A&A manuscript no.
(will be inserted by hand later)

Your thesaurus codes are:
09.13.2, 02.13.4, 02.18.7

ASTRONOMY
AND
ASTROPHYSICS
25.5.2001

Suggestions for an interstellar cyclopropene search*

A.K. Sharma and **S. Chandra*****

School of Physical Sciences, Swami Ramanand Teerth Marathwada University, Nanded 431 606, India

Received ; accepted

Abstract. Following tentative detection of cyclopropene (C_3H_4) in Sgr B2 through its transition 3_{22} - 2_{21}, several attempts for its confirmation in astronomical objects (including Sgr B2 itself) have been made. We suggest that cyclopropene may be observed in astronomical objects through its transition 2_{20} - 2_{21} at 3.67218 GHz, in absorption, even against the cosmic 2.7 K background, in a region having low density, and low kinetic temperature.

Key words: interstellar molecules - cyclopropene - molecular data

With the discovery of cyclopropenylidene (C_3H_2) in a large number of astronomical objects (see, e.g., Madden et al., 1989), cyclopropene (C_3H_4) has become a plausible candidate for its detection in astronomical object(s). A weak line at 106.86 GHz in Sgr B2 observed by Thaddeus et al. (1985) coincided with one of the predicted strongest lines, the 3_{22} - 2_{21} transition, of C_3H_4. Following this tentative detection of cyclopropene in Sgr B2, several attempts for its confirmation in astronomical objects (including Sgr B2 itself) have been made.

In order to provide rotational frequencies of cyclopropene throughout the radio spectrum to an accuracy sufficient for astronomical purposes, Vrtilek et al. (1987) reported radio spectrum of cyclopropene. In Sgr B2, a search with the Bell Laboratories 7 m telescope for the 5_{15} - 4_{14} and 5_{05} - 4_{04} ortho-para line pair at 149.279 GHz and 149.549 GHz, respectively, resulted in an upper limit of column density 5 x 10^{14} cm^{-2}, assuming a line width of 24 km s^{-1} and a rotational temperature of 11 K (Vrtilek et al., 1987). This upper limit was found to lie below the tentative detection (which implied a column density of C_3H_4 to be 1.3 x 10^{15} cm^{-2}), but still somewhat above the measurement for C_3H_2 (6 x 10^{13} cm^{-2}).

Cyclopropene is a cyclic, asymmetric top molecule with the electric dipole moment of 0.45 D (Kasai et al., 1958) along the a-axis of inertia. In the present investigation, the NLTE occupation numbers of the C_3H_4 molecules 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 the volume element, emitting the line(s), is the cosmic 2.7 K background only.

The molecular data required as input for the present investigation are: (i) Einstein coefficients for various radiative transitions between the rotational energy levels accounted for, and (ii) the rate coefficients for collisional transitions between the levels due to collisions with H_2 molecules. The details for calculation of Einstein A-coefficients for a-type rotational transitions in an asymmetric top molecule have been discussed by Chandra and Rashmi (1998). These transitions are governed by the selection rules:

J:	$\triangle$ J = 0, $\pm$ 1	
k_a, k_c:	odd, odd $\longleftrightarrow$ odd, even	ortho-transitions
	even, even $\longleftrightarrow$ even, odd	para-transitions

The Einstein A-coefficients for the rotational transitions between the levels up to 70 cm^{-1} have been calculated by using the molecular and distortional constants derived by Vrtilek et al. (1987), and have been reported in Tables 1A and 1B, for ortho- and para-C_3H_4, respectively, which are available in the electronic form via anonymous ftp 130.79.128.5 at the CDS. (Though Vrtilek et al. (1987) reported line-intensities for a number of lines of C_3H_4, but for a complete and consistent set of radiative transition probabilities, the Einstein A-coefficients are calculated in the present investigation.)

As of today, knowledge of the collisional transitions, particularly in asymmetric top molecules, is very poor. Further, there are no data for the collisional rates for cyclopropene available in the literature. In absence of any knowledge for collisional rates, we assumed that the collisional rate coefficient for a downward transition $J'k'_ak'_c \rightarrow Jk_ak_c$ at temperature T (K) is given by

$$C(J'k'_ak'_c \rightarrow Jk_ak_c) = [1\text{x}10^{-11}/(2J'+1)]\sqrt{T/30}. \quad (1)$$

Rate coefficient for the corresponding upward transition $Jk_ak_c \rightarrow J'k'_ak'_c$ has been calculated with the help of the detailed equilibrium equation.

