Hindawi Publishing Corporation
Journal of Spectroscopy
Volume 2013, Article ID 820635, 6 pages
http://dx.doi.org/10.1155/2013/820635

Research Article

Complements to the Theoretical Treatments of the Electron Collision with Co^{3+}: An *R*-Matrix Approach

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Received 29 June 2012; Accepted 13 August 2012

Academic Editor: D. Sajan

This paper presents new refined results from the theoretical treatment of electron collision with the Fe-peak element Co^{3+}. We have investigated the relevance of relativistic effects on the accurate representation of the target electron wave functions within the *Breit-Pauli R*-matrix approach. The calculated values for fine-structure levels are compared with the available experimental data in Atomic Structure Database of the National Institute for Standards and Technology. The agreement between the calculated and the experimental data is reasonably good, the energy difference average percentage of the low-lying levels usually agreeing to within 3.6% of each other. For completeness, we summarize herein the existing theoretical *R*-matrix treatments intended specifically to explore the role of including configuration interaction wave functions both in the target-state expansion, and in the $(N+1)$-electron quadratically integrable function expansion. To the best of our knowledge, the work reported herein describes for the first time a detailed calculation for this atomic system, and the results are relevant to the laboratory and astrophysical plasmas.

1. Introduction

The present work aims to provide atomic data and electron collision data for the Fe-peak element Co IV and to supply with additional information the studies on astrophysical opacities. The electron collision data for Fe, Ni, and Co elements, and their ions are important in line identification in stellar objects or in tokamak plasmas, since the collisional rate of deexcitation for metastable levels may be lower than the decay rate by magnetic dipole or electric quadrupole transitions, which become observable. Due to a lack of precise abundance values these data are of importance in the analysis of many astronomical spectra. The needed atomic data can be obtained in various approximations that differ in their demands on resources by several orders of magnitude. Ranges of validity of expansions and applicability of perturbation treatments must be established in order to obtain reliable data with the most economical methods. The *R*-matrix approach has enabled vast amounts of accurate electron and photon collision data which have had wide applications. The recent volume by Burke [1] provides both a general review of the *R*-matrix method as applied to atomic and molecular collision processes and a very extensive bibliography. The *R*-matrix treatments [2–9] have provided results for electron collision with most of the ions of Fe, Ni and Co such as: Fe I, Fe II, Fe III, Fe IV, Fe V, Fe VI, Fe VII, Co V, Co VI, Co II, Ni II, Ni III, Ni V, Ni VI, and Ni VII. Apart from our recent work [10], there is no other *R*-matrix calculation on Co IV ion. In the absence of experimental data on the electron-impact excitation cross-sections for Co IV, the need for accurate collision data can be accomplished only through detailed and accurate target description and atomic level energy data calculation. The calculation reported here is part of a general investigation which started with studies of collision strengths for the electron-impact excitation of forbidden transitions between 136 terms arising from $3d^6$, $3d^5 4s$, and $3d^5 4p$ configurations of Co^{3+} [10]. In particular, for Co IV ion, $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6\ ^5\mathrm{D}$ ground configuration, the energies of the $3d^5 4p$ terms are lying between $3d^6$ and $3d^5 4s$ states but overlapping both. Therefore, in our earlier work, the accuracy of a series of models for the target terms was considered which forms the basis of the *R*-matrix collision calculations. It was found that

