Collisional Transitions in Interstellar Asymmetric Top Molecules

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- It is well known that for the study of a molecule in a cosmic object, we have to account for a multi-level system in the molecule.

- These energy levels are connected through radiative as well as collisional transitions.

- The NLTE effects in the molecule arrive in the picture only when the collisional transitions are present.

Plan of the talk

- Classification of molecules
- Molecules in cosmic objects
- Anomalous Phenomenon in cosmic molecules
- Modeling
- Radiative transition probabilities
- Collisional rate coefficients
- Results for some molecules
- Applications

Classification of Molecules

- Each molecule has three mutually perpendicular axes passing through the center-of-mass.
- Moments of inertia about these three axes can be calculated.
- These axes are named as *a*, *b* and *c* according to the condition $I_a \leq I_b \leq I_c$
- For oblate top symmetric top molecules: $I_a = I_b \leq I_c$
- For prolate top symmetric top molecules: $I_a \leq I_b = I_c$
- For diatomic molecules: $I_a = 0$, $I_b = I_c$
- For spherical top molecules: $I_a = I_b = I_c$
- **For asymmetric top molecules: $I_a < I_b < I_c$**
- **Large number of molecules in cosmic molecules are asymmetric top molecules**

After the discovery of radio window in 1932, the first molecule OH was identified in some cosmic objects in 1963. Since then more than 180 molecules have been identified in the cosmic objects

List of molecules observed in interstellar space

Molecules of two atoms

AlCl, CO, CP, CS, H_2 HD, HCl, N_2, NH, AlF, C_2, CH, CH^+, CN, KCl, NO, NaCl, PN, SO^+, SiN, NS, OH, SO, SiC, SiC, SiS, CO^+, NO^+, HF, PO, FeO, SH

Molecules of three atoms

C_2H, C_2S, H_3^+, HCN, HNC, HCO, HCO^+, DCO^+, HNO, H_2O, N_2H^+, OCS, SO_2, HCS^+, H_2S, c-SiC_2, H_2D^+, NaCN, NaOH, HDO, C_3, CO_2, HCO^+, CCS, CH_2, N_2O, CNO, MgCN, HOC^+, SiCN, SiNC, MgNC, D_2H^+, HCP, CCD, DCN, DNC, AlNC

Molecules of four atoms

C_2H_2, l-C_3H, c-C_3H, C_3O, $HCNH^+$, H_2CO, CH_3, C_3N, C_3S, H_2CS, HNCS, $HOCO^+$, H_3O^+, NH_3, HNCO, D_2CO, HC_2N, H_2CN, NH_2D, C_2H_2, HCCH, c-SiC_3, C_4, HDCO, HDCS, ND_2H, NCCN

Molecules of five atoms

C_4Si, CH_2CN, HCOOH, HC_3N, H_2CCO, H_2NCN, CH_4, c-C_3H_2, C_4H, H_2CHN, SiH_4, C_3HD, C_4D, H_2C_2S, C_5, H_2COH^+, HCCNC, HNCCC, DC_3N, CH_3D, HCCCN, H_2CCN, CH_2NH, H_2CCC

Molecules of six atoms

C_2H_4, C_5H, CH_3NC, C_5O, C_5S, CH_3CN, CH_3OH, CH_3SH, CH_2C_3, $HCONH_2$, HC_2CHO, HC_2COH, H_2C_4, NH_2CHO, HC_3NH^+, CH_3OD, H_3C_2N, H_3COH, H_2CCH_2, CH_3C_2H, C_5N, H_2CCCC, HC_4N, c-H_2C_3O

Molecules of seven atoms

CH_3CCH, HC_5N, H_6H, CH_3NH_2, CH_2CHCN, $HCOCH_3$, CH_2CHON, CH_2CHOH, H_3C_3H, H_2C_2HCN, H_3C_2HO, c-C_2H_4O, CH_3CHO, CH_3C_2H, C_5H_2 ,c-C_5H_2

Molecules of eight atoms

CH_3C_3N, $HCOOCH_3$, CH_2CHCHO, CH_3COOH, $(NH_2)_2CO$, C_7H, C_3H_3NO, H_2C_6, H_3C_4N, CH_2OHCHO

Molecules of nine atoms

CH_3C_4H, C_2H_5CN, $(CH_3)_2O$, HC_7N, C_2H_5OH, C_8H, H_3C_5H, CH_3CH_2CN, $H(CC)_3CN$, CH_3OCH_3, C_7H_2

Molecules of ten atoms

C_6H_3N, H_3CCOCH_3, CH_3CH_2CHO, CH_7CN

Molecules of more than ten atoms:

HC_9N, $HC_{11}N$, C_6H_6, $CH_3OC_2H_5$, $(CH_2)_6N_4$

- Why do we study molecules in cosmic objects?

1. It provides information about:

- Chemical reactions
- Physical conditions (pressure, temp, density etc.)

2. Molecular regions are associated with:

Star forming regions (Birth of stars)

Circumstellar regions of evolved stars (Death of stars)

There are number of cosmic objects which behave like a factory of molecules.

- Molecules radiate IR, Microwaves, Radio waves

Besides the emission and absorption, two Anomalous Phenomena:

1) Microwave Amplification by Stimulated Emission of Radiation (MASER)

2) Anomalous absorption – Absorption against the Cosmic Microwave Background (CMB)

Quasi-resonance collisional pumping in H_2O masers

D.A. Varshalovich, W.H. Kegel & S. Chandra (1983) Sov. Astron. Lett. 9, 209 (1983)

Prediction of maser emisison from H_2O at 1.635 mm and 922 μ

S. Chandra, W.H. Kegel and D.A. Varshalovich (1985) 148, 145.

Astron. Astrophys. 148, 145–150 (1985)

ASTRONOMY
AND
ASTROPHYSICS

Prediction of maser emission from para-H_2O at 1.635 mm and 922μ

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A NEW SUBMILLIMETER WATER MASER TRANSITION AT 325 GHz

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Anomalous absorption

- Observation of a spectral line in absorption against the CMB is an unusual phenomenon.
- The intensity I_ν of a line generated in an interstellar cloud, with homogeneous excitation condition is

$$I_\nu - I_{\nu,bg} = (S_\nu - I_{\nu,bg})(1 - e^{-\tau_\nu})$$

$$B_\nu(T_B) - B_\nu(T_{bg}) = [B_\nu(T_{ex}) - B_\nu(T_{bg})](1 - e^{-\tau_\nu})$$

- Rayleigh - Jeans limit

$$T_B = T_{ex} + (T_{bg} - T_{ex})e^{-\tau_\nu}$$

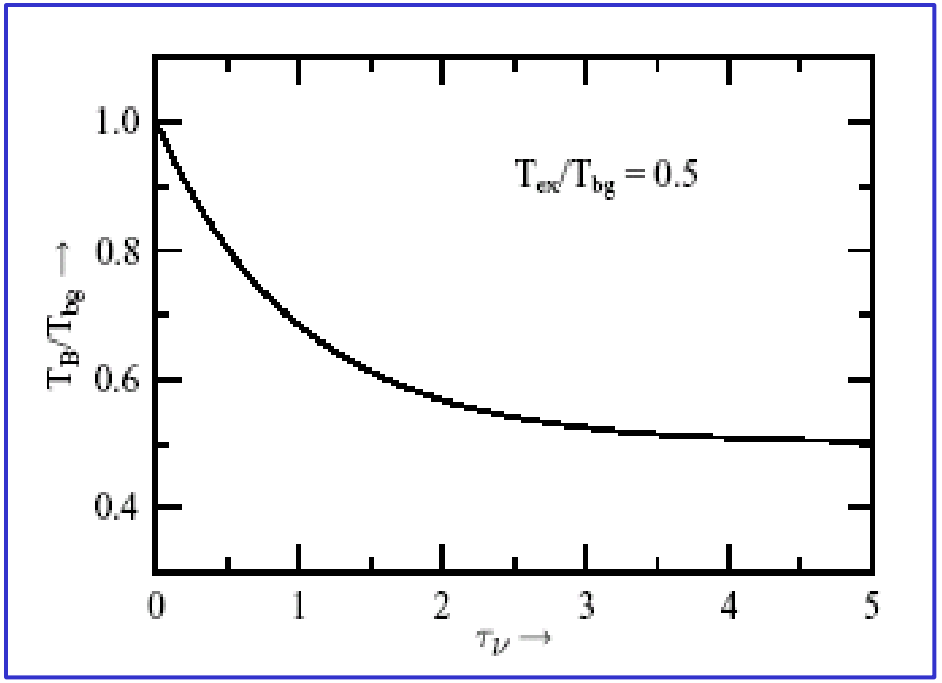
$$T_B = T_{ex} + (T_{bg} - T_{ex})e^{-\tau_\nu}$$

