

Energy levels and transition rates for the boron isoelectronic sequence: Si X, Ti XVIII – Cu XXV^{*,**}

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Received 14 May 2013 / Accepted 14 July 2013

ABSTRACT

Relativistic configuration interaction (RCI) calculations are performed for 291 states belonging to the configurations $1s^22s^22p$, $1s^22s2p^2$, $1s^22p^3$, $1s^22s^23l$, $1s^22s2p3l$, $1s^22p^23l$, $1s^22s^24l'$, $1s^22s2p4l'$, and $1s^22p^24l'$ ($l = 0, 1, 2$ and $l' = 0, 1, 2, 3$) in boron-like ions Si X and Ti XVIII to Cu XXV. Electron correlation effects are represented in the wave functions by large configuration state function (CSF) expansions. States are transformed from jj -coupling to LS -coupling, and the LS -percentage compositions are used for labeling the levels. Radiative electric dipole transition rates are given for all ions, leading to massive data sets. Calculated energy levels are compared with other theoretical predictions and crosschecked against the Chianti database, NIST recommended values, and other observations. The accuracy of the calculations are high enough to facilitate the identification of observed spectral lines.

Key words. atomic data – atomic processes

1. Introduction

The X-ray spectra from L-shell ions are particularly important for astrophysics, as they are in the wavelength range covered by telescopes on board the space observatories *Chandra* and *XMM-Newton* (Landi & Gu 2006). The analysis of high-resolution X-ray spectra requires knowledge of energy levels and a large number of accurate transition rates, either from theory or experiment, to identify spectral lines, produce synthetic spectra, and carry out plasma diagnostics. Similarly, spectra from these ions find applications in the diagnostics and modeling of fusion plasmas. The work on fusion plasma is especially important in relation to the International Thermonuclear Experimental Reactor (ITER).

During the past few years a number of calculations have been carried out to provide more complete sets of energies and transition data for L-shell ions. Merkelis et al. (1995) used the stationary second-order many-body perturbation theory (MBPT) to compute energies for $n = 2$ levels, and transition rates for boron-like ions for $Z = 8$ to 26. The relativistic effects in those calculations were accounted for in the Breit-Pauli approximation. Safronova et al. (1996, 1998, 1999) used relativistic many-body perturbation theory (RMBPT) to compute energies

for $n = 2, 3$ levels and transition rates between $n = 2$ states for boron-like ions with nuclear charges ranging from $Z = 5$ to 100. Gu (2005a) used relativistic configuration interaction and many-body perturbation theory to compute energies of $n = 2$ levels for ions with $Z \leq 60$. The work was later extended to levels in boron-like iron and nickel involving higher n (Gu 2005b, 2007). The calculations by Safronova et al. and Gu are highly accurate and in many cases, give transition wavelengths to within a few mÅ, comparable to what can be obtained in experimental work. Results with high accuracy were obtained by Rynkun et al. (2012) using relativistic configuration interaction (RCI). Energies for $n = 2$ levels and E1, M1, and E2 transition rates were reported for ions with $Z = 7$ to 30. Vilkas et al. (2005) used relativistic multireference many-body perturbation theory (MRMP) to calculate energies in Si X. The energies were accurate enough to unambiguously identify EUV and soft-X-ray spectral lines in old beam-foil spectra. The combined theoretical and experimental work resulted in an extensive data set that is suitable for the validation of different computational methods.

Much work has been focused on iron. Landi & Gu (2006) used the flexible atomic structure code (FAC) to calculate energy levels, transition rates, and electron-ion excitation collision strengths for high-energy configurations in the iron ions Fe XVII to Fe XXIII. Massive calculations have recently also been performed by Jonauskas et al. (2006) and Nahar (2010). These calculations include hundreds of fine-structure levels, but the accuracy of the computed energies is not as high as for the calculations by Safronova et al. (1996, 1998), Gu (2005b, 2007), and Rynkun et al. (2012).

Although theoretical data are available, it is still very difficult to analyze spectra, unambiguously identify transitions, and deduce energy levels with the proper labels. Looking at the

* Research supported in part by the Swedish Research council and the Swedish Institute. Part of this work was supported by the Communauté française of Belgium, the Belgian National Fund for Scientific Research (FRFC/IISN Convention) and by the IUAP-Belgian State Science Policy (BriX network P7/12).

** Tables of energy levels and transition rates (Tables 3–19) are only available at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via <http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/A+A/559/A100>

NIST Atomic Spectra Database (2013), there remain large gaps that need to be filled and misidentifications are present. This paper reports on RCI calculations for 291 states belonging to the configurations $1s^2 2s^2 2p$, $1s^2 2s 2p^2$, $1s^2 2p^3$, $1s^2 2s^2 3l$, $1s^2 2s 2p 3l$, $1s^2 2p^2 3l$, $1s^2 2s^2 4l'$, $1s^2 2s 2p 4l'$, and $1s^2 2p^2 4l'$ ($l = 0, 1, 2$ and $l' = 0, 1, 2, 3$) in boron-like ions Si X, and Ti XVIII to Cu XXV. Energy levels and electric dipole transition rates between the states are given. Results are crosschecked and validated against other theoretical predictions and experimental data. The work is part of a long-term theoretical effort to attain spectroscopic accuracy, i.e. calculated transition energies that are accurate enough to directly confirm or revise experimental identifications. It complements and extends previous work on boron-, carbon-, nitrogen-, oxygen-, and neon-like systems, where energies have been provided with relative inaccuracies of fractions of a per mille (Rynkun et al. 2012; Jönsson et al. 2011, 2013a).

2. Relativistic multiconfiguration calculations

The calculations were performed using the fully relativistic multiconfiguration Dirac-Hartree-Fock (MCDHF) method in jj -coupling (Grant 2007). For practical purposes, a transformation from jj - to LS -coupling (Gaigalas et al. 2003) was done at the end, and in all tables, the quantum states are labeled by the leading LS -percentage composition.

2.1. Multiconfiguration Dirac-Hartree-Fock

Starting from the Dirac-Coulomb Hamiltonian,

$$H_{\text{DC}} = \sum_{i=1}^N \left(c\alpha_i \cdot \mathbf{p}_i + (\beta_i - 1)c^2 + V_i^N \right) + \sum_{i>j}^N \frac{1}{r_{ij}}, \quad (1)$$

where V^N is the monopole part of the electron-nucleus Coulomb interaction, α and β the 4×4 Dirac matrices, and c the speed of light in atomic units, the atomic state functions were obtained as linear combinations of symmetry adapted configuration state functions (CSFs):

$$\Psi(\gamma P J M) = \sum_{j=1}^{\text{NCSF}} c_j \Phi(\gamma_j P J M). \quad (2)$$

Here, J and M are the angular quantum numbers and P is the parity. The label γ_j denotes other appropriate information of the configuration state function j , such as orbital occupancy and coupling scheme. The CSFs were built from products of one-electron Dirac orbitals. Based on a weighted energy average of several states known as the extended optimal level (EOL) scheme (Dyall et al. 1989), both the radial parts of the Dirac orbitals and the expansion coefficients were optimized to self-consistency in the relativistic self-consistent field (RSCF) procedure.

The transverse interaction in the low-frequency limit, or the Breit interaction (McKenzie et al. 1980),

$$H_{\text{Breit}} = - \sum_{i<j}^N \frac{1}{2r_{ij}} \left[\alpha_i \cdot \alpha_j + \frac{(\alpha_i \cdot \mathbf{r}_{ij})(\alpha_j \cdot \mathbf{r}_{ij})}{r_{ij}^2} \right], \quad (3)$$

and leading QED (vacuum polarization and self-energy) were included in subsequent configuration interaction (RCI) calculations. All calculations were performed with the GRASP2K code

(Jönsson et al. 2007, 2013b). To calculate the spin-angular part of the matrix elements, the second quantization method in coupled tensorial form and quasispin technique (Gaigalas et al. 1997) was adopted.

