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Breit–Pauli energy levels, lifetimes and transition data: boron-like spectra

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Abstract. Breit–Pauli results for energy levels, lifetimes and some transition data are reported for all levels up to $2s2p(^3P)3s\ ^2P^o_J$ of the B-like spectrum for $5 \leqslant Z \leqslant 14$. For all but the lowest members of the sequence, these include the $2s^22p$, $2s2p^2$, $2p^3$, $2s^23s$, $2s^23p$, and $2s^23d$ and 2s2p3s configurations, though only the $2s2p(^3P)3s$ terms of the latter. A simultaneous optimization scheme was applied so that a radial basis could be determined for a set of terms that mix in the Breit–Pauli approximation. Convergence of the LS line strength is used as a factor in estimating accuracy as well as the agreement of energy levels and their splitting between theory and experiment. The results are evaluated by comparison with other theoretical results and experiment for transition rates.

1. Introduction

In the past, it has been common practice to perform calculations on small groups of transitions, such as a given transition of an isoelectronic sequence or transitions for a Rydberg series. Often these calculations were totally non-relativistic, with possible scaling to observed transition energies. More recently, calculations for groups of transitions have been reported that include the most important correlation along with Breit–Pauli interactions [1, 2]. The accuracy of the resulting transition rates was in the range of 10–20%, depending on the transition. In a recent paper on the Be sequence [3], systematic, large-scale Breit–Pauli calculations were reported for all allowed E1 transitions between the levels of a portion of the spectrum, including the ground state. A consequence of such an approach is that lifetimes can be reported, which are important when comparing with experimental data for excited states. In some cases, some forbidden transitions were computed as well. At the same time, through comparison with many high-precision experiments and benchmark calculations, estimates of uncertainty were evaluated. The accuracy of the transition rates was often less than 1%, though uncertainties could be larger for very small transition energies or for transitions with extensive cancellation during the calculation of the line strength.

In this paper, we extend the approach to the boron-like sequence by considering all levels up to $2s2p(^3P)3s\ ^2P^o_J$, for $Z = 5, \ldots, 14$. Some results are compared with experiment and recent theory.

2. Computational procedures and optimization strategies

The underlying procedures are the same as those described in the Be-like paper [3] and will not be repeated here.

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Briefly, the non-relativistic multiconfiguration Hartree–Fock (MCHF) approach determines an approximate wavefunction Ψ for the state labelled γLS of the form

$$\Psi(\gamma LS) = \sum_j c_j \Phi(\gamma_j LS) \tag{1}$$

where γ represents the dominant configuration, and any additional quantum numbers required for uniquely specifying the state being considered. The configuration state functions (CSF) $\{\Phi\}$ are built from a basis of one-electron spin–orbital functions

$$\phi_{nlm_l m_s} = \frac{1}{r} P_{nl}(r) Y_{lm_l}(\theta, \varphi) \chi_{m_s}. \tag{2}$$

With the wavefunction expansion is associated an energy functional for *one* LS term and eigenvalue. The traditional MCHF procedure [4] consists of optimizing to self-consistency *both* the radial functions $\{P_{n_j l_j}(r)\}$ and mixing coefficients $\{c_j\}$ of this energy functional. However, in the Breit–Pauli approximation, the wavefunction for a specific J is an expansion over terms. In order to obtain a suitable basis for all these terms, the previous paper introduced the notion of simultaneous optimization of energy expressions derived from several different terms or even several eigenvalues of the same term. Furthermore, the different energy expressions could be weighted according to importance. The result of such an approach is a basis adequate for simultaneously representing the different terms that mix in a Breit–Pauli approximation.

Systematic, large-scale methods were applied in which the wavefunction expansions were obtained from orbital sets of increasing size, allowing for the monitoring of convergence. The model for expansion was a core-polarization model and is best described in terms of a union of two sets, whose members satisfy certain rules in the distribution of principal quantum numbers, as in

$$1s\{1, 2\}\{2, 3\}\{2, 3, \ldots, n \leqslant 6\}^2 \cup 1s^2\{2\}\{2, 3, 4, \ldots, n \leqslant 8\}^2.$$

In this notation, in the first set, the first electron has a principal quantum number of $n = 1$; the second has a principal quantum number of either $n = 1$ or 2, the third either 2 or 3, and the last two electrons have unrestricted principal quantum numbers but with $n \leqslant 6$. The maximum n (and l) characterize a particular expansion in this model. The set of configuration states with a single 1s orbital represents core polarization, whereas those with $1s^2$ are part of the valence correlation. In all cases, correlation in $1s^2$ was neglected so that the computational size could be constrained. Also, all expansions were restricted to $l \leqslant 6$ or i-orbitals. Note that by specifying the expansions by rules that focus on the principal quantum number and include all possible angular quantum numbers, 2s–2p degeneracy effects are automatically included, even though the higher-n virtual orbitals are only doubly occupied.

Once a set of radial orbitals has been obtained, the relativistic corrections can be taken into account within the Breit–Pauli approximation by diagonalizing the Breit–Pauli Hamiltonian [4] to obtain the intermediate coupling wavefunctions

$$\Psi(\gamma J) = \sum_{LS} \sum_j c_j(LS) \Phi(\gamma_j LSJ). \tag{3}$$

Thus the expansion is now the sum of expansions over a set of terms. For all expansions, the iterative Davidson method [5] was used to determine a few of the lowest eigenvalues and eigenvectors [6].

All the results in this paper, unless specifically stated as being LS results, are based on the diagonalization of the Breit–Pauli Hamiltonian in which the orbit–orbit term has been omitted.

This operator does not contribute to the mixing of terms, and behaves like a small correlation correction. Experiments on Li-like atoms [7] have shown that the inclusion of orbit–orbit terms can double the computation times for generating the Breit–Pauli interaction matrix, yet has a negligible effect at the present level of accuracy. For this reason, it has been omitted, as is common practice. In the rest of the paper, we will refer to our results as MCHF results, and only use MCHF+BP for emphasis, when needed.

The oscillator strengths f are calculated using the standard, non-relativistic operators for length and velocity forms (see [3] for details). The non-relativistic line strengths allow us to monitor the convergence between the two forms with the improvement of the wavefunctions. In the Breit–Pauli approximation, the same length form is correct to $O(\alpha^2)$, while the velocity form requires a relativistic correction to the gradient operator [8]. For this reason, it is customary to report both length and velocity results for an LS calculation, but only the length form in the Breit–Pauli calculation. No orthonormality constraints are imposed *between* the two sets of radial functions spanning the total wavefunctions of the initial and final state, allowing *separate* MCHF optimizations for the two states involved.

Table 1. Optimization strategies for groups of terms. Eigenfunctions for a specific term are designated by the dominant configuration. All weights are unity unless designated otherwise in parentheses following the term.

Groups	Additional terms or eigenfunctions
Even	
$2s2p^2\ ^4P, ^2D, ^2S, ^2P$	$2s2p3p\ ^4D$ (0.2)
$2s^23s\ ^2S$	$2p^23s\ ^2S, ^2P$ (0.1), ^4P (0.1)
$2s^23d\ ^2D$	$2p^23d\ ^2D, ^2P$ (0.2), ^4D (0.1)
Odd	
$2s^22p\ ^2P^o, ^2D^o, ^4S^o, ^2P^o$	$2p^3\ ^4S^o, ^2D^o, ^2P^o$
$2s^23p\ ^2P^o$	$2p^23p\ ^2P^o, ^4D^o$ (0.1), $^2S^o$ (0.1), $^4P^o$ (0.1)
$2s2p3s\ ^4P^o$, $2s2p(^3P)3s\ ^2P^o$	$2s^22p\ ^2P^o$, $2p^3\ ^4S^o, ^2D^o, ^2P^o$, $2s^23p\ ^2P^o$ (all 0.2)

The different states of boron and B-like ions were grouped together and a radial basis determined for a set of terms and/or eigenvalues that were deemed to be important for the relativistic effects. In table 1, on the left are the group of terms for which accurate Breit–Pauli results are required. However, because these may mix with additional terms, the latter are listed in the second group. Sometimes these are different eigenfunctions of the same terms and this is indicated by the configuration. Mixing with some of the terms may not be particularly strong. In such cases these LS eigenstates had a smaller weight as indicated in table 1. In all cases, the 1s orbital was obtained from simultaneous optimization at the $n = 3$ level of all the terms as indicated in table 1, but using a special expansion model with distribution $1s^2\{2\}^2\{2, 3\}$, i.e. $1s^2$ with at least two $n = 2$ orbitals. After that, for the expansions described earlier with $n \leqslant 5$, all orbitals except 1s were varied; for $n = 6$, all but 1s, 2s, 2p were varied, for $n = 7$ all but 1s, 2s, 2p, 3s, 3p, 3d, and for $n = 8$, all but 1s, 2s, 2p, ..., 4s, 4p, 4d, 4f. The neutral atom was treated similarly to the ions, though fewer states needed to be determined since all $2p^3$ states lie well above the ionization limit.

