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Atomic data from the Iron Project*

LIV. Relativistic calculations for allowed and forbidden fine structure transitions in Fe XX

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Abstract. An extensive set of oscillator strengths (f), line strengths (S) and radiative decay rates (A) for dipole allowed, intercombination and forbidden transitions in Fe XX is presented. Results include 1792 bound fine structure levels of total angular momenta $J = 1/2$–$19/2$ of even and odd parities, with $2 \leq n \leq 10$, $0 \leq l \leq 14$, orbital angular momenta, $0 \leq L \leq 14$, and total spin multiplicities 2S+1 = 2,4,6, yielding to about 3.8×10^5 allowed and 13,874 forbidden transitions in Fe XX. These results far exceed the available data in literature. The existing data compiled by the National Institute for Standards and Technology (NIST) are available for little over one hundred transitions, and the previously calculated data under the Opacity Project includes 75 590 LS multiplets. The present ab initio calculations are carried out in the close coupling approximation using the relativistic Breit-Pauli R-matrix method for allowed and intercombination E1 transitions. The wavefunction expansion includes 20 fine structure levels of configurations $2s^22p^2$, $2s2p^3$, and $2p^4$ of the core ion Fe XXI. Computed energy levels are identified spectroscopically using a newly developed procedure based on quantum defects and channel contributions. All 55 observed levels have been identified and are in agreement to much less than 1% with most of the calculated values. Coefficients for radiative decays for the forbidden E2, E3, M1 transitions are obtained through atomic structure calculations including relativistic terms in the Breit-Pauli approximation using the code SUPERSTRUCTURE. The theoretical transition probabilities are compared with available values, with varying degree of agreement.

Key words. atomic data

1. Introduction

Highly charged ions of iron are observed in a variety of high-temperature astrophysical sources, ranging from the UV to the X-ray. Spectral analysis and modeling of these spectra require accurate radiative data. However, currently available data is inadequate and incomplete for these purposes. While laboratory work has been carried out for some transitions, such measurements are generally very limited in scope and usually entail only the low-lying transitions. Systematic calculations with high precision have not yet been done for most of the iron ions. On the other hand, recent observations from space based UV and X-ray observatories, such as the HST, FUSE, Chandra and XMM-Newton, show a plethora of high excitation/high ionization lines of most ionization stages of iron. In order to address the great and growing need, work has been initiated to compute radiative data for Fe ions under the Iron Project (Hummer et al. 1993).

In this report large scale datasets for oscillator strengths (f-values), line strengths (S), and transition probabilities (A-values) for E1 (dipole allowed and intercombination), and forbidden electric quadrupole (E2) and octupole (E3), and magnetic dipole (M1) fine structure transitions in nitrogen-like Fe XX are presented. Calculations are carried out using the relativistic Breit-Pauli R-matrix method developed under the Iron Project for the $E1$ transitions, and configuration interaction atomic structure calculations using the code SUPERSTRUCTURE (Eissner et al. 1974; Nahar et al. 2003) for the forbidden $E2$, $E3$, and $M1$ transitions. All together these data should comprise a reasonably complete set of transitions for all practical applications involving Fe XX.

Currently, a limited number of 124 transitions in Fe XX are found in the evaluated compilation of results, obtained by various investigators using different methods, from the web based database of the National Institute for Standards and Technology (NIST). The most extensive previous calculations for oscillator strengths for Fe XX were carried out by VM Burke and DJ Lennon, under the Opacity Project (OP 1995, 1996), that are now accessible through the OP database, TOPbase (Cunto et al. 1993). However, the OP f-values were obtained for

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* Complete electronic files for energies (e.g. Tables 3a, 3b, 7) and transition probabilities (e.g. Tables 4, 5, 8) are available at the CDS via anonymous ftp to `cdsarc.u-strasbg.fr (130.79.128.5)` or via `http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/413/779`

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75 590 dipole allowed multiplets in LS coupling; neglect of fine structure in the OP work was not crucial in the calculation of mean stellar opacities. But fine structure is of paramount importance in spectral line diagnostics of highly charged ions. The present work reports both the allowed and the forbidden transitions for Fe XX including fine structure, of potential importance not only for more accurate plasma opacities, but also in the synthesis of spectral models and in experimental or observational spectral analysis.

2. Theory

The Breit-Pauli R-matrix (BPRM) method, developed under the Iron Project (IP, Hummer et al. 1993; Berrington et al. 1987, 1995) includes relativistic effects in the Breit-Pauli approximation (Scott & Burke 1980; Scott & Taylor 1982). It enables calculation of both the dipole allowed ($\Delta S = 0$) and the intercombination ($\Delta S \neq 0$) E1 transition probabilities in intermediate coupling, in contrast to the OP work in *LS* coupling where only dipole allowed multiplet transitions could be considered. Also, incorporation of the relativistic effects in the close coupling R-matrix method yields a large number of fine structure transition probabilities with higher accuracy.

Many relevant theoretical details of the relativistic BPRM method are discussed in previous works, such as in the first large scale relativistic BPRM calculations for bound-bound transitions in Fe XXIV and Fe XXV (Nahar & Pradhan 1999) and for other ions (Nahar & Pradhan 2000 for Fe V, Nahar et al. 2000 for Fe V, Nahar 2002a for C II and C II, Nahar 2002b for Fe XXI and Ar XIII, Nahar et al. 2003 for Fe XVII). A detailed description of atomic structure calculations for the forbidden transitions, involving the various terms in the Breit-Pauli Hamiltonian, are presented in Nahar et al. (2003). Below, we outline the salient features of these calculations.

In the CC approximation the wavefunction expansion, $\Psi(E)$, for a $(N+1)$ electron system with total spin and orbital angular momenta symmetry $SL\pi$ or total angular momentun symmetry $J\pi$, is described in terms of the target ion states as:

$$\Psi_E(\mathrm{e+ion}) = A\sum_i \chi_i(\mathrm{ion})\theta_i + \sum_j c_j\Phi_j(\mathrm{e+ion}), \tag{1}$$

where χ_i is the target ion wavefunction in a specific state $S_iL_i\pi_i$ or level $J_i\pi_i$, and θ_i is the wavefunction for the interacting $(N+1)$th electron in a channel labeled as $S_iL_i(J_i)\pi_i\, k_i^2\ell_i(SL\pi\ or\ \ J\pi)$ where k_i^2 is the incident kinetic energy. In the second sum the Φ_j's are correlation wavefunctions of the $(N+1)$ electron system that (a) compensate for the orthogonality conditions between the continuum and the bound orbitals, and (b) represent additional short-range correlation that is often of crucial importance in scattering and radiative CC calculations for each $SL\pi$.

The relativistic $(N+1)$-electron Hamiltonian for the N-electron target ion and a free electron in the Breit-Pauli approximation, as adopted in the IP BPRM codes, is

$$H^{\mathrm{BP}}_{N+1} = H_{N+1} + H^{\mathrm{mass}}_{N+1} + H^{\mathrm{Dar}}_{N+1} + H^{\mathrm{so}}_{N+1}, \tag{2}$$

where H_{N+1} is the non-relativistic Hamiltonian,

$$H_{N+1} = \sum_{i=1}^{N+1}\left\{-\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N+1}\frac{2}{r_{ij}}\right\}. \tag{3}$$

added by the one-body mass correction term (H^{mass}_{N+1}), the Darwin term (H^{Dar}_{N+1}), and the spin-orbit interaction term (H^{so}_{N+1}). The mass-correction and Darwin terms improve the energies while the spin-orbit interaction term splits the energies into fine structure components. Present Hamiltonian does not include the two-body spin-spin and spin-other-orbit terms. The set of $SL\pi$ are recoupled to obtain (e + ion) states with total $J\pi$, following the diagonalization of the $(N+1)$-electron Hamiltonian,

$$H^{BP}_{N+1}\Psi = E\Psi. \tag{4}$$

Substitution of the wavefunction expansion introduces set of coupled equations that are solved using the *R*-matrix approach. At negative total energies ($E < 0$), the solutions of the close coupling equations occur at discrete eigenvalues of the (e + ion) Hamiltonian that correspond to pure bound states Ψ_B.

