Methanol as a diagnostic tool of interstellar clouds

I. Model calculations and application to molecular clouds

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Abstract. We present a detailed analysis of the diagnostic properties of methanol, (CH₃OH), in dense molecular clouds, made possible by the availability of new (CH₃OH-He) collisional rate coefficients. Using a spherical Large Velocity Gradient (LVG) model, the dependence on kinetic temperature and spatial density of various millimeter and submillimeter line bands is investigated over a range of physical parameters typical of high- and low-mass star-forming regions. We find CH₃OH to be a good tracer of high-density environments and sensitive to the kinetic temperature. Using our LVG model, we have also developed an innovative technique to handle the problem of deriving physical parameters from observed multi-line spectra of a molecule, based on the simultaneous fit of all the lines with a synthetic spectrum, finding the best physical parameters using numerical methods.

Key words. ISM: molecules – ISM: clouds – molecular processes

1. Introduction

Kinetic temperature and density are fundamental parameters for our understanding of the interstellar medium (ISM). However, since the main gas-phase molecular component, H₂, is not directly observable under “normal” conditions, one has to rely on other molecules to trace the physical state of an interstellar cloud. Usually, symmetric rotors such as NH₃ are used to probe a cloud’s kinetic temperature (Walmsley & Ungerechts 1983; Danby et al. 1988), while linear molecules, e.g. CS, are used to determine its density (e.g., Snell et al. 1984; Beuther et al. 2002). However, different spatial distributions of the tracers (“chemistry”) often complicate the picture, (see, e.g., Tafalla et al. 2002) as they often trace physically different and spatially non-coexisting gas components. It is thus desirable to trace all relevant physical parameters with a single molecule.

Promising candidates exist among slightly asymmetric rotors, which have properties qualifying them as tracers for physical conditions. Since they are almost symmetric, they share a strong sensitivity to kinetic temperature with symmetric molecules, but they also allow determinations of spatial density (for a detailed discussion of H₂CO, see Mundy et al. 1987; Mangum & Wootten 1993).

Methanol, CH₃OH, a slightly asymmetric rotor, is a proven tracer of high-density environments (e.g. Menten et al. 1988), but up to now an extremely poor knowledge of the CH₃OH collisional rates and of their propensity rules has prevented realistic systematic studies exploiting methanol’s full potential as an interstellar tracer. Recently, this situation has changed with the calculation of collisional rate coefficients by Pottage et al. (2001, 2002), which we have integrated in a “standard” Large Velocity Gradient program aimed at modelling methanol excitation. Here, we present an application of our model calculations to observations of clouds without IR radiation, while extensive modelling of a variety of evolved star-forming regions as well as Class I methanol masers will be discussed in accompanying papers. In Sect. 2 we discuss a detailed analysis of the tracing properties of CH₃OH in dense molecular clouds; in Sect. 3 we present a new approach to derive physical parameters from CH₃OH spectral lines.

2. Excitation of CH₃OH

Due to the threefold symmetry of its hindering potential, CH₃OH occurs as A- and E-symmetry states. The E-type, \(-J \leq k \leq J\), is vibrationally doubly degenerate: the \(E_1, k \geq 0\) states are degenerated with \(E_2, k \leq 0\). In the A-type, \(0 \leq K \leq J\),
for \( K \geq 0 \) there are doublets split by asymmetry which are labelled \( A^+ \) and \( A^- \) (Lees & Baker 1968). For radiative transport purposes, its \( A^- \) and \( E^- \)-type symmetry states can be considered as two different molecules, since interconversion can happen only through proton exchange reactions, which happen on timescales so long that the excitation is unaffected. Transitions between \( A^+ \) and \( A^- \) levels occur.

\( \text{CH}_3\text{OH} \) is ubiquitous and associated with different regimes of star formation, from quiescent, cold (\( T \sim 10 \) K), dark clouds, where its abundance relative to \( \text{H}_2 \) is only \( \sim 10^{-9} \) (Friberg et al. 1988), to “hot core” sources near high-mass (proto) stellar objects, where \([\text{CH}_3\text{OH}/\text{H}_2]\) values \( \sim 10^{-7} - 10^{-6} \) are observed (Menten et al. 1986, 1988).

