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A DETAILED INVESTIGATION OF CERTAIN ELECTRONIC TRANSITIONS OF THE BaD MOLECULE FOR ASTROPHYSICAL APPLICATIONS [**]

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The spectroscopic and ro-vibrational constants, FCFs and r-centroids have been evaluated in the present study for $A\,^2\Pi_{1/2}$–$X\,^2\Sigma$, $A\,^2\Pi_{3/2}$–$X\,^2\Sigma$, $B\,^2\Sigma$–$X\,^2\Sigma$, $E\,^2\Pi_{1/2}$–$X\,^2\Sigma$, $E\,^2\Pi_{3/2}$–$X\,^2\Sigma$, $F\,^2\Sigma$–$X\,^2\Sigma$, *and* $L\,^2\Pi$–$X\,^2\Sigma$ *band systems of the barium deuteride (BaD) molecule by adopting a reliable numerical integration procedure. The physical and astrophysical significances of the evaluated FCFs and r-centroids are discussed for all these band systems. The effect of vibration rotation interaction (VRI) on FCFs for the bands of the chosen band systems of BaD molecule is also studied. It is found from the results that the effect of VRI on FCFs is not so significant for the rotational quantum number (J) up to* $J = 50$. *For higher values of J like* $J = 100$, *there is a slight change in the value of FCFs due to the VRI effect.*

Keywords: *BaD molecule, Franck–Condon factors, r-centroids, VRI effect, Celestial environment.*

ДЕТАЛЬНОЕ ИССЛЕДОВАНИЕ НЕКОТОРЫХ ЭЛЕКТРОННЫХ ПЕРЕХОДОВ МОЛЕКУЛЫ BaD ДЛЯ АСТРОФИЗИЧЕСКИХ ПРИМЕНЕНИЙ

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Спектроскопические и колебательно-вращательные константы, факторы Франка–Кондона и r-центроиды для системы полос $A\,^2\Pi_{1/2}$–$X\,^2\Sigma$, $A\,^2\Pi_{3/2}$–$X\,^2\Sigma$, $B\,^2\Sigma$–$X\,^2\Sigma$, $E\,^2\Pi_{1/2}$–$X\,^2\Sigma$, $E\,^2\Pi_{3/2}$–$X\,^2\Sigma$, $F\,^2\Sigma$–$X\,^2\Sigma$ *и* $L\,^2\Pi$–$X\,^2\Sigma$ *молекулы дейтерида бария (BaD) рассчитаны с использованием методов численного интегрирования. Обсуждается важность полученных факторов Франка–Кондона и r-центроид для физических и астрофизических приложений. Из расчетов следует, что влияние колебательно-вращательного взаимодействия на факторы Франка–Кондона несущественно для враща-*

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тельных квантовых чисел $J < 50$. Для более высоких J, например $J = 100$, наблюдаются небольшие изменения факторов Франка–Кондона из-за эффекта колебательно-вращательного взаимодействия.

Ключевые слова: *молекула BaD, факторы Франка–Кондона, r-центроиды, эффект колебательно-вращательного взаимодействия, небесный объект.*

Introduction. The study of the spectra of diatomic molecules is of great importance in many research areas from physical chemistry to astrophysics and nuclear physics [1]. It is widely known that because of the high reactivity of diatomic molecules, many diatomic species are produced from gaseous or solid precursors which are frequently probed via astronomical observations. Among the astrophysically significant diatomic molecules, the light diatomic deuterides and in particular alkaline earth metal deuterides are of great importance for the understanding of chemical bonding and for the estimation of physical conditions of the astrophysical sources emitting the radiation. They have been the subject of many experimental and theoretical investigations [2].

