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Jönsson, Per; Johansson, S. G; Fischer, C. F

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PO Box 117
221 00 Lund
+46 46-222 00 00

ACCURATE CALCULATION OF THE ISOTOPE SHIFT AND HYPERFINE STRUCTURE IN THE BORON (B II) LINE AT 1362 Å

PER JÖNSSON

Department of Physics, Lund Institute of Technology, P.O. Box 118, S-221 00 Lund, Sweden

SVENERIC G. JOHANSSON

Department of Physics, University of Lund, Sölvegatan 14, S-223 62 Lund, Sweden

AND

CHARLOTTE FROESE FISCHER

Department of Computer Science, Vanderbilt University, Box 1679B, Nashville, TN 37235

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ABSTRACT

An extensive multiconfiguration Hartree-Fock (MCHF) calculation of the isotope shift and hyperfine structure in the resonance line of B II at 1362 Å has been performed. The calculated ^{11}B – ^{10}B isotope shift is 13.3 mÅ with an estimated uncertainty of 1%. The calculated interaction constants A and B give a hyperfine structure splitting of less than 0.45 mÅ for both isotopes. The size of the isotope shift in the B II line is similar to the limit of detection in high-resolution observations with the Goddard High Resolution Spectrograph aboard the *Hubble Space Telescope* when side A becomes operational after the service mission.

Subject headings: atomic data — line: identification — Galaxy: evolution — ultraviolet: general

1. INTRODUCTION

The cosmic abundance of the light elements lithium, beryllium, and boron is of particular interest as they are not natural products of nucleosynthesis reactions inside stars. Spallation by cosmic rays and primordial (big bang) nucleosynthesis are two probable processes suggested for the generation of these elements. In the case of boron, the relative abundance of the two stable isotopes (^{10}B and ^{11}B) provides additional information to check the proposed production processes; for example, supernovae are supposed to be major suppliers of ^{11}B to the Galaxy (see, e.g., Duncan, Lambert, & Lemke 1992). The size of the isotope shift of ground-term transitions of B I and B II is of the order of 10–30 mÅ. The low abundance of boron and the absence of metastable states at low excitation potential means that only transitions from the ground term (resonance lines) are observed in astrophysical spectra. All such lines in B I and B II appear below 3000 Å and require space observations at high signal-to-noise ratio and high resolution. Recent observations with the Goddard High Resolution Spectrograph (GHRS) of the *Hubble Space Telescope* have been aimed at studies of the B I resonance lines at 2497 Å (Duncan et al. 1992; Edvardsson et al. 1994) at medium (25,000) and high (90,000) spectral resolution, respectively. Johansson et al. (1993) measured the isotope shift in these lines to be only 11 mÅ and suggested that the B I lines at 2090 Å, having an isotope shift of 25 mÅ, would be better candidates for the study of isotopic ratios. However, the ionization balance in moderate temperature stars as well as in the ISM suggests that B II would be more abundant than B I and therefore B II would be the suitable diagnostic tool. The resonance line of B II appears at 1362 Å, and it was recently observed in medium-resolution GHRS spectra of the interstellar medium toward ζ Ophiuchi (Federman et al. 1993). The outcome of the Service Mission to *HST* in 1993 December will soon show if it will be possible to observe the B II line with *HST*/GHRS in the high-resolution mode.

Recent progress in large-scale variational calculations,

together with today's powerful computers, has made it possible to calculate spectroscopic properties of light atoms with very high accuracy (Tong, Jönsson, & Froese Fischer 1993; Jönsson & Froese Fischer 1993; Carlsson et al. 1994). In the present *Letter* we have calculated the isotope shift splitting of the B II $1s^2 2s^2 \ ^1S$ – $1s^2 2s 2p \ ^1P$ resonance line at 1362 Å with an estimated uncertainty of less than 1%. This should be compared with the previous theoretical value (Clark 1984), for which the uncertainty was estimated to be about 10%–20%, which is not sufficiently accurate to examine the feasibility for measurements of the isotope shift with GHRS. The hyperfine structure (hfs) splitting of the $1s^2 2s 2p \ ^1P$ state has also been calculated for both isotopes, and it turns out to be much smaller than the isotope shift.

