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EVALUATION OF ASTROPHYSICALLY USEFUL PARAMETERS FOR STRONTIUM MONOHYDRIDE AND DEUTERIDE

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SUMMARY: The Franck-Condon factors and r-centroids which are very closely related to transition probabilities, have been evaluated by the more reliable numerical integration procedure for the band systems $B^2\sum - X^2\sum$, $C^2\sum - X^2\sum$ and $F^2\sum - X^2\sum$ of astrophysical molecules strontium monohydride and strontium deuteride using an adequate potential. The Franck-Condon factors are more intense, particularly for the $\Delta\nu = 0$ bands, for all the systems examined here. Thus the bands of the molecules are expected to be present in sunspot spectra, SC-stars, cool M-giant stars and other prominent astrophysical sources.

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

1. INTRODUCTION

Hydrogen is the most abundant element in the universe, and the second group metals are also fairly abundant. Thus hydrides of group II metals are expected to be present in sunspots, stars, nebulae, and the interstellar medium. Among these species, the mono-hydrides of the alkaline-earth metal have received considerable attention from both the experimentalists and the theoreticians, because the monohydrides of Sr, Mg and Ca are relatively easy to synthesize in the gas-phase and have interesting ground states. Due to astrophysical significance of these molecules there arises a renewed interest.

Pande et al. (1969) and Tsuji (1964) reported the presence of SrH molecule on the molecular abundances in sunspots based on Zwaan's sunspot model. Pande pointed out that the partial pressures thus obtained were used to calculate the required molecular concentrations at various geometrical depths in Zwaan's sunspot model. Further the sunspots are dynamic phenomena with a variety of flows and changes in the magnetic field (Gokhale and Zwaan 1972). The molecular lines are particularly useful since they are uncontaminated by photosphere light which has practically no molecular line features in the visible spectrum, due to the difference in effective temperature, between the umbra and the photosphere. Greene (1972) reported the presence of SrH molecule in SC-stars and under the conditions of temperature and pressure similar to those present on cool M-giant stars. Sauval and Tatum (1984) have noted the presence of SrH molecules in the stellar and the cometary spectra. Johnson and Sauval (1982) have predicted the presence of SrH molecule in cool M-giant stars and list the molecular column densities for 248 astrophysical molecules in red-giant stars. Based on the estimates of solar elemental abundances of Sr (Lambert and Warner 1968), the hydrogen isotopes are easily bonding with Sr. Lambert (1980)

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has noted that the group II elements do have hydrides with a predicted increase of column density in the S-type stars. Hence SrH and SrD molecules are expected to be present in stars and sunspot spectra.

The estimates of relative abundances of these metallic species are important for understanding the evolutionary phases of the stars observed and are also essential inputs in modeling the stellar atmospheres of the late type stars. Their relative abundances in interstellar medium give estimates of stellar activity like supernovae in the region observed. Similarly, their abundance variations in cometary spectra can be used to study the interaction of solar wind with cometary material. Also, the relative abundances of these metallic species are useful in studying the cosmic recipe in these pristine objects. Evaluation of molecular parameters for SrH and SrD is therefore useful for many astrophysical studies.

Many systems of bands in the visible and ultraviolet regions of the spectrum of SrH and SrD have been the subject of the study of many investigators. The theoretical study of relationship between the molecular parameters of diatomic molecules has a long and venerable history. The knowledge of vibrational transition probabilities is required to explain the intensity distribution in a molecular band system. An assessment of such transition probability parameters has been the subject of a number of reviews related to astronomy and astrophysics. To a good approximation, the Franck-Condon (FC) factors are proportional to these transition probabilities. Accurate values of the FC factors and related quantities are essential to obtain radiative lifetime and vibrational temperature for the astrophysical molecules and also determining the density and temperature of the solar corona during solar flares and in studying energy loss in controlled thermo-nuclear plasmas.

To the best of our knowledge, there has been no report on the Franck - Condon factors and r-centroids for the band systems $B^2\sum -X^2\sum$, $C^2\sum -X^2\sum$ and $F^2\sum -X^2\sum$of astrophysical molecules SrH and SrD in literature. Therefore the reliable values of the FC factors and r-centroids for these band systems of the molecules SrH and SrD have been determined by the numerical integration procedure, using the Morse potential.

