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Transfer of radiation through cyclopropenylidene and ethylene oxide⋆

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Abstract. Cyclopropenylidene and ethylene oxide molecules are of astronomical importance as their observed lines, distributed throughout the observable microwave region, have a number of pairs having nearly equal frequencies, but different excitation energies and/or belonging to two different species of the molecule. Hence, these molecules may play important role in detecting physical conditions in cosmic objects. Therefore, in order to calculate intensities of the lines, we have investigated transfer of radiation through a cosmic object containing the molecule at a kinetic temperature of 10 K. Our results show that some lines of the molecule may be found in absorption against the cosmic 2.7 K background.

Key words. ISM: molecules – molecular data – radiative transfer

1. Introduction

Cyclopropenylidene (C_3H_2), in astronomical objects, was identified by Thaddeus et al. (1985); they reported twelve emission lines of the molecule, distributed throughout the observable microwave region. Ethylene oxide (C_2H_4O) has been observed by Dickens et al. (1997) in Sgr B2N; twelve emission lines of the molecule, distributed throughout the observable microwave region, have been reported by them. These observable lines of the molecules have line-pairs which may play an important role for finding out physical conditions in astronomical objects.

Therefore, in order to calculate intensities of lines, we have investigated transfer of radiation through an astronomical object containing the molecule at a kinetic temperature of 10 K.

2. Basic formulation and molecular data

NLTE occupation numbers of energy levels of the molecule under investigation are calculated in an on-the-spot approximation by using the escape probability method (see, e.g., Rausch et al. 1996), where the external radiation field, impinging on a volume element, and emitting the lines, is the cosmic 2.7 K background only. In the present investigation, we accounted for 47 and 48 rotational energy levels for ortho- and para-C_3H_2, respectively, and 52 rotational energy level for ortho- and para-C_2H_4O.

The molecular data required as input for the present investigation are: (i) Einstein A-coefficients for radiative transitions between the rotational energy levels accounted for, and (ii) rate coefficients for collisional transitions between the energy levels due to collisions with H_2 molecules.

Both cyclopropenylidene and ethylene oxide are *b*-type asymmetric top molecules having a large electric dipole moment of 3.325 D and 1.88 D, respectively, along their *b*-axis of inertia. Details for calculation of Einstein A-coefficients for *b*-type rotational transitions in an asymmetric top molecule have been discussed by Chandra et al. (1984).

Very accurate values for the molecular and distortional constants for cyclopropenylidene have been reported by Bogey et al. (1987), and for ethylene oxide have been reported by Pan et al. (1998). These constants are used here for calculation of a consistent set of Einstein A-coefficients for rotational transitions between the levels accounted for. The Einstein A-coefficients, used here, are reported in Tables 1A, and 1B, respectively, for ortho- and para-C_3H_2, and in Tables 1C, and 1D, respectively, for ortho- and para-C_2H_4O. These tables are available in electronic form at the CDS.

Collisional rate coefficients for downward transitions between the lowest 16 levels of ortho- and between the lowest 17 levels of para-C_3H_2 for a kinetic temperature $T = 10$ K are taken from Avery & Green (1989). For other transitions, $J'k'_ak'_c \rightarrow Jk_ak_c$ at a kinetic temperature T, collisional rate coefficients are given by Sharma & Chandra (2001)

$$C\,(J'k'_ak'_c \rightarrow Jk_ak_c) = 1 \times 10^{-11}\,\sqrt{T/30}/\,(2J'+1)\,. \qquad (1)$$

No data are, however, available in the literature for the collisional rate coefficients for ethylene oxide. In the absence of any

⋆ Tables 1A, 1B, 1C, and 1D are only available in electronic form at the CDS via anonymous ftp to
cdsarc.u-strasbg.fr (130.79.128.5) or via
http://cdsweb.u-strasbg/cgi-bin/qcat?J/A+A/402/1

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Table 2A. Lines of cyclopropenylidene observed in cosmic objects.