A practical advantage is that, because of its complex energy level structure, it has groups of several transitions close together in wavelength space throughout the millimeter and submillimeter region that can be observed simultaneously, thus minimizing relative calibration uncertainties, and a multitude of its transitions is observable with ground-based telescopes.

Methanol has in the past been used as a probe of spatial density in dense molecular clouds, (cf. Friberg et al. 1988; Walmsley et al. 1988; Menten et al. 1988; Kalenskii et al. 1997; Bachiller et al. 1998); however, uncertainties in the derived densities are expected since these authors modelled the \( \text{CH}_3\text{OH} \) excitation using collisional rates based upon the experiments by Lees & Haque (1974) for \( \text{CH}_3\text{OH} \) with \( \text{He} \), for low states of \( \text{CH}_3\text{OH}-E \) only.

The \( \text{CH}_3\text{OH} \) spectrum up to 500 GHz is shown in Fig. 1 for two different sets of physical parameters typical for the ISM calculated with our LVG program. Rest frequencies are from the Cologne Database for Molecular Spectroscopy, (http://www.cdms.de, Müller et al. 2001), which includes new measurements by Xu & Lovas (1997).
2.1. \( \text{CH}_3\text{OH}-\text{He} \) collisional rates

Only recently (see Pottage et al. 2001, 2002), rate coefficients for collisions of methanol with helium, for both \( \text{CH}_3\text{OH}-\text{A} \) and \( \text{CH}_3\text{OH}-\text{E} \), have been computed for levels up to \((J,k^1) = 9\) at kinetic temperatures up to 200 K. Calculations of rate coefficients for collisions with para-\( \text{H}_2 \) have been recently carried out and comparisons of our results with this new dataset will be analysed in a forthcoming paper. With this new set of collisional rates, we have carried out statistical equilibrium calculations on both \( \text{A} \)- and \( \text{E} \)-types for the torsional ground state, using the Large Velocity Gradient (LVG) method with spherical geometry in the derivation of de Jong et al. (1975). Since the new calculations on collisional rates have been computed only for the torsional ground state, we limit our study to those sources in which the only external radiation field is the cosmic background radiation, in order to avoid any effect due to infrared pumping. We estimate differences in the interaction potentials between \( \text{He} \) and \( \text{H}_2 \) to be likely more important than those due to their different reduced masses and did not scale the \( \text{CH}_3\text{OH}-\text{He} \) collisional rates by any factor related to the masses.

Our calculations are extended to the first 100 levels for each state, for which the collisional rates from Pottage et al. (2001, 2002) are available; the coverage in energy is thus incomplete above 100 K, (see Figs. 2a,b), and does not allow a reliable estimation of the partition function at high temperatures. We compared our LTE values for the partition function with the one obtained with a more complete set of levels, \((J \leq 26, k \leq 14)\), for which energies are calculated using global fit parameters reported in Xu & Hougen (1995), and we expect no significant uncertainties in our results up to 50 K, where the deviation from the most accurate value of \( Q \) is close to 10%. Since our sample of sources is not expected to show temperatures higher than 50 K, the inaccuracy in the partition function should not affect our calculations. All allowed radiative transitions for the levels up to \((J,k) = 9\) have been included in our model, even the weak \( \Delta k \geq 2 \) lines. Line strengths are from Mekhtiev et al. (1999).

2.2. First test – dark clouds

Pottage et al. (2001) have compared their results with the ones from Lees & Haque (1974) and tested the accuracy of their collisional rates by modelling the \( 2_0 \rightarrow 3_{-1} \) \( \text{E} \) transition at 12.18 GHz. They find a generally good agreement with the measurements of Lees & Haque (1974), with exceptions, for example, in the \( \Delta k = 3m \) transitions, (where \( m \) is an integer). We extended the tests to other transitions observed in dark clouds, where any external radiation field but the cosmic
2.3. CH$_3$OH as a probe of interstellar physical conditions

The richness of the CH$_3$OH spectrum prevents us from a systematic study of all its transitions: taking into account only the energy levels with $(J, K) \leq 9$, the $E$ state alone has more than 300 lines, (see Figs. 1a, b). Therefore, we restricted our study to only some bands observable from ground based telescope and not showing any maser action: the $2_k \rightarrow 1_k$-A and -E type lines near 96 GHz, the $5_1 \rightarrow 4_1$-A and -E lines near 241 GHz, the $7_k \rightarrow 6_k$-A and -E lines near 338 GHz. Even if promising candidates to trace kinetic temperature are in the submillimeter bands, with current collisional rates, we cannot reliably analyse higher transitions because the level set is incomplete above 100 K, (see Figs. 2a, b).

