ISSN 1384-1076

New·Astronomy

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Fine structure transitions in Fe XIV

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HIGHLIGHTS

- ▶ Al like iron ion, Fe XIV, is seen in astronomical objects: the sun, Seyfert galaxies.
- ▶ Radiative transitions in Fe XIV cause spectral lines and stellar opacities.
- ▶ The largest set of energy levels and parameters for radiative transitions is reported.
- ▶ Present results from relativistic Breit-Pauli R-matrix method are of high accuracy.
- ▶ These should determine more precise stellar abundances, diagnostics, pulsations etc.

ARTICLE INFO

ABSTRACT

Results are reported for Fe XIV energy levels and transitions obtained from the ab initio relativistic Breit–Pauli R-matrix (BPRM) method. BPRM method developed under the Iron Project is capable of calculating very large number of fine structure energy levels and corresponding transitions. However, unlike in the atomic structure calculations, where levels are identified spectroscopically based on the leading percentage contributions of configurations, BPRM is incapable of such identification of the levels and hence the transitions. The main reason for it is that the percentage contributions can not be determined exactly from the large number of channels in the R-matrix space. The present report describes an identification method that uses considerations of quantum defects of channels, contributions of channel from outer regions, Hund's rule, and angular momenta algebra for addition and completeness of fine structure components. The present calculations are carried out using a close coupling wave function expansion that included 26 core excitations from configurations $2s^2 2p^6 3s^2$, $2s^2 2p^6 3s 3p$, $2s^2 2p^6 3p^2$, $2s^2 2p^6 3s 3d$, and $2s^2 2p^6 3p 3d$. A total of 1002 fine structure levels with $n \leqslant 10$, $l \leqslant 9$, and $0.5 \leqslant J \leqslant 9.5$ with even and odd parities and the corresponding 130,520 electric dipole allowed (E1) fine structure transitions, a most complete set for astrophysical modelings of spectral analysis and opacities, is presented. Large number of new energy levels are found and identified. The energies agree very well, mostly in less than 1% with the highest being 1.9%, with the 68 observed fine structure levels. While the high lying levels may have some uncertainty, an overall accuracy of energy levels should be within 10%. BPRM transitions have been benchmarked with the existing most accurate calculated transition probabilities with very good agreement for most cases. Based on the accuracy of the method and comparisons, most of the transitions can be rated with A ($\leqslant 10\%$) to C ($\leqslant 30\%$).

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1. Introduction

Fe XIV, the aluminum like iron ion, exists in many astronomical objects, such as, in the sun (e.g. Edlen, 1942), in Seyfert galaxies (e.g. Ferguson et al., 1997). The ion is most known for its green emission line at 5303 Å due to the forbidden transition $3s^2 3p^2 P^o_{1/2} - 3s^2 3p^2 P^o_{3/2}$ in the ground configuration. The line, first identified in the optical coronal spectrum by Edlen (1942), is used as a diagnostic line (e.g. Brickhouse et al., 1995; Brosius et al., 1998). This and few other low-lying forbidden lines due to transitions, particularly among the levels of $3s3p^2(^4P_J)$ and of $3s3p3d(^4F^o_J)$, have been under considerable study both experimentally (e.g. Trabert et al., 1988; Beiersdorfer et al., 2003; Trabert, 2010; Brenner et al., 2007) and theoretically (e.g. Santana et al., 2009; Hao et al., 2010). Other spectral lines of Fe XIV have been seen in the soft X-ray and extreme-ultraviolet (EUV) in the solar corona (e.g. Acton et al., 1985; Thomas and Neuport, 1994; Brosius et al., 1998; Brown et al., 2008) and studied theoretically

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by investigators, such as, using MCDF method by Gupta and Msezane (2001); Fischer et al. (2006)), for n = 3–4 allowed transitions by Wei et al. (2008), for levels up 4d by Tayal (2008); Jian-Zhong et al. (2012), and Thomas–Fermi approximation by Storey et al. (2000); Liang et al. (2010), and ab initio multireference Moller–Plesset perturbation theory by Santana et al. (2009). A relatively large list of publications for these lines are available at the National Institute for Standards and Technology (NIST) website. The evaluated compilation of Fe XIV transitions by NIST includes about 70 energy levels from Sugar and Corliss, (1985), Shirai et al. (2000), and 151 transitions from Shirai et al. (2000), Fawsett et al. (1972), Huang (1986), and Garstang (1962); Redfors and Litzen (1989) also measured number of energy levels of Fe XIV.

In contrast to most of the earlier atomic structure calculations, the present theoretical study on Fe XIV transitions employs the ab initio Breit–Pauli R-matrix (BPRM) method in the close coupling (CC) approximation (Hummer et al., 1993; Scott and Burke, 1980; Scott and Taylor, 1982; Berrington et al., 1995) for the first time for this ion. Hence the results benchmark the BPRM method with earlier experimental as well as other accurate theoretical approximations. In addition, using the computational capability of the CC approximation with the R-matrix method, a large number of fine structure transitions for n going up to 10 have been considered. Such large scale computation is needed for astrophysical models such as producing synthetic spectra, calculations of plasma opacities etc. (e.g. Seaton et al., 1994) which require more complete set of transitions. For example, we still do not have accurate iron abundance in the sun due to lack of accurate opacity (e.g. Bailey et al., 2009). One major difficulty of BPRM method is to carry out the spectroscopy of levels and transitions. Identification of the levels and transitions is important for various diagnostic applications. This report will discuss the identifications along with new results of the levels and electric dipole allowed transitions in iron ion, Fe XIV.

2. Theory

Breit–Pauli R-matrix method (Hummer et al., 1993, Scott and Burke, 1980, Scott and Taylor, 1982, Berrington et al., 1995) is the relativistic extension of the R-matrix method used under the Opacity Project (The Opacity Project Team, 1995, 1996). The relativistic effects are considered through Breit–Pauli approximation. The wave functions are represented in close-coupling approximation which allows consideration of large number of core excitations. In the CC approximation the atomic system is represented as the 'target' or the 'core' ion of N-electrons interacting with the $(N + 1)$th electron. In the electron–ion system, the $(N + 1)$th electron may be bound or in the continuum depending on its energy. The total wave function, Ψ_E, of the $(N + 1)$-electron system in a symmetry $J\pi$ is expressed as an expansion over the eigenfunctions of the target ion, χ_i in specific level $S_iL_i(J_i)\pi_i$, coupled with the $(N + 1)$th electron function, θ_i:

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

where the first sum is over the ground and excited states of the target or the core ion. A is the anti-symmetrization operator. The $(N + 1)$th electron with kinetic energy k_i^2 corresponds to a channel labeled $S_iL_i(J_i)\pi_i k_i^2 \ell_i(SL(J)\pi)$. The Φ_js in the second term are bound channel functions of the $(N + 1)$-electron system that account for short range correlation not considered in the first term and the orthogonality between the continuum and the bound electron orbitals of the target. The core orbitals of $(N + 1)$ electrons system are the same as those of N-electron system.

