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 (C₃H₄) in Sgr B2 through its transition 3ₜ₁ - 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 2₀ - 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 (C₃H₂) in a large number of astronomical objects (see, e.g., Madden et al., 1989), cyclopropene (C₃H₄) 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 3ₜ₁ - 2₁ transition, of C₃H₄. 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 5₁ₕ - 4₁ₕ and 5ₕₗ - 4ₕₗ ortho-para line pair at 149.279 GHz and 149.549 GHz, respectively, resulted in an upper limit of column density 5 x 10⁵ 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 C₃H₄ to be 1.3 x 10⁶ cm⁻²), but still somewhat above the measurement for C₃H₂ (6 x 10⁵ cm⁻²).

Cyclopropene is a cyclic, asymmetric top molecule with the electric dipole moment of 0.45 D (Kassi et al., 1988) along the s-axis of inertia. In the present investigation, the NLTE occupation numbers of the C₃H₄ 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 H₂ molecules. The details for calculation of Einstein A-coefficients for α-type rotational transitions in an asymmetric top molecule have been discussed by Chandra and Rashmi (1998). These transitions are governed by the selection rules:

\[ \Delta J = 0, \pm 1 \]

\[ k_n, k_p: \text{odd, odd } \leftrightarrow \text{odd, even} \]

\[ \text{Even, even } \leftrightarrow \text{odd, para-transitions} \]

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-C₃H₄, 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 C₃H₄, 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 \( J'k'_{\alpha}k'_{\beta} \rightarrow Jk_{\alpha}k_{\beta} \) at temperature T (K) is given by

\[ C(J'k'_{\alpha}k'_{\beta} \rightarrow Jk_{\alpha}k_{\beta}) = \frac{1.1 \times 10^{-11}}{(2J' + 1)} \sqrt{T/30}. \]  

(1)

Rate coefficient for the corresponding upward transition \( Jk_{\alpha}k_{\beta} \rightarrow J'k'_{\alpha}k'_{\beta} \) 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 \( 10^6 \text{ cm}^{-3} \) to \( 10^9 \text{ cm}^{-3} \), and the calculations are performed for the kinetic temperatures of 10, 20 and 30 K. The transition 2₀ - 2₁ at 3.67218 GHz, proposed for detection in astronomical objects, belongs to para-C₃H₄. For para-C₃H₄, we
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 $n_{\text{H}_2}$, and $n_{\text{C}_3\text{H}_4} = \frac{\Delta n(r)}{dr}$, where $n_{\text{C}_3\text{H}_4}$ is the density of $\text{C}_3\text{H}_4$ and $(\Delta n(r)/dr)$ the velocity gradient. The intensity, $I_\nu$, of a line generated in an interstellar cloud, with homogeneous excitation conditions, is given by

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

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

Fig. 2 shows the iso-lines for intensity for the transition $2_00 - 2_21$, in the units of Planck's function $[(I_\nu - I_{\nu,\text{bg}})/B_\nu(T)]$, 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 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 $2_0 - 2_1$ 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 $(I_v - I_{v,bg})/B_v(T)$ 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 $2_0 - 2_1$ 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


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