one could obtain a better representation for the 136 Co IV levels arising from the $3d^6$, $3d^5 4s$, and $3d^5 4p$ manifolds by allowing double-electron promotions from the $3p$-shell into the $3d$-shell and single-electron promotion into the $4s$ and $4p$-shell. In order to explore the effect of including of additional states, we have performed additional collision calculation including a further 136 states which arise from the inclusion of the fourth $3d^5 4d$ configuration in the $\boldsymbol{R}$-matrix expansion. Section 2 gives a summary of our previously reported results. At this level of accuracy, the key conclusion is that the interaction between the lowest even configurations and the perturbation on odd parity configurations play an important role in such calculations. Therefore, we have decided to study the relativistic effects on the accurate representation of target electron wave-functions. Section 3 gives the results from semirelativistic *Breit-Pauli* R-matrix computation of the fine-structure splitting in Co^{3+}. The calculated theoretical data are compared with the available experimental data in Atomic Structure Database (ASD) of the National Institute for Standards and Technology [11]. The ASD data is based on the compilation of Co ions by Sugar and Corliss [12]. In their work, all energy levels are given in units of cm^{-1}, beginning with a value of zero for the ground levels. Although uncertainties are not provided with these extrapolated values, the levels uncertainty is presumed $\pm 0.5\ cm^{-1}$. Section 4 gives our concluding remarks and the future directions of research.

2. The Electron Collision with Co^{3+}: An R-Matrix Approach

In our earlier work [10] we have initiated a study of electron-impact excitation of Co^{3+}, $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6\ (^5D^e)$ ground configuration, considering the forbidden transitions which arise between the 136 terms of the $3d^6$, $3d^5 4s$ and $3d^5 4p$ configurations. The following excitation ways have been considered:

$$\begin{aligned} e^- + Co^{3+}\left(3p^6 3d^6\,{}^5D\right) \longrightarrow Co^{2+*} &\downarrow \left(3p^5 3d^8, 3p^5 3d^7 4s \text{ or } 3p^5 3d^7 4p\right) \\ Co^{3+} &\left(3p^6 3d^6, 3p^6 3d^5 4s \text{ or } 3p^6 3d^5 4p\right) + e^- \end{aligned} \tag{1}$$

In the first stage of the calculation, we used CIV3 program [13] to obtain accurate target state energies and wave functions which are used in the following stages of the R-matrix calculations. The target wave functions and the $(N + 1)$-electron quadratically integrable functions were constructed with a common set of one-electron spin-orbital functions. In the second stage of calculation we used RMATRXI program by Berrington et al. [14] to solve the electron-atom collision problem in the R-matrix internal region. In the asymptotic region, the radius is propagated to a new distance, chosen large enough that the radial functions which represent the colliding electron can be accurately represented by an asymptotic expansion. In the third stage of calculation we used FARM [15] to solve the electron-atom collision problem in the R-matrix external and asymptotic regions. These programs enable the K-matrix, S-matrix, and hence collision strengths to be determined. The K-matrix elements and the S-matrix elements, and therefore, the collision strengths Ω_{ij} can be calculated by matching the solution of the inner and outer regions at the R-matrix boundary radius $r = a$. For completeness, the expression for the electron scattering cross section is given herein. The expressions for the S-matrix and T-matrix as related to the K-matrix are

$$S = (1 + iK)(1 - iK)^{-1}, \qquad T = S - 1, \tag{2}$$

where these matrices have particular total J and π values. The partial collision strength which contributes to the cross-section for a transition of the target from state r to a state s is a summation over the channels $\alpha_r J_r^t j_r$ to $\alpha_s J_s^t j_s$ that are coupled to them. α represents all the other quantum numbers that uniquely identify a target state. The total collision strength is a sum of the partial collision strengths for each symmetry as follows:

$$\Omega_{rs}^{J\pi} = \frac{g}{2} \sum_{j_r j_s} |T_{rs}|^2, \qquad \Omega_{rs} = \sum_{J\pi} \Omega_{rs}^{J\pi}, \tag{3}$$

where $g = 2J + 1$ for jj coupling, and Ω_{rs} should be symmetric. Then, the total cross section for this transition is given by

$$\sigma_{r \to s} = \frac{\pi a_0^2}{k_r^2 g_r} \Omega_{rs}, \tag{4}$$

where $g_r = 2J_r^t + 1$ and a_0 is the Bohr radius to convert from atomic units.

