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Fourier-transform infrared emission spectroscopy of BO

G. Li, R.J. Hargreaves, J.-G. Wang, P.F. Bernath *

Department of Chemistry, University of York, Heslington, York YO10 5DD, UK

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ABSTRACT

The Fourier-transform infrared emission spectra of BO were recorded using a Bruker IFS 125 HR spectrometer. The observed spectrum of BO in the 1200–2100 cm^{-1} region contains three bands: the fundamental bands of ^{11}BO and ^{10}BO and a hot band of ^{11}BO with band origins measured to be 1861.9242(97), 1915.3071(09) and 1838.3773(68) cm^{-1}, respectively.

1. Introduction

The semi-metal boron has a very rich chemistry and its compounds have many potential applications such as solid state fuel for air-breathing rockets [1], hydrogen storage materials [2], and the proton boron-11 fusion reaction [3]. As an intermediate product formed during the boron combustion process, boron monoxide (BO) has been extensively studied since 1925 when two emission band systems, $A\ ^2\Pi$–$X^2\Sigma^+$ and $B^2\Sigma^+$–$X^2\Sigma^+$ were first identified by Mulliken [4]. The two most important high resolution measurements on these electronic band systems were carried out by Coxon et al. [5] and Mélen et al. [6].

In 1985 the microwave spectrum of BO was recorded by Tanimoto et al. [7]. More recently, an infrared measurement of the BO fundamental band was performed by Stancu et al. [8] using diode laser spectroscopy. However, the microwave and diode laser measurements only probed the $v = 0$ and $v = 1$ vibrational levels of the ground state of BO. Moreover, in the infrared laser study, only 19 lines and 12 lines for the fundamental bands of $^{11}B^{16}O$ and $^{10}B^{16}O$ were observed, respectively, and no hot bands were detected.

The Fourier transform measurements presented here contained the fundamental bands of both isotopic species, ^{11}BO and ^{10}BO, along with one hot band of the main isotopologue ^{11}BO with 95, 72 and 64 lines, respectively. In the previous infrared work [8] the $O + BCl_3$ reaction was used to synthesize BO, which required very specific experimental conditions.

2. Experimental

A full description of the high temperature tube furnace experiment setup can be found elsewhere [9]. In the present study, an alumina boat containing a mixture of equal amounts of boron pieces and boron oxide (B_2O_3) powder was placed in the centre of an alumina tube. The system was evacuated and steadily heated to 1400 °C over a period of 4 h. A piece of zirconia felt was placed between the alumina boat and the tube furnace to prevent the reaction of the reactant with the tube wall. The pumping speed was controlled using a valve and 2 Torr of argon buffer gas was introduced into the tube.

Initially the strong HBO v_3 band [10] was observed at temperatures above 1300 °C. The hydrogen atoms needed to form HBO presumably came from water impurities. BO molecules were then produced by applying a DC discharge (3 kV, 333 mA) to the tube containing HBO. The HBO molecule was the precursor of BO because the HBO signal decreased when the discharge was applied and BO was synthesised. A few mTorr of water vapor was introduced into the tube by passing the argon carrier gas through a glass bubbler to facilitate the production of HBO and BO. High resolution infrared emission spectra of ^{11}BO and ^{10}BO were recorded using a Bruker IFS 125 HR spectrometer using a CaF_2 beam splitter and a MCT detector with a 2200 cm^{-1} long pass filter to cover the 1200–2100 cm^{-1} spectral range.

3. Results and discussion

Fig. 1 shows an expanded portion of the BO spectrum. The figure shows lines from the fundamental bands of ^{11}BO and ^{10}BO and the 2–1 hot band of ^{11}BO with the rotational line assignments marked above. Other unassigned features in this spectrum are due to HBO. It should be noted that the ^{11}BO lines are much more intense than the ^{10}BO lines due to the 4:1 natural abundance ratio of the ^{11}B and ^{10}B isotopes. The observed lines display no spin doubling.

* Corresponding author. Fax: +44 1904 432516.
E-mail address: pfb500@york.ac.uk (P.F. Bernath).

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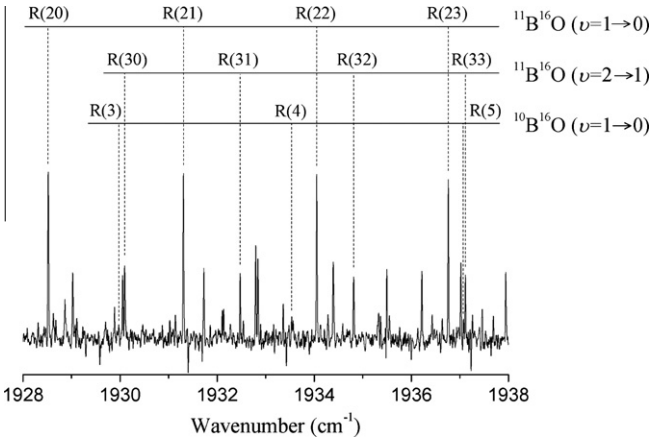

Fig. 1. Emission lines from the two fundamental bands of $^{11}B^{16}O$ and $^{10}B^{16}O$, and the v = 2–1 hot band of the main isotopologue $^{11}B^{16}O$ recorded by Fourier transform spectroscopy. The unmarked features are due to HBO.

