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Energy Levels and Radiative Rates for Transitions in Fe X

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Abstract

Energy levels, radiative rates, oscillator strengths, line strengths, and life-times among 54 levels of the ($1s^22s^22p^6$) $3s^23p^5$, $3s3p^6$, $3s^23p^43d$ and $3s3p^53d$ configurations of Fe X have been calculated using the GRASP code. Comparisons are made with results available in the literature. Our energy levels are assessed to be accurate to better than 3 %, whereas results for other parameters are probably accurate to better than 20 %.

Keywords:

energy level, radiative rate, oscillator strength, line strength, life-time

1. Introduction

Iron is an abundant element, particularly in solar and fusion plasmas, and its emission lines are observed in almost all ionization stages. Emission lines of Fe X in the EUV and UV ranges have been observed in the spectra of the solar atmosphere and late-type stars, and provide useful plasma diagnostics. Therefore, in this paper we report energies for 54 levels of the ($1s^22s^22p^6$) $3s^23p^5$, $3s3p^6$, $3s^23p^43d$ and $3s3p^53d$ configurations, and radiative rates, oscillator strengths, and line strengths for electric and magnetic dipole and quadrupole transitions among these levels. Additionally, life-times of the excited levels are calculated and compared with the available measured values.

The earlier available similar results are of Bhatia & Doschek (BD: [1]), and Deb *et al.* (DGM: [2]). BD have included configuration interaction (CI) among the basic 4 configurations only, but DGM have included extensive CI, and therefore, their results should be the most accurate available to date. However, their energies for the highest 28 levels (27 – 54) are consistently lower than those of BD, and the highest 8 levels of the $3s3p^53d$ configuration differ up to 11 % (≤ 0.9 Ry) - see Table 1 of [1]. Therefore, our aim is to explain these differences, and to assess the accuracy of the available atomic data. Additionally, DGM have reported radiative rates for only electric dipole (E1) transitions, whereas corresponding results for other types of transitions (namely, electric quadrupole E2, magnetic dipole M1 and magnetic quadrupole M2) are also required in the modelling of plasmas. Therefore, in this paper we report radiative rates for all types of transitions.

2. Energy levels

To calculate our results, we have adopted the fully relativistic GRASP code [3] with the option of *extended average level* (EAL). Our calculations are in the jj coupling scheme, and Breit and QED corrections have been included. A test calculation performed with only the above 4 configurations produced energy levels which closely agree (within 1 %) with those of BD. However, inclusion of additional CI with the $3p^63d$, $3s3p^43d^2$, $3s^23p^33d^2$ and $3s^23p^23d^3$ configurations, especially of $3s^23p^33d^2$, is quite pronounced, and this lowers the energies by ~ 0.7 Ry. Therefore, our conclusion is that for a reasonably accurate calculation of energy levels for Fe X, inclusion of CI among the $3s^23p^5$, $3s3p^6$, $3s^23p^43d$, $3s3p^53d$, $3p^63d$, $3s3p^43d^2$, $3s^23p^33d^2$ and $3s^23p^23d^3$ configurations is necessary, and the effect of other neglected configurations is insignificant. Our calculated (lowest 38) energy levels obtained with CI among 669 levels of the above 8 configurations are listed in Table 1. Also listed in this table are the available experimental energies from NIST, and the theoretical energies of BD and DGM.

The agreement between present theoretical and experimental energy levels is within 3 %, and their orderings are also nearly the same. However, the energy levels of BD are clearly higher by up to 11 %, and also differ in ordering in a few instances, such as levels 19 and 21. This is because of the exclusion of CI with additional configurations as stated earlier. The agreement between our CI calculations and those of DGM is also within 3 % for all levels, and the ordering is also the same for a majority of these. However, DGM sus-

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Table 1 Energy levels (in Ry), radiative rates (s^{-1}), and life-times (s) for Fe X. ($a \pm b \equiv a \times 10^{\pm b}$)