In our preliminary work, three target-model calculations have been developed: (a) a *three-LS-coupled* R-matrix calculation including $3d^6$, $3d^5 4s$, and $3d^5 4p$ states in the N-electron-wave function expansion; (b) *a six-target*-model calculation, where electron correlation effects were explored by carrying out separate calculations with six configurations $3d^6$, $3d^5 4s$, $3d^5 4p$, $3p^4 3d^8$, $3p^4 3d^7 4s$, and $3p^4 3d^7 4p$ in the target state expansion and the configurations $3d^7$, $3d^6 4s$, $3d^6 4p$, $3d^5 4s^2$, $3d^5 4s4p$, $3d^5 4p^2$, $3p^5 3d^8$, $3p^4 3d^9$, $3p^5 3d^8$, $3p^4 3d^9$, $3p^4 3d^8 4s$, and $3p^6 3d^5 4s^2$ in the $(N + 1)$-electron quadratically integrable function expansion; and (c) *a nine-target*-model calculation. Starting with the 136-level model, we have included in the R-matrix expansion all 184 LS-coupled states which arise from nine-target configurations $3d^6$, $3d^5 4s$, $3d^5 4p$, $3p^4 3d^8$, $3p^4 3d^7 4s$, $3p^4 3d^7 4p$, $3p^5 3d^7$, $3p^5 3d^6 4s$, and $3p^5 3d^6 4p$. The 136 LS target states arising

from the *three*, *six*, and *nine* basis configurations above, were optimally represented by configuration interaction type expansions in terms of eight orthogonal basis orbitals. Figure 1 shows the graphical abstraction of the *R*-matrix H-file as output from HBrowse, a Graphical *R*-matrix Atomic Collision environment, GRACE, tool [16]. This H-file was used to convey information from the inner-region to the outer-region in the six-target model calculation. In order to have a consistent set of wave functions for the N- and $(N+1)$-electron wave functions, the $(N+1)$-electron configuration data have been obtained by adding one electron to the N electron configurations in all possible ways. Hence, we can include these $(N+1)$-electron configurations in the collision wave function by including the configuration interaction wave functions with configuration $3p^5 3d^7$ in the basis set used in the CI expansion of the N-electron target states.

For collision calculations, a number of systematic checks on Co^{3+} have been performed. We have investigated the position of $3d^5 4d$ and $3d^4 4s^2$ terms including the configurations $3d^5 4s^2$, $3d^5 4p^2$, $3d^5 4d^2$, $3d^5 4s4p$, and $3d^5 4p4d$ in the $(N+1)$-electron quadratically integrable function expansion. The $3d^5 4d$ terms are lying between $3d^5 4p$ and $3d^4 4s^2$ states but overlapping both. We have carried out a first calculation in which 272 *LS terms* of the four configurations $3d^6$, $3d^5 4s$, $3d^5 4p$, and $3d^5 4d$ with a maximum 841 channels which includes the $3p^6 3d^5 4d$ configuration, are included in the *R*-matrix expansion. Figure 2 presents a comparison between the collision strengths as outputs from two different calculations where 136 terms arising from the $3d^6$, $3d^5 4s$, and $3d^5 4p$ manifolds [10], and 272 terms arising from $3d^6$, $3d^5 4s$, $3d^5 4p$, and $3d^5 4d$ manifolds are included into the *R*-matrix expansion, respectively. The inclusion of additional states affects the resonance structure in the collision strengths. The collision-strength results correspond to the transition from the ground state $3d^6(^5\mathrm{D}^e)$ to the first excited state $3d^6(^3\mathrm{P}^e)$, $^4\mathrm{F}^e$ symmetry. As shown in Figure 2, the resonance positions are pushed to lower scattered electron energies.

