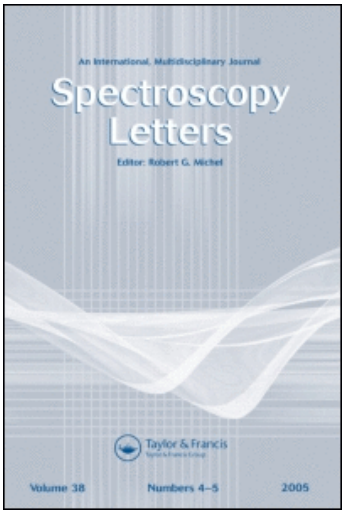

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Vibrational Constants of the B-X System of LaO Using Rotational Data

Carlos B. Suarez[a]
[a] Departamento de Fisica, Universidad Nacional de La Plata and Consejo Nacional de Investigaciones Cientificas y Tecnicas, La Plata, ARGENTINA

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VIBRATIONAL CONSTANTS OF THE B-X SYSTEM OF LaO USING ROTATIONAL DATA.

Key words: Spectroscopy-Diatomics- Vibrational constants.

Carlos B. Suarez
Departamento de Fisica, Universidad Nacional de La Plata and Consejo Nacional de Investigaciones Cientificas y Tecnicas, C.C. 67, 1900 La Plata, ARGENTINA.

In order to derive precise vibrational constants of diatomic molecules the usual procedure needs the origins of rotationally analysed bands. However,the knowledge of these origins is a very hard task,and most commonly only a few bands are known with such a detail. For that reason, we have chosen a procedure suggested by Jenkins and McKellar [1], that we followed with corresponding branches of the 1-0, 0-0 and 0-1 bands of the B-X system of LaO. For consistency, only measurements reported by Åkerlind [2] were used throughout.

The number of rotationally analysed bands were not sufficient to obtain w_e and $w_e x_e$ directly. We then used the Pekeris [3] relation,with which both constants were fixed after a few iterations.

The values obtained for the B and X states are given in Table 1, together with the other necessary molecular parameters. A comparison with previous reported figures is in order,and Table 2 shows results from Schoonveldt and Sundaram [4], Green [5] and Huber and Herzberg [6].

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TABLE 1

Spectroscopic Constants of LaO B-X Band System: σ_e =17837.80 cm^{-1}

State	w_e	$w_e x_e$	B_e	α_e	$\Delta G_{1/2}$
B	735.71	2.65	0.3414	0.00170	730.40
X	817.23	2.24	0.3526	0.00139	812.74

TABLE 2

Comparison of Vibrational Constants

	ref.6		ref.5		ref.4		this work	
X	812.75	2.22	817.26	3.097 #	817.22 a	2.21	817.23	2.24
					815.67 b	2.549		
B	730.40	2.04	-	-	734.59	2.06	735.71	2.65

using a three-term polynomial.
a from A-X and B-X transitions.
b from C-X transition.

TABLE 3

Centrifugal Distorsion Constants D_v ($\times 10^6$)

State	D_0	D_1	D_2	remarks
B	0.295	0.293	0.292	calc.,this work
	0.25	0.2		Åkerlind[2]
	0.2914	0.285		B and S, ref.7
X	0.263	0.265	0.266	calc.,this work
	0.26	0.26		Åkerlind[2]
	0.2579	0.2667		B and S, ref.7

In order to check the values obtained in this work, we have performed a numerical integration to obtain the centrifugal distorsion constants D_v which requires as input of the calculation the vibrational constants proposed here, apart of the rotational constants. The results are given in Table 3 and are compared with the graphically obtained by Åkerlind [2], and with the values reported by Bernard and Sibai [7] from a global treatment of all the data known for LaO .The agreements found are very good.

To summarize, we think that whenever possible, this method using rotational data is to be preferred because it leads to improved vibrational constants.

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