TRANSFER OF RADIATION IN H_2CS MOLECULE IN INTERSTELLAR SPACE

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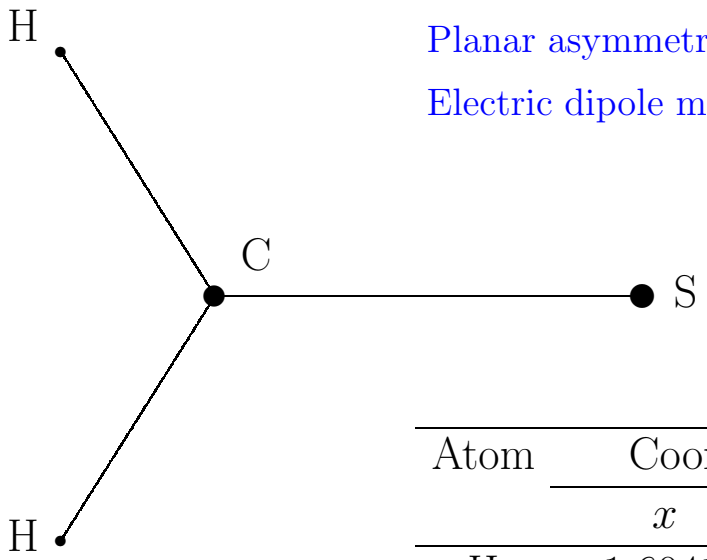
1 Structure



Planar asymmetric top molecule

Electric dipole moment 1.6491 Debye

Atom	Coordinates (Å)	
	x	y
H	−1.604144	0.920748
H	−1.604144	−0.920748
C	−1.025473	0.000000
S	0.585070	0.000000

- Structure of H_2CS is very similar to that of H_2CO which has been identified in a large number of cosmic objects.
- Though cosmic abundance of sulpher is much smaller than that of carbon and oxygen, but H_2CS has been identified in some cosmic objects.
- Some other sulpher-bearing molecules identified in cosmic objects are CS, NS, SO, SiS, C_2S, OCS, SO_2, H_2S, CCS, C_3S, HNCS, H_2C_2S, C_5S, CH_3SH

2 Laboratory study

1. D.R. Johnson, F.X. Powell, 1970. Science 169, 679.
2. D.R. Johnson, F.X. Powell, W.H. Kirchhoff, 1971. J. Mol. Spectrosc. 39, 136.
3. Y. Beers, G.P. Klein, W.H. Kirchhoff, D.R. Johnson, 1972. J. Mol. Spect. 44, 553.
4. A. Maeda, I.R. Medvedev, M. Winnewisser, F.C. De Lucia, E. Herbst, H.S.P. Müller, M. Koerber, C.P. Endres, S. Schlemmer, 2008, ApJS 176, 543.

$\Longrightarrow$ Derived rotational and distortional constants for H_2CS

Parameter[a]	in MHz
A	$2.916133419858 \times 10^{5}$
B	$1.76989948807 \times 10^{4}$
C	$1.66524986641 \times 10^{4}$
D_J	$19.0210847 \times 10^{-3}$
D_{JK}	$522.283353 \times 10^{-3}$
D_K	23.344325
d_1	$-1.2084913 \times 10^{-3}$
d_2	$-0.17734329 \times 10^{-3}$
H_J	-3.3329×10^{-9}
H_{JK}	1.487734×10^{-6}
H_{KJ}	$-28.222103 \times 10^{-6}$
H_K	5.95849×10^{-3}
h_1	3.085179×10^{-9}
h_2	1.65623×10^{-9}
h_3	0.32731×10^{-9}
L_{JK}	0.19622×10^{-9}
L_{KKJ}	-20.7881×10^{-9}
L_K	-2.1726×10^{-6}
l_1	-0.37662×10^{-12}

[a] Maeda et al. (2008)

- These parameters are required for obtaining transition probabilities between rotational levels.