As a first step, we analysed line ratios from transitions close together in frequency space, in order to find diagnostic tests of kinetic temperature and density which are not affected by beam-size differences, pointing and absolute calibration uncertainties. A slight asymmetry in the abundances of the A and E subspecies, due to a difference in their ground state energies, has been suggested and indeed observed (see Friberg et al. 1988; Menten et al. 1988). Since their relative abundance can vary from 0.69 in dark clouds, (Friberg et al. 1988), to 2 in OMC-2, (Menten et al. 1988), comparisons between CH$_3$OH-E and -A lines are not taken into account to avoid any uncertainties in deriving physical parameters due to an inaccurate knowledge of the A/E ratio.

From the CH$_3$OH-E selected transitions, we found several ratios to be calibration-independent tracers of density: the $T_R(2_1 \rightarrow 1_1)/T_R(2_1 \rightarrow 1_2)$ and the $T_R(2_0 \rightarrow 1_0)/T_R(2_2 \rightarrow 1_1)$ in the 96 GHz band; the $T_R(5_0 \rightarrow 4_0)/T_R(5_1 \rightarrow 4_1)$, the $T_R(5_1 \rightarrow 4_1)/T_R(5_1 \rightarrow 4_2)$, the $T_R(5_2 \rightarrow 4_2)/T_R(5_1 \rightarrow 4_1)$, and the $T_R(5_2 \rightarrow 4_2)/T_R(5_1 \rightarrow 4_1)$ in the 241 GHz band. They all show a dependence on temperature in the range 5−15 K that suggest their use as temperature tracer in dark clouds. However, no line ratios in the 1 mm and the 3 mm bands show a pure dependence on the kinetic temperature, while for several ratios in the 1 mm band we found a strong sensitivity to both density and temperature.

The submillimeter band we analysed, at 338 GHz, shows a behaviour very similar to the 1 mm series, with several line ratios being sensitive to both kinetic temperature and spatial density. However, some line ratios can be used as calibration-independent tracers of density, (e.g. the $T_R(7_0 \rightarrow 6_0)/T_R(7_1 \rightarrow 6_0)$ and the $T_R(7_1 \rightarrow 6_1)/T_R(7_1 \rightarrow 6_2)$). A pure dependence on kinetic temperature is found in line ratios with $|l| \geq 3$, but mainly at low density ($n$(H$_2$) $\leq 10^5$ cm$^{-3}$) where these lines are very weak (see Figs. 6a, b). However, given the sensitivity to both kinetic temperature and spatial density of several line ratios in the 5 and 7$_k$ bands and the pure dependence on density of others, the simultaneous observations of several lines from these series allows determining both the physical parameters.

Figures 4−6 show LVG model predictions for line ratios in logarithmic scale as function of density and temperature at different column densities. The submillimeter bands are studied only at high column densities (10$^{14}$−10$^{16}$ cm$^{-2}$/(km s$^{-1}$)).
Results of statistical equilibrium calculations for CH$_3$OH. The $T_{\text{ch}}$($2_0 \rightarrow 1_0$)/$T_{\text{ch}}$($2_{-1} \rightarrow 1_{-1}$) line ratio is shown in logarithmic scale, as function of H$_2$ density and temperature at $N$(CH$_3$OH)/$\Delta v = 10^{13}$, a) $N$(CH$_3$OH)/$\Delta v = 10^{14}$, b) $N$(CH$_3$OH)/$\Delta v = 10^{15}$, c) and $N$(CH$_3$OH)/$\Delta v = 10^{16}$ cm$^{-2}$/(km s$^{-1}$). d) The black contours range from $-1.5$ to $0$ by steps of $0.1$. The whole $T$–$n$ plane is accessible to observations.

where their brightness temperatures become significant. Our results are summarized in the following guidelines:

- line ratios in the $2_k \rightarrow 1_k$ and the $5_k \rightarrow 4_k$ bands at 96 and 241 GHz are tracers of densities higher than $10^5$ cm$^{-3}$, with a weak dependence on temperatures up to 15 K;
- line ratios in the $5_k \rightarrow 4_k$ at 241 GHz and $7_k \rightarrow 6_k$ at 338 GHz are sensitive to kinetic temperature and spatial density, with some examples of pure density tracers;
- information on kinetic temperature is recovered when lines with an excitation temperature close to the expected kinetic temperature of the source are observed.

