АСТРОФИЗИКА

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METHANIMINE IN COOL COSMIC OBJECTS USING ACCURATE COLLISIONAL RATE COEFFICIENTS

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Accurate collisional rate coefficients for collisional transitions between 15 rotational levels of methanimine, colliding with p-H_2 molecule, are available. Methanimine is a planar, asymmetric top molecule having electric dipole moment with components $\mu_a = 1.3396$ Debye and $\mu_b = 1.4461$ Debye, and thus, producing both the *a* and *b* type spectral lines of nearly equal intensities. Therefore, all the rotational levels need to be considered together. Between 15 rotational levels, 105 collisional transitions are considered in an investigation by others. We have discussed that each level is not connected with all others through the collisions, and therefore, there should be 77 instead of 105 collisional transitions between 15 levels of methanimine. With availability of accurate collisional rate coefficients, it is worth to perform the Sobolev analysis of methanimine. We have found six weak MASER transitions, 1_{10}-1_{11}, 2_{11}-2_{12}, 3_{12}-3_{13}, $4_{1,3}$-$4_{1,4}$, 3_{03}-2_{12} and $4_{0,4}$-$3_{1,3}$, and one transition 1_{11}-2_{02}, showing anomalous absorption. These seven lines may play important role for the methanimine.

Keywords: *ISM: molecules: methanimine: MASER action and radiative transfer*

1. *Introduction*. Methanimine (CH_2NH) is an important prebiotic molecules, as it is considered as precursor of glycine (NH_2CH_2COOH) [1,2]

$$CH_2NH \xrightarrow{2H} CH_3NH_2 \xrightarrow{CO_2} CH_2NH_2COOH\,.$$

According to Strecker's synthesis [3], the methanimine can be produced through the combination of ammonia (NH_3) [4] and formaldehyde (H_2CO) [5], which are well known abundant species in the interstellar medium (ISM):

$$NH_3 + H_2CO \rightarrow CH_2NH + H_2O\,.$$

Faure et al. [6] have calculated accurate collisional rate coefficients for collisional transitions between 15 rotational levels of methanimine due to collisions with p-H_2 molecule. They [6] have considered 105 collisional transitions between 15 levels, considering that each level is connected to all other levels through collisions. By considering the symmetries, we have discussed that there should be 77 instead of 105 collisional transitions between 15 levels of methanimine.

Gorski et al. [7] have discovered methanimine megamasers toward compact obscured galaxy nuclei at 5.29 GHz through the transition 1_{10}-1_{11}. As the accurate

collisional rate coefficients are available, we have performed the Sobolev analysis of methanimine. Six weak MASER transitions, 1_{10}-1_{11}, 2_{11}-2_{12}, 3_{12}-3_{13}, $4_{1.3}$-$4_{1.4}$, 3_{03}-2_{12} and $4_{0.4}$-$3_{1.3}$, and one transition 1_{11}-2_{02}, showing anomalous absorption have been found. These seven lines may be found significant for the investigation of methanimine.

2. *Methanimine (CH_2NH).* The methanimine is a planar asymmetric top molecule having electric dipole moment with components $\mu_a = 1.3396$ Debye and $\mu_b = 1.4461$ Debye [8]. Thus, it has both *a* and *b* type radiative transitions of nearly equal intensities. Godfrey et al. [9] have reported the first detection of methanimine in gas phase in the molecular cloud Sgr B2 towards the Galactic center. Subsequently, it has been found in Sgr B2 [10-15], in molecular cloud L183 [16], in Orion-KL nebula [17-19], in W51 [17,18], in Ori 3N, G34.3+0.15 [17] in G10.47+0.03, G34.3+0.2, G31.41+0.3, G19.6-0.23, NGC6334F, DR21(OH) [18], in G19.61- 0.23 [20], in IRC+10216 [21], and in ultra-luminous infrared galaxy Arp 220 [22]. Bourgalais et al. [23] have predicted the existence of methanimine in the atmosphere of Titan. The results of Yuen et al. [24] have supported the formation of methanimine in the massive star formation regions.

