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Energy levels, lifetimes and branch fractions for Fe XI

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ABSTRACT

We present transition energies, probabilities and branching ratios for the electric dipole allowed (E1) and forbidden (M1, E2, M2) lines of the $3s^23p^4$, $3s3p^5$ and $3s^23p^33d$ configurations of Fe XI. Large-scale multiconfiguration Dirac–Fock wavefunctions are applied to include the effects of relativity, correlation and rearrangement of the electron density consistently within the same (computational) model. From the transition probabilities, lifetimes of the 46 lowest-lying excited levels are derived, and the prospects for experimental verification are discussed. An M2 transition is identified in the solar extreme ultraviolet spectrum.

Key words: atomic data – atomic processes – line: identification – methods: numerical – Sun: UV radiation – ultraviolet: general.

1 INTRODUCTION

Sounding rockets and then satellites revealed that the Sun radiates brightly in spectral regions like the vacuum ultraviolet (VUV) and extreme ultraviolet (EUV) that are not accessible by ground observations. One of the first large-scale investigations of the solar VUV spectrum employed the High Resolution Telescope and Spectrograph (HRTS) and the *Skylab* Apollo Telescope Mount (ATM). It revealed rich spectra that took more than a decade to evaluate, and many lines in those spectra remain unidentified. For example, on the basis of these observations, Sandlin et al. (1986) provided a catalogue of 3250 lines in the interval 1175–1710 Å, of which 49 per cent remained unclassified. Since its launch in 1995, the *Solar and Heliospheric Observatory* (*SOHO*) spacecraft has helped considerably to broaden our knowledge about the Sun.[1] Among *SOHO*'s instruments is SUMER, a VUV spectrometer that has delivered numerous highly resolved spectra of the solar atmosphere. The outermost part of this atmosphere, the corona, forms a plasma of charged particles, which continue to flow throughout the Solar system as the solar wind. Based on the SUMER spectra, Feldman et al. (1997) presented a catalogue that lists about 900 lines in the range 500–1610 Å, of which again a considerable fraction have not yet been identified. Another satellite, the *Far Ultraviolet Spectroscopic Explorer* (*FUSE*), was launched in 1999 for studying the wavelength band 905–1195 Å in astrophysical sources away from the Sun.[2]

Many of the solar VUV and EUV spectral lines arise from highly charged ions, as was to be expected even before the satellite missions made direct observation possible. Edlén (1942) confirmed an earlier suggestion that some prominent coronal lines in the visible spectrum arise from transitions between levels of the ground complex in highly charged ions of Ca and Fe. Correspondingly, the line spectra of iron and neighbouring elements have been observed not only in the Sun (Malinovsky & Heroux 1973; Feldman, Doschek & Seely 1988; Feldman et al. 1997) but also in a number of other astronomical objects, for instance in the spectra of late-type stars (Haiche, Drake & Schmitt 1994; Drake, Laming & Widing 1995). More spectra with high spectral resolution are expected from the aforementioned *FUSE* mission in the near future.

The presence of such ions (which require a high-temperature environment) in a location above a much cooler photosphere forced a revolution in our understanding of the solar corona. At typical coronal temperatures, one of the most abundant elements, Fe, would be expected to be prominent in charge states 9+ and 10+, i.e. giving rise to spectra Fe X and Fe XI. Therefore, these two spectra have attracted a lot of interest during the past decades. However, after all these efforts, most of the levels in the low-lying configurations $3s3p^6$ and $3s^23p^43d$ of Fe X are known, but knowledge of the corresponding $3s3p^5$ and $3s^23p^33d$ of Fe XI still remains fragmentary (Shirai et al. 1990; Träbert 1998).

For multiply charged ions of the iron group, many of the observed lines arise from the $3s3p^n$ and $3s^23p^{n-2}3d$ ($n = 2, \ldots, 6$) configurations. In order to provide theoretical guidance – at least for the dominant lines of these spectra – Fawcett (1986, 1987,

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[1] *SOHO* homepage at http://sohowww.nascom.nasa.gov/

[2] *FUSE* homepage at http://fuse.pha.jhu.edu/

1991) carried out a series of (semi-empirically scaled) relativistic Hartree–Fock computations as well as some ab initio Dirac–Fock calculations. These calculations describe most of the strong transitions fairly well. Unfortunately, much less information and data – either theoretical or experimental – are available for the medium and weak lines of these spectra, including the 'forbidden' magnetic dipole (M1) and electric quadrupole (E2) transitions. In the absence of competing decay branches, these transitions are often the ones which are observed. The incompleteness of experimental wavelength observations as well as insufficiently reliable calculations have so far hampered a more complete assignment of forbidden lines in the solar spectrum (see e.g. Smitt 1976; Mason & Nussbaumer 1977). Although a number of calculations have treated Fe XI in the past (Mendoza & Zeippen 1983; Fawcett 1986; Saloman & Kim 1989; Verner, Verner & Ferland 1996; Bhatia & Doschek 1996; Chou et al. 1996; Deb & Tayal 1998), only a few of these computations, however, covered transition probabilities of the weak and forbidden lines as well as the lifetimes of the low-lying levels. We recently demonstrated for weak and medium lines (and even for some strong ones) that accurate transition probabilities and lifetimes are only obtained by applying large-scale wavefunctions that include the effects of relativity, correlation and rearrangement of the bound electron density within the same computational model (Kohstall et al. 1998, 1999; Dong et al. 1999). In addition, lines that are often called *weak* as a result of their low transition probabilities may appear prominent in some observations, depending on the presence (or absence) of competing decay channels and on the physical environment, i.e. population and depopulation processes.

In the following, we report on an elaborate computation of the electric dipole *allowed* (E1) and *forbidden* (M1, E2, M2) transitions among the 47 levels of the $3s^23p^4$, $3s3p^5$ and $3s^23p^33d$ configurations of Fe^{10+} ions. Such transitions – including intensity ratios for the decay of some of the lower-lying levels – have been observed from a rocket-based spectrograph by Thomas & Neupert (1994). We applied relativistic multiconfiguration Dirac–Fock (MCDF) wavefunctions in order to provide a consistent and improved data set for all transitions among the low-lying levels of the Fe XI spectrum and to derive intensity ratios and lifetimes from these data. The present investigation continues our recent work on the Fe X spectrum (Dong et al. 1999), which helped, with continuing effort, in identifying further forbidden lines in Fe X (Jupén & Träbert, in preparation) and prompted the demand for an equivalent data set for Fe XI. We therefore hope that the data supplied for the low-lying spectrum of Fe XI will be found similarly useful for the interpretation of current as well as future astrophysical observations.

