Can HeH⁺ molecule be present in solar photosphere

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Abstract. The equivalent widths of the P and R branch lines of the fundamental vibration-rotation band arising from the ground state of HeH⁺ have been calculated in a chosen photospheric model. The resulting equivalent widths suggest that the solar spectrum in the infrared region should be searched for resolving the question regarding the presence or absence of HeH⁺ in the sun.

Key words: HeH⁺ molecule—solar spectrum

1. Introduction

In view of the large abundance of helium and ionised hydrogen under variety of astrophysical conditions, Dabrowski & Herzberg (1977) predicted fundamental (1-0), (2-1) and (3-2) band lines of HeH⁺. The ground state of HeH⁺ is $X^1\Sigma^+$. The first excited state $A^{1}\Sigma^{+}$ which is 103243 cm⁻¹ above the ground state has a shallow potential with minimum at 2.9 Å. The transition from the ground state to $A^{1}\Sigma^{+}$ is very difficult to observe. Hence line absorption of HeH⁺ which may take place only as vibration-rotation band lines in the infrared spectral region of the sun and stars should be searched for. In sun the two identified molecules CO and HCl with ground state as $X^{1}\Sigma^{+}$ show vibration-rotation band lines in IR regions. Molecule CO has the highest dissociation energy ($D_0^0 = 11.096$ eV) among all identified molecules in the sun and as such CO once formed will be difficult to dissociate. Molecule CO shows largest abundance after H2 in the sun. The possibility of detecting HCl in the sun was independently indicated by Lambert et al. (1971) and Gaur & Pande (1972). Hall & Noyes (1972) identified (1-0) and (2-1) vibration-rotation lines of HCl. The runs of abundances of HeH⁺ and HCl with depth in the photospheric model by Vernazza et al. (1981) (abbreviated as VAL-81) show that HCl abundance is many orders more at and around the temperature minimum region, but in the deeper layers the abundance of molecule HeH+ exceeds that of HCl and shows a monotonic increase. The above result is a consequence of higher dissociation energy of HCl $(D_0^0 = 4.33 \text{ eV})$ as compared to that of HeH $(D_0^0 = 1.845 \text{ eV})$ and also due to partial pressures of the constituent atoms with depth. The dipole moment of HeH⁺ ($\mu_0 = 1.66$ and $\mu_1 = 4.29$ Debye), being more as compared to HCl ($\mu_0 = 1.092$ and $\mu_1 = 0.953$ Debye) results in higher values of line strengths of fundamental band lines of HeH⁺. Thus it seems that under photospheric conditions HeH⁺ abundance and line strengths may produce detectable absorption lines. To explore the above possibility we have calculated the equivalent widths of P and R branch lines of (1-0) band arising from the $X^1\Sigma^+$ ground state of HeH⁺ molecule. The results of such an investigation will be presented here.

2. Equivalent width calculations

Under photospheric conditions, the maximum populated rotation level by HeH^+ molecule is expected to be around J=7. The predicted wavenumbers of P and R branch lines of (1-0) vibration-rotation band by Dabrowski & Herzberg (1977) are up to J=10. The molecular constants of Bernath & Amano (1981) which predict wavenumbers of lines very close to the observed values were used to derive wavenumbers of P and R branch lines up to J=18. Lines arising from K=J=0 to 18 were chosen for calculations. The calculated wavenumbers are listed in table 1.

Table 1. Computed equivalent widths of P and R branch lines of (1-0) band of HeH⁺

(1-0)		P Branch			R Branch	
Band						
K	(cm ⁻¹)	$f.S_{ m J}$	W (mÅ)	(cm ⁻¹)	$f.S_{ m J}$	W (mÅ)
0		_	_	2972.57	1.5944E-04	14
1	2843.90	5.0846E-05	15	3028.37	1.0340E-04	16
2	2771.80	5.6783E-05	16	3077.99	9.0111E-05	18
3	2695.05	5.6358E-05	17	3121.08	8.2704E-05	19
4	2614.03	5.3875E-05	21	3157.30	7.7091E-05	21
5	2529.13	5.0526E-05	25	3186.35	7.2177E-05	22
6	2440.74	4.6782E-05	27	3207.95	6.7551E-05	22
7	2349.21	4.2872E-05	28	3221.86	6.3036E-05	21
8	2254.90	3.8927E-05	28	3227.87	5.8550E-05	20
9	2158.12	3.5026E-05	28	3225.81	5.4059E-05	19
10	2059.19	3.1222E-05	26	3215.55	4.9551E-05	17
11	1958.37	2.7554E-05	25	3197.03	4.5032E-05	15
12	1855.89	2.4050E-05	22	3170.21	4.0512E-05	13
13	1751.95	2.0730E-05	20	3135.13	3.6012E-05	11
14	1646.69	1.7611E-05	17	3091.89	3.1555E-05	9
15	1540.22	1.4705E-05	15	3040.62	2.7164E-05	7
16	1432.58	1.2023E-05	12	2981.56	2.2866E-05	5
17	1323.77	9.5721E-06	10	2914.99	1.8686E-05	4
18	1213.70	7.3601E-06	7	2841.28	1.4654E-05	3

For calculating the line strengths, $f.S_J$, or vibration-rotation line oscillator strengths, we made use of Penner (1959) formulations and dipole moment value of Dabrowski & Herzberg (1977). The details for calculating $f.S_J$ and the equivalent widths are given in our earlier work (Gaur & Pande 1972).

The model atmosphere used by us is VAL-81 (Vernazza et al. 1981). The partition functions and dissociation constants of HeH⁺ molecule, to derive partial pressure of HeH⁺ at various optical depths, were adopted from Gaur & Tripathi (1985). The continuous opacity sources considered were H⁻ ion, neutral hydrogen, electron and Rayleigh scatterings. Formulations by Tsuji (1966) were used for continuous opacity calculations.

The calculated equivalent widths of the chosen lines are listed in table 1.

3. Concluding remarks

It is obvious from table 1 that both P and R branch lines of the (1-0) vibration-rotation band of HeH⁺ can be easily detected in the infrared photospheric spectrum.

The above conclusion is based on two assumptions: (i) The molecular constants of Bernath & Amano (1981) which were derived from the measured laboratory wavenumbers of nine observed (1-0) band lines can be extrapolated to obtain the wavenumbers of lines chosen by us. These lines were R(4), R(3), R(2), R(1), R(0), P(1), P(2), P(3) and P(4). (ii) The electronic dipole moment values (μ_0 and μ_1) adopted from Debrowski & Herzberg (1977) are correct.

Higher values of dipole moment compared to that of HCl resulted in higher line strengths and consequently in appreciable equivalent widths of HeH⁺ lines. Even if the equivalent widths are reduced by a factor of 2 to 4 due to uncertainties in the model and assumptions involved in the calculations the (1-0) band lines of HeH⁺ remain detectable with heterodyne technique such as given by Demings et al. (1986). Hence it may be desirable to investigate the photospheric spectrum so as to resolve the question of presence or absence of HeH⁺ in sun in an incontrovertible manner.

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