The main result we found is that, for all the analysed millimeter bands, ratios between lines in the same band are strongly sensitive to density, with a weaker dependence on temperature.

This is explained by the high probability of the $a$-type$^2$ radiative transitions to occur, ($A_{ij} \propto \mu^2$, $\mu_a = 0.896$, $\mu_b = 1.412$, Sastry et al. 1981). Even if CH$_3$OH is only slightly asymmetric, ($\kappa = -0.98$ for CH$_3$OH, while $\kappa = -1$ for a prolate symmetric rotor, where $\kappa$ is the Ray’s asymmetry parameter, Ray 1932; Townes & Schawlow 1996), the $\Delta k \neq 0$ radiative lines are strongly allowed and not mainly dependent on the collisions as the structural similarity of asymmetric molecules with symmetric rotors would suggest. However, in the submillimeter regime, several transitions show a strong dependence on the kinetic temperature in the range up to 100–150 K. Nevertheless, since several line ratios in the $5_k \rightarrow 4_k$ and in the $7_k \rightarrow 6_k$ band are strongly dependent on kinetic temperature and

\footnote{Using standard asymmetric rotor nomenclature, $a$-type transitions have $\Delta k = 0$, while $b$-type transitions have $\Delta k = \pm 1$.}
Fig. 5. Results of statistical equilibrium calculations for CH\textsubscript{3}OH-E. The $T_{\text{ex}}(5 \rightarrow 4)/T_{\text{ex}}(5 \rightarrow 4)$ line ratio in logarithmic scale is shown as function of H\textsubscript{2} density and temperature at $N$(CH\textsubscript{3}OH)/$\Delta v = 10^{13}$, a) $N$(CH\textsubscript{3}OH)/$\Delta v = 10^{14}$, b) $N$(CH\textsubscript{3}OH)/$\Delta v = 10^{15}$, c) and $N$(CH\textsubscript{3}OH)/$\Delta v = 10^{16}$ cm$^{-2}$/km s$^{-1}$. d) The black contours range from −1.5 to 0 by steps of 0.1 in a), b) and c); from −0.5 to 0.1 by steps of 0.05 in d). The whole $T$–$n$ plane is accessible to observations.

spa\textsubscript{t}ial density, both the parameters can be derived when a rich CH\textsubscript{3}OH spectrum is available, with lines in different frequency and excitation ranges. Line ratios from the $5_k \rightarrow 4_k$ band with the $7_k \rightarrow 6_k$ series show a dependence on temperature up to 50–80 K, at high density, $n$(H\textsubscript{2}) $\geq 10^6$ cm$^{-3}$, (see Figs. 7a,b), since they have different excitation energies.

3. Analysis technique

The traditional approach for deriving physical parameters such as kinetic temperature and spatial density from an observed spectrum involves “by-hand” Gaussian fitting of the lines with multiple components and $\chi^2$ analysis comparing the measured quantities with statistical equilibrium calculations (see Olmi et al. 1993; Mangum & Wootten 1993). Better results are obtained if the analysed quantities are ratios between lines close together in frequency space and observed simultaneously with the same receiver, because uncertainties due to absolute calibration and to the beam filling factor are minimized. The main drawback is the loss of information on the column density. On the other hand, when working with line intensities, uncertainties due to absolute calibration and to the beam filling factor play a major role in making the determination of physical parameters less reliable. In general, this kind of analysis also ignores upper limits on lines too weak to be detected, because of the non-physical fitting procedure. For complex sources, the technique also requires decomposing line profiles, a tedious and, for strongly blended lines, very unreliable process. When applied to large multi-line datasets, like line surveys of a source
or systematic multi-frequency studies of a molecule, by-hand fitting is impractical. With sensitive receivers available nowadays and in view of the next generation of instruments, which will provide copious amounts of data in a short time, new methods of data analysing and modelling are required.