3 Search for H_2CS in cosmic objects

Unsuccessful attempts:

1. N.J. Evans, C.H. Townes, H.F. Weaver, D.R.W. Williams, 1970. Science 169, 680.

2. R.D. Davies, R.S. Booth, A. Pedlar, 1971. Mon. Not. Roy. Astr. Soc. 152, 7p.

First successful attempt:

1. M.W. Sinclair, N. Fourikis, J.C. Ribes, B.J. Robinson, R.D. Brown, P.D. Godfrey, 1973. Austral. J. Phys. 26, 85.

   ($2_{11} \rightarrow 2_{12}$ transition at 3.19 GHz in Sgr B2)

$\Longrightarrow$ **The cosmic objects where H_2CS is found and may be found are cool cosmic objects having kinetic temperature of few tens of Kelvin. Thus, we are concerned with rotational levels in the ground vibrational and ground electronic states.**

4 Rotational energy levels

- For rotational levels of H_2CS (asymmetric top molecule) wave functions can be expressed in terms of wave functions for symmetric top molecule as (Chandra et al. (2011) New Astronomy 16, 152)

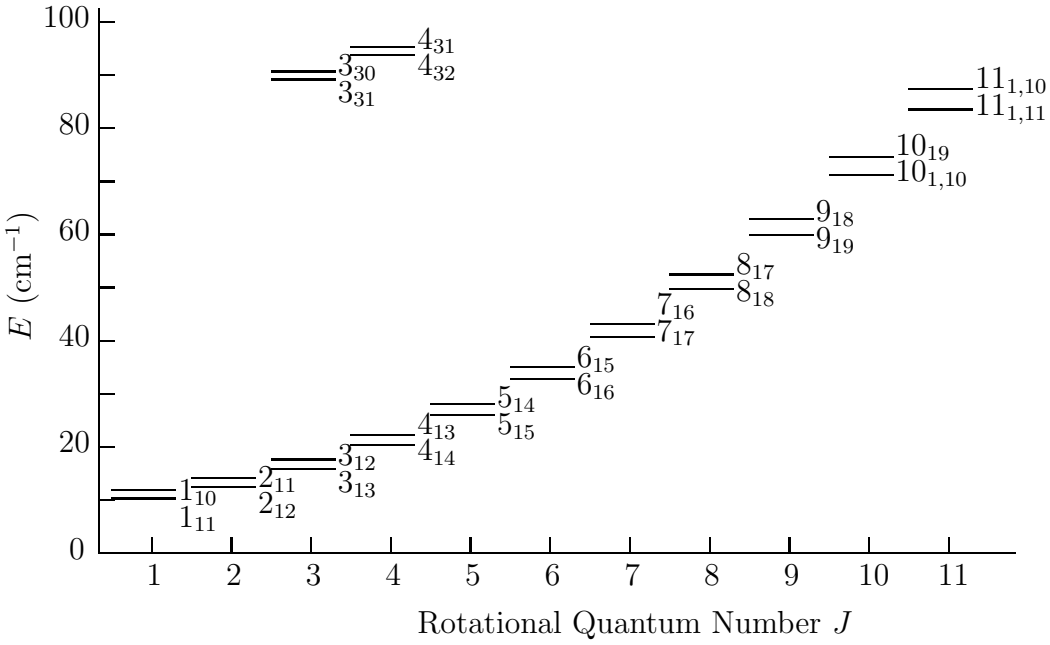
$$\psi_{J\tau M}(\alpha,\beta,\gamma) = \sqrt{\frac{2J+1}{8\pi^2}} \sum_{K=-J}^{J} g^J_{\tau K} D^J_{MK}(\alpha,\beta,\gamma)$$

  where $g^J_{\tau K}$ are expansion coefficients; J rotational quantum number; pseudo quantum number $\tau = k_a - k_c$; quantum numbers k_a and k_c can assume independently integer values 1, 2, ..., J.

- Owing to parallel and anti-parallel orientations of nuclear spins of two hydrogen atoms in H_2CS, there are ortho ($I = 1$) and para ($I = 0$) species. These two species behave as if they are two distinct molecules and there are no transitions between them.

- Using molecular and distortional constants, lowest 26 rotational energy levels of ortho H_2CS are given in Table and shown in the energy level diagram (not to the scale).

