# A POSSIBLE PRESENCE OF HeH+ IN WHITE DWARFS

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**Abstract.** The equivalent width calculations for the fundamental vibration rotation band lines of HeH<sup>+</sup> have been carried out for a non-DA white dwarf model with an effective temperature of 12000 K. Both P and R branch lines with rotational quantum numbers J=3 to 18 were included in the calculations. A search for these lines in helium rich white dwarfs is suggested.

### 1. Introduction

Black (1978) showed that significant abundance of simple molecules like H<sub>2</sub>, H<sub>2</sub><sup>+</sup>, HeH<sup>+</sup>, OH, and CH<sup>+</sup> can exist in planetary nebulae as conditions of partial ionization and moderate temperature ( $10^3 \le T \le 10^4 \text{ K}$ ) expected in transition zones are conducive to the efficient formation of these molecules. He suggested that molecular lines near 3μ may be due to HeH <sup>+</sup> and OH. Earlier, Dabrowski and Herzberg (1977) had shown that predicted emission spectrum of HeH+ can fairly well match the position and shapes of features at 3.09 and  $3.4\mu$  observed in planetary nebula NGC 7027. From expected line strengths Scrimger et al. (1978) concluded that previously observed feature at 3.4 $\mu$  in NGC 7027 cannot be due to R(16) 4–2 transition of HeH<sup>+</sup>. However, Black (1978) suggested that the reason for not yet definitely identified HeH $^+$  lines near 3 $\mu$  may be due to low-resolution spectrum of NGC 7027. Flower and Roueff (1979) evaluated rates of radiative association and photodissociation of HeH + under physical conditions prevailing in gaseous nebulae. They found that the destruction of HeH+ by EUV radiation field around the nebula is much faster than the creation by recombination resulting in lower equilibrium abundance of HeH+. Dust-mixed ionized gas could substantially reduce photodissociation and lead to detectable emission from J = 1-0transition at  $149\mu$  of HeH <sup>+</sup> molecule. Roberge and Dalgarno (1982) suggested that with higher sensitivity or spectral resolution emission at  $149\mu$  from H II blisters and at  $3.364\mu$ from high-density planetary nebulae should be detectable. Dense atmosphere, high temperature and high abundance of H and He in non-DA white dwarfs may be conducive to the formation of HeH<sup>+</sup>. With this in view, the molecular dissociation equilibrium calculations were earlier carried out (Gaur et al., 1988). We found appreciable abundances of HeH + in non-DA white dwarf models with effective temperatures in the range 12 000 to 20 000 K. On the basis of this, the search for molecular lines of HeH <sup>+</sup> in helium-rich white dwarfs was suggested. To know the possibility of detectability of fundamental-vibration rotation band lines of HeH+, we carried out equivalent width calculations for some chosen P and R branch lines of this band in a selected white-dwarf model. Here we present the results of these calculations.

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## 2. Equivalent Width Calculations

The ground state of HeH<sup>+</sup> is  $X^1\Sigma^+$ . The first excited state  $A^1\Sigma^+$  lies by 103 243 cm above  $X^1\Sigma^+$  and has a shallow potential curve. As HeH<sup>+</sup> in ground state has fairly large dipole moment ( $\mu = 1.66$  Debye) an ordinary vibration-rotation spectrum in infrared region may play a role in astronomical spectra (Dabrowski and Herzberg, 1977).

For white-dwarf models with effective temperatures between 12 000 to 20 000 K, the most populated rotational quantum level will be J = 10 to J = 14. Thus, in equivalent width calculations of (1-0) vibration-rotation band lines, originating from J = 10 or more should also be included. Dabrowski and Herzberg (1977) predicted wave numbers of lines up to J = 10. Hence it was necessary to calculate the wave numbers of lines with higher rotational quantum numbers. Using the molecular constants of Bernath and Amano (1981) and the following expression, we calculated the wave numbers of P and R branch lines up to K = J = 18

$$w = B_{v'}K'(K'+1) - D_{v'}K'^{2}(K'+1)^{2} + H_{v'}K'^{3}(K'+1)^{3} - B_{v''}K''(K''+1) + D_{v''}K''^{2}(K''+1)^{2} - H_{v''}K''^{3}(K''+1)^{3},$$

where the symbols with the single prime denote the upper level, while the double prime stands for the lower level. For the P branch K' - K'' = -1 and for the R branch K' - K'' = 1.

