Calculations of Oscillator Strengths for Singly Ionized Iron Group Elements by Means of the Orthogonal Operator Approach

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1   Introduction

The relatively high abundances of iron group elements in stellar objects stimulates interest in these elements. The need for accurate laboratory data is further increased due to the launch of high dispersive space laboratories such as the Goddard High Resolution Spectrograph on board the Hubble Space Telescope [1].

Being an odd-Z number element cobalt is far less abundant than the even-Z iron group elements, Cr, Fe and Ni. However, Co II lines appear up to OB-type stars and are observed in absorption in the interstellar medium (ISM). This requires accurate transition probabilities (oscillator strengths) for transitions from the low lying levels in the $(3d^8 + 3d^7 4s)$ system, which is responsible for the absorption lines.

State of the art experimental values from radiative lifetimes and branching fractions are accurate, but restricted to a limited number of transitions [2].

Advanced computer codes exist to calculate energy level values and wave functions *ab initio*. These codes allow the introduction of very many interacting configurations. Ab-initio calculations are powerful in relatively simple systems with one term outside the closed shell only. In that case the system is dominated by electrostatic interactions, mixing levels of different configurations having the same term names.

In iron group and other transition group elements, in which we deal with several d-electrons the systems show many terms of different multiplicity and total angular orbital moment (L) within a relatively small energy range. Including more and more correlation is not the point in calculations of transition elements. These systems are dominated by magnetic interactions, of which the Spin-Orbit interaction is strongest. These magnetic interactions are responsible for the mixing of levels with the same total angular momentum J, but with different multiplicity (2S+1) or different orbital angular momentum (L). This effect strongly affects transition probabilities or oscillator strengths and is responsible for the appearance of intercombination lines. Therefore, for the iron group elements, it is far more important to describe well the magnetic mixing that appears from the spacing between levels of the same J-value and the non-diagonal magnetic matrix element between them, than to include more configurations.

The orthogonal operator approach, developed over the last years [3], provides the possibility to describe spacings between levels far more accurate by than other computational methods. The orthogonal operator approach is a semi-empirical method, in which the eigenvalues of the Hamiltonian are fitted to experimental energy values by adjusting the electrostatic and magnetic interactions of the Hamiltonian. The method is basically founded on the Slater-Condon Theory. However, their interactions, as used by the Cowan method, are orthogonalized in our method. This stabilizes the

fitting, makes the operators as independent as possible and offers the possibility of adding higher order electrostatic and magnetic effects; thus far, these interactions had to be left out as they corrupted the least squares fitting procedure. The extension of the Hamiltonian results in a far smaller average deviation. This implies a better description of the level structure, i.e. the spacings between the levels, resulting in optimal eigenvector compositions. These intermediate eigenvectors are used to sandwich the pure LS-transition probabilities. Afterwards these quantities are multiplied by the electric dipole transition integrals. The latter (see Table 1) are obtained by means of the MCDF code of Parpia et al. [4] and corrected for core-polarization.

2 Results

As input for the fitting procedure, level values obtained by Pickering et al. [5] were used. The levels included covered $(3d^8 + 3d^7 4s + 3d^6 4s^2 + 3d^7 4d + 3d^7 5s + 3d^7 5d + 3d^7 6s)$ for the even system and $(3d^7 4p + 3d^6 4s4p + 3d^5 4s^2 4p + 3d^7 5p + 3d^7 4f)$ for the odd system. For studying the resonance transitions in the $(3d^8 + 3d^7 4s)$ - $3d^7 4p$ transition array only the three lowest configurations in both systems are relevant. In the even system the mean deviation, the average deviation between the calculated eigenvalues and the experimental energy values, is 39 cm^{-1}, mainly due to some larger deviations in the 4d- and 5d configuration. For most of the levels in the the lowest even configurations the deviation is only a few cm^{-1}. In the odd system the mean deviation is 19 cm^{-1}. Using the level values and eigenvector compositions of the two lowest even and the lowest odd configuration results in a large number of oscillator strengths and wavelengths, which will be published elsewhere [6]. Here we restrict ourselves to giving the oscillator strengths for lines from the lowest even multiplets recently measured by Mullman et al. [2] and kindly provided to us by Lawler, present at the ICAMDATA conference. In Table 2 our values are given together with the experimental values of Mullman et al. and values from the Kurucz database [7]. Our results agree very well with those of Mullman et al., solving some large discrepancies between Mullman and Kurucz data. These discrepancies not only concern weak intercombination lines but also the strong resonance transitions between the lowest even term $3d^8$ ^{3}F levels and $3d^7(^4$F$)4p$ ^{3}F and ^{3}G levels (see lines at 2027.040 Åand 2025.760 Å). For sixteen of the twenty-eight lines, given by Mullman et al. [2], our values are within Mullmans error bars, and nineteen are within 10%. Only a few weaker lines with log(gf) values around -2.0 show larger deviations.

Acknowledgements

Table 1: Values for the electric dipole transition integrals in Co II calculated by means of MCDF including core polarization

	$3d^8$	$3d^7 4s$	$3d^6 4s^2$	$3d^7 4d$	$3d^7 5s$	$3d^7 5d$	$3d^7 6s$
$3d^7 4p$	.79	-2.65	-	-3.20	2.13	-0.79	0.57
$3d^6 4s4p$	-	0.65	-2.44	-	-	-	-
$3d^5 4s^2 4p$	-	-	0.55	-	-	-	-
$3d^7 5p$	0.22	0.03	-	4.88	-6.41	-6.00	4.89
$3d^7 4f$	0.19	-	-	-5.56	-	7.32	-

Table 2: Comparison between theory and experiment[a] of log(gf)-values for the $(3d^8+3d^74s) \rightarrow 3d^74p$ transitions involving the lowest even multiplets.