The absorption spectra of such free radicals have been detected in different stars, comets, and interstellar medium (ISM); therefore, laboratory or theoretical spectroscopic investigations of these absorption spectra serve as a powerful tool to find correlation between these observations [3]. It is not surprising to find the presence of deuterium-containing species in astrophysical sources, and in fact molecules containing the deuterium atoms are sensitive probes for the conditions in the environments of solar system [4]. However, in the literature, there is a lag in the search for barium deuteride (BaD) molecule in celestial environment due to the unavailability of extensive sets of spectroscopic parameters derived from both theoretical and experimental observations.

The laboratory absorption spectrum of barium deuteride was extensively studied in the visible and ultraviolet (UV) regions by various researchers. Edvinsson et al. [5] had studied the absorption spectra of BaD molecule in the region 2500–3500 Å by observing the (0,0) and (1,0) bands of the *F–X* system. By investigating the various bands of *C–X* and *D–X* systems, the rotational analysis of the perturbed C and D states of BaD molecule was done by Kopp et al. [6]. Kopp et al. [7] studied the absorption spectra of BaD in the region 9200–11200 Å by recording the *A–X* band system using a concave grating spectrograph. Kopp and Wirhed [8] reported a detailed study on the rotational lines of the *B–X* band system. The rotational lines analysis of various bands of *E–X* system was performed, and the molecular constants of the electronic states of BaD molecule were also reported by Kopp and Wirhed [9]. Khan [10] reinvestigated the *F–X* band system of BaD molecule, and he reported a detailed rotational line analysis of the bands (0,1) and (1,0). A high-resolution absorption spectrum of BaD was recorded, and few intense bands of *K–X* and *L–X* were observed in the ultraviolet region by Baig et al. [11].

Though experimental studies on certain band systems of BaD molecule were reported in the literature, there is a lack of knowledge of their spectroscopic constants and transition probability parameters. In view of spectroscopy and astrophysics, parameters like molecular constants, Franck–Condon factors (FCFs), and *r*-centroids for the band systems *A*, *B*, *E*, *F*, *L–X* of BaD molecule have been evaluated in the present study by employing the numerical integration method, as of BaD molecule may be found in celestial objects like stars, comets, ISM, etc. A study related to the vibration rotation interaction (VRI) effect on FCFs has also not yet appeared in the literature for the band systems of BaD molecule, hence the present study also focuses on the effect of VRI on FCFs. In the present study, the band systems *C–X* and *K–X* are not considered, since the number of experimentally observed upper and lower vibrational levels (v', v'') for these two systems is (1,0) [9, 11] is not sufficient to compute the FCF matrix or array.

Theory. Franck–Condon factors and *r*-centroids: FCFs play an important role in theoretical modeling and interpreting the experimental observations for irradiative processes like electronic spectra of UV-Vis absorption and fluorescence as well as non-radiative processes like electron and energy transfer [12]. During a radiative transition from one electronic state to another electronic state in a diatomic molecule, the intensity of each individual transition between vibrational levels for an allowed electronic transition is mainly governed by the probability of overlap of vibrational wave functions of the upper and lower states ($\Psi_{v'}$ and $\Psi_{v''}$). Such expectation value or probability is termed FCFs. Mathematically, the FCF can be written as [1]

$$q_{v',v''} = |\langle\Psi_{v'}|\Psi_{v''}\rangle|^2, \qquad (1)$$

Another spectroscopic parameter called *r*-centroid is also found to be of much importance as it can be used i) in the interpretation of intensity measurements of many band systems of astrophysically important molecules; ii) in the determination of the variation of the electronic transition moment with inter-nuclear separation; and thereby iii) in the derivation of band strengths and other molecular transition probability parameters [13]. It is known that the expression for the r-centroid is [1]

$$\tilde{r}_{v'v''} = \frac{< \Psi_{v'} \,|\, r \,|\, \Psi_{v''} >}{< \Psi_{v'} \,|\, \Psi_{v''} >}, \tag{2}$$

where r is the internuclear distance (in Å). The physical meaning of r-centroid may be understood from the above equation. The r-centroid is seen to be a weighted average with respect to $\Psi_{v'}\Psi_{v''}$ of the range of r values experienced by the molecule during an electronic transition.

