A comprehensive set of UV and x-ray radiative transition rates for Fe XVI

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Abstract

Sodium-like Fe XVI is observed in collisionally ionized plasmas such as stellar coronae and coronal line regions of active galactic nuclei including black hole-accretion disc environments. Given its recombination edge from neon-like Fe XVII at ~ 25 Å, the Fe XVI bound–bound transitions lie in the soft x-ray and EUV (extreme ultraviolet) range. We present a comprehensive set of theoretical transition rates for radiative dipole allowed E1 transitions including fine structure for levels with $n\ell(SLJ) \leqslant 10$, $\ell \leqslant 9$ using the relativistic Breit–Pauli R-matrix (BPRM) method. In addition, forbidden transitions of electric quadrupole (E2), electric octupole (E3), magnetic dipole (M1) and magnetic quadrupole (M2) type are presented for levels up to $5g(SLJ)$ from relativistic atomic structure calculations in the Breit–Pauli approximation using code SUPERSTRUCTURE. Some of the computed levels are autoionizing, and oscillator strengths among those are also provided. BPRM results have been benchmarked with the relativistic coupled cluster method and the atomic structure Dirac–Fock code GRASP. Levels computed with the electron collision BPRM codes in bound state mode were identified with a procedure based on the analysis of quantum defects and asymptotic wavefunctions. The total number of Fe XVI levels considered is 96, with 822 E1 transitions. Tabulated values are presented for the oscillator strengths f, line strengths S and Einstein radiative decay rates A. This extensive dataset should enable spectral modelings up to highly excited levels, including recombination-cascade matrices.

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1. Introduction

Highly charged iron ions exist in a variety of high-temperature astrophysical sources emitting or absorbing radiation from the optical to the x-ray range. The spectral lines of these ions provide information about physical conditions and chemical abundances in many sources. Iron, including Fe XVI, lines have been recently identified in XMM observations of the narrow-line Seyfert 1 galaxy MKN335, currently in a historically low state of x-ray flux from black hole accretion [10]. The analysis and modeling of these spectra require accurate and extensive radiative data. Coronal iron ions are of special interest because they provide temperature and density diagnostics. Their presence implies a high degree of ionization and could also be a discriminant between photoionized and

collisionally ionized environments. Spectral lines of Ne-like Fe XVII are signatures of most coronal plasmas. It follows that in collisional ionization equilibrium adjacent ionization stages, Na-like Fe XVI and F-like Fe XVIII, would also be present; indeed, all three ions are often observed. However, the energetics of the three ions differ significantly. Whereas the strongest x-ray lines of Fe XVII and Fe XVIII lie around 15 Å, the Fe XVI lines are found in the softer x-ray region below the recombination edge

$$\text{Fe XVII } (2p^6 \, {}^1S_0) + e(k^2 \rightarrow 0) \longrightarrow \text{Fe XVI } (n\ell; SLJ) + h\nu, \tag{1}$$

at 25.3 Å, hence photo-excitations or bound–bound transitions at $\lambda > 25$ Å may be detected. They span a wavelength region from soft x-rays to the EUV. For example Fe XVI lines from solar active regions due to transitions among low $n(SLJ)$ levels are observed around 300 Å on the one hand, and from

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Table 1. Binding energies E_c calculated by BPRM for Fe XVI (with magnetic interaction between electrons that can be absorbed into ζ) and comparison with observed energies E_o from NIST. I_J is the positional level index in the given symmetry $J\pi$, K or K + L telling that closed shells $1s^2$ or $1s^2 2s^2 2p^6$ are screening *all* spin–orbit parameters ζ. Case K + L computed with `NRANG2=15` basis functions while `RA=4.03`.

