# Two-electron–one-photon M1 and E2 transitions between the states of the $2p^3$ and $2s^2 2p$ odd configurations for B-like ions with $18 \leq Z \leq 92$



2010 J. Phys. B: At. Mol. Opt. Phys. 43 035005

(http://iopscience.iop.org/0953-4075/43/3/035005)

J. Phys. B: At. Mol. Opt. Phys. **43** (2010) 035005 (11pp) doi:10.1088/0953-4075/43/3/035005

# Two-electron–one-photon M1 and E2 transitions between the states of the $2p^3$ and $2s^22p$ odd configurations for B-like ions with $18 \leqslant Z \leqslant 92$

**Jiguang Li[1], Per Jönsson[2], Chenzhong Dong[1,3] and Gediminas Gaigalas[4,5]**

[1] College of Physics and Electronic Engineering, Northwest Normal University, Lanzhou 730070, People's Republic of China
[2] Nature, Environment, Society, Malmö University, Malmö S-20506, Sweden
[3] Joint Laboratory of Atomic and Molecular Physics, NWNU and IMP CAS, Lanzhou 730070, People's Republic of China
[4] Department of Physics, Vilnius Pedagogical University, Studentų 39, Vilnius LT-08106, Lithuania
[5] Institute of Theoretical Physics and Astronomy, A Goštauto 12, Vilnius LT-01108, Lithuania

E-mail: Dongcz@nwnu.edu.cn

Received 22 October 2009, in final form 25 November 2009
Published 20 January 2010
Online at stacks.iop.org/JPhysB/43/035005

**Abstract**
Two-electron–one-photon (TEOP) M1 and E2 transition energies, line strengths and transition probabilities between the states of the $2p^3$ and $2s^22p$ odd configurations for B-like ions with $18 \leqslant Z \leqslant 92$ have been calculated using the GRASP2K package based on the multiconfiguration Dirac–Hartree–Fock (MCDHF) method. Employing active-space techniques to expand the configuration list, we have systematically considered the valence, core–valence and core–core electron correlation effects. Breit interaction and quantum electrodynamical (QED) effects were also included to correct atomic state wavefunctions and the corresponding energies. Influences of electron correlation, Breit interaction and QED effects on transition energies and line strengths of the TEOP M1 and E2 transitions were analysed in detail. The present results were also compared with other theoretical and experimental values.

## 1. Introduction

B-like ions attract wide attention since they are often found in astrophysical [1–4] and thermal nuclear fusion plasmas [5–7]. Transitions within the $n = 2$ complex of ions in the B-like isoelectronic sequence, including forbidden and resonance lines, play key roles in diagnosing temperatures, densities and ionic abundances of plasma [8–15]. As well-known examples, Cheng *et al* first theoretically calculated relevant atomic properties for isoelectronic ions from Li-like to F-like in 1976 [16]. Later, Edlén made systematic comparisons of the theoretical results of Cheng *et al* and experimental values [8]. For all transitions studied, Edlén derived $Z$-dependent functions to represent the relatively small differences between experimental and theoretical energies. From these functions recommended values for transition wavelengths were obtained. Since then, additional studies on energy structures, transition probabilities and other atomic properties of B-like ions have been made in order to supply more accurate data [17–22] and to explore electron correlation effects [22–25] and quantum electrodynamical (QED) effects [26–28]. Meanwhile, some experiments with high precision have been carried out, for example, using electron-beam ion trap (EBIT) devices at Lawrence Livermore National Laboratory [29–31] and at the Max-Plank-Institut für Kernphysik [32, 33] and heavy-ion storage ring measurements at TSR in Heidelberg [34]. These measurements provided benchmarks for theoretical approaches.

In the present work we calculated the two-electron–one-photon (TEOP) M1 and E2 transition energies, line strengths and transition probabilities between the states of

 

**Table 1.** Energy separation (in $cm^{-1}$) of the states in the $2s^22p$ and $2p^3$ odd configurations relative to the ground state $2s^22p(J = 1/2)$ in $Ar^{13+}$ from calculations with increasing active sets (AS).

| AS | $2s^22p_{3/2}$ $(J = 3/2)$ | $2p_{1/2}2p_{3/2}^2$ $(J = 3/2)$ | $2p_{1/2}^2 2p_{3/2}$ $(J = 3/2)$ | $2p_{3/2}^3$ $(J = 5/2)$ | $2p_{3/2}^3$ $(J = 1/2)$ | $2p_{3/2}^3$ $(J = 3/2)$ |
|---|---|---|---|---|---|---|
| VV | | | | | | |
| $n = 2$ | 22 693 | 717 695 | 823 226 | 841 048 | 923 780 | 927 927 |
| $n = 3$ | 22 563 | 721 368 | 816 511 | 818 342 | 915 417 | 919 618 |
| $n = 4$ | 22 554 | 722 173 | 815 535 | 817 405 | 913 523 | 917 774 |
| $n = 5$ | 22 554 | 722 500 | 815 341 | 817 222 | 913 053 | 917 314 |
| $n = 6$ | 22 554 | 722 585 | 815 301 | 817 185 | 912 934 | 917 198 |
| $n = 7$ | 22 554 | 722 617 | 815 294 | 817 180 | 912 896 | 917 161 |
| $n = 8$ | 22 554 | 722 630 | 815 292 | 817 178 | 912 879 | 917 145 |
| CV | 22 619 | 720 053 | 813 314 | 815 217 | 911 206 | 915 491 |
| CC | 22 606 | 719 621 | 812 898 | 814 802 | 910 667 | 914 957 |
| QED | 22 653 | 717 830 | 811 103 | 813 017 | 908 942 | 913 242 |
| Edlén[a] | 22 653 | 717 895 | 810 913 | 812 907 | 908 573 | 912 906 |
| MCDF[b] | 22 362 | 718 557 | 819 317 | 821 036 | 919 614 | 923 661 |
| MBPT[c] | 22 670 | 718 148 | 810 423 | | 908 086 | |
| MCDF[d] | 22 975 | 716 054 | 821 268 | 823 056 | 920 264 | 924 533 |
| NIST[e] | 22 658 | 718 900 | 810 200 | 812 800 | 908 700 | 913 000 |

VV: valence correlation, CV: core–valence correlation, CC: core–core correlation; these results labelled by VV, CV, CC have included Breit interaction, QED: QED effects, $n$: the largest principal quantum number of the active set.
[a] Edlén [8],
[b] Galavís *et al* [11],
[c] Safronova *et al* [14],
[d] Cheng *et al* [16],
[e] NIST [40].

**Table 2.** Line strength (in au) of M1 transitions of $Ar^{13+}$ from calculations with increasing active sets (AS).

| AS | 3–1 | 3–2 | 4–1 | 4–2 | 5–2 | 6–2 | 7–1 | 7–2 |
|---|---|---|---|---|---|---|---|---|
| VV | | | | | | | | |
| $n = 2$ | 1.979[−5] | 8.062[−5] | 2.085[−5] | 5.122[−5] | 2.788[−5] | 2.391[−5] | 1.526[−5] | 2.403[−7] |
| $n = 3$ | 2.025[−5] | 8.088[−5] | 2.136[−5] | 5.275[−5] | 2.864[−5] | 2.466[−5] | 1.542[−5] | 2.575[−7] |
| $n = 4$ | 1.993[−5] | 7.925[−5] | 2.110[−5] | 5.210[−5] | 2.819[−5] | 2.432[−5] | 1.509[−5] | 2.493[−7] |
| $n = 5$ | 1.986[−5] | 7.886[−5] | 2.101[−5] | 5.191[−5] | 2.808[−5] | 2.423[−5] | 1.499[−5] | 2.512[−7] |
| $n = 6$ | 1.984[−5] | 7.878[−5] | 2.100[−5] | 5.190[−5] | 2.805[−5] | 2.422[−5] | 1.499[−5] | 2.496[−7] |
| $n = 7$ | 1.984[−5] | 7.875[−5] | 2.100[−5] | 5.189[−5] | 2.805[−5] | 2.421[−5] | 1.499[−5] | 2.495[−7] |
| $n = 8$ | 1.984[−5] | 7.874[−5] | 2.099[−5] | 5.189[−5] | 2.804[−5] | 2.420[−5] | 1.499[−5] | 2.493[−7] |
| CV | 1.992[−5] | 7.916[−5] | 2.107[−5] | 5.208[−5] | 2.816[−5] | 2.430[−5] | 1.499[−5] | 2.553[−7] |
| CC | 1.991[−5] | 7.909[−5] | 2.105[−5] | 5.202[−5] | 2.812[−5] | 2.428[−5] | 1.497[−5] | 2.557[−7] |
| QED | 2.020[−5] | 8.023[−5] | 2.135[−5] | 5.275[−5] | 2.852[−5] | 2.459[−5] | 1.515[−5] | 2.594[−7] |

