J. Plasma Fusion Res. SERIES, Vol.7 (2006) 282-285

Excitation Energies, Oscillator Strengths, and Transition Rates in B I, Al I, Ga I, In I, and Tl I

SAFRONOVA Ulyana I.

Physics Department, University of Nevada, Reno, Reno NV 89557, USA

(Received: 4 October 2004 / Accepted : 28 May 2005)

Abstract

The energies of the ground np states and the lowest ns and nd states in neutral B, Al, Ga, In and Tl are obtained by using the relativistic many-body perturbation theory (RMBPT) method. First-, second-, third-order, and 'all order' Coulomb energies and first- and second-order Breit energies are calculated. Reduced matrix elements, oscillator strengths, and transition rates are determined for the possible $nl_j - n'l'_{j'}$ electric-dipole transitions.

Keywords:

relativistic many-body perturbation theory, excitation energy, Breit, electric-dipole transition

1. Introduction

Energy levels and dipole matrix elements for low-lying $ns_{1/2}$, $np_{1/2}$, and $np_{3/2}$ states in alkali-metal atoms were studied systematically using the relativistic single-double (SD) method in which single and double excitations of the Dirac-Hartree-Fock (DHF) wave functions were included to all orders of perturbation theory. The SD method was applied previously to study properties of Li and Be^+ in Ref. [1], Cs in Ref. [2], Na-like ions with Z ranging from 11 to 16 in Ref. [3], alkali-metal atoms Na, K, Rb, and Cs in Ref. [4], and Au-like ions in Ref. [5]

The ground-state energy of thallium was treated as a one-electron system in Refs. [6,7] using third-order and all-order calculations in many-body perturbation theory, respectively. In that case the three-electron state $6s^26p$ with the 78 electrons in core (closed $n = 1 - 4$ shells [Nd] and three closed subshells $5s^25p^65d^{10}$) was considered as the one-electron state $6p$ with 80 electrons in the core [Nd] $5s^25p^65d^{10}6s^2$. In the present paper we use those presentations of three-electron systems as one-electron systems. We treat the $1s^22s^2nl$ states in B I as the nl one-electron state with [He] $2s^2$ core, the [Ne] $3s^2nl$ states in Al I as the nl one-electron state with [Ne] $3s^2$ core, the [Ni] $4s^2nl$ states in Ga I as the nl one-electron state with [Ni] $4s^2$ core, the [Pd] $5s^2nl$ states in In I as the nl one-electron state with [Pd] $5s^2$ core, and the [Nd] $5s^25p^65d^{10}6s^2nl$ states in Tl I as the nl one-electron state with [Nd] $5s^25p^65d^{10}6s^2$ core.

Energies of low-lying excited states of neutral atoms with three electrons above the core (Al I. Tl I, and Bi 1) were presented in Ref. [8]. Results were obtained to second order in relativistic many-body perturbation theory using frozen-core Dirac-Hartree-Fock orbitals as a basis set. Combination of the many-body perturbation theory with the configuration-interaction method was presented in Ref. [9] to evaluate in Tl I ionization potential and the first few energy intervals. The same method was used recently by Kozlov *et al*. [10] to calculate the energies, hyperfine constants for the seven low-lying states, and the dipole matrix elements between those states.

2. Calculations of energies

In Table 1, we present DHF energies $E^{(1)}$, single-double Coulomb energies E_{SD}, E_{3extra}, and first- and second-order Breit energies $B^{(n)}$, $n = 1, 2$. The values E_{SD} are evaluated by using the all-order single-double method described in detail in Refs. [1-5]. The SD equations are set up in a finite basis and solved iteratively to give the single- and double-excitation coefficients and the correlation energy E_{SD}. The basis orbitals used to define the single-particle states are linear combinations of B-splines. For each angular momentum state, the basis set consists of 50 (B I, Al I, Ga I, In I) or 40 (Tl I) B-splines of order 8. In our iterative calculations, we used only 40 of the 50 orbitals (B I, Al I, Ga I, In I) or 35 of the 40 orbitals (Tl I). The B-spline basis orbitals were interpolated onto a 500 point nonlinear radial grid. All orbitals were constrained to a large spherical cavity; the cavity radii chosen to be 60 a.u. for B I, 90 a.u. for Al I, 100 a.u. for Ga I and In I and, 65 a.u. for Tl I. Such