The relativistic Hamiltonian in the BPRM method is given by

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

where the last three terms are relativistic corrections, respectively:

mass correction term, $\quad H_{N+1}^{mass} = -\frac{\alpha^2}{4}\sum_i p_i^4,$

Darwin term, $\quad H_{N+1}^{Dar} = \frac{Z\alpha^2}{4}\sum_i \nabla^2(\frac{1}{r_i}),$ $\qquad$ (3)

spin−orbit interaction term, $\quad H_{N+1}^{so} = Z\alpha^2\sum_i \frac{\mathbf{l}_i.\mathbf{s}_i}{r_i^3}.$

The spin–orbit interaction H_{N+1}^{so} splits LS energy into fine structure levels. Total Briet–Pauli Hamiltonian has more terms, but they are relatively weaker two-body interactions terms (e.g. Pradhan and Nahar, 2011). Only part of those contributions is included in the BPRM calculations.Substitution of $\Psi_E(e + ion)$ in the Schrodinger equation

$$H_{N+1}\Psi_E = E\Psi_E \tag{4}$$

introduces a set of coupled equations that are solved using the R-matrix method (e.g. Pradhan and Nahar, 2011). In the R-matrix method, the space is divided in two regions, the inner and the outer regions, of a sphere of radius r_a with the ion at the center. The R-matrix boundary, r_a, is chosen to be large enough for electron–electron interaction potential to be zero outside it. The wave function beyond the R-matrix boundary $r > r_a$ is then Coulombic due to perturbation from the long-range multipole potentials. In the inner region, the partial radial wave function F_i of the interacting electron is expanded in terms of a basis set, called the R-matrix basis, $F_i = \sum a_k u_k$, which satisfies

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + V(r) + \epsilon_{lk}\right]u_{lk} + \sum_n \lambda_{nlk}P_{nl}(r) = 0. \tag{5}$$

and are made continuous at the boundary by matching with the Coulomb functions outside the boundary. The solution is a continuum wave function Ψ_F for an electron with positive energies (E > 0), or a bound state Ψ_B at a negative total energy (E ⩽0).

The transition matrix element for radiative transition to an excited state is given by

$$\langle \Psi_B \|\mathbf{D}\| \Psi_{B'} \rangle, \tag{6}$$

where $\mathbf{D} = \sum_i r_i$ is the dipole operator and the sum is over the number of electrons; Ψ_B and $\Psi_{B'}$ are the initial and final bound wave functions. The transition matrix element can be reduced to generalized line strength as

$$\mathbf{S} = |\langle \Psi_j \|\mathbf{D}\| \Psi_i \rangle|^2 = \left| \left\langle \psi_f \mid \sum_{j=1}^{N+1} r_j \mid \psi_i \right\rangle \right|^2, \tag{7}$$

where Ψ_i and Ψ_f are the initial and final state wave functions. The line strengths are energy independent quantities. The oscillator strength (f_{ij}) and radiative decay rate or Einstein's A-coefficient for an E1 transition are given by

$$f_{ij} = \frac{E_{ji}}{3g_i}S(ij), \quad A_{ji}(a.u.) = \frac{1}{2}\alpha^3 g_i/g_j E_{ji}^2 f_{ij}. \tag{8}$$

E_{ji} is the energy difference between the initial and final states, α is the fine structure constant, and g_i, g_j are the statistical weight factors of the initial and final states, respectively.The lifetime of a level can be computed as

$$\tau_k = \frac{1}{A_k}, \tag{9}$$

where $A_k == \sum_i A_{ki}$ is the total radiative transition probability in atomic unit for level k. In time unit,

$$g_i A_{ki}(s^{-1}) = 2.6774 \times 10^9 \; s^{-1}(E_i - E_k)^3 S(ik) \tag{10}$$

3. Computation

The close coupling wave function expansion, Eq. (1), of Fe XIV included 26 levels of the core ion Fe XV. This means that the BPRM calculations will find the possible bound levels of Fe XIV where the core ion can be in the ground level or in one of the 25 possible excited levels. The core levels belong to configurations $3s^2, 3s3p, 3p^2, 3s3d$ and $3p3d$ with filled inner shells $1s^2 2s^2 2p^6$. These levels are given in Table 1.

The wave functions of the target or core orbitals are obtained from atomic structure calculations using the later version (Nahar et al., 2003) of code SUPERSTRUCTURE (SS) (Eissner et al. (1974)). SS employs Thomas-Fermi–Dirac–Amaldi approximation. Eighteen configurations of core Fe XV, given in Table 1, were optimized along with the Thomas–Fermi scaling parameters (λ_{nl}) for the orbitals. These configurations and values of λ_{nl} are given in the Table 1. The calculated energies E_c (Table 1) are very close to the observed values compiled at NIST website, the largest difference being within 5% for the level $3p^2(^1S_0)$. Some improvement in accuracy $(N+1)$-electron energies can be achieved by replacing the calculated core level energies with observed energies during diagonalization of the $(N+1)$-electron Hamiltonian. No optimization of wave functions is carried out, that is, the same calculated orbitals functions are used.

The second sum in the wave function expansion, the bound-channel expansion, in Eq. (1) includes 63 configurations of the $(N+1)$-electron system as specified by a range of minimum and maximum occupancies (listed within parentheses after the orbitals) as: $2p(5-6), 3s(0-2), 3p(0-3), 3d(0-2), 4s(0-2), 4p(0-2), 4d(0-1), 4f(0-1), 5s(0-1), 5p(0-1), 5d(0-1)$. All $SLJ\pi$ symmetries of the electron–ion system formed from the target states coupled with an interacting electron with continuum partial waves $0 \leqslant l \leqslant 12$ are considered.

Steps of computations for transition parameters of other atomic systems using BPRM codes (Berrington et al., 1995) can be found in earlier papers (e.g. Nahar et al., 2003). STG1 of the BPRM codes carries out computation of radiative integrals while STG2 computes the coefficients of angular algebra of the Hamiltonian. Stage RECUPD carries out the intermediate coupling calculations for the fine structure components and STGH forms the Hamiltonian matrix and dipole transition matrices. The energy eigenvalues are computed by STGB and the levels are searched by scanning through the poles in the Hamiltonian using a very fine quantum defect mesh, Δq going as small as 0.00025. The energy levels are identified spectroscopically using code PRCBPID (Nahar and Pradhan, 2000; Nahar, 2000) as explained in the next section. STGBB calculates the oscillator strengths. The R-matrix results for energies and oscillator strengths are processed using codes PBPRAD (Nahar, 2003)

4. Spectroscopic designation of energy levels

The spectroscopy for identification of energy levels and transitions in BPRM method is different from the atomic structure structure calculations. In the multi-configuration interaction, a state usually has contributions from a number of states of same symmetry but from various configurations. For example, the $^2P^o$ state of Fe XIV can have contributions from $3s^23p(^2P^o), 3p^3(^2P^o), 3s3p3d(^2P^o), 3s^24p(^2P^o)$ etc. The lowest energy state $^2P^o$ will have the maximum (usually 100%) contribution from the ground state, $3s^23p(^2P^o)$, while the first excited $^2P^o$ state will have maximum contribution from $3p^3(^2P^o)$, second excited $^2P^o$ state will have from $3s^24p(^2P^o)$, and so on. These percentage contributions from various configurations or the mixing coefficients are determined while the Hamiltonian matrix is optimized. Atomic structure calculation designates the energy state by the spectroscopic state which has the highest or the leading percentage contribution.

In contrast to atomic structure, close coupling approximation treats the electron–ion system as channels of interaction such that the solution of the multi-configuration Hartree–Fock equation is a continuum wave function Ψ_F for an electron with positive energies (E > 0) or a bound state Ψ_B at a negative total energy (E $\leqslant$ 0). Each energy level will have contributions from a number of channels and the dominating channels determine the spectroscopic designation of it. However, determination of channel contributions in the R-matrix method is more involved since each channel has contributions from inner and outer regions of the R-matrix sphere. As explained earlier that in the inner region, an orbital radial wave function is expanded by the R-matrix basis set and extended outward up to the R-matrix boundary where it is matched with the outer region wave function. The BPRM method provides percentage contributions of channels from outer region. Hence these contributions may not reflect the highest contributing channels. However, a level designation often corresponds to one of the first two/three channels with highest percentage contributions. The theoretical spectroscopy for identification of the levels from these channels are built in the program PRCBPID (Nahar and Pradhan, 2000; Nahar, 2000) as summarized below. The method is based on quantum defect analysis, channel contributions, rules of angular momenta algebra, correspondence between LS and fine structure components, and Hund's rule as a guidance. A set of spectroscopically identified levels are given in Table 2.