$\tau_\nu \rightarrow 0$, we have $T_B = T_{bg}$

$\tau_\nu \rightarrow \infty$, we have $T_B = T_{ex}$

For anomalous absorption

$$0 < T_{ex} < T_B < T_{bg}$$

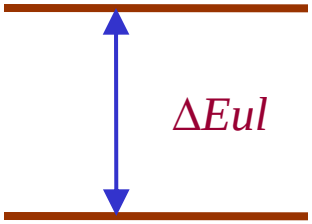


Variation of τ_ν with T_B/T_{bg} for T_{ex}/T_{bg}= 0.5

- For a molecule in LTE the population densities of energy levels are related through the relation

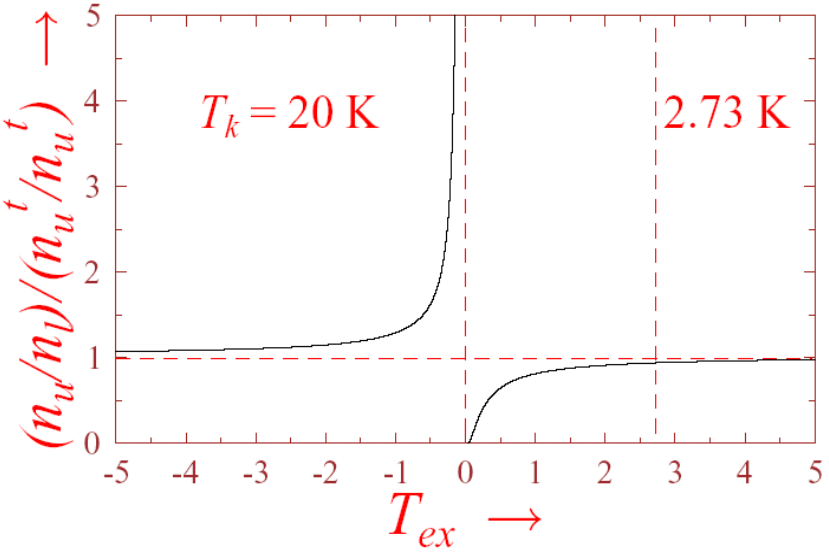
$$\frac{n_u^t}{n_l^t} = \frac{g_u}{g_l} \exp(-\Delta E_{ul}/kT_k)$$

- For Non-LTE the population densities of energy levels are related through the relation



$$\frac{n_u}{n_l} = \frac{g_u}{g_l} \exp(-\Delta E_{ul}/kT_{ex})$$

$$\frac{n_u/n_l}{n_u^t/n_l^t} = \exp\left[\frac{\Delta E}{k}\left(\frac{1}{T_k} - \frac{1}{T_{ex}}\right)\right]$$

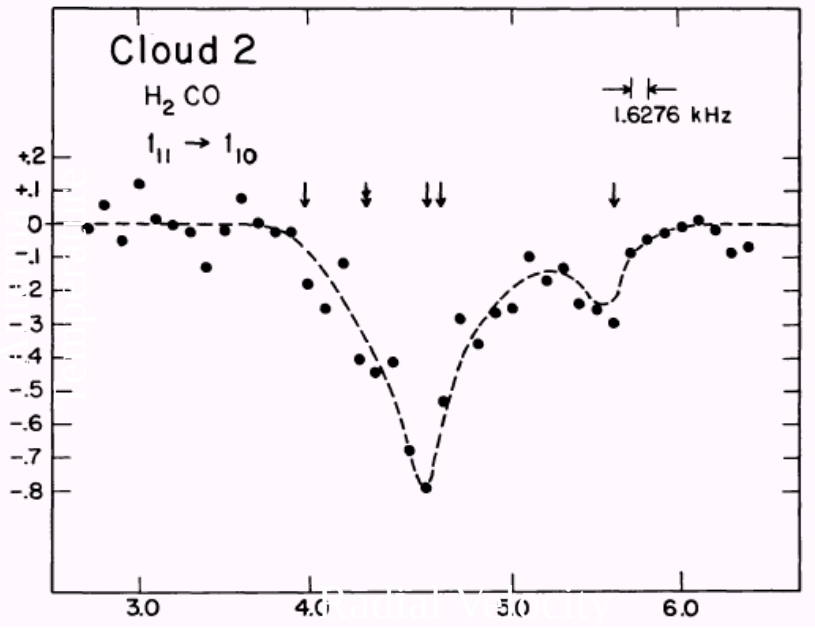


Variation of $(n_u/n_l)/(n^t_u/n^t_l)$ versus T_{ex} for the line of 4.83 GHz at (T_k =20 K).

- For anomalous absorption, T_{ex} is in between the vertical dotted lines ($0 < T_{ex} < 2.73$ K) and the brightness temp. is in between T_{ex} and 2.73 K ($T_{ex} < T_B < 2.73$ K).

- Negative value of excitation temperature corresponds to the MASER action

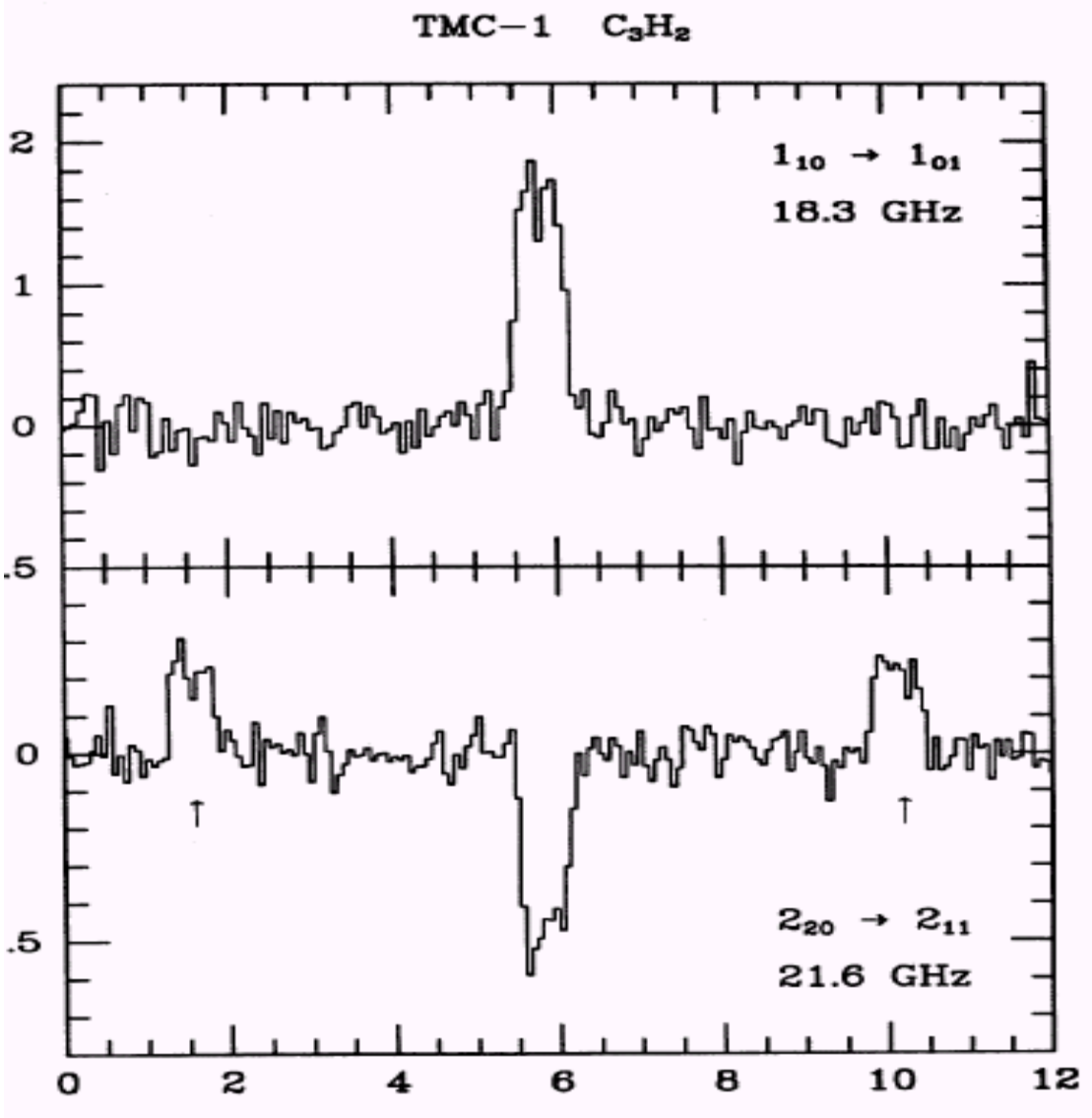
Spectrum of H_2CO Palmer *et al.* (1969)



- H_2CO is the first organic molecule identified in a number of cosmic objects through its transition 1_{11} - 1_{10} at 4.831 GHz. in absorption (Snyder *et al.*, 1969) .