Transition	Frequency (GHz)	Excitation energy (K)
$1_{10}-1_{01}$	18.3431	0.9
$2_{20}-2_{11}$	21.5874	9.7
$2_{11}-2_{02}$	46.7556	8.7
$2_{02}-1_{11}$	82.0936	6.4
$3_{12}-3_{03}$	82.9662	13.7
$3_{22}-3_{13}$	84.7277	16.1
$2_{12}-1_{01}$	85.3389	4.1
$4_{32}-4_{23}$	85.6564	26.7
$4_{04}-3_{13}$	150.8207	19.3
$4_{14}-3_{03}$	150.8519	17.0
$6_{06}-5_{15}$	217.8220	38.6
$6_{16}-5_{05}$	217.8222	36.3
$4_{41}-3_{30}$	265.7595	29.9

Table 2B. Lines of ethylene oxide observed in Sgr B2N.

Transition	Frequency (GHz)	Excitation energy (K)
$1_{11}-0_{00}$	39.5816	1.9
$4_{22}-4_{13}$	41.5794	20.5
$4_{41}-4_{32}$	47.0950	21.6
$5_{50}-5_{41}$	47.5569	33.6
$3_{12}-2_{21}$	104.6886	9.9
$6_{34}-5_{23}$	219.5128	38.6
$8_{08}-7_{17}$	235.1061	52.4
$8_{18}-7_{07}$	235.1061	50.7
$5_{41}-4_{32}$	249.1616	31.3
$5_{50}-4_{41}$	249.6236	33.6
$8_{17}-7_{26}$	254.2318	59.3
$8_{27}-7_{16}$	254.2357	57.5

knowledge for collisional rate coefficients, we assumed that the rate coefficient for a downward transition $J'k'_ak'_c \rightarrow Jk_ak_c$ at the kinetic temperature T is given by Eq. (1). For upward collisional rate coefficients, for C_3H_2 as well as C_2H_4O, we accounted for the fact that downward and upward collisional rate coefficients are related through the detailed equilibrium.

3. Observations

Observed lines of cyclopropenylidene and ethylene oxide are given in Tables 2A and 2B, respectively.

The spectral line $1_{10}-1_{01}$ of C_3H_2 at 18.343 GHz was easily detectable in a wide range of objects throughout the galaxy. The sources where this transition was found include cold dust clouds, circumstellar envelopes, complex molecular clouds in vicinity of H II regions, and the spiral arm clouds towards the supernova remnant Cas A. The most interesting feature of the line $2_{20}-2_{11}$ of C_3H_2 at 21.5874 GHz has been its absorption even against the cosmic 2.7 K background, in all cosmic objects investigated by Madden et al. (1989). However, Cox et al. (1987) found this line in emission in the planetary nebula NGC 7027.