Index	Configuration	Level	NIST	GRASP	BD [1]	DGM [2]	A (s^{-1})	τ (s)
1......	$3s^23p^5$	$^2P^o_{3/2}$	0.0000	0.0000	0.0000	0.0000	....	....
2......	$3s^23p^5$	$^2P^o_{1/2}$	0.1429	0.1426	0.1322	0.1426	6.892+01	1.451-02
3......	$3s3p^6$	$^2S_{1/2}$	2.6358	2.6024	2.6329	2.5927	4.274+09	2.340-10
4......	$3s^23p^4$ (^{3}P)3d	$^4D_{5/2}$	3.5422	3.5473	3.5564	3.5448	6.751+06	1.481-07
5......	$3s^23p^4$ (^{3}P)3d	$^4D_{7/2}$	3.5422	3.5468	3.5569	3.5446	5.877+01	1.702-02
6......	$3s^23p^4$ (^{3}P)3d	$^4D_{3/2}$	3.5544	3.5587	3.5661	3.5545	6.370+06	1.570-07
7......	$3s^23p^4$ (^{3}P)3d	$^4D_{1/2}$	3.5681	3.5724	3.5784	3.5682	8.742+06	1.144-07
8......	$3s^23p^4$ (^{3}P)3d	$^4F_{9/2}$	3.8059	3.8407	3.8263	3.8077	1.294+01	7.727-02
9......	$3s^23p^4$ (^{1}D)3d	$^2P_{1/2}$	......	3.8608	3.8904	3.7636	3.138+08	3.186-09
10......	$3s^23p^4$ (^{3}P)3d	$^4F_{7/2}$	3.8528	3.8876	3.8693	3.8549	1.771+01	5.647-02
11......	$3s^23p^4$ (^{3}P)3d	$^4F_{5/2}$	3.8890	3.9220	3.9005	3.8925	4.511+07	2.217-08
12......	$3s^23p^4$ (^{3}P)3d	$^4F_{3/2}$	3.9029	3.9345	3.9150	3.9373	2.395+08	4.175-09
13......	$3s^23p^4$ (^{1}D)3d	$^2P_{3/2}$	3.9360	3.9375	3.9585	3.8949	3.147+08	3.178-09
14......	$3s^23p^4$ (^{1}D)3d	$^2D_{3/2}$	3.9605	3.9942	4.0056	3.9710	3.311+08	3.020-09
15......	$3s^23p^4$ (^{3}P)3d	$^4P_{1/2}$	3.9622	3.9992	3.9978	3.9833	3.322+08	3.011-09
16......	$3s^23p^4$ (^{3}P)3d	$^4P_{3/2}$	......	4.0435	4.0450	4.1171	5.750+06	1.739-07
17......	$3s^23p^4$ (^{3}P)3d	$^4P_{5/2}$	4.0265	4.0615	4.0652	4.0303	1.134+08	8.820-09
18......	$3s^23p^4$ (^{3}P)3d	$^2F_{7/2}$	4.0172	4.0716	4.1517	4.0274	7.305+01	1.369-02
19......	$3s^23p^4$ (^{1}D)3d	$^2D_{5/2}$	......	4.0836	4.0871	4.0532	5.871+07	1.703-08
20......	$3s^23p^4$ (^{1}D)3d	$^2G_{9/2}$	4.1075	4.1612	4.1440	4.1116	7.774+01	1.286-02
21......	$3s^23p^4$ (^{1}D)3d	$^2G_{7/2}$	4.1106	4.1660	4.0649	4.1249	7.580+01	1.319-02
22......	$3s^23p^4$ (^{3}P)3d	$^2F_{5/2}$	4.1256	4.1935	4.1866	4.1513	2.182+07	4.582-08
23......	$3s^23p^4$ (^{1}D)3d	$^2F_{5/2}$	......	4.4664	4.4638	4.5386	1.662+08	6.018-09
24......	$3s^23p^4$ (^{1}D)3d	$^2F_{7/2}$	4.4286	4.5020	4.4981	4.5689	2.193+02	4.560-03
25......	$3s^23p^4$ (^{1}S)3d	$^2D_{3/2}$	4.6639	4.7243	4.7849	4.7120	8.724+08	1.146-09
26......	$3s^23p^4$ (^{1}S)3d	$^2D_{5/2}$	......	4.7618	4.8234	4.9266	3.073+08	3.254-09
27......	$3s^23p^4$ (^{1}D)3d	$^2S_{1/2}$	4.9380	5.0228	5.2766	4.9886	1.760+11	5.681-12
28......	$3s^23p^4$ (^{3}P)3d	$^2P_{3/2}$	5.1414	5.2727	5.3219	5.2806	1.644+11	6.084-12
29......	$3s^23p^4$ (^{3}P)3d	$^2P_{1/2}$	5.1941	5.3243	5.3762	5.3628	1.603+11	6.237-12
30......	$3s^23p^4$ (^{3}P)3d	$^2D_{5/2}$	5.2211	5.3428	5.4723	5.3950	1.977+11	5.058-12
31......	$3s^23p^4$ (^{3}P)3d	$^2D_{3/2}$	5.3422	5.4633	5.5857	5.5132	1.946+11	5.139-12
32......	$3s3p^5$(^{3}P)3d	$^4P^o_{1/2}$	......	6.2252	6.4777	6.1094	3.511+09	2.848-10
33......	$3s3p^5$(^{3}P)3d	$^4P^o_{3/2}$	......	6.2485	6.5033	6.1323	3.537+09	2.827-10
34......	$3s3p^5$(^{3}P)3d	$^4P^o_{5/2}$	......	6.2905	6.5485	6.1760	3.578+09	2.795-10
35......	$3s3p^5$(^{3}P)3d	$^4F^o_{9/2}$	6.3484	6.5516	6.6584	6.3568	6.410+09	1.560-10
36......	$3s3p^5$(^{3}P)3d	$^4F^o_{7/2}$	6.3742	6.5771	6.6857	6.3834	6.460+09	1.548-10
37......	$3s3p^5$(^{3}P)3d	$^4F^o_{5/2}$	6.4024	6.6044	6.7131	6.4115	6.534+09	1.530-10
38......	$3s3p^5$(^{3}P)3d	$^4F^o_{3/2}$	6.4283	6.6293	6.7369	6.4366	6.596+09	1.516-10

