

International Atomic Energy Agency

and

United Nations Educational Scientific and Cultural Organization

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

HARTREE-FOCK ENERGIES OF THE DOUBLY EXCITED STATES
OF THE BORON ISOELECTRONIC SEQUENCE *

Th.M. El-Sherbini **, H.M. Mansour **, A.A. Farrag **

International Centre for Theoretical Physics, Trieste, Italy

and

A.A. Rahman

Physics Department, Faculty of Science, Cairo University, Egypt.

ABSTRACT

Hartree-Fock energies of the $1s^2 2s 2p ns({}^4P)$, $1s^2 2s 2p np({}^4P, {}^4D)$ and $1s^2 2s 2p nd({}^4P, {}^4D)$; $n = 3 - 6$ states in the boron isoelectronic sequence are reported. The results show a fairly good agreement with the experimental data of Bromander for O IV.

MIRAMARE - TRIESTE

August 1985

* To be submitted for publication.

** Permanent address: Physics Department, Faculty of Science, Cairo University, Egypt.

1. INTRODUCTION

The study of doubly excited quartet states in the isoelectronic sequence of light atoms and ions is of particular interest. The relatively high populations of these states in the beam-fail light source [1,2] and the high purity of the mass-analyzed beam have enabled many new state classifications to be made in these systems. These states are metastable against autoionization in the non-relativistic limit because they cannot interact with the underlying continua by electrostatic interaction due to conservation of spin multiplicity. Thus, such states may have lifetimes longer than 10^{-8} sec., and can therefore, undergo radiative dipole transitions to the low lying doubly excited quartet states of appropriate orbital symmetry and parity. Holoien and Geltman [3] have calculated energies of low lying 4P and 4S states of the lithium isoelectronic sequence for LiI to Ne VII by using explicitly correlated basis functions. Their results have been used to classify the narrow lines arising from such transitions. Junker and Bardsley [4] used a limited configuration interaction approach to calculate the energies of a large number of metastable states of lithium-like, beryllium-like and boron-like, oxygen and fluorine atoms. Recently Lunell [5] and Ali [6] have reported Hartree-Fock energy calculations of 4P and 4D states in the lithium isoelectronic sequence.

As far as we know, in the case of the boron isoelectronic sequence there are no such calculations available in the literature. Therefore, in the present article we have extended the previous studies on LiI to BI isoelectronic sequence. The numerical Hartree-Fock code of Froese-Fischer [7] was used for calculating the energies of the $1s^2 2s 2p ns({}^4P)$, $1s^2 2s 2p np({}^4P, {}^4D)$ and $1s^2 2s 2p nd({}^4P, {}^4D)$; $n = 3-6$ states in the boron sequence. The method of calculation was explained in our previous publications[8,9].

2. RESULTS AND DISCUSSIONS

For the quartet states in the BI sequence (similar to those in the LiI sequence), three electrons move in three different spatial orbitals with radial localization in different regions of configuration space and also can be assigned "parallel spins". Correlation of electron motion due

to the antisymmetry of the wave function for electron interchange, as dictated by the Pauli principle, would simulate somewhat the desired correlation of electron motion due to electrostatic repulsion and thus a rather simple "ansatz" for the wavefunctions as a Hartree-Fock wavefunction might yield a satisfactory description of such states. This is justified by the work of Lunell [5], who reported a rather small difference between the Hartree-Fock energy and the configuration interaction energy of the $1s\ 2s\ 3p\ ^4P$ and $1s\ 2s\ 4p\ ^4P$ states of lithium.

Our calculated Hartree-Fock energies of the $1s^2\ 2s\ 2pns(^4P)$, $1s^2\ 2s\ 2pnp(^4P)$, $1s^2\ 2s\ 2p\ np(^4D)$, $1s^2\ 2s\ 2p\ nd(^4P)$ and $1s^2\ 2s\ 2p\ nd(^4D)$ states, with $n = 3-6$ and for BI to Mg VIII are listed in tables 1-5. There are no experimental as well as theoretical data available in literature for doubly excited states in BI isoelectronic sequence for comparison, except the experimental analysis of Bromander [10] for O IV. In table 6, we list his values together with our data, where a satisfactorily good agreement between both results is obtained.

In conclusion, our calculations of the Hartree-Fock energies of the quartet states in the BI sequence are useful in identifying spectral lines observed experimentally in transitions between these states.

ACKNOWLEDGMENTS

Three of the authors (EL-S., A.A.F. and H.M.M.) would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste.

REFERENCES

- [1] C. Jupen, L. Engstrom, S. Huldt, A. Trigueiros, J.O. Ekberg, U. Litzen and I. Martison, Physica Scripta 29 (1984) 226.
- [2] M. Agentoft, T. Andersen, K.T. Chung and B.F. Davis, Physica Scripta 31 (1985) 74.
- [3] E. Holoien and S. Geltman, Phys. rev. 153 (1967) 81.
- [4] B.R. Junker and J.N. Bardsley, Phys. Rev. A8 (1973) 1345.
- [5] S. Lunell, Physica Scripta 16 (1977) 13.
- [6] M.A. Ali, J. Quant. Spectrosc. Radiat. Transfer 20 (1978) 565.
- [7] C. Froese-Fischer, Comp. Phys. Comm. 4 (1972) 107.
- [8] Th.M. El-Sherbini and S.H. Allam, Ann. Physik 39 (1982) 107.
- [9] Th.M. El-Sherbini and A.A. Rahman, Ann. Physik 39 (1982) 333.
- [10] J. Bromander, Arkiv Fysik 40 (1969) 257.