2. ISOTOPE SHIFT AND HYPERFINE STRUCTURE

The starting point for nonrelativistic atomic calculations is the zero-order Hamiltonian

$$H_0 = \sum_{i=1}^N \left(-\frac{\nabla_i^2}{2m} - \frac{Z}{r_i} \right) + \sum_{i < j}^N \frac{1}{r_{ij}}, \quad (1)$$

where the nucleus is assumed to be a point charge of infinite mass. When the effects of the finite nuclear mass and size are taken into account, the calculated energy levels are slightly shifted. Energy levels of different isotopes of an element are shifted differently, leading to the so-called level isotope shift. In general, the atomic nucleus possesses higher order electromagnetic moments, not included in the zero-order Hamiltonian, that interacts with the electrons. The inclusion of these interactions leads to the hyperfine structure splitting of the calculated levels. All the above effects are small and can to a very good approximation be treated in first-order perturbation theory.

2.1. Isotope Shift

For a finite nuclear mass, M , the kinetic energy of the nucleus must be considered. Using the momentum conserva-

TABLE 1
SPECIFIC MASS SHIFT PARAMETER, ELECTRON DENSITY AT THE NUCLEUS AND TOTAL ENERGY (in a.u.) FOR THE
1s²2s²1S AND 1s²2s2p¹P TERMS IN B II AS A FUNCTION OF THE INCREASING ACTIVE SET OF ORBITALS

ACTIVE SET	1s ² 2s ² 1S				1s ² 2s2p ¹ P			
	S (a.u.)	\psi(0) ²	E ₀ (a.u.)	Ncfg ^a	S (a.u.)	\psi(0) ²	E ₀ (a.u.)	Ncfg ^a
hf	0.00000	72.629	-24.237575	1	-0.40398	70.752	-23.912873	1
2s1p	-0.02017	72.452	-24.296413	5	-0.40107	70.748	-23.913062	4
3s2p1d	0.62518	72.490	-24.334812	63	0.29144	70.692	-23.988668	98
4s3p2d1f	0.62481	72.497	-24.342409	460	0.25636	70.714	-24.001844	713
5s4p3d2f1g	0.60169	72.501	-24.346046	1066	0.27732	70.712	-24.008886	2300
5s4p3d2f1g ^b	0.60166	72.501	-24.346052	2432	0.27734	70.712	-24.008921	5654
6s5p4d3f2g1h	0.59803	72.503	-24.347410	2306	0.27459	70.717	-24.011624	5211
7s6p5d4f3g2h1i	0.59709	72.504	-24.347943	4200	0.27330	70.719	-24.012990	9772

NOTE.—The total energy has been calculated from the zero-order Hamiltonian.

^a Number of configuration state functions in the wavefunction expansion.

^b Complete active space CI calculation. No restriction on the excitations.

tion law in the center-of-mass coordinate system, the operator for the internal kinetic energy of an N -electron atom becomes

$$H_{\text{kin}} = - \sum_{i=1}^N \frac{\nabla_i^2}{2\mu} - \frac{1}{M} \sum_{i<j}^N \nabla_i \cdot \nabla_j. \quad (2)$$

The first term includes a correction to the electron mass in which the mass m is replaced by the reduced mass, $\mu = Mm/(M+m)$.¹ This correction to the electron mass can be accounted for by multiplying the energy levels E_0 , calculated from the zero-order Hamiltonian, by $M/(M+m)$. The resulting energy correction to the level E_0 is then given by

$$E_{\text{nms}} = -E_0 \frac{m}{M+m}. \quad (3)$$

This is the normal mass shift (nms). The inclusion of the second term leads to an additional energy correction known as the specific mass shift (sms):

$$E_{\text{sms}} = -\langle \psi | \frac{1}{M} \sum_{i<j}^N \nabla_i \cdot \nabla_j | \psi \rangle. \quad (4)$$

In Tables 1 and 2 the specific mass shift parameter S is given:

$$S = -\langle \psi | \sum_{i<j}^N \nabla_i \cdot \nabla_j | \psi \rangle. \quad (5)$$

This parameter represents the expectation value of the mass-independent factor of the specific mass shift operator.