- This transition 1_{11} - 1_{10} was also observed in anomalous absorption in a large number of cosmic objects (Palmer *et al.*, 1969).

Spectrum of c-C_3H_2 Maddan *et al.* (1989)



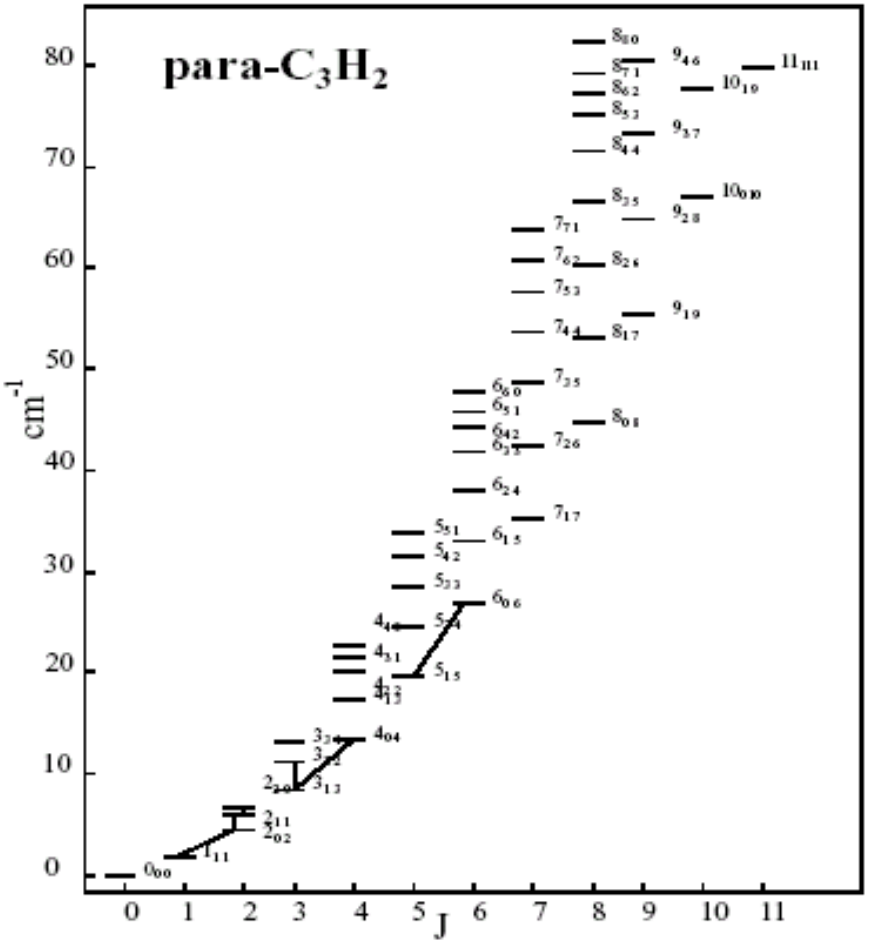
Modeling

In our model, the CMB is the only background to the cosmic object under investigation

CMB 2.73 K Cosmic object Observer

Since the kinetic temperature in dark molecular clouds is rather low, 10-20 K, only rotational transitions in the ground electronic and ground vibrational states can take place.

Energy level diagram of para-C_3H_2



Set of linear equations coupled with equations of radiative transfer is solved through iterative procedure.

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

Optically allowed transitions

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

Optically forbidden transitions

$$P_{ij} = n_{H_2}\ C_{ij}$$

$$A_{ul} = \frac{2h\nu^3}{c^2}\ B_{ul} \qquad B_{ul} = \frac{g_l}{g_u}\ B_{lu}$$

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

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

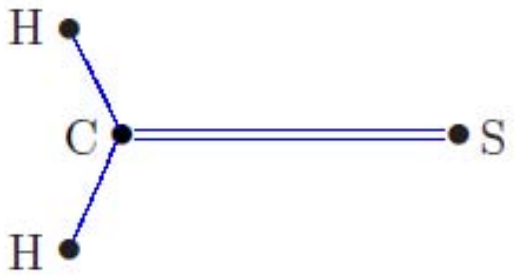
In order to include a large number of cosmic objects where molecule may be found, numerical calculation are carried out for wide ranges of physical parameters $\gamma \equiv n_{mol}/(dv_r/dr)$ and hydrogen density n_{H2}

Asymmetric top molecules

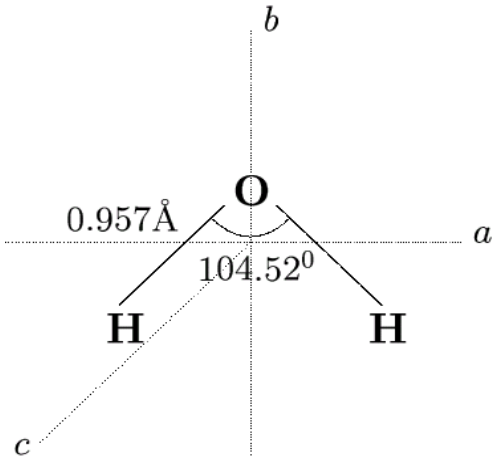
Depending on the direction of the electric dipole moment, asymmetric top molecules are classified in to *a*-type and *b*-type asymmetric top molecules.

a-type examples: H_2CO, H_2CS, etc.

b-type examples: H_2O, H_2S, C_3H_2 etc.



a-type molecule



b-type molecule

Treatment of asymmetric top molecules is quite complicated as they have no preferential direction for quantization and the energy matrix is non-diagonal.

Rotational wave functions for an asymmetric top molecule can be described by linear combination of symmetric top wave functions (Chandra et al., 1984)

$$A_{J\tau M}(\alpha,\beta,\gamma) = \sqrt{\frac{2J+1}{8\pi^2}} \sum_{K=-J}^{J} g_{\tau K}^{J} D_{MK}^{J}(\alpha,\beta,\gamma)$$

Einstein A-Coefficients

➢ *a*-type radiative transitions are governed by the selection rules

$$J : \Delta J = 0, \pm 1$$

$$k_a , k_c : \text{ even, odd } \leftrightarrow \text{ even, even}$$

$$\text{odd, even } \leftrightarrow \text{ odd, odd}$$

➢ In the representation where the axis of quantization is along the *a*-axis of inertia, Einstein *A*-coefficient for *a*-type transition $J'\tau' \rightarrow J\tau$ is

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

C - the Clebsch-Gordon coefficient, g - expansion coefficients

b-type radiative transitions are governed by the selection rules

$$J : \Delta J = 0, \pm 1$$

$$k_a , k_c : \text{ even, odd } \leftrightarrow \text{ odd, even}$$

$$\text{even, even } \leftrightarrow \text{ odd, odd}$$

In the representation where the axis of quantization is along the *a*-axis of inertia, Einstein *A*-coefficient for *b*-type transition $J'\tau' \rightarrow J\tau$ is

$$A(J'_{\tau'} \rightarrow J_{\tau}) = \frac{32\pi^4\nu^3\mu_b^2(2J+1)}{3hc^3(2J'+1)} \times \left[\sum_{K=-J}^{J} g_{\tau K}^{J} \left(g_{\tau' K+1}^{J'} C_{JK11}^{J'K+1} + g_{\tau' K-1}^{J'} C_{JK1,-1}^{J'K-1}\right)\right]^2$$

We have used the very accurate molecular and distortional constants of Maeda et al. (2008)