3. Comparison of models and effects on line strengths

For allowed transitions in B I and C II, the J-dependent relativistic corrections from a Breit–Pauli calculation are essentially negligible, and so it is informative to compare the present results from our model, appropriate for transition studies, with other models that have been

used for isotope shift and hyperfine structure calculations, sensitive not only to correlation in the outer portion of the wavefunction but also to regions closer to the nucleus.

Jönsson *et al* [9] have reported transition data, including the line strength, for several allowed $2s^2 2p–2s2p^2$ transitions in B I and C II. Their model was quite different from the one used in this paper. For each LS term, single and double replacements were made from a multireference set, including the core, a model referred to as SD-MR. Orbitals were optimized for these expansions, systematically, up to $n = 8$ at which point relativistic shift corrections (to be described later) were added as well as triple and quadruple (TQ) excitations for the $n = 5$ orbital set. The final expansions ranged from 20 338 to 94 358 CSFs, depending on the term. The triple and quadruple excitations significantly improved both the agreement with the observed transition energy for the multiplet and the agreement between length and velocity forms of the oscillator strength. A comparison with this model provides a check on the accuracy of this paper as well as a check on our method for estimating the uncertainty proposed earlier [3].

Table 2. Comparison of (a) the SD-MR model of computation followed by triple and quadruple excitations and simple relativistic effects [9] with (b) present work, (c) experimental energies from NIST tabulations. All energies are in cm^{-1} and all transitions are from the $2s^2 2p\ ^2P^o$ ground state.

			Non-relativistic			Relativistic		
	Upper term		ΔE	S_l	S_v	ΔE	S_l	S_v
B I	$2s^2 3s\ ^2S$	(a)	39 756	3.6833	3.9580	40 017	3.7876	3.9019
		(b)	40 010	3.8608	3.8634	39 994	3.8613	
		(c)				40 029		
	$2s2p^2\ ^2D$	(a)	47 991	1.9865	1.9607	47 910	1.9433	1.9368
		(b)	48 026	1.9639	1.9375	48 032	1.9462	
		(c)				47 846		
C II	$2s2p^2\ ^2S$	(a)	96 571	2.4276	2.3408	96 478	2.4183	2.4166
		(b)	96 597	2.4228	2.4149	96 668	2.4175	
		(c)				96 451		
	$2s2p^2\ ^2P$	(a)	110 534	8.8965	8.8057	110 569	8.9075	8.8784
		(b)	110 689	8.8998	8.8767	110 825	8.8977	
		(c)				110 610		
	$2s2p^2\ ^2D$	(a)	74 872	3.3718	3.3404	74 842	3.3917	3.3887
		(b)	74 959	3.3895	3.3692	75 044	3.3865	
		(c)				74 889		

Table 2 presents data for the SD-MR model followed by TQ excitations. Unlike this paper, where Breit–Pauli corrections with term mixing are included, in their work only the LS-dependent relativistic shift corrections are taken into account. These are the J-independent corrections that include the mass–velocity correction, one- and two-body Darwin terms and spin–spin contact. For the non-relativistic calculations, the agreement between the length and velocity forms of the line strength is notably better in this paper. After relativistic corrections have been added (as explained above) Jönsson *et al*'s [9] results with TQ excitations are generally in better agreement with the observed transition energies [10] than present work. As for the line strength, the agreement between the length and the velocity forms is markedly better in this paper for boron, and somewhat better for C II, with the length form in better agreement than the two velocity forms. When relativistic corrections are added, the length form from the two models comes into excellent agreement (one or two parts per thousand) except for the transition to $2s^2 3s\ ^2S$ in boron where the SD-MR model appears not to be as

Table 3. Theoretical lifetimes (in s) for excited states up to 2s2p3s ^{4}P^o of B-like systems for $Z = 5, \ldots, 14$.

Term	J	$Z=5$	$Z=6$	$Z=7$	$Z=8$	$Z=9$	$Z=10$	$Z=11$	$Z=12$	$Z=13$	$Z=14$
$2s^2 2p\ ^2P^o$	$\frac{1}{2}$										
	$\frac{3}{2}$	3.049E+07	4.306E+05	2.075E+04	1.916E+03	2.663E+02	4.931E+01	1.128E+01	3.039E+00	9.320E−01	3.177E−01
$2s2p^2\ ^4P$	$\frac{1}{2}$	6.167E+00	7.654E−03	1.374E−03	3.380E−04	1.045E−04	3.808E−05	1.571E−05	7.138E−06	3.499E−06	1.825E−06
	$\frac{3}{2}$	1.562E+00	9.693E−02	1.369E−02	2.999E−03	8.657E−04	3.022E−04	1.212E−04	5.405E−05	2.621E−05	1.360E−05
	$\frac{5}{2}$	3.999E−01	2.234E−02	3.559E−03	8.377E−04	2.527E−04	9.044E−05	3.667E−05	1.634E−05	7.836E−06	3.983E−06
$2s2p^2\ ^2D$	$\frac{5}{2}$	2.290E−08	3.451E−09	1.996E−09	1.406E−09	1.082E−09	8.771E−10	7.351E−10	6.309E−10	5.506E−10	4.517E−10
	$\frac{3}{2}$	2.285E−08	3.441E−09	1.985E−09	1.396E−09	1.066E−09	8.579E−10	7.125E−10	6.044E−10	5.201E−10	4.865E−10
$2s2p^2\ ^2S$	$\frac{1}{2}$		4.523E−10	3.584E−10	2.790E−10	2.256E−10	1.886E−10	1.613E−10	1.399E−10	1.226E−10	1.080E−10
$2s2p^2\ ^2P$	$\frac{1}{2}$		2.445E−10	1.762E−10	1.380E−10	1.134E−10	9.617E−11	8.332E−11	7.337E−11	6.545E−11	5.918E−11
	$\frac{3}{2}$		2.445E−10	1.762E−10	1.379E−10	1.133E−10	9.594E−11	8.297E−11	7.285E−11	6.468E−11	5.803E−11
$2p^3\ ^4S^o$	$\frac{3}{2}$		2.944E−10	2.056E−10	1.579E−10	1.280E−10	1.074E−10	9.228E−11	8.064E−11	7.136E−11	6.371E−11
$2p^3\ ^2D^o$	$\frac{5}{2}$		1.834E−09	8.841E−10	5.850E−10	4.352E−10	3.449E−10	2.839E−10	2.399E−10	2.062E−10	1.807E−10
	$\frac{3}{2}$		1.835E−09	8.848E−10	5.857E−10	4.360E−10	3.458E−10	2.849E−10	2.410E−10	2.074E−10	1.795E−10
$2p^3\ ^2P^o$	$\frac{1}{2}$		4.966E−10	2.931E−10	2.179E−10	1.697E−10	1.380E−10	1.156E−10	9.885E−11	8.596E−11	7.529E−11
	$\frac{3}{2}$		4.961E−10	2.935E−10	2.182E−10	1.701E−10	1.384E−10	1.161E−10	9.942E−11	8.659E−11	7.600E−11
$2s^2 3s\ ^2S$	$\frac{1}{2}$	3.996E−09	2.266E−09	3.194E−10	1.240E−10	6.050E−11	3.355E−11	2.025E−11	1.300E−11	8.753E−12	6.117E−12
$2s^2 3p\ ^2P$	$\frac{1}{2}$	5.006E−08	8.973E−09	4.410E−09	1.387E−09	6.713E−10	3.705E−10	2.226E−10	1.424E−10	9.571E−11	6.697E−11
	$\frac{3}{2}$	5.004E−08	8.963E−09	4.400E−09	1.386E−09	6.705E−10	3.670E−10	2.222E−10	1.421E−10	9.543E−11	6.672E−11
$2s^2 3d\ ^2D$	$\frac{3}{2}$	4.629E−09	3.493E−10	7.938E−11	2.824E−11	1.270E−11	6.593E−12	3.774E−12	2.322E−12	1.508E−12	1.023E−12
	$\frac{5}{2}$	4.631E−09	3.494E−10	7.945E−11	2.828E−11	1.273E−11	6.612E−12	3.788E−12	2.333E−12	1.517E−12	1.031E−12
$2s2p3s\ ^4P^o$	$\frac{1}{2}$		1.188E−09	2.307E−10	9.835E−11	4.949E−11	2.780E−11	1.691E−11	1.092E−11	7.381E−12	5.183E−12
	$\frac{3}{2}$		1.187E−09	2.305E−10	9.820E−11	4.938E−11	2.772E−11	1.684E−11	1.085E−11	7.327E−12	5.135E−12
	$\frac{5}{2}$		1.187E−09	2.300E−10	9.791E−11	4.917E−11	2.755E−11	1.671E−11	1.074E−11	7.228E−12	5.048E−12
$2s2p(^3P)3s\ ^2P^o$	$\frac{1}{2}$		4.966E−10	3.864E−10	1.418E−10	6.813E−11	3.743E−11	2.321E−11	1.896E−11	9.692E−12	6.784E−12
	$\frac{3}{2}$		4.961E−10	3.851E−10	1.411E−10	6.758E−11	3.699E−11	2.244E−11	1.794E−11	9.386E−12	6.506E−12

