New Astronomy 48 (2016) 1–4

Contents lists available at ScienceDirect

New Astronomy

journal homepage: www.elsevier.com/locate/newast

Very low probability of detection of TiH_2 molecule in a cosmic object

M.K. Sharma[a], M. Sharma[a], S. Chandra[b,c,*]

[a] School of Studies in Physics, Jiwaji University, Gwalior 474011, India
[b] Department of Physics, Lovely Professional University, Phagwara 144411, India
[c] Zentrum für Astronomie und Astrophysik, Technische Universität Berlin, Hardenbergstrasse 36, D-10623 Berlin, Germany

HIGHLIGHTS

- Energies of rotational levels of TiH_2 are calculated.
- Einstein *A*-coefficients for transitions between the levels in TiH_2 are calculated.
- For normal densities up to $10^{4.5}$ cm^{-3}, no transitions are found to show significant brightness temperature.

ARTICLE INFO

Article history:
Received 1 August 2015
Revised 7 March 2016
Accepted 19 March 2016
Available online 6 April 2016

Keywords:
ISM: Molecules
TiH_2
Einstein *A*-coefficients
Radiative transfer

ABSTRACT

In the year 1979, identification of TiH and TiO in the atmosphere of cool M-type stars has been historical, as the Titanium was first time discovered in a cosmic object. Third Titanium-bearing molecule, TiO_2, also is identified in the red supergiant VY CMa. Thus, there is a natural question about the detection of TiH_2 molecule, as the cosmic abundance of hydrogen is approximately 2000 times larger than that of the oxygen. The large abundance of H as compared to O may not suffice as, for example, the probability of formation of CO is much larger than that of CH. Without going into the details of Chemistry, we have discussed that the probability of detection of TiH_2 in a cosmic object is very low, though it has a large electric dipole moment.

1. Introduction

Identification of TiH (Yerle, 1979) and TiO (Clegg et al., 1979) in the atmosphere of cool M-type stars has been historical, as the Titanium was first time discovered in a cosmic object. Tentative detection of TiO_2 in the atmosphere of red supergiant VY CMa was reported by Brünken et al. (2008). Presence of TiO_2 in the environment of the red supergiant VY CMa is confirmed by Kaminski et al. (2013a, 2013b) and De Beck et al. (2015). There is a natural question about the detection of TiH_2, as the cosmic abundance of hydrogen is approximately 2000 times larger than that of the oxygen.

The large abundance of H as compared to O may not suffice as, for example, the probability of formation of CO is much larger than that of CH. Without falling into the trap of Chemistry, we have solved a set of statistical equilibrium equations coupled with the equations of radiative transfer, and have found that the probability of detection of TiH_2 in a cosmic object is very low, though it has large electric dipole moment $\mu = 2.792$ Debye.

2. Molecular and computational details

For understanding how a spectrum forms in a cosmic object, one considers an appropriate number of energy levels of the molecule of interest. These levels are connected through radiative and collisional transitions. For getting information about the energies of levels and the radiative transition probabilities (Einstein *A*-coefficients) among the levels, one requires the rotational and centrifugal distortion constants, and the electric dipole moment of the molecule. To the best of our knowledge, no information about the spectroscopic study of TiH_2 is available in the literature or in the following databases:

http://home.strw.leidenuniv.nl/~moldata
http://www.astro.uni-koeln.de/cdms/catalog#description
http://spec.jpl.nasa.gov/ftp/pub/catalog/catdir.html
http://basecol.obspm.fr

Under such circumstances, the theoretical laboratories, such as GAUSSIAN, MOLPRO, NWCHEM, may play important role. We have optimized the molecule TiH_2 with the help of GAUSSIAN 2009,

* Corresponding author at: Department of Physics, Amity Institute of Applied Sciences, Amity University Campus, Sector - 125, NOIDA 201313, India. Tel.: +919915519345; fax: +911824506111.
E-mail address: suresh492000@yahoo.co.in (S. Chandra).

http://dx.doi.org/10.1016/j.newast.2016.03.005
1384-1076/

Table 1
Rotational and centrifugal distortion constants.

Parameter	Value (MHz)	Parameter	Value (MHz)
A	2.8589602×10^5	Φ_J	$2.037108491 \times 10^{-3}$
B	1.2520818×10^5	Φ_{JK}	$-1.928681064 \times 10^{-2}$
C	8.707408×10^4	Φ_{KJ}	$-1.946479675 \times 10^{-2}$
Δ_J	6.004343468	Φ_K	$5.110638046 \times 10^{-1}$
Δ_{JK}	-4.186548023×10^1	ϕ_J	$1.014000418 \times 10^{-3}$
Δ_K	2.549058853×10^2	ϕ_{JK}	$-3.557138924 \times 10^{-3}$
δ_J	2.465123434	ϕ_K	$1.085768474 \times 10^{-1}$
δ_K	2.332384340		