Level		J	I_J	E_c/Ry		E_o/Ry	ν_o
				K	K + L		
$2p^6 3s$	^{2}S	0.5	1	35.9570	35.9517	35.9611	
3p	^{2}P^o	1.5	1	33.2342	33.2344	33.2442	
3p	^{2}P^o	0.5	1	33.4269	33.4208	33.4351	
3d	^{2}D	2.5	1	29.7436	29.7494	29.7790	2.93 201
3d	^{2}D	1.5	1	29.7853	29.7767	29.8055	2.93 070
4s	^{2}S	0.5	2	18.9363	18.9415	18.9410	
4p	^{2}P^o	1.5	2	17.8566	17.8677	17.8665	
4p	^{2}P^o	0.5	2	17.9324	17.9407	17.9394	
4d	^{2}D	2.5	2	16.5695	16.5836	16.5879	3.92 848
4d	^{2}D	1.5	2	16.5879	16.5965	16.5992	3.92 714
4f	^{2}F^o	3.5	1	16.0472	16.0524	16.0462	
4f	^{2}F^o	2.5	1	16.0544	16.0572	16.0503	
5s	^{2}S	0.5	3	11.6932	11.6856	11.7032	
5p	^{2}P^o	1.5	3	11.1648	11.1523	11.1641	
5p	^{2}P^o	0.5	3	11.1997	11.1888	11.2004	
5d	^{2}D	2.5	3	10.5448	10.5335	10.5494	4.92 695
5d	^{2}D	1.5	3	10.5538	10.5403	10.5545	4.92 495
5f	^{2}F^o	3.5	2	10.2719	10.2671	10.2734	
5f	^{2}F^o	2.5	2	10.2754	10.2695	10.2761	
5g	^{2}G	4.5	1	10.2407	10.2410	10.2379	
5g	^{2}G	3.5	1	10.2428	10.2424	10.2388	
6s	^{2}S	0.5	4	7.92865	7.92884	7.93052	
6p	^{2}P^o	1.5	4	7.62529	7.62755	7.63071	
6p	^{2}P^o	0.5	4	7.64675	7.64840	7.65350	
6d	^{2}D	2.5	4	7.27514	7.28139	7.28653	5.92 734
6d	^{2}D	1.5	4	7.28069	7.28539	7.29200	5.92 511
6f	^{2}F^o	3.5	3	7.12545	7.12931	7.13599	
6f	^{2}F^o	2.5	3	7.12755	7.13072	7.13654	
7s	^{2}S	0.5	5	5.73268	5.73174	5.67969	
7p	^{2}P^o	1.5	5	5.54563	5.54512	5.51567	
7d	^{2}D	2.5	5	5.32979	5.33174	5.33523	6.92 697
7d	^{2}D	1.5	5	5.33325	5.33426	5.33797	6.92 519
7f	^{2}F^o	3.5	4	5.23597	5.23697	5.24165	
7f	^{2}F^o	2.5	4	5.23727	5.23783	5.24037	
8p	^{2}P^o	1.5	6	4.21396	4.21377	4.17610	
8d	^{2}D	2.5	6	4.07158	4.07258	4.07586	7.92 520
8d	^{2}D	1.5	6	4.07386	4.07426	4.07768	7.92 343
8f	^{2}F^o	3.5	5	4.00876	4.00914	4.01390	
8f	^{2}F^o	2.5	5	4.00965	4.00972	4.01481	
9p	^{2}P^o	1.5	7	3.31016	3.31001	3.27395	
9d	^{2}D	2.5	7	3.21126	3.21171	3.20105	8.94 280
9d	^{2}D	1.5	7	3.21283	3.21289	3.16460	8.99 416
9f	^{2}F^o	3.5	6	3.16713	3.16723	3.15548	
9f	^{2}F^o	2.5	6	3.16774	3.16764	3.15548	

Table 2. $\Delta\mu_\ell = \nu_{\ell+1/2} - \nu_{\ell-1/2}$ for lower n from data in table 1.

$n\ell$	K	K + L	Obs
3p	0.00801	0.00775	0.00793
4p	0.00801	0.00770	0.00770
3d	0.00208	0.00134	0.00131
4d	0.00218	0.00154	0.00134
4f	0.00090	0.00059	0.00051
i.e.	7.2 mRy	4.7 mRy	4.1 mRy