Computational procedure. It is clear from the above mathematical expressions that the accuracy of $q_{v'v''}$ and $\tilde{r}_{v'v''}$ depends mainly on the wave functions $\Psi_{v'}$ and $\Psi_{v''}$ which in turn depend on the potential energy curves used to solve the Schrodinger wave equation. Hence it is essential to follow the proper procedure to obtain the potential energy curves for both electronic states involved in the electronic transition. The various potential functions are available in the literature for the purpose of the calculation of FCFs and r-centroids. Among them, the Morse function is the most popular empirical potential function because of its simple form, and in many cases the Morse approach provides a good approximation and yields reliable FCFs and r-centroids. Therefore, the Morse procedure is adopted to construct the potential energy curves for the electronic states involved in the present study [14]. The spectroscopic constants ω_e, $\omega_e x_e$, r_e, and B_e are calculated by fitting the obtained energy values around the equilibrium position to a polynomial in terms of the internuclear distance. These values are displayed in Table 1 along with the constants available in the literature, and they are discussed in the following section.

TABLE 1. Spectroscopic Constant for the Electronic States of the BaD Molecule

State		r_e, in Å	ω_e, cm^{-1}	B_e, cm^{-1}
X	Experimental data [11,16]	2.230	829.77	1.7071
	Present study	2.231	840.74	1.7047
$A_{1/2}$	Experimental data [11,16]	2.259	788.85	1.6475
	Present study	2.224	836.27	1.7175
$A_{3/2}$	Experimental data [11, 16]	2.259	791.23	1.6598
	Present study	2.264	810.62	1.6567
B	Experimental data [11, 16]	2.298	772.99	1.6355
	Present study	2.301	819.31	1.6033
$E_{1/2}$	Experimental data [11, 16]	2.186	867.82	1.7653
	Present study	2.180	854.49	1.7897
$E_{3/2}$	Experimental data [11, 16]	2.186	872.19	1.7874
	Present study	2.189	885.29	1.7713
F	Experimental data [11, 16]	2.149	860.60	1.8376
	Present study	2.157	843.06	1.8224
L	Experimental data [11, 16]	2.162	921.70	1.8180
	Present study	2.155	912.27	1.8280

r_e – internuclear distance; ω_e – vibrational frequency; B_e – rotational constant.

From the dataset of potential energy curves, the values of maximum and minimum internuclear distance are calculated for all the experimentally observed vibrational levels involved in the electronic transition. The vibrational wave functions for all the vibrational levels in the electronic states involved in the present study are then calculated at the interval of 0.01 Å, having the lower and upper limits, say, 1.953 and 2.660 Å for $A\,^2\Pi_{1/2}$–$X\,^2\Sigma$, 1.953 and 2.653 Å for $A\,^2\Pi_{3/2}$–$X\,^2\Sigma$, 1.910 and 2.778 Å for $B\,^2\Sigma$–$X\,^2\Sigma$, 1.917 and 2.606 Å for $E\,^2\Pi_{1/2}$–$X\,^2\Sigma$, 1.911 and 2.606 Å for $E\,^2\Pi_{3/2}$–$X\,^2\Sigma$, 1.930 and 2.511 Å for $F\,^2\Sigma$–$X\,^2\Sigma$, and 1.900 and 2.528 Å for $L\,^2\Pi$–$X\,^2\Sigma$ band systems, respectively. After obtaining the vibrational wave functions, the values of $q_{v'v''}$ and $\tilde{r}_{v'v''}$ are obtained by solving Eqs. (1) and (2) using the Bates' method [15] of numerical integration, and they are given in Tables 2–6. The experimentally derived molecular constants used in the present study are taken from [11, 16].