3. Semirelativistic *Breit-Pauli R*-Matrix Calculation of the Fine-Structure Splitting

The *R*-matrix theory commences by partitioning configuration space into three regions describing the scattering of an electron by an N-electron atom or ion: an internal region, an external region, and an asymptotic region. The solutions obtained in each of these regions are related by the *R*-matrix which corresponds to the inverse of the logarithmic derivative of the wavefunction on the boundary of the two regions. One important point to note is that, in the *R*-matrix method, the inner region solution is obtained only once, and then cross-sections for any number of energy points are readily available. In the asymptotic region, the radius is propagated to a new distance, chosen large enough that the radial functions which represent the colliding electron can be accurately represented by an asymptotic expansion. The RMATXI package of codes [14] includes relativistic effects in the *Breit-Pauli* approximation (BPRM) [17, 18]. The Hamiltonian is written as follows:

$$H_{N+1}^{\mathrm{BP}} = H_{N+1}^{\mathrm{NR}} + H_{N+1}^{\mathrm{mass}} + H_{N+1}^{\mathrm{DAR}} + H_{N+1}^{\mathrm{so}}, \quad (5)$$

where H_{N+1}^{NR} is the nonrelativistic Hamiltonian, H_{N+1}^{mass} is the one-body mass-velocity term, H_{N+1}^{DAR} is the Darwin term, and H_{N+1}^{so} is the spin-orbit term. This last term breaks *LS* symmetry leading to fine-structure levels $J\pi$ of total angular momentum quantum number J at parity π. In relativistic BPRM calculations, sets of collisional symmetry $SL\pi$ are recoupled to obtain the states of the $(N+1)$ atomic system with total $J\pi$, followed by diagonalization of the $(N+1)$-electron Hamiltonian. Details of diagonalizing H_{N+1}^{BP} at the *R*-matrix boundary are given in [17], as is the outward propagation. In our BPRM calculations, we have constructed an eigenfunction expansion over the three configurations $3d^6$, $3d^5 4s$, and $3d^5 4p$ of Co^{3+}, yielding 136 fine-structure levels corresponding to 43 *LS* terms. Eight orthogonal one-electron orbitals $1s$, $2s$, $2p$, $3s$, $3p$, $3d$, $4s$, and $4p$ were used both in the definition of the target states and also for the $(N+1)$-electron quadratically integrable functions. In all of the models, the $1s$, $2s$, $2p$, $3s$, $3p$, and $3d$ radial functions have been taken from the Hartree-Fock ground state $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6\ ^5\mathrm{D}$, given in the tables of Clementi and Roetti [19]. Using the nonrelativistic Schrödinger Hamiltonian, we have established the wave functions by optimizing further three orbitals on various $L = 2$, 3, and 4 states. Full details of the three-target model calculation have been reported in our previous work [10]. The one- and two-electron radial integrals are computed by STG1 of the BPRM codes using one-electron target orbitals. The calculation considers all possible bound levels for $0 \le J \le 8$ with $0 \le L \le 7$, and $(2S+1) = 1, 3, 5, 7$ even and odd parities. The intermediate coupling calculations are carried out on recoupling the *LS* symmetries in a pair-coupling representation in stage RECUPD. The (electron + core) Hamiltonian matrix is diagonalized for each resulting $J\pi$ in STGH. The number of coupled channels was 1024 and the Hamiltonian matrix size was 20502. Table 1 gives results for the 47 lowest even parity energy levels and the comparison with ASD data. Agreement between theory and experiments is reasonably good, the energy difference average percentage of the low-lying levels usually agreeing to within 3.6% of each other.

4. Conclusions

We have carried out the first detailed calculation on the electron scattering with Fe-peak element Co IV where 272 LS terms arising from configurations $3d^6$, $3d^5 4s$, $3d^5 4p$, and $3d^5 4d$ have been included in the *R*-matrix expansion. Given detailed calculation provided here and comparison with our earlier work [10], we estimate that the accuracy of our data is within 20% for transitions within the $3d^6$ manifold. Due to the lack of experimental data for electron-impact excitation on this complex ion, there is no way to fully assess the accuracy of our earlier and present calculations. We expect that these data on Co IV and that from our previous

Table 1: Comparison between the calculated theoretical levels energy and the experimental data from ASD, in Rydberg units.

