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Research Paper

Suggestion for search of cyclopropenone (c-C_3H_2O) in a cosmic object

M.K. Sharma[a], M. Sharma[b], S. Chandra[c,*]

[a] Physics Department, Dream Valley College, Sitholi, Gwalior 474005, India
[b] School of Studies in Physics, Jiwaji University, Gwalior 474011, India
[c] Amity Center for Astronomy & Astrophysics, Amity Institute of Applied Sciences, Amity University, Sector - 125, Noida 201313, India

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ABSTRACT

Following Minimum Energy Principle, out of the three isomers of chemical formula C_3H_2O, the cyclopropenone (c-C_3H_2O) is the most stable and therefore may be the most abundant and easily detectable in a cosmic object. The cyclopropenone is detected in Sgr B2(N). Owing to half-spin of each of two hydrogen atoms, the c-C_3H_2O has two distinct ortho and para species. Using the rotational and centrifugal distortion constants along with the electric dipole moment, we have calculated energies of 100 rotational levels of each of the ortho and para species of c-C_3H_2O and the Einstein A-coefficients for radiative transitions between the levels. The values of Einstein A-coefficients along with the scaled values for collisional rate coefficients are used for solving a set of statistical equilibrium equations coupled with the equations of radiative transfer.

Brightness temperatures of seven rotational transitions of each of the ortho and para species of c-C_3H_2O are investigated. Out of fourteen transitions, seven are found to show anomalous absorption and rest seven are found to show emission feature. We find that the transitions $1_{10} - 1_{11}$ (1.544 GHz) may play important role in identification of cyclopropenone in a cosmic object.

1. Introduction

The chemical formula C_3H_2O has three isomers, namely, propynal (HCCCHO), l-propadienone (CH_2CCO) and cyclopropenone (c-C_3H_2O). According to the Minimum Energy Principle, out of these three isomers, the cyclopropenone is the most stable (Loomis et al., 2015) and therefore may be most abundant and easily detectable in a cosmic object. Further, owing to its large electric dipole moment (4.39 Debye), the intensities of its lines are more than those of other two isomers. Therefore, in order to search for the cyclopropenone in a cosmic object, its laboratory spectrum was first recorded by Benson et al. (1973). Benson et al. (1973) determined the rotational constants, electric dipole moment, structure and molecular g-values where the molecule was taken as a rigid rotator.

Because of the consideration for rigid structure, the uncertainties for the predicted frequencies were quite large and were not accurate enough as required by the astronomers. In order to provide better frequencies, Guillemin et al. (1990) recorded spectrum of cyclopropenone and derived rotational and centrifugal distortion constants, given in Table 1 (column 2).

Hollis et al. (2006) identified 6 transitions of c-C_3H_2O in Sgr B2(N) (See Table 2), which may be produced by the gas-phase oxygen addition reaction.

$$c\text{-}C_3H_2 + O \rightarrow c\text{-}C_3H_2O \quad (1)$$

However, this reaction (Eq. 1) may have a barrier because the electronic spin is not conserved, as atomic oxygen lies in a triplet state. On the other hand, it is suggested that the reaction

$$c\text{-}C_3H_2 + O_2 \rightarrow c\text{-}C_3H_2O + O \quad (2)$$

may be important, because both the molecular and atomic oxygen have triplet ground states, so that the electronic spin is conserved. The reaction (Eq. 2) is expected to have a small barrier if it is exothermic.

The cyclopropenylidene (c-C_3H_2) has been found ubiquitous (Madden et al., 1989). Maluendes et al. (1993) explained about much larger abundances of c-C_3H_2 relative to l-C_3H_2 in interstellar clouds as due to differences in the depletion rates. The c-C_3H_2 has an unbounded pair of electrons that makes it highly reactive in a laboratory (Thaddeus et al., 1985). However, in the interstellar environment, c-C_3H_2 may not be as reactive as l-C_3H_2 (Maluendes et al., 1993).