Table 1

Energy levels, calculated (E_c) and observed (E) (NIST), of the core ion Fe XV included in the eigenfunction expansion of Fe XIV. The core was optimized with a set of 18 configurations with closed K-shell: $2s^22p^63s^2(1)$, $2s^22p^63s3p(2)$, $2s^22p^63p^2(3)$, $2s^22p^63s3d(4)$, $2s^22p^63p3d(5)$, $2s^22p^63s4s(6)$, $2s^22p^63s4p(7)$, $2s^22p^63s4d(8)$, $2s^22p^63s4f(9)$, $2s^22p^63s5s(10)$, $2s^22p^63s5p(11)$, $2s^22p^63s5d(12)$, $2s^22p^63p4s(13)$, $2s^22p^63p4p(14)$, $2s^22p^63p4d(15)$, $2s^22p^63p4f(16)$, $2s^22p^53s3p(17)$, $2s^22p^53s3d(18)$.

i	Configuration	Term	$2J$	E(Ry)	E_c(Ry)
1	$2p^63s^2$	^1S	0	0.0	0.0
2	$3s3p$	$^3P^o$	0	2.1315	2.1834
3	$3s3p$	$^3P^o$	2	2.1839	2.2353
4	$3s3p$	$^3P^o$	4	2.3129	2.3578
5	$3s3p$	$^1P^o$	2	3.2068	3.3002
6	$3p^2$	^3P	0	5.0532	5.1726
7	$3p^2$	^1D	4	5.0995	5.1747
8	$3p^2$	^3P	2	5.1447	5.2541
9	$3p^2$	^3P	4	5.3007	5.3969
10	$3p^2$	^1S	0	6.0110	6.3052
11	$3s3d$	^3D	2	6.1854	6.2770
12	$3s3d$	^3D	4	6.1947	6.2931
13	$3s3d$	^3D	6	6.2095	6.3178
14	$3s3d$	^1D	4	6.9447	7.1840
15	$3p3d$	$^3F^o$	4	8.4588	8.5441
16	$3p3d$	$^3F^o$	6	8.5488	8.6369
17	$3p3d$	$^1D^o$	4	8.6435	8.7422
18	$3p3d$	$^3F^o$	8	8.6539	8.7421
19	$3p3d$	$^3D^o$	2	8.9566	9.0891
20	$3p3d$	$^3P^o$	4	8.9624	9.0995
21	$3p3d$	$^3D^o$	6	9.0658	9.2072
22	$3p3d$	$^3P^o$	0	9.0752	9.1896
23	$3p3d$	$^3P^o$	2	9.0784	9.1982
24	$3p3d$	$^3D^o$	4	9.0819	9.2109
25	$3p3d$	$^1F^o$	6	9.6824	9.8995
26	$3p3d$	$^1P^o$	2	9.7951	10.043

λ_{nl} = 1.38(1s), 1.25(2s), 1.15(2p), 1.15(3s), 1.1(3p), 1.0(3d), 1.0(4s), 1.0(4p), 1.0(4d), 1.0(4f), 1.0(5s), 1.0(5p).1.0(5f)

Table 2
Sample set of fine structure energy levels of Fe XIV, grouped as components of LS terms.

$C_t(S_tL_t\pi_t)$		J_t	nl	$2J$	E (Ry)	ν	$SL\pi$
$Nl\nu$ = 2, $^2L^o$:P (3 1)/2							
$2p63s2$	(1Se)	0	$3p$	1	−2.88230E+01	2.64	2Po
$2p63s2$	(1Se)	0	$3p$	3	−2.86520E+01	2.62	2Po
$Nl\nu$ (c) = 2: set complete							
Eqv electron/unidentified levels, parity: e							
$3s3p2$				1	−2.68030E+01	2.70	4Pe
$3s3p2$				3	−2.67330E+01	2.71	4Pe
$3s3p2$				5	−2.66410E+01	2.71	4Pe
$Nl\nu$ (c) = 3: set complete							
$Nl\nu$ = 9, $^2L^e$: S(1)/2P(31)/2D(53)/2F(75)/2G(97)/2							
$3p2$	(1De)	2	$3d$	5	−1.96549E+01	2.84	2DFe
$3p2$	(1De)	2	$3d$	7	−1.95955E+01	2.83	2FGe
$3p2$	(1De)	2	$3d$	7	−1.94588E+01	2.85	2FGe
$3p2$	(1De)	2	$3d$	9	−1.94215E+01	2.84	2Ge
$3p2$	(1De)	2	$3d$	3	−1.94120E+01	2.83	2De
$3p2$	(1De)	2	$3d$	5	−1.93740E+01	2.85	2De
$3p2$	(1De)	2	$3d$	1	−1.88526E+01	2.85	2SPe
$3p2$	(1De)	2	$3d$	1	−1.87559E+01	2.86	2SPe
$3p2$	(1De)	2	$3d$	3	−1.87283E+01	2.88	2PDe
$Nl\nu$ (c) = 9: set complete							

A channel is described as $(C_t)^{2S_t+1}L_{t_jj_t}^{\pi_t}nl$ where C_t is the target (core) configuration, $^{2S_t+1}L_{t_jj_t}^{\pi_t}$ is the target state and l is the orbital angular momentum of the valence electron. The principle quantum number n is to be determined. The BPRM method calculates sets of energies belonging to various symmetries $J\pi$. The symmetry provides the total angular momentum J and parity π of the levels. Hence, each level of the $J\pi$ set has contributions from all possible channels with all possible states that form total angular momentum J which is the sum of angular momenta of the target level and of the valence electron. The program PRCBPID Nahar, 2000 picks the first two most contributing channels to the level as a start and determines the total number of possible spectroscopic designations $^{2S+1}L_J^\pi$ for the final state for each channel (e.g. as given in the last column of energy levels of Table 2). For these, following Hund's rule as a guide for the energy positions of the levels, two assumptions are made. In the first assumption the lower levels are given higher spin-multiplicity $2S_t + 2$ and the higher ones lower spin-multiplicity $2S_t$. (We note that there is no multiplicity $2S_t$ with a singlet core state). The second assumption is, again following Hund's rule, that levels with higher total orbital angular momentum L with the same $2S + 1$ lie lower than those with lower L. However, in case of existing accurate identifications, such as those of NIST, BPRM levels are matched with their identification for consistency.

The principle quantum number of the valence electron, n, is determined next from the quantum defect (μ), its orbital angular momentum (l), and principle quantum number n_t of the outer electron of the target or the core state. BPRM method provides table of effective quantum numbers $(\nu_{nl} = n_l - \mu_l)$ of the valence electron for each contributing channel. ν_l of various channels can be studied along the energy levels to identify a Rydberg series. For a Rydberg series of levels with a particular angular momentum (l) of the valence electron, the quantum defect μ_l remains about the same, especially for higher levels while the effective quantum number ν_{nl} increases approximately by unity with higher levels. μ_l follows the order $\mu_s > \mu_p > \mu_d > \mu_f$ and so on. For high l, μ_l is almost zero. For example, the first energy set in Table 2 indicates that μ_p is about 0.35. The value of μ_l becomes more consistent with higher energy levels. Hence analyzing ν_{nl} of the channels, a Rydberg series and its μ_l can be recognized. For such an identified Rydberg series of levels with same $J\pi$, the lowest level with orbital angular momentum l is assigned with the principle quantum number n

of the next unoccupied orbital of the core. Hence, for the first p-electron of the set of Table 2 it is $n = n_t = 3$ since this is first unoccupied orbital. Then n of higher levels of the series are assigned with increasing numbers differing by unity. Similarly μ_l of other series are determined. Once μ_l of various s, p, d etc. found, they are used as guidance for determination of the nl of other levels with different core states and configuration, especially for a series with a single level.