The primary quantity expressing radiative excitation or de-excitation in a weak field is the line strength

$$S^{\mathrm{X}\lambda}(ij) = \left|\left\langle \Psi_j \middle\| O^{\mathrm{X}\lambda} \middle\| \Psi_i \right\rangle\right|^2, \qquad S(ji) = S(ij), \tag{5}$$

for various multipole transitions $\mathrm{X}\lambda(ij)$ (Nahar et al. 2003). The oscillator strength, f_{ij}, for electric dipole (E1) transition, for example, is obtained as

$$f_{ij} = \frac{E_{ji}}{3g_i}S^{E1}, \tag{6}$$

where E_{ji} is the transition energy in Rydberg between states i and j and S^{E1} is the line strength. The coefficient for radiative decay, A_{ji} (or the transition probability) is defined as

$$A_{ji}(\mathrm{a.u.}) = \frac{1}{2}\alpha^3\frac{g_i}{g_j}E_{ji}^2 f_{ij}, \tag{7}$$

where α is the fine structure constant, and g_i, g_j are the statistical weight factors of the initial and final states, respectively. The A-values or the Einstein coefficients for spontaneous decay by higher order multipole radiation are as follows:

electric quadrupole (E2) and magnetic dipole (M1)

$$g_jA^{\mathrm{E2}}_{ji} = 2.6733\times10^{3}\mathrm{s}^{-1}\,(E_j-E_i)^5 S^{\mathrm{E2}}(i,j) \tag{8}$$

$$g_jA^{\mathrm{M1}}_{ji} = 3.5644\times10^{4}\mathrm{s}^{-1}\,(E_j-E_i)^3 S^{\mathrm{M1}}(i,j); \tag{9}$$

and for electric octopole (E3)

$$g_jA^{\mathrm{E3}}_{ji} = 1.2050\times10^{-3}\mathrm{s}^{-1}\,(E_j-E_i)^7 S^{\mathrm{E3}}(i,j). \tag{10}$$

The lifetime of a level can be obtained from the A-values as,

$$\tau_k(s) = \frac{1}{A_k}, \tag{11}$$

where A_k is the total radiative transition probability for the level k, i.e., $A_k = \sum_i A_{ki}(\mathrm{s}^{-1})$, and $A_{ji}(\mathrm{s}^{-1}) = A_{ji}(\mathrm{a.u.})/\tau_0$, $\tau_0 = 2.4191\times10^{-17}$ s is the atomic unit of time.

3. Calculations

The CC calculations using the BPRM method proceed in several stages. Below we describe these as they pertain to Fe XX.

Table 1. Fine structure levels and the relative energies of the target (core) ion Fe XXI in wavefunction expansion of Fe XX. The atomic structure calculations for the wavefunction employs spectroscopic set of configurations: $2s^22p^2$, $2s2p^3$, $2p^4$, $2s^22p3s$, $2s^22p3p$, $2s^22p3d$, $2s2p^23s$, $2s2p^23p$, $2s2p^23d$, $2p^33s$, and correlation configurations: $2p^33p$, $2p^33d$, $2p^34s$, $2p^34p$, $2p^34d$, $2s^22p4s$, $2s^22p4p$, $2s^22p4d$, $2s2p^24s$, $2s2p^24p$, $2s2p^24d$, and the Thomas-Fermi scaling parameters for the orbitals: λ_{nl} = 1.42(1s), 1.25(2s), 1.15(2p), 1.25(3s), 1.15(3p), 1.17(3d), –1.20(4s), –1.20(4p), –1.2(4d).

	Term	J_t	E_t (Ry)
1	$2s^22p^2(^3P)$	0	0.0
2	$2s^22p^2(^3P)$	1	0.67297
3	$2s^22p^2(^3P)$	2	1.0694
4	$2s^22p^2(^1D)$	2	2.2286
5	$2s^22p^2(^1S)$	0	3.3890
6	$2s2p^3(^5S^o)$	1	4.4374
7	$2s2p^3(^3D^o)$	1	7.0785
8	$2s2p^3(^3D^o)$	2	7.0837
9	$2s2p^3(^3D^o)$	3	7.3260
10	$2s2p^3(^3P^o)$	0	8.3507
11	$2s2p^3(^3P^o)$	1	8.4281
12	$2s2p^3(^3P^o)$	2	8.5871
13	$2s2p^3(^3S^o)$	1	9.9838
14	$2s2p^3(^1D^o)$	2	10.268
15	$2s2p^3(^1P^o)$	1	11.491
16	$2s2p^4(^3P)$	2	15.002
17	$2s2p^4(^3P)$	1	15.861
18	$2s2p^4(^3P)$	0	15.817
19	$2s2p^4(^1D)$	2	16.560
20	$2s2p^4(^1S)$	0	18.665

3.1. Wavefunction expansion

The most important initial step is to construct an accurate representation of the target or core ion eigenstates. The wavefunction expansion for the Fe XX → (e + Fe XXI) system consists of 20 fine strucuture levels (Table 1) of the target ion Fe XXI from configurations $2s^22p^2$, $2s2p^3$, $2p^4$. The target wavefuctions were obtained from atomic structure calculations using SUPERSTRUCTURE (Eissner et al. 1974). Table 1 lists the set of spectroscopic and correlation configurations, and the values of Thomas-Fermi scaling parameters for individual orbitals λ_{nl} employed in the atomic structure calculations. All orbitals up to the 3d were treated as spectroscopic, i.e. included in the total Fe XX wavefunction expansion. The relative energies given in Table 1 are the measured values in the NIST database that are used in the BPRM calculations for radiative data.

The bound-channel term of the wavefunction, the second term in Eq. (1), includes all possible $(N + 1)$-configurations from vacant orbitals to maximum occupancies $2s^2$, $2p^6$, $3s^2$, $3p^2$, and $3d^2$.

3.2. The allowed and intercombination E1 transitions

As mentioned, the BPRM calculations involve several stages and begin with the wavefunctions of the target or the core eigenstates. The one-electron orbitals from SUPERSTRUCTURE are used as the input for the BPRM codes to compute the one- and two-electron radial integrals, in STG1. The (e + ion) algebraic and angular coefficients are computed in STG2. The intermediate coupling calculations are enabled on recoupling the LS symmetries in a pair-coupling representation in stage RECUPD. The (e + core) Hamiltonian matrix is diagonalized for each resulting $J\pi$ in STGH.

Calculations for Fe XX transitions included all possible bound levels for $1/2 \leq J \leq 19/2$ of even and odd parities, with $n \leq 10$, $l \leq 12$, $0 \leq L \leq 14$, and $(2S + 1) = 2, 4, 6$. The fine structure bound levels are obtained on scanning through the poles in the (e + ion) Hamiltonian with a fine mesh of effective quantum number ν, at $\Delta\nu = 0.001$ or less. The mesh is orders of magnitude finer than the typical $\Delta\nu = 0.01$ generally employed in the OP work to obtain the LS energy terms. This is one of the main reasons that the BPRM calculations require orders of magnitude more CPU time and memory than LS coupling. Since the fine structure components lie in smaller energy gaps, a very fine mesh is essential to avoid any missing levels and to obtain accurate energies for high-lying levels.

