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TRANSITION 2_{12}-3_{03} MAY HELP FOR DETECTION OF METHYLENE IN A COOL COSMIC OBJECT

M.K.SHARMA[1], S.CHANDRA[2]

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Methylene is an important astrochemical compound. Though its laboratory spectrum was analyzed in 1982, its first unambiguous detection could be feasible after more than one decade in the hot core of Orion-KL nebula and the approximate molecular cloud of the continuum source W51M through its emission line 4_{04}-3_{13}. Since then waiting of its further detection has now broken as it has been detected in W51 E, W51 M, W51 N, W49 N, W43, W75 N, DR21, and S140 star forming regions, and in W3 IRS5 through the same transition 4_{04}-3_{13}. To find potential lines of methylene, we have performed Sobolev LVG analysis of each of the ortho and para species of methylene, considering 10 rotational levels having energy up to 324 cm^{-1}. We have found only three lines, 4_{04}-3_{13}, 5_{05}-4_{14} and 2_{12}-3_{03} of methylene, which may help for its detection in a cosmic object. The line 2_{12}-3_{03} lying at the lowest energy may be more helpful in a cosmic object having low kinetic temperature.

Keywords: *ISM: molecules: methylene: Sobolev LVG analysis: radiative transition*

1. *Introduction*. Methylene radical CH_2 is one of the lightest polyatomic molecules found in interstellar medium. It has great importance both in chemistry and in spectroscopy. In the spectroscopy, it is the simplest neutral polyatomic molecule with a triplet electronic ground state (its electronic ground state is $X\ ^3B_1$). In the chemistry, it is the prototypical carbene. Methylene has considerable astrophysical importance also, as it is both produced and destroyed at an early stage in the sequence of the ion-molecule reactions, which govern the interstellar chemistry (e.g., Godard et al. [1] and references therein). Further, CH_2 has been speculated to play important role in the photo-dissociation sequence of methane (CH_4) in the cometary ice mantles [2].

Formation of methylene in the interstellar medium (ISM) has been proposed through the dissociative recombination [3-5]:

$$CH_3^+ + e \rightarrow \begin{cases} CH_2 + H \\ CH + 2H\,. \end{cases} \qquad (1)$$

The dissociative recombination reaction has been studied by Vejby-Christensen [6] and is shown to produce methylene as dominant product. The destruction of methylene occurs mainly via reaction with O atoms except in poorly shielded regions. Therefore, predictions of the abundance of methylene in the diffuse clouds

as well as in the dense clouds should be reasonably reliable, and the observed abundances should be a strong test of ion-molecule models.

Some authors, for example, references cited by Boland [7], have discussed for the formation of CH2 as the following:

$$CH_3 + \text{photon} \rightarrow CH_2 + H \quad (2)$$

$$CH_4 + \text{photon} \rightarrow CH_2 + H_2 \quad (3)$$

For both the dense and diffuse interstellar clouds, in the gas-phase chemical models, the methylene plays key role, where it is produced early in the sequence of ion-molecule reactions through the processes such as [8]

$$C + H_3^+ \rightarrow CH^+ + H_2 \quad (4)$$

$$CH^+ + H_2 \rightarrow CH_2^+ + H \quad (5)$$

$$C^+ + H_2 \rightarrow CH_2^+ + h\nu \quad (6)$$

$$CH_2^+ + H \rightarrow CH_3^+ + H \quad (7)$$

$$CH_3^+ + e^- \rightarrow CH_2^+ + H \quad (8)$$

It is found that a high formation rate of CH_2 is unavoidable. Further reactions of these molecules with atomic oxygen produce more complex molecules in the ISM.

Despite its importance and large predicted abundances, methylene is not yet detected in comets and only few detections have been made in the ISM.

Considering the importance of methylene, scientists have analyzed its laboratory spectrum from time to time [9-13]. Rotational and centrifugal distortion constants derived by Michael et al. [12] in the A-reduced Watson Hamiltonian with I^r representation have been used in the present analysis. Methylene has small electric dipole moment 0.57 Debye [14] along the *b*-axis of inertia.