Table 1. Parameters of H_2CS and H_2CO in MHz

Parameter	H_2CS^a	H_2CO^b
A	$2.916133419858 \times 10^5$	$2.81970554688 \times 10^5$
B	$1.76989948807 \times 10^4$	$3.88339890137 \times 10^4$
C	$1.66524986641 \times 10^4$	$3.40042453613 \times 10^4$
D_J	$19.0210847 \times 10^{-3}$	$70.3210068 \times 10^{-3}$
D_{JK}	$522.283353 \times 10^{-3}$	$1321.10115 \times 10^{-3}$
D_K	23.344325	19.3908972
d_1	$-1.2084913 \times 10^{-3}$	$-10.4379818 \times 10^{-3}$
d_2	$-0.17734329 \times 10^{-3}$	$-2.50146158 \times 10^{-3}$
H_J	-3.3329×10^{-9}	3.9247×10^{-9}
H_{JK}	1.487734×10^{-6}	7.45331×10^{-6}
H_{KJ}	$-28.222103 \times 10^{-6}$	10.7216×10^{-6}
H_K	5.95849×10^{-3}	4.02125×10^{-3}
h_1	3.085179×10^{-9}	3.23314×10^{-9}
h_2	1.65623×10^{-9}	4.78713×10^{-9}
h_3	0.32731×10^{-9}	1.594631×10^{-9}
L_{JJK}	-	-94.21×10^{-12}
L_{JK}	0.19622×10^{-9}	0.3310×10^{-9}
L_{KKJ}	-20.7881×10^{-9}	-4.5282×10^{-9}
L_K	-2.1726×10^{-6}	-0.5919×10^{-6}
l_1	-0.37662×10^{-12}	-
l_2	-	-0.30793×10^{-12}
l_3	-	-0.42735×10^{-12}
l_4	-	$-0.137543 \times 10^{-12}$

[a] Maeda et al. (2008)

[b] Brünken et al. (2003); the signs of L_{KKJ} and L_K are corrected.

Table 3. Einstein A-coefficients and $\mu^2 S(2I+1)$ for transitions

Transition	A-coeff (s^{-1})	$3\mu^2 S$ (D^2)	Transition	A-coeff (s^{-1})	$3\mu^2 S$ (D^2)
$1_{1,0} \rightarrow 1_{1,1}$	1.814E-11	12.20	$2_{1,2} \rightarrow 1_{1,1}$	2.941E-06	12.20
$2_{1,1} \rightarrow 1_{1,0}$	3.222E-06	12.20	$2_{1,1} \rightarrow 2_{1,2}$	1.632E-10	6.80
$3_{1,3} \rightarrow 2_{1,2}$	1.260E-05	21.80	$3_{3,1} \rightarrow 2_{1,2}$	1.098E-07	0.00
$3_{1,2} \rightarrow 2_{1,1}$	1.381E-05	21.80	$3_{3,0} \rightarrow 2_{1,1}$	1.093E-07	0.00
$3_{1,2} \rightarrow 3_{1,3}$	6.529E-10	4.80	$3_{3,0} \rightarrow 3_{1,3}$	9.588E-08	0.00
$4_{1,4} \rightarrow 3_{1,3}$	3.267E-05	30.60	$4_{3,2} \rightarrow 3_{1,3}$	2.684E-07	0.00
$4_{3,2} \rightarrow 3_{3,1}$	1.596E-05	14.30	$4_{1,3} \rightarrow 3_{1,2}$	3.579E-05	30.60
$4_{1,3} \rightarrow 4_{1,4}$	1.814E-09	3.70	$5_{1,5} \rightarrow 4_{1,4}$	6.681E-05	39.20
$5_{1,4} \rightarrow 4_{1,3}$	7.320E-05	39.20	$5_{1,4} \rightarrow 5_{1,5}$	4.080E-09	3.00
$6_{1,6} \rightarrow 5_{1,5}$	1.187E-04	47.60	$6_{1,5} \rightarrow 5_{1,4}$	1.301E-04	47.60
$6_{1,5} \rightarrow 6_{1,6}$	7.995E-09	2.50	$7_{1,7} \rightarrow 6_{1,6}$	1.920E-04	55.90
$7_{1,6} \rightarrow 6_{1,5}$	2.103E-04	55.90	$7_{1,6} \rightarrow 7_{1,7}$	1.421E-08	2.20
$8_{1,8} \rightarrow 7_{1,7}$	2.903E-04	64.30	$8_{1,7} \rightarrow 7_{1,6}$	3.181E-04	64.30
$8_{1,7} \rightarrow 8_{1,8}$	2.349E-08	1.90	$9_{1,9} \rightarrow 8_{1,8}$	4.173E-04	72.50
$9_{1,8} \rightarrow 8_{1,7}$	4.573E-04	72.50	$9_{1,8} \rightarrow 9_{1,9}$	3.669E-08	1.70
$10_{1,10} \rightarrow 9_{1,9}$	5.767E-04	80.80	$10_{1,9} \rightarrow 9_{1,8}$	6.318E-04	80.80
$10_{1,9} \rightarrow 10_{1,10}$	5.480E-08	1.60	$11_{1,11} \rightarrow 10_{1,10}$	7.720E-04	89.00
$11_{1,10} \rightarrow 10_{1,9}$	8.458E-04	89.00	$11_{1,10} \rightarrow 11_{1,11}$	7.889E-08	1.40

The value of $\mu^2 S(2I+1)$ for the transition $1_{10} - 1_{11}$ is twice of that for the transition $2_{11} - 2_{12}$ (through which the molecule was identified).

Hence, the transition $1_{10} - 1_{11}$ has large probability for its detection.

Collisional rate coefficients

Computation of collisional rate coefficients is quite cumbersome task. However, in absence of them, qualitative investigations can be carried out by choosing some scaling laws for the rate coefficients, which do not favour any anomalous behaviour from their own.

In our investigation for some molecules, scaled values of the rate coefficients for downward transitions $C(J'\tau' \rightarrow J\tau)$ are used

For the upward transitions we have accounted for the fact that the rate coefficients for downward transitions and upward transitions are related through the detailed equilibrium equation

$$C(J_{k_a k_c} \rightarrow J'_{k'_a k'_c}) = C(J'_{k'_a k'_c} \rightarrow J_{k_a k_c}) \frac{2J'+1}{2J+1} \exp\left(-\frac{\Delta E}{kT_K}\right)$$

- Collisional rate coefficient for the rotational transition $J\tau \rightarrow J'\tau'$ at kinetic temperature T, averaged over Maxwellian distribution

$$C(J\tau \rightarrow J'\tau'|T) = \left(\frac{8kT}{\pi\mu}\right)^{1/2}\left(\frac{1}{kT}\right)^{2}\int_{0}^{\infty}\sigma(J\tau \rightarrow J'\tau'|E)\, E e^{-E/kT} dE$$

where cross section $\sigma(J\tau \rightarrow J'\tau'|E)$ for the transition is given by

$$\sigma(J\tau \rightarrow J'\tau'|E) = (2J'+1)\sum_{LMM'} S(J,\tau,J',\tau'|L,M,M')\, q(L,M,M'|E).$$

q(L,M,M'|E) are calculated by MOLSCAT

$$S(J,\tau,J',\tau'|L,M,M') = \sum_{p,p',q,q'} g^{p}_{J\tau} g^{q}_{J\tau} g^{p'}_{J'\tau'} g^{q'}_{J'\tau'} (-1)^{p'+q'} \begin{pmatrix} J & L & J' \\ -p & M & p' \end{pmatrix}\begin{pmatrix} J & L & J' \\ -q & M' & q' \end{pmatrix}.$$

Collisional rates for asymmetric top molecules
S. Chandra and W.H. Kegel, Astron. Astrophys. Suppl. 142, 113-118 (2000)

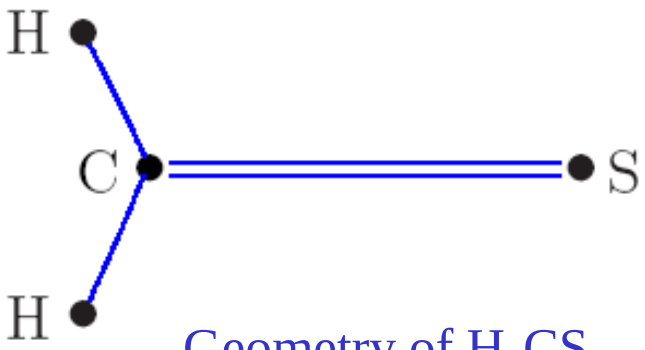
MOLSCAT

- For are now using MOLSCAT, written by S. Green and J.M.Hutson in FORTRAN language.