The large number of theoretically computed fine structure energy levels are identified using a newly developed spectroscopic identification procedure encoded in the code PRCBPID (Nahar & Pradhan 2000). The levels obtained from the BPRM calculations occur at eigenvalues of the BP Hamiltonian, labeled only by the total angular momentum and parity, i.e. by $J\pi$, which is insufficient for unique identification. The computed energies however yield quantum defects relative to the parent target level $S_iL_iJ_i$ to which a given Rydberg series of bound levels $(S_iL_iJ_i)n\ell$ belongs. The identification procedure coded in PRCBPID employs quantum defect analysis of levels computed up to effective quantum number $\nu \approx 10$, together with an analysis of the wavefunction components of all coupled channels. However, often a level can be assiged to a multiple spectroscopic identification. The spectroscopic identification of low lying levels are reconfirmed by comparing with those of available levels, especially those found in the NIST database. The remaining energy levels, following Hund's rule, are assigned notation such that a level with higher angular orbital momentum L and/or higher spin multiplicity lies below the lower L and/or lower spin multiplicity. The final designation assignment is given as $C_t(S_tL_t\pi_t)J_tnlJ(SL)\pi$, where C_t, $S_tL_t\pi_t$, J_t are the configuration, LS term and parity, and total angular momentum of the target, nl are the principal and orbital quantum numbers of the outer or the valence electron, and J and $SL\pi$ are the total angular momentum, LS term and parity of the $(N+1)$-electron system. In addition the level identification procedure establishes a unique correspondence between the fine structure levels and their LS terms such that exact number of fine structure levels are accounted for each LS term.

3.3. Forbidden transitions

Forbidden transition are considered through configuration interaction atomic structure calculations using the code SUPERSTUCTURE (Eissner et al. 1974). The code has been updated to consider electric octupole (E3) and magnetic quadrupole (M2) transitions in addition to electric dipole (E1) and quadrupole (E2) and magnetic dipole (M1) in Breit-Pauli approximation (Nahar et al. 2003). First reported results on higher multipole transitions are on Fe XVII (Nahar et al. 2003). A^{E2}, A^{E3}, and A^{M1} are obtained for almost 14 000 forbidden transitions among the first 215 levels of Fe XX.

4. Results and discussion

Computed data are presented and discussed separately for energy levels, oscillator strengths for E1 transitions, and forbidden transitions.

4.1. Theoretical energy levels

1792 fine structure levels are found theoretically. Oscillator strengths, line strengths, and transition probabilities for the bound-bound allowed and forbidden transitions among these levels in Fe XX are computed. The energy levels correspond to total angular momenta $1/2 \leq J \leq 19/2$ of even and odd parities, and levels up to $n \leq 10$ and $0 \leq l \leq 14$, with total orbital angular momenta $0 \leq L \leq 14$ and spin multiplicities $2S + 1 = 2, 4, 6$.

A total of 63 levels (55 from energy table and 8 from the transition table) are available from the NIST compilation. Each of them has been identified in the theoretical dataset. Table 2 presents comparison between calculated BPRM energies and the measured values. Most of the calculated levels are well within 1% of the measured energies, with the largest discrepancy being 3.4% for the level $2s^22p^2(^3P)4d(^4P_{5/2})$. The measured value for this component, $^4P_{5/2}$, is relatively larger compared to the other two components $^4P_{3/2}$ and $^4P_{1/2}$, where the differences are less than 1%. The level index, I_J, in the table, is the position of the calculated level in the given $J\pi$ symmetry. This establishes the correspondence between the calculated and the observed levels, useful in applications.

The complete set of calculated energy levels of Fe XX is availabe eletronically. Following previous works, (e.g. Nahar et al. 2000) the energies are presented in two formats, (i) where levels are ordered as components of a LS term showing spectroscopic completeness of the set, and (ii) in ascending energy order for each $J\pi$ symmetry for practical applications.

4.1.1. LSJ term format

In the LS term format the fine structure components LSJ are grouped together according to the same configuration $CLSJ$, useful for spectroscopic diagnostics. It also provides the check for completeness of sets of energy levels that should belong to the corresponding LS term, and detects any missing level. Table 3a presents a sample set of Fe XX levels in this format. The columns provide the core information, $C_t(SL\pi\ J)_t$, the configuration of the outer electron, nl, total angular momentun, J, energy in Rydbergs, the effective quantum number of the valence electron, ν (= $z/\sqrt{(E - E_t)}$, where E_t is the next immediate target threshold energy), and possible LS term designations of the level. No effective quantum number is assigned for an equivalent electron state. The top line of each set provides the expected number of fine structure levels (Nlv) for the $^{(2S+1)}L^{\pi}$ terms, where spin multiplicity $(2S+1)$ and parity π are defined. Values of L and of total angular momentum J associated with each L are specified within parentheses next to L. The line is followed by set of BPRM energy levels of same configurations. $Nlv(c)$ at the end of the set specifies total number of calculated J-levels obtained. If $Nlv = Nlv(c)$ for

Table 2. Comparison of calculated BPRM absolute energies, E_c, with the observed ones, E_o, for Fe XX. I_J is the level index for calculated energy position in symmetry $J\pi$. The asterisk next to a J-value indicates that the term has incomplete set of observed fine structure levels.

Level		J	I_J	E_o (Ry)	E_c (Ry)
2s22p3	$^4S^o$	1.5	1	115.735	115.80
2s22p3	$^2D^o$	2.5	1	114.080	114.19
2s22p3	$^2D^o$	1.5	2	114.451	114.54
2s22p3	$^2P^o$	1.5	3	112.741	112.85
2s22p3	$^2P^o$	0.5	1	113.324	113.43
2s2p4	^4P	2.5	1	108.833	108.94
2s2p4	^4P	1.5	1	108.225	108.32
2s2p4	^4P	0.5	1	108.024	108.12
2s2p4	^2D	2.5	2	106.002	106.16
2s2p4	^2D	1.5	2	106.161	106.30
2s2p4	^2S	0.5	2	104.752	104.91
2s2p4	^2P	1.5	3	104.314	104.48
2s2p4	^2P	0.5	3	103.421	103.59
2p5	$^2P^o$	1.5	4	97.8132	97.989
2p5	$^2P^o$	0.5	2	96.8164	97.008
2s22p2(3P)3s	^4P	2.5*	3	49.4420	49.287
2s22p2(3P)3s	^4P	0.5*	4	50.4616	50.243
2s22p2(1D)3s	^2D	2.5*	4	48.1968	48.093
2s22p2(1S)3s	^2S	0.5	6	46.9768	46.963
2s22p2(3P)3d	^4F	1.5*	8	45.3824	45.888
2s22p2(3P)3d	^4D	0.5*	7	45.3140	45.159
2s22p2(3P)3d	^4P	2.5*	8	44.6892	44.703
2s22p2(3P)3d	^4P	1.5*	10	44.5820	44.703
2s22p2(3P)3d	^2F	3.5*	3	44.3800	44.539
2s22p2(3P)3d	^2D	2.5	9	44.1632	44.329
2s22p2(3P)3d	^2D	1.5	11	44.1718	44.184
2s22p2(1D)3d	^2D	2.5	11	43.4728	43.691
2s22p2(1D)3d	^2D	1.5	13	43.5112	43.637
2s22p2(1D)3d	^2F	3.5	6	43.2888	43.491
2s22p2(1D)3d	^2F	2.5	13	43.0104	43.054
2s22p2(1D)3d	^2P	1.5*	15	42.9780	43.199
2s22p2(1D)3d	^2S	0.5	12	43.0172	42.944
2s22p2(1S)3d	^2D	2.5*	14	42.2322	42.470
2s22p2(1S)3d	^2D	1.5	16	42.1436	42.343
2s22p2(3P)4d	^4P	2.5	38	24.8966	25.767
2s22p2(3P)4d	^4P	1.5	48	24.4402	24.591
2s22p2(3P)4d	^4P	0.5	35	24.6935	24.591
2s22p2(3P)4d	^4F	2.5*	39	24.6674	25.202
2s22p2(3P)4d	^4D	2.5*	40	24.6004	24.746
2s22p2(3P)4d	^2F	3.5	18	24.4444	24.500
2s22p2(3P)4d	^2F	2.5	41	24.3594	25.001
2s22p2(3P)4d	^2D	2.5	42	24.1820	24.500
2s22p2(3P)4d	^2D	1.5	50	24.2070	24.281
2s22p2(1D)4d	^2D	2.5	44	23.2710	23.379
2s22p2(1D)4d	^2D	1.5	52	23.2687	23.489
2s22p2(1D)4d	^2G	3.5*	20	23.3784	23.379
2s22p2(1D)4d	^2F	2.5*	45	23.1110	23.315
2s22p2(1D)4d	^2P	1.5*	53	23.0968	23.315
2s22p2(1S)4d	^2D	2.5	46	22.0780	22.040
2s22p2(1S)4d	^2D	1.5	54	21.9918	22.222
2s22p2(3P)5d	^4P	2.5	71	16.0034	16.198
2s22p2(3P)5d	^4P	1.5	87	15.0865	15.123
2s22p2(3P)5d	^4P	0.5	61	15.0444	15.123
2s22p2(3P)5d	^4F	2.5*	74	15.5370	15.615
2s22p2(3P)5d	^2F	3.5	45	15.1991	15.132
2s22p2(3P)5d	^2F	2.5	75	15.4288	15.579
2s22p2(3P)5d	^2D	2.5*	79	15.1586	15.233
2s22p2(3P)5d	^4D	2.5*	81	15.0284	15.123
2s22p2(1D)5d	^2G	3.5*	53	14.0875	14.166
2s22p2(1D)5d	^2D	2.5	88	14.0321	14166
2s22p2(1D)5d	^2D	1.5	94	14.1017	14.103
2s22p2(1D)5d	^2F	2.5*	89	13.9920	14.021
2s22p2(1D)5d	^2P	1.5*	95	14.0277	14.021