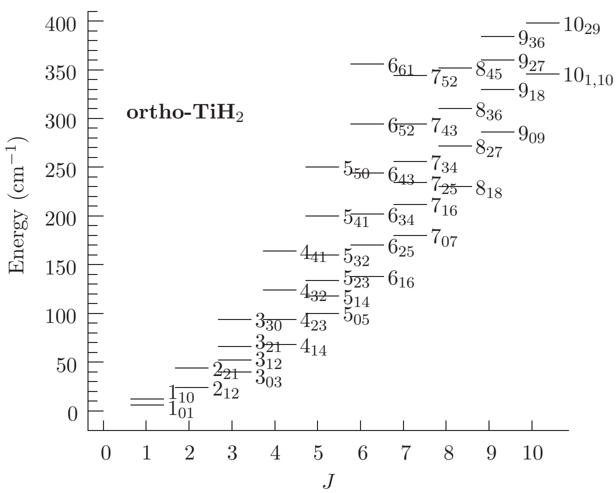

Fig. 1. Energy level diagram for 40 levels of ortho-TiH_2.

where B3LYP method and cc-pVTZ basis-set are used. The rotational and centrifugal distortion constants obtained are given in Table 1.

The TiH_2 is asymmetric top molecule with the Ray parameter $\kappa = -0.6164$. It is a planar molecule having electric dipole moment $\mu = 2.792$ Debye along the b-axis of inertia. Its bond length Ti-H is ∼1.7077 Å and the angle H-Ti-H is ∼111.9°. Owing to the 1/2 value of spin of each of the two hydrogen atoms, the TiH_2 has two distinct species: (i) ortho (with parallel spins) and (ii) para (with anti-parallel spins). These two species behave as if they are two independent molecules, because there are no transitions between their levels.

For calculation of energies of the levels and Einstein A-coefficients between the levels, we have employed the software ASROT (http://info.ifpan.edu.pl/~kisiel/prospe.htm#use), where we have used the rotational and centrifugal distortion constants, given in Table 1 and electric dipole moment $\mu = 2.792$ Debye. We have considered 40 levels of each of the ortho and para species, shown in Figs. 1 and 2, respectively. These levels are connected through radiative and collisional transitions. Collisional transitions do not follow any selection rules, but the radiative transitions are governed by the selection rules:

$$\begin{array}{lll} J: & \Delta J = 0, \pm 1 & \\ k_a, k_c: & \text{odd, even} \longleftrightarrow \text{even, odd} & \text{(ortho transitions)} \\ & \text{even, even} \longleftrightarrow \text{odd, odd} & \text{(para transitions)} \end{array}$$

Here, J is the rotational quantum number, and k_a and k_c are the projections of J on the axis of symmetry in case of symmetric top molecules. There are 89 and 88 radiative transitions between the ortho levels and para levels, respectively. The values of the Einstein A-coefficients are rather large as compared to those of a molecule,

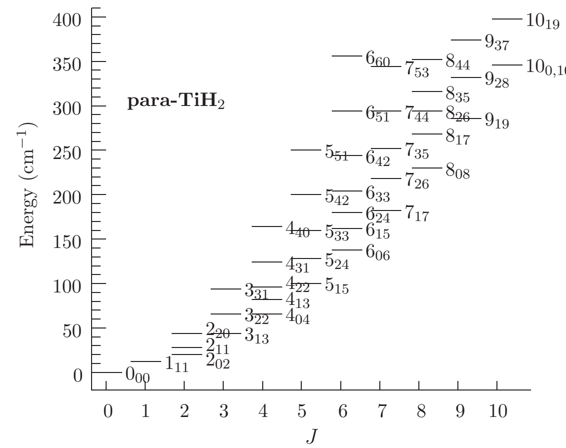

Fig. 2. Energy level diagram for 40 levels of para-TiH_2.

in general. Out of the said number of radiative transitions, 85 ortho and 83 para transitions have Einstein A-coefficient larger than 10^{-5} s^{-1}. The Einstein A-coefficients get value up to 1.1 s^{-1}.

3. Details of model

The model used here is the same as discussed by Chandra and Shinde (2008), Sharma et al. (2012). A set of statistical equilibrium equations coupled with the equations of radiative transfer is written as the following:

$$n_i \sum_{\substack{j=1 \\ j \neq i}}^{40} P_{ij} = \sum_{\substack{j=1 \\ j \neq i}}^{40} n_j P_{ji} \qquad i = 1, 2, \ldots, 40$$

where n denotes the population density of energy level and the parameter P is as the following:

(i) For a radiatively allowed transition

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

(ii) For a radiatively forbidden transition

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

Here, A and B are the Einstein coefficients, C the rate coefficient for collisional transition and n_{H_2} the density of molecular hydrogen. The escape probability β for the transition is

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

where optical thickness τ_ν has been expressed as

$$\tau_\nu = \frac{hc}{4\pi\,(dv_r/dr)}\left[B_{lu} n_l - B_{ul} n_u\right]$$

where (dv_r/dr) denotes the velocity gradient in the cloud. This is non-linear set of equations.

We have solved this set of equations for each of the ortho and para species of TiH_2. The external radiation field impinging on the volume element, generating the lines, is the cosmic microwave background (CMB) only, which corresponds to the background temperature $T_{bg} = 2.73$ K (Sharma et al., 2016). The parameter γ is expressed as $\gamma = n_{mol}/(dv_r/dr)$. Here, n_{mol} is the density of TiH_2 and (dv_r/dr) the velocity gradient in the object.

The required input data are the radiative transition probabilities and the collisional rate coefficients for the transitions between