Corresponding author's e-mail: ulyanas@unr.edu

Table 1 DHF energies $E^{(1)}$, single-double Coulomb energies E_{SD}, E_{3extra}, and first- and second-order Breit corrections $B^{(1)}$ and $B^{(2)}$. Units, cm^{-1}.

nlj	$E^{(1)}$	$B^{(1)}$	$B^{(2)}$	E_{SD}	E_{3extra}
		B I			
$2p_{1/2}$	−60546	10	−6	−6448	294
$2p_{3/2}$	−60528	5	−6	−6447	294
$3s_{1/2}$	−25138	1	0	−1946	53
$4s_{1/2}$	−11370	0	0	−571	14
$5s_{1/2}$	−6489	0	0	−288	6
$6s_{1/2}$	−4194	0	0	−85	3
$3d_{3/2}$	−12327	0	0	−891	28
$4d_{3/2}$	−6934	0	0	−486	13
$5d_{3/2}$	−4432	0	0	−309	7
$6d_{3/2}$	−3074	0	0	−249	4
		Al I			
$3p_{1/2}$	−42824	18	−15	−5392	244
$3p_{3/2}$	−42714	12	−16	−5387	244
$4s_{1/2}$	−21312	2	−2	−1754	84
$5s_{1/2}$	−10130	1	0	−485	25
$6s_{1/2}$	−5938	0	0	−217	11
$7s_{1/2}$	−3903	0	0	−99	13
$3d_{3/2}$	−12709	0	0	−2421	79
$4d_{3/2}$	−7142	0	0	−1069	34
$5d_{3/2}$	−4548	0	0	−580	17
$6d_{3/2}$	−3144	0	0	−357	10
		Ga I			
$4p_{1/2}$	−43033	58	−79	−5610	176
$4p_{3/2}$	−42294	42	−77	−5534	191
$5s_{1/2}$	−21936	7	−10	−1909	65
$6s_{1/2}$	−10332	2	−4	−528	18
$7s_{1/2}$	−6028	1	−1	−229	7
$8s_{1/2}$	−3951	1	0	−112	4
$4d_{3/2}$	−12423	1	−2	−1264	74
$5d_{3/2}$	−6981	0	−1	−568	32
$6d_{3/2}$	−4457	0	0	−301	16
$7d_{3/2}$	−3089	0	0	−173	9
		Tl I			
$6p_{1/2}$	−43824	259	−421	−5759	694
$6p_{3/2}$	−36636	135	−291	−5298	807
$7s_{1/2}$	−21109	26	−46	−2065	266
$8s_{1/2}$	−10040	9	−15	−570	79
$9s_{1/2}$	−5893	4	−7	−246	35
$10s_{1/2}$	−3878	2	−4	−155	23
$6d_{3/2}$	−12218	3	−8	−1223	154
$7d_{3/2}$	−6864	2	−4	−533	65
$8d_{3/2}$	−4391	1	−2	−273	35
$9d_{3/2}$	−3049	1	−1	−271	35

Table 2 Comparison of the SD energies of the nl states with NIST data [11]. The difference between the SD and NIST data are shown. Units: cm^{-1}.