Considering the dipole moment  $\mu$  as a function of internuclear distance r as

$$\mu = \mu_0 + \mu_1 (r - r_e)$$
,

where  $\mu_1 = 4.29$  Debye and  $r_e = 0.7743$  Å and by use of the expression (2-20) (7-85a) and (7-85b) of Penner (1959), the line intensity factor,  $fS_{T}$  for R and P branches of the fundamental vibration-rotation band arising from  $X^{1}\Sigma^{+}$  electronic state can be expressed, respectively, as

$$fS_{J} = \frac{8\pi^{2}m_{e}c^{2}}{3he^{2}} \frac{\mu_{1}^{2}}{2\alpha} \frac{K+1}{2K+1} w \left[ 1 - \frac{4\mu_{0}}{\mu_{1}r_{e}} \gamma(K+1) \right]$$

$$fS_{L} = \frac{8\pi^{2}m_{e}c^{2}}{2\kappa} \frac{\mu_{1}^{2}}{2\kappa} \frac{K}{2K+1} w \left[ 1 - \frac{4\mu_{0}}{\mu_{1}r_{e}} \gamma(K+1) \right]$$

$$fS_{J} = \frac{8\pi^{2}m_{e}c^{2}}{3he^{2}} \frac{\mu_{1}^{2}}{2\alpha} \frac{K}{2K+1} w \left[1 - \frac{4\mu_{0}}{\mu_{1}r_{e}} \gamma K\right]$$

where  $\alpha = \omega_e/[2B_e r_e^2]$  and  $\gamma = 2B_e/\omega_e$ .

The calculated wave numbers and line intensity factors of the (1-0) band lines for both the P and R branches are given in Table I. If we follow Schadee (1968), the equivalent width W of the chosen line can be expressed as

$$W = \frac{\pi e^2}{m_{\rm H} m_e c^2} \lambda^2 f S_{\rm J} \int_0^\infty \frac{G(\tau') p({\rm HeH^+})}{K_\lambda \rho k T Q} e^{-F_{\rm J} h c/(kT)} d\tau,$$

		TABLE	3 I				
Computed	equivalent	widths	of P	and	R	branch	lines

(1–0) band <i>K</i>	P branch			R branch				
	$(cm^{-1})$	$fS_{\mathtt{J}}$	W (mÅ)	(cm <sup>-1</sup> )	$fS_{\mathtt{J}}$	W (mÅ)		
3	2695.05	5.6358E - 05	14	3121.08	8.2704E - 05	15		
4	2614.03	5.3875E - 05	18	3157.30	7.7091E - 05	17		
5	2529.13	5.0526E - 05	21	3186.35	7.2177E - 05	18		
6	2440.74	4.6782E - 05	23	3207.95	6.7551E - 05	18		
7	2349.21	4.2872E - 05	24	3221.86	6.3036E - 05	18		
8	2254.90	3.8927E - 05	25	3227.87	5.8550E - 05	17		
9	2158.12	3.5026E - 05	24	3225.81	5.4059E - 05	16		
10	2059.19	3.1222E - 05	23	3215.55	4.9551E - 05	15		
11	1958.37	2.7554E - 05	22	3197.03	4.5032E - 05	13		
12	1855.89	2.4050E - 05	20	3170.21	4.0512E - 05	12		
13	1751.95	2.0730E - 05	17	3135.13	3.6012E - 05	10		
14	1646.69	1.7611E - 05	14	3091.89	3.1555E - 05	9		
15	1540.22	1.4705E - 05	10	3040.62	2.7164E - 05	7		
16	1432.58	1.2023E - 05	5	2981.56	2.2866E - 05	6		
17	1323.77	9.5721E - 05	1	2914.99	1.8686E - 05	4		
18	1213.70	7.3601E - 05	1	2841.28	1.4654E - 05	3		