radiative transition probabilities for a number of iron ions as well as astrophysical applications and spectral modeling (www.astronomy.ohio-state/~pradhan). With particular relevance to the present work transition rates for *all* levels up to high-$n(SLJ)$ are needed in such models. For example, recently, we have developed a general spectral modeling (GSM) code for transient, quasi-steady state, and steady-state laboratory and astrophysical plasmas [18]. One of the features of GSM is the computation of a *collision-less transition matrix* that requires a complete set of transition rates in order to compute recombination-cascade matrices. The first application of GSM, to interpret hard x-ray spectra from He-like Ca, Fe and Ni, revealed significant and unexpected discrepancies with previous work for well-known and widely used line ratios as diagnostics of high-temperature plasmas [19, 20]. The new models employed BPRM level-specific unified recombination rates for $n(SLJ) \leqslant 10$, including radiative and dielectronic recombination in an *ab initio* and self-consistent manner, and BPRM radiative transition rates (e.g. [16]). Similarly, we plan to investigate the accuracy and completeness of spectral models of other important ionization stages, namely the Na-, Ne- and F-like iron ions.

The National Institute for Standards and Technology (NIST; (http://physics.nist.gov/PhysRefData/ASD/index.html) provides the evaluated and compiled table of transitions for Fe XVI from earlier calculations. Among forbidden transitions, it includes only E2 transitions by Tull *et al* [29], who calculated them in a frozen-core Hartree–Fock approximation. Later Charro *et al* [5] calculated radiative decay rates for E2 transitions of Fe XVI using a relativistic quantum defect orbital formalism. In the absence of accurate fine structure transitions, NIST has carried out fine structure splitting of LS multiplets for some transitions.

This report provides radiative data obtained from the first R-matrix calculation for Fe XVI-levels. It is part of a project at OSU for a systematic study of iron and iron-group atoms and ions by Nahar *et al* (e.g. Fe V [14, 17], Fe XVII [15], Fe XX [13], Fe XXI [12], Fe XXIV and Fe XXV [16]). We also benchmark the present results against other elaborate relativistic calculations using the multi-configuration Dirac–Fock code (MCDF—GRASP2, e.g. [21]) and relativistic coupled cluster theory (RCC, e.g. [27, 28]).

2. Formulation

The relativistic Breit–Pauli R-matrix method with close coupling (CC) approximation, described in a number of papers [2, 3, 11, 22, 23, 26], enables calculation of a large number of fine structure E1 transitions with high accuracy. In

higher levels between $25\,\text{Å} < \lambda < 80\,\text{Å}$ on the other hand (e.g. [6, 7]).

Multi-wavelength spectroscopy of ions such as Fe XVI requires a reasonably complete set of atomic parameters. Generally, these are obtained from large-scale calculations of high accuracy, such as those being carried out under the Iron Project (IP: [11]), and extensions thereof such as the RmaX Network (viz. www.astronomy.ohio-state/~nahar). These calculations require a great deal of effort and computational resources. The Ohio State University (OSU) group has been engaged in calculations of such extensive datasets of

Table 3. Sample table of fine structure energy levels of Fe XVI as sets of LS term components. C_t is the core configuration, ν is the effective quantum number.

$C_t(S_t L_t \pi_t)$	J_t	nl	$2J$	E/Ry	ν	$SL\pi$
$Nlv = 1, {}^2L^e$: S (1)/2						
$\quad$ $2s^2 2p^6$ ($^1S^e$)	0	3s	1	$-3.59570E+01$	2.67	2 S e
$\quad$ $Nlv(c) = 1$:set complete						
$Nlv = 2, {}^2L^o$: P (3 1)/2						
$\quad$ $2s^2 2p^6$ ($^1S^e$)	0	3p	1	$-3.34269E+01$	2.77	2 P o
$\quad$ $2s^2 2p^6$ ($^1S^e$)	0	3p	3	$-3.32342E+01$	2.78	2 P o
$\quad$ $Nlv(c) = 2$:set complete						
$Nlv = 2, {}^2L^e$: D(5 3)/2						
$\quad$ $2s^2 2p^6$ ($^1S^e$)	0	3d	3	$-2.97853E+01$	2.93	2 D e
$\quad$ $2s^2 2p^6$ ($^1S^e$)	0	3d	5	$-2.97436E+01$	2.93	2 D e
$\quad$ $Nlv(c) = 2$:set complete						

Table 4. Sample output of fine structure energy levels of Fe XVI.