Due to the finite size of the nucleus the potential inside the nuclear charge distribution deviates from the potential of a point charge Z . For light atoms, where nonrelativistic wavefunctions can be used, the resulting energy correction to the level E_0 is given by

$$E_{\text{fs}} = \frac{2\pi}{3} Z |\psi(0)|^2 \langle r^2 \rangle, \quad (6)$$

where $\langle r^2 \rangle$ is the mean square radius of the nucleus. This is the so-called field shift (fs). For a discussion of the different isotope shift operators, see, for example, Froese Fischer et al. (1993).

¹ In atomic units (a.u.) $m = 1$, but we include it explicitly to avoid misunderstandings. The nuclear mass M is usually given in units of the unified atomic mass (u) and must be converted to atomic units before being used in the above formulas. $1 \text{ u} = 1822.88851 \text{ a.u.}$

2.2. Hyperfine Structure

Hyperfine structure is due to the interaction between the electrons and nuclear magnetic dipole and electric quadrupole moments. The interaction couples the nuclear, I , and electronic, J , angular momenta to a total momentum $F = I + J$, and leads to a splitting of the fine-structure levels. The interaction energy is conventionally written in terms of the magnetic dipole and electric quadrupole interaction constants A_J and B_J :

$$W_{\text{hfs}}(J) = \frac{1}{2} A_J C + B_J \frac{(3/4)C(C+1) - I(I+1)J(J+1)}{2I(2I-1)J(2J-1)}, \quad (7)$$

where $C = F(F+1) - J(J+1) - I(I+1)$.

3. METHOD OF CALCULATION

The wavefunctions were generated with the multi-configuration Hartree-Fock (MCHF) atomic structure package of Froese Fischer (1991), where the wavefunction, ψ , for a state labeled γLS is expanded in terms of configuration state functions (CSFs) with the same LS term

$$\psi(\gamma LS) = \sum_j c_j \phi_j(\gamma_j LS). \quad (8)$$

In the numerical MCHF approach the CSFs are sums of products of spin-orbitals, where the radial part of the spin-orbital is represented by its numerical values at a number of

TABLE 2
DIFFERENCE OF SPECIFIC MASS SHIFT PARAMETERS, ELECTRON DENSITIES
AT THE NUCLEUS, AND TOTAL ENERGIES (in a.u.) FOR THE 1s²2s2p¹P
AND 1s²2s²1S TERMS IN B II AS A FUNCTION OF THE INCREASING
ACTIVE SET OF ORBITALS

Active Set	ΔS (a.u.)	$\Delta \psi(0) ^2$	ΔE_0 (a.u.)
hf	-0.40398	-1.877	0.324702
2s1p	-0.38090	-1.704	0.383351
3s2p1d	-0.33374	-1.798	0.346144
4s3p2d1f	-0.36844	-1.783	0.340564
5s4p3d2f1g	-0.32437	-1.790	0.337160
5s4p3d2f1g ^a	-0.32433	-1.790	0.337131
6s5p4d3f2g1h	-0.32344	-1.786	0.335786
7s6p5d4f3g2h1i	-0.32379	-1.785	0.334953
Experiment ^b			0.334420

^a Complete active space CI calculation. No restriction on the excitations.

^b Olme 1970.

grid points. In the multiconfigurational self-consistent field (MC SCF) procedure both the orbitals and the expansion coefficients are optimized to self-consistency. The calculations of the specific mass shift parameter and the hyperfine structure constants from the MCHF wavefunctions were done with the isotope shift and hyperfine structure programs (Froese Fischer et al. 1993; Jönsson, Wahlström, & Froese Fischer 1993) that are part of the MCHF atomic structure package.

The configuration expansions were obtained with the active space method (Roos, Taylor, & Siegbahn 1980; Olsen et al. 1988), where CSFs of a particular parity and *LS* symmetry are generated by excitations from the reference configuration to an active set of orbitals. The active set is then increased in a systematic way, allowing the convergence of the specific mass shift and hyperfine parameters to be studied. If all possible excitations to the active set are allowed, the configuration state expansion, referred to as the complete active space (CAS), grows very rapidly with the increasing active set. Many of these configurations, obtained mainly from three- and four-particle excitations, have very small expansion coefficients and contribute little to the total energy or to the studied parameters. By imposing different restrictions on the allowed excitations, the number of configuration states can be kept down but with only a small change of the final results (Tong et al. 1993; Froese Fischer 1993). In our calculations we included only configurations where at least two of the orbitals had principal quantum numbers $n < 4$.