Though its laboratory spectrum was analyzed by Sears et al. [9] in 1982, but for more than one decade its unambiguous detection was not there and its first detection was given by Hollis et al. [15] through its emission line 4_{04}-3_{13} generated in the hot core of Orion-KL nebula and the approximate molecular cloud of the continuum source W51M. After that it remained elusive and now has been detected by Jacob et al. [16] through the same transition 4_{04}-3_{13} in W51 E, W51 M, W51 N, W49 N, W43, W75 N, DR21, and S140 star forming regions, and in W3 IRS5. However, Polehampton et al. [17] have detected methylene in far-infrared through the hyperfine transitions, 1_{11}-0_{00} $J = 1 - 1$ 127.85823 μm and 1_{11}-0_{00} $J = 2 - 1$ 127.64614 μm. No other lines of methylene have been detected in any cosmic object. Lyu et al. [18] have reported search of CH_2 toward HD 154368 and ζ Ophiuchi in the UV molecular bands.

Using rotational and centrifugal distortion constants, and energies of rotational levels, we have calculated Einstein *A*-coefficients for radiative transitions between the levels. The radiative transition probabilities along with the scaled values of collisional rate coefficients, we have performed the Sobolev LVG analysis of both species, separately and have found only 3 potential lines: two MASER lines, 4_{04}-3_{13} and 5_{05}-4_{14}, and one anomalous absorption line 2_{12}-3_{03}. These lines may help in the detection of methylene in a cosmic object. Line 2_{12}-3_{03} lying at the lowest energy may be more helpful in a cosmic object having low kinetic temperature.

2. *Rotational levels*. Planar molecule CH_2 has para and ortho species because of two equivalent hydrogen atoms. These species are independent of each other, as there are no transitions (radiative as well as collisional) between them. Sears et al. [9] have reported energies of fine-structure components of rotational levels (their Table VIII). Energies of 10 rotational levels for each species (Table 1) have been taken from Chandra [19], which have been derived from the data given by Sears et al. [9]. The same energies have been used by Jacob et al. [16] in their Fig.1.

Table 1

ENERGIES (cm^{-1}) OF ROTATIONAL LEVELS

Level	Energy	Level	Energy
1_{01}	15.5319	0_{00}	0.0000
1_{10}	79.5749	2_{02}	46.8528
3_{03}	93.6629	1_{11}	78.3634
2_{12}	108.4476	2_{11}	112.0324
3_{12}	160.7819	3_{13}	153.6331
4_{14}	213.8307	4_{04}	155.9426
5_{05}	233.6137	4_{13}	225.7113
2_{21}	276.3092	2_{20}	276.3279
5_{14}	306.7614	5_{15}	289.0015
3_{21}	323.5423	3_{22}	323.4496

3. *Radiative transitions*. For the electric dipole moment lying along the b-axis of inertia, the radiative transitions are governed by the following selection rules, given for an asymmetric top molecule:

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

$$K_a, K_c: \quad \text{even, even} \leftrightarrow \text{odd, odd} \quad \text{ortho transition}$$

$$\text{even, odd} \leftrightarrow \text{odd, even} \quad \text{para transition}.$$

For an ortho level, the $(K_a + K_c)$ is an even integer, whereas for a para level, the $(K_a + K_c)$ is an odd integer. It may be noted that the "ortho" and "para" designations are opposite to the standard *b*-type case because of the unusual electronic symmetry

of the state, which is antisymmetric to the exchange of protons.

For the para CH_2, the energy level diagram for 10 rotational levels is given in Fig.1, where the transitions 5_{05}-4_{14} and 2_{12}-3_{03} are shown. Between these 10 rotational levels, there are 13 radiative transitions (Table 2). For the ortho CH_2,

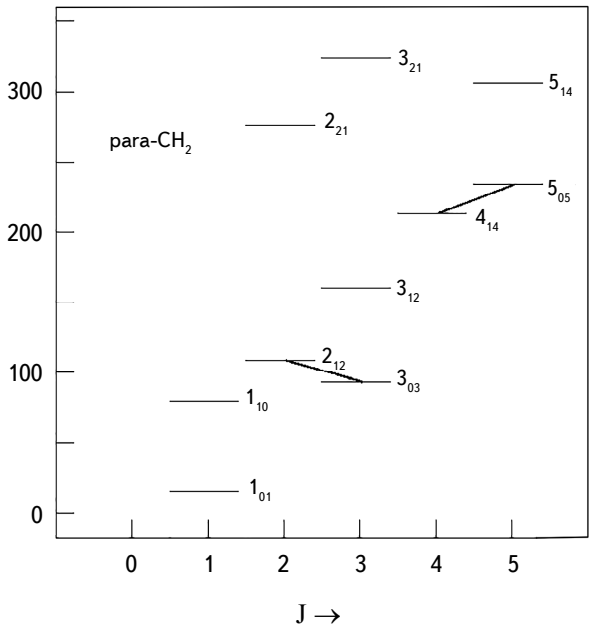

Fig.1. Energy level diagram of 10 para levels of CH_2, where the transitions 5_{05}-4_{14}, and 2_{12}-3_{03}, are shown.