Effect of VRI on FCFs. The present study is mainly towards the prediction of the existence of BaD molecular lines in the spectra of sunspot. To predict the existence of a diatomic molecule in sunspot, one can therefore use vibrational data like transition probability parameters, oscillator strength, vibrational temperature, etc. However, it is necessary to ensure that the FCF value is not get affected by the energy associated with the rotational movement of a diatomic molecule. Such influence is sometimes called vibration rotation interaction (VRI) effect. The intensity of a vibration-rotation line of a diatomic molecule can be significantly influenced by VRI [17]. In the literature one can find reports on the investigation of the dependence of wave functions and FCFs on the rotational quantum number J [18, 19]. Under VRI condition, the minimum of the effective potential can be shifted from r_e to r_0, as shown by the formula given by Shumaker [19]:

$$r_0 = r_e[1 + 4B_e^2 J(J + 1)/\omega_e^2], \tag{3}$$

where r_e is the equilibrium internuclear distance, in Å, B_e is the rotational constant, cm^{-1}, and ω_e is the vibrational frequency, cm^{-1}. Knowledge of the value of $|\Delta r - \Delta r_e|$ during a transition helps us to infer the effect of VRI on FCFs because the FCF depends on the change in r_0 with J [20]. This VRI effect is sometimes negligible in the case of few diatomic molecules, especially for relatively lower rotational quantum numbers. However, the influence of VRI on FCFs for higher values of J may be appreciable. Hence, it is essential to verify this dependence using the above equation, for further application of the derived vibrational probability parameters. Pertaining to this aspect, the present study deals with the effect of VRI on FCFs for certain band systems of BaD molecule using the available molecular constants [16], and the results are discussed in the following section.

Results and discussion. A comparison between the values for the internuclear distance r_e, the vibrational frequency ω_e and the rotational constant B_e calculated from the Morse potential energy curve and the experimental data available in the literature are given in Table 1. The experimental and the theoretical values for r_e are in excellent agreement, where the relative error for r_e among the different states varies from 0.04% for state X to 1.54% for state $A_{1/2}$. The relative error of r_e for the remaining states is 0.22, 0.13, 0.27, 0.13, 0.37, and 0.29% for states $A_{3/2}$, B, $E_{1/2}$, $E_{3/2}$, F, and L, respectively. Values of r_e are relatively close from one state to the other; for example r_e differs from the ground state by only 0.0074 Å for state $A_{1/2}$. The state L has the farthest minimum from that of the ground state, with the distance between corresponding minima equal to 0.076 Å. Such information can be valuable for radiative and nonradiative excitation experiments, pertaining to laser cooling and atom/molecule trapping.

The expression of the vibrational levels of BaD atomic molecules is generally given by

$$E_v = \omega_e(v + 1/2) - \omega_e x_e(v + 1/2)^2 + \omega_e y_e(v + 1/2)^3. \tag{4}$$

Values for the vibrational frequency ω_e are in very good agreement with experiment where the relative error values vary from 1.02% (state L) to about 6% (state B). Values of ω_e usually describe the shape of the potential energy curve, the steeper the curve: the higher the values of ω_e. The obtained curves in the present study were so steep that the values of the vibrational frequencies reached values as high as 912 cm^{-1} (for state L). Six states have relative error values for ω_e that are less than 3% (X, $A_{3/2}$, $E_{1/2}$, $E_{3/2}$, F, L), while the two remaining states present corresponding relative errors close to 6%.

On the other hand, two acceptable values were obtained for $\omega_e x_e$, i.e., with a relative error that is less than 10% (states L and $E_{1/2}$). Such results are generally not alarming, since such a high amount of precision rarely occurs in the calculation for the second order terms in the expression of the vibrational energy to match closely that of experiment.