2.2. Transition parameters

The evaluation of spontaneous transition rates, A , between two states, $\gamma' P' J' M'$ and $\gamma P J M$, built on different and independently optimized orbital sets is non-trivial. The transition rates, or probabilities, can be expressed in terms of the transition moment, which is defined as

$$\langle \Psi(\gamma P J) \| \mathbf{T} \| \Psi(\gamma' P' J') \rangle = \sum_{j,k} c_j c'_k \langle \Phi(\gamma_j P J) \| \mathbf{T} \| \Phi(\gamma'_k P' J') \rangle, \quad (4)$$

where \mathbf{T} is the transition operator (Cowan 1981). The calculation of the transition moment breaks down to the task of summing up reduced matrix elements between different CSFs. The reduced matrix elements can be evaluated using standard techniques assuming that both left and right hand CSFs are formed from the *same* orthonormal set of spin-orbitals. This constraint is severe, since a high-quality and compact wave function requires orbitals optimized for specific electronic states from which orbital non-orthogonalities arise in the calculation of transition amplitudes (Fritzsche et al. 1994). To get around the problems, the wave functions of the two states, $\gamma' P' J' M'$ and $\gamma P J M$, were separately optimized, and their representations were transformed in such a way that the orbital sets became biorthonormal (Olsen et al. 1995). Standard methods were then used to evaluate the matrix elements between the transformed CSFs.

For electric dipole (E1) transitions, there are two forms of the transition operator, the length, and velocity form (Grant 1974). The length form is usually the preferred one. The agreement between transition rates computed in the two forms can be used as an indicator of the accuracy of the underlying wave functions (Froese Fischer 2009). In this work, we introduce the ratio, R , between the transition rates, A , in length and velocity forms as the indicator.

2.3. Validation for Si X

Si X holds a prominent position among boron-like ions because many energy levels are known with a high accuracy from the combined theoretical and experimental work by Vilkas et al. (2005). The ion is thus an excellent testing ground. To validate current computational methods and strategies, calculations were performed for the lowest states belonging to the configurations $1s^2 2s^2 2p$, $1s^2 2s 2p^2$, $1s^2 2p^3$, $1s^2 2s^2 3l$, $1s^2 2s 2p 3l$, and $1s^2 2p^2 3l$ ($l = 0, 1, 2$) in Si X. We describe the calculations for the odd states. The calculations for the even parity states were done in a similar manner.

As a starting point, an RSCF calculation was performed in the EOL scheme for the weighted average of the odd parity reference states. To include electron correlation, this calculation was followed by two calculations where the CSF expansions were obtained by allowing single and double (SD) excitations from all shells of the odd parity reference configurations to active orbital sets with principal quantum numbers up to $n = 4$ and 5 , respectively. Additional RSCF calculations were performed for CSF expansions obtained by allowing SD excitations from the outer shells of the odd reference configurations to active orbital sets that were systematically enlarged from $n = 6$ up to $n = 9$

and with orbital angular momenta up to $l = 6$. The RSCF calculations generated a well balanced active orbital set. In a final step, an RCI calculation was performed. The expansion was obtained by allowing SD excitations from all shells of the reference configurations to the largest active orbital set. The resulting expansion that accounted for core-core, core-valence, and valence-valence electron correlation effects consisted of 474 000 CSFs distributed over the $J = 1/2, 3/2, \dots, 9/2$ angular symmetries. The same computational strategy applied to the even parity states yielded a final RCI expansion that consisted of 503 000 CSFs. Tests indicated that the calculated properties were well converged with respect to the active orbital sets.

2.4. Calculations for Ti XVIII to Cu XXV

For the ions Ti XVIII to Cu XXV, that is the focus of this paper, we considered the levels belonging to the configurations $1s^2 2s^2 2p$, $1s^2 2s 2p^2$, $1s^2 2p^3$, $1s^2 2s^2 3l$, $1s^2 2s 2p 3l$, $1s^2 2p^2 3l$, $1s^2 2s^2 4l'$, $1s^2 2s 2p 4l'$, and $1s^2 2p^2 4l'$ ($l = 0, 1, 2$ and $l' = 0, 1, 2, 3$). The calculations for these ions were done in a similar way as for Si X, generating active orbital sets with orbitals up to $n = 9$ and $l = 6$. The final RCI calculations were based on expansions obtained by allowing SD excitations from all shells of the reference configurations to the largest active orbital sets. Due to a larger number of reference states for Ti XVIII to Cu XXV, as compared with Si X, the expansions were now larger. For the odd parity states, there were 982 000 CSFs distributed over the $J = 1/2, 3/2, \dots, 11/2$ angular symmetries. For the even parity states, there were 971 000 CSFs. For Ti XVIII to Cu XXV, the orbital set spans more states compared with Si X. However, tests indicated that the calculated properties were well converged with respect to the active orbital sets also in this case.

2.5. Labeling of states

The wave functions in the present work were obtained as expansions over jj -coupled CSFs, and it is convenient to give the states the same labels as the dominating CSFs. The states were, however, not well described in jj -coupling, and in the expansions, many CSFs had nearly the same weight. To adhere to the labeling in the NIST database and in other sources, the states should instead be given in LS -coupling. As discussed by Safronova et al. (1998), LS -coupling is neither a good labeling system nor is it straightforward to assign labels. Safronova et al. (1998) used a number of rules to perform the task, but these were sometimes not consistent with the experimental labels, thus, causing confusion. In this work, we used a module in the latest release of the GRASP2K code (Jönsson et al. 2013b) to transform from jj - to LS -coupling to obtain the leading LS -percentage composition. This gave a label system compatible with the one used by experimentalists, which often relied on calculations using the HFR suite of codes Cowan (1981) for their analysis. It also corresponded to the labels obtained from non-relativistic calculations with relativistic corrections in the Breit-Pauli approximation (Jonas et al. 2006; Nahar 2010). It should be noted that there were also states with the same leading LS -percentage composition in LS -coupling, and for these states, a more complete composition should be used as the label.

3. Results and discussion

3.1. Energies for Si X

The calculations for Si X serve as validation. In Table 1, we compare energies in Si X from the final RCI calculation with

observed and calculated energies by Vilkas et al. (2005) and from the Chianti database (Landi et al. 2012). The calculations by Vilkas et al. are based on relativistic multireference many-body perturbation theory (MRMP). The experimental energies in the Chianti database are all reassessed from the original wavelength measurements. There are, however, only small differences compared with the experimental energies given by Vilkas et al. The theoretical energies given in the Chianti database are from R-matrix calculations by Liang et al. (2009). In Table 1, there are also energies from RMBPT calculations by Safronova et al. (1996, 1998). Labels from the latter calculations in some cases did not match the labels from the RCI calculations. From the J quantum number and the computed energies, it was however possible to correctly match all the levels. Except for the R-matrix calculation that was optimized for electron-ion collisional data, which requires a comparatively small target, there is an excellent agreement between the different sets of calculations and observations. The mean relative energy differences between calculations and observations are 0.018% for RCI, 0.029% for MRMP, and 0.068% for RMBPT. Looking at Table 1 more closely, it is seen that two many-body perturbation theory-based calculations (MRMP and MBPT) yield values that are too low, but the third (RMBPT) yields values that are too high. To quantify this, we computed the mean level deviation (MLD) between the observed and calculated energy levels. The MLD is given by

$$MLD = \frac{1}{N} \sum_{i=1}^N |E_{\text{obs}}(i) - E_{\text{calc}}(i) + ES|, \quad (5)$$

where the energy shift (ES) is chosen to minimize the sum. The MLD and ES are 236 cm^{-1} and 12 cm^{-1} for RCI, 258 cm^{-1} and -47 cm^{-1} for MRMP, and 770 cm^{-1} and 804 cm^{-1} for RMBPT. Although not very large, there is a positive bias of the predicted energy levels from the RMBPT calculations.