Table 4. Comparison of the computed spectrum for O IV with tabulated NIST [11] data.

			Level (cm^{-1})			Splitting (cm^{-1})		
Configuration	Term	J	Theory	Obs.	Diff.	Theory	Obs.	Diff.
$2s^22p$	$^2P^o$	$\frac{1}{2}$						
		$\frac{3}{2}$	387.22	385.9	1.32	387.22	385.9	1.32
$2s2p^2$	^4P	$\frac{1}{2}$	71 521.87	71 439.8	82.07			
		$\frac{3}{2}$	71 653.75	71 570.1	83.65	131.88	130.30	1.58
		$\frac{5}{2}$	71 838.32	71 755.5	82.82	316.45	315.70	0.75
	^2D	$\frac{5}{2}$	127 160.10	126 936.3	223.80			
		$\frac{3}{2}$	127 173.62	126 950.2	223.42	13.52	13.90	−0.38
	^2S	$\frac{1}{2}$	164 743.52	164 366.4	377.12			
	^2P	$\frac{1}{2}$	180 699.39	180 480.8	218.59			
		$\frac{3}{2}$	180 943.38	180 724.2	219.18	243.98	243.40	0.58
$2p^3$	$^4S^o$	$\frac{3}{2}$	231 804.66	231 537.5	267.16			
	$^2D^o$	$\frac{5}{2}$	255 508.26	255 155.9	352.36			
		$\frac{3}{2}$	255 536.62	255 184.9	351.72	28.36	29.00	−0.64
	$^2P^o$	$\frac{1}{2}$	289 546.21	289 015.4	530.81			
		$\frac{3}{2}$	289 555.50	289 023.5	532.00	9.29	8.10	1.19
$2s^23s$	^2S	$\frac{1}{2}$	357 724.81	357 614.3	110.51			
$2s^23p$	^2P	$\frac{1}{2}$	390 505.04	390 161.2	343.84			
		$\frac{3}{2}$	390 592.30	390 248.0	344.30	87.27	86.80	0.47
$2s^23d$	^2D	$\frac{3}{2}$	419 756.15	419 533.9	222.25			
		$\frac{5}{2}$	419 772.73	419 550.6	222.13	16.59	16.70	−0.11
$2s2p3s$	$^4P^o$	$\frac{1}{2}$	439 047.29	438 849.0	198.29			
		$\frac{3}{2}$	439 182.67	438 983.9	198.77	135.38	134.90	0.48
		$\frac{5}{2}$	439 430.24	439 230.9	199.34	382.94	381.90	1.04
$2s2p(^3P)3s$	$^2P^o$	$\frac{1}{2}$	453 280.99	452 806.6	474.39			
		$\frac{3}{2}$	453 546.26	453 071.5	474.76	265.27	264.9	0.37

satisfactory. It is likely that the SD orbital basis, also optimized on core correlation, did not adequately represent the outer portion of the wavefunction which does not contribute as much to the energy as correlation in the core. This may account for the fact that the present results are in better agreement with the SD-MR velocity form. Thus the present model seems to be well suited to the computation of transition rates for the boron-like sequence, including also transitions to the $2s^23l$ states, and the length form is the more accurate line strength. This suggests that the error in the line strength is less than the difference between the two forms would imply.

4. Breit–Pauli results

The orbital basis from simultaneous optimization may be used to determine J-dependent energy levels and transition rates. In table 3 we report the lifetimes of all the levels of the configurations considered in this work. These are based primarily on the allowed E1 transitions between the different states but the M2 transitions, $2s^22p\ ^2P^o_J$–$2s2p^2\ ^4P_{J'}$ were also computed as well as the E2 and M1 transitions $2s^22p\ ^2P^o_{1/2}$–$2s^22p\ ^2P^o_{3/2}$, which contribute to the lifetime

Table 5. Comparison of computed spectrum for O IV with tabulated NIST [11] data and other theories. The second line is the difference in % between theory and observed.

Configuration	Term	J	Obs.	Present work	IRON[a]	SJS[b]	MVGK[c]
O IV							
$2s^2 2p$	$^2P^o$	$\frac{1}{2}$					
		$\frac{3}{2}$	385.9	387.22	383	389	372
				0.34	−0.75	0.80	−3.60
$2s2p^2$	^4P	$\frac{1}{2}$	71 439.8	71 521.87	67 925	72 107	70 106
				0.11	−5.04	0.93	−1.88
		$\frac{3}{2}$	71 570.1	71 653.75	68 059	72 241	70 235
				0.12	−5.03	0.93	−1.88
		$\frac{5}{2}$	71 755.5	71 838.32	68 246	72 434	70 413
				0.12	−5.01	0.94	−1.88
	^2D	$\frac{5}{2}$	126 936.3	127 160.10	130 936	126 098	121 908
				0.18	3.10	−0.66	−4.04
		$\frac{3}{2}$	126 950.2	127 173.62	130 945	126 110	121 923
				0.18	3.10	−0.66	−4.04
	^2S	$\frac{1}{2}$	164 366.4	164 743.52	169 367	164 788	160 426
				0.23	3.00	0.26	−2.43
	^2P	$\frac{1}{2}$	180 480.8	180 699.39	188 768	179 035	179 375
				0.12	4.49	−0.80	−0.61
		$\frac{3}{2}$	180 724.2	180 943.38	189 008	179 284	179 608
				0.12	4.48	−0.80	−0.61
$2p^3$	$^4S^o$	$\frac{3}{2}$	231 537.5	231 804.66	232 226	231 813	229 755
				0.12	0.30	0.12	−0.77
	$^2D^o$	$\frac{5}{2}$	255 155.9	255 508.26	262 131	253 849	243 729
				0.14	2.70	−0.51	−4.58
		$\frac{3}{2}$	255 184.9	255 536.62	262 167	253 873	243 770
				0.14	2.70	−0.51	−4.58
	$^2P^o$	$\frac{1}{2}$	289 015.4	289 546.21	299 326	289 700	278 883
				0.18	3.50	0.24	−3.57
		$\frac{3}{2}$	289 023.5	289 555.50	299 328	289 712	278 883
				0.18	3.50	0.24	−3.57
Si X							
$2s^2 2p$	$^2P^o$	$\frac{1}{2}$					
		$\frac{3}{2}$	6 990	7 047.75	6 907	7 000	6 874
				0.82	−1.19	0.14	−1.67
$2s2p^2$	^4P	$\frac{1}{2}$	161 010	161 689.07	157 244	161 437	160 718
				0.42	−2.37	0.26	−0.18
		$\frac{3}{2}$	163 490	164 205.82	159 728	163 925	163 201
				0.43	−2.33	0.27	−0.18
		$\frac{5}{2}$	167 060	167 784.68	163 310	167 511	166 754
				0.43	−2.27	0.27	−0.18
	^2D	$\frac{5}{2}$	287 850	288 822.32	292 392	287 448	286 178
				0.34	1.57	−0.14	−0.58
		$\frac{3}{2}$	287 880	288 838.81	292 473	287 460	286 245
				0.33	1.58	−0.15	−0.57
	^2S	$\frac{1}{2}$	367 670	368 785.69	372 843	367 741	365 775
				0.30	1.40	0.02	−0.52

Table 5. Continued.