VV: valence correlation, CV: core–valence correlation, CC: core–core correlation; these results labelled by VV, CV, CC have included Breit interaction, QED: QED effects, $n$: the principal quantum number of the active set.
Designations: 1: $1s^22s^22p_{1/2}$ $(J = 1/2)$, 2: $1s^22s^22p_{3/2}$ $(J = 3/2)$, 3: $1s^22p_{1/2}2p_{3/2}^2$ $(J = 3/2)$,
4: $1s^22p_{1/2}^2 2p_{3/2}$ $(J = 3/2)$, 5: $1s^22p_{3/2}^3$ $(J = 5/2)$, 6: $1s^22p_{3/2}^3$ $(J = 1/2)$, 7: $1s^22p_{3/2}^3$ $(J = 3/2)$.

the $2p^3$ and $2s^22p$ odd configurations for B-like ions with $18 \leqslant Z \leqslant 92$ using the GRASP2K package [35] based on the multiconfiguration Dirac–Hartree–Fock method. The TEOP transitions are classified as forbidden transitions. Involving two electrons the transition probabilities are zero in the single-configuration approximation, where all relativistic orbitals in initial and final states are orthogonal [36]. These transitions are good candidates not only for testing the quality of the wavefunctions and further checking many-body atomic theory, but also for providing tools for plasma diagnostics. In this paper, we also presented the influence of electron correlation effects, Breit interaction and QED effects on the TEOP M1, E2 transition energies and probabilities. It was found that the TEOP transitions are sensitive to these effects. Recommendations of atomic data including wavelengths, line strengths and transition probabilities were provided for B-like Ar, Fe, Kr, Mo, Xe, Eu, W, Hg, U ions.

## 2. Theory

The multiconfiguration Dirac–Hartree–Fock method is explained in detail in a recent monograph by Grant [37] and

**Table 3.** Line strength in au of E2 transitions of $Ar^{13+}$ in Babushikin (B) and Coulomb (C) gauges from calculations with increasing active sets (AS).

| | 3–1 | | 4–1 | | 4–2 | | 5–1 | | 5–2 | | 6–2 | | 7–1 | | 7–2 | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AS | B | C | B | C | B | C | B | C | B | C | B | C | B | C | B | C |
| $n=2$ | 3.870[−6] | 3.239[−10] | 8.104[−4] | 2.590[−10] | 5.026[−4] | 1.766[−10] | 4.340[−4] | 0.000[0] | 1.574[−3] | 1.680[−9] | 3.651[−4] | 2.477[−10] | 2.149[−4] | 1.490[−10] | 5.049[−4] | 1.145[−12] |
| $n=3$ | 6.493[−6] | 4.657[−6] | 1.275[−3] | 9.693[−4] | 7.904[−4] | 6.243[−4] | 6.860[−4] | 5.281[−4] | 2.471[−3] | 1.921[−3] | 5.577[−4] | 3.706[−4] | 3.213[−4] | 2.081[−4] | 7.852[−4] | 5.370[−4] |
| $n=4$ | 6.460[−6] | 5.884[−6] | 1.241[−3] | 1.138[−3] | 7.678[−4] | 7.047[−4] | 6.673[−4] | 6.121[−4] | 2.403[−3] | 2.201[−3] | 5.377[−4] | 4.925[−4] | 3.071[−4] | 2.806[−4] | 7.600[−4] | 6.961[−4] |
| $n=5$ | 6.554[−6] | 6.266[−6] | 1.249[−3] | 1.208[−3] | 7.712[−4] | 7.470[−4] | 6.713[−4] | 6.490[−4] | 2.415[−3] | 2.333[−3] | 5.426[−4] | 5.202[−4] | 3.096[−4] | 2.965[−4] | 7.675[−4] | 7.378[−4] |
| $n=6$ | 6.577[−6] | 6.405[−6] | 1.253[−3] | 1.233[−3] | 7.733[−4] | 7.614[−4] | 6.733[−4] | 6.622[−4] | 2.422[−3] | 2.378[−3] | 5.437[−4] | 5.327[−4] | 3.100[−4] | 3.038[−4] | 7.695[−4] | 7.555[−4] |
| $n=7$ | 6.588[−6] | 6.471[−6] | 1.255[−3] | 1.245[−3] | 7.743[−4] | 7.685[−4] | 6.743[−4] | 6.685[−4] | 2.425[−3] | 2.400[−3] | 5.447[−4] | 5.380[−4] | 3.106[−4] | 3.070[−4] | 7.710[−4] | 7.633[−4] |
| $n=8$ | 6.590[−6] | 6.497[−6] | 1.255[−3] | 1.249[−3] | 7.746[−4] | 7.711[−4] | 6.745[−4] | 6.709[−4] | 2.426[−3] | 2.409[−3] | 5.448[−4] | 5.404[−4] | 3.106[−4] | 3.083[−4] | 7.712[−4] | 7.666[−4] |
| CV | 6.533[−6] | 6.401[−6] | 1.247[−3] | 1.234[−3] | 7.696[−4] | 7.619[−4] | 6.701[−4] | 6.637[−4] | 2.411[−3] | 2.384[−3] | 5.413[−4] | 5.336[−4] | 3.085[−4] | 3.043[−4] | 7.662[−4] | 7.569[−4] |
| CC | 6.525[−6] | 6.365[−6] | 1.246[−3] | 1.228[−3] | 7.687[−4] | 7.576[−4] | 6.694[−4] | 6.600[−4] | 2.408[−3] | 2.371[−3] | 5.408[−4] | 5.308[−4] | 3.081[−4] | 3.026[−4] | 7.657[−4] | 7.530[−4] |
| QED | 6.583[−6] | 6.424[−6] | 1.251[−3] | 1.233[−3] | 7.707[−4] | 7.600[−4] | 6.714[−4] | 6.624[−4] | 2.416[−3] | 2.379[−3] | 5.425[−4] | 5.327[−4] | 3.087[−4] | 3.034[−4] | 7.682[−4] | 7.559[−4] |

VV: valence correlation, CV: core–valence correlation and CC: core–core correlation, these results labelled by VV, CV, CC have included Breit interaction, QED: QED effects, $n$: the principal quantum number of the active set.