nlj	B	Al	Ga	In	Tl
	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$
$(n)p_{1/2}$	187	249	−172	403	91
$(n)p_{3/2}$	187	246	−181	353	100
$(n+1)s_{1/2}$	−147	−56	−194	−155	−154
$(n+2)s_{1/2}$	−9	−2	−43	−25	−22
$(n+3)s_{1/2}$	10	−10	−21	−7	−11
$(n+4)s_{1/2}$	170	16	−4	0	−46
$(n)d_{3/2}$		786	−14	−12	−151
$(n+1)d_{3/2}$	−1033	−2136	65	−84	−85
$(n+2)d_{3/2}$	−475	−1000	70	5	−41
$(n+3)d_{3/2}$	−293	−558	63	76	−122

large cavities were needed to accommodate the highly excited states considered here. The DHF energies of the lowest three to four ns and nd states were represented to five or more significant digits by the B-spline basis functions. Generally, the larger values of n had lower accuracy, which is unimportant owing to the decreasing size of correlation correction with increasing n. Terms in the angular momentum decomposition with angular momentum l are from 0 to 6. The contributions with E_{3extra} headings presented in Table 1 give the part of the third-order RMBPT correction that it is not included in the SD energy [1-5].

In Table 2, the deviation (δE) of our SD *ab-initio* results from the recommended NIST data [11] are shown. The values of δE for the ionization potential given in Table 2 are in the range 0.2 % for Tl I, 0.35 % for B I and Ga I, 0.5 % for Al I and up to 0.86 % for In I. The best agreement (0 - 20 cm^{-1}) is for 4s, 5s states in B I, for 5s, 6s, 7s states in Al I, 6s, 7s, 8s states in Ga I, 7s, 8s, 9s states in In I, and 8s, 9s states in Tl I. Larger disagreements are found for the nd states. Those disagreement for $nd_{3/2}$ states could be explained by strong mixing of the $2s2p^2 + 2s^23d$ states in B I, the $3s3p^2 + 3s^23d$ states in Al I, the $4s4p^2 + 4s^24d$ states in Ga I, and the $5s5p^2 + 5s^25d$ states in In I. Such mixing is less important for the $6s^26d$ in Tl I since the first term of the $6s6p^2$ configuration is situated near the $6s^210s$ and $6s^29d$ states and so it does not give the large correction for the lowest $6s^26d$ state. The largest disagreement in Tl I is 150 cm^{-1} for 7s and $6d_{3/2}$ states and as a result the values of δE in Tl I are in the range from 0.2 % up to 0.68 %. Comparing the value for $6p_{3/2}$ - $6p_{1/2}$ splitting (7802 cm^{-1} and 7793 cm^{-1}), we obtain 0.12 % for the deviation in Tl I.

3. Calculations of electric-dipole matrix elements, oscillator strengths, and transition rates

Transition matrix elements provide another test of quality of atomic-structure calculations and another measure of the size of correlation corrections. Reduced matrix elements of the dipole operator in first-, second-, third- and 'all order'- perturbation theory between low-lying states of B I and Ga I are presented in Table 3. The first-order reduced matrix elements $Z^{(1)}$ are obtained from length-form DHF calculations. Length-form and velocity-form matrix elements differ typically by 10 %. Second-order matrix elements in the table, $Z^{(2)}$, which include $Z^{(1)}$, are extended to include all high-order corrections associated with the random-phase approximation (RPA). These second-order calculations are practically gauge independent.

The third-order matrix elements $Z^{(3)}$ include $Z^{(RPA)}$ plus Brueckner-orbital $Z^{(BO)}$, structural radiation $Z^{(SR)}$, and a normalization correction $Z^{(NORM)}$ described, for example in Refs. [3,4]. It is found that RPA corrections are very large, $10-40$ %, being smallest for $np_{3/2}-(n+1)s_{1/2}$ transitions with $n = 2$ for B I, $n = 3$ for Al I, $n = 4$ for Ga I (see, Table 3), $n = 5$ for In I, and $n = 6$ for Tl I. Third-order corrections are smaller, $2-15$ %, being smallest for $np_{1/2} - nd_{3/2}$ transitions with $n = 3$ for Al I, $n = 4$ for Ga I, $n = 5$ for In I, and $n = 6$ for Tl I.

Table 3 Reduced matrix elements of the dipole operator in first-, second-, third- and 'all order'- perturbation theory in B I, Al I, and Ga I.