Configuration	Term	J	Obs.	Present work	IRON[a]	SJS[b]	MVGK[c]
	^{2}P	$\frac{1}{2}$	390 040	390 729.09	399 416	389 928	389 343
				0.18	2.38	−0.03	−0.18
		$\frac{3}{2}$	394 030	394 730.53	403 458	393 889	393 294
				0.18	2.36	−0.02	−0.19
$2p^3$	^{4}S^o	$\frac{3}{2}$	509 330	510 841.65	510 174	509 543	508 580
				0.30	0.17	0.04	−0.15
	^{2}D^o	$\frac{5}{2}$	575 430	577 255.29	583 822	574 823	571 902
				0.32	1.45	−0.11	−0.61
		$\frac{3}{2}$	575 450	577 310.99	583 853	574 863	571 928
				0.32	1.45	−0.11	−0.61
	^{2}P^o	$\frac{1}{2}$	646 760	649 306.20	658 272	646 133	643 250
				0.39	1.76	−0.10	−0.54
		$\frac{3}{2}$	647 390	649 944.81	658 833	646 775	643 825

[a] IRON [2].
[b] SJS [12].
[c] MVGK [13].

of the latter. In other cases, the contributions from forbidden transitions to the lifetime are negligible but calculations were also performed for $2s2p^2\ ^4P_J$–$2s2p^2\ ^4P_{J'}$. A complete set of transition data (transition energies, line strength, oscillator strengths, transition rates) is available at http://www.vuse.vanderbilt.edu/∼cff/mchf_collection This site also reports LS convergence trends, including the length and velocity forms of the line strength. As shown in our earlier paper [3] the latter can be used in the estimation of accuracy. All other reported data are based on Breit–Pauli line strengths in the length form. For each atom or ion, an ascii file may be viewed or downloaded that contains all the information about the transitions in floating point form, suitable for processing.

5. Accuracy of Breit–Pauli energies

The accuracy of computed oscillator strengths and transition rates depends not only on the line strength but also on the transition energies. The latter can often be measured more accurately than computed, and computed transition data can be improved through scaling so that, in effect, the observed transition energy is used. However, for the production of large amounts of data, this is not practical since, particularly for more highly ionized systems, the data may not be available. Our aim in this paper is to predict transitions to within a fraction of a per cent. This, of course, is more easily achieved when the transition energy is large than when it is small.

Table 4 compares the computed spectrum with observation for O IV, where both correlation and relativistic effects are important. The difference in the excitation energies (theory − observed) appears to be largest for $2p^3\ ^2P^o_J$, possibly because of the neglect of core correlation, since $2p^5$ is an allowed configuration for this term. The discrepancies for $2s2p(^3P)3s\ ^2P^o_J$ are almost as large. In all other cases, the difference is a few 100 cm^{-1}, ranging from 80 to 377 cm^{-1}. The splitting is also reported. It is defined here to be the energy with respect to the lowest level of the multiplet so that this value for the highest level gives the spread of the multiplet. The latter is a useful measure of the adequacy of the Breit–Pauli approximation, as was described in the Be-like paper [3]. All the theoretical energies and splittings were computed from variational total energies with somewhat more precision than displayed in this table.

Table 6. Accuracy indicators for allowed transitions. The first line shows the differences between S_v and S_l in per cent and the second line the differences (in %) between computed Breit–Pauli transition energies and transition energies from NIST data (average for each term).

Transition	5	6	7	8	9	10	11	12	13	14
$2s^22p\ ^2P^o$–$2s2p^2\ ^2D$	1.35	0.60	0.47	0.29	0.24	0.23	0.21	0.20	0.15	0.13
	0.39	0.22	0.22	0.18	0.15	0.16	0.19	0.21	0.25	0.33
$2s^22p\ ^2P^o$–$2s2p^2\ ^2S$		0.33	0.24	0.23	0.50	0.24	0.14	0.14	0.12	0.11
		0.22	0.24	0.23	0.27	0.24	0.21	0.24	0.25	0.30
$2s^22p\ ^2P^o$–$2s2p^2\ ^2P$		0.26	0.18	0.15	0.14	0.13	0.12	0.11	0.11	0.10
		0.20	0.12	0.18	0.15	0.16	0.19	0.21	0.25	0.33
$2s^22p\ ^2P^o$–$2s^23s\ ^2S$	−0.07	0.41	0.44	0.15	0.09	0.06	0.02	0.01	−0.003	−0.01
	−0.09	−0.02	0.02	0.03	0.03	0.04	0.03	0.05	0.05	0.08
$2s^22p\ ^2P^o$–$2s^23d\ ^2D$	−0.09	−0.01	0.15	−0.08	−0.09	−0.06	−0.05	−0.05	−0.05	−0.04
		−0.03	0.06	0.05	0.05	0.01	0.04	0.02	0.02	0.01
$2s2p^2\ ^4P$–$2p^3\ ^4S^o$		0.11	−4.83	−3.90	0.11	0.11	0.09	0.10	0.10	0.09
		0.13	0.13	0.12	0.10	0.11	0.12	0.15	0.18	0.23
$2s2p^2\ ^4P$–$2s2p3s\ ^4P^o$		0.31	0.88	0.42	0.35	0.30	0.26	0.24	0.21	0.20
		0.02	0.04	0.03	0.03	0.04	0.02	0.03	0.03	0.03
$2s2p^2\ ^2D$–$2p^3\ ^2D^o$		0.14	0.11	0.19	0.19	0.16	0.11	0.09	0.10	0.09
		0.09	0.06	0.10	0.11	0.16	0.12	0.16	0.23	0.30
$2s2p^2\ ^2D$–$2p^3\ ^2P^o$		−0.16	0.09	0.11	0.13	0.10	0.11	0.10	0.11	0.25
		−0.04	0.18	0.18	0.20	0.20	0.22	0.27	0.30	0.44
$2s2p^2\ ^2D$–$2s2p(^3P)3s\ ^2P^o$			−0.60	0.00	0.12	0.17	0.15	0.11	0.10	0.10
			0.11	0.08	0.08	0.05	0.06	0.05	0.05	0.05
$2s2p^2\ ^2S$–$2p^3\ ^2P^o$		2.73	4.02	2.24	1.46	1.24	0.84	0.84	0.81	0.68
		−0.04	−0.04	0.05	0.02	0.02	−0.01	0.21	0.25	0.34
$2s2p^2\ ^2S$–$2s^23p\ ^2P^o$		−0.43	0.23	−0.13	0.15	0.14	0.14	0.10	0.08	0.29
		−0.12	0.14	0.12	0.05	0.11	0.20	0.25	0.32	0.51
$2s2p^2\ ^2S$–$2s2p(^3P)3s\ ^2P^o$			0.30	−0.16	0.55	0.29	0.36	0.20	0.18	0.18
			0.07	0.03	0.02	0.02	0.04	0.04	0.04	0.04
$2s2p^2\ ^2P$–$2p^3\ ^2D^o$		−1.56	−1.93	−0.28	0.20	0.04	0.36	0.36	0.47	0.36
		−0.20	−0.13	−0.01	−0.07	−0.02	−0.02	0.23	0.25	0.30
$2s2p^2\ ^2P$–$2p^3\ ^2P^o$		1.03	0.97	1.01	0.86	0.78	0.62	0.59	0.53	0.48
		0.05	0.19	0.18	0.16	0.27	0.23	0.25	0.34	0.62
$2s2p^2\ ^2P$–$2p^3\ ^2P^o$		−1.58	0.16	0.21	0.22	0.24	−0.28	0.27	0.24	0.43
		−0.15	0.33	0.29	0.28	0.29	0.33	0.38	0.42	0.73
$2s2p^2\ ^2P$–$2s^23p\ ^2P^o$		−21.3	8.23	−8.46	−7.85	−5.78	−4.50	−3.74	−3.10	−0.55
		−0.34	0.01	0.06	0.02	0.03	−0.01	0.16	0.20	0.18
$2s2p^2\ ^2P$–$2s2p(^3P)3p\ ^2P^o$			−1.79	−1.50	−1.05	−1.01	−1.03	−1.02	−0.97	−1.34
			0.17	0.09	0.09	0.02	0.07	0.06	0.05	0.07
$2p^3\ ^2D^o$–$2s^23d\ ^2D$		141	−17.5	−0.37	−5.04	−1.79	−0.12	−1.23	0.04	−0.88
		4.78	−0.18	−0.08	−0.04	−0.11	−0.03	−0.07	−0.08	−0.10
$2p^3\ ^2P^o$–$2s^23s\ ^2S$		65.7	44.2	−44.5	−12.3	0.63	5.40	4.42	5.08	3.98
		0.29	4.48	−0.62	−0.24	−0.14	−0.13	−0.11	−0.10	0.39