the energy level diagram for 10 rotational levels is given in Fig.2, where the transition 4_{04}-3_{13}, is shown. Between these 10 rotational levels, there also are 13 radiative transitions (Table 2).

We have interest in the rotational transitions of CH_2, as the observations in cosmic objects have been made for the rotational transitions [15,16] only. However, the rotational levels have fine and hyperfine splittings. Information about such splitting for the transitions 2_{12}-3_{03} and 4_{04}-3_{13} may be found in Table 1 of Jacob et al. [16]. The radiative transition probabilities for the rotational transitions in the methylene are not available in literature. Dagdigian & Lique [20] have given Einstein A-coefficients for the transitions between some fine-structure levels of CH_2. For the rotational transitions, using the rotational and centrifugal distortion constants of Michael et al. [12], we have calculated line strengths for the radiative transitions between the levels using the software ASROT [22]. The line-strength $S_{ul}(=S_{lu})$ is related to the Einstein A-coefficient, A_{ul}, through the relation

$$A_{ul} = \frac{64\pi^4 \nu^3 \mu^2}{3 g_u h c^3} S_{ul} \qquad (9)$$

Table 2

EINSTEIN *A*-COEFFICIENTS (s^{-1}) FOR TRANSITIONS

Transition	*A*-coefficient	Transition	*A*-coefficient
1_{10}-1_{01}	1.338E-02	1_{11}-0_{00}	1.635E-02
2_{12}-1_{01}	2.452E-02	1_{11}-2_{02}	5.460E-04
2_{21}-1_{10}	2.328E-01	2_{20}-1_{11}	2.350E-01
2_{21}-2_{12}	8.030E-02	2_{11}-2_{02}	1.398E-02
2_{21}-3_{12}	5.421E-03	2_{20}-2_{11}	7.740E-02
2_{12}-3_{03}	6.887E-05	3_{13}-2_{02}	3.560E-02
3_{21}-2_{12}	2.348E-01	2_{20}-3_{13}	6.145E-03
3_{12}-3_{03}	1.505E-02	3_{22}-2_{11}	2.292E-01
3_{21}-3_{12}	9.597E-02	3_{22}-3_{13}	1.032E-01
4_{14}-3_{03}	4.979E-02	3_{22}-4_{13}	5.348E-03
3_{21}-4_{14}	6.892E-03	4_{04}-3_{13}	2.235E-07
5_{05}-4_{14}	1.570E-04	4_{13}-4_{04}	1.659E-02
5_{14}-5_{05}	1.867E-02	5_{15}-4_{04}	6.725E-02

where g_u $(= 2J_u + 1)$ denotes the statistical weight of upper level with rotational quantum number J_u, μ is the electric dipole moment and ν the frequency of transition. There are well known relations between the Einstein *A* and *B*

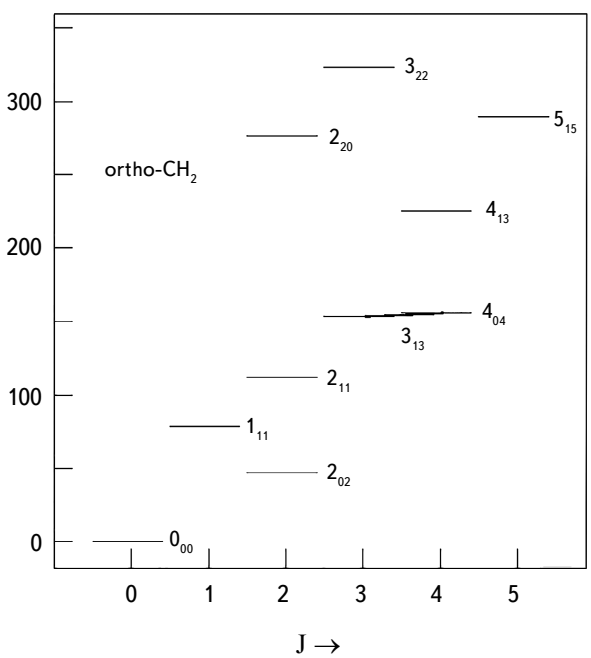

Fig.2. Energy level diagram of 10 ortho levels of CH_2, where the transition 4_{04}-3_{13} is shown.