In the terrestrial laboratories, the methanimine has been analyzed from time to time [25-30]. The rotational and centrifugal distortion constants derived by Motoki et al. [29] are used in the present work for calculation of energies of rotational levels, and radiative transitions probabilities for the radiative transitions between the levels. Sharma et al. [31] have investigated analytically weak MASER action of 1_{10}-1_{11} transition of methanimine. Sil et al. [32] have performed the chemical modeling for prediction of abundances of aldimines and amines in hot cores. Luthra et al. [33] have predicted the gas-phase methanimine abundance in cold cores.

2.1. *Collisional transitions.* The 15 rotational levels considered by Faure et al. [6] and their energies are given in Table 1. The selection rules for the *J* for non-radiative (collisional) transitions are:

$$\Delta J = 0, \pm 1, \pm 2, \pm 3, ...$$

Table 1

LEVELS AND THEIR ENERGIES IN cm^{-1}

No.	Level	Energy	No.	Level	Energy	No.	Level	Energy
1	000	0.00	6	212	11.61	11	404	21.27
2	101	2.13	7	211	12.14	12	414	25.91
3	202	6.40	8	303	12.78	13	413	27.67
4	111	7.52	9	313	17.74	14	221	28.29
5	110	7.69	10	312	18.80	15	220	28.29

Let us consider the collisional transitions only for k_a, k_c levels. Each of the pseudo quantum number, k_a and k_c can independently assume even (e) and odd (o) positive integer values, including zero. When the electric dipole moment is along the *a*-axis of inertia, the following collisional transitions for $k_a k_c$ are not allowed.

$$(e,o) \leftrightarrow (o,e) \qquad (e,e) \leftrightarrow (o,o) \tag{1}$$

$$(e,o) \leftrightarrow (o,o) \qquad (e,e) \leftrightarrow (o,e). \tag{2}$$

These rules divide the rotational levels into the ortho and para species. The allowed collisional transitions are:

$$(o,e) \leftrightarrow (o,o) \qquad (o,o) \leftrightarrow (o,o) \qquad (o,e) \leftrightarrow (o,e) \qquad (\text{Group I}) \tag{3}$$

$$(e,o) \leftrightarrow (e,e) \qquad (e,o) \leftrightarrow (e,o) \qquad (e,e) \leftrightarrow (e,e) \qquad (\text{Group II}) \tag{4}$$

The above can be verified from the papers published for *a*-type molecules. When the electric dipole moment is along the *b*-axis of inertia, the following collisional transitions for k_a, k_c are not allowed.

$$(e,o) \leftrightarrow (e,e) \qquad (o,e) \leftrightarrow (o,o) \tag{5}$$

$$(e,o) \leftrightarrow (o,o) \qquad (o,e) \leftrightarrow (e,e) \tag{6}$$

These rules divide the rotational levels into the ortho and para species. The allowed collisional transitions are:

$$(e,o) \leftrightarrow (o,e) \qquad (e,o) \leftrightarrow (e,o) \qquad (o,e) \leftrightarrow (o,e) \qquad (\text{Group III}) \tag{7}$$

$$(e,e) \leftrightarrow (o,o) \qquad (e,e) \leftrightarrow (e,e) \qquad (o,o) \leftrightarrow (o,o) \qquad (\text{Group IV}). \tag{8}$$

The above can be verified from the papers published for *b*-type molecules.

The present molecule methanimine has both *a* and *b* components of electric dipole moment. Consequently, the transitions (5) are allowed due to *b* component of dipole moment, and the transitions (1) are allowed due to a component of dipole moment. However, still the transitions (6) and transitions (2) are not allowed. These transitions (6 and 2) are the blank positions in Table 3.