2 BRIEF OUTLINE OF THE COMPUTATIONS

Here, we shall restrict ourselves to a brief account of the computational procedure; details on the (rather frequently) applied multiconfiguration Dirac–Fock method have been presented in a number of case studies by various groups [for details regarding the theoretical background, we refer to Grant (1988), and to Dong et al. (1999) for our work on Fe X]. Again, the (relativistic) wavefunctions for our computations below have been obtained from the atomic structure package GRASP92 (Parpia, Froese Fischer & Grant 1996). This package implements the MCDF method in which an atomic state is approximated by a superposition of configuration state functions (CSF) of the same symmetry:

$$\psi_\alpha(PJM) = \sum_{r=1}^{n_c} c_r(\alpha)|\gamma_r PJM\rangle. \qquad (1)$$

The major difference among the various relativistic computations concerns the number of CSF, n_c, in equation (1). This size of the wavefunction expansions typically reflects the extent to which electron correlations are taken into account. Wavefunction expansions (1) of several (ten) thousand CSF are nowadays applied in order to obtain a sufficiently accurate description of the level structure and transition properties. In GRASP92, the CSF are antisymmetrized products of a common set of *orthonormal* orbitals which are optimized self-consistently on the basis of the Dirac–Coulomb Hamiltonian. Further relativistic corrections to the electron–electron interaction are added in a second step by diagonalizing the Dirac–Coulomb–Breit Hamiltonian matrix; we also estimated the contributions from quantum electrodynamics (QED) but found them negligible at the present level of accuracy.

In the wavefunction expansion (1), the number of CSF, n_c, increases very rapidly as virtual excitations of electrons from the (spectroscopically) occupied shells into unoccupied subshells are taken into account. In the present computations we included excitations from the 3s, 3p and 3d subshells but kept the neon-like core ($1s^22s^22p^6$) unaffected. The restriction to account for only *valence–valence* correlations has been found to be a sufficient approximation if, say, more than four or five valence electrons occur (Fritzsche, Froese Fischer & Fricke 1998).

In the lower-lying spectrum of Fe XI, there are five even-parity levels of the $3s^23p^4$ ground configuration with total angular momenta $J = 0$, 1 and 2. A single (low-lying) replacement of one of the valence electrons leads to the two odd-parity configurations $3s3p^5$ and $3s^23p^33d$, which comprise altogether 42 levels with $J = 0, \ldots, 5$. From these excited levels only those with $J \leq 3$ can decay by allowed E1 transitions to the ground configuration. While the five excited $J = 4$ levels are still coupled to the ground states via forbidden M2 transitions, the $J = 5$ level of $3s^23p^33d$ is (practically) stable against the ground-state levels. Instead, these $J = 4$ and $J = 5$ levels (mainly) decay by forbidden M1 and E2 transitions to lower-lying levels of the same parity. All these forbidden lines are included in the present study. When compared with the strong dipole-allowed transitions, the M1, E2 and M2 line strengths are suppressed by several orders of magnitude. Accordingly, the $J = 4$ and $J = 5$ levels exhibit typical lifetimes of a few (tens of) milliseconds, which are shorter by only a factor of about 10 compared with the lifetimes of the four excited levels of the ground configuration.

Table 1. Number of CSF used in the atomic state function expansion (1) for different level groups.

Parity	J	Level numbers	$3l$	$5l$	$6l'^a$
odd	0, 1, 2	5	583	6817	8333
even	0	5	86	4952	8643
	1	11	228	13496	16064
	2	11	298	18480	22511
	3	9	294	19211	24372
	4	5	227	16461	18617
	5	1	140	1194	13476

[a] For excitations into the $6l$ subshells, we incorporated beyond the 5SD approximation ($5l$) all excitations of type $3l6l'$ but only the *pure* double excitations of type $nl6l$ with $n = 4$, 5 and 6.

Table 2. Excitation energies and lifetimes for the low-lying levels of the $3s^2 3p^4$, $3s3p^5$ and $3s^2 3p^3 3d$ configurations for Fe XI.

No.	J^P	Energy (cm^{-1}) This work	Energy (cm^{-1}) Experiment	Lifetime (s) Length	Lifetime (s) Velocity	Lifetime (s) Experiment
1	2+	0.0	0.0			
2	1+	12512	12668[a]	2.37(−2)		
3	0+	14273	14312[a]	3.60		
4	2+	38565	37744[a]	9.81(−3)		
5	0+	82166	80815[a]	1.01(−3)		
6	2−	283983	283558[a]	3.33(−10)	2.64(−10)	
7	1−	293678	293158[a]	3.14(−10)	3.19(−10)	
8	0−	299113	299163[a]	3.14(−10)	3.20(−10)	
9	1−	363653	361842[a]	1.20(−10)	1.18(−10)	
10	0−	387246	387760[b]	8.69(−9)	8.55(−9)	1.33(−8)[c]
11	1−	387694	388015[b]	9.85(−9)	1.00(−8)	1.5(−8)[c]
12	2−	387707	388280[b]	1.37(−8)	1.30(−8)	1.3(−8)[c]
13	3−	387916	388712[b]	4.12(−8)	4.00(−8)	6…7(−8)[c]
14	4−	388784	389590[d]	2.82(−2)		
15	2−	413674		2.82(−8)	2.48(−8)	
16	3−	415913		3.60(−7)	2.56(−7)	
17	1−	417969		2.90(−8)	2.94(−8)	
18	2−	423780		4.73(−8)	4.60(−8)	
19	0−	426123		1.77(−8)	1.64(−8)	
20	3−	426927		4.24(−8)	4.27(−8)	
21	4−	431363		7.99(−3)		
22	3−	450841		1.07(−8)	1.02(−8)	1.2(−8)[c]
23	4−	452425		4.32(−2)		
24	5−	454538		9.58(−2)	9.71(−2)	
25	4−	461966		1.59(−2)	1.36(−2)	
26	2−	468571		8.40(−10)	7.84(−10)	
27	0−	484609		2.64(−9)	2.31(−9)	
28	1−	484662		6.28(−10)	6.06(−10)	
29	1−	487464		3.38(−10)	3.21(−10)	
30	3−	487501		3.76(−9)	3.65(−9)	
31	2−	488729		9.78(−9)	9.35(−9)	
32	4−	488789		1.50(−3)		
33	2−	492064		5.58(−10)	5.39(−10)	
34	2−	496300	496090[a]	1.72(−10)	1.61(−10)	
35	3−	499911		2.04(−9)	1.98(−9)	
36	3−	529964		1.08(−9)	1.04(−9)	
37	1−	537200	526480[a]	9.71(−12)	9.51(−12)	
38	2−	538134	531290[a]	8.05(−12)	7.81(−12)	
39	1−	540715	533450[a]	8.67(−12)	8.45(−12)	
40	1−	548756	541390[a]	8.12(−12)	7.92(−12)	
41	0−	548663	541720[a]	7.52(−12)	7.30(−12)	
42	3−	560935	554300[a]	7.09(−12)	6.89(−12)	
43	2−	568259	561610[a]	7.28(−12)	7.08(−12)	
44	1−	573284	566380[a]	7.11(−12)	6.95(−12)	
45	2−	585545	578861[a]	8.91(−12)	8.74(−12)	
46	3−	602120	594030[a]	6.48(−12)	6.31(−12)	
47	1−	631221	623080[a]	7.81(−12)	7.70(−12)	