Equivalent electron states can not be identified in the above manner since their quantum defects are not well defined in BPRM calculations. These states are worked out separately from possible equivalent electron configurations of $(N + 1)$ electrons system. These configurations are formed by adding one electron in the outer orbital of the target configurations. For example, for Fe XIV, addition of an electron gives the possible equivalent configurations are $3s3p^2$, $3p^3$, $3s3d^2$, and $3p3d^2$. Using angular algebra, all possible LS states and their fine structure components are obtained separately by hand. These levels are then searched in the calculated energy levels with same J, π. They often lie in the low energy region. As mentioned above, they do not have well defined quantum defects μ or effective quantum number ν, and do not fit any Rydberg state. For these levels the effective quantum number ν can be estimated by using the formula

$$\nu = z/\sqrt{E}.$$

The total higher or lower spin and angular momenta for these levels are assigned following the similar criteria mentioned above for non-equivalent electron states. An example set of levels for an equivalent state $3s3p^2(^4P)$ is given in second set of Table 2.

After the initial assignments, all calculated levels from all $J\pi$ are sorted out to group them into sets of fine structure components for the LS terms. Each set is sorted with same configuration $((C_t)nl)$, same core state $(S_tL_t\pi_t)$, same total spin multiplicity $2S + 1$ and parity π but has all possible corresponding L and J values. The possible L values are listed at the top of the energy set and the corresponding J values are listed within parentheses next to the L value as shown in Table 2. Each set of levels is checked for complete number of fine structure levels $^{2S+1}L_J^o$ defined as $Nl\nu$ in Table 2. The program PRCBPID writes the message on completeness if the calculated levels $Nl\nu(c)$ matches the expected number of levels $Nl\nu$, otherwise specifies the J values of the missing levels. Missing levels are often found as extra or duplicate levels belonging to some other sets. They indicate mixing of various configurations contributing to the levels. Identification of these levels are then adjusted from the contributing channels and following above criteria. Thus a unique correspondence is made between the fine structure levels and their LS terms such that exact number of fine structure levels are accounted for each LS term.

The last energy set of configuration $3p^2(^1D)3d$ in Table 2 is expected to have 9 levels. The top line specifies the set of $^2L^e$ where for the particular configuration and doublet spin multiplicity, the L values are S, P, D, F and G, and the corresponding J-values are as given within parentheses next to the L values. These J-values add to a total number of 9 levels, that is, 1 level from state $^2S^e$, 2 from $^2P^e$, 2 from $^2D^e$, 2 from $^2F^e$, and 2 from $^2G^e$. The number of calculated levels for the set is also found to be 9 and hence the calculated set is complete as indicated at the bottom line. In this set, it is also seen that there is a single L value for some levels, but more than one possible L-values for some other energy levels (last column). A level with more than one possible L-values can have a preferred L-value for a unique correspondence to a term, such as the level with higher angular momentum may lie lower. Following the criteria explained above, the first level with two possible L-values, D and F, F can be chosen since it is higher than D. Hence, the first and the third levels can form the term $^2F^e$ The second level

Table 3
Comparison of calculated absolute energies, E_c, of Fe-XIV with the measured values E_o (NIST and Refors and Litzen 1989). The negative sign for the energies is omitted for convenience. i_j indicates position of the calculated level for symmetry J. An asterisk indicates incomplete set of observed energies for the LS multiplet.

Conf	Term	$J : i_j$	E_o(Ry)	E_c(Ry)
$3s23p$	$^2P^o$	0.5: 1	28.8230	28.8316
$3s23p$	$^2P^o$	1.5: 1	28.6520	28.6656
$3s3p2$	$^4P^e$	2.5: 1	26.6410	26.5415
$3s3p2$	$^4P^e$	1.5: 1	26.7330	26.6205
$3s3p2$	$^4P^e$	0.5: 1	26.8030	26.6813
$3s3p2$	$^2D^e$	2.5: 2	26.0760	25.9949
$3s3p2$	$^2D^e$	1.5: 2	26.0960	26.0121
$3s3p2$	$^2S^e$	0.5: 2	25.5000	25.3640
$3s3p2$	$^2P^e$	1.5: 3	25.2100	25.0888
$3s3p2$	$^2P^e$	0.5: 3	25.2830	25.1570
$3s23d$	$^2D^e$	2.5: 3	24.4930	24.4416
$3s23d$	$^2D^e$	1.5: 4	24.5110	24.4594
$3p3$	$^2D^o$	2.5: 1	23.5360	23.4455
$3p3$	$^2D^o$	1.5: 2	23.5710	23.4726
$3p3$	$^4S^o$	1.5: 3	23.4820	23.3460
$3p3$	$^2P^o$	1.5: 5	22.9420	22.8222
$3p3$	$^2P^o$	0.5: 2	22.9700	22.8444
$3s3p(3Po)3d$	$^4F^o$	4.5*: 1	22.8070	22.7052
$3s3p(3Po)3d$	$^4F^o$	3.5*: 1	22.8820	22.7732
$3s3p(3Po)3d$	$^4F^o$	2.5*: 2	22.9370	22.8230
$3s3p(3Po)3d$	$^4P^o$	2.5: 3	22.5330	22.3805
$3s3p(3Po)3d$	$^4P^o$	1.5: 6	22.4060	22.3609
$3s3p(3Po)3d$	$^4P^o$	0.5: 4	22.4100	22.3473
$3s3p(3Po)3d$	$^4D^o$	3.5: 2	22.4380	22.2672
$3s3p(3Po)3d$	$^4D^o$	2.5: 4	22.4070	22.2668
$3s3p(3Po)3d$	$^4D^o$	1.5: 7	22.5110	22.2711
$3s3p(3Po)3d$	$^4D^o$	0.5: 3	22.4980	22.2781
$3s3p(3Po)3d$	$^2D^o$	2.5: 5	22.2820	22.1398
$3s3p(3Po)3d$	$^2D^o$	1.5: 8	22.2880	22.1455
$3s3p(3Po)3d$	$^2F^o$	3.5: 3	21.8990	21.7521
$3s3p(3Po)3d$	$^2F^o$	2.5: 6	22.0350	21.8734
$3s3p(3Po)3d$	$^2P^o$	1.5*: 9	21.4680	21.2572
$3s3p(1Po)3d$	$^2F^o$	3.5: 4	21.3730	21.1774
$3s3p(1Po)3d$	$^2F^o$	2.5: 7	21.3460	21.1551
$3s3p(1Po)3d$	$^2P^o$	1.5:11	21.1350	20.9391
$3s3p(1Po)3d$	$^2P^o$	0.5: 5	21.1730	20.9779
$3s3p(1Po)3d$	$^2D^o$	2.5: 8	21.1280	20.9261
$3s3p(1Po)3d$	$^2D^o$	1.5:10	21.1620	20.9544
$3p2(3P)3d$	$^4F^e$	4.5*: 1	19.8570	19.7588
$3p2(3P)3d$	$^4F^e$	3.5*: 1	19.9180	19.9293
$3p2(3P)3d$	$^4F^e$	2.5*: 4	19.9750	19.9904
$3p2(3P)3d$	$^4D^e$	3.5: 2	19.6820	19.8193
$3p2(3P)3d$	$^4D^e$	2.5: 5	19.7450	19.8744
$3p2(3P)3d$	$^4D^e$	1.5: 6	19.7490	19.7625
$3p2(1D)3d$	$^2D^e$	2.5: 7	19.3740	19.2462
$3p2(1D)3d$	$^2D^e$	1.5: 7	19.4120	19.6604
$3p2(3P)3d$	$^4P^e$	2.5: 8	19.3000	19.1466
$3p2(3P)3d$	$^4P^e$	1.5: 8	19.3040	19.2144
$3p2(3P)3d$	$^4P^e$	0.5: 5	19.3080	19.5906
$3p2(1S)3d$	$^2D^e$	2.5*: 9	18.8330	18.6442
$3p2(3P)3d$	$^2F^e$	3.5: 5	18.7540	18.5942
$3p2(3P)3d$	$^2F^e$	2.5:10	18.8000	18.6312
$3s3d2(3F)$	$^4F^e$	3.5*: 6	18.6590	18.3515
$3p2(3P)3d$	$^2D^e$	2.5*:12	18.3260	18.0539
$3s3d2(3G)$	$^2G^e$	4.5: 4	17.8870	17.6259
$3s3d2(3G)$	$^2G^e$	3.5: 7	17.8900	17.6284
$3s3d2(3F)$	$^2F^e$	3.5: 8	17.4770	17.1460
$3s3d2(3F)$	$^2F^e$	2.5:15	17.4890	17.1601
$3s24s$	$^2S^e$	0.5:12	15.7470	15.8272
$3s24p$	$^2P^o$	1.5:20	14.4800	14.7102
$3s24p$	$^2P^o$	0.5:12	14.5270	14.7686
$3s3p(3Po)4s$	$^4P^o$	2.5*:20	13.5560	13.4596
$3s3p(3Po)4s$	$^4P^o$	1.5*:23	13.6700	13.9034
$3s24d$	$^2D^e$	2.5:16	13.3570	13.3252
$3s24d$	$^2D^e$	1.5:17	13.3680	13.3363
$3s24f$	$^2F^o$	3.5:14	12.5260	12.5028
$3s24f$	$^2F^o$	2.5:21	12.5240	12.5060
$3s3p(3Po)4f$	$^4G^e$	5.5*: 1	10.2880	10.2105