- It has about 40000 lines

- MOLSCAT works only on Main Frame Computer.

- Optimization of molecule



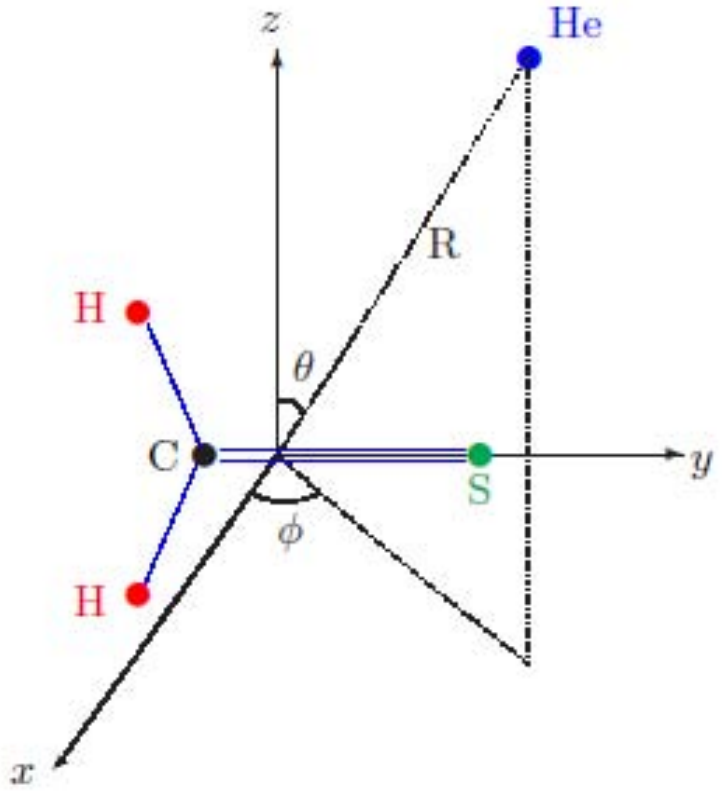
Geometry of H_2CS

Table 2: coordinates of atoms in H_2CS in Å

Atom	*x*	*y*	*z*
S	0.0	0.0	0.585083
C	0.0	0.0	- 1.025413
H	0.0	0.920713	- 1.604425
H	0.0	- 0.920713	- 1.604425

- Potential energy of H_2CS = -437.5138022 eV
- Potential energy of He = -2.9145066 eV

We calculated the interaction potential between the molecule and He using the method B3LYP and basis cc-pVTz.



Interaction potential between the H_2CS and He atom

R	*θ*	*Φ*	Potential
4.5	0	0	-440.379128
4.5	15	30	-440.38251
4.5	45	60	-440.392736
4.5	60	90	-440.4003792
4.5	90	0	-440.4188597
4.5	120	30	-440.4124326
4.5	150	60	-440.209587
4.5	180	90	-440.2214068

- The potential is fitted in terms of the spherical harmonics:

where, $Y_{lm}(\theta, \phi)$ are spherical harmonics.

$$V(R, \theta, \phi) = \sum_{lm} v_{lm}(R) \left[Y_{lm}(\theta, \phi) + (-1)^m Y_{l-m}(\theta, \phi) \right]$$

Table. Values of the coefficients $v_{lm}(R)$ of H_2CS+He

R^a	V_{00}	V_{10}	V_{20}	V_{22}	V_{30}	V_{32}
4.5	33502.66	-22658.55	30857.94	-4342.43	-15087.48	5951.42
5.0	14167.83	-9725.29	12977.89	-1821.00	-6351.28	2378.60
5.5	5725.21	-3992.57	5214.01	-749.38	-2573.22	942.30
6.0	2206.49	-1541.75	1987.89	-294.05	-1000.00	353.87
6.5	812.17	-557.74	715.24	-108.09	-366.59	124.08
7.0	290.73	-187.61	240.23	-35.49	-126.46	39.60
7.5	104.37	-53.23	81.34	-10.15	-37.90	10.81
8.0	36.19	-15.52	22.29	-1.62	-12.92	1.97

R^a	V_{40}	V_{42}	V_{44}	V_{50}	V_{52}	V_{54}
4.5	1587.34	-12251.19	655.87	4115.77	7387.12	-1388.57
5.0	657.45	-4892.31	223.24	1537.61	2825.58	-486.20
5.5	159.10	-1983.44	78.16	657.06	1117.75	-185.03
6.0	5.79	-779.67	23.51	275.63	431.01	-69.31
6.5	-12.08	-292.44	3.69	113.38	159.57	-25.42
7.0	-15.59	-103.21	-3.37	39.98	55.99	-5.25
7.5	-6.94	-32.64	-5.97	14.51	18.04	-2.43
8.0	-3.59	-9.19	-6.83	6.43	4.94	-0.23

[a]Distances in atomic units (1 au = 0.52917706 Å) and energies in units of cm^{-1}.

Collisional rate coefficients

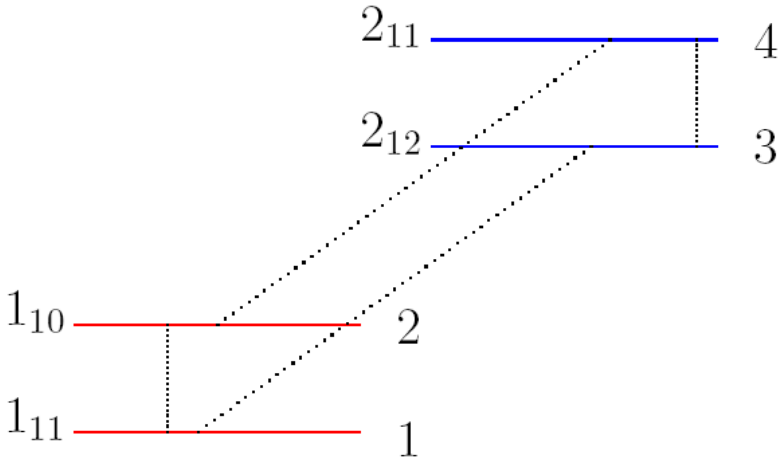
$$C\left(J'_{k'_a k'_c} \rightarrow J_{k_a k_c}\right) = 1x10^{-11}(2J+1)\sqrt{\frac{T_k}{30}}$$

- These are scaled values.
- We want to improve collisional rates.

For anomalous absorption, the excitation temperature T_{ex}, brightness temperature TB and the background temperature T_{bg} satisfy the condition $\mathbf{0 < T_{ex} < T_B < T_{bg}}$. Here, the CMB temperature is 2.73 K.

Let us try to find out the requirement for the anomalous absorption for the transition $1_{11} - 1_{10}$.

For this transition, the levels of the doublet $J = 1$ are radiatively connected to the levels of $J = 2$ doublet only, as shown in the following figure.



The radiatively allowed transitions between the levels are shown by the dotted lines.

In the optically thin limit ($n_{H_2}C_{ul} << A_{ul}$), for these four energy levels, the statistical equilibrium equations may be expressed as the following

$$\frac{n_2}{n_1} = \frac{C_{14}}{C_{23}}$$

For anomalous absorption, we require $n_2 < n_1$, showing that $C_{14} < C_{23}$.

This shows that the transition between the levels 1_{11} and 1_{10} would show absorption against the CMB provided $C_{14} < C_{23}$.

Since our scaled values give $C_{14} = C_{23}$, we have to modify either C_{14}, C_{23} or both of them in order to get anomalous absorption

RESULTS AND DISCUSSION

In the present investigation, we have taken $\gamma = 10^{-6}$ cm^{-3} $(km/s)^{-1}$ pc and 10^{-5} cm^{-3} $(km/s)^{-1}$ pc.

The condition $C_{14} < C_{23}$ can be produced either by increasing the collision rates between the levels 1_{10} and 2_{12} by some positive factor greater than 1 or by reducing the collision rates between the levels 1_{11} and 2_{11} by a positive factor greater than 1 or by doing both.