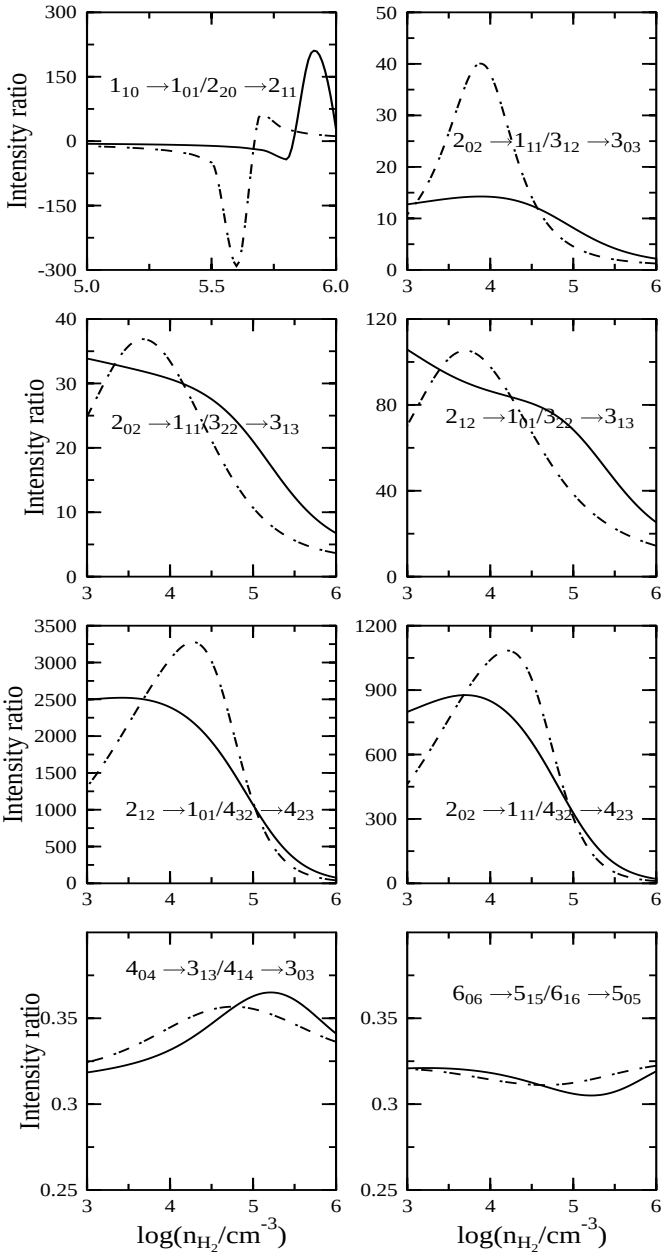

Fig. 1. Variation of the ratio of intensities of pairs of lines of C_3H_2, measured in the unit of Planck's function at a kinetic temperature of 10 K. Solid line is for $\gamma = 10^{-6}$ cm^{-3} (km s^{-1})$^{-1}$ pc, and the dotted line for $\gamma = 10^{-5}$ cm^{-3} (km s^{-1})$^{-1}$ pc. For the ratio $1_{10} \rightarrow 1_{01}/2_{20} \rightarrow 2_{11}$, the graph is shown for a part of the molecular hydrogen density. For low density, which is not shown in the figure, the graph extends almost horizontally.

4. Numerical results and discussion

In order to include a large number of cosmic objects, numerical calculations are carried out for wide ranges for physical parameters. The molecular hydrogen density n_{H_2} has been varied over the range from 10^3 cm^{-3} to 10^6 cm^{-3}, and calculations are performed for a kinetic temperature of 10 K. In the calculations, free parametres are the hydrogen density n_{H_2}, and $\gamma \equiv n_{mol}/(dv_r/dr)$, where n_{mol} is density of the molecule, and dv_r/dr the velocity gradient.

4.1. Absorption lines

Besides the line 2_{20}–2_{11} of C_3H_2, a number of other lines of C_3H_2, and of C_2H_4O are found in absorption against the cosmic 2.7 K background. We (Chandra & Kegel 2001) predicted that besides the line 2_{20}–2_{11}, the lines 3_{30}–3_{21}, and 3_{31}–3_{22} of C_3H_2, and three lines 2_{20}–2_{11}, 3_{30}–3_{21}, and 3_{31}–3_{22} of C_2H_4O may be observed in absorption against the cosmic 2.7 K background.

The present investigation is in agreement that the line 2_{20}–2_{11} of C_3H_2 appears in absorption even against the cosmic 2.7 K background, observed by Madden et al. (1989). The line has positive intensity at large hydrogen density, showing that density in the planetary nebula NGC 7027, where the emission feature was observed, has been more than about $10^{5.6}$ cm^{-3}. Calculations of Avery and Green (1989) found two lines 3_{30}–3_{21} and 3_{21}–3_{12}, in absorption against the cosmic 2.7 K background. In the present investigation, we also found the same.

4.2. Line-ratios

The observed lines (Tables 2A and 2B) have a number of line-pairs having nearly equal frequencies, but different excitation energies and/or belonging to two different species. These pairs of lines may be used for diagnostic purposes. The advantage of using such pairs is that two lines of the pair may be observed almost simultaneously with a common telescope, and thus, in forming ratio of the line intensities, systematic errors involving source coupling efficiency, calibration uncertainty, and atmospheric absorption, are canceled out.