can be $^2G^e_{7/2}$ to combine with the fourth for $^2G^e$. The seventh and ninth can form $^2P^e$ while the eighth level is $^2S^e$.

Identification procedure is repeated with different contributing channels for missing levels as well as for removing duplicate identities until all levels have been identified uniquely. All assigned spectroscopic levels, equivalent and single valence electron, are compared with the available energies and transitions, for consistency. These identifications of levels are then used to define those of fine structure transitions.

BPRM identification of levels are needed mainly for guidance in diagnostics and other applications. However, spectroscopy of level identification is one of the most laborious tasks. It also involves some judgment. While low lying or weakly interacting levels can be more definitely identified, others may contain some uncertainty from mixed configuration interaction whose dominance is the main determining factor for identification. As noted earlier for the R-matrix method, the mixing coefficients are less defined because of two contributions, from the inner and the outer regions. Atomic structure calculations do not have the space divided and levels are defined with dominant configuration. Hence some differences from different approximations in identifications arising due to differences in the most contributing configuration do not necessarily indicate an error, rather indicate of other possible designations with different leading percentage contributions.

5. Results and discussion

The results of Fe XIV and the discussions are divided into four following subsections, fine structure energy levels, oscillator strengths for E1 transitions, lifetimes, and estimation of accuracy.

5.1. Fine structure energy levels

The present BPRM calculation has obtained a total of 1002 fine structure levels with $n \leqslant 10$, $l \leqslant 9$, and $0.5 \leqslant J \leqslant 9.5$ with even and odd parities. While NIST compilation lists only 68 observed levels, other calculations have found more energy levels. However, the present calculation has found the largest number of new levels. These levels have been identified spectroscopically as $C_t(^{2S_t+1}L^{\pi_t}_{t\ J_t})nl^{2S+1}L^\pi_J$ using the numerical procedure explained in the above section. Table 2 presents a sample set of identified energies grouped together as components LSJ of LS terms. The consistency of energy values $E(Ry)$ of each set of the same configuration and $J\pi$ indicate consistency in their identification. The format of Table 2 is similar to that of the NIST and is useful for spectroscopic diagnostics.

The ion has a relatively larger number of equivalent electron states from the configurations $3s3p^2, 3p^3, 3s3d^2$, and $3p3d^2$. While $3s3p^2$ give four states, ^4P, ^2P, ^2D, ^2S, and $3p^3$ gives three states $^4P^o$, $^2D^o$, $^2G^o$, the other two give more states due to ^1S, ^1D, ^1G, ^3P, ^3F states of $3d^2$ configuration. Hence $3s3d^2$ gives ^2G, ^4F, ^2F, ^2D, ^4P, ^2P, and ^2S, and $3p3d^2$ gives $^2H^o$, $^2G^o$, $^2H^o$, $^4G^o$, $^4F^o$, $^4D^o$, $^2G^o$, $^2F^o$, $^2D^o$, $^2F^o$, $^2D^o$, $^2P^o$, $^4D^o$, $^4P^o$, $^4G^o$, $^2D^o$, $^2P^o$, $^2S^o$, $^2S^o$. The configuration $3p3d^2$ often does not form bound states in other elements. However, the strong attractive nuclear potential of highly charged Fe XIV causes the orbitals pulled into these bound levels.

BPRM energies of Fe XIV are compared in Table 3 with the available 68 measured energies (Sugar and Corliss, 1985; Shirai et al., 2000) and those of Redfors and Litzen, 1989). They are ordered in energy from the ground to higher excited LS terms. The negative sign for the energies has been omitted for convenience. The BPRM energies agree very well, mostly in less than 1% and the highest being 1.9% for $3s3d^2(^3F)$ levels, with the measured fine structure levels. The number next to the J-value in Table 3 is the relative position of the level in the calculated set of levels of the $J\pi$ symmetry.

5.2. Oscillator strengths for E1 transitions

From the 1002 fine structure energy levels of Fe XIV with $0.5 \leqslant J \leqslant 9.5$ a total of 130,520 electric dipole (E1) transitions is obtained. The E1 transitions correspond to both the same spin multiplicity (dipole allowed) as well as different spin multiplicity (intercombination) transitions. These can be identified spectroscopically through those of the fine structure levels. The file containing all the transitions is available electronically.

The R-matrix codes calculates oscillator strengths (f) both in length and in velocity forms. However, only the length form f-values are treated to be more accurate and are used. The integral for a f-value varies as $1/r$ in length form and as $1/r^2$ for velocity form. Hence it depends on the contributions from over a much larger radial distance in length form than that of the velocity form. Except for hydrogen and helium like ions for which wave function can be almost exact, f in two forms usually do not agree well. The other exception is with central-field approximation, which does not have any angular dependence and can not account for correlation effect properly, can give similar f-values in both forms. With proper treatment of angular dependence and configuration interactions of multi-electron systems, the difference becomes more prominent. The wave function in the R-matrix method, which has inner and outer regions, extends over a large distance and the outer region contributes more accurately to the transition integral in length form than to that in velocity form.

A subset of the Fe XIV transitions has been reprocessed with the observed energies where the calculated BPRM line strengths (S) are multiplied by the observed transition energies. This is a common method practiced by the NIST for its compiled transition tables. Since the observed energies are more accurate, the processed values are useful for diagnostics where exact observed transition energies are used for line identifications. A sample set of these transitions of Fe XIV, formatted similar to that of the NIST, is presented in Table 4. The transitions are grouped together as fine structure components of the LS multiplets. The transitions with same spin multiplicity are statistically averaged over to obtain the LS multiplets. However, such average is carried out only for same-spin transitions.

Current NIST table contains a small set of 151 transitions in Fe XIV. The latest published results also consider only limited number of transitions, with highest n to be 4. However, astrophysical modeling requires all possible transitions going up to very high n. The present work provides the most complete set of transitions for all practical purposes. For modeling the present oscillator strengths are available electronically in sets of $J\pi - J'\pi'$ (similar to the format given in earlier publications, e.g. Nahar 2010).

The BPRM transition probabilities are benchmarked with the earlier results compiled by NIST as well as with recent calculations in Table 5. NIST includes transitions from Shirai et al. (2000); Fawcett et al. (1972), and Huang (1986) and rates them with alphabetic letters, mostly D and E, for accuracies. However, comparison in Table 5 shows that the present A-values in very good agreement with most of those in the NIST compiled table. Similar is the case with other work not compared in the table. For example, for the first transition in the table, $3s^23p(^2P_{1/2}^o) - 3s3p^2(^2S_{1/2})$, Liang et al.