3.2. Energies for Fe XXII

In Table 2, we give calculated energies for the levels belonging to the configurations $1s^2 2s^2 2p$, $1s^2 2s 2p^2$, $1s^2 2p^3$, $1s^2 2s^2 3l$, $1s^2 2s 2p 3l$, and $1s^2 2p^2 3l$ ($l = 0, 1, 2$) in Fe XXII. The full data set comprising of levels with $n = 4$ is given in Table 7. In Table 2, calculated and observed energies from the Chianti database (Landi et al. 2012) are also given. Calculated energies held by the Chianti database are from Landi & Gu (2006). The observed levels are from different sources and all the references are given in the database. In addition, energies from RMBPT calculations by Safronova et al. (1996, 1998) and (Gu 2005b, 2007) are given. Due to inconsistencies in the labels, the RMBPT results by Safronova et al. (1996, 1998) in several cases were matched using J quantum numbers and computed energies. There is an excellent agreement between the energies from the RCI calculations and the RMBPT calculations. Similar to Si X, the energies from the RMBPT calculations are higher than the energies from the RCI calculations. The agreement with the calculated energies from the Chianti database (Landi et al. 2012) is very good but not on the same level as for the RMBPT calculations. In most cases, there is a satisfactory agreement with the observed energies. The lack of experimental data, however, makes it difficult to distinguish between different theories, and we need to fall back on the results from Si X to draw any conclusions about the accuracy of the calculated energies. Undoubtedly, the combined energy levels from the RCI and RMBPT calculations provide a very good starting point for further identifications of observed lines.

Table 1. Energies in cm^{-1} for levels in Si X.

No.	Configuration	LS	J	$E(\text{RCI})$	$E(\text{EXP})$	$E(\text{MRMP})$	$E(\text{RMBPT})$	$E(\text{CHI}_{\text{exp}})$	$E(\text{CHI}_{\text{calc}})$	$E(\text{MBPT})$
1	2s(2).2p	2P	1/2	0	0	0	0	0	0	0
2	2s(2).2p	2P	3/2	6 990	6 991	6 961	7 000	6 991	7 290	6 874
3	2s.2p(2)3P	4P	1/2	161 022	161 010	160 813	161 437	161 028	157 687	160 718
4	2s.2p(2)3P	4P	3/2	163 453	163 490	163 286	163 925	163 503	160 324	163 201
5	2s.2p(2)3P	4P	5/2	167 044	167 060	166 847	167 511	167 069	164 438	166 754
6	2s.2p(2)1D	2D	3/2	288 100	287 850	287 727	287 448	287 851	294 258	286 178
7	2s.2p(2)1D	2D	5/2	288 117	287 880	287 754	287 467	287 860	294 455	286 245
8	2s.2p(2)1S	2S	1/2	368 007	367 670	367 623	367 741	367 658	375 537	365 775
9	2s.2p(2)3P	2P	1/2	390 395	390 040	390 501	389 298	390 050	400 444	389 343
10	2s.2p(2)3P	2P	3/2	394 369	394 030	394 504	393 257	394 027	404 878	393 294
11	2p(3)4S	4S	3/2	509 213	509 330	509 165	509 543	509 289	511 830	508 580
12	2p(3)2D	2D	3/2	575 538	575 430	575 133	574 823	575 427	586 864	571 928
13	2p(3)2D	2D	5/2	575 564	575 450	575 158	574 863	575 456	587 281	571 902
14	2p(3)2P	2P	1/2	646 972	646 760	646 691	646 133	646 760	661 395	643 250
15	2p(3)2P	2P	3/2	647 589	647 390	647 250	646 775	647 390	662 243	643 835
16	2s(2).3s	2S	1/2	1 821 975	1 822 000	1 821 859	1 823 343	1 822 004	1 815 605	
17	2s(2).3p	2P	1/2	1 902 444	1 902 100	1 902 494	1 903 801		1 896 879	
18	2s(2).3p	2P	3/2	1 904 304	1 903 957	1 904 352	1 905 665		1 898 664	
19	2s(2).3d	2D	3/2	1 979 272	1 979 260	1 979 457	1 980 633	1 979 260	1 975 596	
20	2s(2).3d	2D	5/2	1 979 762	1 979 730	1 979 944	1 981 124	1 979 730	1 976 124	
21	2s.2p_3P.3s	4P	1/2	1 992 698	1 992 850	1 992 728	1 994 133	1 992 860	1 987 010	
22	2s.2p_3P.3s	4P	3/2	1 994 989	1 995 140	1 995 016	1 996 432	1 995 153	1 989 420	
23	2s.2p_3P.3s	4P	5/2	1 999 276	1 999 580	1 999 293	2 000 715	1 999 580	1 993 714	
24	2s.2p_3P.3s	2P	1/2	2 031 112	2 031 070	2 031 025	2 032 013	2 031 060	2 029 150	
25	2s.2p_3P.3s	2P	3/2	2 035 800	2 035 860	2 035 692	2 036 700	2 035 860	2 033 938	
26	2s.2p_3P.3p	2P	1/2	2 064 373	2 064 770	2 064 333	2 065 321	2 064 590	2 063 696	
27	2s.2p_3P.3p	2P	3/2	2 066 510	2 066 600	2 066 470	2 067 465	2 066 750	2 064 727	
28	2s.2p_3P.3p	4D	1/2	2 068 522		2 068 488	2 069 556		2 059 572	
29	2s.2p_3P.3p	4D	3/2	2 069 516		2 069 481	2 070 055		2 061 793	
30	2s.2p_3P.3p	4D	5/2	2 070 743		2 070 725	2 071 935		2 065 470	
31	2s.2p_3P.3p	4D	7/2	2 074 525		2 074 502	2 075 720		2 069 208	
32	2s.2p_3P.3p	4S	3/2	2 085 441		2 085 399	2 086 792		2 079 378	
33	2s.2p_3P.3p	4P	1/2	2 095 426		2 095 274	2 096 880		2 090 773	
34	2s.2p_3P.3p	4P	3/2	2 097 476		2 097 329	2 098 935		2 092 807	
35	2s.2p_3P.3p	4P	5/2	2 099 483		2 099 337	2 100 939		2 095 022	
36	2s.2p_3P.3p	2D	3/2	2 105 583	2 105 750	2 105 297	2 106 140	2 105 800	2 103 702	
37	2s.2p_3P.3p	2D	5/2	2 110 094	2 110 260	2 109 773	2 110 659	2 110 260	2 108 207	
38	2s.2p_3P.3d	4F	3/2	2 131 375		2 131 548	2 132 998		2 127 778	
39	2s.2p_3P.3p	2S	1/2	2 132 461	2 132 700	2 132 289	2 132 857	2 132 500	2 132 024	
40	2s.2p_3P.3d	4F	5/2	2 132 726		2 132 895	2 134 355		2 129 237	
41	2s.2p_3P.3d	4F	7/2	2 134 759		2 134 922	2 136 394		2 131 381	
42	2s.2p_3P.3d	4F	9/2	2 137 677		2 137 824	2 139 316		2 134 382	
43	2s.2p_3P.3d	4D	1/2	2 150 711	2 150 900	2 150 882	2 152 278	2 150 919	2 146 486	
44	2s.2p_3P.3d	4D	3/2	2 150 921	2 150 900	2 151 105	2 152 488	2 150 920	2 146 707	
45	2s.2p_3P.3d	4D	5/2	2 151 357	2 151 360	2 151 561	2 152 918	2 151 377	2 147 165	
46	2s.2p_3P.3d	4D	7/2	2 153 615	2 153 830	2 153 782	2 155 194	2 153 837	2 149 526	
47	2s.2p_3P.3d	2D	3/2	2 153 671	2 153 700	2 153 800	2 154 783	2 153 700	2 151 636	
48	2s.2p_3P.3d	2D	5/2	2 154 450	2 154 480	2 154 603	2 155 637	2 154 480	2 152 077	
49	2s.2p_1P.3s	2P	1/2	2 158 254	2 158 087	2 158 381	2 158 891		2 162 678	
50	2s.2p_1P.3s	2P	3/2	2 158 498	2 158 330	2 158 624	2 159 097	2 158 330	2 162 831	
51	2s.2p_3P.3d	4P	5/2	2 160 667	2 160 920	2 160 688	2 162 652	2 160 928	2 155 784	
52	2s.2p_3P.3d	4P	3/2	2 161 866	2 162 100	2 161 922	2 163 898	2 162 191	2 156 515	
53	2s.2p_3P.3d	4P	1/2	2 162 702	2 162 770	2 162 752	2 164 752		2 162 831	
54	2s.2p_3P.3d	2F	5/2	2 188 725	2 188 590	2 189 222	2 188 637	2 188 594	2 189 496	
55	2s.2p_3P.3d	2F	7/2	2 193 061	2 193 120	2 193 558	2 192 958	2 193 093	2 193 926	
56	2s.2p_3P.3d	2P	3/2	2 199 160	2 199 200	2 199 553	2 200 720	2 199 200	2 198 590	
57	2s.2p_3P.3d	2P	1/2	2 201 712	2 201 790	2 202 131	2 203 226	2 201 790	2 201 058	
58	2s.2p_1P.3p	2D	3/2	2 236 095	2 237 640	2 237 399	2 236 148		2 243 158	