The expression for the rotational constant of a diatomic molecule is given by

$$B_v = B_e - \alpha_e(v + 1/2) + ... \tag{5}$$

In our case, the calculated values for B_e are in excellent agreement with the experimental ones, where three of the states have relative error values for B_e that are less that 0.6% (X, $A_{3/2}$, and L), two have corresponding error values that are less than 1% ($E_{3/2}$ and F), and two with values less than 1.5% (B and $E_{1/2}$). The largest relative error that we obtained for B_e was for the state $A_{1/2}$, which had a value of 4.25%. Just as in the case of $\omega_e x_e$ for vibrational levels, the obtained values for the second term in the expression for the rotational constant (α) did not show agreement with experiment. This is also common as it rarely occurs that such a second term matches with its corresponding experimental value.

The remarkable correspondence between experiment and theoretical values for r_e, ω_e, and B_e shows that the Morse potential and the corresponding potential energy curves we used for our calculation are actually very accurate and reflect well the behavior of the BaD molecule, for both ground and excited states.

As rightly pointed out in [21–23] the FCF helps to specify the intensity of a vibronic transition and is defined by the square of the vibrational overlap of Eq. (1). Hence knowledge of accurate FCFs can yield band intensity data and other related important parameters. Tables 2–5 lists the values of FCFs and *r*-centroids with the corresponding experimental band wavelengths of various electronic transitions of BaD molecule. To avoid any chance of errors in FCFs as a result of the breakdown of the *r*-centroid approximation, FCFs smaller than 0.001 are ignored and are not included in the Tables. The experimentally available wavelengths of the bands are also included in the respective Tables [6–10]. The FCFs for the systems $A\,^2\Pi_{1/2}$–$X\,^2\Sigma$, $A\,^2\Pi_{3/2}$–$X\,^2\Sigma$, $B\,^2\Sigma$–$X\,^2\Sigma$, $E\,^2\Pi_{1/2}$–$X\,^2\Sigma$, $E\,^2\Pi_{3/2}$–$X\,^2\Sigma$, $F\,^2\Sigma$–$X\,^2\Sigma$, and $L\,^2\Pi$–$X\,^2\Sigma$ of the BaD molecule reveal that the (0,0) band is more intense than other bands. It is of interest to note that the next most prominent bands are (1,1) of $A_{1/2}$–X, (1,1) and (2,2) of $A_{3/2}$–X, (1,1) and (2,2) of B–X, (1,1) and (2,2) of $E_{1/2}$–X, (1,1) and (2,2) of $E_{3/2}$–X, (1,1) of F–X, and (1,1) of L–X, while all other bands are relatively weak. It is also found that the diagonal values of FCFs of all the band systems of the BaD molecule are greater than the others. In other words, the condon parabola degenerates into a straight line because the $\Delta v = 0$ sequence bands are more intense than $\Delta v = \pm1$ and ±2 sequence bands. Such kind of parabola degeneracy in the FCF array was observed in [24] for many diatomic molecules of astrophysical interest.

TABLE 2. Franck-Condon Factors and *r*-centroids of $A\,^2\Pi_{1/2}$–$X\,^2\Sigma$ and $A\,^2\Pi_{3/2}$–$X\,^2\Sigma$ Band System

v'/v''	Parameter	0	1	2	0	1	2
		$A\,^2\Pi_{1/2}$–$X\,^2\Sigma$			$A\,^2\Pi_{3/2}$–$X\,^2\Sigma$		
0	$q_{v'v''}$	0.979	0.021	*	0.979	0.021	*
	$\tilde{r}_{v'v''}$, Å	2.260	2.977		2.260	2.974	
	λ, Å	10443.22			10064.26		
1	$q_{v'v''}$	0.020	0.921	0.044	0.020	0.920	0.044
	$\tilde{r}_{v'v''}$, Å	1.562	2.291	2.956	1.565	2.291	2.954
	λ, Å	9695.00	10497.36		9339.80	10105.80	
2	$q_{v'v''}$	*	0.040	0.803	*	0.041	0.792
	$\tilde{r}_{v'v''}$, Å		1.637	2.321		1.650	2.319
	λ, Å			10552.95		9388.70	10148.52

* $q_{v'v''} \cong 0$.