An innovative technique to handle the problem, proposed by Schilke et al. (1999) and recently improved by Comito et al. (2004), is based on the simultaneous fit of all the lines in a spectrum with a synthetic spectrum computed under Local Thermodynamic Equilibrium (LTE) conditions. Here we propose an extension to this technique using the LVG approximation: this development is necessary and fully justifies the computing-time involved in such an analysis because we expect prominent departures from LTE in the sources of our sample and in many other astrophysical scenarios. To allow for complexity in the physical conditions along a line of sight, our model handles multiple components, which are assumed not to interact, i.e. the intensities simply add up. The free parameters for each component are kinetic temperature, molecular hydrogen density, source size and column density. To take into account the possibly different abundance between A and E states, CH$_3$OH-A and CH$_3$OH-E column densities are treated as two independent free parameters. Line width, $\Delta v$, and LSR velocity, $v_{LSR}$, are fixed parameters and assumed to be the same for all the lines in each component. The fitting is done by minimizing the $\chi^2$ between the data and the model spectrum using
the Levenberg-Marquardt method from Press et al. (1992). The $\chi^2$ analysis is however not trivial, given the high number of fitted channels. We assume the degrees of freedom to be given by $\nu_d = N_o - N_f$, where $N_o$, the number of observed quantities, is here the number of all the channels in which CH$_3$OH transitions fall, even if not detected, plus the observed velocity and line width of each components. $N_f$ is the number of free parameters. Frequencies for the line identification are from the Cologne Database for Molecular Spectroscopy. In the current implementation, 100 000 lines can be fitted simultaneously and data from different telescopes can be combined easily.

All the levels for which the collisional rates from Pottage et al. (2002) are available are used for the calculations; however, at low temperatures ($T_{\text{kin}} \lesssim 30$ K) the program runs into numerical problems due to the depopulation of the most excited levels in this regime. Therefore, only a subset of transitions is used in this range.

We assume the following representation of the spectrum:

$$ T_v = \sum_c \eta_c \phi_c \left[ J(T_{\text{ex}}^c) - J(T_{\text{bg}}) \right] \left( 1 - e^{-\tau_c} \right) $$

(1)

with

$$ \tilde{T}_v = \sum \eta_c \phi_c \left[ J(T_{\text{ex}}^c) - J(T_{\text{bg}}) \right] \left( 1 - e^{-\tau_c} \right) $$

(2)


$$ J(T_{\text{ex}}^c) = \sum \eta_c \phi_c \frac{J(T_{\text{ex}}^c)}{\sum \eta_c \phi_c \tau_c} $$

(3)

where $T_{\text{ex}}$ and $\tau$ are given by the LVG results, $\eta$ is the beam filling factor and $\phi$ the line profile. The sums are computed on both $A$ and $E$ states; the indices $l$ and $c$ correspond to lines and spatial components. In Eq. (2), $n^l_{\text{low}}$ and $n^c_{\text{up}}$ are the fractional populations of the lower and upper levels for the transition $l$ in the component $c$ and depend on the set of levels used for the calculations.

An implicit assumption, when solving the radiative transport equation with the escape probability method, is that different lines do not overlap locally. This is not true for molecules with a complex spectrum, especially for CH$_3$OH, whose $A$ and $E$ transitions are often very close in the frequency space. Following Cesaroni & Walmsley (1991), we define an average optical depth and brightness temperature by means of the previous expressions Eqs. (2) and (3) when lines have a frequency separation $v_l - v_j \leq \Delta v_l + \Delta v_j$.

Equation (3) is equivalent to Eq. (13) of Cesaroni & Walmsley (1991) in units of temperature. In the optically thin limit, Eq. (3) is equal to the traditional approach of convolving a line with several Gaussians. On the other hand, it better describes situations in which both optically thin and optically thick lines are present: photons emitted from the optically thin transition are locally absorbed by the optically thick emission. The intensities of the lines do not simply add up like in the optically thin limit, but the intensity at the overlapping frequencies is mainly described by the optically thick emission. In the simplest case of one component and two transitions, both optically thin, Eq. (1) can be approximated by

$$ T_v = \eta_1 \phi_1 \left[ J(T_{\text{ex}}^1) - J(T_{\text{bg}}) \right] \frac{\tau_1}{\tau_1 + \tau_2} + \eta_2 \phi_2 \left[ J(T_{\text{ex}}^2) - J(T_{\text{bg}}) \right] \frac{\tau_2}{\tau_1 + \tau_2} $$

while when one of the two lines, e.g. line 1, is optically thick

$$ T_v = \frac{1}{\tau_1} \eta_1 \phi_1 \left[ J(T_{\text{ex}}^1) - J(T_{\text{bg}}) \right] \frac{\tau_1}{\tau_1 + \tau_2} + \frac{1}{\tau_2} \eta_2 \phi_2 \left[ J(T_{\text{ex}}^2) - J(T_{\text{bg}}) \right] \frac{\tau_2}{\tau_1 + \tau_2} $$