**Table 4.** The contributions of electronic correlation, Breit interaction and QED effects to energy separation of the $2s^2 2p$ and $2p^3$ odd configurations related to the ground state for $Ar^{13+}$, $Kr^{31+}$, $Xe^{49+}$, $Hg^{69+}$ and $U^{87+}$ in $cm^{-1}$.

| | $2s^2 2p_{3/2}$ ($J = 3/2$) | | $2p_{1/2} 2p_{3/2}^2$ ($J = 3/2$) | | $2p_{1/2}^2 2p_{3/2}$ ($J = 3/2$) | | $2p_{3/2}^3$ ($J = 5/2$) | | $2p_{3/2}^3$ ($J = 1/2$) | | $2p_{3/2}^3$ ($J = 3/2$) | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Model | This work | CKD | This work | CKD | This work | CKD | This work | CKD | This work | CKD | This work | CKD |
| $Ar^{13+}$ | | | | | | | | | | | | |
| DF | 23 815 | 23 921 | 717 699 | 718 417 | 822 766 | 823 199 | 825 643 | 826 119 | 923 260 | 922 119 | 928 013 | 926 972 |
| EC | −78 | | 2003 | | −10 166 | | −10 039 | | −12 849 | | −12 701 | |
| BI | −1131 | −1136 | −131 | −47 | 187 | 385 | −913 | −752 | 153 | 428 | −469 | −165 |
| VP | −3 | | 135 | | 134 | | 134 | | 131 | | 131 | |
| SE | 51 | | −1876 | | −1819 | | −1808 | | −1752 | | −1732 | |
| QED | 47 | 10 | −1742 | −2316 | −1685 | −2316 | −1674 | −2311 | −1621 | −2283 | −1601 | −2274 |
| Total | 22 653 | 22 795 | 717 830 | 716 054 | 811 103 | 821 268 | 813 017 | 823 056 | 908 942 | 920 264 | 913 242 | 924 533 |
| Edlén[a] | 22 653 | | 717 895 | | 810 913 | | 812 907 | | 908 573 | | 912 906 | |
| MBPT[b] | 22 670 | | 718 148 | | 810 423 | | | | 908 086 | | | |
| NIST[c] | 22 658 | | 718 900 | | 810 200 | | 812 800 | | 908 700 | | 913 000 | |
| $Kr^{31+}$ | | | | | | | | | | | | |
| DF | 503 467 | 503 571 | 2273 518 | 2273 751 | 2658 644 | 2659 382 | 2770 739 | 2771 381 | 2962 203 | 2961 297 | 3348 906 | 3348 779 |
| EC | 123 | | −5072 | | −5072 | | −9631 | | −12 004 | | −9469 | |
| BI | −11 609 | −11 696 | 10 793 | 10 933 | 3250 | 3475 | −6238 | −6184 | 5104 | 5552 | −8726 | −8426 |
| VP | 32 | | 2490 | | 2524 | | 2527 | | 2501 | | 2523 | |
| SE | 751 | | −24 983 | | −24 429 | | −24 397 | | −24 098 | | −23 266 | |
| QED | 783 | −1052 | −22 493 | −27 321 | −21 905 | −27 242 | −21 870 | −27 241 | −21 598 | −27 059 | −20 743 | −26 817 |
| Total | 492 772 | 490 823 | 2256 746 | 2257 363 | 2634 918 | 2635 615 | 2733 001 | 2737 956 | 2933 705 | 2939 790 | 3309 968 | 3313 536 |
| Edlén[a] | 492 596 | | 2252 774 | | 2648 185 | | 2736 647 | | 2935 423 | | 3314 969 | |
| MBPT[b] | 492 491 | | 2255 499 | | 2633 444 | | | | 2931 644 | | | |
| MCDF[d] | 491 789 | | 2266 564 | | 2643 753 | | 2744 543 | | 2849 242 | | 3322 091 | |
| NIST[c] | 492 560 | | | | | | 2743 300 | | | | 3306 800 | |

**Table 4.** (Continued.)

| Model | $2s^2 2p_{3/2}$ $(J = 3/2)$ | | $2p_{1/2} 2p_{3/2}^2$ $(J = 3/2)$ | | $2p_{1/2}^2 2p_{3/2}$ $(J = 3/2)$ | | $2p_{3/2}^3$ $(J = 5/2)$ | | $2p_{3/2}^3$ $(J = 1/2)$ | | $2p_{3/2}^3$ $(J = 3/2)$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | This work | CKD | This work | CKD | This work | CKD | This work | CKD | This work | CKD | This work | CKD |
| $Xe^{49+}$ | | | | | | | | | | | | |
| DF | 2935 068 | 2935 120 | 5935 087 | 5935 025 | 8606 331 | 8607 372 | 8802 394 | 8803 245 | 9072 192 | 9071 535 | 11 808 513 | 11 808 921 |
| EC | 452 | | −8489 | | −2986 | | −9426 | | −11 276 | | −7414 | |
| BI | −46 290 | −46 709 | 48 596 | 49 389 | 5445 | 5449 | −25 464 | −25 630 | 15 358 | 16 162 | −41 219 | −41 115 |
| VP | 402 | | 14 710 | | 15 138 | | 15 137 | | 15 097 | | 15 379 | |
| SE | 3203 | | −108 774 | | −105 745 | | −105 737 | | −105 396 | | −101 064 | |
| QED | 3605 | −15 753 | −94 064 | −121 722 | −90 606 | −122 409 | −90 600 | −122 411 | −90 299 | −122 227 | −85 684 | −121 946 |
| Total | 2892 835 | 2872 658 | 5881 130 | 5862 692 | 8518 183 | 8490 412 | 8676 904 | 8655 204 | 8985 975 | 8965 470 | 11 674 197 | 11 645 860 |
| MBPT[b] | 2889 909 | | 5875 725 | | 8510 206 | | 8668 460 | | 8977 354 | | 11 662 874 | |
| Exp.[e] | 2893 527 | | | | | | | | | | | |
| $Hg^{75+}$ | | | | | | | | | | | | |
| DF | 17 116 580 | 17 116 180 | 22 533 382 | 22 532 782 | 39 197 188 | 39 198 478 | 39 491 563 | 39 492 704 | 39 879 448 | 39 879 180 | 56 697 472 | 56 698 251 |
| EC | 1234 | | −10 941 | | −2973 | | −9503 | | −10 756 | | −5959 | |
| BI | −196 596 | −198 486 | 179 644 | 182 042 | −19 541 | −20 571 | −125 897 | −127 535 | 13 284 | 14 196 | −214 798 | −216 727 |
| VP | 6188 | | 102 169 | | 108 490 | | 108 484 | | 108 450 | | 113 984 | |
| SE | 4829 | | −486 081 | | −481 357 | | −481 347 | | −481 136 | | −471 513 | |
| QED | 11 017 | 13 778 | −383 912 | −405 106 | −372 867 | −420 313 | −372 864 | −420 359 | −372 686 | −420 282 | −357 529 | −432 340 |
| Total | 16 932 234 | 16 931 472 | 22 318 137 | 22 309 718 | 38 801 806 | 38 757 594 | 38 983 300 | 38 944 810 | 39 509 291 | 39 473 094 | 56 119 187 | 56 049 184 |
| MBPT[b] | 16 917 425 | | 22 302 136 | | 38 770 777 | | 38 951 632 | | 39 478 323 | | 56 072 806 | |
| $U^{87+}$ | | | | | | | | | | | | |
| DF | 33 350 044 | 33 349 278 | 40 227 906 | 40 220 806 | 73 025 310 | 73 020 445 | 73 360 970 | 73 355 943 | 73 809 414 | 73 803 056 | 106 857 517 | 106 851 517 |
| EC | 2117 | | −12 678 | | −2935 | | −9418 | | −10 363 | | −5363 | |
| BI | −348 908 | −352 308 | 287 489 | 291 342 | −79 676 | −81 919 | −244 571 | −247 798 | −29 113 | −28 597 | −421 799 | −426 146 |
| VP | 20 059 | | 229 042 | | 249 442 | | 249 426 | | 249 400 | | 268 434 | |
| SE | −13 595 | | −872 159 | | −885 829 | | −885 816 | | −885 653 | | −891 708 | |
| QED | 6464 | 4391 | −643 118 | −692 185 | −636 387 | −734 074 | −636 391 | −734 127 | −636 253 | −734 067 | −623 274 | −771 854 |
| Total | 33 009 716 | 33 001 361 | 39 859 600 | 39 819 963 | 72 306 313 | 72 204 452 | 72 470 589 | 72 374 018 | 73 133 685 | 73 040 392 | 105 807 082 | 105 653 517 |
| MBPT[b] | 32 958 993 | | 39 787 509 | | 72 182 938 | | 72 346 257 | | 73 010 341 | | 105 631 703 | |

DF: MCDHF calculations within $n = 2$ complex, EC: MCDHF and RCI calculations including all electron correlations as mentioned in article, BI: Breit interaction, VP: Vacuum polarization, SE: Self-energy, QED: VP + SE. CKD: Theoretical results by Cheng *et al* [16].

