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Strengths of rotational lines from H_2CC molecule: Addressing tentative detection

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ABSTRACT

Though H_2C, H_2CCC, H_2CCCC, H_2CCO, H_2CO, H_2CS molecules have been identified in cool interstellar clouds, identification of H_2CC is still awaited. Formation of H_2CC in the interstellar medium is quite probable as the cosmic abundance of carbon is 20 times larger than that of the sulphur, and the molecule H_2CS has already been identified in the interstellar medium. To our knowledge, no laboratory study for H_2CC is available in literature. Physical conditions in the interstellar medium are quite different as compared to those in a terrestrial laboratory. Using the rotational and centrifugal distortion constants for H_2CC, we have calculated the energies of rotational levels and the strengths of lines between the levels up to 270 cm^{-1}. We have found that 88 and 87 lines of ortho-H_2CC and para-H_2CC, respectively have Einstein *A*-coefficient larger than 10^{-5} s^{-1}. These lines may help in the identification of H_2CC in the interstellar medium. Tentative detection of H_2CC has been addressed.

1. Introduction

Formaldehyde (H_2CO) is the first organic molecule identified in a number of galactic and extragalactic radio sources through its transition $1_{10} - 1_{11}$ at 4.830 GHz in absorption (Snyder et al., 1969). Later on, widespread distribution of H_2CO and of carbon monoxide (CO) was found in the interstellar medium (ISM), and subsequent discovery of CS, the sulpher analogue of CO, in a number of radio sources, suggested that the thioformaldehyde (H_2CS), the sulpher analogue of H_2CO, might be present in the interstellar medium. After some unsuccessful attempts, the first success for the identification of H_2CS was reported by Sinclair et al. (1973) through its transition $2_{11} - 2_{12}$ at 3.139 GHz in Sgr B2 in absorption. The H_2CC molecule is very similar to H_2CO and H_2CS, as all these three: (i) are a-type asymmetric top molecules, (ii) have C_{2v} symmetry. Further, all the C,S and O atoms have nuclear spin zero and due to two hydrogen atoms, the energy levels of these molecules are divided into ortho and para species. Identification of H_2CC in the ISM is quite probable as the cosmic abundance of carbon is 20 times larger than that of the sulpher.

Other similar molecules identified in the ISM are H_2C (Nakajima et al., 2011), H_2CCC (Cernicharo et al., 1991a), H_2CCCC (Cernicharo et al., 1991b; Kawaguchi, 1991), H_2CCO (Irvine, 1989; Matthews and Sears, 1986; Ohishi, 1991; Turner, 1977). After identification of these six molecules, non-identification of H_2CC in the ISM appears quite astonishing. Chandra et al. (2011) and Sharma et al. (2013) have proposed that H_2CC may be identified in a cool cosmic object through its transition $1_{10} - 1_{11}$ at 4.89 GHz. However, the Einstein *A*-coefficient for this transition is quite small ($A = 4.15 \times 10^{-9}$ s^{-1}). That is, the radiative life-time of upper level of this transition is 2.4096×10^8 s = 7.64 years. We, therefore, have attempted to look for other transitions of H_2CC for which the radiative life-time is small and therefore the Einstein *A*-coefficient is quite large; larger than 10^{-5} s^{-1}. Rotational levels are denoted by $J_{k_a k_c}$, where *J* stands for the rotational quantum number, and k_a and k_c are the projections of *J* on the axis of symmetry in case of prolate and oblate symmetric tops, respectively. Owing to the parallel and anti-parallel orientations of nuclear spins of two hydrogen atoms, the H_2CC can have two species, known as the ortho-H_2CC ($I = 1$, parallel spins) and para-H_2CC ($I = 0$, anti-parallel spins). These two species behave as if they are two distinct molecules, as there are no transitions between them.

2. Computational methods

The H_2CC is a planar *a*-type asymmetric top molecule having large electric dipole moment 2.4661 Debye along the *a*-axis of inertia. Quantum theoretical calculations on H_2CC have been performed using a density functional (DFT) approach with the help of GAUSSIAN 2009, (Frisch, 2010). We have employed the Becke three parameter hybrid functional in conjunction with the Lee-Yang-Parr non-local correlation functional (B3LYP) (Becke, 1993; Lee et al., 1988) in conjunction with

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Table 1
Rotational and centrifugal distortion constants of H_2CC in MHz.