4. RESULTS AND DISCUSSION

In Table 1 the value of the specific mass shift parameter, the electron density at the nucleus and the total energy, calculated from the zero-order Hamiltonian, for the $1s^2 2s^2 {}^1S$ and $1s^2 2s 2p {}^1P$ terms of B II are shown as a function of the increasing active set of orbitals. The notation for the active set follows the conventions used in quantum chemistry. The set $3s 2p 1d$, for example, contains three *s*-orbitals, two *p*-orbitals, and one *d*-orbital. It is seen that the specific mass shift parameter for the 1S term has converged to within 0.2%. The final value $S = 0.59709$ a.u. is in very good agreement with the theoretical value $S = 0.5975$ a.u. of Chung, Zhu, & Wang (1993). To see the effect of the neglected configurations in the expansion, a CAS calculation was performed for the $5s 4p 3d 2f 1g$ orbital set. The change in the specific mass shift parameter compared with the smaller expansion is only 3×10^{-5} a.u. and is of no significance. The specific mass shift parameter for the 1P term changes with 0.5% when going from the $6s 5p 4d 3f 2g 1h$ to the $7s 6p 5d 4f 3g 2h 1i$ active set, indicating a little slower convergence compared with the 1S term.

Since the isotope shift in a transition is determined by the difference of the level isotope shift for the upper and lower level, it is interesting to monitor the difference of the specific mass shift parameters, the electron densities at the nucleus and the energies for the two levels. In Table 2 these differences for the 1P and 1S terms are shown as a function of the increasing active set of orbitals. Although the individual specific mass shift parameters for the upper and lower state change very much with the increasing active set of orbitals, the difference is comparatively constant, and even rather small expansions give acceptable values. The transition energy has not yet converged but shows a monotonous trend toward the experimental value of Ölme (1970).

From the parameters in Table 2 the $1s^2 2s^2 {}^1S - 1s^2 2s 2p {}^1P$

transition energies in atomic units for ${}^{11}\text{B}$ and ${}^{10}\text{B}$ were calculated as

$$\Delta E = \Delta E_0 - \Delta E_0 \frac{m}{M+m} + \frac{\Delta S}{M} + \frac{2\pi}{3} Z \Delta |\psi(0)|^2 \langle r^2 \rangle, \quad (9)$$

where M is the nuclear mass of the isotope and $\langle r^2 \rangle$ the mean square nuclear radii, both expressed in atomic units. The root mean square nuclear radii of the isotopes, needed for the evaluation of the field shift, were taken from pionic and muonic X-ray measurements of Olin et al. (1981); ${}^{10}\text{B}$, $\langle r^2 \rangle^{1/2} = 2.44(6)$ fm and ${}^{11}\text{B}$, $\langle r^2 \rangle^{1/2} = 2.38(4)$ fm. From the transition energies in atomic units the wavenumbers and wavelengths were calculated and are shown in Table 3, from which an isotope shift of 0.718 cm^{-1} or 13.3 mÅ can be deduced. Based on the convergence trends of Table 2, the error in the calculated isotope shift is estimated to be below 1%. It should be noted that it is only the wavelength shift between the lines that can be calculated with an accuracy 0.1 mÅ and not the wavelengths of the lines themselves. The laboratory wavelength, which represents the center of gravity value for the solar composition of boron, is $1362.461 \pm 0.010 \text{ Å}$ (Ölme 1970).

B II is a computationally favorable case in two ways: first, the parameters of the upper and lower levels show very similar convergence trends, leaving differences rather constant; and second, the normal and specific mass shift contributions have the same sign and add to the total shift. For the neutral first row atoms, the situation is more complicated. Here the levels are in general affected very differently by correlation, making accurate calculations of the specific mass shift difficult. In cases where the normal and specific mass shift have different sign, the inaccuracy of the latter can give a large error in the total shift. An example of these difficulties is the $1s^2 2s^2 2p^2 P - 1s^2 2s^2 3s^2 S$ transition in B I where the isotope shift of 0.094 cm^{-1} from a third-order MBPT calculation (Veseth 1985) differs substantially from the experimental shift of 0.174 cm^{-1} (Johansson et al. 1993). Generally, to obtain reliable values for the isotope shift, one has to perform very extensive calculations, in which the specific mass shift parameter for both the upper and lower levels are well converged.

