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Examining barium deuteride molecules in sunspots

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Diatomic molecules in space have been studied for many years; in particular alkaline earth-free radicals like mono-halides, hydrides, and deuterides have been the subject of many experimental and theoretical investigations (Berg et al. 1997). Mashonkina & Gehren (2000) reported that the elemental ratios [Ba/Fe], [Eu/Fe], and [Eu/Ba] influence stars differently in different Galactic populations. They also discovered that barium is produced by the s-process in evolved low mass stars. Andrievsky et al. (2009) reported that barium is a key element in constraining the evolution of the r-process in the first galactic stars. As yet, Ba abundances in these very metal-poor stars have mainly been measured under the Local Thermodynamical Equilibrium (LTE) assumption. It is not surprising to find deuterium in astrophysical sources and in fact molecules containing the deuterium atom are sensitive probes for observing the environmental conditions of the solar system (Schelmer et al. 2014). Experimental studies exist of certain band systems of the barium deuteride (BaD) molecule; yet there is no prediction of the BaD molecule in sunspots. This study focuses on the search for BaD molecular lines in the sunspot spectra using the line identification technique (Karthikeyan et al. 2010).

To examine the abundance of the BaD molecule in sunspots, we carried out a careful search for BaD molecular lines using high-resolution Fourier Transform Spectra (FTS) of sunspots provided by Wallace et al. (1998) and Wallace et al. (2000). The rotational lines of the A–X band system were recorded by Kopp et al. (1966). The nine bands corresponding to the B–X system between 10100 and 11840cm^{-1} were investigated by Kopp and Wirhed (1966). Later, the E–X and E–X band systems of BaD were recorded in the range 13750-16210 cm^{-1} by Kopp and Wirhed (1967). It is noteworthy that there is no available ultraviolet sunspot spectrum in the respective region of the F, L–*X* system. As a result we chose only

five band systems in our search for the BaD molecular lines in sunspot spectra using the line identification technique. The number of chance coincidences (*C*) and *I*-parameter for the bands of the A–X, B–X, E–X system of the BaD molecule were calculated using the formula available in the literature (Karthikeyan et al. 2010; Shanmugapriya et al. 2015).

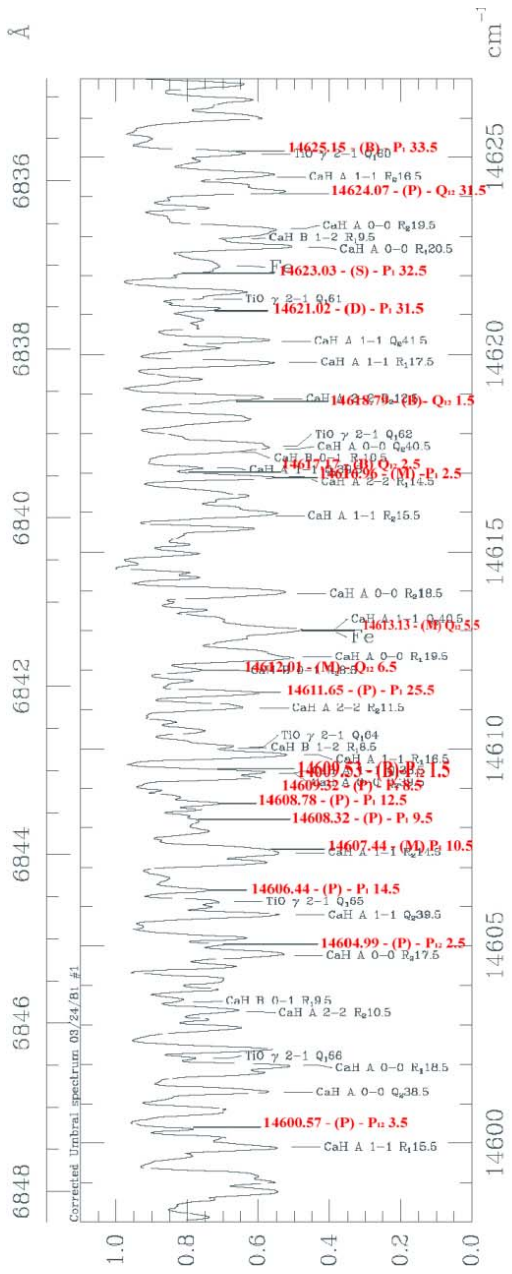

Figure 1(a)