The BO spectrum was calibrated with the NIST CO line list [11] and the absolute accuracy of this calibration is better than 0.0002 cm^{-1}. The lines were fitted with a Voigt lineshape function using M. Carleer's WSpectra program [12]. The general accuracy of strong blended lines is better than 0.0004 cm^{-1}, but many lines are overlapped by HBO and were de-weighted. A Loomis-Wood program was then used to identify the bands with the J values assigned using lower state combination differences. The measured wavenumbers of the lines together with the microwave data and the diode laser data were then fitted as $^1\Sigma$–$^1\Sigma$ transition. The accuracy of unblended infrared lines was taken as 0.0004 cm^{-1} and the accuracy of the microwave lines was taken as 0.03 MHz.

Band origins from Stancu et al. [8], 1861.92409(13) and 1915.30674(14) cm^{-1}, for ^{11}BO and ^{10}BO respectively, are in very good agreement with our fitted results, 1861.9242(97) and 1915.3071(09) cm^{-1} (Table 1). Furthermore, the 2–1 band of ^{11}BO was measured for the first time and the origin was derived from the least-squares fit to be 1838.3773(68) cm^{-1}. The vibrational parameters, ω_e and $\omega_e x_e$, for ^{11}BO were determined to be 1885.4712(27) and 11.7734(65) cm^{-1}, respectively, which are listed in Table 2. For comparison, molecular parameters derived from previous diode laser and electronic spectral measurements are also provided in Table 2. The previously measured values for ω_e do not satisfactorily agree each other (see Table 2), presumably partly because different numbers of vibrational levels were included in their determination from the lower resolution electronic spectra.

Table 1
Fitted molecular parameters (in cm^{-1}) for BO ($X^2\Sigma^+$).

	Present work	Infrared laser[a]	Electronic[b]	Microwave[c]
	$^{11}B^{16}O$			
B_0	1.7734100(72)	1.773421(10)	1.772861(79)	1.77341071(15)
D_0	$6.3486(37) \times 10^{-6}$	$6.42(3) \times 10^{-6}$	$6.236(35) \times 10^{-6}$	$6.3871(9) \times 10^{-6}$
B_1	1.7568518(36)	1.756845(9)	1.756263(83)	
D_1	$6.3465(91) \times 10^{-6}$	$6.33(2) \times 10^{-6}$	$6.189(39) \times 10^{-6}$	
B_2	1.7402701(15)	–	1.739767(82)	
D_2	$6.3462(75) \times 10^{-6}$	–	$6.253(38) \times 10^{-6}$	
v_0	1861.9242(97)	1861.92409(13)	1861.965	
v_1	1838.3773(68)	–		
	$^{10}B^{16}O$			
B_0	1.8776711(80)	1.877680(22)	1.87714(10)	1.87767255(22)
D_0	$7.1151(16) \times 10^{-6}$	$7.10(13) \times 10^{-6}$	$6.983(60) \times 10^{-6}$	$7.1986(12) \times 10^{-6}$
B_1	1.8596270(04)	1.859662(25)	6.854(72) $\times 10^{-6}$	
D_1	$7.1133(63) \times 10^{-6}$	$7.28(17) \times 10^{-6}$	6.854(72) $\times 10^{-6}$	
v_0	1915.3071(09)	1915.30674(14)	1915.36	

[a] Ref. [8].
[b] Ref. [6].
[c] Ref. [7].

Table 2
Derived molecular parameters (in cm^{-1}) for BO($X^2\Sigma^+$).

	Present work	Infrared laser[a]	Mélen et al.[b]	Coxon et al.[c]
	$^{11}B^{16}O$			
ω_e	1885.4712(27)	1885.552(28)[d]	1885.286(41)	1885.579(32)
$\omega_e x_e$	11.7734(65)	–	11.694(11)	11.825(14)
B_e	1.7816989(75)	1.781709(7)	1.781110(31)	1.781366(50)
D_e	$6.3489(40) \times 10^{-6}$	$6.47(1) \times 10^{-6}$	$6.247(14) \times 10^{-6}$	
α_e	$1.65699(78) \times 10^{-2}$	$1.6576(14) \times 10^{-2}$	$1.6516(17) \times 10^{-2}$	$1.6444(19) \times 10^{-2}$
r_e(Å)	1.2045531(45)	1.204550(4)	–	–
	$^{10}B^{16}O$			
ω_e	–	1940.202(38)[d]	1940.308(23)	1940.218(41)
$\omega_e x_e$	–	–	12.4873(42)	12.433(19)
B_e	1.8866932(68)	1.886689(17)	1.886154(46)	1.886250(82)
D_e	$7.1159(93) \times 10^{-6}$	$7.01(10) \times 10^{-6}$	$6.928(20) \times 10^{-2}$	–
α_e	$1.80441(76) \times 10^{-2}$	$1.8018(34) \times 10^{-2}$	$1.8107(13) \times 10^{-2}$	$1.7894(77) \times 10^{-2}$
r_e(Å)	1.2045605(87)	1.204561(9)	–	–

[a] Ref. [8].
[b] Ref. [6].
[c] Ref. [5].
[d] Ref. [8]. (Note: this value was calculated by using the anharmonicity parameter from Coxon et al.).

The rotational constant, B_0 of 1.7734100(72) and 1.8776711(80) cm^{-1} for ^{11}BO and ^{10}BO, respectively, have been derived from the least-squares fit. Both results are in very good agreement with the values 1.77341071(15) and 1.87767255(22) cm^{-1} determined from the microwave measurements [7]. These results are also in good agreement with the infrared laser results, which are also listed in Table 1. By assuming the usual linear dependence of B_v with respect to v [13], the B_e and α_e parameters were derived and the results are given in Table 2. The equilibrium bond length r_e were derived for both isotopic species, which are 1.2045531(45) and 1.2045605(87) Å for ^{11}BO and ^{10}BO, respectively.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.jms.2010.07.006.

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