Both ${}^{10}\text{B}$ and ${}^{11}\text{B}$ have a nonzero nuclear spin leading to a hyperfine structure splitting of the $1s^2 2s 2p {}^1P_1$ state. The hyperfine structure constants have been calculated with the nuclear magnetic dipole moments of Raghavan (1989) and the electric quadrupole moments of Pykkö & Li (1993). The values are ${}^{10}\text{B}$, $I = 3$, $\mu = 1.80064475(57)\mu_B$, and $Q = 0.08459(24)$ barn and ${}^{11}\text{B}$, $I = 3/2$, $\mu = 2.6886489(10)\mu_B$ and $Q = 0.04059(10)$ barn. The convergence for the hyperfine structure constants is shown in Table 4. The magnetic dipole interaction constant is rather insensitive to correlation and is very well described by the Hartree-Fock value whereas the

TABLE 3
CALCULATED SPECTROSCOPIC DATA FOR THE RESONANCE TRANSITION IN B II

Transition	Wavenumber (cm^{-1})	Wavelength ^a (Å)	Shift (Å)	Isotope
$1s^2 2s^2 {}^1S - 1s^2 2s 2p {}^1P \dots$	73505.735	1360.4381	0.0133	10
$1s^2 2s^2 {}^1S - 1s^2 2s 2p {}^1P \dots$	73506.453	1360.4248		11

NOTE.—Wavenumbers and wavelengths are given for the two stable isotopes ${}^{10}\text{B}$ and ${}^{11}\text{B}$.

^a The laboratory wavelength, which represents the center of gravity value for the solar composition of boron, is $1362.461 \pm 0.010 \text{ Å}$ (Ölme 1970).

TABLE 4

MAGNETIC DIPOLE AND ELECTRIC QUADRUPOLE INTERACTION CONSTANTS (in MHz) FOR THE $1s^22s2p\ ^1P_1$ STATE IN B II AS A FUNCTION OF THE INCREASING ACTIVE SET OF ORBITALS

ACTIVE SET	^{10}B		^{11}B	
	A_1 (MHz)	B_1 (MHz)	A_1 (MHz)	B_1 (MHz)
hf	60.06	8.338	179.36	4.001
2s1p	60.22	8.360	179.83	4.011
3s2p1d	60.98	8.193	182.11	3.932
4s3p2d1f	60.05	7.677	179.34	3.684
5s4p3d2f1g	60.48	7.764	180.62	3.725
5s4p3d2f1g ^a	60.48	7.761	180.60	3.724
6s5p4d3f2g1h	60.85	8.052	181.71	3.864
7s6p5d4f3g2h1i	60.81	8.002	181.60	3.840

NOTE.—Interaction constants are given for the two stable isotopes ^{10}B and ^{11}B .

^a Complete active space CI calculation. No restriction on the excitations.

electric quadrupole interaction constant decreases slightly with increasing active sets. From the interaction constants the energy splitting between the hfs components can be calculated. The splitting between the $F = I + J$ and $F = |I - J|$ components for ^{11}B is 0.446 mÅ. The corresponding splitting for ^{10}B is 0.261 mÅ. These splittings are small compared with the isotope shift and can be neglected.

5. CONCLUSIONS

In the present *Letter* we report on an accurate calculation of the isotope shift and hyperfine structure of the resonance line of B II at 1362 Å. The transition isotope shift between the stable ^{10}B and ^{11}B isotopes is 13.3 mÅ, and the convergence pattern in the calculations implies an uncertainty of less than 1%. The hyperfine splitting is about a factor of 30 smaller than the isotope shift. Determination of the boron abundance in various objects and in the interstellar medium is of great astrophysical and cosmological significance. Our results now provide the possibility of including the isotope shift in detailed modeling of the B II resonance line in high-resolution spectra, whereas the hyperfine structure can be neglected. The ratio between wavelength and isotope shift is 102,000, which is about the maximum spectral resolution of the echelle grating of the Goddard High Resolution Spectrograph aboard the *Hubble Space Telescope*. However, the Doppler broadening will be a serious limiting factor.

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