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Collisional excitation of thioformaldehyde and of Silylidene

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Abstract

For analysis of spectrum of a molecule in the interstellar medium, radiative and collisional transition probabilities for rotational transitions in the molecule are required. We have calculated collisional rate coefficients for rotational transitions in ortho and para thioformaldehyde (H_2CS), and in ortho and para Silylidene (H_2CSi) due to collisions with He atom for kinetic temperatures 10, 20, 30, 40 and 50 K, following the procedure discussed in our earlier work. The accuracy of collisional rate coefficients may be within a factor of 2.
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1. Introduction

H_2CS was first identified by Sinclair et al. (1973) through its $2_{11} - 2_{12}$ transition at 3.139 GHz in the direction of Sgr B2 in absorption. Since then it has been observed in many molecular clouds (see e.g., Minh et al. (1991), Kaifu et al. (2004)) as well as in the envelope of IRC + 10216 (Agundez et al., 2008). Out of the molecules identified in the interstellar space, some are Si-bearing. The Si-bearing molecules identified in the cosmic objects are SiN, SiC, SiO, SiS, c-SiC$_2$, SiCN, SiNC, c-SiC$_3$, C$_4$Si, SiH$_4$. The search for identification of H_2CSi in the interstellar medium has been unsuccessful (Izuha et al., 1996).

In most regions of interstellar space, the excitation of molecules (and atoms) deviates strongly from that under the local thermal equilibrium (LTE) conditions. Therefore, a quantitative interpretation of observed interstellar molecular lines requires the simultaneous solution of statistical equilibrium equations coupled with the equations of radia-

tive transfer for a large number of lines. As the input parameters, one has to know the radiative and collisional transition probabilities. Information about a number of molecules is available on some databases. However, no collisional data about H_2CS and about H_2CSi are available in those databases.

We have calculated collisional rate coefficients for transitions between 23 rotational levels in each of ortho and para H_2CS, and 25 rotational levels in each of ortho and para H_2CSi, colliding with He atoms, using the method used by Sharma et al. (2014a,b). The colliding partner is assumed to be structureless and we have taken it as the He atom. Wave functions and the energy levels have been obtained by using the rotational and distortional constants derived by Maeda et al. (2008) for H_2CS, and by Izuha et al. (1996) for H_2CSi.

2. Wave functions

The required rotational and distortional constants for H_2CS have been obtained by Maeda et al. (2008) and for H_2CSi have been obtained by Izuha et al. (1996). The energies E and g-coefficients for positive values of K for

Table 1
Wave functions and energies for ortho-H_2CS.

No.	Level	$E(\text{cm}^{-1})$	$\epsilon_{J\tau}$	$g_{J\tau}^1$	$g_{J\tau}^3$	$g_{J\tau}^5$	$g_{J\tau}^7$	$g_{J\tau}^9$	$g_{J\tau}^{11}$
1	1_{11}	10.274713	+	0.7071068					
2	1_{10}	10.309596	−	0.7071068					
3	2_{12}	12.529841	+	0.7071068					
4	2_{11}	12.634487	−	0.7071068					
5	3_{13}	15.912434	+	0.7071065	0.0006517				
6	3_{12}	16.121722	−	0.7071065	0.0006536				
7	4_{14}	20.422377	+	0.7071055	0.0013344				
8	4_{13}	20.771175	−	0.7071055	0.0013408				
9	5_{15}	26.059512	+	0.7071034	0.0021765	0.0000012			
10	5_{14}	26.582682	−	0.7071034	0.0021921	0.0000012			
11	6_{16}	32.823645	+	0.7070996	0.0031815	0.0000032			
12	6_{15}	33.556036	−	0.7070995	0.0032135	0.0000033			
13	7_{17}	40.714546	+	0.7070934	0.0043491	0.0000069	0.0000000		
14	7_{16}	41.690986	−	0.7070930	0.0044075	0.0000070	−0.0000000		
15	8_{18}	49.731943	+	0.7070840	0.0056781	0.0000126	−0.0000000		
16	8_{17}	50.987239	−	0.7070832	0.0057764	0.0000129	−0.0000000		
17	9_{19}	59.875532	+	0.7070705	0.0071667	0.0000210	0.0000000	0.0000055	
18	9_{18}	61.444461	−	0.7070689	0.0073221	0.0000216	−0.0000000	−0.0000602	
19	$10_{1,10}$	71.144970	+	0.7070518	0.0088129	0.0000327	0.0000001	0.0000732	
20	10_{19}	73.062270	−	0.7070489	0.0090469	0.0000339	0.0000000	−0.0000202	
21	$11_{1,11}$	83.539882	+	0.7008340	0.0105212	0.0000482	0.0000001	0.0000338	0.0933863
22	$11_{1,10}$	85.840241	−	0.7048117	0.0109190	0.0000505	0.0000001	−0.0000203	−0.0558684
23	3_{31}	89.136782	+	−0.0006517	0.7071065				