No	Level	$E(\mathrm{cm}^{-1})$	No	Level	$E(\mathrm{cm}^{-1})$
1	1_{11}	10.275	14	7_{16}	41.691
2	1_{10}	10.310	15	8_{18}	49.732
3	2_{12}	12.530	16	8_{17}	50.987
4	2_{11}	12.634	17	9_{19}	59.876
5	3_{13}	15.912	18	9_{18}	61.444
6	3_{12}	16.122	19	$10_{1,10}$	71.145
7	4_{14}	20.422	20	10_{19}	73.062
8	4_{13}	20.771	21	$11_{1,11}$	83.540
9	5_{15}	26.060	22	$11_{1,10}$	85.840
10	5_{14}	26.583	23	3_{31}	89.137
11	6_{16}	32.824	24	3_{30}	89.137
12	6_{15}	33.556	25	4_{32}	93.716
13	7_{17}	40.715	26	4_{31}	93.716



- These energy levels are connected through radiative as well collisional transitions.
- Though collisional transitions are between all levels, but radiative transitions follow selection rules.

5 Basic equations

• We solved statistical equilibrium equations coupled with equations of radiative transfer.

$$n_i \sum_{\substack{j=1 \\ j\neq i}}^{26} P_{ij} = \sum_{\substack{j=1 \\ j\neq i}}^{26} n_j\, P_{ji} \qquad i = 1, 2, \ldots, 26$$

where n's are the population densities of levels and P's are expressed as the following. (i) For optically allowed transitions

$$P_{ij} = \begin{cases} (A_{ij} + B_{ij}\ I_{\nu,bg})\beta_{ij} + n_{H_2}\ C_{ij} & i > j \\ B_{ij}\ I_{\nu,bg}\beta_{ij} + n_{H_2}\ C_{ij} & i < j \end{cases}$$

(ii) For optically forbidden transitions $P_{ij} = n_{H_2}\ C_{ij}$

A's and B's are Einstein coefficients, C's the collisional rate coefficients, n_{H_2} the density of hydrogen molecules, and the escape probability β for the transition is

$$\beta_{lu} = \beta_{ul} = \frac{1 - \exp(-\tau_\nu)}{\tau_\nu}$$

for spherically symmetric geometry. Here optical thickness τ_ν is

$$\tau_\nu = \frac{hc}{4\pi(\mathrm{d}v_r/\mathrm{d}r)}\ [B_{lu}n_l - B_{ul}n_u]$$

where $(\mathrm{d}v_r/\mathrm{d}r)$ is velocity-gradient in the region.

- It is non-linear set of equations which can be solved through iterative procedure.
- The iterative procedure starts with thermal populations of energy levels.
- Here, external radiation field, impinging on a volume element generating the lines, is the CMB only.
- This set of equations is solved through iterative procedure for the given values of n_{H_2} and $\gamma \equiv n_{\rm mol}/(dv_r/dr)$, where $n_{\rm mol}$ is density of the molecule.
- Input parameters are radiative transition probabilities and collisional transition probabilities.

6 Radiative transition probabilities

- The radiative transitions are governed by the selection rules:

$$\begin{aligned} J: &\quad \Delta J = 0, \pm 1 \\ k_a, k_c: &\quad \text{even, odd} \longleftrightarrow \text{even, even} \\ &\quad \text{odd, even} \longleftrightarrow \text{odd, odd.} \end{aligned}$$

In I^r representation, Einstein A-coefficient for the transition $J'_{\tau'} \rightarrow J_\tau$ is

$$A(J'_{\tau'} \rightarrow J_\tau) = \frac{64\pi^4\nu^3\mu^2(2J+1)}{3hc^3(2J'+1)} \left[\sum_{K=-J}^{J} g^J_{\tau K} g^{J'}_{\tau' K} C^{J'K}_{JK10}\right]^2$$