Index	Configuration	$^{2S+1}L_J$	ASD (Ryd)	BPRM (Ryd) this work	Diff.
1	$3d^6$	(^{5}D$_4$)	0.000 000	0.000 000	0.000
2		(^{5}D$_3$)	0.005 824	0.006 295	−0.000 471
3		(^{5}D$_2$)	0.009 8207	0.010 694	−0.000 874
4		(^{5}D$_1$)	0.012 369	0.013 519	−0.001 151
5		(^{5}D$_0$)	0.013 611	0.014 904	−0.001 293
6	$3d^6$	(^{3}P$_2$)	0.208 528	0.262 571	−0.054 043
7		(^{3}P$_1$)	0.225 349	0.281 125	−0.055 776
8		(^{3}P$_0$)	0.231 906	0.288 584	−0.056 678
9	$3d^6$	(^{3}H$_6$)	0.215 783	0.240 697	−0.024 915
10		(^{3}H$_5$)	0.218 994	0.243 895	−0.024 901
11		(^{3}H$_4$)	0.221 183	0.246 191	−0.025 008
12	$3d^6$	(^{3}F$_4$)	0.231 425	0.275 361	−0.043 937
13		(^{3}F$_3$)	0.234 523	0.278 996	−0.044 473
14		(^{3}F$_2$)	0.236 647	0.281 725	−0.045 08
15	$3d^6$	(^{3}G$_5$)	0.264 466	0.304 026	−0.039 56
16		(^{3}G$_4$)	0.269 664	0.310 104	−0.040 441
17		(^{3}G$_3$)	0.272 173	0.312 593	−0.040 421
18	$3d^6$	(^{1}I$_6$)	0.327 534	0.363 430	−0.035 896
19	$3d^6$	(^{3}D$_2$)	0.331 227	0.393 652	−0.062 425
20		(^{3}D$_3$)	0.333 109	0.395 464	−0.062 355
21	$3d^6$	(^{1}G$_4$)	0.334 283	0.384 288	−0.050 005
22	$3d^6$	(^{1}S$_0$)	0.377 646	0.446 562	−0.068 917
23	$3d^6$	(^{1}D$_2$)	0.385 847	0.477 492	−0.091 645
24	$3d^6$	(^{1}F$_3$)	0.461 375	0.550 697	−0.089 322
25	$3d^6$	(^{3}P$_2$)	0.547 657	0.664 605	−0.116 948
26	$3d^6$	(^{3}F$_2$)	0.544 471	0.650 163	−0.105 692
27		(^{3}F$_4$)	0.545 286	0.650 668	−0.105 382
28		(^{3}F$_3$)	0.545 874	0.651 393	−0.105 519
29	$3d^6$	(^{1}G$_4$)	0.618 814	0.735 491	−0.116 677
30	$3d^5 4s$	(^{7}S$_3$)	0.825 192	0.897 493	−0.072 302
31	$3d^6$	(^{1}D$_2$)	0.831 243	1.282 181	−0.450 937
32	$3d^5 4s$	(^{5}S$_2$)	0.936 5447	1.049 445	−0.112 900
33	$3d^5 4s$	(^{5}G$_6$)	1.176 756	1.282 621	−0.105 864
34		(^{5}G$_5$)	1.177 313	1.282 732	−0.105 419
35		(^{5}G$_2$)	1.177 559	0.992 645	0.184 914
36		(^{5}G$_4$)	1.177 573	1.282 640	−0.105 067
37		(^{5}G$_3$)	1.177 619	1.282 411	−0.104 791
38	$3d^5 4s$	(^{5}D$_4$)	1.242 630	1.383 941	−0.141 310
39	$3d^5 4s$	(^{3}G$_5$)	1.250 996	1.383 927	−0.132 931
40		(^{3}G$_3$)	1.251 403	1.372 491	−0.121 087
41		(^{3}G$_4$)	1.251 501	1.370 295	−0.118 794
42	$3d^5 4s$	(^{3}I$_6$)	1.349 569	1.460 891	−0.111 321
43		(^{3}I$_5$)	1.349 637	1.460 601	−0.110 963
44		(^{3}I$_7$)	1.349 641	1.461 431	−0.111 789
45	$3d^5 4s$	(^{1}H$_4$)	1.443 082	1.526 961	−0.083 878
46		(^{1}H$_5$)	1.443 660	1.526 581	−0.082 920
47		(^{1}H$_6$)	1.447 518	1.511 332	−0.063 812

