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ASTROPHYSICALLY USEFUL PARAMETERS FOR CERTAIN BAND SYSTEMS OF BeH, BeD AND BeT MOLECULES

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SUMMARY: The vibronic (vibration-electronic) transition probability parameters such as Franck-Condon (FC) factors and r-centroids of diatomic molecular species could be useful in the identification of molecular bands and in the estimation of relative abundance of the emitted species in astrophysical sources. In this study, they have been evaluated for the electronic transitions $A^2\Pi_r - X^2\Sigma^+$, $B^2\Pi_r - X^2\Sigma^+$ and $C^2\Sigma^+ - X^2\Sigma^+$ systems of BeH, $A^2\Pi_r - X^2\Sigma^+$ and $C^2\Sigma^+ - X^2\Sigma^+$ system of BeD and $A^2\Pi_r - X^2\Sigma^+$ system of BeT molecules using a suitable potential.

Key words. Molecular data – Methods: numerical – Sun: abundances.

1. INTRODUCTION

The overabundance of beryllium and its value of Be/H greater than ∼200 times the solar value in almost fourty three Hg-Mn stars were elaborately discussed by Boesgaard et al. (1982). Sargent et al. (1962) surveyed ten Mn stars, of which x Cancri, 112 Herculis, μ Leporis and υ Herculis have very strong BeII lines and hence reported a Be abundance about 100 times that in the Sun. The observations have been made by Boesgaard et al. (1981) for the presence of the BeII resonance lines in the bright AO star Gamma Geminorum, which set a goal to clarify whether γ -Gem resembles the normal star or the hot AM star in its Be content. IUE (International Ultraviolet Explorer) observations of the Be II lines in ten early type peculiar stars, including five Hg-Mn stars, have been made by Sadakane and Jugaku (1981). With the IUE satellite, Parthasarathy et al. (1984) noted that the spectra of the G-band stars readily suggest that the Be contents of these stars are comparable to that of α Cas and the Hyades K giants. Model atmosphere calculations for red giant star of solar composition show a significant elemental abundance for Be. Further, mono hydrides are among the most readily formed diatoms in a variety of astrophysical contexts (Johnson and Sauval 1982).

With only five electrons, the BeH molecule is perhaps of most interest in its group, since it belongs to the homologous mono hydrides (Colin et al. 1983) with MgH, CaH, SrH and BaH molecules which are extensively studied astrophysical molecules. For instance, recently, the presence of MgH in solar and cool stellar atmospheres (Weck et al. 2003, Mohan Rao and Rangarajan 1999), the intensity of CaH lines in cool dwarfs (Barbuy 1993), and the molecular abundances of SrH in SC-stars (Green 1972) have been reported. Certainly, one very likely class of compounds to be present in space are the BeH molecule and its isotopologues BeD and BeT.

Gaur et al. (1973) have showed that several diatomic molecular species, including BeH, form in sunspots based on Zwaan's sun spot model. Sauval and Tatum (1984) reported the possible presence of BeH molecule in stellar and cometry spectra. Singh

(1988) noted the presence of BeH molecule in cosmic object spectra. Wöhl (1971) analyzed the certainty of the identification and confirmation of the presence of many diatoms in the Umbral spectra on the basis of the W-index and classified the molecules studied as present, presence questionable, presence excludable, or not identifiable. The BeH is one among the listed molecules of presence questionable category. Bailer (1973) has discussed the importance of beryllium and its compounds in environmental science due to their biological activity of highly toxic character in dust, smoke or aerosol form in detail elsewhere. And hence there is considerable interest in the BeD and BeT molecules.

The intensity distribution of the vibrational bands within an electronic transition is largely controlled by the square modulus of the vibrational overlap integral, the so-called Franck-Condon (FC) factor. Since the FC factors and related quantities, such as r-centroids, are proportional to the transition probabilities, a precise knowledge of these parameters provides direct information about the electronic transition moment, band strengths, radiative lifetimes, populations of particular molecular quantum states, vibrational temperature of the source and the kinetics of energy transfer (Kuzmanovic et al. 2005). Evaluation of reliable FC factors is therefore necessary especially for the identification of the presence of many diatomic molecules in spectra of variety of the above astrophysical sources. For instance, despite its suspected presence suggested by the observations of Wöhl (1971), Bagare et al. (2006) have made a fresh search for the presence of AlF lines using the significant values of transition probabilities computed by Balachandra Kumar et al. (2002, 2003, 2004) and reported without doubt that the bands of AlF are present in the umbral spectrum.