λ(Å)	experiment[a]	present	Kurucz[b]	J_f	E_f(cm^{-1})	even	J_i	E_i(cm^{-1})	odd
2693.091	-2.20	-2.09	-1.94	2.0	13260.69*	$1|^3_2$P)	3.0	50381.72*	$1|^4_3$F)^{3}F
2587.220	0.037	0.028	-0.49	3.0	10708.33*	$2|^4_3$F)^{3}F	4.0	49348.30*	$1|^4_3$F)^{3}G
2580.326	0.36	0.39	0.43	4.0	9812.86*	$2|^4_3$F)^{3}F	5.0	48556.05*	$1|^4_3$F)^{3}G
2564.034	0.07	0.072	0.31	3.0	10708.33*	$2|^4_3$F)^{3}F	4.0	49697.68*	$1|^4_3$F)^{3}F
2559.405	-0.21	-0.17	0.17	2.0	11321.86*	$2|^4_3$F)^{3}F	3.0	50381.72*	$1|^4_3$F)^{3}F
2546.160	-1.61	-1.64	-1.61	2.0	11651.28*	$1|^1_2$D)	2.0	50914.32*	$1|^4_3$F)^{3}F
2528.616	0.06	0.10	0.32	4.0	9812.86*	$2|^4_3$F)^{3}F	4.0	49348.30*	$1|^4_3$F)^{3}G
2524.974	-0.06	0.003	0.005	2.0	11321.86*	$2|^4_3$F)^{3}F	2.0	50914.32*	$1|^4_3$F)^{3}F
2519.823	-0.14	-0.11	-0.76	3.0	10708.33*	$2|^4_3$F)^{3}F	3.0	50381.72*	$1|^4_3$F)^{3}F
2506.464	0.05	0.062	-0.47	4.0	9812.86*	$2|^4_3$F)^{3}F	4.0	49697.68*	$1|^4_3$F)^{3}F
2486.441	-0.54	-0.51	-0.48	3.0	10708.33*	$2|^4_3$F)^{3}F	2.0	50914.32*	$1|^4_3$F)^{3}F
2464.199	-0.42	-0.39	-0.66	4.0	9812.86*	$2|^4_3$F)^{3}F	3.0	50381.72*	$1|^4_3$F)^{3}F
2245.129	-0.35	-0.29	-0.51	4.0	4028.99*	$2|^4_3$F)^{5}F	5.0	48556.05*	$1|^4_3$F)^{3}G
2232.072	-1.08	-1.06	-1.89	3.0	4560.79*	$2|^4_3$F)^{5}F	4.0	49348.30*	$1|^4_3$F)^{3}G
2214.793	-1.02	-1.03	-0.97	3.0	4560.79*	$2|^4_3$F)^{5}F	4.0	49697.68*	$1|^4_3$F)^{3}F
2211.428	-1.21	-1.22	-1.38	5.0	3350.49*	$2|^4_3$F)^{5}F	5.0	48556.05*	$1|^4_3$F)^{3}G
2200.421	-1.45	-1.45	-1.39	2.0	4950.06*	$2|^4_3$F)^{5}F	3.0	50381.72*	$1|^4_3$F)^{3}F
2188.999	-2.08	-1.96	-1.80	4.0	4028.99*	$2|^4_3$F)^{5}F	4.0	49697.68*	$1|^4_3$F)^{3}F
2187.039	-2.03	-1.91	-1.97	1.0	5204.70*	$2|^4_3$F)^{5}F	2.0	50914.32*	$1|^4_3$F)^{3}F
2173.335	-1.81	-1.98	-1.85	5.0	3350.49*	$2|^4_3$F)^{5}F	4.0	49348.30*	$1|^4_3$F)^{3}G
2156.950	-2.09	-2.08	-2.67	5.0	3350.49*	$2|^4_3$F)^{5}F	4.0	49697.68*	$1|^4_3$F)^{3}F
2065.542	-1.07	-1.11	-0.85	3.0	950.32*	$1|^3_2$F)	4.0	49348.30*	$1|^4_3$F)^{3}G
2058.817	-1.17	-1.24	-0.93	4.0	.00*	$1|^3_2$F)	5.0	48556.05*	$1|^4_3$F)^{3}G
2027.040	-0.57	-0.57	-0.29	2.0	1597.20*	$1|^3_2$F)	2.0	50914.32*	$1|^4_3$F)^{3}F
2025.760	-0.95	-0.98	-0.26	4.0	.00*	$1|^3_2$F)	4.0	49348.30*	$1|^4_3$F)^{3}G
2022.354	-0.49	-0.48	-0.44	3.0	950.32*	$1|^3_2$F)	3.0	50381.72*	$1|^4_3$F)^{3}F
2011.516	-0.48	-0.40	-0.38	4.0	.00*	$1|^3_2$F)	4.0	49697.68*	$1|^4_3$F)^{3}F
2000.793	-2.15	-1.92	-1.68	3.0	950.32*	$1|^3_2$F)	2.0	50914.32*	$1|^4_3$F)^{3}F

[a] Mullman et al. [2] [b] Kurucz [7]

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