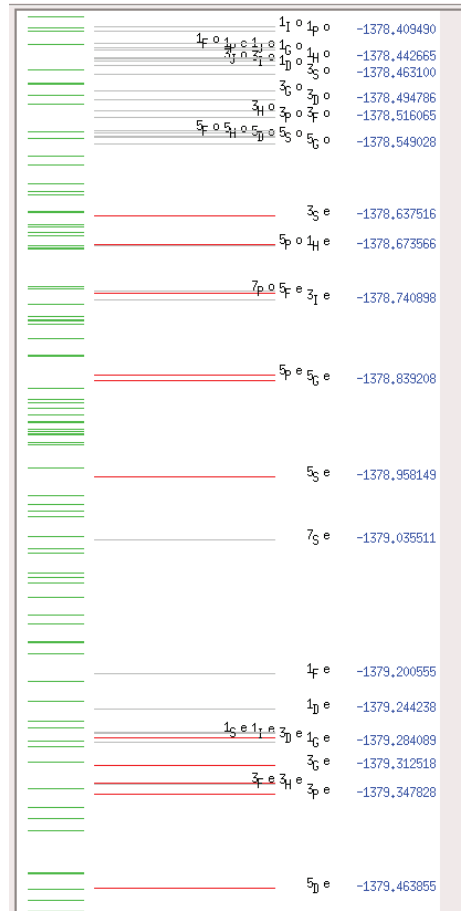

Figure 1: The graphical abstraction of the *R*-matrix H-file as given from HBrowse code, a Graphical *R*-matrix Atomic Collision environment: six *LS*-coupled states are included into the *R*-matrix expansion: $3p^6 3d^6$, $3p^6 3d^5 4s$, $3p^6 3d^5 4p$, $3p^4 3d^8$, $3p^4 3d^7 4s$, and $3p^4 3d^7 4p$, total angular quantum number $0 < L < 9$, $2 < (2S + 1) < 8$, maximum number of channels 18, *R*-matrix radius 15 a.u, Hamiltonian size 290, and scattering symmetry $^4F^e$.

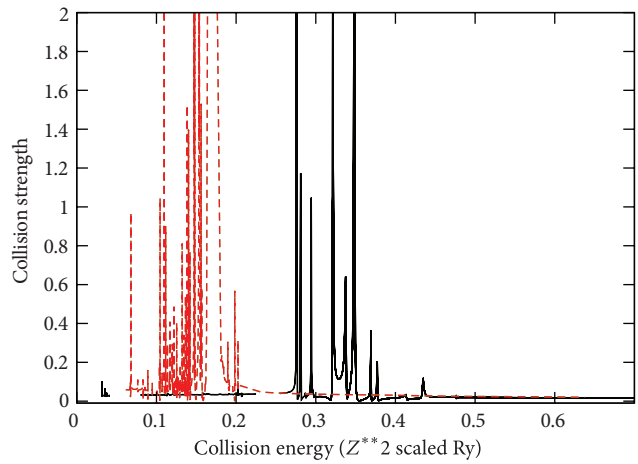

Figure 2: Collision strengths for the $^5D^e$-$^3P^e$ transition of Co^{3+}. The full curve corresponds to the calculation where 136 states arising from the $3d^6$, $3d^5 4s$, and $3d^5 4p$ manifolds are included into the scattering process. The broken curve corresponds to the calculation where 272 states arising from $3d^6$, $3d^5 4s$, $3d^5 4p$, and $3d^6 4d$ configurations are included into the scattering process. Scaled units are used for the collision energy: for positively charged ions energies are scaled by a factor $1/Z^2$, with $Z = 3$ for Co^{3+} ion.

study [10] on this system will be of fundamental value in gauging the accuracy of future calculations for electron impact excitation on this Fe-peak element.

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