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Search for 1_{11}–1_{10} and 2_{11}–2_{12} transitions of H_2CCO, H_2CCC and H_2CCCC in cosmic objects

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Abstract

Formaldehyde (H_2CO) is the first molecule observed in absorption against the cosmic microwave background (CMB) through its transition 1_{11}–1_{10} at 4.829 GHz in several cosmic objects. The second line observed in a large number of cosmic objects is 2_{11}–2_{20} transition at 21.59 GHz of cyclopropenylidene (c-C_3H_2) in absorption against the CMB. The phenomenon of anomalous absorption can take place under rather peculiar conditions developed in a molecule generating the line. In the present investigation, for H_2CCO, H_2CCC and H_2CCCC in cool cosmic objects, we have accounted for kinetic temperature of 10, 20, 30 and 40 K. For each of these three molecules, we have taken 30 rotational energy levels connected by 66 radiative transitions and solved the set of statistical equilibrium equations coupled with equations of radiative transfer through iterative method. We found that relative values of collisional rates can produce anomalous absorption of transitions 1_{11}–1_{10} and 2_{11}–2_{12} in these molecules. Anomalous absorption of 1_{11}–1_{10} and 2_{11}–2_{12} transitions may help in the identification of molecules in cool cosmic objects.

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Keywords: Interstellar molecules – H_2CCO, H_2CCC, H_2CCCC; Molecular processes and interactions; Radiative transfer; Molecular data and transition probabilities

1. Introduction

Transitiion 1_{11}–1_{10} at 4.829 GHz of formaldehyde has been observed in anomalous absorption against CMB in several directions (Palmer et al., 1969). Since the energy level scheme and relative values of radiative transition probabilities for transitions between the levels in H_2CCO, H_2CCC and H_2CCCC are very similar to those for H_2CO (Table 1), in the present investigation we have discussed about the phenomenon of anomalous absorption of transitions 1_{11}–1_{10} and 2_{11}–2_{12} in these molecules. It has been found that a mechanism responsible for anomalous absorption depends on relative values of collisional rate coefficients. To get anomalous absorption in 1_{11}–1_{10} transition, the rate coefficient for $1_{10} \rightarrow 2_{12}$ transition should be larger than that for $1_{11} \rightarrow 2_{11}$ transition. It is possible to get anomalous absorption in 2_{11}–2_{12} transition.

2. Observations

Ketene (H_2CCO) is detected in Sgr B2, TMC-1 and L134N by Turner et al. (1977), Matthews and Sears (1986), Irvine et al. (1989), Ohishi et al. (1991) through its transitions 4_{14}–3_{13}, 4_{04}–3_{03}, 4_{13}–3_{12}, 5_{15}–4_{14}, 5_{05}–4_{04}, 5_{14}–4_{13}, 1_{01}–0_{00}, 2_{02}–1_{01}, 2_{12}–1_{11} and 2_{11}–1_{10}. Molecular and distortional constants for this molecule are taken from Johns and Stone (1972) and are given in Table 2.

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Table 1
Energy in cm^{-1} of rotational levels of ortho species and electric dipole moment

$J_{k_a k_c}$	H_2CCO	H_2CCC	H_2CCCC
1_{11}	9.6705	9.9723	9.6365
1_{10}	9.6831	9.9851	9.6390
2_{12}	11.0061	11.3465	10.2299
2_{11}	11.0438	11.3850	10.2374
3_{13}	13.0094	13.4079	11.1199
3_{12}	13.0849	13.4849	11.1349
4_{14}	15.6805	16.1563	12.3067
4_{13}	15.8063	16.2846	12.3316
5_{15}	19.0192	19.5917	13.7901
5_{14}	19.2081	19.7842	13.8274
6_{16}	23.0257	23.7142	15.5701
6_{15}	23.2901	23.9837	15.6225
7_{17}	27.6999	28.5236	17.6469
7_{16}	28.0523	28.8829	17.7166
8_{18}	33.0416	34.0200	20.0203
8_{17}	33.4948	34.4820	20.1100
9_{19}	39.0509	40.2032	22.6669
9_{18}	39.6174	40.7804	22.7790
$10_{1,10}$	45.7278	47.0732	25.6770
10_{19}	46.4202	47.7791	25.8103
3_{31}	85.0676	87.6697	85.8459
3_{30}	85.0676	87.6697	85.8459
4_{32}	87.7629	90.4427	87.0374
4_{31}	87.7629	90.4427	87.0374
5_{33}	91.1319	93.9090	88.5267
5_{32}	91.1319	93.9090	88.5267
6_{34}	95.1748	98.0685	90.3138
6_{33}	95.1748	98.0685	90.3138
7_{35}	99.8915	102.9211	92.3988
7_{34}	99.8915	102.9211	92.3988
μ (Debye)	1.41	4.1	4.5