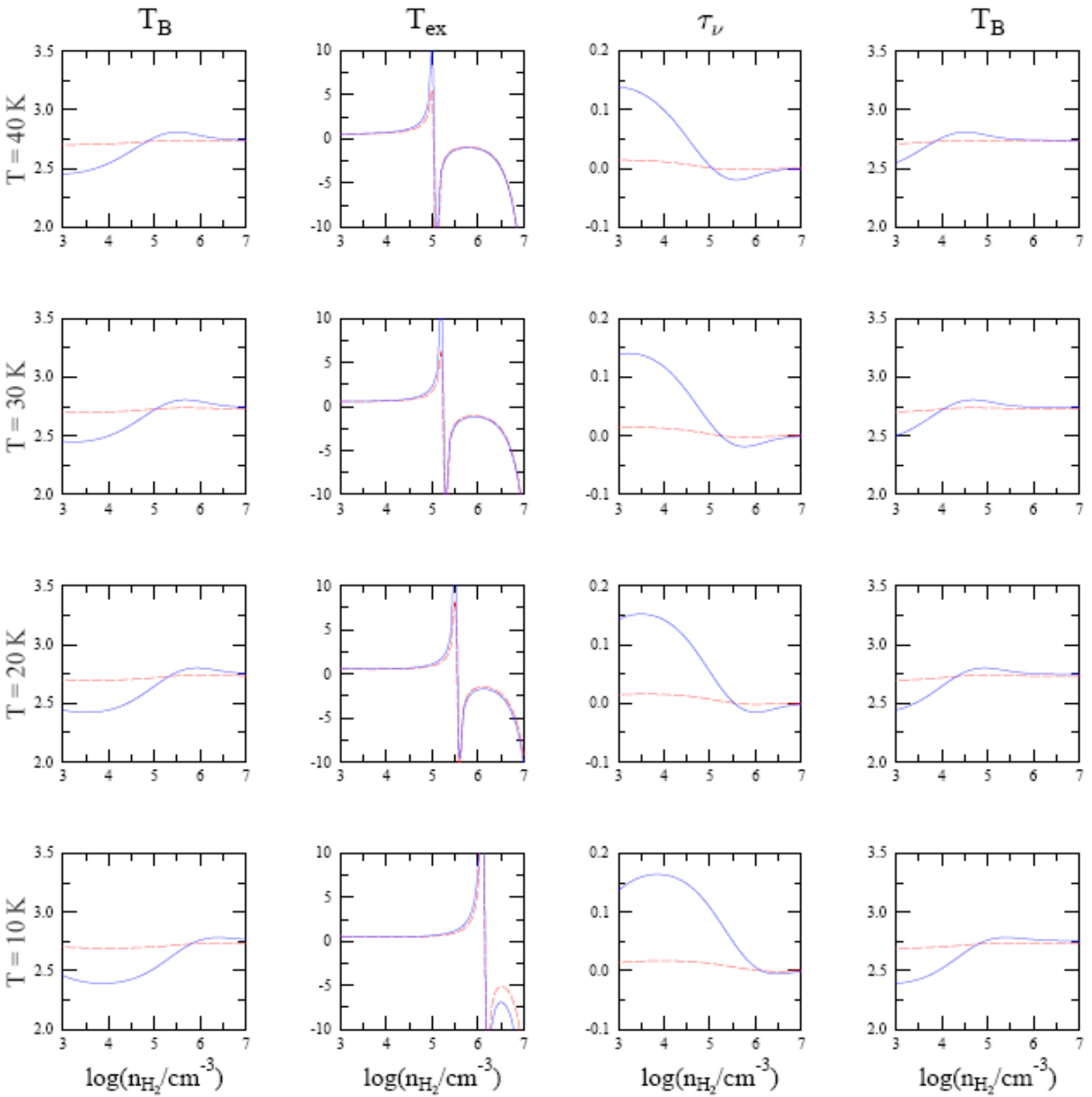


Figure 1: Variation of brightness temperature T_B (K) (column 1), excitation temperature T_{ex} (K) (column 2) and the optical depth τ_ν (column 3) versus hydrogen density n_{H2} for kinetic temperatures of 10 K, 20 K, 30 K and 40 K for transition $1_{10} - 1_{11}$ at 1.0465 GHz of H_2CS. Solid line is for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc, and the dotted line for $\gamma = 10^{-6}$cm^{-3} (km/s)$^{-1}$ pc. For these results, the collisional rates between the levels 1_{10} and 2_{12} are increased by a factor of 2. The brightness temperature T_B (K) (column 4) is when the rates for the transitions with $\Delta k_a = 0$ are enhanced by a factor of 10.

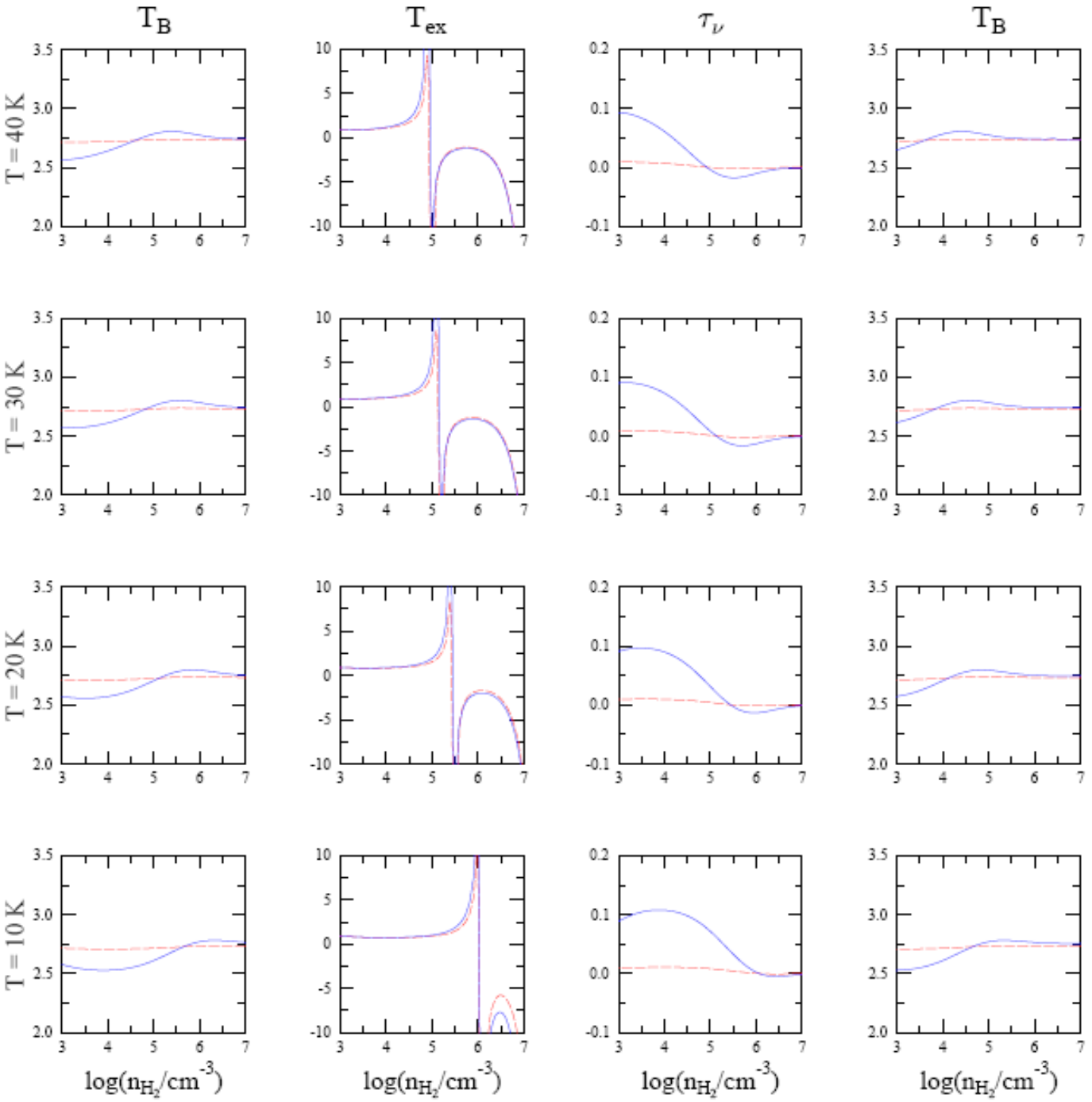


Figure 2: Variation of brightness temperature T_B (K) (column 1), excitation temperature T_{ex} (K) (column 2) and optical depth τ_ν (column 3) versus hydrogen density n_{H2} for kinetic temperatures of 10 K, 20 K, 30 K and 40 K for transition $1_{10} - 1_{11}$ at 1.0465 GHz of H2CS. Solid line is for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc, and the dotted line for $\gamma = 10^{-6}$cm^{-3} (km/s)$^{-1}$pc. For these results, the collisional rates between the levels 1_{11} and 2_{11} are reduced by a factor of 2. The brightness temperature T_B (K) (column 4) is when the rates, for the transitions with $\Delta k_a = 0$ are enhanced by a factor of 10.