Between these 15 levels, there are 35 radiative transitions (Table 2) and 77 collisional transitions (Table 3). In Tables 2 and 3, the first row indicates the upper level and the first column indicates the lower level of transition. Cross indicates transition between levels corresponding to the row and column of the cross. Table 3 obviously indicates that each level is not connected to other levels through collisions.

3. *Details of model.* For 15 levels, we have constituted 15 steady state statistical equilibrium equations, coupled with 35 equations of radiative transfer. The background of the cosmic object generating the lines is taken as the Cosmic Microwave Background (CMB), which corresponds to the background temperature

of 2.73 K. Hence, no spectral line is supposed to have excitation temperature less than 2.73 K. Further, details of the model is discussed by Chandra & Sharma

Table 2

RADIATIVE TRANSITIONS BETWEEN 15 LOWER ROTATIONAL LEVELS OF METHANIMINE. CROSS INDICATES TRANSITION BETWEEN LEVELS CORRESPONDING TO ROW AND COLUMN OF THE CROSS

	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	x		x											
2		x		x	x									x
3			x			x	x	x					x	
4				x	x									x
5						x							x	
6						x	x	x					x	
7									x					x
8									x	x	x			x
9									x	x	x			x
10												x	x	
11												x		
12												x		
13														
14														x

Table 3

COLLISIONAL TRANSITIONS BETWEEN 15 LOWER ROTATIONAL LEVELS OF METHANIMINE. CROSS INDICATES TRANSITION BETWEEN LEVELS CORRESPONDING TO ROW AND COLUMN OF THE CROSS

	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	x	x	x			x	x	x		x		x	x	x
2		x		x	x		x		x	x	x		x	x
3			x			x	x	x		x		x	x	x
4				x	x	x		x	x	x	x	x		x
5					x	x	x	x	x		x	x	x	
6						x	x	x	x		x	x	x	
7								x	x	x	x	x		x
8									x	x	x		x	x
9									x	x	x	x		x
10											x	x	x	
11												x	x	x
12												x	x	
13														x
14														x

[34] and Sharma, Chandra [35,36]. When the excitation temperature of a spectral line is less than 2.73 K, the situation is known as the anomalous absorption, i.e., the absorption against the CMB.

The required input data for the investigation are the radiative transition probabilities (Einstein *A* and *B* coefficients) and the collisional rate coefficients for the collisional transitions.

3.1. *Collisional rate coefficients*. Accurate collisional rate coefficients have been calculated under the CoupledStates (CS) approximation by Faure et al. [6]. Though these collisional rate coefficients are available for the kinetic temperature T up to 30 K, but considering the highest value (28.3 cm^{-1}) of energy, we have used their data for $T = 5,\ 10,\ 15$ K.

4. *Results and discussion*. On solving the set of statistical equilibrium equations coupled with the equations of radiative transfer (Sobolev analysis), we have obtained nonthermal population densities of the levels as a function of the density of colliding partner p-H_2, n_{H_2}, kinetic temperature T, and parameter $\gamma\left[= n_{mol}/\left(d\upsilon_r/dr\right)\right]$, where n_{mol} denotes the density of the methanimine, and $d\upsilon_r/dr$ the velocitygradient in the molecular region. The γ is used as a parameter in the investigation.

To make our results applicable to various types of cosmic objects, in the analysis, we have considered wide ranges of physical parameters. The molecular hydrogen density n_{H_2} is taken from 10^2 to 10^6 cm^{-3}; the kinetic temperatures T are taken 5, 10, 15 K. For γ, we have taken two values as 10^{-5} and 10^{-6} cm^{-3} $(km/s)^{-1}$ pc. However, in Fig.1, we have plotted results for $\gamma = 10^{-5}$ cm^{-3} $(km/s)^{-1}$ pc, as the results for the two sets are very close to each other.

The excitation temperature T_{ex} for a line between an upper level *u* and a lower level *l* is expressed as

$$T_{ex} = -\frac{\Delta E_{ul}}{k \ln\left(n_u g_l / n_l g_u\right)}.$$

where *n* denotes the population density, *g* the statistical weight, *k* the Boltzmann constant, and ΔE_{ul} the energy difference between the two levels.