Transition	$Z^{(1)}$	$Z^{(2)}$	$Z^{(3)}$	$Z^{(SD)}$
B I				
$2p_{3/2} - 3s_{1/2}$	1.732	1.660	1.460	1.749
$2p_{3/2} - 4s_{1/2}$	0.576	0.572	0.517	0.805
$2p_{3/2} - 5s_{1/2}$	0.329	0.307	0.277	0.481
$2p_{3/2} - 6s_{1/2}$	0.249	0.232	0.207	0.113
$2p_{1/2} - 3d_{3/2}$	1.340	1.102	1.012	0.988
$2p_{1/2} - 4d_{3/2}$	0.822	0.605	0.553	0.495
$2p_{1/2} - 5d_{3/2}$	0.595	0.402	0.358	0.162
$2p_{1/2} - 6d_{3/2}$	0.617	0.380	0.324	0.739
Ga I				
$4p_{3/2} - 5s_{1/2}$	3.105	2.844	2.464	2.690
$4p_{3/2} - 6s_{1/2}$	0.875	0.733	0.665	0.716
$4p_{3/2} - 7s_{1/2}$	0.485	0.402	0.366	0.389
$4p_{3/2} - 8s_{1/2}$	0.328	0.266	0.244	0.240
$4p_{1/2} - 4d_{3/2}$	2.851	2.499	2.348	2.412
$4p_{1/2} - 5d_{3/2}$	1.492	1.240	1.130	1.032
$4p_{1/2} - 6d_{3/2}$	0.968	0.779	0.695	0.578
$4p_{1/2} - 7d_{3/2}$	0.701	0.554	0.485	0.441

Electric-dipole matrix elements evaluated in the SD approximation are given in the last column of Table 3. The values Z^{SD} are evaluated by using the all-order single-double method described in detail in Refs. [1-5]. It should be noted that the SD matrix elements Z^{SD} include $Z^{(3)}$ plus the part of fourth-order and all higher-order corrections. As can be seen in Table 3, Z^{SD} values are differ less from the $Z^{(2)}$ values than from the $Z^{(3)}$ values for $p_{3/2} - s_{1/2}$ transitions, $2-6$ %, and opposite for $p_{1/2} - d_{3/2}$ transitions. The values Z^{SD} are smaller than $Z^{(2)}$ values and larger than $Z^{(3)}$ values for $p_{3/2} - s_{1/2}$ transitions but the values Z^{SD} are the smallest than than $Z^{(2)}$ and $Z^{(3)}$ values for $p_{1/2} - d_{3/2}$ transitions.

We compare our SD data ($Z^{(SD)}$) reduced matrix elements of the dipole operator in Tl I with theoretical ($Z^{(theor.)}$) and experimental ($Z^{(expt.)}$) data given by Kozlov et al. in Ref. [10]. It is found that our SD data are in excellent agreement with experimental data and theoretical data obtained by combination of the many-body perturbation theory with the configuration-interaction (CI) method in Refs. [9,10].

Transition rates A_r (s^{-1}) and oscillator strengths (f) for transitions in Ga I and Tl I evaluated in the SD approximation are summarized in Table 4. For convenience, we present also wavelengths calculated using the SD approximation in Table 4. The largest oscil-

Table 4 Wavelengths λ (Å), transition rates A_r (s^{-1}), and oscillator strengths (f) for transitions in Ga I and Tl I calculated using the SD all-order method. Numbers in brackets represent powers of 10.