There has been no report on the FC factors and r-centroids for, $A^2\Pi_r - X^2\Sigma^+$, $B^2\Pi_r - X^2\Sigma^+$ and $C^2\Sigma^+ - X^2\Sigma^+$ systems of BeH, $A^2\Pi_r - X^2\Sigma^+$ and $C^2\Sigma^+ - X^2\Sigma^+$ systems of BeD and $A^2\Pi_r - X^2\Sigma^+$ system of BeT molecules in the literature. However for the $A - X$ system of BeH alone some rough values/relative FC factors are available (Popkie 1971, Machado et al. 1999). Therefore, the reliable values of FC factors and r-centroids for these band systems of BeH, BeD and BeT molecules have been evaluated by a numerical integration procedure using a suitable potential.

2. FRANCK - CONDON FACTORS AND r-CENTROIDS

Mathematically, one can write expression for the intensity ($I_{v'v''}$) of a molecular band for a ($v' - v''$) electronic transition in emission as

$$I_{v'v''} = DN_{v'}E^4_{v'v''}R^2_e(\overline{r}_{v'v''})q_{v'v''}\,, \qquad (1)$$

where D is a constant partly depending on the geometry of the apparatus, $N_{v'}$ is the population of the level v', $E_{v'v''}$ is the quantum energy which is the difference between the energies of upper vibrational level v' and lower vibrational level v'', $q_{v'v''}$ is the Franck-Condon factor, $\bar{r}_{v'v''}$ is the r- centroid and R_e is the electronic transition moment.

The square of the overlap integral is termed as FC factor

$$q_{v'v''} = |\langle\psi_{v'}|\psi_{v''}\rangle|^2\,, \qquad (2)$$

where $\psi_{v'}$ and $\psi_{v''}$ are the vibrational wave functions for the upper and lower states, respectively.

The r-centroid is a unique value of internuclear separation, which may be associated with a ($v' - v''$) band and is defined as

$$\bar{r}_{v'v''} = \frac{\langle\psi_{v'}|r|\psi_{v''}\rangle}{\langle\psi_{v'}|\psi_{v''}\rangle}\,. \qquad (3)$$

In astrophysical studies, the determination of FC factors and r-centroids is so important because they can be used to determine the band strengths such as

$$P_{v'v''} = R^2_e(\overline{r}_{v'v''})q_{v'v''}\,, \qquad (4)$$

where $R_e(\overline{r}_{v'v''})$ is the variation of electronic transition moment. Having these band strengths, one can estimate the temperature of the emitting source and classify the astrophysical sources in the temperature sequence.

The Morse (1929) potential yields considerably reliable FC factors especially for vibrational transition involving low quantum numbers (Partal et al. 2000). The computation of the FC factor is made by Bates' (1949) method of numerical integration according to the detailed procedure provided by Rajamanickam et al. (2001). Morse wave functions are calculated at intervals of 0.01Å for the range of r from 0.95Å to 2.24 Å, from 1.04Å to 1.86Å and 0.94Å to 2.93Å for the $A - X$, $B - X$ and $C - X$ systems of BeH, from 1.00Å to 1.95Å and 0.93Å to 2.50Å for $A - X$ and $C - X$ systems of BeD and from 1.08Å to 1.71Å for $A - X$ system of BeT molecules. Integrals in the Eqs. (2) and (3) for the FC factors $q_{v'v''}$ and r-centroids $\overline{r}_{v'v''}$ are computed numerically and the results are presented respectively in Tables 1, 2 and 3 for $A - X$, $B - X$ and $C - X$ systems of BeH, in Table 4 and 5 for $A - X$ and $C - X$ systems of BeD and in Table 6 for $A - X$ system of BeT molecule. The available experimental wavelengths data (Olsson 1932, Colin et al. 1983, Horne and Colin 1972, De Greef and Colin 1974) for the band systems are also entered in the respective Tables. The molecular constants used in the present study are collected from the compilation of Huber and Herzberg (1979) and also from the works of Colin et al. (1983) and Henriet and Verhaegen (1986).

3. RESULTS AND DISCUSSION

Popkie (1971) has reported a set of relative FC factors for $A-X$ system of BeH by using relatively crude multiconfiguration (MC) wave functions. Machado et al. (1999) have also given an array of FC factors where the significant $\Delta\upsilon = 0$ sequence values are simply 1.00 that is impractical due to the variation of population in successive levels. In both cases, the corresponding r-centroid values were not calculated. In the present study, $q_{v'v''}$ and $\overline{r}_{v'v''}$ have been evaluated by numerical integration method using the revised values of molecular constants and, therefore, reliable and satisfactory.

For the band systems $A-X$ and $B-X$ of BeH, $A-X$ of BeD and $A-X$ of BeT molecules, the FC factors indicate that the $\Delta\upsilon = 0$ sequence bands are most intense.

It is of interest to note that the $\bar{r}_{00}$ value for these systems is found to be greater than $(r'_e + r''_e)/2$ by 0.01Å and hence the potentials are very anharmonic. For $A-X$ system of BeH, since $r'_e < r''_e$, the r-centroid values increase with a decrease in wavelength, which is expected in the violet degraded band system, but reverse is the case which causes a overturn of red shading after (4,4) band. The $A-X$ systems of BeD and BeT are expected to be purely violet degraded band systems.