[a] Fuhr et al. (2000).
[b] Träbert (1998), Jupén & Träbert (in preparation).
[c] Träbert et al. (1993), measured on blended lines.
[d] This work.

In carrying out large-scale computations, one can benefit a great deal from exploiting the symmetries of the atomic levels. Hence, the natural start-up is to divide the levels into groups of the same angular momentum and parity. As previously, we split the excited levels into six groups according to the total angular momentum values $J = 0, \ldots, 5$. In order to keep the calculations feasible, however, and to account for the relatively small splitting within the ground-state configuration, the five ground-state levels have been held together to form an (additional) level group. An independent variation of the wavefunctions for the various level groups then automatically includes a significant part of the electron relaxation. However, it also yields orbital functions for each group that are not quite orthogonal to the orbitals of any other group and, hence, require special care. In order to incorporate these relaxation effects into our transition probability calculations, we applied two (new) components of the RATIP package (Fritzsche et al. 1999), which we adapted to allow for wavefunction expansions of several ten thousand CSF (Fritzsche

Table 3. E1 transition energies, emission rates A and oscillator strengths for the $3s^23p^4$–$3s3p^5$ and $3s^23p^4$–$3s^23p^33d$ lines of Fe XI. The level numbers of the lower and upper level refer to Table 2. The weighted oscillator strength (gf) for emission is displayed in length gauge only; br denotes the branching fraction of this line for the corresponding upper level.

Trans.	J_F	J_I	Type	Wavenumber (cm^{-1})	Wavelength (Å)	A (s^{-1}) Length	Velocity	gf	br
5–7	1	0	E1	211514	472.782	1.37(+7)	1.45(+7)	1.38(−3)	0.00
4–6	2	2	E1	245421	407.463	6.78(+7)	7.38(+7)	8.44(−3)	0.01
4–7	1	2	E1	255115	391.980	1.92(+6)	2.79(+6)	1.32(−4)	0.00
2–6	2	1	E1	271473	368.361	6.98(+8)	7.36(+8)	7.10(−2)	0.23
3–7	1	0	E1	279407	357.901	9.62(+8)	9.48(+8)	5.46(−2)	0.30
2–7	1	1	E1	281167	355.661	7.54(+8)	7.43(+8)	4.29(−2)	0.24
1–6	2	2	E1	283985	352.131	2.23(+9)	2.32(+9)	2.07(−1)	0.74
5–9	1	0	E1	281489	355.254	2.43(+8)	2.28(+8)	1.38(−2)	0.03
2–8	0	1	E1	286604	348.913	3.15(+9)	3.13(+9)	5.75(−2)	1.00
1–7	1	2	E1	293679	340.508	1.45(+9)	1.42(+9)	7.59(−2)	0.46
5–11	1	0	E1	305528	327.302	3.80(+4)	4.67(+4)	1.83(−6)	0.00
4–9	1	2	E1	325090	307.607	7.81(+9)	7.95(+9)	3.32(−1)	0.94
5–17	1	0	E1	335805	297.792	1.87(+6)	2.11(+6)	7.46(−5)	0.00
4–11	1	2	E1	349129	286.427	4.01(+5)	3.95(+5)	1.48(−5)	0.00
4–12	2	2	E1	349145	286.414	5.26(+5)	5.46(+5)	3.24(−5)	0.00
4–13	3	2	E1	349353	286.243	1.66(+5)	1.77(+5)	1.43(−5)	0.00
3–9	1	0	E1	349382	286.220	3.11(+5)	6.04(+5)	1.15(−5)	0.00
2–9	1	1	E1	351142	284.785	1.64(+7)	1.57(+7)	5.97(−4)	0.00
1–9	1	2	E1	363654	274.987	2.74(+8)	2.78(+8)	9.32(−3)	0.03
3–11	1	0	E1	373421	267.794	1.17(+7)	1.28(+7)	3.77(−4)	0.12
2–10	0	1	E1	374733	266.857	1.15(+8)	1.17(+8)	1.12(−3)	1.00
2–11	1	1	E1	375181	266.538	3.21(+7)	3.41(+7)	1.03(−3)	0.32
4–15	2	2	E1	375111	266.588	2.71(+3)	2.82(+4)	1.44(−7)	0.00
2–12	2	2	E1	375196	266.527	8.68(+6)	1.02(+7)	4.62(−4)	0.12
4–16	3	2	E1	377349	265.007	7.28(+5)	8.99(+5)	5.36(−5)	0.26
4–17	1	2	E1	379406	263.570	6.99(+5)	6.68(+5)	2.18(−5)	0.00
4–18	2	2	E1	385217	259.594	8.47(+5)	1.03(+6)	4.28(−5)	0.04
1–11	1	2	E1	387693	257.936	5.77(+7)	5.29(+7)	1.73(−3)	0.57
1–12	2	2	E1	387709	257.925	6.42(+7)	6.68(+7)	3.20(−3)	0.88
1–13	3	2	E1	387917	257.787	2.43(+7)	2.50(+7)	1.69(−3)	1.00
4–20	3	2	E1	388363	257.491	1.21(+7)	1.21(+7)	8.40(−4)	0.51
2–15	2	1	E1	401162	249.276	6.79(+6)	8.75(+6)	3.16(−4)	0.00
3–17	1	0	E1	403697	247.711	2.46(+4)	2.00(+5)	6.79(−7)	0.00
5–28	1	0	E1	402497	248.449	5.29(+7)	5.49(+7)	1.47(−3)	0.03
2–17	1	0	E1	405475	246.624	1.51(+7)	1.41(+7)	4.12(−4)	0.44
5–29	1	0	E1	405299	246.731	3.37(+6)	3.49(+6)	9.22(−5)	0.00
2–18	2	1	E1	411269	243.150	7.31(+4)	5.70(+4)	3.19(−7)	0.00
1–15	2	2	E1	413675	241.736	4.13(+7)	4.04(+7)	1.81(−3)	1.00
4–22	3	2	E1	412277	242.555	5.68(+7)	5.93(+7)	3.51(−3)	0.61
2–19	0	1	E1	413611	241.773	5.66(+7)	6.11(+7)	4.96(−4)	1.00
1–16	3	2	E1	415913	240.435	2.05(+6)	3.00(+6)	1.24(−4)	0.74
1–17	1	2	E1	417970	239.252	1.94(+7)	1.99(+7)	4.99(−4)	0.56
1–18	2	2	E1	423781	235.971	2.03(+7)	2.07(+7)	8.47(−4)	0.96
1–20	3	2	E1	426926	234.233	1.15(+7)	1.13(+7)	6.62(−4)	0.49
4–26	2	2	E1	430008	232.554	1.02(+9)	1.09(+9)	4.13(−2)	0.86
4–28	1	2	E1	446098	224.166	3.38(+8)	3.50(+8)	7.65(−3)	0.21
4–29	1	2	E1	448900	222.767	2.98(+8)	3.01(+8)	6.65(−3)	0.11
4–30	3	2	E1	448938	222.748	6.83(+7)	6.99(+7)	3.56(−3)	0.26
4–31	2	2	E1	450164	222.141	1.00(+8)	1.05(+8)	3.71(−3)	0.98
1–22	3	2	E1	450840	221.808	3.68(+7)	3.83(+7)	1.90(−3)	0.39
4–33	2	2	E1	453500	220.507	9.90(+7)	9.67(+7)	3.61(−3)	0.06
5–37	1	0	E1	455037	219.762	2.29(+8)	2.42(+8)	4.98(−3)	0.00
2–26	2	1	E1	456060	219.269	4.32(+7)	4.58(+7)	1.56(−3)	0.04
4–34	2	2	E1	457766	218.452	1.64(+8)	1.81(+8)	5.88(−3)	0.03
5–39	1	0	E1	458551	218.078	2.14(+9)	2.29(+9)	4.58(−2)	0.02
4–35	3	2	E1	461347	216.757	5.93(+7)	5.94(+7)	2.92(−3)	0.12
5–40	1	0	E1	466590	214.321	4.42(+9)	4.68(+9)	9.14(−2)	0.04