Notes. The labels of the table are values from the following sources: $E(\text{RCI})$ this work, $E(\text{EXP})$ experimental energies by [Vilkas et al. \(2005\)](#), $E(\text{MRMP})$ relativistic multireference Møller-Plesset many-body perturbation calculations by [Vilkas et al. \(2005\)](#), $E(\text{RMBPT})$ relativistic many-body perturbation calculations by [Safronova et al. \(1996, 1998\)](#), $E(\text{CHI}_{\text{exp}})$ experimental energies from the Chianti database by [Landi et al. \(2012\)](#), $E(\text{CHI}_{\text{calc}})$ theoretical results from the Chianti database based on the calculations by [Liang et al. \(2009\)](#), and $E(\text{MBPT})$ many-body perturbation calculations by [Merkelis et al. \(1995\)](#). There seems to be an inconsistency in the labeling of states 58 and 61 between the current calculations and the work by [Vilkas et al. \(2005\)](#).

Table 1. continued.

No.	Configuration	<i>LS</i>	<i>J</i>	<i>E</i> (RCI)	<i>E</i> (EXP)	<i>E</i> (MRMP)	<i>E</i> (RMBPT)	<i>E</i> (CHI _{exp})	<i>E</i> (CHI _{calc})	<i>E</i> (MBPT)
59	2s.2p_1P.3p	2P	1/2	2 236 475	2 236 200	2 236 522	2 236 889	2 236 200	2 240 488	
60	2s.2p_1P.3p	2D	5/2	2 236 805	2 236 400	2 236 731	2 236 815	2 236 400	2 243 290	
61	2s.2p_1P.3p	2P	3/2	2 238 058	2 236 400	2 236 682	2 238 445		2 241 613	
62	2s.2p_1P.3p	2S	1/2	2 253 603	2 253 121	2 253 659	2 254 360	2 253 121	2 264 624	
63	2p(2)3P.3s	4P	1/2	2 284 877		2 284 809	2 285 899		2 280 893	
64	2p(2)3P.3s	4P	3/2	2 287 364		2 287 355	2 288 439		2 283 455	
65	2p(2)3P.3s	4P	5/2	2 291 136		2 291 118	2 292 191		2 287 508	
66	2s.2p_1P.3d	2F	7/2	2 299 933	2 299 900	2 299 891	2 299 975	2 299 890	2 310 646	
67	2s.2p_1P.3d	2F	5/2	2 300 109	2 299 900	2 300 052	2 300 142	2 299 891	2 310 796	
68	2s.2p_1P.3d	2D	3/2	2 310 748	2 310 530	2 311 223	2 311 118	2 310 530	2 319 362	
69	2s.2p_1P.3d	2D	5/2	2 311 464	2 311 390	2 311 943	2 311 839	2 311 390	2 320 123	
70	2p(2)_3P.3s	2P	1/2	2 323 216		2 322 666	2 323 564		2 328 471	
71	2s.2p_1P.3d	2P	1/2	2 323 391		2 323 844	2 323 664		2 334 457	
72	2s.2p_1P.3d	2P	3/2	2 323 923	2 323 820	2 324 376	2 324 215		2 335 213	
73	2p(2)3P.3s	2P	3/2	2 327 400		2 326 861	2 327 751		2 332 902	
74	2p(2)3P.3p	2S	1/2	2 339 997		2 340 074	2 341 171		2 336 064	
75	2p(2)1D.3s	2D	5/2	2 347 203		2 346 689	2 347 181		2 353 236	
76	2p(2)1D.3s	2D	3/2	2 347 351		2 346 831	2 347 364		2 353 366	
77	2p(2)3P.3p	4D	1/2	2 349 696	2 349 960	2 349 758	2 350 778		2 346 091	
78	2p(2)3P.3p	4D	3/2	2 351 202	2 351 487	2 351 285	2 352 306		2 347 621	
79	2p(2)3P.3p	4D	5/2	2 353 724	2 354 035	2 353 833	2 354 853		2 350 222	
80	2p(2)3P.3p	4D	7/2	2 357 163	2 357 463	2 357 261	2 358 274		2 353 892	
81	2p(2)3P.3p	4P	1/2	2 361 188		2 361 277	2 362 361		2 357 818	
82	2p(2)3P.3p	4P	3/2	2 362 053		2 362 122	2 363 177		2 358 865	
83	2p(2)3P.3p	4P	5/2	2 364 104		2 364 198	2 365 216		2 361 178	
84	2p(2)3P.3p	2D	3/2	2 369 768		2 369 698	2 370 363		2 369 720	
85	2p(2)3P.3p	2D	5/2	2 374 695		2 374 623	2 375 314		2 374 684	
86	2p(2)3P.3p	2P	3/2	2 389 244	2 390 320	2 390 048	2 389 727	2 390 320	2 390 797	
87	2p(2)3P.3p	2P	1/2	2 389 965	2 389 320	2 389 833	2 390 492		2 391 261	
88	2p(2)3P.3p	4S	3/2	2 391 186	2 390 416	2 390 242	2 392 471	2 390 416	2 389 919	
89	2p(2)3P.3d	4F	3/2	2 409 325		2 409 112	2 411 067		2 407 672	
90	2p(2)3P.3d	4F	5/2	2 410 664		2 410 471	2 412 429		2 409 134	
91	2p(2)1D.3p	2F	5/2	2 412 504		2 412 050	2 412 367		2 419 039	
92	2p(2)3P.3d	4F	7/2	2 412 609		2 412 429	2 414 392		2 411 263	
93	2p(2)1D.3p	2F	7/2	2 413 820	2 413 600	2 413 377	2 413 680	2 413 600	2 420 301	
94	2p(2)3P.3d	4F	9/2	2 415 202		2 414 998	2 416 965		2 414 141	
95	2p(2)3P.3d	4D	3/2	2 424 678		2 424 574	2 426 350		2 425 542	
96	2p(2)3P.3d	4D	1/2	2 425 065		2 424 952	2 426 942		2 422 738	
97	2p(2)3P.3d	4D	5/2	2 426 345		2 426 235	2 428 068		2 424 680	
98	2p(2)3P.3d	4D	7/2	2 427 276		2 427 159	2 429 055		2 425 920	
99	2p(2)3P.3d	2P	3/2	2 427 770		2 427 682	2 429 484		2 422 259	
100	2p(2)3P.3d	2F	5/2	2 430 387		2 430 062	2 431 338		2 432 909	
101	2p(2)3P.3d	2P	1/2	2 431 387		2 431 332	2 432 949		2 428 981	
102	2p(2)1D.3p	2D	5/2	2 435 354	2 435 260	2 434 828	2 435 504		2 443 217	
103	2p(2)3P.3d	2F	7/2	2 435 482		2 435 133	2 436 409		2 438 137	
104	2p(2)1D.3p	2D	3/2	2 435 574	2 435 480	2 435 048	2 435 713		2 443 314	
105	2p(2)3P.3d	4P	5/2	2 444 419	2 444 460	2 444 609	2 445 954	2 444 423	2 441 588	
106	2p(2)3P.3d	4P	3/2	2 446 095	2 446 000	2 446 301	2 447 629	2 445 960	2 443 294	
107	2p(2)3P.3d	4P	1/2	2 446 963	2 446 877	2 447 178	2 448 486		2 444 190	
108	2p(2)1D.3p	2P	1/2	2 451 503		2 451 115	2 451 452		2 463 812	
109	2p(2)1D.3p	2P	3/2	2 454 522		2 454 082	2 454 523		2 466 801	
110	2p(2)1S.3s	2S	1/2	2 455 499		2 455 285	2 455 530		2 461 840	
111	2p(2)1D.3d	2G	7/2	2 473 069		2 471 997	2 472 992		2 480 185	
112	2p(2)1D.3d	2G	9/2	2 473 575		2 472 482	2 473 462		2 480 747	
113	2p(2)3P.3d	2D	5/2	2 474 296		2 474 527	2 474 914		2 479 335	
114	2p(2)3P.3d	2D	3/2	2 474 302		2 474 666	2 474 912		2 479 261	
115	2p(2)1D.3d	2D	3/2	2 492 078		2 491 801	2 492 746		2 496 240	
116	2p(2)1D.3d	2D	5/2	2 492 500		2 492 517	2 492 077		2 498 177	
117	2p(2)1D.3d	2F	7/2	2 493 331		2 493 453	2 492 206		2 502 927	
118	2p(2)1D.3d	2F	5/2	2 496 155		2 496 068	2 496 126		2 504 448	
119	2p(2)1D.3d	2P	1/2	2 509 755		2 509 581	2 510 578		2 518 769	
120	2p(2)1D.3d	2P	3/2	2 511 607		2 511 513	2 512 459		2 520 593	