2. FRANCK - CONDON FACTORS AND R-CENTROIDS

The wave mechanical formulation of the Franck-Condon principle leads the emission intensity ($I_{v'v''}$) of a molecular band for an ($v' - v''$) electronic transition is proportional to the product of number of molecules present in the particular state, the photon energy and the rate of spontaneous emission. Thus,

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

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 intensities of diatomic molecular bands in emission are controlled by the square of the overlap integral. The square of the coefficients used in the linear combination tells us about the degree of overlap between the excited state wave function and the ground state wave function. The square of the overlap integral is termed as Franck-Condon 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, between which the transition takes place.The r-centroid is a unique value of internuclear separation associated with a ($v' - v''$) band and defined as

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

Morse (1929) potential energy curves for diatomic molecules are required in order to evaluate the Franck-Condon factors especially for vibrational transition involving between their various low quantum number electronic states (Sri Ramachandran et al. 2004). The computation of the Franck-Condon factor is made by Bates's (1949) method of numerical integration according to the detailed procedure provided by Partel et al. (2000). The Morse wave functions are calculated at intervals of 0.01 A for the range of r respectively from 1.82 A to 2.51 A , from 1.76 A to 2.63 A and from 1.80 A to 2.51 A for every observed vibrational level of $B^2\sum -X^2\sum$, $C^2\sum -X^2\sum$ and $F^2\sum -X^2\sum$ states of SrH molecule and 1.86 A to 2.45 A , from 1.85 A to 2.45 A , and 1.83 A to 2.45 A for every observed vibrational level of $B^2\sum -X^2\sum$, $C^2\sum -X^2\sum$ and $F^2\sum -X^2\sum$ states of SrD molecule. Integrals in the Equations (1) and (2) for the Franck-Condon factors $q_{v'v''}$ and r-centroids $\bar{r}_{v'v''}$ are computed numerically and the results are presented respectively in Tables 1, 2 and 3 for the systems $B^2\sum -X^2\sum$, $C^2\sum -X^2\sum$ and $F^2\sum -X^2\sum$ of SrH molecule and Table 4, 5 and 6 for the $B^2\sum -X^2\sum$, $C^2\sum -X^2\sum$ and $F^2\sum -X^2\sum$ states of SrD molecule. The wavelengths $\lambda_{v'v''}$ data (More et al. 1938, Gunnar Edvinsson et al. 1963, Aslam Khan 1963, 1966 and Aslam Khan et al. 1968) 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).

3. RESULTS AND DISCUSSION

The FC factors for the $B^2\sum -X^2\sum$, $C^2\sum -X^2\sum$ and $F^2\sum -X^2\sum$ systems of SrH indicate that the $\triangle\upsilon = 0$ bands are more intense than the other bands. Therefore these bands are readily observable in sunspots and other astrophysical sources where the molecules are expected to be present under favorable physical conditions and temperature.

For the $B^2\sum -X^2\sum$, $C^2\sum -X^2\sum$ and $F^2\sum -X^2\sum$ of SrD, the FC factors show that the $\triangle\upsilon = 0$ bands are more intense and all other bands are comparatively weak.

The sequence difference for all the systems of SrH is found to be constant except for$\triangle\upsilon = -1$ sequence bands. The sequence difference is found to be a constant for all the band systems of SrD molecule.

Another interesting feature in studying these isotopic molecules SrH & SrD evolves with a fact that its main band (0,0) is more intense. So, as is to be expected from the probable near equality of the frequencies of vibration in the two electronic states of each molecule,the $B^2\sum -X^2\sum$, $C^2\sum -X^2\sum$ and $F^2\sum -X^2\sum$ band of SrD have even more perturbations than the corresponding SrH bands and is found at almost exactly the same wavelength. Hence SrD is likely to be present in sunspot spectra.

The FC factor ratio of the corresponding bands of isotopic molecules gives the abundance ratio of the molecules. From our computation, we have obtained, for (0,0) band of system, the Franck-Condon factors' ratio of isotopic molecules SrH and SrD as 1:0.9260. This ratio shows that the possibility of occurrence of both SrH and SrD are more or less equal in the same astrophysical source.