a given term, the calculated energy set is complete. The correspondence of coupled channel wavefunctions and completeness of levels is obtained by the program PRCBPID, which also detects the missing levels. Each level is further identified by all possible *LS* terms in the last column. In case of multiple assignment of *LS* terms, spectroscopic identification of the level can be reduced to the most probable but approximate one by application of Hund's rule mentioned above. It may be noted that levels in the table are grouped consistently, in closely spaced energy ranges and in effective quantum numbers, confirming further the proper designation of the *LS* terms on the whole.

4.1.2. Energy order format

In this format the fine structure levels are presented as sets, ordered in descending energies, belonging to various $J\pi$ symmetries. A sample is shown in Table 3b. The format is convenient for easy implementation in astrophysical models requiring large number of energy levels and corresponding transitions. At the top of each set the total number of energy levels *Nlv* and the symmetry $J\pi$ are specified. For example, the table shows that there are 127 fine structure levels of Fe XX with $J\pi = 1/2^{\rm e}$. The levels are identified by the configuration and *LS* term designation of the parent core, the outer electron quantum numbers (*nl*), absolute energy in Rydberg, the effective quantum number (ν), and the final *LS* term designation. A level may be assigned to one or more *LS* terms in the last column. If the number of possible terms is more than one, all are specified. However, the assigned term may be determined from a variation of Hund's rule as a guideline, as mentioned before,: the term with higher angular momentum lies lower in energy. One reason for specifying all possible terms is that the order of calculated energy levels may not match exactly with that of the measured ones. The other reason is that Hund's rule often does not apply to all cases in complex ions, especially the low lying ones; nonetheless, we find it is useful to establish completeness and order.

4.2. Oscillator strengths for allowed E1 transitions

The allowed E1 ($\Delta J = 0, \pm 1$) transitions are treated with the BPRM method. The 1792 fine structure levels of Fe XX yield approximately 3.8×10^5 allowed E1 (dipole allowed and intercombination) transitions. The table of oscillator strengths of complete set of fine structure transitions is available electronically. The table contains calculated transition probabilities, oscillator strengths, and line strengths alongwith the level energies. Although *A*, the *f*, and the *S* are related, all three are listed since different applications require one or the other quantity.

Table 3a. Sample table of fine structure energy levels of Fe XX as sets of *LS* term components. $C_{\rm t}$ is the core configuration, ν is the effective quantum number.

$C_{\rm t}(S_{\rm t}L_{\rm t}\pi_{\rm t})$		$J_{\rm t}$	*nl*	2*J*	*E* (Ry)	ν	$SL\pi$
Eqv electron/unidentified levels, parity: o							
2s22p3				3	–1.15735E+02		4 S o
Nlv(*c*) = 1 : set complete							
Eqv electron/unidentified levels, parity: o							
2s22p3				3	–1.14451E+02		2 D o
2s22p3				5	–1.14080E+02		2 D o
Nlv(*c*) = 2 : set complete							
Eqv electron/unidentified levels, parity: o							
2s22p3				1	–1.13324E+02		2 P o
2s22p3				3	–1.12741E+02		2 P o
Nlv(*c*) = 2 : set complete							
Eqv electron/unidentified levels, parity: e							
2s2p4				5	–1.08833E+02		4 P e
2s2p4				3	–1.08225E+02		4 P e
2s2p4				1	–1.08024E+02		4 P e
Nlv(*c*) = 3 : set complete							
Eqv electron/unidentified levels, parity: e							
2s2p4				3	–1.06161E+02		2 D e
2s2p4				5	–1.06002E+02		2 D e
Nlv(*c*) = 2 : set complete							
Eqv electron/unidentified levels, parity: e							
2s2p4				1	–1.04752E+02		2 S e
Nlv(*c*) = 1 : set complete							
Eqv electron/unidentified levels, parity: e							
2s2p4				3	–1.04314E+02		2 P e
2s2p4				1	–1.03421E+02		2 P e
Nlv(*c*) = 2 : set complete							
Nlv = 3, $^4L^e$: P (5 3 1)/2							
2s22p2	(3Pe)	1	3s	1	–5.04616E+01	2.80	4 P e
2s22p2	(3Pe)	1	3s	3	–4.98576E+01	2.81	4 P e
2s22p2	(3Pe)	2	3s	5	–4.94420E+01	2.81	4 P e
Nlv(*c*) = 3 : set complete							
Nlv = 2, $^2L^e$: P (3 1)/2							
2s22p2	(3Pe)	0	3s	1	–4.95776E+01	2.84	2 P e
2s22p2	(3Pe)	2	3s	3	–4.81072E+01	2.85	2 P e
Nlv(*c*) = 2 : set complete							
Nlv = 2, $^2L^e$: D (5 3)/2							
2s22p2	(1De)	2	3s	3	–4.91520E+01	2.79	2 D e
2s22p2	(1De)	2	3s	5	–4.81968E+01	2.82	2 D e
Nlv(*c*) = 2 : set complete							
Nlv = 8, $^4L^o$: S (3)/2 P (5 3 1)/2 D (7 5 3 1)/2							
2s22p2	(3Pe)	1	3p	1	–4.86256E+01	2.85	4 PD o
2s22p2	(3Pe)	1	3p	3	–4.82304E+01	2.86	4 SPD o
2s22p2	(3Pe)	0	3p	1	–4.80568E+01	2.88	4 PD o
2s22p2	(3Pe)	2	3p	3	–4.77760E+01	2.86	4 SPD o
2s22p2	(3Pe)	2	3p	5	–4.76976E+01	2.86	4 PD o
2s22p2	(3Pe)	2	3p	5	–4.74888E+01	2.87	4 PD o
2s22p2	(3Pe)	1	3p	3	–4.73964E+01	2.88	4 SPD o
2s22p2	(3Pe)	2	3p	7	–4.72804E+01	2.88	4 D o
Nlv(c)= 8 : set complete							