Table 3 – *continued*

Trans.	J_F	J_I	Type	Wavenumber (cm^{-1})	Wavelength (Å)	A (s^{-1}) Length	Velocity	gf	br
1–26	2	2	E1	468572	213.414	1.27(+8)	1.39(+8)	4.33(−3)	0.11
3–28	1	0	E1	470389	212.590	9.47(+8)	9.81(+8)	1.92(−2)	0.59
2–27	0	1	E1	472097	211.821	3.79(+8)	4.32(+8)	2.55(−3)	1.00
2–28	1	1	E1	472149	211.798	1.17(+8)	1.19(+8)	2.36(−3)	0.07
3–29	1	0	E1	473192	211.331	9.21(+7)	1.07(+8)	1.85(−3)	0.03
2–29	1	1	E1	474952	210.548	5.89(+6)	9.32(+6)	1.17(−4)	0.00
2–31	2	1	E1	476216	209.989	4.95(+5)	5.38(+5)	1.64(−5)	0.00
2–33	2	1	E1	479552	208.528	1.40(+9)	1.45(+9)	4.56(−2)	0.78
2–34	2	1	E1	483788	206.702	1.07(+9)	1.15(+9)	3.42(−2)	0.18
1–28	1	2	E1	484661	206.330	1.38(+8)	1.44(+8)	2.64(−3)	0.09
1–29	1	2	E1	487464	205.143	2.56(+9)	2.69(+9)	4.84(−2)	0.86
1–30	3	2	E1	487501	205.128	1.97(+8)	2.04(+8)	8.72(−3)	0.74
1–31	2	2	E1	488728	204.613	2.25(+6)	1.93(+6)	7.07(−5)	0.02
4–36	3	2	E1	490403	203.914	2.22(+7)	2.68(+7)	9.67(−4)	0.02
1–33	2	2	E1	492064	203.226	2.92(+8)	3.08(+8)	9.05(−3)	0.16
5–44	1	0	E1	491118	203.617	1.41(+7)	1.62(+7)	2.63(−4)	0.00
1–34	2	2	E1	496300	201.491	4.58(+9)	4.88(+9)	1.39(−1)	0.79
4–38	2	2	E1	499570	200.172	1.73(+9)	1.79(+9)	5.18(−2)	0.01
4–37	1	2	E1	498638	200.546	2.44(+8)	2.49(+8)	4.42(−3)	0.00
1–35	3	2	E1	499911	200.036	4.32(+8)	4.45(+8)	1.81(−2)	0.88
4–39	1	2	E1	502151	199.143	5.74(+10)	5.88(+10)	1.02	0.50
4–40	1	2	E1	510191	196.005	5.18(+10)	5.29(+10)	8.94(−1)	0.42
3–37	1	0	E1	522929	191.231	5.03(+7)	4.78(+7)		0.00
4–42	3	2	E1	522372	191.434	1.10(+8)	1.14(+8)	4.21(−3)	0.00
2–38	2	1	E1	525622	190.251	2.15(+10)	2.22(+10)	5.83(−1)	0.17
2–37	1	1	E1	524689	190.589	4.99(+9)	5.06(+9)	8.16(−2)	0.05
3–39	1	0	E1	526443	189.954	2.16(+10)	2.22(+10)	3.51(−1)	0.19
2–39	1	1	E1	528203	189.321	2.95(+10)	3.02(+10)	4.76(−1)	0.26
1–36	3	2	E1	528967	189.048	9.03(+8)	9.34(+8)	3.38(−2)	0.98
4–43	2	2	E1	529695	188.788	3.34(+9)	3.39(+9)	8.93(−2)	0.02
3–40	1	0	E1	534482	187.097	2.88(+10)	2.95(+10)	4.53(−1)	0.23
4–44	1	2	E1	534719	187.014	4.83(+8)	5.00(+8)	7.59(−3)	0.00
2–41	0	1	E1	536150	186.515	1.33(+11)	1.37(+11)	6.94(−1)	1.00
2–40	1	1	E1	536242	186.483	3.07(+10)	3.14(+10)	4.80(−1)	0.25
1–38	2	2	E1	538134	185.827	1.01(+11)	1.04(+11)	2.60	0.81
1–37	1	2	E1	537201	186.150	9.75(+10)	9.95(+10)	1.52	0.95
1–39	1	2	E1	540715	184.940	4.75(+9)	4.89(+9)	7.31(−2)	0.04
1–40	1	2	E1	548775	182.224	7.48(+9)	7.72(+9)	1.12(−1)	0.06
4–45	2	2	E1	546981	182.822	1.05(+11)	1.07(+11)	2.63	0.94
5–47	1	0	E1	549057	182.130	1.26(+11)	1.28(+11)	1.88	0.98
2–43	2	1	E1	555747	179.938	1.05(+11)	1.08(+11)	2.56	0.76
3–44	1	0	E1	559011	178.887	8.02(+10)	8.19(+10)	1.15	0.57
2–44	1	1	E1	560771	178.326	5.74(+10)	5.87(+10)	8.22(−1)	0.41
1–42	3	2	E1	560935	178.274	1.41(+11)	1.45(+11)	4.71	1.00
4–46	3	2	E1	563556	177.445	1.54(+11)	1.58(+11)	5.11	1.00
1–43	2	2	E1	568259	175.976	2.91(+10)	2.98(+10)	6.76(−1)	0.21
1–44	1	2	E1	573283	174.434	2.62(+9)	2.67(+9)	3.58(−2)	0.02
2–45	2	1	E1	573033	174.510	7.17(+9)	7.33(+9)	1.64(−1)	0.06
1–45	2	2	E1	585545	170.781	1.58(+7)	1.38(+7)	3.46(−4)	0.00
4–47	1	2	E1	592608	168.746	9.75(+8)	6.86(+8)	1.25(−2)	0.01
1–46	3	2	E1	602120	166.080	3.68(+8)	3.74(+8)	1.06(−2)	0.00