Table 2. Energies in cm^{-1} for levels in Fe XXII.

No.	Configuration	<i>LS</i>	<i>J</i>	<i>E</i> (RCI)	<i>E</i> (CHI _{exp})	<i>E</i> (CHI _{calc})	<i>E</i> (RMBPT1)	<i>E</i> (RMBPT2)	<i>E</i> (MBPT)
1	2s(2).2p	2P	1/2	0	0	0	0	0	0
2	2s(2).2p	2P	3/2	118 285	118 263	117 691	118 267	118 303	115 443
3	2s.2p(2)3P	4P	1/2	403 673	404 549	401 951	404 549	405 010	403 328
4	2s.2p(2)3P	4P	3/2	459 298	460 192	456 917	460 213	460 689	458 172
5	2s.2p(2)3P	4P	5/2	512 431	513 255	510 139	513 342	513 833	510 567
6	2s.2p(2)1D	2D	3/2	735 905	736 426	740 839	735 993	736 617	732 518
7	2s.2p(2)1D	2D	5/2	758 770	759 211	762 917	758 910	759 515	755 453
8	2s.2p(2)3P	2P	1/2	853 381	853 577	861 488	853 294	854 093	
9	2s.2p(2)1S	2S	1/2	978 159	978 348	985 776	978 150	978 634	
10	2s.2p(2)3P	2P	3/2	992 046	992 314	999 926	991 853	992 581	984 644
11	2p(3)4S	4S	3/2	1 255 316	1 255 688	1 257 805	1 255 463	1 256 519	1 249 923
12	2p(3)2D	2D	3/2	1 395 701	1 396 175	1 403 908	1 395 219	1 396 072	1 390 162
13	2p(3)2D	2D	5/2	1 426 030	1 426 499	1 433 892	1 425 551	1 426 488	1 420 124
14	2p(3)2P	2P	1/2	1 569 636	1 569 672	1 581 306	1 568 918	1 569 861	1 561 491
15	2p(3)2P	2P	3/2	1 627 555	1 627 666	1 637 761	1 626 918	1 627 869	1 618 534
16	2s(2).3s	2S	1/2	8 117 237	8 113 590	8 107 918	8 119 175	8 118 833	
17	2s(2).3p	2P	1/2	8 297 806	8 291 579	8 290 445	8 298 803	8 298 649	
18	2s(2).3p	2P	3/2	8 330 997	8 325 224	8 323 527	8 331 985	8 331 884	
19	2s.2p_3P.3s	4P	1/2	8 477 586		8 470 458	8 478 834	8 478 875	
20	2s(2).3d	2D	3/2	8 494 421	8 496 579	8 489 631	8 496 093	8 496 196	
21	2s(2).3d	2D	5/2	8 504 335	8 506 821	8 499 379	8 506 037	8 505 854	
22	2s.2p_3P.3s	4P	3/2	8 507 625		8 500 768	8 508 849	8 508 916	
23	2s.2p_3P.3s	2P	1/2	8 577 839	8 575 450	8 574 382	8 578 754	8 578 907	
24	2s.2p_3P.3s	4P	5/2	8 590 691		8 583 029	8 591 955	8 592 049	
25	2s.2p_3P.3p	4D	1/2	8 634 984	8 633 711	8 629 951	8 636 514	8 636 797	
26	2s.2p_3P.3p	4D	3/2	8 661 616	8 662 351	8 656 847	8 663 142	8 663 477	
27	2s.2p_3P.3s	2P	3/2	8 665 237		8 661 295	8 666 145	8 666 218	
28	2s.2p_3P.3p	2P	3/2	8 699 412	8 695 599	8 695 467	8 700 904	8 701 228	
29	2s.2p_3P.3p	2P	1/2	8 708 547	8 702 587	8 704 575	8 709 914	8 710 340	
30	2s.2p_3P.3p	4D	5/2	8 711 916	8 709 329	8 707 343	8 713 508	8 713 770	
31	2s.2p_3P.3p	4P	1/2	8 735 480		8 732 712	8 737 145	8 737 226	
32	2s.2p_3P.3p	2D	3/2	8 751 179	8 751 203	8 748 249	8 752 584	8 752 928	
33	2s.2p_3P.3p	4D	7/2	8 787 043		8 781 416	8 788 651	8 788 939	
34	2s.2p_3P.3p	4P	3/2	8 794 361	8 791 290	8 791 428	8 795 842	8 796 124	
35	2s.2p_3P.3p	4P	5/2	8 811 873	8 809 528	8 807 654	8 813 455	8 813 718	
36	2s.2p_3P.3d	4F	3/2	8 813 116		8 809 126	8 814 320	8 813 935	
37	2s.2p_3P.3p	4S	3/2	8 813 390	8 821 484	8 809 256	8 814 919	8 815 018	
38	2s.2p_3P.3d	4F	5/2	8 832 018	8 827 880	8 826 855	8 833 236	8 832 982	
39	2s.2p_3P.3p	2D	5/2	8 858 898		8 856 919	8 860 182	8 860 506	
40	2s.2p_3P.3d	4F	7/2	8 862 578	8 862 591	8 857 727	8 863 787	8 863 687	
41	2s.2p_3P.3d	4P	5/2	8 872 459	8 876 992	8 868 570	8 873 674	8 873 675	
42	2s.2p_3P.3d	4D	3/2	8 882 077	8 881 280	8 878 302	8 883 268	8 883 606	
43	2s.2p_3P.3d	4D	1/2	8 884 770	8 887 033	8 881 341	8 885 905	8 886 620	
44	2s.2p_1P.3s	2P	1/2	8 888 581	8 890 193	8 887 792	8 889 196	8 889 184	
45	2s.2p_3P.3p	2S	1/2	8 888 687		8 891 467	8 889 759	8 890 082	
46	2s.2p_1P.3s	2P	3/2	8 890 352		8 892 629	8 891 016	8 891 145	
47	2s.2p_3P.3d	2D	3/2	8 918 139	8 917 459	8 916 811	8 919 035	8 919 198	
48	2s.2p_3P.3d	4F	9/2	8 931 269		8 925 131	8 932 542	8 932 569	
49	2s.2p_3P.3d	2D	5/2	8 932 260	8 932 540	8 930 632	8 933 066	8 933 530	
50	2s.2p_3P.3d	4D	7/2	8 959 880		8 955 299	8 961 095	8 961 183	
51	2s.2p_3P.3d	4D	5/2	8 970 507	8 971 812	8 966 256	8 971 704	8 971 998	
52	2s.2p_3P.3d	4P	3/2	8 976 869		8 971 917	8 978 211	8 978 346	
53	2s.2p_3P.3d	4P	1/2	8 980 393		8 975 179	8 981 781	8 981 788	
54	2s.2p_3P.3d	2F	5/2	9 005 923	8 999 018	9 005 266	9 006 538	9 006 409	
55	2s.2p_3P.3d	2P	3/2	9 043 525		9 043 425	9 044 576	9 044 727	
56	2s.2p_3P.3d	2F	7/2	9 060 410	9 055 901	9 061 793	9 060 690	9 061 356	
57	2s.2p_1P.3p	2P	1/2	9 064 724		9 070 402	9 065 703	9 066 333	
58	2s.2p_1P.3p	2D	3/2	9 069 665		9 076 756	9 070 487	9 071 092	
59	2s.2p_3P.3d	2P	1/2	9 078 403		9 078 652	9 079 504	9 079 465	
60	2s.2p_1P.3p	2D	5/2	9 089 086		9 095 912	9 089 857	9 090 348	
61	2s.2p_1P.3p	2P	3/2	9 099 693		9 105 308	9 100 659	9 101 122	