96 = number of levels, $n \leqslant 10, l \leqslant 9$

i_e	J	i_J	E/Ry	Config	${}^{2S+1}L^\pi$	$J\pi$ index
1	0.5e	1	$-3.59611E+01$	$2p^6 3s$	$^2S^e$	100001
2	0.5e	2	$-1.89410E+01$	$2p^6 4s$	$^2S^e$	100002
3	0.5e	3	$-1.17032E+01$	$2p^6 5s$	$^2S^e$	100003
4	0.5e	4	$-7.93052E+00$	$2p^6 6s$	$^2S^e$	100004
5	0.5e	5	$-5.67969E+00$	$2p^6 7s$	$^2S^e$	100005
6	0.5e	6	$-4.33725E+00$	$2s^2 2p^6\,^1S^e 8s$	$^2S^e$	100006
7	0.5e	7	$-3.39566E+00$	$2s^2 2p^6\,^1S^e 9s$	$^2S^e$	100007
8	0.5e	8	$-2.73047E+00$	$2s^2 2p^6\,1S^e\,10s$	$^2S^e$	100008
9	0.5o	1	$-3.34351E+01$	$2p^6 3p$	$^2P^o$	110001
10	0.5o	2	$-1.79394E+01$	$2p^6 4p$	$^2P^o$	110002
11	0.5o	3	$-1.12004E+01$	$2p^6 5p$	$^2P^o$	110003
12	0.5o	4	$-7.65350E+00$	$2p^6 6p$	$^2P^o$	110004
13	0.5o	5	$-5.55871E+00$	$2s^2 2p^6\,^1S^e 7p$	$^2P^o$	110005
14	0.5o	6	$-4.22249E+00$	$2s^2 2p^6\,^1S^e 8p$	$^2P^o$	110006
15	0.5o	7	$-3.31599E+00$	$2s^2 2p^6\,^1S^e 9p$	$^2P^o$	110007
16	0.5o	8	$-2.67295E+00$	$2s^2 2p^6\,^1S^e 10p$	$^2P^o$	110008
17	1.5e	1	$-2.98055E+01$	$2p^6 3d$	$^2D^e$	300001
18	1.5e	2	$-1.65992E+01$	$2p^6 4d$	$^2D^e$	300002
19	1.5e	3	$-1.05545E+01$	$2p^6 5d$	$^2D^e$	300003
20	1.5e	4	$-7.29200E+00$	$2p^6 6d$	$^2D^e$	300004
21	1.5e	5	$-5.33797E+00$	$2p^6 7d$	$^2D^e$	300005
22	1.5e	6	$-4.07768E+00$	$2p^6 8d$	$^2D^e$	300006

the CC approximation the wavefunction expansion Ψ_E for a $(N + 1)$-electron system with total orbital angular momentum L, spin multiplicity $(2S + 1)$ and total angular momentum symmetry $J\pi$, is expanded in terms of the states of the N-electron target ion as

$$\Psi_E(\text{e}+\text{ion}) = \mathcal{A} \sum_i \chi_i(\text{ion})\theta_i + \sum_j c_j \Phi_j(\text{e}+\text{ion}), \quad (2)$$

where the multi-configuration wavefunction χ_i describes the target in specific states of $S_i L_i \pi_i$ or $J_i \pi_i$, and θ_i is the suitably vector coupled wavefunction of the 'collisional' electron in a channel labelled $S_i L_i(J_i)\pi_i k_i^2 \ell_i (SL\pi$ or $J\pi)$, at channel energies k_i^2 taken from the total energy balance

$$E = E_i^{\text{target}} \begin{cases} +k_i^2 & \text{if} \geqslant 0 \quad \text{i.e. an open channel,} \\ -z^2/v_i^2 & \text{otherwise} \quad (\text{and } z = Z - N). \end{cases} \quad (3)$$

The quantities Φ_j are correlation wavefunctions composed of $(N + 1)$ electrons orbital functions 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 $SL\pi$.