TABLE 3. Franck–Condon Factors and *r*-centroids of $B\,^2\Sigma$–$X\,^2\Sigma$ Band System

v'/v''	Parameter	0	1	2
0	$q_{v'v''}$	0.896	0.103	0.003
	$\tilde{r}_{v'v''}$, Å	2.279	2.599	3.054
1	$q_{v'v''}$	0.095	0.699	0.196
	$\tilde{r}_{v'v''}$, Å	1.979	2.312	2.616
2	$q_{v'v''}$	0.008	0.164	0.515
	$\tilde{r}_{v'v''}$, Å	1.730	2.011	2.350
3	$q_{v'v''}$	0.001	0.019	0.204
	$\tilde{r}_{v'v''}$, Å	1.474	1.744	2.054

TABLE 4. Franck–Condon Factors and *r*-centroids of $E\,^2\Pi_{1/2}$–$X\,^2\Sigma$ and $E\,^2\Pi_{3/2}$–$X\,^2\Sigma$ Band Syster 156-6

v'/v''	Parameter	0	1	2	0	1	2
		$E\,^2\Pi_{1/2}$–$X\,^2\Sigma$			$E\,^2\Pi_{3/2}$–$X\,^2\Sigma$		
0	$q_{v'v''}$	0.954	0.043	0.002	0.954	0.044	0.002
	$\tilde{r}_{v'v''}$, Å	2.223	1.768	1.374	2.223	1.775	1.362
	λ, Å	6881.93	7277.11		6664.67	7038.64	
1	$q_{v'v''}$	0.046	0.857	0.077	0.047	0.856	0.081
	$\tilde{r}_{v'v''}$, Å	2.692	2.254	1.800	2.687	2.253	1.810
	λ, Å	6515.44	6856.66	7250.72	6318.58	6646.93	7114.80
2	$q_{v'v''}$	*	0.084	0.716	*	0.087	0.719
	$\tilde{r}_{v'v''}$, Å		2.713	2.281		2.710	2.280
	λ, Å		6506.36	6841.16		6309.83	6629.87

* $q_{v'v''} \cong 0$.

TABLE 5. Franck–Condon Factors and *r*-centroids of $F\,^2\Sigma$–$X\,^2\Sigma$ and $L\,^2\Pi$–$X\,^2\Sigma$ Band System

v'/v''	Parameter	0	1	0	1
		$L\,^2\Pi$–$X\,^2\Sigma$		$F\,^2\Sigma$–$X\,^2\Sigma$	
0	$q_{v'v''}$	0.886	0.107	0.843	0.131
	$\tilde{r}_{v'v''}$, Å	2.209	1.945	2.204	1.968
	λ, Å	27174.67			3344
1	$q_{v'v''}$	0.108	0.658	0.147	0.542
	$\tilde{r}_{v'v''}$, Å	2.506	2.234	2.448	2.233
	λ, Å	28078.27	27264.71	3166	
2	$q_{v'v''}$	0.003	0.165		
	$\tilde{r}_{v'v''}$, Å	2.875	2.526		
	λ, Å		28151.00		

Estimated values of *r*-centroid for the band systems $A_{1/2}$–*X*, $A_{3/2}$–*X*, and *B*–*X*, of the BaD molecule are found to increase with wavelength following $r_e' > r_e''$ which indicates that the bands are red degraded. In the case of $E_{3/2}$–*X*, *F*–*X*, and *L*–*X* band systems, *r*-centroid estimates are found to decrease with increasing wavelengths ($r_e' < r_e''$), which is likely to happen for blue degraded band system. It is worth mentioning that Kopp and Wirhed [9] also reported that the bands of *E*–*X* system are blue degraded.