Table 6. Continued.

Transition	5	6	7	8	9	10	11	12	13	14
$2p^3\ ^2P^o$–$2s^23d\ ^2D$		168	−12.2	−30.8	−11.7	−2.49	2.81	3.07	2.93	3.61
		0.58	−0.79	−0.23	−0.13	−0.16	−0.09	−0.11	−0.12	−0.17
$2s^23s\ ^2S$–$2s^23p\ ^2P^o$	9.37	1.29	−0.33	0.35	−0.12	−0.24	−0.38	−0.43	−0.42	−0.47
	4.94	1.10	0.52	0.71	0.30	0.26	0.03	0.05	0.05	0.39
$2s^23s\ ^2S$–$2s2p(^3P)3s\ ^2P^o$			1.61	0.80	0.63	0.41	0.28	0.21	0.16	0.12
			0.52	0.38	0.37	0.27	0.39	0.32	0.33	
$2s^23p\ ^2P^o$–$2s^23d\ ^2D$	−7.69	−1.18	1.42	−0.08	0.18	0.41	0.40	0.39	0.35	0.47
		−1.09	−0.01	−0.42	−0.04	−0.79	0.25	0.02	0.02	0.02
$2s^23d\ ^2D$–$2s2p(^3P)3s\ ^2P^o$			3.29	1.28	3.11	0.03	2.03	0.12	0.38	0.02
			0.89	0.75	0.97	1.46	1.03	1.64	1.95	2.73

Table 5 compares present transitions energies for O IV and Si X, with observation and similar results from other theories. The error in per cent is given below each quoted energy. This paper is totally *ab initio*. The average error is about 0.2% in O IV, but increases somewhat in Si X because of higher-order relativistic corrections. The IRON project [2] work includes semi-empirical term energy corrections. Even so the errors are still a few per cent. The RMBPT results of Safronova *et al* [12] employ a Z-dependent theory and, indeed, the errors in the energy decrease with Z. Merkelis *et al*'s [13] values also are Z-dependent though errors generally are larger than those of Safronova *et al*.

The accuracy of our computed transition rates depends on the accuracy of the energy as well as the discrepancy in the length and velocity forms of the line strength. In table 6, these accuracy indicators for allowed transitions are reported, first the difference in the length and velocity forms of the line strength (in per cent with respect to the average $(S_l + S_v)/2$) of the LS line strength and then the error (in per cent) in the transition energy from the Breit–Pauli calculation. Here we see an improving trend in the line strength as Z increases as well as the variation in this accuracy depending on the transition. Note the particularly large discrepancy for the $2p^3\ ^2P^o_J$–$2s^23s\ ^2S_{J'}$ transition which arises largely from correlation with $2p^23s$ in the upper state, accompanied by cancellation in the 2p–3s transition matrix element. The largest error in a transition energy occurs for $2s^23p\ ^2P^o_J$–$2s^23d\ ^2D_{J'}$ in boron where the transition energy is small. For the ions, the error in the transition energy (as well as excitation energy) is below the 1% level but now the errors first decrease with increasing Z, then, in quite a few instances, begin a slow increase, indicating the limitations of Breit–Pauli for high Z.

As an example of some of the data available at the internet site, table 7 shows a portion of the E1 line list and associated data for O IV. Omitted are some of the intercombination lines with small transition rates. In this table are included the fully *ab initio* data and the energy scaled transition rates along with uncertainty estimates. The latter, in per cent, are the error in the energy plus the discrepancy in the forms of the non-relativistic line strength, also in per cent. This formula provided reasonable estimates of the uncertainties in our earlier paper [3].

6. Comparison with previous results, experiment and semi-empirical evaluations

Doubly ionized nitrogen is one of the important ions in astrophysics. Since the early study by Nussbaumer and Storey [16], relatively few theoretical studies have been undertaken until

Table 7. A portion of the computed line list data for O IV, along with scaled transition rates that included uncertainty estimates. We have omitted some of the intercombination lines with small transition rates.