TABLE 1

Hartree-Fock energies (in a.u.) of the doubly excited $1s^2 2s 2p ns(^4P)$ states; $n=3-6$ of the boron isoelectronic sequence.

Ion	$2s 2p 3s(^4P)$	$2s 2p 4s(^4P)$	$2s 2p 5s(^4P)$	$2s 2p 6s(^4P)$
BI	0.29137	0.35632	0.37906	0.38969
C II	0.69103	0.87931	0.95172	0.98731
N III	1.2327	1.5946	1.7402	1.8136
O IV	1.9152	2.5002	2.7420	2.8656
F V	2.7380	3.5953	3.9562	4.1423
Ne VI	3.7011	4.8798	5.3824	5.6435
Na VII	4.8045	6.3537	7.0207	7.3691
Mg VIII	6.0485	8.0172	8.8714	9.3193

TABLE 2

Hartree-Fock energies (in a.u.) of the doubly excited $1s^2 2s 2p np(^4P)$ states; $n = 3-6$ of the boron isoelectronic sequence.

Ion	$2s 2p 3p(^4P)$	$2s 2p 4p(^4P)$	$2s 2p 5p(^4P)$	$2s 2p 6p(^4P)$
B I	0.32686	0.36845	0.38480	0.39299
C II	0.77052	0.90818	0.96556	0.99511
N III	1.3573	1.6410	1.7627	1.8262
O IV	2.0850	2.5643	2.7732	2.8832
F V	2.9529	3.6770	3.9961	4.1650
Ne VI	3.9612	4.9791	5.4305	5.6711
Na VII	5.1010	6.4708	7.0783	7.4018

TABLE 3

Hartree-Fock energies (in a.u.) of the doubly excited $1s^2 2s 2p np(^4D)$ states; $n = 3-6$ of the boron isoelectronic sequence.

Ion	$2s 2p 3p(^4D)$	$2s 2p 4p(^4D)$	$2s 2p 5p(^4D)$	$2s 2p 6p(^4D)$
B I	0.32207	0.36632	0.38353	0.39206
C II	0.75544	0.90244	0.96259	0.99327
N III	1.3304	1.6314	1.7579	1.8234
O IV	2.0460	2.5508	2.7667	2.8794
F V	2.9018	3.6598	3.9879	4.1602
Ne VI	3.8979	4.9583	5.4212	5.6654
Na VII	5.0344	6.4462	7.0667	7.3952
Mg VIII	6.3117	8.1239	8.9246	9.3496

TABLE 4

Hartree-Fock energies (in a.u.) of the doubly excited $1s^2 2s 2p nd(^4P)$ states; $n = 3-6$ of the boron isoelectronic sequence.

Ion	$2s 2p 3d(^4P)$	$2s 2p 4d(^4P)$	$2s 2p 5d(^4P)$	$2s 2p 6d(^4P)$
B I	0.35413	0.37786	0.38901	0.39510
C II	0.83167	0.92952	0.97541	1.0004
N III	1.4492	1.6734	1.7779	1.8345
O IV	2.2059	2.6076	2.7937	2.8944
F V	3.1021	3.7315	4.0221	4.1794
Ne VI	4.1382	5.0448	5.4628	5.6887
Na VII	5.3148	6.5478	7.1156	7.4226
Mg VIII	6.6322	8.2407	8.9810	9.3812

TABLE 5

Hartree-Fock energies (in a.u.) of the doubly excited $1s^2 2s 2p nd(^4D)$ states; $n = 3-6$ of the boron isoelectronic sequence.

Ion	$2s 2p 3d(^4D)$	$2s 2p 4d(^4D)$	$2s 2p 5d(^4D)$	$2s 2p 6d(^4D)$
B I	0.35128	0.37681	0.38851	0.39482
C II	0.82423	0.92728	0.97445	0.99986
N III	1.4387	1.6705	1.7767	1.8338
O IV	2.1931	2.6042	2.7923	2.8937
F V	3.0875	3.7274	4.0204	4.1784
Ne VI	4.1221	5.0402	5.4608	5.6876
Na VII	5.2972	6.5426	7.1133	7.4213
Mg VIII	6.6132	8.2348	8.9783	9.3798

TABLE 6

A comparison between numerical Hartree-Fock energy calculations of doubly excited quartet states of O IV and the experimental results of Bromander [10]

State	Energy in a.u.	
	This work	Experiment [10]
$1s^2 2s 2p 3s(^4P)$	1.9152	1.9998
$2s 2p 4s(^4P)$	2.5002	2.5925
$2s 2p 3p(^4P)$	2.0850	2.1822
$2S 2p 3p(^4D)$	2.0460	2.1342
$2s 2p 3d(^4D)$	2.1931	2.2775
$2s 2p 3d(^4P)$	2.2059	2.2972
$2s 2p 4d(^4D)$	2.6042	2.7036
$2s 2p 4d(^4P)$	2.6076	2.6973
$2s 2p 5d(^4D)$	2.7923	2.8916
$2s 2p 5d(^4P)$	2.7937	2.8900

