K-shell binding energies of B and C

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K-shell binding energies in free atoms for B and C have been determined with high accuracy by recalibrating the projectile Auger spectra of Bisgaard, Bruch, Dahl, Fastrup, and Rødbro. These results are then compared with theoretical predictions based on the unrestricted Hartree-Fock self-consistent-field method and previous experimental data and theoretical results.

Recent measurements of free-atom K-shell binding energies of light elements[1] have stimulated great theoretical interest in various many-body theories.[2–4] In this work we present the most accurate experimental results on the $1s$ binding energy (BE) of boron and carbon. The accuracy of experimental BE is considerably increased by means of a recalibration procedure which is described in detail elsewhere.[5,6] We also present new theoretical results on the $1s$ binding energies of B and C based on the unrestricted Hartree-Fock (UHF) self-consistent field (SCF) method[7] and electron pair correlation energies.[8] The numerical techniques used by Chung and Davis[9,10] in previous calculations, including the use of interelectronic coordinates to represent the effects of electron correlation, are difficult to apply to core-excited states with more than three electrons. Therefore, the effects of electron correlation were treated in this study using the non-closed-shell many-electron theory (NCMET) of Sinanoğlu.[6,8] It has been shown[11,12] that the UHF-SCF procedure is a special case of the saddle-point variational method[9] for an atom or molecule containing a vacancy in the most tightly bound orbital. The application of this method to core-excited atomic and molecular systems has led to very satisfactory results so far.[6,9]

Our results of the recalibrated K-shell binding energies and the UHF-SCF calculations are presented in Table I together with those of Bisgaard *et al.*[1] and values listed by Sevier.[13] We note that the free-atom K-shell binding energy of 194 ± 1 eV (see also Ref. 15) as tabulated by Sevier deviates significantly from our recalibrated energy of 200.78 ± 0.2 eV. On the other hand the previous theoretical result of Huang *et al.*[14] is in excellent agreement with the experimental value of Ref. 1. We also note that our correlation corrected UHF-SCF binding energy of 200.94 eV is slightly higher than the one of Huang and co-workers but still in very good agreement with the recalibrated data point. For the C case the projectile Auger spectroscopy measurement has yielded a BE of 296.07 ± 0.2 eV. This value is very close to the value from our correlation corrected UHF-SCF calculation, whereas the $1s$ BE given by Huang *et al.*[14] differs by about 0.87 eV (see also Ref. 13) from our experimental result.

From Table I it appears that very good agreement

TABLE I. Experimental $1s$ binding energies of B and C and comparison with theoretical data (in eV).

		Experiment		Sevier (Ref. 13)		
Z	Element	Bisgaard *et al.* (Ref. 1)	Recalibrated data (this work)	Free atom (Ref. 15)	Previous calculations (Ref. 14)	Theory (this work)[a]
5	B	200.8 ± 0.5	200.78 ± 0.2	194 ± 1	200.82	200.94
6	C	296.2 ± 0.5	296.07 ± 0.2		296.94	296.02

[a]Unrestricted Hartree-Fock (UHF) self-consistent field (SCF) method and electron pair correlation energies, this work.

between experimental and theoretical K-shell binding energies of B and C has been achieved. Based on this result the semiempirical free-atom BE value of 194 ± 1 eV as derived by Shirley *et al.*[15] should probably be replaced by 200.78 ± 0.2 eV. Such highly accurate $1s$ binding-energy data may be useful in studying chemical shifts in molecular and solid-state samples.

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