(5)

3.1. Tests on the convergence criterion

Although the simultaneous fit of a spectrum has been demonstrated to be a powerful technique to derive physical parameters (Comito et al. 2004), it does imply several approximations. The assumption behind the analysis is that the CH$_3$OH emission can be reasonably well approximated by a small number of non-interacting components, thus ignoring any alignments between them. This assumption is fully justified when no information on the morphology is available, but it fails in well reproducing the observed spectra if the components are related, leading, for example, to overestimate line intensities when self-absorption happens. The LVG approach adds other uncertainties to the obtained results, since it assumes only one set of physical parameters for each component used for fitting the source and implicitly neglects any local and non-local overlap between the lines; a more detailed model, including density and temperature distributions within each component, would be desirable. However, fitting large datasets with a Monte Carlo synthetic spectrum and minimizing all the free parameters would involve an enormous amount of computing time and it is practically impossible to be applied to a sample of sources. In fact, most (if not all) published Monte Carlo fits used manual fitting of the parameters, with no control over reading a globally best fit, or assessment to the uniqueness of the fit (e.g., Hogerheijde & van der Tak 2000). Moreover, since several spectral windows can be fitted simultaneously, calibration uncertainties still render the determination of physical parameters less reliable. Another drawback is the uniqueness of the $\chi^2$ minimization, which is not a priori guaranteed. Indeed the minimum found occasionally depends on the input parameters. A better control on the fit results is assured when plausible input parameters are used. Particularly important is the information on the source size, which helps in solving the degeneracy between source size, temperature and column density for certain parameter ranges. In the worst situation, no information at all is available in the literature on the source to be modelled and the number of free parameters is $5 \times N_c$, where $N_c$ the number of components. To investigate whether the found solution is local or global, an analysis of the $\chi^2$ distribution as function of the different free parameters in an interval reasonably close to the minimum is desirable.
Table 1. CH$_3$OH model results.

<table>
<thead>
<tr>
<th>Source</th>
<th>$\Delta v$ (km s$^{-1}$)</th>
<th>$T_K$ (K)</th>
<th>$n$(H$_2$) (cm$^{-3}$)</th>
<th>$N$(CH$_3$OH-A) (cm$^{-2}$)</th>
<th>$N$(CH$_3$OH-E) (cm$^{-2}$)</th>
<th>Source size ($''$)</th>
<th>$\chi^2_{df}$</th>
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<tbody>
<tr>
<td>G19.30P1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3</td>
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<tr>
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<td>3.0</td>
<td>44</td>
<td>$10^6$</td>
<td>$7.5 \times 10^{15}$</td>
<td>$3 \times 10^{15}$</td>
<td>5</td>
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<tr>
<td>Outflow</td>
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<td>$1.8 \times 10^5$</td>
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<td></td>
<td>1$\sigma$ fit range</td>
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<tr>
<td>Core</td>
<td>25–320</td>
<td>1.2 $\times 10^5$–3 $\times 10^6$</td>
<td>$3.6 \times 10^{15}$–1.6 $\times 10^{16}$</td>
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<td>1$\sigma$ fit range</td>
<td></td>
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<tr>
<td>Outflow</td>
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<td>4.5 $\times 10^5$–3 $\times 10^6$</td>
<td>$1.4 \times 10^{15}$–3 $\times 10^{15}$</td>
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<tr>
<td>G79.3P1</td>
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<tr>
<td></td>
<td>12–52</td>
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<td>$3.6 \times 10^{13}$–8.1 $\times 10^{15}$</td>
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However, one should be aware of the limits in determining the physical parameters of a source which are intrinsic to this technique. Unless lines with $\tau \ll 1$ and $\tau \gg 1$ are available, solving the degeneracy between source size and column density in the optically thin limit, $(T(\nu) = \sum \eta[J(T_{\nu}) - J(T_{bg})])$, where the information on the temperature is recovered when several optically thin lines are available, or between temperature and source size, in the optically thick case, $(T(\nu) = \sum \eta[J(T_{\nu}) - J(T_{bg})])$, is impossible. Plotting the optical depth for each fitted line gives a better idea on which of the obtained parameters is more affected by uncertainties. Also, fitting CH$_3$OH spectra assures a reliable determination of kinetic temperature only when many lines are fitted, thus covering different excitation ranges, and/or when millimeter and submillimeter data are available, (see Sect. 2.3).