For low density in a region, the collisional rates are very small as compared to the radiative transition rates, and the population densities of levels are governed by the radiative transitions. Therefore, the excitation temperature tends to the CMB temperature of 2.73 K.

One transition 1_{11}-2_{02} is found to show anomalous absorption i.e., the absorption against the CMB. Information about this transition is given in Table 4, where we have given the frequency, Einstein *A* coefficient, energy of upper level of transition, and radiative life-times of upper and lower levels of the transition. For this

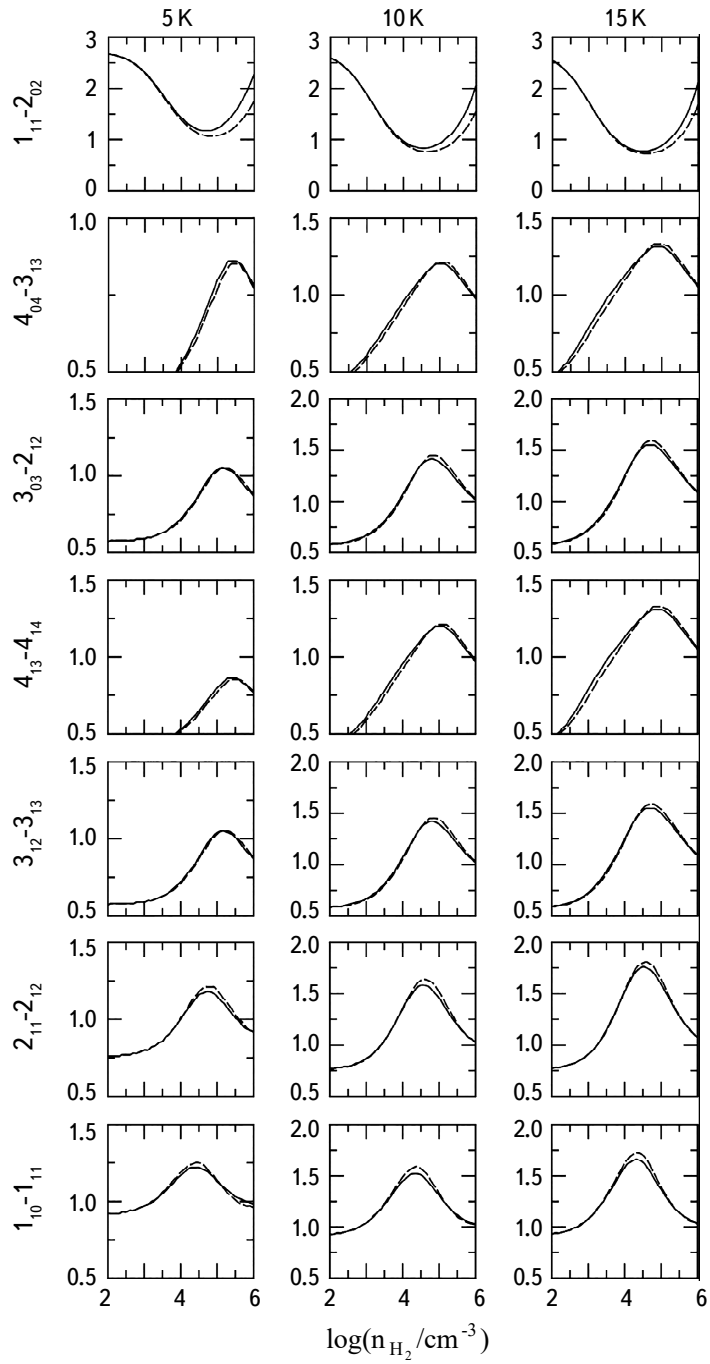

Fig.1 Variation of $n_u g_l / n g_u$ versus molecular hydrogen density n_{H_2} for six transitions 1_{10}-1_{11}, 2_{11}-2_{12}, 3_{12}-3_{13}, $4_{1,3}$-$4_{1,4}$, 3_{03}-2_{12} and $4_{0,4}$-$3_{1,3}$, and variation of excitation temperature T_{ex} (K) versus molecular hydrogen density n_{H_2} for the transition 1_{11}-2_{02}, for kinetic temperatures of 5, 10, 15 K (written at the top) for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc. The solid line is for the present investigation. whereas the dotted line is for the transitions considered by [6].