coefficients:

$$A_{ul} = \frac{2h\nu_{ul}^3}{c^2} B_{ul} \quad \text{and} \quad B_{ul} = \frac{g_l}{g_u} B_{lu} \tag{10}$$

where g_l denotes the statistical weight of the lower level.

4. *Collisional transitions and model.* Besides the radiative transitions, rotational levels are connected through the collisional transitions as well. Though the rate coefficients for collisional transitions due to collisions with He atom have been reported by Dagdigian & Lique [20], and due to collisions with hydrogen molecule have been reported by Dagdigian [21], but the required data for rotational transitions are not available, as we have interest in the rotational transitions, without any fine or hyperfine structure splittings. Here, we have calculated the deexcitation rate coefficients with the help of the following expression for a kinetic temperature T [23,24]:

$$C\left(J'_{k'_a,k'_c} \to J_{k_a,k_c}\right) = \frac{1\cdot 10^{-11}}{2J'+1}\sqrt{T}\,. \tag{11}$$

This expression can be considered as the cross-section times the relative velocity between the species of CH_2 and H_2 molecule, which is the most abundant in a molecular region. The collisional rate coefficients for excitation have been calculated using the detailed equilibrium. These collisional rate coefficients do not produce any kind of anomalous phenomenon from their own. The LVG analysis is carried out in accordance with the procedure used by Sharma [25-27]. The only external radiation field, impinging on a volume element producing radiation lines, is the Cosmic Microwave Background (CMB) with the background temperature $T_{bg} = 2.73$ K.

5. *Results and discussion.* For each species of CH_2, Sobolev LVG analysis is carried out by using the values of radiative transition probabilities and the collisional rate coefficients (obtained from the scaling law) through iterative procedure, where the initial population densities are taken as the thermal values, corresponding to the kinetic temperature T in the region. In order to include different kinds of cosmic objects, where methylene radical may be found, the calculations are performed for 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 10, 20, 50, 100 and 150 K, values of γ are taken as 10^{-6} and 10^{-5} cm^{-3} (km/s)$^{-1}$ pc. The parameter γ, is expressed as $\gamma = n_{mol}/\left(d\,v_r/dr\right)$, where n_{mol} is the density of the species of CH_2 and $(d\,v_r/dr)$ the velocity-gradient in the region. Thus, the γ depends on the column density of the species of CH_2. Here, γ is used as a parameter.

Using Einstein A-coefficients, we have calculated radiative life-time of rotational levels. In general, the radiative life-time of upper level is smaller than that

of the lower level. But for MASER transitions, the reverse is found. Larger life-time of upper level is not sufficient for a MASER action. For a MASER action, population inversion ($n_u g_l / n_l g_u > 1$) between the upper level u and lower level l is also required. Here, n denotes the population density of level, and g denotes the statistical weight. For a radiative transition to be a weak MASER, we have considered two criteria:

1. Radiative life-time of upper level is larger than that of the lower level.
2. There is population inversion between the levels of transition.

Out of 26 spectral lines, two lines, 4_{04}-3_{13}, 5_{05}-4_{14} have been found to have MASER action. Information about these transitions is given in Table 3, where we have given frequency and Einstein A-coefficient of transition, energy of upper level, life-times of upper and lower levels. For these transitions, variation of $n_u g_l / n_l g_u$ versus molecular hydrogen density n_{H_2} is shown in Fig.3, for kinetic temperatures T of 10, 20, 50, 100 and 150 K, written on the top, for the transitions, written on the left.