A sample set of transitions in Fe XX is presented in Table 4. The top of the table specifies the nuclear charge ($Z = 26$) and number of electrons in the ion ($N_{\rm elc} = 7$). Then sets of oscillator strengths belonging to various pairs of symmetries $J_i\pi_i - J_k\pi_k$ are given. The transition symmetries are expressed in the form of $2J_i$, π_i ($\pi = 0$ for even and $\pi = 1$ for odd parity), $2J_k$ and π_k to make whole numbers, at the top of the set. Hence Table 4 presents partial transitions of symmetries $J = 1/2^{\rm e} - J = 1/2^{\rm o}$. The next line gives the number of bound levels belonging to each symmetry, N_{Ji} and N_{Jk}. The line is followed by the number of transitions, $N_{Ji} \times N_{Jk}$. The first two columns are level indices I_i and I_k whose identification can be found from the energy table, the third and the fourth columns provide the energies E_i and E_k in Rydbergs. The fifth column is gf_L, where f_L is the oscillator strength in length formulation and $g = 2J + 1$ is

Table 3b. Sample table for calculated fine structure energy levels of Fe XX in $J\pi$ energy order. *Nlv* is the total number of levels of the symmetry.

Level				E (Ry)	ν	$SL\pi$
		Nlv = 127,		$J\pi$ = 1/2 e		
1	2s2p4		1/2	–1.08024E+02		^{4}Pe
2	2s2p4		1/2	–1.04752E+02		^{2}Se
3	2s2p4		1/2	–1.03421E+02		^{2}Pe
4	$2s22p2(^3P^e_0)$	3s	1/2	–5.04616E+01	2.80	^{4}Pe
5	$2s22p2(^3P^e_0)$	3s	1/2	–4.95776E+01	2.84	^{2}Pe
6	$2s22p2(^1S^e_0)$	3s	1/2	–4.69768E+01	2.82	^{2}Se
7	$2s22p2(^3P^e_0)$	3d	1/2	–4.53140E+01	2.95	^{4}PDe
8	$2s22p2(^3P^e_0)$	3d	1/2	–4.45636E+01	2.96	^{4}PDe
9	$2s22p2(^3P^e_0)$	3d	1/2	–4.44980E+01	2.96	^{2}Pe
10	$2s22p2(^1D^e_0)$	3d	1/2	–4.33144E+01	2.96	^{2}SPe
11	$2s2p3(^5S^o_0)$	3p	1/2	–4.31856E+01	2.90	^{4}Pe
12	$2s22p2(^1D^e_0)$	3d	1/2	–4.30172E+01	2.97	^{2}SPe
13	$2s2p3(^3D^o_0)$	3p	1/2	–4.14220E+01	2.87	^{4}PDe
14	$2s2p3(^3D^o_0)$	3p	1/2	–4.08576E+01	2.89	^{4}PDe
15	$2s2p3(^3D^o_0)$	3p	1/2	–4.04084E+01	2.90	^{2}Pe
16	$2s2p3(^3P^o_0)$	3p	1/2	–3.99518E+01	2.88	^{4}PDe
17	$2s2p3(^3P^o_0)$	3p	1/2	–3.95238E+01	2.89	^{2}SPe
18	$2s2p3(^3P^o_0)$	3p	1/2	–3.94558E+01	2.89	^{4}PDe
19	$2s2p3(^3P^o_0)$	3p	1/2	–3.86848E+01	2.91	^{2}SPe
20	$2s2p3(^3S^o_0)$	3p	1/2	–3.83062E+01	2.89	^{4}Pe

Table 4. Sample set of f-, S and A-values for allowed E1 transitions in Fe XX in $J\pi$ order. $a \pm b$ means $a10^{\pm b}$.

26		7				
1	0	1 1				
127	127	E_i (Ry)	E_j (Ry)	gf_L	S	A_{ji}(s^{-1})
1	1	–1.08023+2	–1.13324+2	1.900-03	1.075-03	2.144+08
1	2	–1.08023+2	–9.68163+1	–1.733-03	4.639-04	8.741+08
1	3	–1.08023+2	–4.86257+1	–4.849-04	2.449-05	6.870+09
1	4	–1.08023+2	–4.80570+1	–2.105-06	1.053-07	3.040+07
1	5	–1.08023+2	–4.75759+1	–5.056-04	2.509-05	7.419+09
1	6	–1.08023+2	–4.66197+1	–3.312-05	1.618-06	5.015+08
1	7	–1.08023+2	–4.56718+1	–2.164-04	1.041-05	3.379+09
1	8	–1.08023+2	–4.47343+1	–1.260-05	5.973-07	2.027+08
1	9	–1.08023+2	–4.32132+1	–6.243-02	2.890-03	1.053+12
1	10	–1.08023+2	–4.19287+1	–3.098-02	1.406-03	5.435+11
1	11	–1.08023+2	–4.17340+1	–2.782-04	1.259-05	4.910+09
1	12	–1.08023+2	–4.12909+1	–2.152-05	9.674-07	3.849+08
1	13	–1.08023+2	–4.06591+1	–3.596-01	1.601-02	6.554+12
1	14	–1.08023+2	–3.99533+1	–2.294-05	1.011-06	4.269+08
1	15	–1.08023+2	–3.86727+1	–1.844-01	7.977-03	3.562+12
1	16	–1.08023+2	–3.85828+1	–3.515-03	1.519-04	6.806+10
1	17	–1.08023+2	–3.85125+1	–8.555-03	3.692-04	1.660+11
1	18	–1.08023+2	–3.81759+1	–4.145-02	1.780-03	8.122+11
1	19	–1.08023+2	–3.79580+1	–1.365-02	5.845-04	2.692+11
1	20	–1.08023+2	–3.72398+1	–4.954-01	2.100-02	9.969+12
1	21	–1.08023+2	–3.71249+1	–3.061-01	1.295-02	6.179+12
1	22	–1.08023+2	–3.63955+1	–9.049-02	3.790-03	1.864+12
1	23	–1.08023+2	–3.58123+1	–2.348-01	9.755-03	4.918+12
1	24	–1.08023+2	–3.50086+1	–7.204-04	2.960-05	1.542+10
1	25	–1.08023+2	–3.47494+1	–4.352-05	1.782-06	9.383+08
...	...	...	...	...	...	...

the statistical weight factor of the initial or the lower level. The sign of gf indicates the upper and lower levels such that a negative value means that i is the lower level, while a positive value means k is the lower level. Column six is line strength S, and the last column is transition probability A_{ki} (s^{-1}). Spectroscopic notation of the transition can be obtained from Table 3b by referrring to the values of $J_i\pi_i$, I_i, $J_k\pi_k$, and I_k.

A subset of BPRM transition probabilities for Fe XX has been reprocessed using observed energy differences rather than the calculated ones to obtain the f- and A-values from the line strengths (S). The S-values are energy independent quantities. As the observed energies have lower uncertainties than the calculated ones, use those instead of the calculated energies improves the accuracy of the f- and A-values for the relevant transitions. (This is a common procedure and is used in the NIST compilation.) The astrophysical models also attempt to use observed transition energies to compute f- and A-values. For any comparison with experimental measurement, observation or spectral diagnostics therefore, values from these sets should be used if given.

The reprocessing of f- and A-values has been carried out for all the allowed transitions ($\Delta J = 0, \pm 1$) among observed levels. This subset consists of 289 transitions of Fe XX (also available electronically). The reprocessed transitions are further ordered in terms of their configurations and LS terms. This enables one to obtain the f-values for LS multiplets and check the completeness of the set of fine structure components belonging to a given multiplet. However, the completeness depends also on the observed set of fine structure levels since the transitions correspond only to the observed levels. The LS multiplets are useful for various comparisons with other calculations and experiments where fine structure transitions can not be resolved. A partial set of these transitions is presented in Table 5. The level index, I_i, for each energy level in the tables is given next to the J-value for easy access to the complete f-file.