Table 2
Wave functions and energies for para-H_2CS.

No.	Level	$E(\text{cm}^{-1})$	$\epsilon_{J\tau}$	$g_{J\tau}^0$	$g_{J\tau}^2$	$g_{J\tau}^4$	$g_{J\tau}^6$	$g_{J\tau}^8$	$g_{J\tau}^{10}$
1	0_{00}	0.000000	+	1.0000000					
2	1_{01}	1.145047	+	1.0000000					
3	2_{02}	3.435027	+	0.9999986	0.0011676				
4	3_{03}	6.869708	+	0.9999932	0.0026107				
5	4_{04}	11.448748	+	0.9999796	0.0045217	0.0000028			
6	5_{05}	17.171684	+	0.9999523	0.0069064	0.0000085			
7	6_{06}	24.037945	+	0.9999046	0.0097659	0.0000191	−0.0000000		
8	7_{07}	32.046840	+	0.9998284	0.0130995	0.0000366	0.0000000		
9	2_{21}	40.013951	−	0.0000000	0.7071068				
10	2_{20}	40.014050	+	−0.0016512	0.7071058				
11	8_{08}	41.197570	+	0.9997141	0.0169060	0.0000634	0.0000001	0.0000766	
12	3_{22}	43.448614	−	0.0000000	0.7071068				
13	3_{21}	43.449112	+	−0.0036921	0.7071019				
14	4_{23}	48.028017	−	0.0000000	0.7071065	0.0005945			
15	4_{22}	48.029510	+	−0.0063946	0.7070921	0.0005945			
16	9_{09}	51.489220	+	0.9995512	0.0211832	0.0001021	0.0000002	0.0000032	
17	5_{24}	53.752034	−	0.0000000	0.7071058	0.0011676			
18	5_{23}	53.755516	+	−0.0097672	0.7070721	0.0011675			
19	6_{25}	60.620504	−	0.0000000	0.7071044	0.0018461	0.0000009		
20	6_{24}	60.627467	+	−0.0138111	0.7070369	0.0018460	0.0000009		
21	$10_{0,10}$	62.920765	+	0.9967047	0.0258599	0.0001555	0.0000003	−0.0000210	−0.0511971
22	7_{26}	68.633239	−	0.0000000	0.7071019	0.0026348	0.0000024		
23	7_{25}	68.645769	+	−0.0185256	0.7069805	0.0026346	0.0000024		

23 rotational levels of ortho and para of H_2CS, and 25 rotational levels of ortho and para of H_2CSi have been calculated following (Sharma et al., 2014a,b) and are presented in Tables 1 and 2 for ortho and para, respectively, and in Tables 3 and 4 for ortho and para H_2CSi, respectively. For a given rotational quantum number J, the K is the projection of J on the axis of symmetry and can assume the values from $-J$ to $+J$ with increment of one.

The τ is a pseudo quantum number which also can assume the values from $-J$ to $+J$ with increment of one. For negative values of K, we have the relation:

$$g_{J\tau}^{-K} = \epsilon_{J\tau}\, g_{J\tau}^K$$

where the value of the phase factor $\epsilon_{J\tau}$ for the level is given in the tables.