Multiplet	J_i–J_k	E (cm^{-1})	S	gf	A_{ki}
$2s^2 3p\ ^2P^o$–$2s^2 3d\ ^2D$	$\frac{3}{2}$–$\frac{3}{2}$	29 163.84	1.3138	0.116 39	1.6508(0.0082)E+07
	$\frac{3}{2}$–$\frac{5}{2}$	29 180.43	11.8279	1.048 40	9.9243(0.0500)E+07
	$\frac{1}{2}$–$\frac{3}{2}$	29 251.11	6.5665	0.583 45	8.3247(0.0415)E+07
$2s^2 3s\ ^2S$–$2s^2 3p\ ^2P^o$	$\frac{1}{2}$–$\frac{1}{2}$	32 780.23	3.6573	0.364 17	1.3051(0.0137)E+08
	$\frac{1}{2}$–$\frac{3}{2}$	32 867.50	7.3162	0.730 42	1.3182(0.0138)E+08
$2s2p^2\ ^2P$–$2p^3\ ^2D^o$	$\frac{3}{2}$–$\frac{5}{2}$	74 564.88	1.8389	0.416 50	2.5744(0.0305)E+08
	$\frac{3}{2}$–$\frac{3}{2}$	74 593.24	0.1981	0.044 89	4.1652(0.0493)E+07
	$\frac{1}{2}$–$\frac{3}{2}$	74 837.23	1.0332	0.234 86	2.1934(0.0259)E+08
$2s2p^2\ ^2P$–$2p^3\ ^2P^o$	$\frac{3}{2}$–$\frac{1}{2}$	108 602.84	0.3346	0.110 39	4.3426(0.0218)E+08
	$\frac{3}{2}$–$\frac{3}{2}$	108 612.13	1.7013	0.561 29	1.1042(0.0055)E+09
	$\frac{1}{2}$–$\frac{1}{2}$	108 846.82	0.6853	0.226 56	8.9532(0.0449)E+08
	$\frac{1}{2}$–$\frac{3}{2}$	108 856.11	0.3184	0.105 27	2.0802(0.0104)E+08
$2s2p^2\ ^2S$–$2p^3\ ^2P^o$	$\frac{1}{2}$–$\frac{1}{2}$	124 802.70	0.1961	0.074 33	3.8614(0.0135)E+08
	$\frac{1}{2}$–$\frac{3}{2}$	124 811.99	0.4220	0.159 98	4.1557(0.0146)E+08
$2s^2 2p\ ^2P^o$–$2s2p^2\ ^2D$	$\frac{3}{2}$–$\frac{5}{2}$	126 772.88	1.0339	0.398 15	7.1135(0.0330)E+08
	$\frac{3}{2}$–$\frac{3}{2}$	126 786.40	0.1119	0.043 11	1.1557(0.0054)E+08
	$\frac{1}{2}$–$\frac{3}{2}$	127 173.62	0.5784	0.223 43	6.0257(0.0278)E+08
$2s2p^2\ ^2D$–$2p^3\ ^2D^o$	$\frac{3}{2}$–$\frac{5}{2}$	128 334.64	0.1387	0.054 06	9.8977(0.0288)E+07
	$\frac{5}{2}$–$\frac{5}{2}$	128 348.16	1.8951	0.738 84	1.3531(0.0039)E+09
	$\frac{3}{2}$–$\frac{3}{2}$	128 363.00	1.2080	0.471 02	1.2942(0.0038)E+09
	$\frac{5}{2}$–$\frac{3}{2}$	128 376.52	0.1419	0.055 33	1.5207(0.0044)E+08
$2s2p^2\ ^4P$–$2p^3\ ^4S^o$	$\frac{5}{2}$–$\frac{3}{2}$	159 966.34	1.5243	0.740 67	3.1606(0.1266)E+09
	$\frac{3}{2}$–$\frac{3}{2}$	160 150.91	1.0163	0.494 40	2.1146(0.0847)E+09
	$\frac{1}{2}$–$\frac{3}{2}$	160 282.80	0.5082	0.247 42	1.0600(0.0426)E+09
$2s2p^2\ ^2D$–$2p^3\ ^2P^o$	$\frac{3}{2}$–$\frac{1}{2}$	162 372.60	0.6628	0.326 93	2.8747(0.0086)E+09
	$\frac{3}{2}$–$\frac{3}{2}$	162 381.89	0.1356	0.066 86	2.9399(0.0088)E+08
	$\frac{5}{2}$–$\frac{3}{2}$	162 395.41	1.1806	0.582 37	2.5611(0.0077)E+09
$2s^2 2p\ ^2P^o$–$2s2p^2\ ^2S$	$\frac{3}{2}$–$\frac{1}{2}$	164 356.30	0.5177	0.258 47	2.3286(0.0106)E+09
	$\frac{1}{2}$–$\frac{1}{2}$	164 743.52	0.2772	0.138 70	1.2555(0.0057)E+09
$2s^2 2p\ ^2P^o$–$2s2p^2\ ^2P$	$\frac{3}{2}$–$\frac{1}{2}$	180 312.17	0.4170	0.228 40	2.4767(0.0674)E+09
	$\frac{3}{2}$–$\frac{3}{2}$	180 556.15	2.0269	1.111 63	6.0432(0.0165)E+09
	$\frac{1}{2}$–$\frac{1}{2}$	180 699.39	0.7977	0.437 83	4.7679(0.0130)E+09
	$\frac{1}{2}$–$\frac{3}{2}$	180 943.38	0.4020	0.220 98	1.2065(0.0033)E+09
$2s2p^2\ ^2D$–$2s^2 3p\ ^2P^o$	$\frac{3}{2}$–$\frac{1}{2}$	263 331.42	0.0267	0.021 32	4.9314(0.1128)E+08
	$\frac{3}{2}$–$\frac{3}{2}$	263 418.69	0.0053	0.004 25	4.9207(0.1126)E+07
	$\frac{5}{2}$–$\frac{3}{2}$	263 432.21	0.0479	0.038 32	4.4347(0.1015)E+08
$2s^2 2p\ ^2P^o$–$2s^2 3s\ ^2S$	$\frac{3}{2}$–$\frac{1}{2}$	357 337.59	0.1164	0.126 35	5.3808(0.0097)E+09
	$\frac{1}{2}$–$\frac{1}{2}$	357 724.81	0.0579	0.062 91	2.6851(0.0048)E+09

Table 7. Continued.

Multiplet	J_i–J_k	E (cm^{-1})	S	gf	A_{ki}
2s2p^2 ^{4}P–2s2p3s ^{4}P^o	$\frac{5}{2}$–$\frac{3}{2}$	367 344.35	0.1824	0.203 51	4.5794(0.0208)E+09
	$\frac{3}{2}$–$\frac{1}{2}$	367 393.54	0.1686	0.188 20	8.4722(0.0386)E+09
	$\frac{1}{2}$–$\frac{1}{2}$	367 525.42	0.0337	0.037 63	1.6954(0.0078)E+09
	$\frac{3}{2}$–$\frac{3}{2}$	367 528.92	0.0540	0.060 28	1.3579(0.0062)E+09
	$\frac{5}{2}$–$\frac{5}{2}$	367 591.91	0.4261	0.475 80	7.1474(0.0326)E+09
	$\frac{1}{2}$–$\frac{3}{2}$	367 660.80	0.1687	0.188 36	4.2459(0.0194)E+09
	$\frac{3}{2}$–$\frac{5}{2}$	367 776.48	0.1825	0.203 88	3.0657(0.0140)E+09
2s^{2}2p ^{2}P^o–2s^{2}3d ^{2}D	$\frac{3}{2}$–$\frac{3}{2}$	419 368.93	0.1574	0.200 52	5.8808(0.0079)E+09
	$\frac{3}{2}$–$\frac{5}{2}$	419 385.51	1.4155	1.803 24	3.5259(0.0047)E+10
	$\frac{1}{2}$–$\frac{3}{2}$	419 756.15	0.7855	1.001 53	2.9427(0.0039)E+10

the work by the Belfast group, the latest publication being by Bell *et al* [1]. Their method is not unlike the present one except for the fact that Slater-type orbitals are used for radial functions and their correlation orbitals are limited to 4p, 5p, 4d, 5d, 4f, with the other orbitals, 2p, 3s, 3p, 3d, being occupied in at least one of the states. To improve the accuracy of their final results, term-energy corrections were used that shift LS blocks during the diagonalization of the Breit–Pauli Hamiltonian to bring energies into close agreement with observation. No conclusion was reached on accuracy.

In table 8, our energy-scaled transition rates with uncertainties are compared with those of Bell *et al* [1] (BHSB), recently reported relativistic many-body perturbation results by Safronova *et al* [15] (SJL), and the 1979 results obtained by Nussbaumer and Storey [16] (NS). The latter are remarkably accurate given that they were computed 20 years ago. Safronova *et al*'s [15] values appear on the whole not to be as accurate. This is not unexpected since N^{2+} is still a relatively lowly ionized system. Agreement with the Belfast results, on the whole, is excellent. Their method appears to be accurate to a few per cent. The uncertainty estimates quoted for our results are derived from an uncertainty in per cent, where the latter is the sum of the error in the energy plus the discrepancy in length and velocity forms of the oscillator strength, all in per cent. The largest uncertainty is for the 2s2p^2 ^{4}P–2p^3 ^{4}S^o multiplet where this value is as large as 6%. On the other hand, the difference with BHSB is only 1–2%. Most other uncertainties are a fraction of a per cent. Note that the uncertainties in the table are given as absolute values (not per cent) with the same exponent as the transition rate itself.

Of particular importance in astrophysics are the intercombination lines from the multiplet, 2s^{2}2p ^{2}P^o–2s2p^2 ^{4}P for which a number of theoretical results have been reported as well as recent results from high-precision experiments. These are compared in table 9 for C II, N III, and O IV. Results reported as theory are from Breit–Pauli calculations, except Merkelis *et al*'s [13] results which are derived from a Z-dependent theory, with O IV being their lowest ion. The present adjusted values, were obtained by rediagonalizing the interaction matrices of the states involved and shifting diagonal energies to agree with observation. The quoted uncertainties are the difference between these adjusted values and the original, *ab initio* ones plus the error in the line strength for 2s^{2}2p ^{2}P^o–2s2p^2 ^{2}D, which had the largest discrepancy for allowed transitions between these configurations. The agreement with the results reported by Brage *et al* [21, 20] is excellent but the methodologies are also similar. Our results with uncertainties overlap with some of the most recent experimental values [18, 19]. In C II, there is good agreement with transition rates from an upper level with different experiments, but not the

Table 8. *Ab initio* energy data for transitions in N III, along with scaled transition rates (A_{ki}) that included uncertainty estimates (un). Omitted are some of the intercombination lines with small transition rates.