The BPRM A-values for Fe XX are compared with other calculations in Table 6 (adopted from the compiled table by NIST). The alphabetic notation next to A-values in NIST column are accuracy estimation (Ac) by the NIST. Cheng et al. (1979) employed multiconfiguration Dirac-Fock (MCDF) method for the $2s^22p^3$–$2s2p^4$ and $2s2p^4$–$2p^5$ transitions in Fe XX, where they included the Breit interaction and the Lamb shift. However, in the early stage of their code development they carried out single configuration calculations for Fe XX and most of the correlation was omitted. Mason & Bhatia (1983) employed a scaled Thomas-Fermi approach with configuration interactions and relativistic effects for $2p^3$–$2p^23s$ and $2p^3$–$2s^23d$ transitions using an earlier version of SUPERSTRUCTURE. Their calculations also omitted much of the correlation as they included only three configurations (a relatively large calculation at that time). The NIST compilation lists 124 transitions, mainly from these two publications. Table 6 compares transitions of the type $2J$–$2J'$ = 4–6, 4–4, and 4–2. A wide range of scatter can be noticed between the present BPRM and previous A-coefficients for spontaneous radiative decays. Among the $2J$–$2J'$ = 4–6 transitions, BPRM A-values show good agreement with Cheng et al. (1979) for transitions such as $2s^22p^3(^4S^o)$–$2s2p^4(^4P)$, but shows a large difference for the $2s^22p^3(^2D^o)$–$2s2p^4(^2D)$ transition.

4.3. Oscillator strengths for forbidden transitions

The forbidden transitions of higher order electric (E2, E3) and magnetic (M1) transitions are treated through atomic structure calculations using SUPERSTRUCTURE. Forbidden transition probabilities are computed for 13 874 transitions among the lowest 215 fine structure levels of 9 configurations of Fe XX, as given in Table 7. Both this table and the transition table

Table 5. Dipole allowed and intercombination transitions in Fe XX, corrected with the observed energies. The notation *a*(*b*) means $a \times 10^b$.

C_i	C_j	T_i	T_j	g_i	g_j	E_{ij} (Å)	f	A (s^{-1})
2s22p3	2s2p4	$^2P^o$	$^4P^e$	2: 1	2: 1	171.6	9.514E-04	2.15E+08
2s22p3	2s2p4	$^2P^o$	$^4P^e$	4: 3	2: 1	192.7	2.465E-03	8.86E+08
2s22p3	2s2p4	$^2P^o$	$^4P^e$	2: 1	4: 1	178.3	3.075E-05	3.23E+06
2s22p3	2s2p4	$^2P^o$	$^4P^e$	4: 3	4: 1	201.2	6.780E-04	1.12E+08
2s22p3	2s2p4	$^2P^o$	$^4P^e$	4: 3	6: 1	233.1	2.689E-04	2.20E+07
2s2p4	2p5	$^4P^e$	$^2P^o$	2: 1	2: 2	82.0	8.591E-04	8.52E+08
2s2p4	2p5	$^4P^e$	$^2P^o$	2: 1	4: 4	89.9	1.088E-03	4.48E+08
2s2p4	2p5	$^4P^e$	$^2P^o$	4: 1	2: 2	80.6	1.413E-04	2.90E+08
2s2p4	2p5	$^4P^e$	$^2P^o$	4: 1	4: 4	88.2	4.197E-04	3.60E+08
2s2p4	2p5	$^4P^e$	$^2P^o$	6: 1	4: 4	83.2	1.977E-03	2.86E+09
2s22p3	2s2p4	$^2P^o$	$^2S^e$	2: 1	2: 2	107.0	5.884E-02	3.43E+10
2s22p3	2s2p4	$^2P^o$	$^2S^e$	4: 3	2: 2	114.8	1.139E-03	1.15E+09
LS		$^2P^o$	$^2S^e$	6	2		1.950E-02	3.11E+10
2s2p4	2p5	$^2S^e$	$^2P^o$	2: 2	2: 2	115.3	5.177E-03	2.60E+09
2s2p4	2p5	$^2S^e$	$^2P^o$	2: 2	4: 4	131.7	4.324E-02	8.32E+09
LS		$^2S^e$	$^2P^o$	2	6		5.003E-02	7.04E+09
2s22p3	2s2p4	$^2P^o$	$^2P^e$	2: 1	2: 3	92.6	4.495E-03	3.50E+09
2s22p3	2s2p4	$^2P^o$	$^2P^e$	4: 3	2: 3	98.4	5.998E-02	8.26E+10
2s22p3	2s2p4	$^2P^o$	$^2P^e$	2: 1	4: 3	101.8	2.603E-02	8.37E+09
2s22p3	2s2p4	$^2P^o$	$^2P^e$	4: 3	4: 3	108.9	2.023E-02	1.14E+10
LS		$^2P^o$	$^2P^e$	6	6		6.247E-02	3.94E+10
2s2p4	2p5	$^2P^e$	$^2P^o$	2: 3	2: 2	138.4	8.032E-02	2.79E+10
2s2p4	2p5	$^2P^e$	$^2P^o$	2: 3	4: 4	162.7	1.083E-02	1.36E+09
2s2p4	2p5	$^2P^e$	$^2P^o$	4: 3	2: 2	122.0	3.592E-02	3.22E+10
2s2p4	2p5	$^2P^e$	$^2P^o$	4: 3	4: 4	140.4	1.022E-01	3.46E+10
LS		$^2P^e$	$^2P^o$	6	6		1.201E-01	4.10E+10
2s22p3	2s22p2(3P)3s	$^2P^o$	$^4P^e$	2: 1	2: 4	14.4	6.278E-04	2.01E+10
2s22p3	2s22p2(3P)3s	$^2P^o$	$^4P^e$	4: 3	2: 4	14.6	2.905E-03	1.83E+11
2s22p3	2s22p2(3P)3s	$^2P^o$	$^4P^e$	4: 3	6: 3	14.3	1.736E-05	3.76E+08
2p5	2s22p2(3P)3s	$^2P^o$	$^4P^e$	2: 2	2: 4	19.5	5.055E-09	8.88E+04
2p5	2s22p2(3P)3s	$^2P^o$	$^4P^e$	4: 4	2: 4	19.1	1.642E-07	6.01E+06
2p5	2s22p2(3P)3s	$^2P^o$	$^4P^e$	4: 4	6: 3	18.7	5.171E-08	6.57E+05
2s22p3	2s22p2(1S)3s	$^2P^o$	$^2S^e$	2: 1	2: 6	13.7	3.080E-02	1.09E+12
2s22p3	2s22p2(1S)3s	$^2P^o$	$^2S^e$	4: 3	2: 6	13.8	1.231E-02	8.58E+11
LS		$^2P^o$	$^2S^e$	6	2		1.844E-02	1.94E+12
2p5	2s22p2(1S)3s	$^2P^o$	$^2S^e$	2: 2	2: 6	18.2	1.098E-06	2.21E+07
2p5	2s22p2(1S)3s	$^2P^o$	$^2S^e$	4: 4	2: 6	17.9	2.508E-06	1.05E+08
LS		$^2P^o$	$^2S^e$	6	2		2.032E-06	1.26E+08
2s22p3	2s22p2(3P)3d	$^2P^o$	$^4D^e$	2: 1	2: 7	13.3	1.368E-02	5.12E+11
2s22p3	2s22p2(3P)3d	$^2P^o$	$^4D^e$	4: 3	2: 7	13.5	8.281E-03	6.10E+11
2p5	2s22p2(3P)3d	$^2P^o$	$^4D^e$	2: 2	2: 7	17.6	1.163E-06	2.51E+07
2p5	2s22p2(3P)3d	$^2P^o$	$^4D^e$	4: 4	2: 7	17.2	2.089E-06	9.36E+07
2s22p3	2s22p2(1D)3d	$^2P^o$	$^2S^e$	2: 1	2:12	12.9	2.663E-02	1.06E+12
2s22p3	2s22p2(1D)3d	$^2P^o$	$^2S^e$	4: 3	2:12	13.0	6.618E-02	5.20E+12
LS		$^2P^o$	$^2S^e$	6	2		5.307E-02	6.28E+12
2p5	2s22p2(1D)3d	$^2P^o$	$^2S^e$	2: 2	2:12	16.9	1.289E-05	3.03E+08
2p5	2s22p2(1D)3d	$^2P^o$	$^2S^e$	4: 4	2:12	16.6	2.733E-05	1.33E+09
LS		$^2P^o$	$^2S^e$	6	2		2.246E-05	1.62E+09
2s22p3	2s22p2(3P)4d	$^2P^o$	$^4P^e$	2: 1	2:35	10.3	1.880E-03	1.19E+11
2s22p3	2s22p2(3P)4d	$^2P^o$	$^4P^e$	4: 3	2:35	10.3	1.051E-03	1.32E+11
2s22p3	2s22p2(3P)4d	$^2P^o$	$^4P^e$	2: 1	4:48	10.3	1.227E-02	3.89E+11
2s22p3	2s22p2(3P)4d	$^2P^o$	$^4P^e$	4: 3	4:48	10.3	5.010E-04	3.13E+10
2s22p3	2s22p2(3P)4d	$^2P^o$	$^4P^e$	4: 3	6:38	10.5	3.683E-03	1.50E+11
2p5	2s22p2(3P)4d	$^2P^o$	$^4P^e$	2: 2	2:35	12.6	1.108E-05	4.67E+08
2p5	2s22p2(3P)4d	$^2P^o$	$^4P^e$	4: 4	2:35	12.4	1.691E-06	1.46E+08
2p5	2s22p2(3P)4d	$^2P^o$	$^4P^e$	2: 2	4:48	12.6	5.395E-08	1.14E+06
2p5	2s22p2(3P)4d	$^2P^o$	$^4P^e$	4: 4	4:48	12.4	2.652E-07	1.15E+07
2p5	2s22p2(3P)4d	$^2P^o$	$^4P^e$	4: 4	6:38	12.6	3.199E-06	8.94E+07
2s22p3	2s22p2(3P)5d	$^2P^o$	$^4P^e$	2: 1	2:61	9.3	1.679E-02	1.30E+12
2s22p3	2s22p2(3P)5d	$^2P^o$	$^4P^e$	4: 3	2:61	9.3	1.792E-03	2.75E+11
2s22p3	2s22p2(3P)5d	$^2P^o$	$^4P^e$	2: 1	4:87	9.3	4.822E-02	1.87E+12
2s22p3	2s22p2(3P)5d	$^2P^o$	$^4P^e$	4: 3	4:87	9.3	7.071E-03	5.42E+11
2s22p3	2s22p2(3P)5d	$^2P^o$	$^4P^e$	4: 3	6:71	9.4	4.990E-03	2.50E+11