Here, $C^{J'K}_{JK10}$ are Clebsch-Gordon coefficients

$\Longrightarrow$ Calculated values of Einstein A-coefficients

Transition	A-coeff (s^{-1})	Transition	A-coeff (s^{-1})
$1_{10} \rightarrow 1_{11}$	1.814×10^{-11}	$2_{12} \rightarrow 1_{11}$	2.941×10^{-6}
$2_{11} \rightarrow 1_{10}$	3.222×10^{-6}	$2_{11} \rightarrow 2_{12}$	1.632×10^{-10}
$3_{13} \rightarrow 2_{12}$	1.260×10^{-5}	$3_{12} \rightarrow 2_{11}$	1.381×10^{-5}
$3_{12} \rightarrow 3_{13}$	6.529×10^{-10}	$4_{14} \rightarrow 3_{13}$	3.267×10^{-5}
$4_{32} \rightarrow 3_{31}$	1.596×10^{-5}	$4_{13} \rightarrow 3_{12}$	3.579×10^{-5}
$4_{31} \rightarrow 3_{30}$	1.596×10^{-5}	$4_{13} \rightarrow 4_{14}$	1.814×10^{-9}
$5_{15} \rightarrow 4_{14}$	6.681×10^{-5}	$5_{14} \rightarrow 4_{13}$	7.320×10^{-5}
$5_{14} \rightarrow 5_{15}$	4.080×10^{-9}	$6_{16} \rightarrow 5_{15}$	1.187×10^{-4}
$6_{15} \rightarrow 5_{14}$	1.301×10^{-4}	$6_{15} \rightarrow 6_{16}$	7.995×10^{-9}
$7_{17} \rightarrow 6_{16}$	1.920×10^{-4}	$7_{16} \rightarrow 6_{15}$	2.103×10^{-4}
$7_{16} \rightarrow 7_{17}$	1.421×10^{-8}	$8_{18} \rightarrow 7_{17}$	2.903×10^{-4}
$8_{17} \rightarrow 7_{16}$	3.181×10^{-4}	$8_{17} \rightarrow 8_{18}$	2.349×10^{-8}
$9_{19} \rightarrow 8_{18}$	4.173×10^{-4}	$9_{18} \rightarrow 8_{17}$	4.573×10^{-4}
$9_{18} \rightarrow 9_{19}$	3.669×10^{-8}	$10_{110} \rightarrow 9_{19}$	5.767×10^{-4}
$10_{19} \rightarrow 9_{18}$	6.318×10^{-4}	$10_{19} \rightarrow 10_{1,10}$	5.480×10^{-8}
$11_{1,11} \rightarrow 10_{1,10}$	7.720×10^{-4}	$11_{1,10} \rightarrow 10_{19}$	8.458×10^{-4}
$11_{1,10} \rightarrow 11_{1,11}$	7.889×10^{-8}		

7 Collisional transition coefficients

- Though collisional transition coefficients do not follow any selection rules, computation of them is a quite cumbersome task.
- In absence of data for them, we have used the data of H_2CO for downward transitions between 14 lowest levels, as besides the similarity of structure, the energy level scheme is also similar.
- For other transitions, collisional transition coefficients are calculated with the help of the expression

$$C(J'_{\tau'} \rightarrow J_{\tau}) = 1\text{x}10^{-11}(2J+1)\sqrt{\frac{T_k}{30}}$$

- For upward collisional rate coefficients, we accounted for the detailed equilibrium:

$$C(J_{\tau} \rightarrow J'_{\tau'}) = C(J'_{\tau'} \rightarrow J_{\tau})\ \frac{2J'+1}{2J+1}\ \exp(-\frac{\Delta E}{kT_k})$$

8 Results & Discussion

- Figure 1 shows the brightness temperature T_B (K) (columns 1 and 3) and the optical depth τ_ν (columns 2 and 4) as a function of hydrogen density n_{H_2} for kinetic temperatures of 10 K, 20 K, 30 K and 40 K for transitions $1_{10} - 1_{11}$ and $2_{11} - 2_{12}$, respectively, of H_2CS. Solid (red) line is for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc and dotted (blue) line for $\gamma = 10^{-6}$ cm^{-3} (km/s)$^{-1}$ pc.
- The transition $1_{10} - 1_{11}$ shows strong anomalous absorption (brightness temperature less than the CMB temperature).
- Anomalous absorption of $1_{10} - 1_{11}$ transition may help in identification of H_2CS in cool cosmic objects.