Notes. The labels of the table are values from the following sources: *E*(RCI) this work, *E*(CHI_{exp}) experimental energies from the Chianti database by Landi et al. (2012), *E*(CHI_{calc}) theoretical results from the Chianti database based on the calculations by Landi & Gu (2006), *E*(RMBPT1) and *E*(RMBPT2) relativistic many-body perturbation calculations by Safronova et al. (1998) and Gu (2005b), respectively, and *E*(MBPT) many-body perturbation calculations by Merkelis et al. (1995).

Table 2. continued.

No.	Configuration	<i>LS</i>	<i>J</i>	<i>E</i> (RCI)	<i>E</i> (CHI _{exp})	<i>E</i> (CHI _{calc})	<i>E</i> (RMBPT1)	<i>E</i> (RMBPT2)	<i>E</i> (MBPT)
62	2p(2)3P.3s	4P	1/2	9 118 912		9 123 798	9 120 240	9 121 764	
63	2p(2)3P.3s	4P	1/2	9 149 238		9 155 638	9 150 308	9 149 595	
64	2p(2)3P.3s	4P	3/2	9 194 344		9 194 998	9 195 888	9 196 446	
65	2p(2)3P.3s	4P	5/2	9 238 765		9 240 718	9 240 194	9 240 891	
66	2s.2p_1P.3d	2F	7/2	9 244 883	9 241 695	9 252 354	9 244 972	9 245 319	
67	2s.2p_1P.3d	2F	5/2	9 246 944	9 248 513	9 254 997	9 246 969	9 247 798	
68	2p(2)3P.3s	2P	1/2	9 256 453		9 262 733	9 257 524	9 257 795	
69	2s.2p_1P.3d	2D	3/2	9 258 054	9 258 550	9 266 053	9 258 435	9 259 089	
70	2p(2)3P.3p	4D	1/2	9 265 728		9 268 638	9 266 552	9 267 540	
71	2s.2p_1P.3d	2D	5/2	9 271 065		9 279 009	9 271 446	9 271 825	
72	2s.2p_1P.3d	2P	1/2	9 292 028	9 296 158	9 300 317	9 292 202	9 292 610	
73	2p(2)3P.3s	2P	3/2	9 292 781		9 301 672	9 293 740	9 294 161	
74	2s.2p_1P.3d	2P	3/2	9 295 050		9 303 790	9 295 460	9 297 428	
75	2p(2)3P.3p	4D	3/2	9 317 796		9 321 670	9 318 521	9 317 592	
76	2p(2)3P.3p	2S	1/2	9 328 563		9 329 059	9 329 502	9 330 254	
77	2p(2)3P.3p	4P	3/2	9 360 271		9 363 400	9 361 002	9 361 701	
78	2p(2)3P.3p	4D	5/2	9 371 185		9 372 494	9 372 086	9 372 823	
79	2p(2)1D.3s	2D	5/2	9 382 381		9 388 388	9 383 379	9 383 856	
80	2p(2)3P.3p	4P	1/2	9 386 963		9 389 596	9 387 850	9 388 569	
81	2p(2)3P.3p	4P	5/2	9 390 171		9 393 616	9 390 871	9 391 667	
82	2p(2)1D.3s	2D	3/2	9 401 788		9 408 841	9 402 779	9 403 272	
83	2p(2)3P.3p	2D	3/2	9 405 687		9 408 875	9 406 421	9 407 121	
84	2p(2)3P.3p	4D	7/2	9 415 407		9 417 870	9 416 184	9 417 034	
85	2p(2)3P.3d	4F	3/2	9 442 806		9 445 457	9 444 457	9 444 707	
86	2p(2)3P.3p	4S	3/2	9 457 597		9 462 645	9 458 323	9 458 973	
87	2p(2)3P.3d	4F	5/2	9 467 287		9 470 461	9 468 941	9 469 216	
88	2p(2)3P.3p	2P	3/2	9 468 348		9 474 459	9 468 959	9 469 712	
89	2p(2)3P.3p	4P	5/2	9 470 503		9 475 392	9 471 076	9 471 880	
90	2p(2)3P.3p	2P	1/2	9 502 072		9 506 492	9 502 700	9 503 514	
91	2p(2)3P.3d	4F	7/2	9 515 961		9 517 326	9 517 712	9 518 013	
92	2p(2)3P.3d	2P	3/2	9 517 535		9 519 245	9 519 188	9 519 421	
93	2p(2)3P.3d	4F	5/2	9 522 897		9 526 533	9 524 349	9 524 729	
94	2p(2)3P.3d	4D	1/2	9 526 682		9 527 993	9 528 406	9 528 477	
95	2p(2)1D.3p	2F	5/2	9 546 415		9 553 309	9 546 808	9 547 226	
96	2p(2)3P.3d	4D	7/2	9 550 997		9 554 694	9 552 453	9 552 841	
97	2p(2)3P.3d	4F	9/2	9 553 431		9 555 812	9 555 036	9 555 502	
98	2p(2)3P.3d	4D	3/2	9 556 163		9 558 419	9 557 805	9 558 104	
99	2p(2)3P.3d	2F	5/2	9 557 419		9 561 129	9 558 904	9 559 164	
100	2p(2)1D.3p	2F	7/2	9 560 556		9 568 254	9 560 845	9 561 455	
101	2p(2)1D.3p	2D	3/2	9 575 573		9 586 171	9 575 952	9 576 362	
102	2p(2)1D.3p	2D	5/2	9 589 651		9 600 502	9 589 999	9 590 518	
103	2p(2)1S.3s	2S	1/2	9 596 474		9 602 660	9 597 294	9 599 387	
104	2p(2)3P.3d	4P	5/2	9 599 015		9 603 928	9 600 579	9 601 039	
105	2p(2)1D.3p	2P	1/2	9 603 114		9 615 263	9 603 205	9 603 444	
106	2p(2)3P.3d	4P	3/2	9 612 278		9 616 586	9 613 842	9 614 442	
107	2p(2)3P.3d	2P	1/2	9 619 110		9 623 542	9 620 524	9 621 205	
108	2p(2)3P.3d	4P	1/2	9 622 724		9 627 054	9 624 349	9 623 547	
109	2p(2)3P.3d	2F	7/2	9 627 209		9 632 658	9 628 350	9 629 088	
110	2p(2)3P.3d	2D	5/2	9 660 947		9 671 595	9 661 719	9 662 562	
111	2p(2)3P.3d	2D	3/2	9 664 835		9 674 472	9 665 833	9 666 317	
112	2p(2)1D.3p	2P	3/2	9 674 446		9 685 925	9 674 688	9 675 061	
113	2p(2)1D.3d	2G	7/2	9 688 292		9 695 973	9 689 278	9 689 426	
114	2p(2)1D.3d	2G	9/2	9 704 493		9 711 931	9 705 446	9 705 728	
115	2p(2)1D.3d	2D	3/2	9 732 050		9 739 425	9 733 253	9 733 690	
116	2p(2)1D.3d	2D	5/2	9 735 460		9 744 260	9 736 412	9 736 898	
117	2p(2)3P.3d	2F	7/2	9 755 048		9 767 078	9 755 415	9 756 194	
118	2p(2)1D.3d	2P	1/2	9 756 542		9 769 623	9 757 683	9 757 949	
119	2p(2)1S.3p	2P	1/2	9 781 564		9 794 556	9 781 468	9 783 188	
120	2p(2)3P.3d	2D	5/2	9 794 915		9 805 785	9 795 588	9 796 076	
121	2p(2)1D.3d	2S	1/2	9 797 251		9 807 437	9 798 210	9 798 346	
122	2p(2)1D.3d	2P	3/2	9 799 072		9 811 671	9 800 363	9 800 522	
123	2p(2)1S.3p	2P	3/2	9 800 777		9 812 548	9 800 700	9 801 694	
124	2p(2)1S.3d	2D	5/2	9 950 988		9 963 706	9 951 646	9 952 360	
125	2p(2)1S.3d	2D	3/2	9 958 705		9 972 842	9 959 300	9 961 443	