Observations of the $2_k \rightarrow 1_a$ and $-E$ lines near 96 GHz, the $J_0 \rightarrow J_{-1}$- $E$ lines at 157 GHz, the $5_k \rightarrow 4_a$- and $-E$ near 241 GHz were obtained towards a sample of more than 60 sources during a systematic program on CH$_3$OH in high-mass star forming regions at the IRAM 30 m telescope during summer 2002–winter 2003. Details on the observations and analysis of the data are given in a forthcoming paper.

Here we discuss the application of our method to two sources of our sample, G19.30P1 and G79.3P1. They belong to a population of infrared-dark clouds, (hereafter IRDCs), identified by Egan et al. (1998) using the Galactic plane survey from the SPIRIT III telescope aboard the Midcourse Space Experiment, MSX. LVG calculations on H$_2$CO, (Carey et al. 1998), give an average value of $T \leq 20$ K, $n$(H$_2$) $\geq 10^5$ cm$^{-3}$ and $N$(H$_2$CO) $\sim 10^{13}$–$10^{14}$ cm$^{-2}$ for IRDCs. Pillai et al. (2004) derive a kinetic temperature of 17 K for G19.30P1 and 15 K for G79.3P1 from NH$_3$ (1, 1), (2, 2), (1, 1), which trace only the cooler, extended envelope, thus resulting in underestimation of $T_K$. Besides the satisfactory agreement between data and fit ($\chi^2_{\nu} = 3$ for G19.30P1, $\chi^2_{\nu} = 2$ for G79.3P1), some lines, mostly the $2_k \rightarrow 1_a$ band, are underestimated in intensities. This behaviour is more marked for G19.30P1, for which the $\chi^2$ analysis does not allow a reliable estimate of temperature due to the shallow property of the minimum. The source also shows a more complex structure than G79.3P1. Therefore, we attribute these discrepancies mainly to the fact that real sources are more complex than our model can represent, with a finite number of non-interacting components, thus ignoring alignment, self-absorption, a gradual gradient of the temperature due to the shallow property of the minimum. The source also shows a more complex structure than G79.3P1. Therefore, we attribute these discrepancies mainly to the fact that real sources are more complex than our model can represent, with a finite number of non-interacting components, thus ignoring alignment, self-absorption, a gradual gradient of the parameters within the source.

G79.3P1 offers, instead, a better agreement of the fit with the data, probably due to a less complex structure. All the lines are well fitted by our model, even the $2_{-1} \rightarrow 1_{-1}$- $E$ which shows an unusual excitation.

Figure 8 shows the $\chi^2$ distribution for G79.3P1 in the $(T_{\text{kin}}, n$(H$_2$)) plane at the column densities derived for $A$- and $E$-species; 1, 2 and 3$\sigma$ confidence contours, computed from the
Table 2. Line parameters.

<table>
<thead>
<tr>
<th>Transition</th>
<th>ν (GHz)</th>
<th>τ (K)</th>
<th>Tex (K)</th>
<th>τ (K)</th>
<th>Tex (K)</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>Core</td>
<td>Outflow</td>
<td>Core</td>
<td>Outflow</td>
<td>G79.3P1</td>
</tr>
<tr>
<td>2→1 → 1→ - E</td>
<td>96.739</td>
<td>-8.8 x 10^{-4}</td>
<td>-7.2 x 10^{-2}</td>
<td>-13.2</td>
<td>-8.0</td>
</tr>
<tr>
<td>2→0 → 1→ - A</td>
<td>96.741</td>
<td>1.0</td>
<td>4.7 x 10^{-1}</td>
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<td>20.3</td>
</tr>
<tr>
<td>2→0 → 1→ - E</td>
<td>96.744</td>
<td>5.2 x 10^{-1}</td>
<td>2.3 x 10^{-1}</td>
<td>16.3</td>
<td>7.9</td>
</tr>
<tr>
<td>2→1 → 1→ - E</td>
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<td>34.7</td>
<td>9.4</td>
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<tr>
<td>6→0 → 6→ - E</td>
<td>157.048</td>
<td>3.1</td>
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<td>2.9</td>
</tr>
<tr>
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<td>8.1 x 10^{-1}</td>
<td>7.4</td>
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<tr>
<td>4→0 → 4→ - E</td>
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<td>1.6</td>
<td>8.0</td>
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<tr>
<td>2→0 → 2→ - E</td>
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<tr>
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<td>37.4</td>
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<td>7.6</td>
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<td>241.813</td>
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<td>19.8</td>
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<td>12.1</td>
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<td>1.9 x 10^{-3}</td>
<td>28.4</td>
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</table>