Table 4

FREQUENCY ν, *A* COEFFICIENT A_{ul}, ENERGY E_u OF UPPER LEVEL, RADIATIVE LIFE-TIME t_u OF UPPER LEVEL AND t_l OF LOWER LEVEL FOR TRANSITIONS OF METHANIMINE

Transition	ν (MHz)	A_{ul} (s^{-1})	E_u (cm^{-1})	t_u (s)	t_l (s)
MASER lines					
$1_{1.0}$-$1_{1.1}$	5290.123	1.546E-09	7.695	1.77E+04	1.07E+04
$2_{1.1}$-$2_{1.2}$	15869.890	1.391E-08	12.137	1.31E+04	5.58E+03
$3_{1.2}$-$3_{1.3}$	31736.418	5.565E-08	18.798	7.56E+03	3.07E+03
$4_{1.3}$-$4_{1.4}$	52880.576	1.546E-07	27.674	4.09E+03	1.81E+03
$3_{0.3}$-$2_{1.2}$	35065.696	1.621E-07	12.777	1.59E+04	5.58E+03
$4_{0.4}$-$3_{1.3}$	105794.062	5.385E-06	21.267	6.31E+03	3.07E+03
Anomalous absorption line					
$1_{1.1}$-$2_{0.2}$	33704.842	1.63E-07	7.52	1.07E+04	5.73E+04

anomalous absorption transition, the variation of excitation temperature T_{ex} (K) versus the molecular hydrogen density n_{H_2} for the kinetic temperatures, written on the top, is shown in Fig.1, uppermost row.

As expected, Fig.1 (uppermost row) shows that with the decrease of density, the excitation temperature tends to the CBM temperature 2.73 K. The trough of the transition is found around $10^{4.5}$ cm^{-3}, which shifts towards the low density with the increase of kinetic temperature, as expected.

For the MASER action, population inversion ($n_u g_l / n_l g_u > 1$) between the upper level *u* and lower level *l* is required.

$$\frac{n_u g_l}{n_l g_u} > 1.$$

Further, the condition of larger radiative life-time of upper level as compared to that of the lower level is a favourable condition. In the present work, we have taken $n_u g_l / n_l g_u > 1.2$. It makes a little hard criteria for the MASER action. Six lines, 1_{10}-1_{11}, 2_{11}-2_{12}, 3_{12}-3_{13}, $4_{1.3}$-$4_{1.4}$, 3_{03}-2_{12} and $4_{0.4}$-$_{31.3}$, have been found to show the weak MASER action. Information about these transitions also is given in Table 4.

For these MASER transitions, the variation of $n_u g_l / n_l g_u$ versus molecular hydrogen density n_{H_2} for kinetic temperatures of 5, 10, 15 K, are given in Fig.1. MASER action is in the region having $n_u g_l / n_l g_u$ larger than 1. The peak of MASER line is found shifted towards the low density region with the increase kinetic temperature, as expected. The MASER action is found to decrease with the decrease of kinetic temperature. At large densities, the population inversion

is destroyed by the collisions.

In their investigation, Faure et al. [6] considered 31 radiative transitions. They did not take four radiative transitions, 2_{20}-1_{01}, 2_{21}-2_{02}, 2_{20}-2_{21} and 2_{20}-3_{03}. Further, they assumed that each level is connected to all other levels through collisions. Thus, they have 105 collisional transitions, whereas in our investigation, there are 77 collisional transitions. The basis of our 77 collisional transitions is the consideration of the symmetries.