The rotational analysis of the $C-X$ band system for BeH and BeD done by Colin et al. (1983) indicates that in spite of the difficulties in the assignment of its bands which is related to the fact that the $C^2\Sigma^+$ state is strongly perturbed by interaction with $A^2\Pi_r$ state, a final unambiguous identification was made. This gives good reason why the FC factors of $C-X$ band system of both BeH and BeD are less intense.

The intensity ratio of the corresponding bands of isotopic molecules gives the abundance ratio of the molecules (Straughan and Walker 1976). As intensity is proportional to FC factor, FC factor ratios also reflect the same. According to our computation, one can find, for (0,0) band of $A-X$ system, the FC factor ratio of the isotopic species BeH, BeD and BeT as $0.998 : 1.00 : 0.999$ which is approximately $1 : 1 : 1$. This ratio tells us that the possibility of existence of these isotopomers are merely the same. That is, if BeH is present in an astrophysical source, one may predict the presence of BeD and BeT molecules, too, in the same source.

The given dataset of FC factors in the present study will, hence, be useful for the identification and confirmation of the isotopomers BeH, BeD and BeT in various umbral spectra which is a proposed work by the authors in due course.

Table 1. Franck-Condon factors and r-centroids for A–X of BeH.

v', v''	λ(Å)	$q_{v'v''}$			$r_{v'v''}$(Å)
		a	b	c	
0,0	4992.1	0.998	1.000	0.999	1.360
1,1	4987.1	0.984	1.000	0.997	1.403
2,2	4984.2	0.958	1.000	0.995	1.448
3,3	4983.5	0.919	1.000	0.992	1.496
4,4	4984.9	0.861	1.000	0.989	1.546
5,5	4988.5	0.780	1.000	0.985	1.600
6,6	4994.5	0.674	—	—	1.656
7,7	5002.5	0.524	—	—	1.706

a) Present Study
b) Machado et al. (1999)
c) Popkie(1971)

Table 2. Franck-Condon factors and r-centroids for B–X of BeH.

v', v''	λ(Å)	$q_{v'v''}$	$r_{v'v''}$(Å)
0,0	—	0.974	1.350
1,1	—	0.926	1.400
2,2	—	0.897	1.454
3,3	—	0.838	1.502

Table 3. Franck-Condon factors and r-centroids for C–X of BeH.

v', v''	λ(Å)	$q_{v'v''}$	$r_{v'v''}$(Å)
0,4		0.003	2.037
0,5		0.017	2.090
0,6		0.069	2.149
0,7	5475.6	0.181	2.217
0,8	5910.3	0.296	2.298
0,9	6358.4	0.281	2.400
0,10		0.135	2.539
1,3		0.001	1.962
1,4		0.008	2.004
1,5		0.039	2.050
1,6		0.101	2.098
1,7		0.129	2.147
1,8		0.038	2.162
1,9	5981.7	0.030	2.442
1,10	6358.7	0.266	2.467
2,3		0.002	1.938
2,4		0.015	1.977
2,5		0.053	2.017
2,6		0.090	2.058
2,7		0.046	2.086
2,8		0.004	2.349
2,9	5661.9	0.096	2.256
2,10		0.035	2.212

Table 4. Franck-Condon factors and r-centroids for A–X of BeD.

v', v''	λ(Å)	$q_{v'v''}$	$r_{v'v''}$(Å)
0,0	4988.5	1.000	1.352
1,1	4984.5	0.996	1.382
2,2	4981.6	0.994	1.414
3,3		0.992	1.446
4,4		0.990	1.480
5,5		0.981	1.514
6,6		0.928	1.541

Table 5. Franck-Condon factors and r-centroids for C–X of BeD.

v', v''	λ(Å)	$q_{v'v''}$	$r_{v'v''}$(Å)
0,7		0.002	2.051
0,8	5026.2	0.008	2.088
0,9	5325.1	0.027	2.128
0,10	5641.6	0.068	2.172
0,11	5972.4	0.132	2.219
0,12	6310.7	0.194	2.271

Table 6. Franck-Condon factors and r-centroids for A–X of BeT.

v', v''	λ(Å)	$q_{v'v''}$	$r_{v'v''}$(Å)
0,0	4988.5	0.999	1.350
1,1	4985.0	0.993	1.376
2,2	4982.2	0.979	1.402
3,3	4980.4	0.915	1.423

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АСТРОФИЗИЧКИ КОРИСНИ ПАРАМЕТРИ ЗА СИСТЕМЕ ТРАКА BeH, BeD И BeT МОЛЕКУЛА

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Израчунати су Франк-Кондонови фактори за неколико познатих тракастих система BeH, BeD и BeT емитованих у астрофизичким изворима. На основу добијених вредности предвиђени су релативни односи интензитета трака и присуство ових изотопних врста у истим изворима.