Fig. 8. χ² square distribution in the [Tex, n(H2)] plane toward G79.3P1. A black triangle marks the minimum position, Tex = 17 K, n(H2) = 2.5 x 10^5 cm⁻³; stars mark the positions at which spectra of Fig. 11 are taken, which are also labelled by numbers. Overlaid in black the 3σ, 2σ and 1σ confidence contours.

Black stars mark the positions within the 1σ confidence contour for which spectra are shown in Fig. 11 along with the best fit; even if the fits within the 1σ range are still pretty good, major deviations from the observations, mainly at 3 mm and 2 mm, occur. Since the fit solution falls in the temperature range in which both the 2k → 1k and the 5k → 4k bands show a dependence on density and temperature, for G79.3P1 the estimates of Tex and n(H2) and their uncertainties correlate. This is not true at higher temperature, as in G19.30P1, where the bands have a pure dependence on density. In the case of G79.3P1 we have also compared our LVG results with a similar analysis under the LTE assumption. The agreement between data and LTE fit is usually less satisfactory than in the LVG case, with χ² values, particularly in the J₀ → J₋₁-E band at 157 GHz, which is a known Class II maser series of lines, where the predicted spectrum differs significantly from the measured data. The best fit under the LTE approximation is found at T = 10 K and for similar values for column densities. The LTE fit overlaid on the data is shown in Fig. 9.
Fig. 9. (a) Best LTE fit, \(T_{\text{kin}} = 10\) K, \(N(\text{CH}_3\text{OH-}A) = 7 \times 10^{13}\) cm\(^{-2}\), \(N(\text{CH}_3\text{OH-}E) = 4.6 \times 10^{13}\) cm\(^{-2}\)) toward G79.3P1 (J2000 coordinates: RA = 20:32:21.8, Dec = 40°20′08″) overlaid on the real data. For comparison the best LVG fit \(T_{\text{kin}} = 17\) K, \(n(\text{H}_2) = 2.5 \times 10^5\) cm\(^{-3}\), \(N(\text{CH}_3\text{OH-}A) = 7.9 \times 10^{13}\) cm\(^{-2}\), \(N(\text{CH}_3\text{OH-}E) = 5.7 \times 10^{13}\) cm\(^{-2}\)) is shown in (b).

Fig. 10. Spectra toward G19.30P1 (J2000 coordinates: RA = 18°25′58.5″, Dec = −12°03′59″), taken with the IRAM 30 m telescope. The 2 mm and 1 mm data are smoothed for the difference in the beam size with the 3 mm data. Overlaid in black the synthetic spectra resulting from the fit.
Fig. 11. Synthetic spectra corresponding to different positions within the 1σ confidence surface overlaid on the spectra observed toward G79.3P1. For comparison, the best fit spectrum is also shown. Major deviations in the 3 mm and 2 mm lines occur in the fits at the 1σ level.
4. Conclusions

Using a spherical LVG model to describe the molecular excitation, we have carried out a detailed analysis of the tracing properties of CH$_3$OH in the millimeter and submillimeter spectrum. We found that many millimeter line ratios are mainly sensitive to spatial density in the range $10^5$–$10^8$ cm$^{-3}$, while in the submillimeter range a strong dependence on kinetic temperature up to 150 K is found. These two results together strongly suggest the use of CH$_3$OH as tracer of physical conditions in low-, intermediate, and high-mass star forming regions.

We have also presented an innovative way of analysing CH$_3$OH spectra which is based on a simultaneous fitting of all the lines observed towards a given position. The application of this technique to two IRDCs, G19.30P1 and G79.3P1, has been discussed.

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