9 Acknowledgments

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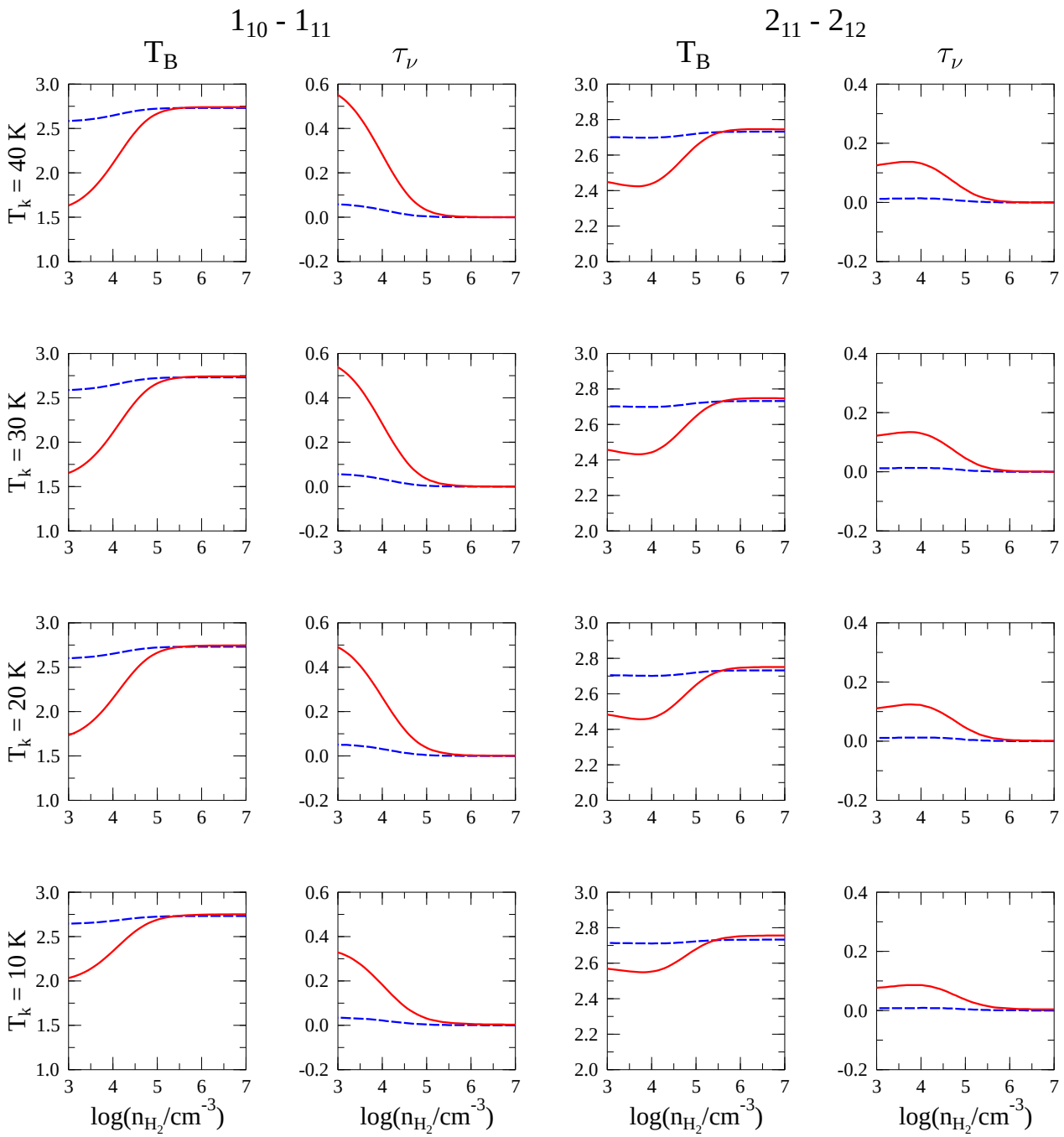

Figure 1: Brightness temperature T_B and optical depth τ for $1_{10} - 1_{11}$ and $2_{11} - 2_{12}$ transitions.