Table 4
Sample set of E1 transition probabilities among the observed levels of Fe XIV, grouped as fine structure transitions of the LS multiplet. I and K represent the calculated energy positions in the corresponding symmetries.

$C_i - C_k$	$T_i - T_k$	g_i:I–g_k:K	E_{ik} (Å)	f	S	A (s^{-1})
$3s^23p-3s3p^2$	2Po–4Pe	2: 1–2: 1	451.12	5.78E−04	1.72E−03	1.89E+07
$3s^23p-3s3p^2$	2Po–4Pe	4: 1–2: 1	492.84	1.33E−04	8.61E−04	7.29E+06
$3s^23p-3s3p^2$	2Po–4Pe	2: 1–4: 1	436.01	2.50E−05	7.19E−05	4.39E+05
$3s^23p-3s3p^2$	2Po–4Pe	4: 1–4: 1	474.87	1.58E−04	9.89E−04	4.68E+06
$3s^23p-3s3p^2$	2Po–4Pe	4: 1–6: 1	453.14	8.90E−04	5.31E−03	1.93E+07
$3s3p^2-3p^3$	4Pe–2Po	2: 1–2: 2	237.74	1.23E−04	1.93E−04	1.45E+07
$3s3p^2-3p^3$	4Pe–2Po	2: 1–4: 5	236.02	2.81E−03	4.37E−03	1.68E+08
$3s3p^2-3p^3$	4Pe–2Po	4: 1–2: 2	242.17	9.72E−05	3.10E−04	2.21E+07
$3s3p^2-3p^3$	4Pe–2Po	4: 1–4: 5	240.38	3.13E−03	9.90E−03	3.61E+08
$3s3p^2-3p^3$	4Pe–2Po	6: 1–4: 5	246.35	9.94E−04	4.84E−03	1.64E+08
$3s3p^2-3s3p(3Po)3d$	4Pe–4Do	2: 1–2: 3	211.68	2.82E−01	3.93E−01	4.20E+10
$3s3p^2-3s3p(3Po)3d$	4Pe–4Do	2: 1–4: 7	212.32	2.42E−03	3.38E−03	1.79E+08
$3s3p^2-3s3p(3Po)3d$	4Pe–4Do	4: 1–2: 3	215.18	1.46E−03	4.13E−03	4.20E+08
$3s3p^2-3s3p(3Po)3d$	4Pe–4Do	4: 1–4: 7	215.84	1.46E−01	4.14E−01	2.08E+10
$3s3p^2-3s3p(3Po)3d$	4Pe–4Do	4: 1–6: 4	210.65	1.20E−01	3.34E−01	1.21E+10
$3s3p^2-3s3p(3Po)3d$	4Pe–4Do	6: 1–4: 7	220.65	5.47E−02	2.38E−01	1.12E+10
$3s3p^2-3s3p(3Po)3d$	4Pe–4Do	6: 1–6: 4	215.23	1.90E−01	8.09E−01	2.74E+10
$3s3p^2-3s3p(3Po)3d$	4Pe–4Do	6: 1–8: 2	216.81	3.91E−01	1.67E+00	4.16E+10
LS	4Pe–4Do	12–20		4.54E−01	3.87E+00	3.92E+10
$3s3p^2-3s3p(3Po)3d$	4Pe–4Po	2: 1–2: 4	207.44	1.46E−03	1.99E−03	2.26E+08
$3s3p^2-3s3p(3Po)3d$	4Pe–4Po	2: 1–4: 6	207.25	4.06E−01	5.54E−01	3.15E+10
$3s3p^2-3s3p(3Po)3d$	4Pe–4Po	4: 1–2: 4	210.80	9.93E−02	2.76E−01	2.98E+10
$3s3p^2-3s3p(3Po)3d$	4Pe–4Po	4: 1–4: 6	210.60	3.76E−02	1.04E−01	5.65E+09
$3s3p^2-3s3p(3Po)3d$	4Pe–4Po	4: 1–6: 3	216.97	2.69E−01	7.70E−01	2.54E+10
$3s3p^2-3s3p(3Po)3d$	4Pe–4Po	6: 1–4: 6	215.18	6.49E−03	2.76E−02	1.40E+09
$3s3p^2-3s3p(3Po)3d$	4Pe–4Po	6: 1–6: 3	221.83	2.45E−02	1.07E−01	3.32E+09
LS	4Pe–4Po	12–12		2.19E−01	1.84E+00	3.21E+10
$3s3p^2-3s3p(1Po)3d$	4Pe–2Po	2: 1–2: 5	161.86	4.71E−04	5.02E−04	1.20E+08
$3s3p^2-3s3p(1Po)3d$	4Pe–2Po	2: 1–4: 11	160.77	2.65E−05	2.80E−05	3.42E+06
$3s3p^2-3s3p(1Po)3d$	4Pe–2Po	4: 1–2: 5	163.90	2.72E−05	5.87E−05	1.35E+07
$3s3p^2-3s3p(1Po)3d$	4Pe–2Po	4: 1–4: 11	162.78	4.87E−06	1.04E−05	1.23E+06
$3s3p^2-3s3p(1Po)3d$	4Pe–2Po	6: 1–4: 11	165.50	3.49E−05	1.14E−04	1.28E+07
$3s^23p-3s3p^2$	2Po–2Se	2: 1–2: 2	274.23	1.91E−01	3.45E−01	1.69E+10
$3s^23p-3s3p^2$	2Po–2Se	4: 1–2: 2	289.11	9.60E−03	3.65E−02	1.53E+09
LS	2Po–2Se	6–2		7.01E−02	3.81E−01	1.85E+10

(2010), who present *gf* values instead of *A*-values from AUTO-STRUCTURE (AS) and FAC codes, obtained 0.401 (AS) and 0.398 (FAC) for *gf* while the present value is 0.382 and for the second transition, $3s^2 3p(^2P^o_{1/2})-3s3p^2(^2D_{3/2})$, they obtained 0.163 (AS) and 0.158 (FAC) compared to present value of 0.153. For the third transition, $3s^2 3p(^2P^o_{3/2})-3s3p^2(^2D_{3/2})$, which is also a weak transition, they obtain for the *gf*, 6.38e−03 (AS) and 6.13e−03 (FAC), and present value is 6.72e−03. However, significant differences are also noted for the present values with others. For example, for transition, $3s^2 3d(^2D_{5/2})-3s^2 4p(^2P^o_{3/2})$ the atomic structure transition probability is $5.1e+10\,s^{-1}$ compared to R-matrix value $3.62e+10\,s^{-1}$. Another case is the fine structure transition $3s3p^2(^2D5/2)-3s3p3d(^2D^o_0)$ for which the present *A*-value is $3.27E+8\,s^{-1}$ while it is $1.9E+08\,s^{-1}$ by Shirai et al. Some difference can be expected from differences in the theoretical approximations, mainly from optimization of the wave functions. Relative to atomic structure calculations, the R-matrix method considers more configuration interactions and predicted transition parame-

ters are in general more accurate, but it can not optimize any selected transitions for improvement. Through optimization, especially for the observed levels, atomic structure calculations can give more accurate transition values for those levels. Another possible reason for difference arises from differences in identification of the states and hence comparing the wroing transition. The mixed states usually have different percentage contributions from the contributing configurations or channels in the two theoretical approximations leading to different spectroscopic identification.

5.3. Lifetimes

With the large set of E1 transitions, lifetimes of excited levels can be obtained accurately from the inverse of the sum of radiative decay rates (A-values). Compared to the allowed transitions, forbidden transitions typically have negligible contributions to lifetimes, except for the low lying metastable levels which decay only through forbidden transitions. Forbidden lines have been

Table 5
Comparison of BPRM *A*-values for E1 transitions in Fe XIV with those by (a) Shirai et al. (2000), (b) Huang (1986), (c) Fawcett et al. (1972), (d)Santana et al. (2009), (e) Tayal (2008), (f)Fischer et al. (2006), (g) Shirai et al., 2000, (h) Gupta and Msezane (2001), (i) Wei et al. (2008).