Table 3

FREQUENCY ν, EINSTEIN A-COEFFICIENT A_{ul}, ENERGY E_u OF UPPER LEVEL, RADIATIVE LIFE-TIME t_u OF UPPER LEVEL AND t_l OF LOWER LEVEL OF TRANSIOTIONS

Transition	ν (MHz)	A_{ul} (s^{-1})	E_u (cm^{-1})	t_u (s)	t_l (s)
$5_{0.5}$-$4_{1.4}$	593079.420	1.570E-04	233.614	6.37E+03	2.01E+01
$4_{0.4}$-$3_{1.3}$	69237.070	2.235E-07	155.943	4.47E+06	2.81E+01
$2_{1.2}$-$3_{0.3}$	443234.160	6.887E-05	108.448	4.07E+01	∞

At low densities, for a transition, brightness temperature and excitation temperature both tend to the CMB temperature of 2.73 K, whereas at high densities, both brightness temperature and excitation temperature tend to the kinetic temperature in the region (thermalization). Meaning that brightness temperature and excitation temperature of an spectral line should not be less than the CMB temperature of 2.73 K. But, one transition 2_{12}-3_{03} has been found to show the excitation temperature less than 2.73 K (anomalous absorption). Information about this transition also is given in Table 3 and variation of excitation temperature versus molecular hydrogen density n_{H_2} is shown in Fig.3, for kinetic temperatures T of 10, 20, 50, 100 and 150 K, written on the top. These 3 lines may play vital role for detection of CH_2 in a cosmic object.

As the kinetic temperature in a molecular region is low (highest value of 150 K is considered here) and the transition 5_{05}-4_{14} lies at high energy (234 cm^{-1}), therefore, the probability of the detection of this transition is not high. It may

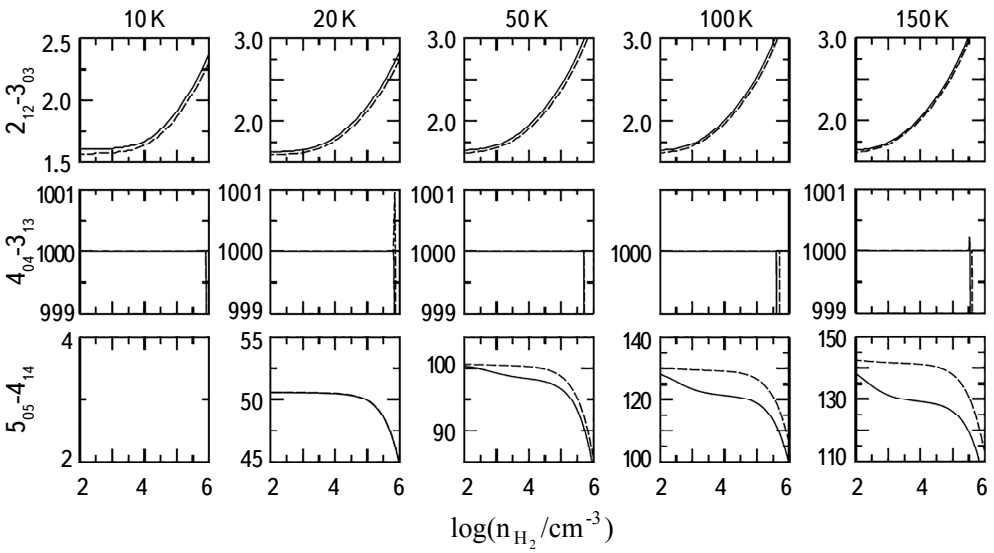

Fig.3. Variation of $n_u g_l / n_l g_u$ versus molecular hydrogen density n_{H_2} for two transitions, 5_{05}-4_{14}, and 4_{04}-3_{13}, and the variation of the excitation temperature Tex versus molecular hydrogen density n_{H_2} for one transition 2_{12}-3_{03}. The plots are for the kinetic temperatures T of 10, 20, 50, 100 and 150 K, written on the top. Solid line corresponds to $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc, whereas the dotted line to $\gamma = 10^{-6}$ cm^{-3} (km/s)$^{-1}$ pc.