Multiplet	J_i–J_k	E (cm^{-1})	A_{ki} (un)	BHSB [1]	SJL [15]	NS [16]
$2s^2 3p\ ^2P^o$–$2s^2 3d\ ^2D$	$\frac{3}{2}$–$\frac{3}{2}$	21 535.78	1.1822(0.0169)E+07	1.337E+07		
	$\frac{3}{2}$–$\frac{5}{2}$	21 541.54	7.0999(0.1020)E+07	8.029E+07		
	$\frac{1}{2}$–$\frac{3}{2}$	21 571.92	5.9391(0.0852)E+07	6.718E+07		
$2s^2 3s\ ^2S$–$2s^2 3p\ ^2P^o$	$\frac{1}{2}$–$\frac{1}{2}$	24 491.04	8.5406(0.0729)E+07	8.730E+07		
	$\frac{1}{2}$–$\frac{3}{2}$	24 527.17	8.5795(0.0732)E+07	8.769E+07		
$2s2p^2\ ^2P$–$2p^3\ ^2D^o$	$\frac{3}{2}$–$\frac{5}{2}$	57 196.64	1.4500(0.0173)E+08	1.527E+08	1.63E+08	1.67E+08
	$\frac{3}{2}$–$\frac{3}{2}$	57 211.16	2.4570(0.0284)E+07	2.503E+07	2.69E+07	2.74E+07
	$\frac{1}{2}$–$\frac{3}{2}$	57 322.09	1.2663(0.0147)E+08	1.290E+08	1.37E+08	1.41E+08
$2s2p^2\ ^2P$–$2p^3\ ^2P^o$	$\frac{3}{2}$–$\frac{1}{2}$	84 698.97	2.8471(0.0141)E+08	2.915E+08	2.92E+08	3.01E+08
	$\frac{3}{2}$–$\frac{3}{2}$	84 703.10	7.1848(0.0356)E+08	7.355E+08	7.34E+08	7.58E+08
	$\frac{1}{2}$–$\frac{1}{2}$	84 809.91	5.7855(0.0287)E+08	5.992E+08	5.91E+08	6.11E+08
	$\frac{1}{2}$–$\frac{3}{2}$	84 814.04	1.3956(0.0069)E+08	1.430E+08	1.44E+08	1.47E+08
$2s2p^2\ ^2S$–$2p^3\ ^2P^o$	$\frac{1}{2}$–$\frac{1}{2}$	99 541.34	2.4382(0.0140)E+08	2.511E+08	2.89E+08	3.09E+08
	$\frac{1}{2}$–$\frac{3}{2}$	99 545.47	2.5347(0.0145)E+08	2.606E+08	2.96E+08	3.19E+08
$2s^2 2p\ ^2P^o$–$2s2p^2\ ^2D$	$\frac{3}{2}$–$\frac{5}{2}$	101 075.31	4.9769(0.0347)E+08	4.977E+08	4.70E+08	5.05E+08
	$\frac{3}{2}$–$\frac{3}{2}$	101 082.12	8.1782(0.0567)E+07	8.188E+07	7.77E+07	8.31E+07
	$\frac{1}{2}$–$\frac{3}{2}$	101 257.13	4.1869(0.0291)E+08	4.187E+08	3.94E+08	4.25E+08
$2s2p^2\ ^2D$–$2p^3\ ^2D^o$	$\frac{3}{2}$–$\frac{5}{2}$	102 106.10	6.6038(0.0109)E+07	6.714E+08	7.17E+07	7.39E+07
	$\frac{5}{2}$–$\frac{5}{2}$	102 112.91	9.1288(0.0143)E+08	9.282E+08	9.94E+08	1.02E+09
	$\frac{3}{2}$–$\frac{3}{2}$	102 120.62	8.7572(0.0150)E+08	8.912E+08	9.56E+08	9.82E+08
	$\frac{5}{2}$–$\frac{3}{2}$	102 127.43	1.0057(0.0017)E+08	1.023E+08	1.08E+08	1.12E+08
$2s2p^2\ ^4P$–$2p^3\ ^4S^o$	$\frac{5}{2}$–$\frac{3}{2}$	129 638.97	2.4194(0.1200)E+09	2.448E+09	2.26E+09	2.50E+09
	$\frac{3}{2}$–$\frac{3}{2}$	129 720.04	1.6161(0.0802)E+09	1.635E+09	1.51E+09	1.67E+09
	$\frac{1}{2}$–$\frac{3}{2}$	129 779.89	8.0921(0.4016)E+08	8.187E+08	7.55E+08	8.36E+08
$2s2p^2\ ^2D^o$–$2p^3\ ^2P$	$\frac{3}{2}$–$\frac{1}{2}$	129 608.44	2.8591(0.0077)E+09	2.337E+09	1.94E+09	2.19E+09
	$\frac{3}{2}$–$\frac{3}{2}$	129 612.57	2.9240(0.0078)E+08	2.362E+08	1.95E+08	2.22E+08
	$\frac{5}{2}$–$\frac{3}{2}$	129 619.37	2.5472(0.0069)E+09	2.092E+09	1.74E+09	1.96E+09
$2s^2 2p\ ^2P^o$–$2s2p^2\ ^2S$	$\frac{3}{2}$–$\frac{1}{2}$	131 149.22	1.8238(0.0089)E+09	1.848E+09	1.85E+09	1.78E+09
	$\frac{1}{2}$–$\frac{1}{2}$	131 324.23	9.4614(0.0459)E+08	9.572E+08	8.26E+08	9.21E+08
$2s^2 2p\ ^2P^o$–$2s2p^2\ ^2P$	$\frac{3}{2}$–$\frac{1}{2}$	145 880.65	1.9080(0.0058)E+09	1.918E+09	1.49E+09	1.91E+09
	$\frac{3}{2}$–$\frac{3}{2}$	145 991.58	4.7134(0.0145)E+09	4.742E+09	3.71E+09	4.71E+09
	$\frac{1}{2}$–$\frac{1}{2}$	146 055.66	3.7457(0.0115)E+09	3.770E+09	2.96E+09	3.775E+09
	$\frac{1}{2}$–$\frac{3}{2}$	146 166.60	9.4216(0.0291)E+08	9.480E+08	7.43E+08	9.42E+08
$2s2p^2\ ^2D$–$2s^2 3p\ ^2P^o$	$\frac{3}{2}$–$\frac{1}{2}$	144 580.39	1.0407(0.0422)E+08	1.065E+08		
	$\frac{3}{2}$–$\frac{3}{2}$	144 616.52	1.0450(0.0424)E+07	1.064E+07		
	$\frac{5}{2}$–$\frac{3}{2}$	144 623.33	9.3771(0.3803)E+07	9.606E+07		
$2s^2 2p\ ^2P^o$–$2s^2 3s\ ^2S$	$\frac{3}{2}$–$\frac{1}{2}$	221 171.47	2.0864(0.0096)E+09	2.050E+09		
	$\frac{1}{2}$–$\frac{1}{2}$	221 346.48	1.0427(0.0047)E+09	1.024E+09		

Table 8. Continued.

Multiplet	J_i–J_k	E (cm^{-1})	A_{ki} (un)	BHSB [1]	SJL [15]	NS [16]
2s2p^2 ^{4}P–2s2p3s ^{4}P^o	$\frac{5}{2}$–$\frac{3}{2}$	230 348.73	1.9493(0.0179)E+09			
	$\frac{3}{2}$–$\frac{1}{2}$	230 367.26	3.6079(0.0331)E+09			
	$\frac{1}{2}$–$\frac{1}{2}$	230 427.11	7.2190(0.0663)E+08			
	$\frac{3}{2}$–$\frac{3}{2}$	230 429.81	5.7792(0.0530)E+08			
	$\frac{5}{2}$–$\frac{5}{2}$	230 464.67	3.0391(0.0279)E+09			
	$\frac{1}{2}$–$\frac{3}{2}$	230 489.66	1.8068(0.0166)E+09			
	$\frac{3}{2}$–$\frac{5}{2}$	230 545.74	1.3033(0.0119)E+09			
2s^{2}2p ^{2}P^o–2s^{2}3d ^{2}D	$\frac{3}{2}$–$\frac{3}{2}$	267 234.42	2.0833(0.0045)E+09	1.859E+09		
	$\frac{3}{2}$–$\frac{5}{2}$	267 240.18	1.2491(0.0027)E+10	1.114E+10		
	$\frac{1}{2}$–$\frac{3}{2}$	267 409.44	1.0419(0.0023)E+10	9.290E+09		

Table 9. Comparison of intercombination transition rates (in s^{-1}) 2s^{2}2p ^{2}P^o_J–2s2p^2 ^{4}P$_{J'}$. Uncertainties are given in units of the last digit quoted.