3.3. Energies for Ti XVIII to Cu XXV

In Tables 3–10, energies from the RCI calculations are given for the levels belonging to the configurations $1s^22s^22p$, $1s^22s2p^2$, $1s^22p^3$, $1s^22s^23l$, $1s^22s2p3l$, $1s^22p^23l$, $1s^22s^24l'$, $1s^22s2p4l'$, and $1s^22p^24l'$ ($l = 0, 1, 2$ and $l' = 0, 1, 2, 3$) in boron-like ions from Ti XVIII to Cu XXV. Energy levels are given in cm^{-1} relative to the ground state $1s^22s^22p\ ^2P_{1/2}$. In addition, the LS -percentage compositions obtained by transforming from jj - to LS -coupling are displayed. It should be carefully noted that some excited levels have the same leading LS -percentage, and in this case, an extended composition should be used as a label. One example is levels 62 and 63 in Fe XXII that are given as $0.41\ 2p^2(^3P)3s\ ^4P + 0.39\ 2s2p(^1P)3p\ ^2S + 0.07\ 2p^2(^1S)3s\ ^2S$ and $0.46\ 2p^2(^3P)3s\ ^4P + 0.42\ 2s2p(^1P)3p\ ^2S + 0.07\ 2s2p(^1P)3p\ ^2P$, respectively. Further, it should be noted that levels of the form $1s^22s^25l$ start to show up far up in the spectra, where the energy separation is small. These levels were not specifically targeted in the RCI calculations, and it is not known how well they are described. The calculated energies are compared with recommended data from the [NIST Atomic Spectra Database \(2013\)](#) and from the Chianti database for Fe XXII ([Landi et al. 2012](#)). The original references are as follows: Ti XVIII, Mn XXI ([Sugar & Corliss 1985](#)); V XIX, Cr XX, Co XXIII, Ni XXIV ([Sugar & Corliss 1985](#); [Shirai et al. 2000](#)); Cu XXV ([Sugar & Musgrove 1990](#)). There is a detailed agreement between calculations and observed energies for the $n = 2$ levels. Observed energies for the more excited levels are lacking to a large extent. For the few available levels and for some ions such as Cr XX, there is good agreement between the calculated and observed energies. However, there are a number of individual levels where theory and experiment can not be reconciled.

Validations in Si X and Fe XXII show that the energies from the RCI calculations are highly accurate. The energies thus serve as benchmarks for other calculations. They are also valuable in further experimental work, both for Fe XXII and for the other ions, as a means to unambiguously identify spectral lines.

3.4. Transition rates

In Table 11, transition rates, A , between the $n = 2$ states in Fe XXII are displayed. In addition, there are some transitions including states with $n = 3$. For the RCI calculations, the ratio R of the transition rates in length and velocity gauges are also shown. The ratio R is used to assess the accuracy of the transition rates. For highly accurate wave functions and strong transitions, R should be close to 1. Values far from 1 indicate that there may be internal cancellations, and weak transitions with values of R far from 1 are generally associated with larger uncertainties. For a deeper discussion about error estimates, see [Froese Fischer \(2009\)](#). The transition rates are compared with values from RMBPT calculations by [Safronova et al. \(1999\)](#), from MBPT calculations by [Merkelis et al. \(1995\)](#), and with values from calculations by [Landi & Gu \(2006\)](#) that are part of the Chianti database. There is a much better consistency between the current rates and the rates by [Merkelis et al. \(1995\)](#) and [Landi & Gu \(2006\)](#) than there is with [Safronova et al. \(1999\)](#); the relative differences being less than 5% for the first two, whereas it is 14% for the RMBPT. Rates from RCI calculations have previously been carefully validated against experiments and other accurate calculations for ions in the boron isoelectronic sequence ([Rynkun et al. 2012](#)). In the studied ions, there was an agreement between different calculations at the 1% level. We thus argue that

the current rates represent an improvement in accuracy compared with available data in the Chianti databases and to the RMBPT calculations by [Safronova et al. \(1999\)](#).