CONCLUSIONS

- We found that the 1_{11} - 1_{10} of H_2CS may show anomalous absorption around the density of 10^4 cm^{-3}.

- This transition may help in identification of the molecule in cool cosmic objects, because the kinetic temperature may not be sufficient for generating the emission spectrum.

- But, the anomalous absorption may be observed as the ground state is always populated.

- Since the value of $\mu^2S(2I+1)$ for the transition 1_{10} - 1_{11} is quite large, the transition 1_{10} - 1_{11} has large probability for its detection.

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Anomalous absorption in thioformaldehyde

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ABSTRACT

Absorption against the Cosmic Microwave Background (CMB), called the anomalous absorption, is an unusual phenomenon. The transition 1_{11}–1_{10} at 4.829 GHz of formaldehyde (H_2CO) was the first one showing the anomalous absorption. The c-C_3H_2 is the second molecule showing anomalous absorption through its transition 2_{20}–2_{11} at 21.590 GHz. Structure of thioformaldehyde (H_2CS) is very similar to that of the H_2CO. Therefore, we have investigated about the physical conditions under which the transition 1_{11}–1_{10} at 1.0465 GHz of H_2CS would be found in anomalous absorption in cool cosmic objects. As in case of H_2CO, the anomalous absorption of 1_{11}–1_{10} of H_2CS is found sensitive to the relative collisional rates and it requires that the collisional rate for the transition 1_{11}–2_{11} must be smaller than that for the transition 1_{10}–2_{12}.

Impact factor 1.732

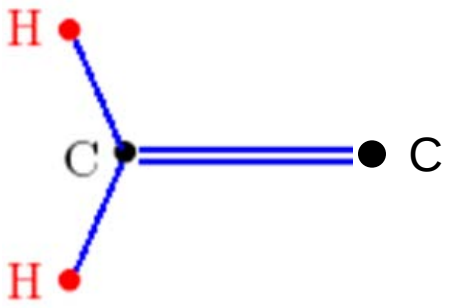
H_2CC

- For the study of H_2CC, we could not find any laboratory information about it.
- In absence of that, the study is nowadays possible with the help of the theoretical laboratories, such as GAUSSIAN, NWCHEM.
- Here, we used the software GAUSSIAN 03 to optimize the geometry of H_2CC.
- We optimized the geometry by using the theory B3LYP/ cc-pVTZ. (Figure 1)
- It is an *a*-type asymmetric top molecule.
- Its electric dipole moment 2.4348 Debye along the axis of the lowest moment of inertia.

Table 2: Optimized coordinates of atoms in H_2CS in Å

Atom	*x*	*y*	*z*
S	0.0	0.0	0.816338
C	0.0	0.0	- 0.474652
H	0.0	0.936624	- 1.025058
H	0.0	- 0.936624	- 1.025058

Figure 1. Structure of H_2CC



• We calculated the interaction potential between the molecule and He using the method B3LYP and basis cc-pVTz.

R	*θ*	*Φ*	Potential
4.5	0	0	-80.1064997
4.5	15	30	-80.1260498
4.5	45	60	-80.1897951
4.5	60	90	-80.2021556
4.5	90	0	-80.2010753
4.5	120	30	-80.1963195
4.5	150	60	-80.1633949
4.5	180	90	-80.1750294

• The potential is fitted in terms of the spherical harmonics:

$$V(R,\theta,\phi) = \sum_{lm} v_{lm}(R)\left[Y_{lm}(\theta,\phi) + (-1)^m Y_{l-m}(\theta,\phi)\right]$$

where, $Y_{lm}(\theta,\phi)$ are spherical harmonics.

R^a	V_{00}	V_{10}	V_{20}	V_{22}	V_{30}	V_{32}
4.5	17093.52	1555.73	12498.92	-1027.11	5465.83	3362.98
5.0	6895.03	983.55	5082.41	-401.98	2265.58	1187.22
5.5	2733.45	567.88	2074.90	-121.84	909.68	417.18
6.0	1037.23	313.72	782.29	-30.69	381.51	140.96
6.5	402.12	149.83	285.99	-2.67	146.30	41.47
7.0	170.41	66.86	100.27	3.79	54.77	9.24
7.5	86.30	29.84	35.83	3.35	17.40	.88
8.0	54.52	14.51	13.79	2.79	7.50	-.70
8.5	38.30	6.49	5.59	3.00	2.12	-1.27
9.0	29.79	4.57	3.54	1.69	.53	-.79
9.5	23.56	4.11	2.36	1.46	1.39	-1.15
10.0	20.00	1.81	.06	1.25	-.08	-1.11

R^a	V_{40}	V_{42}	V_{44}	V_{50}	V_{52}	V_{54}
4.5	2258.02	-1149.35	398.53	2630.55	1321.91	-353.02
5.0	1044.25	-629.00	126.24	1162.38	339.01	-171.03
5.5	457.36	-199.33	42.27	429.43	95.88	-61.25
6.0	184.57	-70.97	13.45	159.78	41.25	-18.44
6.5	77.10	-18.92	1.87	56.18	13.79	-4.97
7.0	32.87	-2.68	-.94	19.98	4.42	-1.23
7.5	13.77	1.68	-1.95	6.58	.97	-.20
8.0	5.59	.89	-1.18	1.95	.70	-.66
8.5	3.13	1.44	-1.69	1.66	-.24	.52
9.0	-1.45	.88	-1.65	-1.35	.28	1.06
9.5	.72	1.00	-1.49	-1.19	.03	.83
10.0	.66	1.01	-1.27	-.50	-.03	.50

[a]Distances in atomic units (1 au = 0.52917706 Å) and energies in units of cm^{-1}.