Constant	cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ
$A \times 10^{-5}$	2.858903384	2.858903384	2.858903384	2.858903384
$B \times 10^{-4}$	3.99341083	3.99341083	3.99341083	3.99341083
$C \times 10^{-4}$	3.50396536	3.50396536	3.50396536	3.50396536
$D_J \times 10^{3}$	42.70790520	43.44087371	44.28356329	44.55227056
D_{JK}	20.98797907	18.94745263	20.44459322	20.41969840
D_K	5.317724694	6.440167938	5.879314400	5.933397632
$d_1 \times 10^{2}$	−1.442126677	−1.373607832	−1.445080323	−1.452037644
$d_2 \times 10^{2}$	−2.675152631	−2.408896481	−2.609261594	−2.613141728
$H_J \times 10^{6}$	−9.085110924	−7.573403608	−8.601743486	−8.655849617
$H_{JK} \times 10^{3}$	2.717970741	2.280665412	2.564823121	2.580959398
$H_{KJ} \times 10^{2}$	−1.854934803	−1.597951879	−1.709596957	−1.731162015
$H_K \times 10^{2}$	2.401038405	2.151628752	2.272677147	2.294269779
$h_1 \times 10^{6}$	−1.524539329	−1.248551723	−1.444404960	−1.443374339
$h_2 \times 10^{6}$	4.698862167	3.929762419	4.456301949	4.485417315
$h_3 \times 10^{6}$	1.651996740	1.367132587	1.571699754	1.572110353

the basis sets, cc- pVTZ, aug-cc-pVDZ, aug-cc-pVTZ and aug-cc-pVQZ. The resulting rotational and centrifugal distortion constants are given in Table 1. These rotational and centrifugal distortion constants are for a Watson's type rotational operator (Watson, 1977), written in I^r representation and with S-type reduction. In absence of laboratory data, use of such data provide reasonably good qualitative results (Sharma et al., 2017,2018). Sharma et al. (2017, 2018) calculated rotational level of c-C_3H_2O and c-C_2H_4O molecules, respectively, by using (i) laboratory data and (ii) data obtained from the optimization using B3LYP method and found that the maximum deviations of the energies obtained from the optimization data was less than 0.8 % as compared to those obtained from the laboratory data. In absence of laboratory information, the use of optimization with the help of B3LYP provides good results which may however be treated as qualitative. Quantum mechanical calculation of PAHs and prebiotic molecules have been done by Mackie et al. (2018) and Skouteris et al. (2017), respectively.

As the electric dipole moment of H_2CC is along the a-axis of inertia, the radiative transitions between the rotational levels are governed by the following selection rules:

J:	$\Delta J = 0, \pm 1$	
k_a, k_c:	odd, even ⟷ odd, odd	(ortho-transition)
	even, even ⟷ even, odd	(para-transition)

We have employed the software ASROT (Kisiel, 2001) where we used the rotational and centrifugal distortion parameters given in Table 1 for aug-cc-pVQZ basis set. The calculated values for energies of levels are given in Table 2 and the Einstein A-coefficients are given in Table 3 for ortho-H_2CC and in Table 4 for para-H_2CC. Einstein A-coefficients for transitions between 23 levels of ortho-H_2CC were calculated and used for the transfer of radiation by Chandra et al. (2011) and Sharma et al. (2013).

3. Results and discussion

Since the kinetic temperature in a cosmic object where H_2CC may be identified might be few tens of Kelvin, we have considered only those rotational levels which lie below 270 cm^{-1}.

For a spectral line to be a strong radio emission line under interstellar conditions, besides a sufficient abundance of the molecule under consideration, two further conditions need to be satisfied:

(i) The upper level must be sufficiently populated. In the interstellar clouds the basic excitation of molecules is dominated in most cases by the collisions. At a given temperature, this limits the energy of upper level. We have chosen the condition for the energy E_j of upper level j of transition:

$E_j < 270$ cm^{-1}

Table 2
Energies of rotational levels.

