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

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

Key words: Spectroscopy-Diatomics- Vibrational constants.

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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<sup>1</sup>, 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<sup>2</sup> were used throughout.

The number of rotationally analysed bands were not sufficient to obtain  $w_3$  and  $w_4$  directly. We then used the Pekeris 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<sup>4</sup>, Green<sup>5</sup> and Huber and Herzberg<sup>6</sup>.

TABLE 1

Spectroscopic Constants of LaO B-X Band System:  $\sigma_e = 17837.80 \text{ cm}^{-4}$

State	w e	w x e e	B e	$\alpha$ 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 <sup>a</sup> 815.67 <sup>b</sup>	2.21 2.24 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 Distortion 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		<sup>a</sup> Akerlind
	0.2914	0.285		B and S, ref. 7
X	0.263	0.265	0.266	calc., this work
	0.26	0.26		<sup>a</sup> Akerlind
	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 distortion 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,<sup>2</sup> and with the values reported by Bernard and Sibai<sup>7</sup> 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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