be noted that in Fig.3, the slide for 10 K for this transition 5_{05}-4_{14} is empty. Lovas et al. [10] have discussed that the energies (155 cm^{-1}) of the levels of 4_{04}-3_{13} transition are rather high for thermal excitation in most of the known molecular clouds, and therefore its detection of this transition would be hampered. The transition 2_{12}-3_{03} at 108 cm^{-1} shows strong anomalous absorption whose strength increases with the decrease of kinetic temperature. The anomalous absorption is quite significant even at 10 K kinetic temperature. The radiative life-time of lower level 3_{03} is infinite, as there is no radiative transition from this level in the downward direction. Further, the level 3_{03} is populated through the radiative transitions 3_{12}-3_{03} and 4_{14}-3_{03}, having large Einstein A-coefficients, $1.505 \cdot 10^{-2}$ s^{-1} and $4.979 \cdot 10^{-2}$ s^{-1}, respectively. It shows that the the population of the level 3_{03} gets quite large as compared to that of the level 2_{12}, leading to the anomalous absorption. The levels 3_{12} and 4_{14} are lower compared to the levels 2_{21} and 3_{21}, which populate the upper level 2_{12}. With the increase of density, the absorption-strength of the transition 2_{12}-3_{03} decreases, as the collisional rate for depopulation of the levels 3_{03} increases. As expected, with the increase of kinetic temperature, the turning in the graphs shifts towards the low density region. This line may be given preference for detection of methylene in a cosmic object having low kinetic temperature. This transition has been suggested by Lovas et al. [10] as well for the detection of CH_2.

We have to state that the present work has been done without any knowledge of the work of Dagdigian [21]. In our work, the anomalous absorption of the transition 2_{12}-3_{03} is found to increase, in particular at high density, with the decrease of kinetic temperature. Dagdigian [21] also obtained weak MASER action of 4_{04}-3_{13} transition and anomalous absorption of 2_{12}-3_{03} transition. There is no mention about the 5_{05}-4_{14} transition.

6. *Conclusions*. Using rotational and centrifugal distortion constants for CH_2, we have calculated line strengths for 13 radiative transitions between 10 rotational levels of each species of CH_2. These line strengths along with the known energies of rotational levels, the radiative transition probabilities (Einstein *A* and *B* coefficients) have been calculated. These radiative transition probabilities in conjunction with the collisional rate coefficients (obtained from scaling law) have been used in the Sobolev LVG analysis. From the analysis, we have found three lines, 4_{04}-3_{13}, 5_{05}-4_{14} and 2_{12}-3_{03} of methylene, which may play important role for its detection. However, the lowest lying line 2_{12}-3_{03} may be given preference in a cosmic object having low kinetic temperature.

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[1] Physics Department, Sunder Deep Group of Institutions, NH-24, Delhi-Hapur Road, Dasna 201001, India, e-mail: mohitkumarsharma32@yahoo.in
[2] Amity Centre for Astronomy & Astrophysics, Amity Institute of Applied Sciences, Amity University, Sector 125, Noida 201313, U.P., India
e-mail: schandra2@amity.edu suresh492000@yahoo.co.in

ВАЖНОСТЬ ПЕРЕХОДА 2_{12}-3_{03} ДЛЯ ОБНАРУЖЕНИЯ МЕТИЛЕНА В ХОЛОДНЫХ КОСМИЧЕСКИХ ОБЪЕКТАХ

М.К.ШАРМА[1], С.ЧАНДРА[2]

Метилен - важное астрохимическое соединение. Хотя его лабораторный спектр был проанализирован в 1982г., он впервые был достоверно обнаружен через более чем одно десятилетие в горячем ядре туманности Орион-KL и близком молекулярном облаке источника непрерывного излучения W51M

через его эмиссионную линию 4_{04}-3_{13}. С тех пор переход 4_{04}-3_{13} был обнаружен в областях звездообразования W51 E, W51 M, W51 N, W49 N, W43, W75 N, DR21 и S140, а также в W3 IRS5. Чтобы найти потенциальные линии метилена, мы провели анализ LVG по Соболеву для каждого из орто- и пара-видов метилена, рассматривая 10 вращательных уровней с энергией до 324 $см^{-1}$. Мы нашли только три линии, 4_{04}-3_{13}, 5_{05}-4_{14} и 2_{12}-3_{03} метилена, которые могут помочь в его обнаружении в космических объектах. Линия 2_{12}-3_{03}, лежащая на самом низком энергетическом уровне, может быть более полезной в случае космических объектов, имеющих низкую кинетическую температуру.

Ключевые слова: *межзвездная среда:молекулы:метилен:анализ LVG Соболева: радиационный переход*

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