Table 6. Comparison of present A-coefficients (in units os 10^8 s^{-1} for Fe XX with those in NIST compilation. Notation $a+b$ means $a \times 10^b$.

A:Ac NIST	A Present	C_i	C_j	$SL\pi$ i	$SL\pi$ j	J_i–J_j
			E1			
$1.3+02^a$:C	1.19+2	2s22p3	2s2p4	$^4S^o$	^4P	3/2–5/2
$1.1+04^b$:D	1.16+4	2s22p3	2p2(3P)3s	$^4S^o$	^4P	3/2–5/2
$3.9+02^b$:E	4.17+2	2s22p3	2p2(1D)3s	$^4S^o$	^2D	3/2–5/2
$1.2+04^b$:E	1.24+3	2s22p3	2p2(1D)3d	$^4S^o$	^2D	3/2–5/2
$6.4\ ^a$:E	5.19+0	2s22p3	2s2p4	$^2D^o$	^4P	3/2–5/2
$2.7\text{-}01^a$:E	1.09-1	2s22p3	2s2p4	$^2D^o$	^2D	3/2–5/2
$5.0+3^b$:D	5.35+3	2s22p3	2p2(1D)3s	$^2D^o$	^2D	3/2–5/2
$1.6+05^b$:D	9.03+4	2s22p3	2p2(1D)3d	$^2D^o$	^2D	3/2–5/2
$2.7\text{-}01^a$:E	2.20-1	2s22p3	2s2p4	$^2P^o$	^4P	3/2–5/2
$1.86+02^a$:C	1.37+2	2s22p3	2s2p4	$^4S^o$	^4P	3/2–3/2
$1.9+01^a$:E	2.87+1	2s22p3	2s2p4	$^4S^o$	^2D	3/2–3/2
$4.6+01^a$:E	8.75+1	2s22p3	2s2p4	$^4S^o$	^2P	3/2–3/2
$1.8\ ^a$:E	1.12	2s22p3	2s2p4	$^2P^o$	^4P	3/2–3/2
$9.4+01^a$:C	1.14+2	2s22p3	2s2p4	$^2P^o$	^2P	3/2–3/2
$2.09+02^a$:C	1.28+2	2s22p3	2s2p4	$^4S^o$	^4P	3/2–1/2
$1.9+01^a$:E	1.48+2	2s22p3	2s2p4	$^4S^o$	^2S	3/2–1/2
$1.2+04^b$:D	3.62+3	2s22p3	2p2(3P)3s	$^4S^o$	^4P	3/2–1/2
$6.2+3^b$:E	4.95+3	2s22p3	2p2(3P)3d	$^4S^o$	^4D	3/2–1/2
3.4^a :E	1.53+1	2s22p3	2s2p4	$^2D^o$	^4P	3/2–1/2
$1.7+3^b$:E	9.14+3	2s22p3	2p2(3P)3s	$^2D^o$	^4P	3/2–1/2
$9.6+02^a$:C	8.26+2	2s22p3	2s2p4	$^2P^o$	^2P	3/2–1/2
$9.8+3^b$:D	8.58+3	2s22p3	2p2(1S)3s	$^2P^o$	^2S	3/2–1/2
$2.0+3^b$:E	9.36-1	2s22p3	2p2(3P)3d	$^2P^o$	^4D	3/2–1/2
			E2			
$1.5+1^a$:E	1.54+1	2s22p3	2s22p3	$^2D^o$	$^2P^o$	5/2–3/2
5.2^a:E	5.40	2s22p3	2s22p3	$^2D^o$	$^2P^o$	3/2–1/2
2.2^c:E	2.15	2p5	2p5	$^2P^o$	$^2P^o$	3/2–1/2
$2.7\text{-}3^a$:E	2.84-3	2s22p3	2s22p3	$^2D^o$	$^2D^o$	3/2–5/2
			M1			
$3.0+4^a$:D	2.91+4	2s22p3	2s22p3	$^4S^o$	$^2P^o$	3/2–3/2
$3.3+4^a$:D	2.97+4	2s22p3	2s22p3	$^4S^o$	$^2P^o$	3/2–1/2
$4.7+4^a$:D	4.34+4	2s22p3	2s22p3	$^2D^o$	$^2P^o$	3/2–3/2
$6.1+3^a$:D	6.06+3	2s22p3	2s22p3	$^2D^o$	$^2P^o$	3/2–1/2

[a] Cheng et al. (1979), [b] Mason & Bhatia (1983).

were processed from SUPERSTRUCTURE output to standard spectroscopic notation. The energies in Table 7 agree with the observed values within 1%. The set of levels and corresponding forbidden transitions data are available electronically. The transitions among levels listed in the observed table have been reprocessed with observed energy difference as in Table 5. Table 8 presents a sample table of forbidden transitions in Fe XX.