3–47	1	0	E1	616950	162.088	6.86(+8)	6.75(+8)	8.11(−3)	0.01
2–47	1	1	E1	618710	161.627	3.69(+8)	3.75(+8)	4.33(−3)	0.00
1–47	1	2	E1	631222	158.423	2.52(+4)	1.74(+4)	2.84(−7)	0.00

& Anton 2000; Fritzsche, Froese Fischer & Dong 2000). Even though these *relaxed-orbital* calculations are computationally expensive when compared to computations within an orthogonal orbital set, this procedure usually improves the results obtained for transition probabilities as well as the mutual agreement of results obtained from different gauges (Babushkin, Coulomb) of the radiation field.

Electron correlations certainly play a crucial role in studying

Table 4. Calculated E1 transition probabilities (s^{-1}, in length gauge) for a few selected $3s^23p^4$–$3s3p^5$ and $3s^23p^4$–$3s^23p^33d$ transitions, compared with previous computations and evaluated data.

Trans.	This work	Fawcett	Bhatia & Doschek (1996)	Deb & Tayal (1998)	Fuhr et al. (2000)
4–6	6.78(+7)		6.28(+7)	6.37(+7)	4.0(+7)
3–7	9.62(+8)	9.17(+8)	1.07(+9)	9.19(+8)	7.1(+8)
2–8	3.15(+9)	2.77(+9)	3.52(+9)	2.90(+9)	2.3(+9)
4–11	4.01(+5)			1.92(+5)	
4–12	5.26(+5)			3.00(+5)	
1–9	2.74(+8)	3.16(+8)	2.15(+8)	2.51(+8)	2.0(+8)
2–41	1.33(+11)	1.40(+11)	2.03(+11)	1.36(+11)	1.40(+11)
5–47	1.26(+11)	1.46(+11)	1.74(+11)	1.22(+11)	1.43(+11)
4–46	1.54(+11)	1.66(+11)	2.22(+11)	1.52(+11)	1.67(+11)
2–45	7.17(+9)	8.41(+9)	1.24(+10)	8.51(+9)	8.6(+9)
1–45	1.58(+7)			2.81(+7)	

the fine structure and transition probabilities of open-shell atoms and ions. These correlations are treated most properly by the active space method, although often at the price of rather sizeable wavefunction expansions. In the present computations, we followed similar lines as demonstrated for Fe x. Outside of the (frozen) neon-like core, we included up to quadruple excitations (SDTQ) of the six valence electrons within the 3s, 3p and 3d subshells as well as single (S) and double (D) excitations into the $4l$ and $5l$ shells. Moreover, to account for the (much) richer fine-structure splitting of Fe^{10+} ions (i.e. the 47 levels in the present study, compared with 31 levels for Fe^{9+}) due to a second 3p hole in their ground configuration, we also added 'pure' double excitations into the $6l$ shells (6s, 6p, 6d and 6f); they include all the excitations of type $3l6l'$ as well as $nl6l$ ($n = 4, 5, 6$). A full account of all single and double excitations into the $6l$ layer would have resulted in wavefunction expansions that are presently not feasible. The selected set of 'pure' double excitations into $6l$ still results in slight improvements of the fine-structure splittings (of about $2000\,cm^{-1}$ for the three highest levels) and, thus, also influences the transition probabilities in the tables below. Table 1 lists the size of the wavefunction expansions for the different level groups; we provide these particular numbers of CSF in the representation of the wavefunctions to make our computations transparent to future studies. To obtain our final results, the expansions from the last column ($6l'$) have been applied.