In the Breit–Pauli approximation relativistic terms of relative magnitude α^2, in the fine structure constant $\alpha \equiv (e^2/\hbar c) \approx 1/137.036$, are added to the non-relativistic Hamiltonian of say N electrons in the field of a nucleus with electric charge number Z:

$$\begin{aligned} H_N^{\text{BP}} = & H_N^{\text{NR}} + H_N^{\text{mass}} + H_N^{\text{d}} + H_N^{\text{so}} \\ & + \frac{1}{2} \sum_{i \neq j}^N \left[g_{ij}(\text{so}+\text{so}') + g_{ij}(\text{ss}') \right. \\ & \left. + g_{ij}(\text{css}') + g_{ij}(\text{d}) + g_{ij}(\text{oo}') \right], \end{aligned} \quad (4)$$

where H_N^{NR} is the non-relativistic Hamiltonian

$$H_N^{\text{NR}} = \sum_{i=1}^N \left\{ -\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^N \frac{2}{r_{ij}} \right\}, \quad (5)$$

assuming $H := H/\text{Ry}$ and $r := r/a_0$, i.e. scaling with the

Table 5. Sample set of f-values, line strengths S and coefficients A for E1 dipole allowed and intercombination transitions in Fe XVI.

I_i	I_k	$\lambda/\text{Å}$	E_i/Ry	E_k/Ry	f	S	$A_{ki} * \text{s}$
1	1	360.75	$-3.5961\text{E}+01$	$-3.3435\text{E}+01$	$-1.210\text{E}-01$	$2.873\text{E}-01$	$6.199\text{E}+09$
1	2	50.56	$-3.5961\text{E}+01$	$-1.7939\text{E}+01$	$-7.854\text{E}-02$	$2.615\text{E}-02$	$2.049\text{E}+11$
1	3	36.80	$-3.5961\text{E}+01$	$-1.1200\text{E}+01$	$-2.276\text{E}-02$	$5.516\text{E}-03$	$1.121\text{E}+11$
1	4	32.19	$-3.5961\text{E}+01$	$-7.6535\text{E}+00$	$-1.173\text{E}-02$	$2.486\text{E}-03$	$7.549\text{E}+10$
1	5	29.97	$-3.5961\text{E}+01$	$-5.5587\text{E}+00$	$-6.351\text{E}-03$	$1.253\text{E}-03$	$4.716\text{E}+10$
1	6	28.71	$-3.5961\text{E}+01$	$-4.2225\text{E}+00$	$-3.817\text{E}-03$	$7.216\text{E}-04$	$3.088\text{E}+10$
1	7	27.91	$-3.5961\text{E}+01$	$-3.3160\text{E}+00$	$-2.487\text{E}-03$	$4.572\text{E}-04$	$2.129\text{E}+10$
1	8	27.38	$-3.5961\text{E}+01$	$-2.6730\text{E}+00$	$-1.720\text{E}-03$	$3.100\text{E}-04$	$1.531\text{E}+10$
2	1	62.87	$-1.8941\text{E}+01$	$-3.3435\text{E}+01$	$6.452\text{E}-02$	$2.671\text{E}-02$	$1.089\text{E}+11$
2	2	909.81	$-1.8941\text{E}+01$	$-1.7939\text{E}+01$	$-1.790\text{E}-01$	$1.072\text{E}+00$	$1.442\text{E}+09$
2	3	117.73	$-1.8941\text{E}+01$	$-1.1200\text{E}+01$	$-7.449\text{E}-02$	$5.774\text{E}-02$	$3.584\text{E}+10$
2	4	80.73	$-1.8941\text{E}+01$	$-7.6535\text{E}+00$	$-3.257\text{E}-02$	$1.732\text{E}-02$	$3.334\text{E}+10$
2	5	68.10	$-1.8941\text{E}+01$	$-5.5587\text{E}+00$	$-1.445\text{E}-02$	$6.476\text{E}-03$	$2.078\text{E}+10$
2	6	61.91	$-1.8941\text{E}+01$	$-4.2225\text{E}+00$	$-7.427\text{E}-03$	$3.028\text{E}-03$	$1.293\text{E}+10$
2	7	58.32	$-1.8941\text{E}+01$	$-3.3160\text{E}+00$	$-4.329\text{E}-03$	$1.662\text{E}-03$	$8.490\text{E}+09$
2	8	56.02	$-1.8941\text{E}+01$	$-2.6730\text{E}+00$	$-2.763\text{E}-03$	$1.019\text{E}-03$	$5.874\text{E}+09$
3	1	41.93	$-1.1703\text{E}+01$	$-3.3435\text{E}+01$	$1.241\text{E}-02$	$3.426\text{E}-03$	$4.707\text{E}+10$
3	2	146.13	$-1.1703\text{E}+01$	$-1.7939\text{E}+01$	$9.760\text{E}-02$	$9.391\text{E}-02$	$3.049\text{E}+10$
3	3	1812.38	$-1.1703\text{E}+01$	$-1.1200\text{E}+01$	$-2.409\text{E}-01$	$2.875\text{E}+00$	$4.891\text{E}+08$
3	4	225.02	$-1.1703\text{E}+01$	$-7.6535\text{E}+00$	$-8.802\text{E}-02$	$1.304\text{E}-01$	$1.160\text{E}+10$
3	5	148.31	$-1.1703\text{E}+01$	$-5.5587\text{E}+00$	$-2.807\text{E}-02$	$2.741\text{E}-02$	$8.511\text{E}+09$
3	6	121.82	$-1.1703\text{E}+01$	$-4.2225\text{E}+00$	$-1.308\text{E}-02$	$1.049\text{E}-02$	$5.879\text{E}+09$
3	7	108.65	$-1.1703\text{E}+01$	$-3.3160\text{E}+00$	$-7.344\text{E}-03$	$5.254\text{E}-03$	$4.150\text{E}+09$
3	8	100.91	$-1.1703\text{E}+01$	$-2.6730\text{E}+00$	$-4.608\text{E}-03$	$3.061\text{E}-03$	$3.018\text{E}+09$
4	1	35.73	$-7.9305\text{E}+00$	$-3.3435\text{E}+01$	$5.561\text{E}-03$	$1.308\text{E}-03$	$2.907\text{E}+10$
4	2	91.05	$-7.9305\text{E}+00$	$-1.7939\text{E}+01$	$3.136\text{E}-02$	$1.880\text{E}-02$	$2.524\text{E}+10$
4	3	278.69	$-7.9305\text{E}+00$	$-1.1200\text{E}+01$	$1.543\text{E}-01$	$2.831\text{E}-01$	$1.325\text{E}+10$
⋮	⋮			……			