[a] Edlén [8].

[b] Safronova *et al* [14].

[c] NIST [40].

[d] Aggarwal *et al* [21].

[e] Träbert *et al* [31].

**Table 5.** Comparison of QED corrections (in $cm^{-1}$) to transition energy between the $2s^22p_{3/2}$ and $2s^22p_{1/2}$ level for B-like Ar, Ke and Xe ions.

| Ions | This work | Reference [28] | Reference [32] |
|---|---|---|---|
| $Ar^{13+}$ | 47 | | 49.5 (7.0) |
| $Kr^{31+}$ | 783 | 795 | |
| $Xe^{49+}$ | 3605 | 3686 | |

here we will just outline the method. Starting from the Dirac–Coulomb Hamiltonian

$$H_{\rm DC} = \sum_{i=1}^{N} \left( c\,\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + (\beta_i - 1)c^2 + V_i^N \right) + \sum_{i>j}^{N} 1/r_{ij}, \qquad (1)$$

where $V^N$ is the monopole part of the electron–nucleus Coulomb interaction, the atomic state functions (ASFs) describing different fine structure levels are obtained as linear combinations of symmetry adapted configuration state functions (CSFs):

$$\Psi(\gamma P J M_J) = \sum_j c_j \Phi(\gamma_j P J M_J). \qquad (2)$$

Here $J$ and $M_J$ are the angular quantum numbers and $P$ is parity. $\gamma$ denotes other appropriate labelling of the configuration state function, for example orbital occupancy and coupling scheme. The configuration state functions are built from products of one-electron Dirac orbitals. In the relativistic self-consistent field procedure both the radial parts of the Dirac orbitals and the expansion coefficients are optimized to self-consistency. Calculations can be done for single levels, but also for a portion of a spectrum in an extended optimal level (EOL) way where optimization is on a weighted sum of energies. In subsequent relativistic configuration interaction (RCI) calculations the transverse photon interaction

$$H_{\rm Breit} = -\sum_{i<j}^{N} \left[ \frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j}{2r_{ij}} + \frac{(\boldsymbol{\alpha}_i \cdot \boldsymbol{r}_{ij})(\boldsymbol{\alpha}_j \cdot \boldsymbol{r}_{ij})}{2r_{ij}^3} \right] \qquad (3)$$

may be included in the Hamiltonian [38]. In the RCI calculations vacuum polarization [38], and self-energy corrections [38], can also be accounted for. In the GRASP2K package self-energy corrections can be added into the diagonal Hamiltonian matrix element so that the effect can be taken into account in the mixing coefficients $c_j$ in equation (2) and then in the atomic state wavefunction.

Once the atomic state functions have been obtained transition parameters, such as line strengths and rates, for multipole transitions between two atomic states $\gamma P J M_J$ and

**Table 6.** The line strength of the TEOP M1 transition including different contributions for $Ar^{13+}$, $Kr^{31+}$, $Xe^{49+}$ and $W^{69+}$ in au.

| Model | 3–1 | 3–2 | 4–1 | 4–2 | 5–2 | 6–2 | 7–1 | 7–2 |
|---|---|---|---|---|---|---|---|---|
| $Ar^{13+}$ | | | | | | | | |
| DF+EC | 2.308[−5] | 9.076[−5] | 2.447[−5] | 6.030[−5] | 3.252[−5] | 2.749[−5] | 1.646[−5] | 3.175[−7] |
| BI | −0.317[−5] | −1.168[−5] | −0.342[−5] | −0.828[−5] | −0.439[−5] | −0.321[−5] | −0.149[−5] | −0.619[−7] |
| VP | −0.001[−5] | −0.005[−5] | −0.001[−5] | −0.003[−5] | −0.002[−5] | −0.001[−5] | −0.001[−5] | −0.001[−7] |
| SE | 0.030[−5] | 0.119[−5] | 0.031[−5] | 0.077[−5] | 0.041[−5] | 0.033[−5] | 0.019[−5] | 0.038[−7] |
| Total | 2.020[−5] | 8.023[−5] | 2.135[−5] | 5.275[−5] | 2.852[−5] | 2.459[−5] | 1.515[−5] | 2.594[−7] |
| $Kr^{31+}$ | | | | | | | | |
| DF+EC | 2.292[−3] | 4.022[−4] | 9.924[−5] | 5.005[−3] | 1.203[−3] | 1.086[−3] | 1.823[−5] | 2.217[−5] |
| BI | −0.198[−3] | −0.060[−4] | 0.056[−5] | −0.442[−3] | −0.101[−3] | −0.087[−3] | 0.048[−5] | −0.052[−5] |
| VP | −0.090[−3] | −0.020[−4] | −0.041[−5] | −0.020[−3] | −0.005[−3] | −0.004[−3] | −0.007[−5] | −0.007[−5] |
| SE | 0.108[−3] | 0.210[−4] | 0.420[−5] | 0.240[−3] | 0.056[−3] | 0.049[−3] | 0.070[−5] | 0.079[−5] |
| Total | 2.192[−3] | 4.153[−4] | 1.036[−4] | 4.783[−3] | 1.153[−3] | 1.043[−3] | 1.933[−5] | 2.236[−5] |
| $Xe^{49+}$ | | | | | | | | |
| DF+EC | 7.345[−3] | 7.524[−5] | 4.757[−6] | 1.553[−2] | 3.635[−3] | 3.508[−3] | 1.291[−6] | 4.066[−6] |
| BI | −0.583[−3] | 0.079[−5] | 0.313[−6] | −0.122[−2] | −0.292[−3] | −0.280[−3] | 0.157[−6] | 0.253[−6] |
| VP | −0.083[−3] | −0.107[−5] | −0.043[−6] | −0.018[−2] | −0.041[−3] | −0.039[−3] | −0.010[−6] | −0.028[−6] |
| SE | 0.716[−3] | 0.891[−5] | 0.333[−6] | 0.153[−2] | 0.353[−3] | 0.339[−3] | 0.073[−6] | 0.218[−6] |
| Total | 7.369[−3] | 8.287[−5] | 5.360[−6] | 1.566[−2] | 3.655[−3] | 3.527[−3] | 1.511[−6] | 4.508[−6] |
| $Hg^{75+}$ | | | | | | | | |
| DF+EC | 9.239[−3] | 7.758[−6] | 6.638[−8] | 1.887[−2] | 4.586[−3] | 4.553[−3] | 1.934[−8] | 0.930[−7] |
| BI | −0.809[−3] | 0.789[−6] | 1.538[−8] | −0.163[−2] | −0.405[−3] | −0.402[−3] | 0.680[−8] | 0.213[−7] |
| VP | −0.310[−3] | −0.345[−6] | −0.119[−8] | −0.064[−2] | −0.154[−3] | −0.152[−3] | −0.028[−8] | −0.011[−7] |
| SE | 1.830[−3] | 2.001[−6] | 0.604[−8] | 0.375[−2] | 0.907[−3] | 0.900[−3] | 0.129[−8] | 0.050[−7] |
| Total | 9.951[−3] | 1.020[−5] | 8.661[−8] | 2.036[−2] | 4.934[−3] | 4.898[−3] | 2.715[−8] | 1.183[−7] |
| $U^{87+}$ | | | | | | | | |
| DF+EC | 8.592[−3] | 2.837[−6] | 0.967[−8] | 1.742[−2] | 4.274[−3] | 4.259[−3] | 2.609[−9] | 1.572[−8] |
| BI | −0.763[−3] | 0.510[−6] | 0.368[−8] | −0.153[−2] | −0.383[−3] | −0.382[−3] | 1.426[−9] | 0.555[−8] |
| VP | −0.457[−3] | −0.204[−6] | −0.025[−8] | −0.093[−2] | −0.227[−3] | −0.226[−3] | −0.061[−9] | −0.022[−8] |
| SE | 2.228[−3] | 1.007[−6] | 0.101[−8] | 0.453[−2] | 1.106[−3] | 1.102[−3] | 0.194[−9] | 0.077[−8] |
| Total | 9.600[−3] | 4.145[−6] | 1.411[−8] | 1.949[−2] | 4.771[−3] | 4.754[−3] | 4.168[−9] | 2.281[−8] |

DF+EC labels results where electron correlations are taken into account. BI, VP and SE mean that Breit interaction, vacuum polarized and self-energy are further considered, respectively.