Transition		λ	A_r	f
$4p_{1/2}$	$5s_{1/2}$	4048	5.234[7]	1.286[−1]
$4p_{3/2}$	$5s_{1/2}$	4186	1.003[8]	1.318[−1]
$4p_{1/2}$	$6s_{1/2}$	2656	1.369[7]	1.449[−2]
$4p_{3/2}$	$6s_{1/2}$	2715	2.574[7]	1.422[−2]
$4p_{1/2}$	$7s_{1/2}$	2368	5.801[6]	4.875[−3]
$4p_{3/2}$	$7s_{1/2}$	2414	1.102[7]	4.814[−3]
$4p_{1/2}$	$4d_{3/2}$	2868	1.249[8]	3.079[−1]
$4p_{3/2}$	$4d_{3/2}$	2936	2.487[7]	3.214[−2]
$4p_{1/2}$	$5d_{3/2}$	2441	3.704[7]	6.616[−2]
$4p_{3/2}$	$5d_{3/2}$	2490	7.365[6]	6.848[−3]
$6p_{1/2}$	$7s_{1/2}$	3808	6.078[7]	1.321[−1]
$6p_{3/2}$	$7s_{1/2}$	5409	7.375[7]	1.618[−1]
$6p_{1/2}$	$8s_{1/2}$	2596	1.634[7]	1.651[−2]
$6p_{3/2}$	$8s_{1/2}$	3253	1.762[7]	1.397[−2]
$6p_{1/2}$	$6d_{3/2}$	2786	1.320[8]	3.072[−1]
$6p_{3/2}$	$6d_{3/2}$	3557	2.268[7]	4.301[−2]
$6p_{1/2}$	$7d_{3/2}$	2389	4.740[7]	8.115[−2]
$6p_{3/2}$	$7d_{3/2}$	2935	7.481[6]	9.659[−3]

lator strengths agree with experimental results within the corresponding uncertainties in many cases. The $8s - 8p_j$ and $9s - 9p_j$ transitions have the largest oscillator strengths; however, the $6p_j - 6d_{j'}$ transitions have the largest transition rates.

4. Conclusion

In summary, a systematic relativistic MBPT study of the energies of ns^2np_j, $ns^2(n+1)s_{1/2}$, $ns^2(n+2)s_{1/2}$, $ns^2(n+3)s_{1/2}$, $ns^2(n)d_{1/2}$, $ns^2(n+1)d_{3/2}$, $ns^2(n+2)d_{3/2}$ states in B I ($n = 2$), Al I ($n = 3$), Ga I ($n = 4$), In I ($n = 5$), and Tl I ($n = 6$) is presented. The energy calculations are in good agreement with existing experimental energy data and provide a theoretical reference database for the line identification. A systematic relativistic MBPT study of reduced matrix elements, oscillator strengths, and transition rates for electric-dipole transitions is conducted. Both length and velocity forms of matrix elements are evaluated. Small differences between length and velocity-form calculations, caused by the nonlocality of the DHF potential, are found in second order. However, including third-order corrections with full RPA leads to complete agreement between the length- and velocity-form results.

The most interesting part of this work is that we treat three-electron system as one-electron system. We found excellent agreement with NIST data for more then 10 states of five atoms with different numbers of electron from 5 up to 81.

We believe that our energies and transition rates will be useful in analyzing existing experimental data and in planning new experiments.

Acknowledgements

This work was supported by DOE/NNSA under UNR grant DE-FC52-01NV14050.

References

[1] S.A. Blundell *et al.*, Phys. Rev. A , **40**, 2233 (1989).

[2] S.A. Blundell *et al.*, Phys. Rev. A , **43**, 3407 (1991).

[3] M.S. Safronova *et al.*, Phys. Rev. A, **58**, 1016 (1998).

[4] M.S. Safronova *et al.*, Phys. Rev. A, **60**, 4476 (1999).

[5] U.I. Safronova and W. R. Johnson, Phys. Rev. A, **69**, 052511 (2004).

[6] S.A. Blundell *et al.*, Phys. Rev. A , **42**, 3751 (1990).

[7] Z.W. Liu and H. P. Kelly, Phys. Rev. A, **45**, R4210 (1992).

[8] W.R. Johnson *et al.*, Phys. Scr., **56**, 252 (1997).

[9] V.A. Dzuba *et al.*, Phys. Rev. A, **54**, 3948, (1996).

[10] M.G. Kozlov *et al.*, Phys. Rev. A, **64**, 052107 (2001).

[11] C.E. Moore, *Atomic Energy Levels - v. III*, NSRDS-NBS 35 (Washington DC, U. S. Government Printing Office, 1971).