hydrogenic ionization energy $\text{Ry} \equiv (\alpha^2/2)m_0 c^2 \approx 13.59\,\text{eV}$ and Bohr radius $a_0 \equiv (\hbar/m_0 c)/\alpha = 0.529 \times 10^{-8}\,\text{cm}$. The BPRM method includes the three one-body terms: mass–velocity correction H_N^{mass}, the Darwin term H_N^{d} and ordinary spin–orbit interaction H_N^{so}. The mutual spin–orbit and spin–other–orbit effects (so + so′) by core electrons enter only via (Blume–Watson) screening of spin–orbit parameters, as (Fe XVII+e) is effectively a one body rather than an $(N+1)$ electron system, and all spin–spin interaction (ss′) among electrons drops out for an unpolarized Ne-like core. Complications by L-shell polarization correlation are discussed in a later section.

This paper is concerned with solutions of

$$\langle \Psi | H | \Psi \rangle = E_{\min} \qquad (6)$$

when *all* channels are closed, i.e. all $k_i^2 < 0$ in equation (3), which is a Hartree–Fock eigenvalue problem with a *discreet* spectrum E, because $\nu = n - \mu$ forms Rydberg series along *integer* n (while the target states χ_i with energies E_i are 'frozen cores'). At eigenvalues E for target and $(N+1)$ electrons in a bound state, and with 'frozen cores' χ_i in the particular case of expansion (2), to which it is moreover applied as a first step.