**Table 7.** The contributions from Breit interaction (BI) and QED effects to the line strength of the E2 transition for $Ar^{13+}$, $Kr^{31+}$, $Xe^{49+}$ and $W^{69+}$ in au.

| Model | 3–1 | 4–1 | 4–2 | 5–1 | 5–2 | 6–2 | 7–1 | 7–2 |
|---|---|---|---|---|---|---|---|---|
| $Ar^{13+}$ | | | | | | | | |
| DF+EC | 7.265[−6] | 1.252[−3] | 7.561[−4] | 6.669[−4] | 2.406[−3] | 5.406[−4] | 2.989[−4] | 7.725[−4] |
| BI | −0.740[−6] | −0.006[−3] | 0.126[−4] | 0.025[−4] | 0.003[−3] | 0.002[−4] | 0.092[−4] | −0.068[−4] |
| VP | −0.001[−6] | <−0.001[−3] | −0.002[−4] | −0.001[−4] | −0.001[−3] | −0.001[−4] | <−0.001[−4] | −0.001[−4] |
| SE | 0.059[−6] | 0.004[−3] | 0.022[−4] | 0.021[−4] | 0.008[−3] | 0.018[−4] | 0.007[−4] | 0.027[−4] |
| Total | 6.583[−6] | 1.251[−3] | 7.707[−4] | 6.714[−4] | 2.416[−3] | 5.425[−4] | 3.087[−4] | 7.682[−4] |
| $Kr^{31+}$ | | | | | | | | |
| DF+EC | 1.901[−5] | 1.510[−5] | 8.764[−6] | 1.137[−5] | 5.625[−5] | 1.329[−5] | 1.271[−7] | 2.013[−5] |
| BI | −0.044[−5] | 0.054[−5] | −0.059[−6] | 0.021[−5] | −0.001[−5] | −0.002[−5] | 0.109[−7] | 0.042[−5] |
| VP | −0.003[−5] | −0.002[−5] | −0.017[−6] | −0.002[−5] | −0.010[−5] | −0.002[−5] | −0.003[−7] | −0.003[−5] |
| SE | 0.041[−5] | 0.022[−5] | 0.188[−6] | 0.016[−5] | 0.111[−5] | 0.027[−5] | 0.026[−7] | 0.026[−5] |
| Total | 1.895[−5] | 1.584[−5] | 8.876[−6] | 1.172[−5] | 5.725[−5] | 1.350[−5] | 1.404[−7] | 2.079[−5] |
| $Xe^{49+}$ | | | | | | | | |
| DF+EC | 2.468[−6] | 4.511[−7] | 0.978[−6] | 5.604[−7] | 5.322[−6] | 1.275[−6] | 2.833[−10] | 0.943[−6] |
| BI | −0.033[−6] | 0.240[−7] | −0.015[−6] | 0.254[−7] | −0.051[−6] | −0.013[−6] | 0.369[−10] | 0.047[−6] |
| VP | −0.016[−6] | −0.012[−7] | −0.006[−6] | −0.014[−7] | −0.034[−6] | −0.008[−6] | −0.016[−10] | −0.002[−6] |
| SE | 0.135[−6] | 0.093[−7] | 0.055[−6] | 0.108[−7] | 0.283[−6] | 0.068[−6] | 0.119[−10] | 0.016[−6] |
| Total | 2.554[−6] | 4.831[−7] | 1.012[−6] | 5.952[−7] | 5.521[−6] | 1.322[−6] | 3.305[−10] | 1.004[−6] |
| $Hg^{75+}$ | | | | | | | | |
| DF+EC | 2.140[−7] | 1.293[−8] | 8.638[−8] | 1.855[−8] | 4.491[−7] | 1.072[−7] | 2.688[−13] | 3.032[−8] |
| BI | −0.065[−7] | 0.133[−8] | −0.265[−8] | 0.182[−8] | −0.134[−7] | −0.032[−7] | 0.642[−13] | 0.313[−8] |
| VP | −0.053[−7] | −0.005[−8] | −0.215[−8] | −0.006[−8] | −0.110[−7] | −0.026[−7] | −0.035[−13] | −0.008[−8] |
| SE | 0.305[−7] | 0.022[−8] | 1.243[−8] | 0.031[−8] | 0.637[−7] | 0.152[−7] | 1.620[−13] | 0.038[−8] |
| Total | 2.327[−7] | 1.444[−8] | 9.401[−8] | 2.060[−8] | 4.884[−7] | 1.166[−7] | 3.474[−13] | 3.375[−8] |
| $U^{87+}$ | | | | | | | | |
| DF+EC | 8.207[−8] | 3.593[−9] | 3.312[−8] | 5.264[−9] | 1.720[−7] | 4.100[−8] | 0.968[−14] | 8.576[−9] |
| BI | −0.302[−8] | 0.458[−9] | −0.120[−8] | 0.646[−9] | −0.063[−7] | −0.149[−8] | 0.122[−14] | 1.104[−9] |
| VP | −0.344[−8] | −0.013[−9] | −0.140[−8] | −0.019[−9] | −0.072[−7] | −0.172[−8] | −0.022[−14] | −0.022[−9] |
| SE | 1.644[−8] | 0.049[−9] | 0.668[−8] | 0.070[−9] | 0.344[−7] | 0.820[−8] | 0.101[−14] | 0.074[−9] |
| Total | 9.204[−8] | 4.086[−9] | 3.720[−8] | 5.961[−9] | 1.930[−7] | 4.600[−8] | 1.169[−14] | 9.731[−9] |

DF+EC labels results where electron correlations are taken into account. BI, VP and SE mean that Breit interaction, vacuum polarized and self-energy are further considered, respectively.

**Table 8.** Wavelength in angstrom, line strength in au and transition probability in $s^{-1}$ for the TEOP M1 and E2 transitions between the $2p^3$ and $2s^22p$ configurations of B-like Ar. The transition rates taken from [11] are summed over M1 and E2 transition rates.

| | | | λ (Å) | | | $A$ ($s^{-1}$) | |
|---|---|---|---|---|---|---|---|
| Transition | $J_f$–$J_i$ | Type | This work | Reference [11] | $S$ (au) | This work | Reference [11] |
| 3–1 | 3/2–1/2 | M1 | 139.31 | 139.17 | 2.020[−5] | 5.038[1] | 9.398[1] |
| | | E2 | | | 6.583[−6] | 3.513[1] | |
| 3–2 | 3/2–3/2 | M1 | 143.85 | 143.70 | 8.023[−5] | 1.818[2] | 2.128[2] |
| 4–1 | 3/2–1/2 | M1 | 123.29 | 122.05 | 2.135[−5] | 7.682[1] | 1.264[4] |
| | | E2 | | | 1.251[−3] | 1.229[4] | |
| 4–2 | 3/2–3/2 | M1 | 126.83 | 125.52 | 5.275[−5] | 1.744[2] | 6.959[3] |
| | | E2 | | | 7.707[−4] | 6.575[3] | |
| 5–1 | 5/2–1/2 | E2 | 123.00 | 121.80 | 6.714[−4] | 4.452[3] | 4.538[3] |
| 5–2 | 5/2–3/2 | M1 | 126.52 | 125.25 | 2.852[−5] | 6.329[1] | 1.440[4] |
| | | E2 | | | 2.416[−3] | 1.391[4] | |
| 6–2 | 1/2–3/2 | M1 | 112.83 | 111.49 | 2.459[−5] | 2.309[2] | 1.697[4] |
| | | E2 | | | 5.425[−4] | 1.661[4] | |
| 7–1 | 3/2–1/2 | M1 | 109.50 | 108.26 | 1.515[−5] | 7.781[1] | 5.616[3] |
| | | E2 | | | 3.087[−4] | 5.491[3] | |
| 7-2 | 3/2–3/2 | M1 | 112.29 | 110.99 | 2.594[−7] | 1.236 | 1.209[4] |
| | | E2 | | | 7.682[−4] | 1.205[4] | |