Out of the data of PRIMOS, Loomis et al. (2015) identified 9 transitions of c-C_3H_2O in Sgr B2(N) (See Table 2). As c-C_3H_2 has

* Corresponding author.
E-mail address: suresh492000@yahoo.co.in (S. Chandra).

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Table 1
Rotational and centrifugal distortion constants.

Constant	Value (MHz)[a]	Value (MHz)[b]
A	32040.734	31894.8500
B	7825.04620	7733.8104
C	6280.68461	6224.5032
Δ_J	1.79362×10^{-3}	$1.651250766 \times 10^{-3}$
Δ_{JK}	33.7882×10^{-3}	$3.271020188 \times 10^{-2}$
Δ_K	50.65×10^{-3}	$4.379488485 \times 10^{-2}$
δ_J	0.38536×10^{-3}	$3.533088298 \times 10^{-4}$
δ_K	22.156×10^{-3}	$2.093510188 \times 10^{-2}$
H_J		$2.937852086 \times 10^{-10}$
H_{JK}		$6.851055671 \times 10^{-8}$
H_{KJ}		$-1.128055614 \times 10^{-7}$
H_K		$9.251718141 \times 10^{-8}$
h_J		$2.362038947 \times 10^{-10}$
h_{JK}		$3.968188988 \times 10^{-8}$
h_K		$1.205246347 \times 10^{-6}$

[a] derived by Guillemin et al. (1990)
[b] values obtained from optimization of c-C_3H_2O molecule.

Table 2
Frequency ν, A-coefficient A_{ul}, energy E_u of upper level, radiative life-time t_u of upper level and t_l of lower level for transitions.

Transition	ν (GHz)	A_{ul} (s^{-1})	E_u (cm^{-1})	t_u (s)	t_l (s)
$3_{12} - 3_{13}$[d,c]	9.263	1.487E-08	3.8070	1.32D+05	1.83D+05
$3_{12} - 2_{11}$[d,c]	44.587	7.573E-06	3.8070	1.32D+05	5.63D+05
$4_{13} - 4_{14}$[d,c]	15.428	4.134E-08	5.7857	5.11D+04	7.11D+04
$1_{10} - 1_{11}$	1.544	4.131E-10	1.3289	2.42D+09	∞
$2_{11} - 2_{12}$[d]	4.633	3.717E-09	2.3207	5.63D+05	7.84D+05
$2_{11} - 1_{10}$[d]	29.756	1.773E-06	2.3207	5.63D+05	2.42D+09
$3_{13} - 2_{12}$[d]	39.957	5.450E-06	3.4982	1.83D+05	7.84D+05
$1_{01} - 0_{00}$[d,c]	14.106	2.099E-07	0.4702	4.76D+06	∞
$3_{03} - 2_{02}$[d,c]	42.032	7.125E-06	2.8093	1.40D+05	5.01D+05
$3_{22} - 2_{21}$[c]	42.316	4.047E-06	6.1528	2.32D+05	2.18D+05
$2_{20} - 2_{21}$	0.071	5.467E-14	4.7446	6.97D+06	9.35D+06
$3_{21} - 3_{22}$	0.356	3.378E-12	6.1647	2.18D+05	2.32D+05
$4_{22} - 4_{23}$	1.063	5.329E-11	8.0671	6.71D+04	7.21D+04
$2_{02} - 1_{01}$[d]	28.140	1.998E-06	1.4082	5.01D+05	4.76D+06

[c] identified by Hollis et al. (2006).
[d] observed by Loomis et al. (2015).

been found ubiquitous (Madden et al., 1989), there is probability of finding c-C_3H_2O in other molecular regions also.

In order to provide information about identification of cyclopropenone in a cosmic object, we have calculated energies of rotational levels and Einstein A-coefficients for radiative transitions between the levels, by using accurate values of rotational and centrifugal distortion constants, and electric dipole moment.

