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SINGLE INNER-ELECTRON $(n-1)d^{10}ns^2 \rightarrow (n-1)d^9ns^2np$ TRANSITIONS IN ZINC $(n=4)$ AND CADMIUM $(n=5)$

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ABSTRACT

In a recent study of the first autoionizing multiplets in e/Zn and e/Cd energy-loss spectra (Predojević *et al*. 2003), the energy levels and line widths are reported. In this paper, the excitation of the same $(n-1)d^9ns^2np$ states of zinc $(n=4)$ and cadmium $(n=5)$ atoms are studied using multiconfiguration Dirac-Fock approximation, without taking connection of discrete states with continuum into account. The energies of 12 relativistic components and optical oscillator strengths for transitions to the states with $J=1$, for both atomic systems are calculated. Influence of various numbers of configurations, which were taken into account, is considered. Calculated quantities and assignments according to LS coupling scheme are compared with experimental results mentioned above.

Keywords: Autoionising states, Configuration interaction, Multiconfiguration Dirack-Fock approximation

Introduction

The subjects of this paper are autoionising states occuring due to electron transition from inner *(n*-1*)d* shell to outer *ns* shell in Zn and Cd atoms, with energies falling between their ionisation thresholds. The number of these states is the number of possible *J* values, that are obtained applying the rule of coupling of momenta, what is 12 for given configuration. These states were observed in electron-impact ionisation of outer s-shell as resonant lines in ionisation cross section [1-3], and those that are 'optically allowed' (i.e. 3 states with $J=1$), were also observed in photoabsorption spectra measurements [4].

The calculation of the autoionising states energies has been accomplished using single configuration Hartree-Fock [5,6] or multiconfiguration Hartree-Fock approximations [7,8]. In both types of calculation, fitting *ab initio* computed average energy of configuration along with scaling *ab initio* obtained Slater-Condon (reducing up to 25%) and spin-orbit (increasing up to 33%) parameters, were performed in order to achieve reasonable agreement with observed positions of autoionising levels. Moreover, in these papers relativistic effects were taken into account only through spin-orbit interaction, although they could have more important influence, especially in Cd atom with Z=48.

In this paper, relativistic treatment of denoted states has been carried out together with configuration mixing effect on their energy values. Computation has been realised using MCDF program package [9] without additional fitting and scaling. Attaineded results are compared with observed ones in order to check validity of applied method of calculation. Although relativistic treatment implies jj coupling, more common LS coupling scheme is used throughout the paper.

Calculations

The energies of autoionising states under consideration were obtained in relativistic multiconfiguration Dirac-Fock approximation by appropriate program package [9]. Before starting computations, check of importance of different configurations were made, and only those configurations that give states with energies close to energies of states of interest, were retained. This check was fulfilled using single configuration Dirac-Fock approximation and some results of this pre-calculation for Cd atom is presented below.

Configuration	Energy range [eV]
$4d^{10}5s5p$	2.534 – 5.294
$4d^{10}5s6p$	5.962 – 6.218
$4d^{10}5p^2$	8.358 – 10.910
$4d^{10}5p6p$	11.896 – 12.489
$4d^{9}5p^3$	22.784 – 26.764

Reported energy values referred to the ground state of Cd. In this way, it is found that the next configurations have to be included in multiconfiguration computation:

a) for Zn atom: $3d^{10}4s^2 + 3d^9 4s^2 4p + 3d^{10}4s4p + 3d^{10}4p5s$

b) for Cd atom: $4d^{10}5s^2 + 4d^9 5s^2 5p + 4d^{10}5p6p + 4d^{10}5p^2$

It is important to mention here that listed configuration are written in nonrelativistic form and that they actually denote 12 relativistic configurations. For example, $4d^{10}5p^2$ is shorter way to write following relativistic configurations: $4d^4_{3/2}4d^6_{5/2}5p_{1/2}5p_{3/2}$, $4d^4_{3/2}4d^6_{5/2}5p^2_{1/2}$ and $4d^4_{3/2}4d^6_{5/2}5p^2_{3/2}$.

Results and discussion

After marking out relevant configurations for both atomic systems, calculations were performed in 'frozen core' approximation and results are tabulated in Table 1, 2 along with observed energies. Squared parenthesis next the values in second column of both tables indicate references, where they are taken from. Reported energies referred to the ground state energy of corresponding atom. Assignment includes only LS terms whose contribution to given state is greater than 0.1%. All terms belong to $(n-1)d^9ns^2np$ configuration, unless it is otherwise indicated in parenthesis by the term symbol. Effect of configuration interaction on positions of autoionising levels and optical oscillator strengths (labelled by f) for transitions from ground $^1S_0$ state is demonstrated for $J=1$ levels in Cd (Table 3).

As it can be seen from Table 1and 2, discrepancy between computed and observed results is greater for Zn atom, than in Cd atom: in the worst case it goes up to 4.1% for Zn, and up to 1.2% for Cd atom. Better agreement was achieved for lower levels in Zn, and for higher levels in Cd. Assignment, given here, distinguishes from that given in [7,8]; difference is particularly noticeable for cadmium. Reason for this disagreement is different set of configurations, included in calculation here and in references [7,8]. Configuration interaction is important (Table 3), because it vary significantly state energies and optical oscillator strengths. Mixing of configurations is particularly of great importance in zinc, where it interchanges

the order of first four levels from $J = 2, 1, 4, 3$ for single configuration approximation to $J = 2, 3, 4, 1$ in multiconfiguration calculation.