Present A-coefficients for forbidden transitions are compared with previous works in Table 6. In contrast to E1 transitions, present results for E2 and M1 transitions, agree well in general with those by Cheng et al. (1979).

5. Conclusion

Accurate and large-scale calculations have been carried out for allowed and forbidden transitions in Fe XX corresponding to 1792 calculated fine structure energy levels upto $n = 10$. All levels have been spectroscopically identified and checked for completenss. The set of results far exceeds the currently available experimental and theoretical data.

Table 7. Sample set of fine strucuture levels of Fe XX and their relative energies for which forbidden transitions are considered. The configuration indices (Cf) correspond to $2s^22p^3$(1), $2s2p^4$(2), $2p^5$(3), $2s^22p^23s$(4), $2s^22p^23p$(5), $2s^22p^23d$(6), $2s2p^33s$(7), $2s2p^33p$(8), $2s2p^33d$(9).

ie	SLp(cf)	g	k*cm	E (Ry)
1	4So(1)	4	0	0.00000E+00
2	2Do(1)	4	142375	1.29742E+00
3	2Do(1)	6	180031	1.64057E+00
4	2Po(1)	2	261233	2.38053E+00
5	2Po(1)	4	322630	2.94002E+00
6	4Pe(2)	6	753923	6.87025E+00
7	4Pe(2)	4	820511	7.47704E+00
8	4Pe(2)	2	842332	7.67589E+00
9	2De(2)	4	1053027	9.59589E+00
10	2De(2)	6	1068512	9.73700E+00
11	2Se(2)	2	1203981	1.09715E+01
12	2Pe(2)	4	1259046	1.14733E+01
13	2Pe(2)	2	1352995	1.23294E+01
14	2Po(3)	4	1972895	1.79783E+01
15	2Po(3)	2	2078476	1.89405E+01
16	4Pe(4)	2	7223242	6.58230E+01
17	4Pe(4)	4	7282550	6.63635E+01
18	2Pe(4)	2	7313778	6.66481E+01
19	4Pe(4)	6	7323735	6.67388E+01
20	2Pe(4)	4	7356044	6.70332E+01
21	4Do(5)	2	7420827	6.76236E+01
22	2De(4)	6	7456435	6.79480E+01
23	4Do(5)	4	7461617	6.79953E+01
24	2De(4)	4	7466086	6.80360E+01
25	4Po(5)	2	7475943	6.81258E+01
26	2Do(5)	4	7506494	6.84042E+01
27	4Do(5)	6	7513283	6.84661E+01
28	2So(5)	2	7526680	6.85882E+01
29	4Po(5)	6	7534287	6.86575E+01
30	4Po(5)	4	7546466	6.87685E+01
		....		

The results are obtained in intermediate coupling, including relativistic effects using the Breit Pauli R-matrix method (BPRM) in the close coupling approximation for allowed E1 transitions and configuration interaction atomic structure calculations using SUPERSTRUCTURE for forbidden electric quadrupole (E2), and octupole (E3), and magnetic quadrupole (M1) transitions. The energies show very good agreement, within 1%, with most of the measured values compiled by the NIST. However, present transition probabilities show varying degree of agreement, especially for E1 transitions, with the previous calculations obtained using lower configurations interactions. The results from the present work should be particularly useful in the analysis of X-ray and Extreme Ultraviolet spectra from astrophysical and laboratory sources where non-local thermodynamic equilibrium (NLTE) atomic models with many excited levels are needed.

All data are available electronically. A subset of f-values has been reprocessed using available observed energies for better accuracy.

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Table 8. Line strength (S) and A-coefficients for the forbidden electric quadrupole (E2) and octupole (E3), and magnetic dipole (M1) transitions in Fe XX. The level numbers ($i,\ j$) and configurations indices (C_i and C_j) correspond to those in Table 7, such as $2s^22p^3$(1), $2s2p^4$(2), $2p^5$(3), $2s^22p^23s$(4), $2s^22p^23p$(5), etc.

i	j	$SL\pi$ $: C_i$	$SL\pi$ $: C_j$	g_i	g_j	λ (Å)	SE2	AE2 s^{-1}	SM1	AM1 s^{-1}
						E2 and M1				
2	1	4So:1	2Do:1	4	4	721.40	3.31E-04	7.11E-01	7.98E-01	1.43E+04
3	1	4So:1	2Do:1	4	6	567.77	6.92E-04	3.28E+00	4.55E-02	1.12E+03
3	2	2Do:1	2Do:1	4	6	2666.08	1.37E-03	2.84E-03	1.78E+00	4.22E+02
4	1	4So:1	2Po:1	4	2	384.21	6.35E-05	6.37E+00	1.25E-01	2.97E+04
4	2	2Do:1	2Po:1	4	2	822.00	2.41E-03	5.40E+00	2.50E-01	6.06E+03
4	3	2Do:1	2Po:1	6	2	1188.40	2.13E-03	7.55E-01	0.00E+00	0.00E+00
5	1	4So:1	2Po:1	4	4	309.27	4.45E-06	6.60E-01	1.28E-01	2.91E+04
5	2	2Do:1	2Po:1	4	4	541.36	8.13E-04	7.34E+00	1.02E+00	4.34E+04
5	3	2Do:1	2Po:1	6	4	679.29	5.30E-03	1.54E+01	5.74E-01	1.24E+04
5	4	2Po:1	2Po:1	2	4	1585.64	6.99E-04	2.93E-02	9.59E-01	1.62E+03
7	6	4Pe:2	4Pe:2	6	4	1468.60	2.15E-03	1.32E-01	3.54E+00	7.54E+03
8	6	4Pe:2	4Pe:2	6	2	1116.08	1.73E-03	8.39E-01	0.00E+00	0.00E+00
8	7	4Pe:2	4Pe:2	4	2	4649.52	2.07E-04	7.99E-05	3.13E+00	4.20E+02
9	6	4Pe:2	2De:2	6	4	345.02	1.35E-04	1.16E+01	8.39E-04	1.38E+02
9	7	4Pe:2	2De:2	4	4	450.97	1.32E-06	2.98E-02	1.45E-01	1.07E+04
9	8	4Pe:2	2De:2	2	4	499.40	9.50E-05	1.28E+00	4.15E-02	2.25E+03
						E3				
i	j	$SL\pi$ $: C_i$	$SL\pi$ $: C_j$	g_i	g_j	λ (Å)	SE3	AE3 s^{-1}		
6	4	4Pe:2	2Po:1	6	2	203.06	4.17E-06	3.07E-05		
8	3	4Pe:2	2Do:1	2	6	150.10	2.91E-08	5.33E-06		
10	4	2De:2	2Po:1	6	2	125.30	1.41E-04	3.05E-02		
11	3	2Se:2	2Do:1	2	6	98.12	1.49E-04	5.35E-01		
13	3	2Pe:2	2Do:1	2	6	85.92	5.42E-04	4.93E+00		
15	6	2Po:3	4Pe:2	2	6	76.37	1.59E-05	3.30E-01		
15	10	2Po:3	2De:2	2	6	99.62	5.72E-04	1.85E+00		
16	3	4Pe:4	2Do:1	2	6	14.25	1.23E-04	3.24E+05		
18	3	2Pe:4	2Do:1	2	6	14.01	9.42E-04	2.80E+06		
19	4	4Pe:4	2Po:1	6	2	14.21	8.80E-05	7.89E+04		
19	15	4Pe:4	2Po:3	6	2	19.10	1.50E-06	1.70E+02		
21	6	4Do:5	4Pe:2	2	6	15.00	1.98E-06	3.65E+03		

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