The *r*-centroid values for (0,0) transition of all the investigated systems are slightly greater than $(r_e' + r_e'')/2$ and are found to have approximately a constant value of 0.01 Å which reveals that the potentials are not much anharmonic [25]. The values of sequence differences of *r*-centroids reflect a valuable information: the potential energy curves involved in the present study are broad because the values of sequence differences for all the band systems are found to be around 0.03 Å.

Table 6 provides the values of Δr_e and $|\Delta r_0 - \Delta r_e|$ for two different rotational quantum numbers. For all the band systems of the BaD molecule, $|\Delta r_0 - \Delta r_e|$ increases with increasing *J* values, which tells us that the FCFs are significantly affected with increasing *J* values. Thus it is advisable to consider the effect of VRI on FCFs at the time of search of the BaD molecular lines in the spectra of celestial object. However, the calculated FCFs for the BaD molecular vibronic transitions may act as supportive evidence or the guiding parameter at the time of searching for the presence of BaD molecule in a chosen astrophysical source.

TABLE 6. Δr_e and $|\Delta r_0 - \Delta r_e|$ Values for Band Systems of the BaD Molecule

Band System	Δr_e, Å	$\|\Delta r_0 - \Delta r_e\|$, Å	
		$J = 50$	$J = 100$
$A\,^2\Pi_{1/2} - X\,^2\Sigma$	0.029	0.00381	0.01628
$A\,^2\Pi_{3/2} - X\,^2\Sigma$	0.029	0.00471	0.01982
$B\,^2\Sigma - X\,^2\Sigma$	0.068	0.00824	0.03382
$E\,^2\Pi_{1/2} - X\,^2\Sigma$	0.044	0.00443	0.01635
$E\,^2\Pi_{3/2} - X\,^2\Sigma$	0.044	0.00305	0.01089
$F\,^2\Sigma - X\,^2\Sigma$	0.080	0.00328	0.01418
$L\,^2\Pi - X\,^2\Sigma$	0.068	0.01091	0.04203

As mentioned in the Introduction, there is no significant result reported in the literature corresponding to the prediction of BaD molecular lines in the spectral atlas of any astrophysical sources. However, several authors made an extensive study on the molecular parameters like partition functions, dissociation energies, etc., for the astrophysically significant diatomic molecules including the hydride and deuteride of barium [26, 27]. Most deuterated molecules detected to date are in the form of either saturated molecules or ions, and their observation could provide an important clue to the formation process of the major deuterated species [28]. Hence, the present study will be helpful towards the search and identification of BaD molecule in the celestial environment following the line identification technique [29, 30].

Conclusion. The electronic properties of the BaD molecule are investigated. The spectroscopic and rovibrational constants have been calculated and compared with experimental data. Contrarily to previous studies [31–33], the constants have been deduced by using the Morse procedure to construct the potential energy curves. Still, the obtained results are in perfect accordance with experiment. The vibronic transition probability parameters FCFs and r-centroids have been calculated for $A^2\Pi_{1/2}$–$X\,^2\Sigma$, $A^2\Pi_{3/2}$–$X\,^2\Sigma$, $B\,^2\Sigma$–$X\,^2\Sigma$, $E\,^2\Pi_{1/2}$–$X\,^2\Sigma$, $E\,^2\Pi_{3/2}$–$X\,^2\Sigma$, $F^2\Sigma$–$X\,^2\Sigma$, and $L^2\Pi$–$X\,^2\Sigma$ band systems of the BaD molecule. The FCF results show that in most of cases were $\Delta v = 0$, sequence bands are more intense, which is quite natural for the absorption spectra of astrophysically significant molecules. It is well known that for applications to the spectroscopy of cooler stellar envelopes, it is compulsory to know which absorption bands of the vibronic transitions of diatomic molecule are strong or more intense. In this aspect, the FCFs and r-centroids derived in the present study along with the line or band wavelengths data are thus useful for molecular identification purposes, as well as for diagnostic purposes and radiative transfer calculations for a celestial object.

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