$\gamma' P' J' M'_J$ can be expressed in terms of the reduced transition matrix element

$$\left\langle \Psi(\gamma P J) \left\| \mathbf{Q}_k^{(\lambda)} \right\| \Psi(\gamma' P' J') \right\rangle, \tag{4}$$

where $Q_{kq}^{(\lambda)}$ is the electromagnetic multipole operator of order $k$ in Coulomb or Babushkin gauges. The superscript designates the type of multipole: $\lambda = 1$ for electric multipoles and $\lambda = 0$

**Table 9.** Wavelength in angstrom, line strength in au and transition probability in $s^{-1}$ for the TEOP M1 and E2 transitions between the $2p^3$ and $2s^22p$ configurations of B-like Fe. The transition rates taken from [11] are summed over M1 and E2 transition rates.

| | | | λ (Å) | | | $A$ ($s^{-1}$) | |
|---|---|---|---|---|---|---|---|
| Transition | $J_f$–$J_i$ | Type | This work | Reference [11] | $S$ (au) | This work | Reference [11] |
| 3–1 | 3/2–1/2 | M1 | 79.64 | 79.71 | 2.890[−4] | 3.859[3] | 5.653[3] |
| | | E2 | | | 1.963[−5] | 1.715[3] | |
| 3–2 | 3/2–3/2 | M1 | 87.92 | 87.84 | 5.034[−4] | 4.994[3] | 5.340[3] |
| 4–1 | 3/2–1/2 | M1 | 71.63 | 71.32 | 1.690[−4] | 3.100[3] | 3.121[4] |
| | | E2 | | | 1.856[−4] | 2.756[4] | |
| 4–2 | 3/2–3/2 | M1 | 78.26 | 77.76 | 6.413[−4] | 9.023[3] | 1.528[4] |
| | | E2 | | | 6.087[−5] | 5.806[3] | |
| 5–1 | 5/2–1/2 | E2 | 70.10 | 69.85 | 8.595[−5] | 9.475[3] | 9.494[3] |
| 5–2 | 5/2–3/2 | M1 | 76.44 | 76.01 | 2.491[−4] | 2.507[3] | 2.735[4] |
| | | E2 | | | 3.371[−4] | 2.410[4] | |
| 6–2 | 1/2–3/2 | M1 | 68.88 | 68.49 | 2.157[−4] | 8.901[3] | 3.724[4] |
| | | E2 | | | 7.758[−5] | 2.802[4] | |
| 7–1 | 3/2–1/2 | M1 | 61.43 | 61.29 | 3.725[−5] | 1.084[3] | 4.318[3] |
| | | E2 | | | 9.818[−6] | 3.143[3] | |
| 7–2 | 3/2–3/2 | M1 | 66.24 | 65.98 | 9.029[−6] | 2.095[2] | 3.080[4] |
| | | E2 | | | 1.406[−4] | 3.087[4] | |

**Table 10.** Wavelength in angstrom, line strength in au and transition probability in $s^{-1}$ for the TEOP M1 and E2 transitions between the $2p^3$ and $2s^22p$ configurations of B-like Kr.

| | | | λ (Å) | | $S$ (au) | | $A$ ($s^{-1}$) | |
|---|---|---|---|---|---|---|---|---|
| Transition | $J_f$–$J_i$ | Type | This work | Reference [21] | This work | Reference [21] | This work | Reference [21] |
| 3–1 | 3/2–1/2 | M1 | 44.31 | 44.12 | 2.192[−3] | 2.088[−3] | 1.699[5] | 1.640[5] |
| | | E2 | | | 1.895[−5] | 1.807[−5] | 3.105[4] | 3.026[4] |
| 3–2 | 3/2–3/2 | M1 | 56.69 | 56.35 | 4.153[−4] | 4.344[−4] | 1.537[4] | 1.638[4] |
| 4–1 | 3/2–1/2 | M1 | 37.95 | 37.83 | 1.036[−4] | 1.107[−4] | 1.278[4] | 1.379[4] |
| | | E2 | | | 1.584[−5] | 1.597[−5] | 5.634[4] | 5.773[4] |
| 4–2 | 3/2–3/2 | M1 | 46.68 | 46.47 | 4.783[−3] | 4.552[−3] | 3.170[5] | 3.059[5] |
| | | E2 | | | 8.876[−6] | 8.600[−6] | 1.121[4] | 1.111[4] |
| 5–1 | 5/2–1/2 | E2 | 36.59 | 36.44 | 1.172[−5] | 1.150[−5] | 3.335[4] | 3.343[4] |
| 5–2 | 5/2–3/2 | M1 | 44.64 | 44.39 | 1.153[−3] | 1.105[−3] | 5.830[4] | 5.678[4] |
| | | E2 | | | 5.725[−5] | 5.588[−5] | 6.029[4] | 6.052[4] |
| 6–2 | 1/2–3/2 | M1 | 40.97 | 40.69 | 1.043[−3] | 9.979[−4] | 2.046[5] | 1.998[5] |
| | | E2 | | | 1.350[−5] | 1.326[−5] | 6.553[4] | 6.657[4] |
| 7–1 | 3/2–1/2 | M1 | 30.21 | 30.10 | 1.933[−5] | 1.976[−5] | 4.728[3] | 4.887[3] |
| | | E2 | | | 1.404[−7] | 1.487[−7] | 1.562[3] | 1.684[3] |
| 7–2 | 3/2–3/2 | M1 | 35.50 | 35.33 | 2.236[−5] | 2.297[−5] | 3.372[3] | 3.513[3] |
| | | E2 | | | 2.079[−5] | 2.054[−5] | 1.033[5] | 1.044[5] |

for magnetic multipoles. Inserting the CSF expansions this reduces to a sum over reduced matrix elements between CSFs. Using Racah algebra techniques these matrix elements, in turn, can be obtained as a sum over radial integrals over the radial one-electron Dirac orbitals [37].