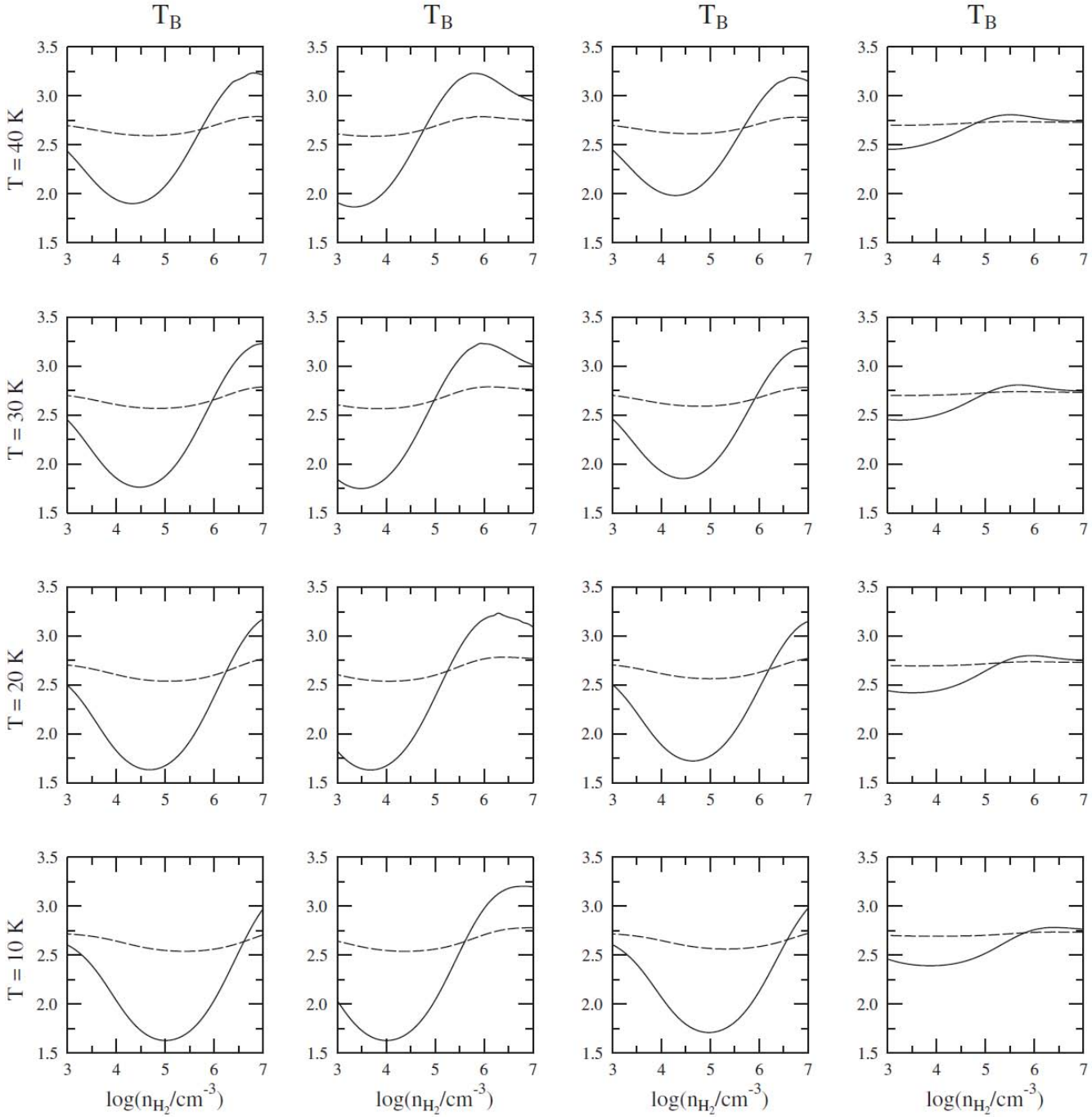


Figure 1: Variation of brightness temperature T_B (K) (column 1), versus hydrogen density n_{H2} for kinetic temperatures of 10 K, 20 K, 30 K and 40 K for transition $1_{10} - 1_{11}$ of H_2CC. Solid line is for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc, and the dotted line for $\gamma = 10^{-6}$cm^{-3} (km/s)$^{-1}$ pc. For these results, the collisional rates between the levels 1_{10} and 2_{12} are increased by a factor of 2. T_B (K) (column 2) is when the rates for the transitions with $\Delta k_a = 0$ are enhanced by a factor of 10. T_B (K) (column 3) of the transition 1_{10} - 1_{11} of H_2CO where rotational and distortional constants of Brünken et al. (2003) are used. T_B (K) (column 4) is for the transition 1_{10} - 1_{11} of H_2CS where the rotational and distortional constants of Maeda et al. (2008) are used.

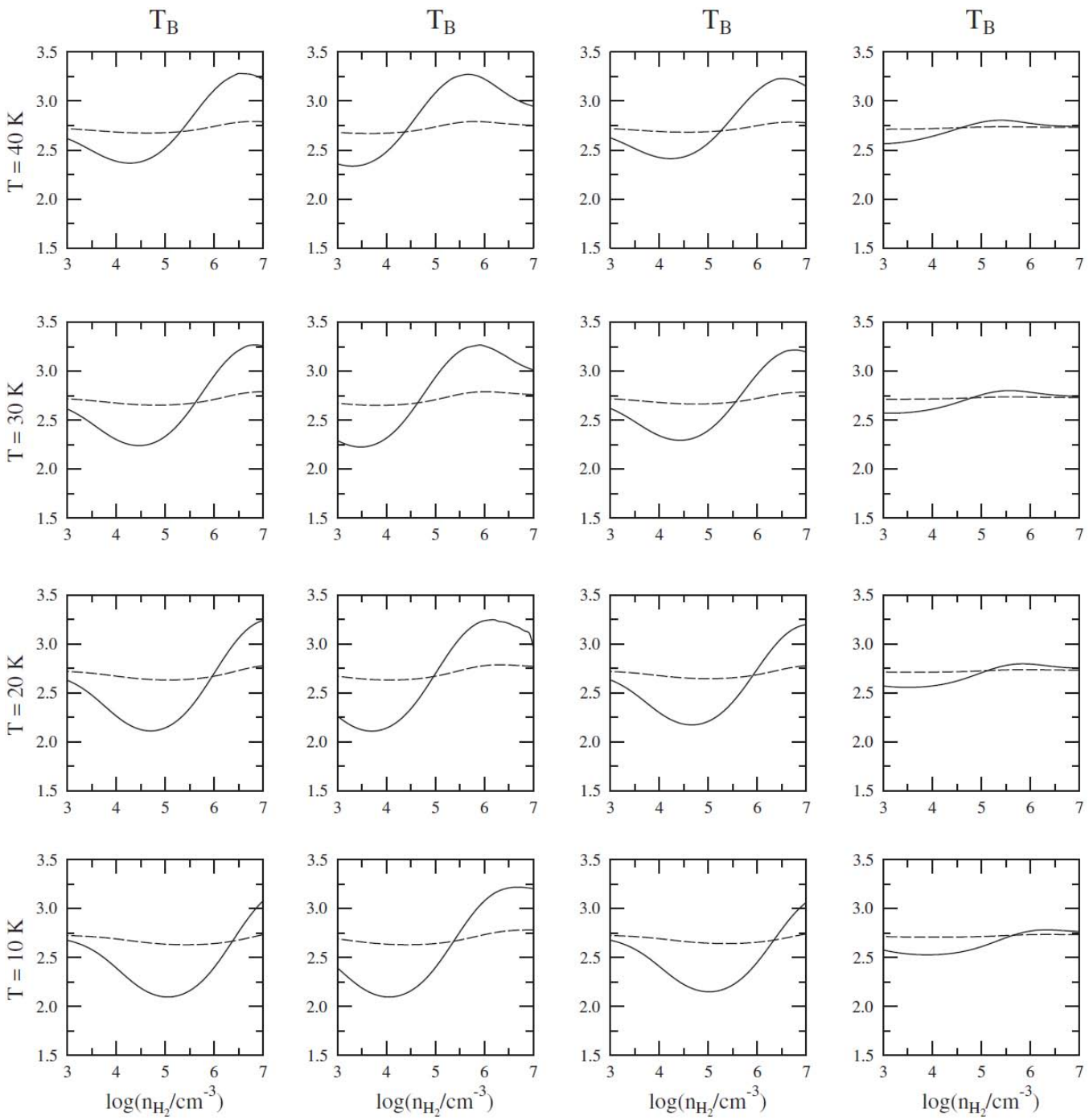


Figure 2: Variation of brightness temperature T_B (K) (column 1) versus hydrogen density n_{H2} for kinetic temperatures of 10 K, 20 K, 30 K and 40 K for transition 1_{10} -1_{11} of H_2CC. Solid line is for $\gamma = 10^{-5}$ cm^{-3} $(km/s)^{-1}$ pc, and the dotted line for $\gamma = 10^{-6} cm^{-3}$ $(km/s)^{-1} pc$. For these results, the collisional rates between the levels 1_{11} and 2_{11} are reduced by a factor of 2. T_B (K) (column 4) is when the rates, for the transitions with $\Delta k_a = 0$ are enhanced by a factor of 10. T_B (K) (column 3) of the transition 1_{10} - 1_{11} of H_2CO where rotational and distortional constants of Brünken et al. (2003) are used. T_B (K) (column 4) is for the transition 1_{10} - 1_{11} of H_2CS where the rotational and distortional constants of Maeda et al. (2008) are used.

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Suggestion for the search of H_2CC in cool cosmic objects

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ABSTRACT

The transition $1_{11} - 1_{10}$ at 4.829 GHz of formaldehyde (H_2CO) was the first one showing the anomalous absorption, *i.e.*, the absorption against the cosmic microwave background. Anomalous absorption is an unusual phenomena. Structure of H_2CC is very similar to that of H_2CO and H_2CS. Both H_2CO and H_2CS have already been identified in a number of cosmic objects. Though H_2CC is not yet identified in the cosmic objects, we propose that H_2CC may be identified in cool cosmic objects through its transition $1_{11} - 1_{10}$ at 4.85 GHz in anomalous absorption.

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Applications

- To identify molecules in cool cosmic objects.
- To find out Physical conditions prevailing in the cosmic objects.
- To get information about chemical reactions going on in the cosmic objects.

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