where the symbols are described in Schadee's referred paper. The weighting factor  $G(\tau')$  is expressed as:

$$G(\tau') = \frac{\int\limits_{\tau'}^{\infty} B(\tau') E_1(\tau') \,\mathrm{d}\tau' - B(\tau') E_2(\tau')}{\int\limits_{0}^{\infty} B(\tau') E_2(\tau') \,\mathrm{d}\tau'} \;,$$

where  $B(\tau')$  is the Planck function at an optical depth  $\tau'$  at the line wavelength and  $E_1(\tau')$  and  $E_2(\tau')$  are integro-exponential functions evaluated from the formulations of Stankiewicz (1968).

The lines were assumed to be formed under LTE by a pure absorption mechanism having a Doppler profile. The quantity  $K_{\lambda}$  is the total continuum opacity per gram. Main contributions to continuum opacity resulted from He<sup>-</sup>, H, and H<sup>-</sup>. Other sources of opacities were also considered but showed negligible contribution (Tsuji, 1966; Mihalas, 1967; Sommerville, 1965).

The partial pressure of HeH<sup>+</sup> were adopted from our earlier work (Gaur *et al.*, 1988). The model selected by us was a non-DA white-dwarf model (Koester, 1984) with an effective temperature of 12000 K for equivalent width calculations as this model amongst all models of its category showed a maximum concentration of HeH<sup>+</sup>. The

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partition functions Q were calculated from the expression given by Gaur and Tripathi (1985). The resulting equivalent widths for the selected model are given in Table I.

#### 3. Conclusions

From Table I it is obvious that the (1-0) vibration-rotation band lines of HeH<sup>+</sup> molecule show appreciable equivalent widths in the chosen model which may be detected by some sophisticated high-resolution technique. Even if the equivalent widths are reduced by a factor of 2 or 3 because of uncertainties in the model, oscillator strength and assumptions involved, the lines may be detected, with heterodyne techniques using largest possible telescope (Deming *et al.*, 1986) or echelle spectrographs of higher resolution and higher sensitivity backed up with CCD detectors. Though we are not experts in the use of large telescope and sophisticated detecting techniques, we feel that it may be desirable to investigate white-dwarfs spectra in the spectral region around  $3\mu$  so as to resolve the possibility of the presence or absence of HeH<sup>+</sup> in helium-rich white-dwarf stars.

### References

Bernath, P. and Amano, T.: 1981, Am. Phys. Soc. 48, 20.

Black, J. H.: 1978, Astrophys. J. 222, 125.

Dabrowski, I. and Herzberg, G.: 1977, Trans. New York Acad. Sci. Ser. 38(II), 14.

Deming, D., Gleaner, D. A., Kauff, H. U., Hill, A. A., and Espenak, F.: 1986, Nature 322, 232.

Flower, D. R. and Roueff, E.: 1979, Astron. Astrophys. 72, 361.

Gaur, V. P. and Tripathi, B. M.: 1985, J. Quant. Spectr. Rad. Trans. 33, 91.

Gaur, V. P., Tripathi, B. M., Joshi, G. C., and Pande, M. C.: 1988, Astrophys. Space Sci. 147, 107.

Koester, D.: 1984 (priv. comm.).

Mihalas, D.: 1967, in B. Alder, S. Fernbach and M. Rotenberg (eds.), *Methods in Computational Physics*, Academic Press, New York, Vol. 7, p. 1.

Penner, S. S.: 1959, Quantitative Molecular Spectroscopy and Gas Emissivities, Pergamon Press Ltd., London.

Roberge, W. and Dalgarno, A.: 1982, Astrophys. J. 255, 489.

Schadee, A.: 1968, Astrophys. J. 151, 239.

Scrimger, J. N., Lowe, R. P., Moorhead, J. M., and Wehlau, W. H.: 1978, Publ. Astron. Soc. Japan 90, 257.

Sommerville, W. B.: 1965, Astrophys. J. 141, 811.

Stankiewicz, A.: 1968, Acta Astron. 18, 289.

Tsuji, T.: 1966, Publ. Astron. Soc. Japan 18, 127.