Level	ortho-H_2CC			para-H_2CC		
No.	Level	E (GHz)	E (cm^{-1})	Level	E (GHz)	E (cm^{-1})
1	$1_{1,1}$	320.883	10.696	$0_{0,0}$	0.000	0.000
2	$1_{1,0}$	325.777	10.859	$1_{0,1}$	74.974	2.499
3	$2_{1,2}$	465.854	15.528	$2_{0,2}$	224.847	7.495
4	$2_{1,1}$	480.536	16.018	$3_{0,3}$	449.474	14.982
5	$3_{1,3}$	683.263	22.775	$4_{0,4}$	748.635	24.954
6	$3_{1,2}$	712.625	23.754	$5_{0,5}$	1122.036	37.401
7	$4_{1,4}$	973.055	32.435	$2_{2,1}$	1217.949	40.598
8	$4_{1,3}$	1021.984	34.066	$2_{2,0}$	1218.020	40.601
9	$5_{1,5}$	1335.159	44.505	$3_{2,2}$	1442.378	48.079
10	$5_{1,4}$	1408.532	46.951	$3_{2,1}$	1442.733	48.091
11	$6_{1,6}$	1769.486	58.983	$6_{0,6}$	1569.317	52.311
12	$6_{1,5}$	1872.165	62.406	$4_{2,3}$	1741.558	58.052
13	$7_{1,7}$	2275.932	75.864	$4_{2,2}$	1742.625	58.087
14	$7_{1,6}$	2412.754	80.425	$7_{0,7}$	2090.055	69.668
15	$3_{3,1}$	2682.830	89.428	$5_{2,4}$	2115.441	70.515
16	$3_{3,0}$	2682.830	89.428	$5_{2,3}$	2117.928	70.598
17	$8_{1,8}$	2854.383	95.146	$6_{2,5}$	2563.966	85.466
18	$4_{3,2}$	2981.381	99.379	$6_{2,4}$	2568.931	85.631
19	$4_{3,1}$	2981.385	99.379	$8_{0,8}$	2683.771	89.459
20	$8_{1,7}$	3030.142	101.005	$7_{2,6}$	3087.057	102.902
21	$5_{3,3}$	3354.629	111.821	$7_{2,5}$	3095.969	103.199
22	$5_{3,2}$	3354.647	111.822	$9_{0,9}$	3349.951	111.665
23	$9_{1,9}$	3504.710	116.824	$8_{2,7}$	3684.627	122.821
24	$9_{1,8}$	3724.143	124.138	$8_{2,6}$	3699.415	123.314
25	$6_{3,4}$	3802.613	126.754	$10_{0,10}$	4088.061	136.269
26	$6_{3,3}$	3802.665	126.756	$9_{2,8}$	4356.576	145.219
27	$10_{1,10}$	4226.777	140.893	$9_{2,7}$	4379.664	145.989
28	$7_{3,5}$	4325.371	144.179	$4_{4,1}$	4716.200	157.207
29	$7_{3,4}$	4325.503	144.183	$4_{4,0}$	4716.200	157.207
30	$10_{1,9}$	4494.539	149.818	$11_{0,11}$	4897.571	163.252
31	$8_{3,6}$	4922.947	164.098	$5_{4,2}$	5087.917	169.597
32	$8_{3,5}$	4923.238	164.108	$5_{4,1}$	5087.917	169.597
33	$11_{1,11}$	5020.440	167.348	$10_{2,9}$	5102.792	170.093
34	$11_{1,10}$	5341.074	178.036	$10_{2,8}$	5137.115	171.237
35	$9_{3,7}$	5595.385	186.513	$6_{4,3}$	5534.029	184.468
36	$9_{3,6}$	5595.967	186.532	$6_{4,2}$	5534.029	184.468
37	$12_{1,12}$	5885.550	196.185	$12_{0,12}$	5777.981	192.599
38	$12_{1,11}$	6263.453	208.782	$11_{2,10}$	5923.148	197.438
39	$10_{3,8}$	6342.726	211.424	$11_{2,9}$	5972.144	199.071
40	$10_{3,7}$	6343.808	211.460	$7_{4,4}$	6054.565	201.819
41	$13_{1,13}$	6821.954	227.398	$7_{4,3}$	6054.566	201.819
42	$11_{3,9}$	7165.006	238.834	$8_{4,5}$	6649.559	221.652
43	$11_{3,8}$	7166.901	238.897	$8_{4,4}$	6649.561	221.652
44	$13_{1,12}$	7261.340	242.045	$13_{0,13}$	6728.841	224.295
45	$5_{5,1}$	7315.789	243.860	$12_{2,11}$	6817.506	227.250
46	$5_{5,0}$	7315.789	243.860	$12_{2,10}$	6885.081	229.503
47	$6_{5,2}$	7759.574	258.652	$9_{4,6}$	7319.047	243.968
48	$6_{5,1}$	7759.574	258.652	$9_{4,5}$	7319.053	243.968
49	$14_{1,14}$	7829.500	260.983	$14_{0,14}$	7749.770	258.326
50	$12_{3,10}$	8062.257	268.742	$13_{2,12}$	7785.714	259.524