λ (Å)	A(s⁻¹) Other	A(s⁻¹) BPRM	$C_i - C_j$	$SL\pi i - j$	$gi - j$
274.23	1.70 + 10^e, 1.72e+10^f,1.78 + 10^g, 1.73e+10^h	1.69E+10	$3s^2 3p-3s3p^2$	$^2P^o-^2S$	2–2
334.16	2.41 + 09^e, 2.46e+09^f,2.38 + 09^g, 2.30e+09^h	2.20E+09	$3s^2 3p-3s3p^2$	$^2P^o-^2D$	2–4
356.52	8.79 + 07^e, 8.67e+07^f, 7.32 + 07^g	8.83E+07	$3s^2 3p-3s3p^2$	$^2P^o-^2D$	4–4
353.75	1.98 + 09^e, 1.99e+09^f, 1.91 + 09^g, 1.85e+09^h	1.83E+09	$3s^2 3p-3s3p^2$	$^2P^o-^2D$	4–6
453.14	2.06e+07^d, 2.33 + 07^e, 2.47 + 07^f, 2.65e+07^g	1.93E+07	$3s^2 3p-3s3p^2$	$^2P^o-^4P$	4–6
474.87	4.851 + 06^d, 5.43 + 06^e, 5.91 + 06^f, 6.22e+06^g	4.68E+06	$3s^2 3p-3s3p^2$	$^2P^o-^4P$	4–4
492.84	7.885 + 06^d, 9.16 + 06^e, 1.01 + 07^f, 9.89e+06^g	7.29E+06	$3s^2 3p-3s3p^2$	$^2P^o-^4P$	4–2
436.01	4.640 + 05^d, 5.68 + 05^e, 5.19 + 05^f, 5.66e+05^g	4.39E+05	$3s^2 3p-3s3p^2$	$^2P^o-^4P$	2–4
451.12	2.230 + 07^d, 2.33e+07^e, 2.60 + 07^f, 2.67e+07^g	1.89E+07	$3s^2 3p-3s3p^2$	$^2P^o-^4P$	2–2
211.331	3.6e+10 D^b	3.62E+10	$3s^2 3p-3s^2 3d$	$^2P^o-^2D$	2–4
69.66	8.9e+10 D^c	8.96E+10	$3s^2 3p-3s^2 4s$	$^2P^o-^2S$	2–2
70.613	1.7e+11 D^c	1.85E+11	$3s^2 3p-3s^2 4s$	$^2P^o-^2S$	4–2
58.963	2.7e+11 C^{a,c}	2.61E+11	$3s^2 3p-3s^2 4d$	$^2P^o-^2D$	2–4
59.579	3.1e+11 C^{a,c}	3.10E+11	$3s^2 3p-3s^2 4d$	$^2P^o-^2D$	4–6
280.739	1.2e+10:D^a	1.23E+10	$3s3p^2-3p^3$	$^4P-^4S^o$	4–4
288.512	1.6e+10:D^a	1.66E+10	$3s3p^2-3p^3$	$^4P-^4S^o$	6–4
274.797	6.2e+09:D^a	6.51E+09	$3s3p^2-3p^3$	$^4P-^4S^o$	2–4
210.615	1.9e+10 D^a	1.59E+10	$3s3p^2-3s3p(^1P^o)3d$	$^2S-^2P^o$	2–2
218.578	2.5e+10:E^a	2.54E+10	$3s3p^2-3s3p(^3P^o)3d$	$^4P-^4P^o$	4–6
223.256	3.0e+09:E^a	3.32E+09	$3s3p^2-3s3p(^3P^o)3d$	$^4P-^4P^o$	6–6
213.176	4.1e+10 D^a, 4.43e+10^i	4.20E+10	$3s3p^2-3s3p(^3P^o)3d$	$^4P-^4D^o$	2–2
216.742	4.5e+08:E^a	4.20E+08	$3s3p^2-3s3p(^3P^o)3d$	$^4P-^4D^o$	4–2
212.154	1.1e+10 D^a, 9.37e+09^i	1.21E+10	$3s3p^2-3s3p(^3P^o)3d$	$^4P-^4D^o$	4–6
216.576	2.7e+10 D^a, 2.99e+10^i	2.74E+10	$3s3p^2-3s3p(^3P^o)3d$	$^4P-^4D^o$	6–6
216.928	4.04e+10:C^a, 4.46e+10^i	4.20E+08	$3s3p^2-3s3p(^3P^o)3d$	$^4P-^4D^o$	6–8
185.099	1.4e+08 E^a	1.69E+08	$3s3p^2-3s3p(^1P^o)3d$	$^2D-^2P^o$	4–2
183.684	3.0e+08 E^a	3.71E+08	$3s3p^2-3s3p(^1P^o)3d$	$^2D-^2P^o$	4–4
184.438	2.7e+08 E^a	2.44E+08	$3s3p^2-3s3p(^1P^o)3d$	$^2D-^2P^o$	6–4
184.661	8.8e+07 E^a	6.13E+07	$3s3p^2-3s3p(^1P^o)3d$	$^2D-^2D^o$	4–4
185.423	1.9e+08 E^a	3.27E+08	$3s3p^2-3s3p(^1P^o)3d$	$^2D-^2D^o$	6–4
192.629	1.4e+09 E^a	1.64E+09	$3s3p^2-3s3p(^1P^o)3d$	$^2D-^2F^o$	6–6
193.752	2.7e+10 E^a	2.94E+10	$3s3p^2-3s3p(^1P^o)3d$	$^2D-^2F^o$	6–8
191.806	2.6e+10 E^a, 2.84e+10^i,	2.80E+10	$3s3p^2-3s3p(^1P^o)3d$	$^2D-^2F^o$	4–6
171.822	3.1e+08 E^a	2.27E+08	$3s3p^2-3s3p(^3P^o)3d$	$^4P-^2P^o$	2–4
193.264	4.2e+08 E^a	3.53E+08	$3s3p^2-3s3p(^1P^o)3d$	$^4P-^2F^o$	6–8
173.851	3.3e+08 E^a	2.73E+08	$3s3p^2-3s3p(^1P^o)3d$	$^4P-^2F^o$	6–8
69.386	7.6e+10:D^a	8.85E+10	$3s3p^2-3s3p(^3P^o)4s$	$^4P-^4Po$	2–4
69.176	5.6e+10:D^a	6.28E+10	$3s3p^2-3s3p(^3P^o)4s$	$^4P-^4Po$	4–6
70.251	8.1e+10 D^a	9.72E+10	$3s3p^2-3s3p(^3P^o)4s$	$^4P-^4P^o$	6–4
69.667	1.3e+11 D^a	1.45E+11	$3s3p^2-3s3p(^3P^o)4s$	$^4P-^4P^o$	6–6
91.273	5.6e+10 D^{a,c}	2.45E+10	$3s^2 3d-3s^2 4p$	$^2D-^2P^o$	4–2
91.009	5.1e+10 D^{a,c}	3.58E+10	$3s^2 3d-3s^2 4p$	$^2D-^2P^o$	6–4
76.152	7.0e+11 C^{a,c}	6.30E+11	$3s^2 3d-3s^2 4f$	$^2D-^2F^o$	6–8
76.022	6.6e+11 C^{a,c}	5.86E+11	$3s^2 3d-3s^2 4f$	$^2D-^2F^o$	4–6
72.80	8.8e+11 D^a	8.26E+11	$3s3p(^3P^o)3d-3s3p(^3P^o)4f$	$presup4F^o-^4G$	10–12

Table 6
Sample set of lifetimes of excited Fe XIV levels obtained from E1 transitions.