In order to include a large number of astronomical objects, where the molecule may be observed, numerical calculations are carried out for wide ranges for the physical parameters. The molecular hydrogen density has been varied over the range from 10^3 cm^{-3} to 10^6 cm^{-3}, and the calculations are performed for the kinetic temperatures of 10, 20 and 30 K. The transition 2_{20} - 2_{21} at 3.67218 GHz, proposed for detection in astronomical objects, belongs to para-C_3H_4. For para-C_3H_4, we

Send offprint requests to: S. Chandra

*Tables 1A and 1B are available only in electronic form via anonymous ftp 130.79.128.5 at the CDS

**Present Address: B.R.C.M. College of Engineering & Technology, Bahal 127 028, India

***Visiting Associate of the Inter-University Centre for Astronomy & Astrophysics, Pune 411 007, India

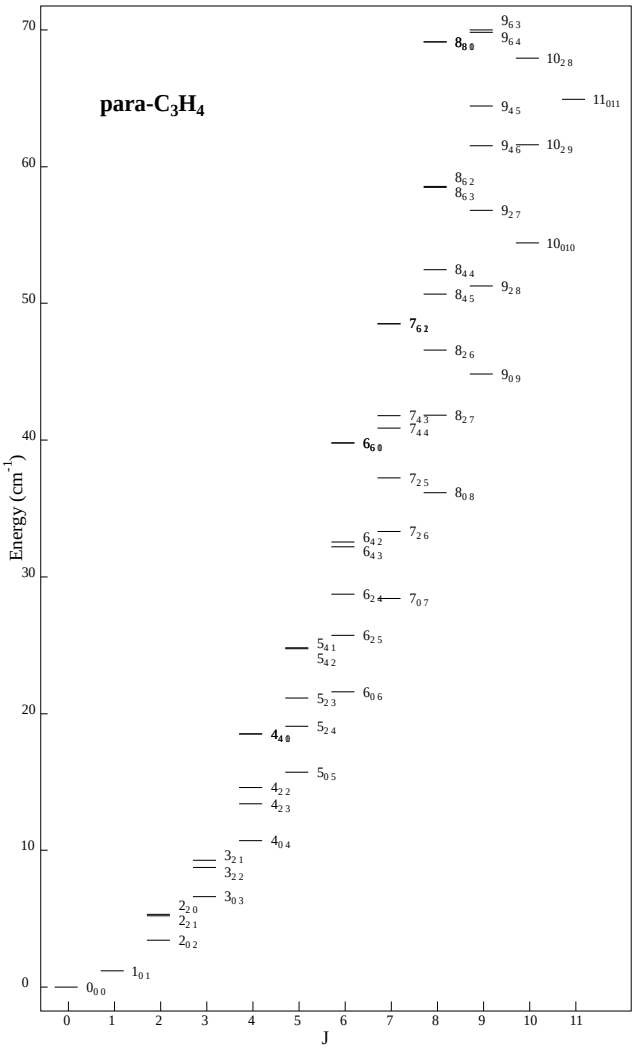

Fig. 1. Rotational energy levels in the ground vibrational state of para-C_3H_4, accounted for in the present investigation.

accounted for 52 rotational energy levels shown in Fig. 1. These levels are connected through 217 radiative transitions for which the Einstein A-coefficients are given in Table 1B. In the calculations, the free parameters are hydrogen density n_{H_2}, and $\gamma \equiv n_{C_3H_4}/(dv_r/dr)$, where $n_{C_3H_4}$ is the density of C_3H_4, and (dv_r/dr) the velocity gradient. The intensity, I_ν, of a line generated in an interstellar cloud, with homogeneous excitation conditions, is given by

$$I_\nu - I_{\nu,bg} = (S_\nu - I_{\nu,bg})(1 - e^{-\tau_\nu})$$

where $I_{\nu,bg}$ is the intensity of the continuum against which the line is observed, τ_ν the optical depth of the line, and S_ν the source function, which is the Planck's function at the excitation temperature T_{ex}, i.e., $S_\nu = B_\nu(T_{ex})$.