The ratio of the intensities observed against the cosmic background in units of Planck's function at a temperature of 10 K, i.e., $(I_\nu - I_{\nu,bg})/B_\nu(10\ \mathrm{K})$, of the pairs of lines for various values of γ are shown in Fig. 1 for C_3H_2, and in Fig. 2 for C_2H_4O. In Fig. 1, for the first frame, we have shown only that part of the graph which is sensitive to the molecular hydrogen density. In calculating the line-ratios, we have used the ratio 3:1 for ortho to para abundances. For other values of the abundance-ratio, the graph can be easily scaled down. As expected, the intensity-ratio of the last two pairs does not vary significantly with the molecular hydrogen density. These pairs may, obviously, be used to find the ratio of ortho to para abundances of C_3H_2. The ratio of the intensities of the lines in the first six pairs may be used to find the molecular hydrogen density in the region, and the density of C_3H_2 for the known velocity gradient.

The first two pairs in Fig. 2 have nearly equal frequencies, but different excitation energies. In these pairs, both the lines belong to the same species. Hence, the intensity-ratio for these pairs is free of the abundance-ratio for ortho to para species. In the last two pairs, the frequencies of the lines are almost equal, and the excitation energies are nearly equal. In these pairs, the lines belong to two distinct species. These four pairs may be used for diagnostic purposes.

In calculating the ratios, we have used the ratio 3:1 for ortho to para abundances. For other values for the abundance-ratio, the graph can be easily scaled down. As expected, the intensity-ratio of the last two pairs does not vary significantly with the molecular hydrogen density. These pairs may, obviously, be used to find the ratio of the ortho to para abundances of C_2H_4O. The ratio of intensities of the lines in the first two pairs may be used to find the molecular hydrogen density in the region. Figure 2 shows that the intensity-ratios are not very sensitive to the value of γ, except for the ratio $1_{11} \rightarrow 0_{00}/4_{22} \rightarrow 4_{13}$ in the low hydrogen density region.

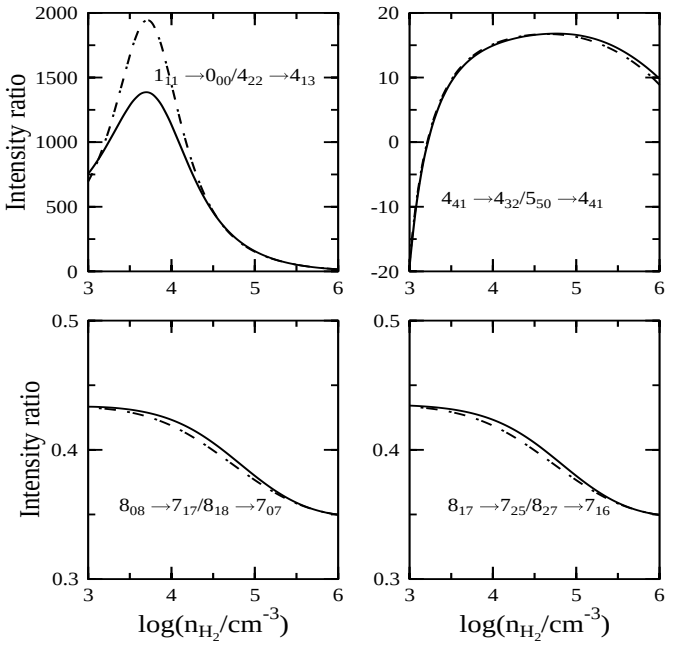

Fig. 2. Variation of the ratio of intensities of pairs of lines of C_2H_4O, measured in the unit of Planck's function at a kinetic temperature of 10 K. Solid line is for $\gamma = 10^{-6}$ cm^{-3} (km s^{-1})$^{-1}$ pc, and the dotted line for $\gamma = 10^{-5}$ cm^{-3} (km s^{-1})$^{-1}$ pc.

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