In the case of $B^2\sum -X^2\sum$, $C^2\sum -X^2\sum$ and $F^2\sum -X^2\sum$ of SrH & SrD molecules, since $r'_e < r''_e$, the r-centroid values increase with decrease in wavelength which is expected in the violet degraded band system and confirms that the potentials are not very anharmonic.

Table 1. Franck-Condon factors, r-Centroids and Wavelengths of B-X bands of SrH

$\upsilon' - \upsilon''$	$\upsilon'' = 0$	$\upsilon'' = 1$
$\upsilon' = 0$	a) 0.9425 b) 2.1398 c) 7018.10	0.0465 1.6320 *
$\upsilon' = 1$	a) 0.0519 b) 2.6449 c) *	0.7869 2.1827 7009.50

Table 2. Franck-Condon factors, r-Centroids and Wavelengths of C-X bands of SrH

$\upsilon' - \upsilon''$	$\upsilon'' = 0$	$\upsilon'' = 1$	$\upsilon'' = 2$
$\upsilon' = 0$	a) 0.8654 b) 2.1210 c) 3809.37	0.1208 1.8318 3987.24	0.0138 1.6067 *
$\upsilon' = 1$	a) 0.1327 b) 2.4414 c) 3629.76	0.6388 2.1687 3790.75	0.1876 1.8628 *
$\upsilon' = 2$	a) 0.0043 b) 2.9603 c) *	0.2271 2.4878 *	0.4574 2.2173 3774.29

Table 3. Franck-Condon factors, r-Centroids and Wavelengths of F-X bands of SrH

$\upsilon' - \upsilon''$	$\upsilon'' = 0$	$\upsilon'' = 1$
$\upsilon' = 0$	a) 0.8788 b) 2.1243 c) 2924.83	0.1062 1.8147 3031
$\upsilon' = 1$	a) 0.1173 b) 2.4627 c) 2814.76	0.6617 2.1734 2914.00

Table 4. Franck-Condon factors, r-Centroids and Wavelengths of B-X bands of SrD

$\upsilon' - \upsilon''$	$\upsilon'' = 0$	$\upsilon'' = 1$
$\upsilon' = 0$	a) 0.9484 b) 2.1381 c) 7020.00	0.0442 1.6962 *
$\upsilon' = 1$	a) 0.0466 b) 2.5926 c) *	0.8067 2.1679 *

Table 5. Franck-Condon factors, r-Centroids and Wavelengths of C-X bands of SrD

$\upsilon' - \upsilon''$	$\upsilon'' = 0$	$\upsilon'' = 1$
$\upsilon' = 0$	a) 0.8979 b) 2.1272 c) 3805.30	0.0928 1.8447 3930.95
$\upsilon' = 1$	a) 0.0959 b) 2.4420 c) 3673.35	0.6891 2.1573 3790.50

Table 6. Franck-Condon factors, r-Centroids and Wavelengths of F-X bands of SrD

$v'-v''$	$v''=0$	$v''=1$
$v'=0$	a) 0.8138 b) 2.1141 c) 2926.98	0.1604 1.9113 *
$v'=1$	a) 0.1751 b) 2.3435 c) 2846.61	0.1604 2.1500 2917.00

In all above Tables,
a) $q_{v'v''}$: Franck-Condon factor
b) $r_{v'v''}$: r-Centroids(Å)
c) $\lambda_{v'v''}$: Wavelength(Å)

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ЕВАЛУАЦИЈА АСТРОФИЗИЧКИ КОРИСНИХ ПАРАМЕТАРА ЗА СТРОНЦИЈУМ МОНОХИДРИД И ДЕУТЕРИД

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Оригинални научни рад

Франк-Кондонови фактори и r-центроиди који су тесно повезани са вероватноћама прелаза, рачунати су поузданом процедуром нумеричке интеграције и коришћењем адекватног потенцијала за системе трака $B^2\sum -X^2\sum$, $C^2\sum -X^2\sum$ и $F^2\sum -X^2\sum$ за астрофизичке молекуле стронцијум монохидрид и стронцијум деутерид. Франк-Кондонови фактори су интензивнији, посебно за $\Delta\nu = 0$ траке, за све овде испитиване системе. Стога се очекује да траке ових молекула буду присутне у спектрима сунчеве светлости, SC-звезда, хладних M-џиновских звезда и других значајних астрофизичких извора.