3 RESULTS AND DISCUSSIONS

Transition probabilities and lifetimes have been calculated for all allowed (E1) and forbidden (M1, E2, M2) transitions among the levels of $3s^23p^4$, $3s3p^5$ and $3s^23p^33d$ configurations in Fe^{10+} ions. Below, we present our results in a number of tables similar to our work on Fe x (Dong et al. 1999). Table 2 shows the excitation energies and lifetimes for the 47 lowest levels of Fe xi; the excitation energies are given relative to the $3s^23p^4$ $J = 2$ ground state. As far as available, the energies are compared to (critically evaluated) data from the NIST Atomic Spectroscopic Database (Fuhr et al. 2000)[3] and to additional data obtained by Jupén, Isler & Träbert (1993) and by Träbert (1998). Table 2 also assigns a level number to each level (in ascending order of energy), which is used in the other tables to denote individual transitions among the levels. While good agreement is found with experiment for the low-lying levels, they become slightly less well represented for higher excitation energies. However, despite a shift of about $8000\,cm^{-1}$ for the highest levels at an excitation energy of $\approx 600\,000\,cm^{-1}$ (which corresponds to an accuracy of better than 2 per cent), the deviations from the evaluated data increase rather gradually, beginning at the low levels, and hence allow for a clear assignment of the levels. Considering this 'systematic' shift, it is surprising to find a single level in the NIST Database at $496\,090\,cm^{-1}$ that practically coincides with the calculated energy; this unexpected coincidence in the face of an otherwise different trend raises the question whether the level has been correctly assigned. However, our calculated excitation energies for levels 10 to 14, the ^5D levels, near $390\,000\,cm^{-1}$, are also very close to the experimentally determined positions (Träbert 1998). Similarly, in earlier work on sextet levels in Cu xiii (Träbert, Fritzsche & Jupén 1998), the best candidate lines for decays of these levels, which are excited, but lowest of their symmetry, suggested energy values very close to prediction. The presently questioned case at $496\,090\,cm^{-1}$, however, seems in no particular way exceptional, and a misassignment seems plausible, considering that the other levels of the same multiplet have not yet been found.

Table 3 displays the transition energies, probabilities and oscillator strengths of the (allowed) E1 transitions of the $3s^23p^4$–$3s3p^5$ and $3s^23p^4$–$3s^23p^33d$ configurations. These transition probabilities are listed in two gauge forms, length and velocity gauge (respectively, Babushkin and Coulomb gauge in relativistic notation), in order to provide an indication of the quality of the data as well as reference for further investigations. Of course, an agreement of the results from different gauges for some individual line does not guarantee the accuracy of these particular data, but the overall agreement (or disagreement) for a whole transition array certainly provides insights into the quality of the approximation. Apart from the transition probabilities, we also list the weighted oscillator strengths for emission from the upper level (in length gauge) as well as the branch fractions (br) for a spontaneous decay of the upper level into the corresponding line. The branch fractions may help in identifying (new) lines and in carrying out lifetime measurements.

Good agreement between the length and velocity gauge results is obtained for the probabilities (and corresponding level lifetimes) for most medium and strong lines. As expected, some larger deviations among these two gauge forms arise for a few of the weaker lines, but they stay within a factor of 2. For a few selected transitions, Table 4 shows a comparison of transition probabilities with previous (semi-empirically adjusted) computations by Fawcett (1986) and Bhatia & Doschek (1996), and with those done by Deb & Tayal (1998). In the last column of this table, we also display data from the NIST Database; as seen from this

[3] NIST homepage at http://physics.nist.gov/PhysRefData/contents.html

Table 5. M1 and E2 transition energies, emission rates A and oscillator strengths gf for lines of the $3s^23p^4$ and $3s^23p^33d$ configurations of Fe XI. Notations are the same as in Table 3.