Fig. 2 shows the iso-lines for intensity for the transition 2_{20} - 2_{21}, in the units of Planck's function $[(I_\nu - I_{\nu,bg})/B_\nu(T)]$, for the kinetic temperatures T = 10, 20, and 30 K. In the figure, we have plotted only negative intensities; in the large density region (on the right-side of iso-lines), the intensity becomes

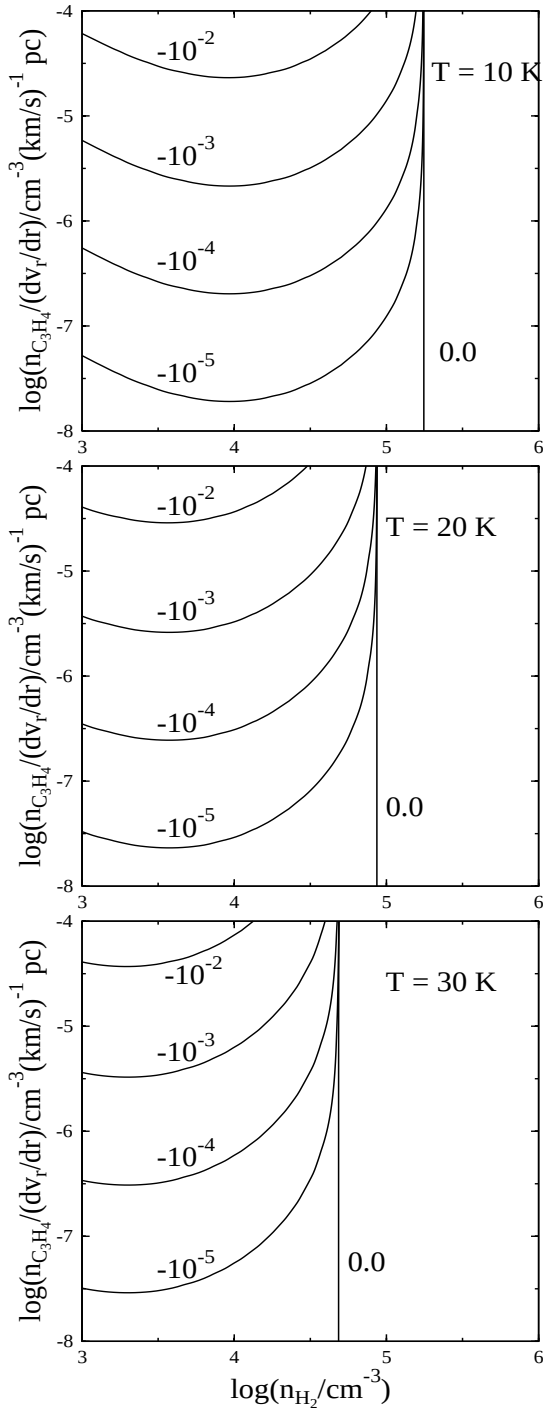

Fig. 2. The iso-lines for intensity against the cosmic 2.7 K background, in the unit of Planck's function at the kinetic temperature of T (K), i.e., $(I_\nu - I_{\nu,bg})/B_\nu(T)$, for the 2_{20} - 2_{21} transition at 3.67218 GHz of para-C_3H_4. Only negative values for the kinetic temperatures T = 10, 20, and 30 K are plotted. For large molecular hydrogen densities (where the iso-lines are not plotted), the value becomes positive.

positive. Thus, the absorption and emission nature of the line may play significant role for providing information about the limiting value of the density in the region. For the low density region, the line 2_{20} - 2_{21} shows absorption, even against the cosmic 2.7 K background, whereas in the large density region, the transition shows an emission against the cosmic 2.7 K background. (If there is some source in the background of the object, the line would show absorption against the background source.) The negative value of $(I_\nu - I_{\nu,bg})/B_\nu(T)$ increases with the decrease of the molecular hydrogen density. Further, it increases with the decrease of the kinetic temperature T. Thus, cyclopropene has large probability for its detection through its transition 2_{20} - 2_{21} in the cosmic object(s) having low density and low kinetic temperature.

Acknowledgements. We are grateful to Prof. Dr. W.H. Kegel of the university of Frankfurt/Main, Germany for his encouragements. Financial support form the D.S.T., New Delhi is thankfully acknowledged. Thanks are due to Mr. Harshal Hayatnagarkar for his valuable help.

References

Chandra, S., Rashmi, 1998, A&AS, **131**, 137
Kasai, P.H., Myers, R.J., Eggers, D.F., Wiberg, K.B., 1958, J. Chem. Phys. **30**, 512
Madden, S.C., Irvine, W.M., Matthews, H.E., Friberg, P., Swade, D.A., 1989, AJ **97**, 1403
Rausch, E., Kegel, W.H., Tsuji, T., Piehler, G., 1996, A&A **315**, 533
Thaddeus, P., Vrtilek, J.M., Gottlieb, C.A., 1985, ApJ **299**, L63
Vrtilek, J.M., Gottlieb, C.A., LePage, T.J., Thaddeus, P., 1987, ApJ **316**, 826

This article was processed by the author using Springer-Verlag LaTeX A&A style file 1990.