## 3. Results and discussions

The success of a calculation relies on a judiciously chosen configuration expansion. To ensure the convergence of a calculated expectation value within a certain correlation model, the configuration expansion must be enlarged in a systematic way. A very efficient way of doing this is to use the active set approach, where $jj$-coupled configuration state functions of a specified parity $P$ and angular momentum $J$ symmetry are generated by excitations from one or more reference configurations to an active set of orbitals. The convergence of the atomic property can then be studied as a function of the size of the active set. To build a reasonable correlation model and control the accuracy we performed tentative calculations on transition energies and line strengths of the TEOP M1, E2 transitions for $Ar^{13+}$. In the calculations the states of the $2s^22p$ and $2p^3$ configurations were simultaneously optimized in an extended optimal level (EOL) scheme. These calculations were followed by calculations with CSF expansions generated by single (S)- and double (D)-excitations from the 2s and 2p shells of the reference configurations $2s^22p$ and $2p^3$ to the active set in order to consider valence-valence (VV) correlations. The active set was systematically increased by adding layers of new orbitals. The largest active set included all relativistic orbitals with

**Table 11.** Wavelength in angstrom, line strength in au and transition probability in $s^{-1}$ for the TEOP M1 and E2 transitions between the $2p^3$ and $2s^22p$ configurations of B-like Mo.

| Transition | $J_f$–$J_i$ | Type | λ (Å) | $S$ (au) | $A$ ($s^{-1}$) |
|---|---|---|---|---|---|
| 3–1 | 3/2–1/2 | M1 | 32.10 | 3.968[−3] | 8.089[5] |
| | | E2 | | 9.883[−6] | 8.117[4] |
| 3–2 | 3/2–3/2 | M1 | 46.50 | 2.366[−4] | 1.586[4] |
| 4–1 | 3/2–1/2 | M1 | 25.58 | 3.934[−5] | 1.585[4] |
| | | E2 | | 4.210[−6] | 1.077[5] |
| 4–2 | 3/2–3/2 | M1 | 33.96 | 8.608[−3] | 1.483[6] |
| | | E2 | | 3.972[−6] | 2.464[4] |
| 5–1 | 5/2–1/2 | E2 | 24.79 | 4.060[−6] | 8.097[4] |
| 5–2 | 5/2–3/2 | M1 | 32.58 | 1.991[−3] | 2.588[5] |
| | | E2 | | 2.395[−5] | 1.218[5] |
| 6–2 | 1/2–3/2 | M1 | 30.26 | 1.850[−3] | 9.004[5] |
| | | E2 | | 5.699[−6] | 1.257[5] |
| 7–1 | 3/2–1/2 | M1 | 19.66 | 9.093[−6] | 8.071[3] |
| | | E2 | | 1.520[−8] | 1.449[3] |
| 7–2 | 3/2–3/2 | M1 | 24.26 | 1.662[−5] | 7.849[3] |
| | | E2 | | 7.097[−6] | 2.365[5] |

**Table 12.** Wavelength in angstrom, line strength in au and transition probability in $s^{-1}$ for the TEOP M1 and E2 transitions between the $2p^3$ and $2s^22p$ configurations of B-like Xe.

| Transition | $J_f$–$J_i$ | Type | λ (Å) | $S$ (au) | $A$ ($s^{-1}$) |
|---|---|---|---|---|---|
| 3–1 | 3/2–1/2 | M1 | 17.00 | 7.369[−3] | 1.014[7] |
| | | E2 | | 2.554[−6] | 5.031[5] |
| 3–2 | 3/2–3/2 | M1 | 33.46 | 8.387[−5] | 1.509[4] |
| 4–1 | 3/2–1/2 | M1 | 11.74 | 5.360[−6] | 2.234[4] |
| | | E2 | | 4.831[−7] | 6.066[5] |
| 4–2 | 3/2–3/2 | M1 | 17.78 | 1.566[−2] | 1.880[7] |
| | | E2 | | 1.012[−6] | 1.596[5] |
| 5–1 | 5/2–1/2 | E2 | 11.52 | 5.952[−7] | 5.464[5] |
| 5–2 | 5/2–3/2 | M1 | 17.29 | 3.655[−3] | 3.179[6] |
| | | E2 | | 5.521[−6] | 6.671[5] |
| 6–2 | 1/2–3/2 | M1 | 16.41 | 3.527[−3] | 1.076[7] |
| | | E2 | | 1.322[−6] | 6.217[5] |
| 7–1 | 3/2–1/2 | M1 | 8.57 | 1.511[−6] | 1.621[4] |
| | | E2 | | 3.305[−10] | 2.006[3] |
| 7–2 | 3/2–3/2 | M1 | 11.39 | 4.508[−6] | 2.059[4] |
| | | E2 | | 1.004[−6] | 1.468[6] |

**Table 13.** Wavelength in angstrom, line strength in au and transition probability in $s^{-1}$ for the TEOP M1 and E2 transitions between the $2p^3$ and $2s^22p$ configurations of B-like Eu.

| Transition | $J_f$–$J_i$ | Type | λ (Å) | $S$ (au) | $A$ ($s^{-1}$) |
|---|---|---|---|---|---|
| 3–1 | 3/2–1/2 | M1 | 10.61 | 9.073[−3] | 5.125[7] |
| | | E2 | | 1.032[−6] | 2.151[6] |
| 3–2 | 3/2–3/2 | M1 | 26.97 | 3.994[−5] | 1.374[4] |
| 4–1 | 3/2–1/2 | M1 | 6.74 | 1.239[−6] | 2.723[4] |
| | | E2 | | 1.240[−7] | 2.489[6] |
| 4–2 | 3/2–3/2 | M1 | 10.98 | 1.891[−2] | 9.642[7] |
| | | E2 | | 4.134[−7] | 7.262[5] |
| 5–1 | 5/2–1/2 | E2 | 6.67 | 1.654[−7] | 2.346[6] |
| 5–2 | 5/2–3/2 | M1 | 10.77 | 4.484[−3] | 1.613[7] |
| | | E2 | | 2.186[−6] | 2.814[6] |
| 6–2 | 1/2–3/2 | M1 | 10.35 | 4.394[−3] | 5.338[7] |
| | | E2 | | 5.231[−7] | 2.461[6] |
| 7–1 | 3/2–1/2 | M1 | 4.80 | 3.694[−7] | 2.257[4] |
| | | E2 | | 2.686[−11] | 2.961[3] |
| 7–2 | 3/2–3/2 | M1 | 6.61 | 1.327[−6] | 3.098[4] |
| | | E2 | | 2.745[−7] | 6.091[6] |

**Table 14.** Wavelength in angstrom, line strength in au and transition probability in $s^{-1}$ for the TEOP M1 and E2 transitions between the $2p^3$ and $2s^22p$ configurations of B-like W.

| Transition | $J_f$–$J_i$ | Type | λ (Å) | $S$ (au) | $A$ ($s^{-1}$) |
|---|---|---|---|---|---|
| 3–1 | 3/2–1/2 | M1 | 6.04 | 9.918[−3] | 3.033[8] |
| | | E2 | | 3.834[−7] | 1.334[7] |
| 3–2 | 3/2–3/2 | M1 | 21.10 | 1.640[−5] | 1.177[4] |
| 4–1 | 3/2–1/2 | M1 | 3.58 | 2.180[−7] | 3.216[4] |
| | | E2 | | 2.923[−8] | 1.400[7] |
| 4–2 | 3/2–3/2 | M1 | 6.19 | 2.040[−2] | 5.798[8] |
| | | E2 | | 1.546[−7] | 4.762[6] |
| 5–1 | 5/2–1/2 | E2 | 3.55 | 4.101[−8] | 1.353[7] |
| 5–2 | 5/2–3/2 | M1 | 6.12 | 4.912[−3] | 9.627[7] |
| | | E2 | | 8.055[−7] | 1.750[7] |
| 6–2 | 1/2–3/2 | M1 | 5.95 | 4.861[−3] | 3.111[8] |
| | | E2 | | 1.925[−7] | 1.444[7] |
| 7–1 | 3/2–1/2 | M1 | 2.49 | 6.769[−8] | 2.950[4] |
| | | E2 | | 1.577[−12] | 4.596[3] |
| 7–2 | 3/2–3/2 | M1 | 3.53 | 2.778[−7] | 4.254[4] |
| | | E2 | | 6.738[−8] | 3.436[7] |

$n \leqslant 8$ and $l \leqslant 4$. Due to stability problems in the relativistic SCF procedure only the outermost layer of orbitals could be optimized each time. Breit interaction as a part of the electron correlations has been taken into account by a relativistic configuration interaction (RCI) calculation in each step. Energies relative to a ground-state energy of zero for $Ar^{13+}$ are presented in table 1. The first column in the table represents the largest principal quantum number of the active set involved in each step of the calculation. As can be seen from table 1, the VV correlations have converged when $n = 7$. The valence calculations were followed by RCI calculations. In these calculations residual core–valence (CV) and core–core (CC) correlation effects were accounted for by including CSFs obtained by excitations also from the 1s shell of the reference configurations to the largest active space ($n = 7, l = 4$). Triple (T) and quadruple (Q) excitations were neglected due to their very small contributions. The leading QED effects were also added in the RCI calculations and the final results are displayed at the end of table 1. Compared with other theoretical data, the largest discrepancies are less than 1%. In tables 2 and 3 we list the line strengths of the TEOP M1 and E2 transitions. Also in this case the values are well converged with respect to the active set and there is a reasonable consistency between the Babushkin (length) and Coulomb (velocity) gauges for the E2 transition. Therefore, we believe that our results are reliable. We would use the Babushkin gauge because it is the more reliable gauge for electric multipole transitions [39]. Based on these results, we performed similar calculations for the other B-like ions. When $Z \geqslant 28$, we only consider the active set of $n \leqslant 6, l \leqslant 4$ since electron correlation effects converge faster with increasing atomic number $Z$.