We have repeated our calculations for the transitions (31 radiative and 105 collisional) considered by Faure et al. [6] and the results are shown in Fig.1. comparison of the two sets of results shows a very little variation. This very little variation may be assigned to small values of collisional rates as compared to the Einstein *A* coefficients. The contribution of four transitions, 2_{20}-1_{01}, 2_{21}-2_{02}, 2_{20}-2_{21} and 2_{20}-3_{03} is not found significant, as they are connecting the highest two levels whose population densities are very low.

The anomalous absorption transition 1_{11}-2_{02} and weak MASER transition 1_{10}-1_{11} have a common level 1_{11}. The appearance of these two anomalous phenomena (anomalous absorption and weak MASER action) simultaneously may be assigned to a large value $0.931 \cdot 10^{-4}$ s^{-1} of Einstein *A*-coefficient for the transition 1_{11}-0_{00}.

5. *Conclusions*. For 15 rotational levels of methanimine, we have discussed that there should be 77 collisional transitions, instead of 105 taken by Faure et al. [6]. It is also found that Faure et al. [6] have not considered four radiative transitions, 2_{20}-1_{01}, 2_{21}-2_{02}, 2_{20}-2_{21} and 2_{20}-3_{03}. A set of statistical equilibrium equations coupled with the equations of radiative transfer has been solved (Sobolev analysis), for wide ranges of physical parameters. We have found six lines, 1_{10}-1_{11}, 2_{11}-2_{12}, 3_{12}-3_{13}, $4_{1.3}$-$4_{1.4}$, 3_{03}-2_{12} and $4_{0.4}$-31.3, having the weak MASER action and one line, 1_{11}-2_{02} having anomalous absorption. Present results have been found to vary very little when the transitions (radiative and collisional) considered by Faure et al. [6] are taken. It may be because of the relative dominance of radiative transitions over the collisional ones.

The anomalous absorption transition 1_{11}-2_{02} and the weak MASER transition 1_{10}-1_{11}, connecting a common level 1_{11}, may be assigned to the large value $0.931 \cdot 10^{-4}$ s^{-1} of Einstein *A* coefficient of the transition 1_{11}-0_{00}.

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МЕТАНИМИН В ХОЛОДНЫХ КОСМИЧЕСКИХ ОБЪЕКТАХ С ИСПОЛЬЗОВАНИЕМ ТОЧНЫХ КОЭФФИЦИЕНТОВ СКОРОСТИ СТОЛКНОВЕНИЙ

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Представлены точные коэффициенты скорости столкновений для переходов между 15 вращательными уровнями метанимина, сталкивающегося с молекулой p-H_2. Метанимин представляет собой плоскую асимметричную молекулу с электрическим дипольным моментом, имеющим компоненты $\mu_a = 1.3396$ Дебая и $\mu_b = 1.4461$ Дебая. Это приводит к образованию спектральных линий типа *a* и *b* с почти одинаковой интенсивностью. Следовательно, все вращательные уровни необходимо рассматривать вместе. В исследованиях других авторов первоначально рассматривались в общей сложности 105 переходов между 15 уровнями метанимина. В данной работе учитывалось, что не каждый уровень связан со всеми другими посредством столкновений, и, следовательно, должно быть 77 вместо 105 переходов между 15 уровнями метанимина. При наличии точных коэффициентов скорости столкновений важно выполнить анализ Соболева для метанимина. В ходе анализа были идентифицированы шесть слабых мазерных переходов: 1_{10}-1_{11}, 2_{11}-2_{12}, 3_{12}-3_{13} $4_{1.3}$-$4_{1.4}$, 3_{03}-2_{12} и $4_{0.4}$-$3_{1.3}$, а также один переход 1_{11}-2_{02}, демонстрирующий аномальное поглощение. Эти семь линий могут играть важную роль в поведении метанимина.

Ключевые слова: *МЗС: молекулы: метанимин: мазеры: перенос излучения*

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