Trans.	J_F	J_I	Type	Wavenumber (cm^{-1})	Wavelength (Å)	A (s^{-1}) Length	Velocity	gf	br
3–23	4	3	M1	1587	63012.0	1.01(−1)		5.42(−2)	0.00
2–3	0	1	M1	1760	56818.2	2.78(−1)		1.35(−7)	1.00
23–24	5	4	M1	2111	47370.9	1.86(−1)		6.87(−7)	0.02
20–21	4	3	M1	4438	22532.7	1.63		1.12(−6)	0.01
23–25	4	4	M1	9540	10482.2	9.64(−2)		1.43(−8)	0.00
1–2	1	2	M1	12512	7992.33	4.22(+1)		1.21(−6)	1.00
16–21	4	3	M1	15451	6472.07	5.41		3.06(−7)	0.04
21–23	4	4	M1	21063	4747.66	5.41		1.64(−7)	0.23
21–24	5	4	M1	23171	4315.74	8.00		2.46(−7)	0.77
2–4	2	1	M1	26052	3838.48	9.90		1.09(−7)	0.10
25–32	4	4	M1	26822	3728.28	4.30(+1)		8.07(−7)	0.06
21–25	4	4	M1	30603	3267.65	3.18		4.58(−8)	0.05
24–32	4	5	M1	34251	2919.62	4.85(+1)		5.58(−7)	0.07
24–32	4	5	E2	34251	2919.62	8.87(−1)	6.37(−1)	1.02(−8)	0.00
23–32	4	4	M1	36363	2750.05	4.74(+1)		4.84(−7)	0.07
23–32	4	4	E2	36363	2750.05	3.71(−1)	3.59(−1)	3.79(−9)	0.00
20–25	4	3	M1	35041	2853.80	3.48		3.82(−8)	0.06
16–23	4	3	M1	36514	2738.68	4.59(−1)		4.65(−9)	0.02
22–32	4	3	M1	37949	2635.12	5.89		5.52(−8)	0.01
1–4	2	2	M1	38564	2593.09	9.19(+1)		4.63(−7)	0.90
1–4	2	2	E2	38564	2593.09	1.56(−1)	1.50(−1)	7.89(−10)	0.00
14–21	4	4	M1	42580	2348.52	3.08(+1)		2.29(−7)	0.25
13–21	4	3	M1	43447	2301.65	1.43		1.02(−8)	0.01
4–5	0	2	E2	43603	2293.42	8.77	9.13	6.92(−9)	0.01
15–25	4	2	E2	48293	2070.69	1.13(−1)	4.38(−1)	6.53(−10)	0.00
21–32	4	4	M1	57426	1741.37	2.44(+1)		9.98(−8)	0.04
21–32	4	4	E2	57426	1741.37	1.48	3.27	6.04(−9)	0.00
20–32	4	3	M1	61863	1616.48	1.20(+1)		4.25(−8)	0.02
14–23	4	4	M1	63643	1571.26	1.32(+1)		4.38(−8)	0.57
14–23	4	4	E2	63643	1571.26	1.00(−1)	1.03(−1)	3.34(−10)	0.00
13–23	4	3	M1	64510	1550.15	1.39		4.50(−9)	0.06
13–23	4	3	E2	64510	1550.15	1.07(−1)	2.35(−1)	3.48(−10)	0.00
14–24	5	4	M1	65754	1520.82	2.05		7.82(−9)	0.19
14–24	5	4	E2	65754	1520.82	2.12(−1)	2.99(−1)	8.09(−10)	0.02
2–5	0	1	M1	69654	1435.67	9.80(+2)		3.03(−7)	0.99
16–32	4	3	M1	72877	1372.18	3.87(+1)		9.83(−8)	0.06
16–32	4	3	E2	72877	1372.18	1.77	4.55	4.49(−9)	0.00
14–25	4	4	M1	73184	1366.42	2.63(+1)		6.63(−8)	0.42
13–25	4	3	M1	74051	1350.42	6.40		1.58(−8)	0.10
15–32	4	2	E2	75115	1331.29	6.01(−2)	3.19(−1)	1.44(−10)	0.00
1–5	0	2	E2	82167	1217.03	1.65	1.75	3.66(−10)	0.00
14–32	4	4	M1	100006	999.940	2.57(+2)		3.46(−7)	0.38
13–32	4	3	M1	100873	991.346	4.84(+1)		6.42(−8)	0.07
12–32	4	2	E2	101081	989.306	2.27(−1)	3.95(−1)	2.99(−10)	0.00
6–14	4	2	E2	104799	954.208	2.55(−1)	3.50(−1)	3.13(−10)	0.00
6–21	4	2	E2	147379	678.523	2.78(+1)	3.69(+1)	1.73(−8)	0.22
6–23	4	2	E2	168442	593.676	3.52(−1)	3.67(−1)	1.67(−10)	0.02
6–25	4	2	E2	177983	561.851	3.16	3.65	1.35(−9)	0.05
6–32	4	2	E2	204805	488.269	1.26(+2)	1.49(+2)	4.06(−8)	0.02

comparison, rather sizeable deviations may arise even for strong transitions. [Further such comparisons have been presented by Deb & Tayal (1998).] Such deviations may amount, for instance for the line 47–5, to 4 per cent and 13 per cent, respectively, if compared with Deb & Tayal (1998) and the NIST Database (Fuhr et al. 2000) – this is within the expected accuracy of both our data and those from NIST – but to as much as 38 per cent in comparison to the predictions given by Bhatia & Doschek (1996). For the strong lines, our transition data generally agree satisfactorily with those of Fawcett (1986) and Deb & Tayal (1998); they are, however, in much less agreement with the recently revised set of E1 transition data given by Bhatia & Doschek (1996). For the weak lines (which were not included by Fawcett), the agreement with Deb & Tayal (1998) is still

satisfactory at the level of a factor of 2–3. For these lines, larger deviations between different gauge forms typically occur in all of the computations. Owing to our 'systematically' enlarged wavefunction expansions and the inclusion of relaxation effects, however, we expect our data to be more consistent than those from semi-empirical studies. On the other hand, these weak lines are known to be sensitive to configuration mixings and, thus, might benefit from semi-empirical adjustments of the Hamiltonian matrix as has been carried out by Fawcett (1986) and Deb & Tayal (1998). The computations by Bhatia & Doschek (1996) are probably less accurate, in particular for medium–intense and weak lines, because only rather small wavefunction expansions were used in those calculations.

The $3s^23p^33d$ excited levels with $J = 4$ and 5 can decay spontaneously only via *forbidden* transitions into lower-lying levels of the same configuration or, for $J = 4$, also into the ground configuration. These metastable levels and their decays have already been discussed by Mason & Nussbaumer (1977). In Table 5, we report the transition probabilities, oscillator strengths and branching ratios for the magnetic dipole (M1) and electric quadrupole (E2) transitions within the $3s^23p^4$, $3s3p^5$ and $3s^23p^33d$ configurations. Only transitions with a transition rate of $A > 10^{-1}\,s^{-1}$ are included in the table. As seen from this table, the decays are predominantly due to M1 transitions, but for some of the lines, the E2 component contributes at the 10 per cent level. Unlike E1 lines, the ('weak') electric quadrupole transitions are sensitive to the applied gauge of the radiation field, and deviations of up to a factor of 5 between the results from using length or velocity gauges are found. The transition probabilities for the magnetic quadrupole lines from the $J = 4$ levels to the two $3s^23p^4$ $J = 2$ levels of the ground configuration are listed in Table 6. These M2 rates are typically of the same order of magnitude as the decay of the $J = 4$ levels to levels within the same configuration. In one case, the ^{5}D level multiplet (levels 10 to 14), however, our calculations show that the M2 decay from level 14 to the ground state dominates by far (Table 6). This insight confirms earlier estimates of a line near 260 Å that were based on simpler calculations (Mason & Nussbaumer 1977). We identify this transition with a line in the solar spectrum, at 256.68 Å, which originally had been assigned to S XI only (Dere 1978). Our new identification completes the multiplet. While our calculated fine-structure splittings for this multiplet differ from the experimental ones by about 20 per cent, the calculated excitation energies are very close (<0.2 per cent) to the measured data (Table 2). For the other $J = 4$ and $J = 5$ levels, an experimental verification is less likely, as they all have several decay branches that therefore will individually be weaker. If, however, those individual transitions could be identified, our data set below makes consistency checks possible. Fortunately for the present new assignment, substantial fractions of the decays of the still unidentified high-J levels point towards this very level 14 and thus boost its decay intensity. At a lifetime of 28 ms, this decay could not be seen by conventional means in the laboratory, but only in the low collision rate environment of the Sun. It may be observable, however, in forthcoming experiments at electron beam ion traps (EBIT).