Table 2
Molecular and distortional constants in MHz

Constants	H_2CCO[a]	H_2CCC[b]	H_2CCCC[c]
A	282,081	288,783	284,468
B	10,293.9772	10,588.639	4503.309
C	9915.2396	10,203.966	4428.616
D_J	3.394×10^{-3}	4.248×10^{-3}	0.5393×10^{-3}
D_{JK}	476.04×10^{-3}	516.4×10^{-3}	144.0×10^{-3}
D_K	23.535	23.535	0.0000
d_1	0.1453×10^{-3}	-0.153×10^{-3}	-0.0157×10^{-3}
H_{JK}	8.4×10^{-6}	7.6×10^{-6}	0.14×10^{-6}
H_{KJ}	-0.7103×10^{-3}	-1.28×10^{-3}	0.35×10^{-3}

[a] Johns and Stone (1972).
[b] Vrtilek et al. (1990).
[c] Killian et al. (1990).

Propadienylidene (H_2CCC) is detected by Cernicharo et al. (1991a), Kawaguchi et al. (1991) in IRC +10216 and TMC-1 through its transitions 1_{01}–0_{00}, 5_{15}–4_{14}, 5_{14}–4_{13}, 7_{16}–6_{15}, 2_{12}–1_{11}, 2_{02}–1_{01}, 2_{11}–1_{10}, 4_{14}–3_{13} and 4_{13}–3_{12}. Molecular and distortional constants for this molecule are taken from Vrtilek et al. (1990) and are given in Table 2.

Carbene (H_2CCCC) is detected by Cernicharo et al. (1991b), Kawaguchi et al. (1991) in IRC +10216 and TMC-1 through its transitions 9_{09}–8_{08}, $10_{1,10}$–9_{19}, $11_{1,11}$–$10_{1,10}$, $11_{0,11}$–$10_{0,10}$, $11_{1,10}$–$10_{1,9}$, $12_{0,12}$–$11_{0,11}$, $12_{1,11}$–$11_{1,10}$, $15_{1,15}$–$14_{1,14}$, $15_{1,14}$–$14_{1,13}$, $16_{1,16}$–$15_{1,15}$, 2_{12}–1_{11}, 2_{02}–1_{01}, 2_{11}–1_{10}, 4_{14}–3_{13}, 4_{04}–3_{03}, 4_{13}–3_{12}, 5_{15}–4_{14}, 5_{05}–4_{04} and 5_{14}–4_{13}. Molecular and distortional constants for this molecule are taken from Killian et al. (1990) and are given in Table 2.

3. Basic formulation

The transitions of our interest, 1_{11}–1_{10} and 2_{11}– 2_{12}, belong to the ortho species of each molecule. In our investigation, NLTE occupation numbers of 30 energy levels for each molecule are calculated in an on-the-spot approximation by using the escape probability method (Rauch et al., 1996; Chandra et al., 2005) where the external radiation field, impinging on a volume element generating lines, is the CMB only. In the present investigation, we solved a set of 30 simultaneous equations coupled with 66 equations of radiative transfer. This system of equations is non-linear and can be solved through iterative method for given values of hydrogen density n_{H_2} and $\gamma \equiv n_{\rm mol}/(dv_r/dr)$, where $n_{\rm mol}$ is density of molecule and dv_r/dr, the velocity gradient in cosmic object. Basic data required in this investigation are Einstein A-coefficients for radiative transitions and collisional rate coefficients between the levels.

4. Einstein A-coefficients

Treatment of an asymmetric top molecule is quite complicated as it has no preferential direction for quantization and the energy matrix is non-diagonal. Rotational wave functions for an asymmetric top molecule can be described by a linear combination of wave functions for a symmetric top molecule (Chandra et al., 1984)

$$\Psi_{J\tau M}(\alpha,\beta,\gamma) = \sqrt{\frac{2J+1}{8\pi^2}} \sum_{K=-J}^{J} g^J_{\tau K} D^J_{MK}(\alpha,\beta,\gamma)$$

where α, β, γ are Euler angles specifying orientation of the molecule, J the rotational quantum number, $g^J_{\tau K}$ the expansion coefficients, D^J_{MK} the Wigner D-function and the pseudo quantum number τ is defined as

$$\tau = k_a - k_c$$

where k_a and k_c are projections of J on the axis of symmetry in case of prolate and oblate symmetric tops, respectively. Rotational levels in an asymmetric top molecule are specified as J_{k_a,k_c} or J_τ. All the three molecules, H_2CCO, H_2CCC and H_2CCCC being a-type asymmetric top, the rotational radiative transitions are governed by selection rules

$$J: \quad \Delta J = 0, \pm 1$$
$$k_a, k_c: \quad \text{even, odd} \leftrightarrow \text{even, even}$$
$$\text{odd, even} \leftrightarrow \text{odd, odd}.$$

In the representation where the axis of quantization is along a-axis of inertia, Einstein A-coefficient for transition $J'_{\tau'} \rightarrow J_\tau$ is given by Chandra and Sahu (1993), Chandra and Rashmi (1998)