pected that the ordering of the $3s^23p^4(^3P)3d\ ^4F_{3/2}$ and $3s^23p^4(^1D)3d\ ^2P_{3/2}$ levels (i.e. 12 and 13) might be misprinted by NIST, but our calculations confirm the NIST ordering to be correct. Moreover, a major anomaly between our calculations and those of DGM is for the ordering of the $3s^23p^4(^3P)3d\ ^4P_{3/2}$ level (16), which is almost pure and does not have any considerable contribution from other levels, in both calculations. To conclude, we may state with confidence that the energy levels of NIST, DGM and our GRASP calculations listed in Table 1 are accurate to $\sim 3\,\%$, and also agree in general in the orderings.

3. Radiative rates

In total we have calculated oscillator strengths (*f*-values), radiative rates (*A*- values), and line strengths

(S- values) for all 460 electric dipole (E1), 590 electric quadrupole (E2), 437 magnetic dipole (M1), and 606 magnetic quadrupole (M2) transitions among the 54 levels of Fe X. CI among the above listed 8 configurations has been included, and the effect of including additional CI with configurations such as: $3s3p^44\ell^2$, $3p^54\ell^2$, $3s^23p^45\ell$ and $3s3p^55\ell$ has been assessed to be insignificant. In Table 1 we present our A- values for only resonance transitions, which are a sum over all types of transitions. A complete set of results for all transitions (among all 54 levels) along with detailed comparisons and discussion is available elsewhere [4]. However, for a majority of E1 transitions, especially the stronger ones, the agreement between our and the DGM's calculations is better than 20 %, but for weaker transitions the differences are sometimes larger.

Finally, in Table 1 we also list our calculated life-times. The corresponding measurements are only available for seven levels, namely $3s^23p^5\ ^2P^o_{1/2}$, $3s3p^6\ ^2S_{1/2}$, $3s^23p^4(^3P)3d\ ^4F_{9/2}$, $3s^23p^4(^3P)3d\ ^4F_{7/2}$, $3s^23p^4(^3P)3d\ ^2F_{7/2}$, $3s^23p^4(^1D)3d\ ^2G_{9/2}$, and $3s^23p^4(^1D)3d\ ^2F_{7/2}$, i.e. levels 2, 3, 8, 10, 18, 20, and 24, respectively - see Table 4 of [4]. Life-times of the $3s^23p^5\ ^2P^o_{1/2}$, $3s^23p^4(^3P)3d^2F_{7/2}$ and $3s^23p^4(^1D)3d\ ^2F_{7/2}$ levels remain stable (within 10 %) among different test calculations, and also agree to better than 10 % with the measurements. The life-time of the $3s3p^6\ ^2S_{1/2}$ level shows the largest variation (between 178 and 403 ps) among different test calculations, but our concluded value of 234 ps agrees within 10 % with the measurements as well as with other theoretical results. Similarly, life-time measurements for the $3s^23p^4(^3P)3d\ ^4F_{9/2}$ level are in agreement with our present theoretical results, but the measured life-times of the $3s^23p^4(^3P)3d\ ^4F_{7/2}$, $3s^23p^4(^1D)3d\ ^2G_{9/2}$, $3s^23p^4(^3P)3d\ ^4F_{7/2}$, and $3s^23p^4(^3P)3d\ ^4F_{9/2}$, levels are overestimated. It may be because the measured estimation is based on the identification of the dominant (M1) transitions alone, whereas our calculations show a significant contribution from other transitions as well - see details in [4]. Therefore, based on this analysis and the possible uncertainty of 10 % – 32 % in the experimental results, we may state in conclusion that the theory and experiment agree well for transitions in Fe X, and hence confirm the accuracy of the presently reported radiative rates.

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