^{2}P^o_J–^{4}P$_{J'}$					Total from ^{4}P$_{J'}$		
$\frac{1}{2}$–$\frac{1}{2}$	$\frac{3}{2}$–$\frac{1}{2}$	$\frac{1}{2}$–$\frac{3}{2}$	$\frac{3}{2}$–$\frac{3}{2}$	$\frac{3}{2}$–$\frac{5}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	Source
C II							
Theory							
61.52(70)	69.46(59)	1.465(12)	8.874(70)	44.89(40)	130.98(129)	10.34(9)	(adjusted) present
71.91	81.89	1.871	10.22	50.31	153.8	12.09	Galavis *et al* (1998) [2]
62.1	68.9	1.43	9.34	45.7	131	10.77	Froese Fischer (1994) [14]
Experiment				51(4)	146(10)	12(2)	Fang *et al* (1993) [17]
				45.35(15)	125.8(9)	9.61(5)	Träbert *et al* (1999) [18]
				50.0(25)	130.0(55)	9.0(10)	Smith *et al* (1999) [19]
N III							
Theory							
358.5(27)	371.4(28)	9.276(72)	63.89(44)	281.6(20)	729.9(56)	73.17(51)	(adjusted) present
417.7	446.2	11.72	69.96	317.1	863.9	81.68	Galavis *et al* (1998) [2]
346.8	361.5	8.781	60.20	266.0	708.3	68.98	Bell *et al* (1995) [1]
360.9	371.7	9.11	65.1	281.8	732.6	74.21	Brage *et al* (1995) [21]
Experiment				308(22)	1019(64)	75(6)	Fang *et al* (1993) [17]
				305(6)	755(35)	71.8(11)	Träbert *et al* (1999) [18]
O IV							
Theory							
1493(8)	1466(8)	39.08(21)	294.4(19)	1194(6)	2959(16)	333.5(21)	(adjusted) present
1724	1762	48.36	314.7	1331	3486	363.1	Galavis *et al* (1998) [2]
1469	1430	38.37	294.2	1172	2899	332.6	Brage *et al* (1996) [20]
1810	1770	22.8	328	1040	3580	350.8	Merkelis *et al* (1996) [13]

same experiment for all upper levels. In N III, there is overlap in the decay rates from $^4P_{1/2}$ and $^4P_{3/2}$ of N III with [18] but not with $^3P_{5/2}$, where their experimental value has a rather small error bar.

Finally, in table 10 we report lifetimes for boron and some boron-like ions for a number of states. For 2s2p^2 ^{2}D$_J$ there appears to be some J dependence in Na VII, but for others

Table 10. Computed lifetimes (in ns) compared with experimental and other theoretical data. In each case, the first line is present work. When only J-independent data are available, these data are included only for the lowest level.

Configuration	Term	J	B I	C II	N III	O VI	Na VII
$2s2p^2$	^{2}D	$\frac{5}{2}$	22.90	3.451	1.996	1.406	0.735
					2.12[l]	1.49[l]	
					2.04(15)[i]		0.70(7)[a]
					2.09(8)[k]		0.680[b]
					2.04[m]		
		$\frac{3}{2}$	22.85	3.441	1.985	1.396	0.713
					2.09(8)[k]		0.69(5)[a]
							0.659[b]
	^{2}S	$\frac{1}{2}$		0.452	0.358	0.279	0.161
					0.411[l]	0.303[l]	
					0.46(6)[i]	0.248[c]	0.155(10)[a]
					0.32(6)[k]	0.36(8)[f]	0.143[b]
					0.356[m]	0.29(20)[e]	
	^{2}P	$\frac{1}{2}$		0.245	0.176	0.138	0.0833
					0.229[l]	0.167[l]	
					0.190(15)[i]		0.073(10)[a]
					0.19(5)[k]		0.083[b]
					0.177[m]		
		$\frac{3}{2}$		0.245	0.176	0.138	0.0830
					0.20(6)[k]		
$2p^3$	^{4}S^o	$\frac{3}{2}$		0.294	0.206	0.158	0.0923
					0.221[l]	0.168[l]	
					0.26(5)[k]		0.095(10)[a]
					0.204[m]		0.088 [b]
	^{2}D^o	$\frac{5}{2}$		1.834	0.884	0.585	0.284
					0.814[l]	0.566[l]	
				1.70(15)[g]			0.28(4)[a]
				1.85[j]	0.862[m]		0.271[b]
		$\frac{3}{2}$		1.835	0.885	0.586	0.285
							0.272[b]
	^{2}P^o	$\frac{1}{2}$		0.497	0.293	0.218	0.116
					0.321[l]	0.229[l]	
					0.282[m]		0.105[b]
		$\frac{3}{2}$		0.496	0.294	0.218	0.116
$2s^23s$	^{2}S	$\frac{1}{2}$	3.996	2.266	0.319	0.124	0.0203
			4.02[h]		0.420(20)[i]	0.131[c]	
					0.334[m]	0.137(10)[d]	
$2s^23p$	^{2}P^o	$\frac{1}{2}$	50.06	8.973	4.410	1.387	0.223
				8.9(3)[g]	4.15[m]		
		$\frac{3}{2}$	50.04	8.963	4.400	1.386	0.222
$2s^23d$	^{2}D	$\frac{3}{2}$	4.629	0.349	0.0794	0.0282	0.0038
		$\frac{5}{2}$	4.631	0.349	0.0795	0.0283	0.0038
			4.60[h]		0.793[m]		

Table 10. Continued.

Configuration	Term	J	B I	C II	N III	O VI	Na VII
2s2p3s	$^4P^o$	$\frac{1}{2}$		1.188	0.231	0.0984	0.0169
						0.0983[c]	
						0.101(5)[d]	
		$\frac{3}{2}$		1.187	0.231	0.0982	0.0168
				1.187	0.230	0.0979	0.0167

[a] [22] (Exp.). [b] [22] (MCDF). [c] [24]. [d] [25]. [e] [26]. [f] [27]. [g] [28]. [h] [29]. [i] [30]. [j] [31]. [k] [32]. [l] [15]. [m] [23].

the J dependence is negligible. For Na VII some interesting recent results have been reported by Tordoir *et al* [22]. The paper includes both new experimental measurements and MCDF calculations that include some correlation. It is interesting to note that, in some instances, this paper is in closer agreement with experiment ($2s2p^2\ ^2D_J$ and $2p^3\ ^4S^o$ and $^2D^o$) than with the MCDF calculations. This may be related in part to the fact that an EAL approximation was used that does not include configuration interaction of orbitals during orbital optimization. Most experiments have relatively large error bars so that theory agrees moderately well. The one exception is the lifetime of $2s^23s\ ^2S$ in N III. Quite a few lifetimes for this system have been reported by Stafford *et al* [23] and the difference in our two values for the $2s^23s\ ^2S$ lifetime is less than 5%. For $2s^23p\ ^2P^o_J$ the difference is closer to 6%, but in other cases the agreement is considerably better. Indeed, in N III, our theoretical values are in closer agreement with Stafford *et al* [23] than other theory or experiment. The accuracy of a lifetime is determined primarily by the largest modes of decay. From tables 7 and 8, we see that the uncertainty in the lifetime of $2s^23p\ ^2P^o_J$ may be as large as 4% and 2% in N III and O IV, respectively, but others are expected to have smaller errors.

7. Conclusions

In this paper we have presented and analysed transition data for a portion of a spectrum in the boron-like isoelectronic sequence. Results are based on simultaneous optimization of orbitals for a number of terms and the diagonalization of the Breit–Pauli Hamiltonian (omitting orbit–orbit terms). By employing systematic, large-scale methods, we are able to monitor the convergence of the line strength. The recommended values are values scaled to the observed transition energy. For allowed transitions, we estimate the uncertainty of such data, in per cent, to be the sum of the discrepancy in the length and velocity form of the line strength plus the error in the transition energy, both also in per cent. Further comparative studies with more accurate theories and experiment are needed to evaluate this assumption.

The large Breit–Pauli calculations were performed on the T3E at the National Energy Research Scientific Computing Center (NERSC) using an MPI version of the code and employing 64 processors for the larger cases.

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