In tables 4–7, contributions from electron correlation, Breit interaction and QED effects to energies and line strengths

**Table 15.** Wavelength in angstrom, line strength in au and transition probability in $s^{-1}$ for the TEOP M1 and E2 transitions between the $2p^3$ and $2s^22p$ configurations of B-like Hg.

| Transition | $J_f$–$J_i$ | Type | λ (Å) | $S$ (au) | $A$ ($s^{-1}$) |
|---|---|---|---|---|---|
| 3–1 | 3/2–1/2 | M1 | 4.48 | 9.951[−3] | 7.459[8] |
| | | E2 | | 2.327[−7] | 3.608[7] |
| 3–2 | 3/2–3/2 | M1 | 18.57 | 1.020[−5] | 1.075[4] |
| 4–1 | 3/2–1/2 | M1 | 2.58 | 8.661[−8] | 3.412[4] |
| | | E2 | | 1.444[−8] | 3.555[7] |
| 4–2 | 3/2–3/2 | M1 | 4.57 | 2.036[−2] | 1.436[9] |
| | | E2 | | 9.401[−8] | 1.317[7] |
| 5–1 | 5/2–1/2 | E2 | 2.57 | 2.060[−8] | 3.463[7] |
| 5–2 | 5/2–3/2 | M1 | 4.53 | 4.934[−3] | 2.378[8] |
| | | E2 | | 4.884[−7] | 4.753[7] |
| 6–2 | 1/2–3/2 | M1 | 4.43 | 4.898[−3] | 7.603[8] |
| | | E2 | | 1.166[−7] | 3.830[7] |
| 7–1 | 3/2–1/2 | M1 | 1.78 | 2.715[−8] | 3.236[4] |
| | | E2 | | 3.474[−13] | 5.414[3] |
| 7–2 | 3/2–3/2 | M1 | 2.55 | 1.183[−7] | 4.799[4] |
| | | E2 | | 3.375[−8] | 8.731[7] |

**Table 16.** Wavelength in angstrom, line strength in au and transition probability in $s^{-1}$ for the TEOP M1 and E2 transitions between the $2p^3$ and $2s^22p$ configurations of B-like U.

| Transition | $J_f$–$J_i$ | Type | λ (Å) | $S$ (au) | $A$ ($s^{-1}$) |
|---|---|---|---|---|---|
| 3–1 | 3/2–1/2 | M1 | 2.51 | 9.600[−3] | 4.100[9] |
| | | E2 | | 9.204[−8] | 2.593[8] |
| 3–2 | 3/2–3/2 | M1 | 14.60 | 4.145[−6] | 8.984[3] |
| 4–1 | 3/2–1/2 | M1 | 1.38 | 1.411[−8] | 3.596[4] |
| | | E2 | | 4.086[−9] | 2.261[8] |
| 4–2 | 3/2–3/2 | M1 | 2.54 | 1.949[−2] | 7.977[9] |
| | | E2 | | 3.720[−8] | 9.761[7] |
| 5–1 | 5/2–1/2 | E2 | 1.38 | 5.961[−9] | 2.224[8] |
| 5–2 | 5/2–3/2 | M1 | 2.53 | 4.771[−3] | 1.318[9] |
| | | E2 | | 1.930[−7] | 3.446[8] |
| 6–2 | 1/2–3/2 | M1 | 2.49 | 4.753[−3] | 4.142[9] |
| | | E2 | | 4.600[−8] | 2.679[8] |
| 7–1 | 3/2–1/2 | M1 | 0.95 | 4.168[−9] | 3.330[4] |
| | | E2 | | 1.169[−14] | 4.340[3] |
| 7–2 | 3/2–3/2 | M1 | 1.37 | 2.182[−8] | 5.678[4] |
| | | E2 | | 9.731[−9] | 5.570[8] |

for the TEOP M1 and E2 transitions are presented. In previous theoretical studies, Cheng *et al* performed similar calculations using the MCDF method developed by Desclaux [16]. These results, labelled CKD, are included in table 4. The agreement on transition energy with the DF model and the contributions from Breit interaction between the results of Cheng *et al* and ours are acceptable along entire isoelectronic sequence, although there exist some differences that result from the restricted electron correlation within the $n = 2$ complex in the calculations by Cheng *et al.* However, large differences in QED corrections were found. Therefore, we further compared the present QED corrections with other theoretical calculations, which are displayed in table 5. As can be seen from this table, the present values of QED effects are in good agreement with other results and thus are reliable. In table 4 we also display Edlén's recommended values and other theoretical and experimental data. Comparing with these data, we see that relatively large differences exist for high-$Z$ ions, which mainly come from the Breit interaction and high-order QED effects.

The line strengths of the TEOP M1 and E2 transitions are zero in single-configuration approximations. Hence, we display only these results in tables 6 and 7, which were calculated by considering electron correlation (EC), Breit interaction (BI), vacuum polarization (VP) and self-energy (SE) effects, respectively. As can be seen from these two tables, line strength of the M1 transition is more sensitive to the Breit interaction than the one of the E2 transitions, even for low-charged ions. With increasing atomic number $Z$ the QED contributions, especially the self-energy corrections, to both of the M1 and E2 line strengths become more important.

Finally, we presented all calculated TEOP M1 and E2 transitions wavelengths, line strengths and probabilities in tables 8–16 for B-like Ar, Fe, Kr, Mo, Xe, Eu, W, Hg and U. Some other theoretical and experimental values were also displayed for comparison.

## 4. Conclusions

Two-electron–one-photon (TEOP) M1 and E2 transition energies, line strengths and transition probabilities between the states of the $2p^3$ and $2s^22p$ odd configurations of B-like ions with $18 \leqslant Z \leqslant 92$ have been calculated using the GRASP2K package based on the multiconfiguration Dirac–Hartree–Fock (MCDHF) method. Electron correlation effects were handled in a systematic way. The Breit interaction and QED effects further corrected the atomic state function and corresponding energy.

The present calculated transition energies were compared with other theoretical and experimental values. Good agreement was found for low- and mid-charged ions, whereas the discrepancies become more obvious with increasing atomic number $Z$. The differences mainly come from the Breit interaction and high-order QED effects. We found that the line strengths of the TEOP M1 transition are more sensitive to the Breit interaction than those of the TEOP E2 transitions. With increasing atomic number $Z$, QED corrections become more important, especially the self-energy effect. Some recommendations of atomic data including wavelengths, line strengths and transition probabilities were supplied for the TEOP transition.

## Acknowledgments

We would like to thank the two (anonymous) referees for pointing our attention to the differences in the QED effect on transition energy. This work is supported by the National Nature Science Foundation of China (grant no 10434100, 10774122), the specialized Research Fund for the Doctoral Program of Higher Education of China (grant no 20070736001) and the Foundation of Northwest Normal University (NWNU-KJCXGC-03-21). Financial support by the Swedish Research Council is gratefully acknowledged.

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