In Tables 12–19, transition energies, wavelengths, transition rates A , weighted oscillator strengths gf , and the ratio R of the transition probabilities in length and velocity gauges are displayed for transitions in Ti XVIII to Cu XXV. The transition rates between the $n = 2$ states agree very well with the previous RCI calculations by [Rynkun et al. \(2012\)](#). Many of the transitions with R far from 1 involve configurations that differ by two or more electrons such as $2s^23p-2s2p^2$ (transition 17–8 in Table 16) or $2s2p3d-2p^23s$ (transition 71–65 in Table 16). These transitions are forbidden in the single configuration approximation and are opened due to configuration interaction. The rates of these transitions are extremely challenging to compute, and for some of them, the values from various calculations differ substantially. These type of transitions have recently been analyzed by [Bogdanovich et al. \(2007\)](#).

4. Conclusions

We have used large scale RCI calculations with expansion sizes of nearly a million CSFs to obtain transition energies for levels belonging to the configurations $1s^22s^22p$, $1s^22s2p^2$, $1s^22p^3$, $1s^22s^23l$, $1s^22s2p3l$, $1s^22p^23l$, $1s^22s^24l'$, $1s^22s2p4l'$, and $1s^22p^24l'$ ($l = 0, 1, 2$ and $l' = 0, 1, 2, 3$) in boron-like ions from Ti XVIII to Cu XXV. The problem of labeling has been discussed, and we used a transformation from jj - to LS -coupling to obtain the leading LS -percentage compositions. The latter are used as labels for the levels. Computational methods and strategies have been validated for Si X, where accurate energies are available ([Vilkas et al. 2005](#)). For Si X, energies from the RCI calculations are in excellent agreement with observations with a mean relative energy difference of only 0.018%. For Fe XXII, the calculated energies are checked against values from the Chianti database ([Landi et al. 2012](#)), RMBPT calculations by [Safronova et al. \(1996, 1998\)](#) and [Gu \(2005b, 2007\)](#), and from MBPT calculations by [Merkelis et al. \(1995\)](#). There is a detailed agreement between the present energies and the energies from the RMBPT calculations. In most cases, there is also a good agreement with observations. However, there are obvious cases where theory and experiment do not match at all. The agreement is also very good between the present energies and the experimental energies for the $n = 2$ levels of ions other than Fe XXII. For these ions, experimental energies for higher levels are largely missing. For the energies that are available, most notably in Cr XX, there is a good consistency with the energies from the RCI calculations in many cases. However, there are several cases where there are obvious experimental misidentifications. The present energies are the most accurate energies available for these ions. They should be of value for future experimental work.

A comparison of the transition rates between the $n = 2$ states in Fe XXII shows that the values are less consistent than could originally be expected. The current transition rates differ from the RMBPT values by 14%, but the agreement is better for the stronger transitions. The agreement with the calculations by [Merkelis et al. \(1995\)](#) and [Landi & Gu \(2006\)](#) is considerably better with a relative difference of around 5%. Rates from RCI calculations have previously been carefully validated against experiments and other accurate calculations for ions in the boron isoelectronic sequence. Rates in the studied ions agreed between different calculations at the 1% level ([Rynkun et al. 2012](#)). We thus argue that the current rates represent an

improvement in accuracy compared with available data in the CHIANTI database and from the RMBPT and MBPT calculations by Safronova et al. (1999) and Merkelis et al. (1995).

References

- Bogdanovich, P., Karpuškieėė, R., & Rancova, O. 2007, *Phys. Scr.*, 75, 669
- Cowan, R. 1981, *The theory of atomic structure and spectra* (Berkeley: University of California Press)
- Dyall, K. G., Grant, I. P., Johnson, C. T., Parpia, F. A., & Plummer, E. P. 1989, *Comput. Phys. Commun.*, 55, 425
- Fritzsche, S., & Grant, I. P. 1994, *Phys. Lett. A*, 186, 152
- Froese Fischer, C. 2009, *Phys. Scr.*, 134, 014019
- Gaigalas, G., Rudzikas, Z., & Froese Fischer, C. 1997, *J. Phys. B At. Mol. Opt. Phys.*, 30, 3747
- Gaigalas, G., Žalandauskas, T., & Rudzikas, Z. 2003, *At. Data Nucl. Data Tables*, 84, 99
- Grant, I. P. 1974, *J. Phys. B*, 7, 1458
- Grant, I. P. 2007, *Relativistic Quantum Theory of Atoms and Molecules* (New York: Springer)
- Gu, M. F. 2005a, *At. Data Nucl. Data Tables*, 89, 267
- Gu, M. F. 2005b, *ApJSS*, 156, 105
- Gu, M. F. 2007, *ApJSS*, 169, 154
- Jonauskas, V., Bogdanovich, P., Keenan, F. P., et al. 2006, *A&A*, 455, 1157
- Jönsson, P., He, X., Froese Fischer, C., & Grant, I. P. 2007, *Comput. Phys. Commun.*, 177, 597
- Jönsson, P., Rynkun, P., & Gaigalas, G. 2011, *At. Data Nucl. Data Tables*, 97, 648
- Jönsson, P., Bergtsson, P., Ekman, J., et al. 2013a, *At. Data Nucl. Data Tables*, in press, <http://dx.doi.org/10.1016/j.adt.2013.06.001>
- Jönsson, P., Gaigalas, G., Bieroń, J., Froese Fischer, C., & Grant, I. P. 2013b, *Comput. Phys. Commun.*, 184, 2197
- Kramida, A., Ralchenko, Yu., Reader, J., & NIST ASD Team 2012, *NIST Atomic Spectra Database* (ver. 5.0), National Institute of Standards and Technology, <http://physics.nist.gov/asd>
- Landi, E., & Gu, M. F. 2006, *ApJ*, 640, 1171
- Landi, E., Del Zanna, G., Young, P. R., et al. 2012, *ApJS*, 744, 99
- Liang, G. Y., Whiteford, A. D., & Badnell, N. R. 2009, *A&A*, 499, 943
- McKenzie, B. J., Grant, I. P., & Norrington, P. H. 1980, *Comput. Phys. Commun.*, 21, 233
- Merkelis, G., Vilkas, M. J., Gaigalas, G., & Kisielius, R. 1995, *Phys. Scr.*, 51, 233
- Nahar, S. N. 2010, *At. Data Nucl. Data Tables*, 96, 26
- Olsen, J., Godefroid, M., Jönsson, P., Malmqvist, P. Å., & Froese Fischer, C. 1995, *Phys. Rev. E*, 52, 4499
- Rynkun, P., Jönsson, P., Gaigalas, G., & Froese Fischer, C. 2012, *At. Data Nucl. Data Tables*, 98, 481
- Safronova, M. S., Johnson, W. R., & Safronova, U. I. 1996, *Phys. Rev. A*, 54, 2850
- Safronova, U. I., Johnson, W. R., & Safronova, M. S. 1998, *At. Data Nucl. Data Tables*, 69, 183
- Safronova, U. I., Johnson, W. R., & Livingston, A. E. 1999, *Phys. Rev. A*, 60, 996
- Shirai, T., Sugar, J., Musgrove, A., & Wisese, W. L. 2000, *J. Phys. Chem. Ref. Data*, Monograph, 8, 1
- Sugar, J., & Corliss, C. 1985, *J. Phys. Chem. Ref. Data*, 14, Suppl. 2, 1
- Sugar, J., & Musgrove, A. 1990, *J. Phys. Chem. Ref. Data*, 19, 527
- Vilkas, M., Ishikawa, Y., & Träbert, E. 2005, *Phys. Scr.*, 72, 181