Level					J	Ij	E (Ry)	Lifetime (sec)	Ntrans
1	3s3p2			4Pe	0.5	1	−2.6803E+01	3.814E−08	2
2	3s3p2			2Se	0.5	2	−2.5500E+01	5.414E−11	2
3	3s3p2			2Pe	0.5	3	−2.5283E+01	2.822E−11	2
4	3p2	3Pe	3d	4De	0.5	4	−1.9726E+01	4.531E−11	16
5	3p2(3P)3d			4Pe	0.5	5	−1.9308E+01	2.942E−11	16
6	3p2	3Pe	3d	2 P e	0.5	6	−1.9141E+01	1.238E−11	16
7	3p2	1De	3d	2 S P e	0.5	7	−1.8853E+01	2.229E−11	16
8	3p2	1De	3d	2 S P e	0.5	8	−1.8756E+01	2.206E−11	16
9	3s3d2			4 P e	0.5	9	−1.8038E+01	1.302E−11	16
10	3s3d2			2 P e	0.5	10	−1.6886E+01	1.045E−11	16
11	3s3d2			2 S e	0.5	11	−1.6754E+01	1.124E−11	16
12	3s24s			2Se	0.5	12	−1.5747E+01	3.635E−12	20
13	3s3p	3Po	4p	4 P D e	0.5	13	−1.2634E+01	6.935E−12	40
14	3s3p	3Po	4p	4 P D e	0.5	14	−1.2530E+01	5.167E−12	40
15	3s3p	3Po	4p	2 S P e	0.5	15	−1.2432E+01	1.693E−11	42

studied extensively as mentioned earlier in the introduction. The present results are for the allowed transitions only.

The lifetimes of 1001 excited levels of Fe XIV using E1 transitions are reported. A sample set of lifetimes is presented in Table 6. The last column (Ntrns) lists the number of E1 transitions contributed for the lifetime of the level.

The present lifetimes should accurate for most excited levels except for the very low lying ones which decay mainly through a single intercombination line. For example, the intercombination transitions, $3s^23p(^2P^o_{1/2})$—$3s3p^2(^4P_{1/2})$ and $3s^23p(^2P^o_{3/2})$—$3s3p^2(^4P_{5/2})$, have been the focus of a larger number of studies since the inverse of the A-values of these transitions give lifetimes of the upper levels $3s3p^2(^4P_{1/2})$, $3s3p^2(^4P_{5/2})$. These lifetimes were measured to be about 29 ns and 39 ns with experimental errors of about 5 ns respectively by Trabert et al. (1988); Trabert et al. (1993)). Compared to present BPRM A-values, the earlier Storey et al. (2000); Fischer et al. (2006); Tayal, 2008; Liang et al. (2010) get larger A-values for these levels, as given in Table 5, and hence should give shorter lifetimes than the present values. They agree better with the experimental measurement. The present lifetimes of these levels are 38 ns and 52 ns respectively. The lifetime of the first level, $3s3p^2(^4P_{1/2})$, with a single decay or transition, is seen in Table 6. It can be noted in Table 5 that the A-values for fine structure components of this multiplet, $3s^23p(^2P^o)$—$3s3p^2(^4P)$, by Santana et al. (2009) who used ab initio multireference Moller–Plesset perturbation theory agree better with the present BPRM values showing consistency in the two calculations. These appear to suggest that the atomic structure calculations may have had specifically optimized to agree with the measured lifetimes.

5.4. Estimation of accuracy

The BPRM method involves large scale computations. The accuracy of the results is a crucial part of the computation and they are considered through a number of ways as explained below.

The accuracy of the energy levels and transitions of the (N + 1)-electron system are dependent on the core or target wave functions. To improve these wave functions for the core Fe XV, various sets of configurations and choice of Thomas–Fermi scaling parameters λ_{nl} are used until the set of calculated energies have overall good agreement with the observed values, as shown in Table 1. These wave functions are the input wave function for the R-matrix calculations where the final wave functions are generated.

The choice on the number of core levels to be included in the first term of the wave function expansion is based on the formation of possible bound states of the ion with the given core excitations. The present calculations included 26 levels of the core Fe XV. The high-lying excited core levels do not form bound states of the electron–ion system, and corresponding channels have insignificant effect on the bound state energies.

The second term in the wave function expansion, Eq. (1), provides the additional configurations for (N + 1) electron system needed for completeness of the orthogonality condition for equivalent electron states. As listed in the computation section, all possible configurations for such states were included. This term also includes some more configurations to consider the short-range electron–electron correlation effects and coupling of channels more accurately. The present calculation includes all these configurations, as listed in the Computation section, with a total of 63 configurations for the term.

Consideration of R-matrix boundary is also an important factor to accuracy to make sure that all correlation effects are well within the boundary so that the wave function is Coulombic outside of it. This implies that the amplitudes of the orbital wave functions are insignificant or almost vanishing at the boundary. The present calculations chose the R-matrix boundary to be $3.5a_o$ where inner orbital wave functions are almost zero, the amplitudes of 3d orbital has value of the order of 10^{-5}.

The calculated target energies were replaced by the observed energies in calculating the Hamiltonian matrix. This improves the positions of the Rydberg series of resonances in photoionization calculations. However, the improvement is not well defined or linear for energies of the (N + 1) electron system since the correlation effect on the wave functions dominates more than that by the slight shift in the core energies. For the present case where the calculated core energies are in good agreement with the observed energies, the improvement in energies could be about 1%.

The bound levels were obtained from the poles in the Hamiltonian using very fine mesh of effective quantum number (Δv=0.001 to 0.00025). Hence all the calculated energy levels within very narrow quantum defects were sorted out. However, there are some missing levels in the very high energy states. These levels require additional configurations with highly excited levels. Inclusion of these additional configurations make the computation very large to handle whereas these highly excited levels can be estimated in hydrogenic approximation. The calculated highly excited levels may have some uncertainties. The accuracy on the splitting of the highly excited levels depends on the relativistic effects. The BPRM method includes the three relativistic one-body correction terms and part of the two-body terms, and higher order terms may contribute to the splitting significantly. Nonetheless, based on the agreement with observed energies in Table 3 and including the possible uncertainties of the higher levels, the BPRM energies are expected to be accurate within 10% for the entire set.

The radiative decay rates for transitions show various degrees of agreement with the existing calculated values. Some differences, especially for transitions with higher levels. can arise from the differences in spectroscopic identification. The caluclated energies of Fe XIV agree very well with the 68 observed values. These observed energies were used to replace the 68 calculated level energies in obtaining the oscillator strengths and radiative decay rates from the calculated line strengths. The purpose is to carry out precise diagnostics where accurate transition energies are used. However, the wave functions in line strengths correspond to the calculated energies and hence such replacement by observed energies may not necessarily improve the radiative decay rates. Considering that the BPRM values for energy levels and transitions have an overall consistency of accuracy, good agreement with existing transition probabilities indicate that BPRM transitions can have an estimated accuracy of A (within 10%) to C (within 30%) for most transitions.

6. Conclusion

Energies and transition parameters for Fe XIV are presented from Breit–Pauli R-matrix method. The theoretical spectroscopy of energy levels and transitions of BPRM method is explained in detail. Although laborious, the identification is unique in proper correspondence between fine structure and LS terms. Through use of powerful computational capability the BPRM method, the present work has resulted in the most complete set of allowed transitions, with n going up to 10, needed for both diagnostics as well as astrophysical modeling. The results have been benchmarked with very good agreement with the existing accurate measured energies in less than 2% and good agreement for most of the existing calculated transitions. Based on the accuracy of the wave function of Fe XIV, the comparison of energy levels and the transitions, and the relativistic Breit–Pauli method used for computation, the estimated accuracy of the large set of energy levels should be within 10% and be A (within 10%) to C (within 30%) for most transitions.

Electronic files for energy levels, oscillator strengths, radiative decay rates, and lifetimes are available electronically from the NORAD-Atomic-Data website: www.astronomy.ohio-state.edu/nahar/nahar_radiativeatomicdata.html.

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