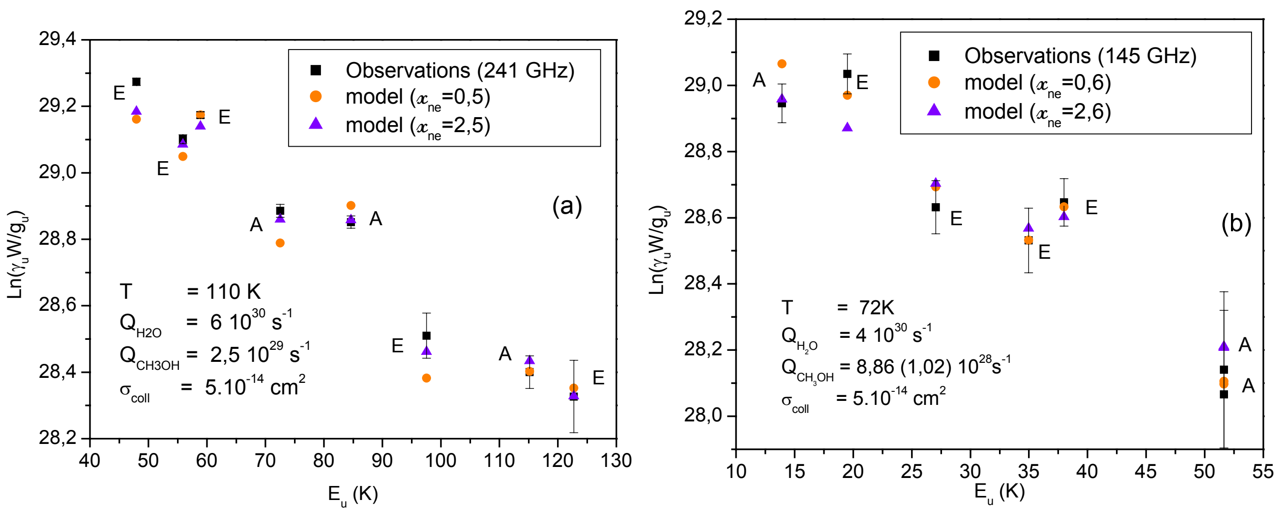

Fig. 3. Comparison between observed and simulated rotational diagrams. a) 12 March 1997. b) 29 May 1997.

4 Results and discussion

As can be seen in Fig. 3, this study is hampered by departures of the population distribution from a thermal distribution. By adjusting the main parameters of the model (σ_{coll}, x_{ne}, $Q_{\mathrm{CH_3OH}}$), the two rotational diagrams could be reasonably reproduced (Fig. 3). The retrieved rotational temperatures from least-square fits are $T_{\mathrm{rot}} = 79.2 \pm 2.7$ K for the data set secured on 12 March 1997, $T_{\mathrm{rot}} = 50.5 \pm 3.8$ K for the data set secured on 29 May 1997. These values are lower than the T_{kin} measured for the same dates, showing that CH_3OH is rotationally relaxed.

The x_{ne} scale factor, employed to take into account the collisions of methanol with electrons, seems to be a crucial parameter. A value lower than 1 correspond to a small contribution whereas a value higher than 1 stands for a more important contribution. The rotational diagrams corresponding to two different values of x_{ne} are shown for the two data sets in Fig. 3. In Fig. 3a, it appears that the observations are better reproduced with a high value of x_{ne}, whereas this is not so clear farther from the Sun in Fig. 3b.

Using together the E and A lines of methanol, we find that the production rate $Q_{\mathrm{CH_3OH}} = 25\pm2.30\times10^{28}$ s^{-1} at a distance of 0.98 AU from the Sun, whereas a smaller value of $8.9 \pm 1.0 \times 10^{28}$ s^{-1} is found at a distance of 1.36 AU. This is close to values obtained in previous studies (Biver et al. 2002).

Then, the E/A ratio is obtained by adjusting separately the observational points relevant to the E or A species and comparing the resulting E and A production rates. This leads to E/A= 1.14 ± 0.28 and 1.30 ± 0.38 for the two sets of data, respectively. The large error bars stem from the failure of the model to reproduce exactly the departures from the thermal distribution, rather than from the signal-to-noise ratio of the lines. The lower bounds are 0.86 and 0.92, leading to $T_{\rm spin} > 15$ K and > 18 K for the two sets of data, respectively.

We note that for the collision rates of methanol with water, we have used a unique *conventional* cross section for all the transitions ($\sigma_{\rm coll} = 5 \times 10^{-14}$ cm^2), without any consideration on the total nuclear spin of the collisional partners or their rotational states. Varying this parameter between 2 and 7×10^{-14} cm^2 only slightly affects the shape of the rotational diagrams. Certainly, a significant improvement of the model in the future would be to use level-dependent cross sections for H_2O–CH_3OH collisions, when available. It is not excluded that the ortho-to-para ratio of water could play an important role in the collisional excitation of methanol if cross sections relative to *ortho*-H_2O are different from *para*-H_2O.

5 Conclusions

In this work, we were able to determine a minimum value of the spin temperature of methanol, which does not contradict the earlier measures made with H_2O, NH_2 and CH_4, leading to a possible important gap between $T_{\rm spin}$ and $T_{\rm kin}$. It has also been possible to show that collisions of methanol with electrons play an important role in order to reproduce observations.

Watanabe et al. (2006) have determined experimentally that methanol can be formed by CO hydrogenation contained in pure or mixed ices, but this process is efficient only at temperatures below 15 K. If the spin temperature limit we obtained is indeed relevant to the formation temperature of methanol, another formation mechanism should be envisaged for this species. Laboratory analyses simulating cometary environments are needed to solve this issue.

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