Table 1. *Comparison of observed (E_{exp}) and calculated (E_{calc}) $4d^9 5s^2 5p$ levels for Zn.*

J	E_{exp}[eV]	E_{calc}[eV]	Assignment
2	10.973 [1]	11.136	97% ^{3}P + 3% ^{3}D
3		11.381	64% ^{3}F + 33% ^{1}F + 3% ^{3}D
4		11.385	100% ^{3}F
1	11.192 [4]	11.409	92% ^{3}P + 4% ^{1}P + 3% ^{3}D
0	11.378 [1]	11.601	99.5% ^{3}P
2		11.635	68% ^{3}F + 15% ^{3}D + 15% ^{1}D + 1% ^{3}P
3	11.538 [1]	11.745	64% ^{3}D + 30% ^{1}F + 5% ^{3}F
2	11.618 [1]	11.846	49% ^{1}D + 30% ^{3}F + 21% ^{3}D
3	11.668 [1]	11.956	36% ^{1}F + 33% ^{3}D + 31% ^{3}F
1	11.804 [4]	12.138	73% ^{3}D + 20% ^{1}P + 6% ^{3}P + 0.5% ^{1}P[$4s4p$]
2		12.180	61% ^{3}D + 36% ^{1}D + 2% ^{3}P + 1% ^{3}F
1	11.876 [4]	12.353	73% ^{1}P + 24% ^{3}D + 1% ^{3}P + 2% ^{1}P [$4s4p$]

Table 2. *Comparison of experimental and calculated $4d^9 5s^2 5p$ levels for Cd.*

J	E_{exp}[eV]	E_{calc}[eV]	Assignment
2	11.605 [3]	11.421	93% ^{3}P + 7% ^{3}D
3	11.805 [3]	11.688	58% ^{3}F + 36% ^{1}F + 6% ^{3}D
4	11.943 [2]	11.834	100% ^{3}F
1	12.062 [3]	11.904	84% ^{3}P + 10% ^{1}P + 6% ^{3}D
2	12.174 [2]	12.123	39% ^{3}F + 32% ^{1}D + 26% ^{3}D + 4% ^{3}P
3	12.313 [2]	12.252	78% ^{3}D + 21% ^{1}F + 1% ^{3}F
0	12.443 [2]	12.324	99.8% ^{3}D + 0.2% ^{3}P [$5p6p$]
2	12.563 [2]	12.433	58% ^{3}F + 36% ^{1}D + 6% ^{3}D
3	12.703 [2]	12.721	42% ^{1}F + 41% ^{3}F + 13% ^{3}D
1	11.810 [3]	12.787	68% ^{1}P + 16% ^{3}D + 15% ^{3}P + 1% ^{1}P[$5p6p$]
1	12.938 [4]	12.918	77.8% ^{3}D + 21% ^{1}P + 0.7% ^{3}P + 0.4% ^{1}P [$5p6p$]
2	12.932 [3]	12.986	61% ^{3}D + 32% ^{1}D + 3% ^{3}F + 3% ^{3}P

Conclusion

Considered autoionising states were treated here as pure discrete states neglecting their interaction with continuum of *ns* shell. It is concluded that mixing configuration is of remarkable importance, so these kinds of calculations always have to be carried out beyond single configuration approximation. Reason for existing discrepancy between observed and computed results, except omitting interaction with continuum, could be applied coupling scheme. Both atoms are placed in the middle of Periodic table (Z=30 for Zn and Z=48 for Cd), so it cannot be claimed certainly that one of LS or jj coupling, that was used here, is dominated, and similar calculation should be performed using come other coupling scheme.

Table 3. *Configuration mixing effect on autoionising levels with $J = 1$ and oscillator strength in Cd. Subscript* a *denotes calculation performed with one configuration included $(4d^9 5s^2 5p)$; subscript* b *stands for two mixing configuration computation $(4d^9 5s^2 5p + 4d^{10} 5p^2)$; no subscripts indicate computation carried out in full configuration mixing $(4d^9 5s^2 5p + 4d^{10} 5p^2 + 4d^9 5p6p)$.*

Level	E_a [eV]	f_a	E_b [eV]	f_b	E [eV]	f

$^3P_1$	13.041	0.019	11.648	0.021	11.904	0.029
$^1P_1$	14.105	0.177	12.635	0.188	12.787	0.208
$^3D_1$	14.162	0.089	12.714	0.055	12.914	0.072

References

[1] C.G. Back, M.D.White, V. Pejčev and K.J. Ross, J. Phys. B **14**, 1981, p. 1497
[2] V. Pejčev, K.J. Ross, D. Rassy and T.W. Ottley, J. Phys. B **10**, 1977, p. 459
[3] B. Predojević, D. Šević, V. Pejčev, B.P. Marinković and D.M. Filipović, J. Phys. B, 2003, to be published
[4] G.W. Marr and J.M. Austin, Proc. Roy. Soc. A **310**, 1969, p. 137
[5] M. Wilson, J. Phys. B **1**, 1968, p. 736
[6] N.L.S. Martin, J. Phys. B **17**, 1984, p. 1797
[7] M.W.D. Mansfield, J. Phys. B **14**, 1981, p. 2781
[8] M.W.D. Mansfield and M.M.Murnane, J. Phys. B **18**, 1985, p. 4223
[9] I.P. Grant, B.J. McKenzie, P.H. Norrington, D.F. Mayers and N.C. Pyper, CPC **21**, 1980, p. 207

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