System	Band	Wavenumber range(cm⁻¹)	N	W	C(cm⁻¹)	I
$E^2\Pi_{1/2}-X^2\Sigma$	(0,0)	14526.79–14894.76	244	3.4	121	65
	(1,1)	14561.24–14923.38	212	3.7	110	77
	(2,2)	14613.37–14885.48	114	3.5	57	26
	(1,0)	14343.92–14703.85	222	3.2	104	77
	(2,1)	15365.32–15658.00	193	2.6	**68**	**70**
	(0,1)	13737.92–14114.43	222	2.2	78	51
	(1,2)	13790.77–14157.72	224	2.2	80	60
$E^2\Pi_{3/2}-X^2\Sigma$	(0,0)	15000.35–15442.36	261	2.2	**93**	**102**
	(1,1)	15040.86–15542.48	248	2.1	84	78
	(2,2)	15079.09–15425.68	134	2.9	62	34
	(1,0)	15821.96–16236.65	256	2.1	86	49
	(2,1)	15843.93–16212.05	227	2.5	89	56
	(0,1)	14205.88–14529.39	243	2.7	100	64
	(1,2)	14258.63–14527.85	183	2.9	81	32
$A^2\Pi_{1/2}-X^2\Sigma$	(0,0)	9080.85–9473.42	261	2.8	111	56
	(1,1)	9523.59–9123.09	197	1.5	**51**	**62**
	(2,2)	9080.85–9473.42	168	2.6	68	45
	(1,0)	9932.78–10311.75	183	2.5	72	25
	(2,1)	9876.00–10249.00	164	2.5	64	30
$A^2\Pi_{3/2}-X^2\Sigma$	(0,0)	9557.00–10024.00	285	2.9	124	81
	(1,1)	9570.00–9976.00	242	2.4	**89**	**91**
	(2,2)	9615.00–9928.00	181	2.9	75	57
	(1,0)	10501.00–10768.00	155	1.2	**30**	**33**
	(2,1)	10497.00–10708.00	146	2.0	33	29
$D^2\Sigma-X^2\Sigma$	(8,0)	23575.90–23892.25	79	1.3	18	17
	(9,0)	24153.97–23564.70	100	1.3	23	18
	(10,0)	23773.38–24385.09	61	1.2	**13**	**21**
$B^2\Sigma-X^2\Sigma$	(0,0)	10666.96–11083.88	197	1.6	**53**	**54**
	(1,0)	11416.50–11870.97	177	2.9	**77**	**78**
	(1,1)	10608.55–11069.93	179	1.5	47	28
	(0,1)	10076.89–10341.81	146	2.1	49	23
	(2,1)	11405.25–11795.75	162	2.9	71	67
	(2,2)	10694.10–11008.45	142	1.4	35	30
	(1,2)	10095.33–10289.62	94	2.0	31	26
	(3,2)	11400.74–11719.16	125	2.8	53	38
	(3,3)	10723.03–10946.26	61	1.5	16	17

Figure 1(b)

Figure 1. (a) A portion of the sunspot spectrum marked with the rotational lines of BaD molecule; (b) C-index and I-parameter values obtained in the chosen range

Out of 6488, 1767 lines including the categories Present (P), Shoulder (S), and Blend (B) were considered to be identified. Figure 1 (a) shows a section view of the sunspot umbral spectrum with rotational lines of the E –X systems of the BaD molecule. Figure 1 (b) shows the calculated *I*-parameter and *C*-index values for the chosen bands of the A–X , B–X and E-X systems. The number of laboratory lines searched (N) and the line density (W) are also displayed in the figure 1(b). The existence of diatomic molecules is assumed only when the *I*-parameter is significantly greater than the *C*-index. However, the number of lines we identified from the observed spectra (I) is slightly higher than the number of chance coincidences (C) for only a few bands of the investigated systems of the BaD molecule. For other bands, the *I*-parameter is slightly lower than the *C*-index. Because sunspots exhibit favorable conditions for the existence of the BaD molecule, results from the chance coincidence technique do not predict the BaD molecule. This may be due to the overlapping of BaD molecular lines with other atomic and molecular lines confirmed in the sunspot spectra. The present study therefore confirms that the presence of the BaD molecule in sunspots is still questionable. Future work on accurate laboratory spectrum may help to resolve this question.

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