In the study of cosmic molecules, calculation of collisional rate coefficients is the most difficult part. Since no data for the collisional rate coefficients are available in literature, we have considered scaled values for collisional rate coefficients. These scaled values for collisional rate coefficients along with the radiative transition probabilities (Einstein A-coefficients) are used for solving the statistical equilibrium equations coupled with the equations of radiative transfer. We have found four ortho lines and three para lines to show anomalous absorption. We suggest that the transition $1_{10} - 1_{11}$ (1.544 GHz) may play important role for identification of cyclopropenone in a cosmic object.

2. Radiative transitions in cyclopropenone

Cyclopropenone is a ring structure molecule having large electric dipole moment of 4.39 Debye (Loomis et al., 2015) along the axis of lowest moment of inertia. Because of half nuclear spin of two hydrogen atoms, there are two species: ortho ($I = 1$, parallel spins) and para ($I = 0$, antiparallel spins). These two species behave as if they are two independent molecules, as there are no transitions between them. Since the kinetic temperature in a cosmic object where cyclopropenone may be found is low, we are concerned with the rotational levels in the ground vibrational and ground electronic states. The rotational levels are connected through radiative and collisional transitions. Though the collisional transitions do not follow any selection rules, the radiative transitions are governed by the selection rules:

$$\begin{aligned} J: &\quad \Delta J = 0, \pm 1 \\ k_a, k_c: &\quad \text{odd, even} \longleftrightarrow \text{odd, odd} \quad \text{(ortho transition)} \\ &\quad \text{even, even} \longleftrightarrow \text{even, odd} \quad \text{(para transition)} \end{aligned}$$

Here, J denotes the rotational quantum number of level, and k_a and k_c are projections of J on the symmetric axis in case of prolate and oblate symmetric top molecules, respectively. For the given values of rotational and centrifugal distortion constants, and electric dipole moment, we have calculated energies of rotational levels and Einstein A-coefficients for radiative transitions between the levels with the help of the software ASROT (Kisiel, 2001). For each of the ortho and para species, we have considered 100 rotational levels which lie up to 81 cm^{-1}. Among these levels, there are 398 transitions in ortho c-C_3H_2O and 395 transitions in para c-C_3H_2O. The frequencies of transitions are accurate and may be used for astronomical observations.

Table 3
Structure of c-C_3H_2O molecule.

Atom	Coordinates (Å)		
	x	y	z
O	0.000000	0.000000	1.543884
C	0.000000	0.000000	0.338745
C	0.000000	0.675654	−0.935196
C	0.000000	−0.675654	−0.935196
H	0.000000	1.557401	−1.580596
H	0.000000	−1.557401	−1.580596

3. Optimization of cyclopropenone

We optimized the cyclopropenone with the help of software GAUSSIAN 2009 where we used B3LYP method and cc-pVDZ basis set. The cyclopropenone is a planar molecule and the coordinates of its atoms are given in Table 3. The rotational and centrifugal distortion constants obtained from the optimization are also given in Table 1 (column 3). We have calculated also the energies of rotational levels by using the rotational and centrifugal distortion constants obtained from the optimization. Energies of all 100 levels of each of the ortho and para species of c-C_3H_2O are found to be less than those obtained in Section 2. The maximum deviation is found to be -1.05%. It shows that when spectroscopic data are not available, qualitative study of molecule may be done with the help of data obtained from the optimization of molecule. However, the frequencies so obtained would not be as accurate as required by astronomers.

4. Details of model

The model used here is the same as discussed by Chandra and Shinde (2008); Sharma et al. (2012), for example, where the external radiation field impinging on the volume element, generating the lines, is the cosmic microwave background (CMB) only, which corresponds to the background temperature $T_{bg} = 2.73$ K. The parameter γ is expressed as $\gamma = n_{mol}/(d\nu_r/dr)$. Here, n_{mol} is the density of cyclopropenone and $(d\nu_r/dr)$ the velocity gradient in the object.

The most difficult part in the study of interstellar molecules is the computation of collisional rate coefficients (Sharma et al.,