Our identification of an M2 transition in Fe XI suggests reconsideration of the search for another M2 transition, $3s^23p^5$ $^2P_{3/2}$–$3s^23p^43d$ $^4D_{7/2}$ in Fe X, that has also been indicated by Mason & Nussbaumer (1977) for the same wavelength range. Combining evidence from solar spectra, tokamak plasmas and beam–foil data, Smitt (1976) and Jupén et al. (1993) identified a line at 257.262 Å with the $3s^23p^5$ $^2P_{3/2}$–$3s^23p^43d$ $^4D_{5/2}$ E1 intercombination transition in Fe X. This line is blended with one of the components of the Fe XI multiplet discussed above, $3s^23p^4$ $^3P_2$–$3s^23p^43d$ $^5D_3$. As the two upper $3s^23p^43d$ ^4D levels with $J = 5/2$ and $J = 7/2$ in Fe X are only narrowly spaced, an E1 decay of the $J = 5/2$ level and an M2 decay of the $J = 7/2$ level will be difficult to resolve spectroscopically, and these lines will normally appear blended with each other. In the laboratory the first component will be dominant and the second will be

Table 6. M2 transition energies, emission rates A and oscillator strengths for the $3s^23p^4$–$3s^23p^3$ 3d lines of Fe XI. Notations are the same as in Table 3.

Trans.	J_F	J_I	Type	Wavenumber (cm^{-1})	Wavelength (Å)	A (s^{-1}) Length	gf	br
1–14	4	2	M2	388764	257.225	3.54(+1)	3.19(−9)	1.00
4–21	4	2	M2	392781	254.595	5.71(+1)	4.99(−9)	0.46
4–23	4	2	M2	413844	241.637	1.31	1.03(−10)	0.06
4–25	4	2	M2	423384	236.192	1.61(+1)	1.21(−9)	0.26
1–21	4	2	M2	431344	231.834	9.80(−1)	7.11(−11)	0.00
1–23	4	2	M2	452407	221.040	7.57(−1)	4.99(−11)	0.03
1–25	4	2	M2	461948	216.475	4.18	2.64(−10)	0.07
1–32	4	2	M2	488770	204.595	1.19(+1)	6.73(−10)	0.02

Table 7. Calculated M1, E2 and M2 forbidden transition probabilities A (s^{-1}) for a few selected lines of the $3s^23p^4$ and $3s^23p^33d$ configurations, compared with previous computations and evaluated data from the NIST Atomic Spectroscopic Database.

Trans.	Type	This work	Mason & Nussbaumer (1977)	Biemont & Hansen (1986)	Fuhr et al. (200)
2–3	M1	2.78(−1)		2.49(−1)	2.26(−1)
1–4	M1	9.19(+1)		9.25(+1)	1.5(−1)
	E2	1.56(−1)		1.54(−1)	1.5(−1)
4–121	M1	3.08(+1)			2.8(+1)
6–25	M1	3.16			1.8
4–21	M2	5.71(+1)	4.0(+1)		4.0(+1)
1–25	M2	4.18	1.3		1.3

practically invisible (because of collisional quenching of the upper level), while in the solar spectrum both levels may contribute to the observed line, but the M2 component will be the stronger one. This implies that, depending on the conditions in the light source, different transitions dominate the observation of what is perceived as the same line.

Unfortunately, hardly any experimental lifetimes are presently available for comparison with our ab initio predictions. The only exceptions are beam–foil lifetime data on the incompletely resolved ground-state intercombination transition multiplet (Träbert et al. 1993) that corroborate our results for several of the $3s^23p^33d\ ^5D_J$ levels. At face value, the measured lifetimes are up to 50 per cent longer than our present predictions. However, the signal level on such long-lived decays was low, and not much more than one decay length (for the 40-ns long-lived component even less than one) was covered. Such a situation poses severe problems for any multi-exponential analysis, and therefore the numerical results of the experimental work should not be overinterpreted. Moreover, our tables show why there is such a lack of further experimental data. A large number of levels feature lifetimes of many nanoseconds or even milliseconds. In many terrestrial light sources, such levels will be too long-lived to be observed. Beam–foil spectroscopy has practical limits for the measurement of lifetimes of such long-lived levels because of geometrical constraints. Also, this technique is ion source and accelerator limited for the necessary signal level above background (Träbert 1997). Even in dilute tokamak plasmas, such long-lived levels may be collisionally quenched rather than the radiative decays be seen (Sugar, Kaufman & Rowan 1987). Consequently, most previous line identifications relate to transitions in the ground complex (from solar observations) and to short-lived (few picosecond lifetimes) levels whose lifetimes can be more accurately predicted than measured.

For a few M1/E2 transitions, a comparison with previous computations and estimates from the NIST Database is presented in Table 7. Considering the spectra of the *SOHO* mission and other such enterprises mentioned above, there certainly is a need to pursue the problem of laboratory measurements on such transitions, so that those lines can be analysed in the near future. In this context, particular hope rests on the progress in the development of electron beam ion trap (EBIT) devices, which have demonstrated their capability to provide not only spectral observation of forbidden transitions like the solar coronal lines, but also to measure radiative lifetimes reliably in the millisecond range (Träbert, Utter & Beiersdorfer 2000a; Träbert et al. 2000b). Once the wavelengths are known, an alternative, very accurate technique to measure millisecond atomic lifetimes is offered by using heavy-ion storage rings (Träbert et al. 1999). Our transition energies and probabilities may propel the analysis of such lines and, possibly, also entire new lifetime measurements. Accurate lifetime data might be of interest first of all for the ground-state configuration, since in many astrophysical and laboratory plasmas these lines will be *optically thin*, and this renders them a very useful tool for plasma diagnostics.

4 CONCLUSIONS

In summary, we have calculated the electric dipole allowed and forbidden transitions in the low-lying spectrum of Fe XI. This work extends a previous study on Fe X, which promoted the identification of forbidden lines and the evaluation of data from recent lifetime measurements. With our systematically enlarged wavefunctions we are able to provide consistent and accurate data not only for the (strong) E1 resonance lines but also for weak and forbidden transitions, and to assign an M2 transition in the solar EUV spectrum. For the other $J = 4$ and $J = 5$ levels, our data might guide future laboratory work using EBIT or a heavy-ion storage ring and help to identify further yet unidentified lines in solar spectra.

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