The primary quantity for radiative transitions is the line strength, for E1-type transitions in the length form the square of a reduced dipole matrix element:

$$S = \left| \left\langle \Psi_{\text{f}} \left\| \sum_{j=1}^{N+1} C^{[1]} r_j \right\| \Psi_{\text{i}} \right\rangle \right|^2, \qquad (7)$$

where Ψ_i and Ψ_f are the initial and final bound wavefunctions (and r scaled in Bohr units a_0). Derived from the line strength, which does not explicitly depend upon the transition energy $E_{ji} = E_j - E_i$, are secondary quantities such as the oscillator strength f_{ij}, which is a pure number going back to classical physics, and the radiative transition probability or Einstein's A-coefficient (E scaled in Ry), an inverse time:

$$f_{ij} = \frac{E_{ji}}{3g_i} S, \qquad A_{ji} * \tau_0 = \alpha^3 \frac{g_i}{g_j} E_{ji}^2 f_{ij}, \qquad (8)$$

where $\tau_0 \equiv \hbar/\text{Ry} = 4.8381 \times 10^{-17}\,\text{s}$ is the time $2a_0/(\alpha c)$ it takes a hydrogenic ground state electron to cross the Bohr orbit, and g_i, g_j are the statistical weight factors of initial and final state.

Radiative data for forbidden transitions of electric quadrupole (E2), octupole (E3) and magnetic dipole (M1), quadrupole (M2) type are computed using configuration interaction atomic structure calculations with code SUPERSTRUCTURE (SS), in the low-Z Breit–Pauli approximation [8, 9, 15]. SS represents the nuclear and electron–electron potential by a statistical Thomas–Fermi–Dirac–Amaldi model potential and includes relativistic one-body terms as well as two-body FS terms in the Breit interaction of equation (3), and ignores the last three two-body terms. Radiative probabilities for 'forbidden' excitation or de-excitation via various modes of higher powers in α and E_{ij} can be obtained with the generalized line strength

$$S^{X\lambda}(ij) = \left| \left\langle \Psi_j \| O^{X\lambda} \| \Psi_i \right\rangle \right|^2, \quad S(ji) = S(ij), \qquad (9)$$

Table 6. Sample table of dipole allowed same-spin and intercombination E1 transitions in Fe XVI, grouped as fine structure components of *LS* multiplets. Calculated energies have been replaced by observed energies.

C_i–C_k	T_i–T_k	g_i : I–g_j : K	E_{ik} (Å)	f	S	A (s^{-1})
2p63s–2p63p	2Se–2Po	2: 1- 2: 1	360.75	1.21E − 01	2.87E − 01	6.20E + 09
2p63s–2p63p	2Se–2Po	2: 1- 4: 1	335.41	2.62E − 01	5.80E − 01	7.78E + 09
LS	2Se–2Po	2- 6		3.83E − 01	8.67E − 01	7.20E + 09
2p63s–2p64p	2Se–2Po	2: 1- 2: 2	50.56	7.85E − 02	2.61E − 02	2.05E + 11
2p63s–2p64p	2Se–2Po	2: 1- 4: 2	50.36	1.47E − 01	4.87E − 02	1.93E + 11
LS	2Se–2Po	2- 6		2.26E − 01	7.48E − 02	1.98E + 11
2p63s–2p65p	2Se–2Po	2: 1- 2: 3	36.80	2.28E − 02	5.52E − 03	1.12E + 11
2p63s–2p65p	2Se–2Po	2: 1- 4: 3	36.75	4.33E − 02	1.05E − 02	1.07E + 11
LS	2Se–2Po	2- 6		6.61E − 02	1.60E − 02	1.08E + 11
2p63s–2p66p	2Se–2Po	2: 1- 2: 4	32.19	1.17E − 02	2.49E − 03	7.55E + 10
2p63s–2p66p	2Se–2Po	2: 1- 4: 4	32.17	2.24E − 02	4.75E − 03	7.23E + 10
LS	2Se–2Po	2- 6		3.41E − 02	7.24E − 03	7.29E + 10
2p63p–2p64s	2Po–2Se	2: 1- 2: 2	62.87	6.45E − 02	2.67E − 02	1.09E + 11
2p63p–2p64s	2Po–2Se	4: 1- 2: 2	63.71	6.83E − 02	5.73E − 02	2.24E + 11
LS	2Po–2Se	6- 2		6.70E − 02	8.40E − 02	3.33E + 11
2p64s–2p64p	2Se–2Po	2: 2- 2: 2	909.81	1.79E − 01	1.07E + 00	1.44E + 09
2p64s–2p64p	2Se–2Po	2: 2- 4: 2	848.09	3.86E − 01	2.15E + 00	1.79E + 09
LS	2Se–2Po	2- 6		5.65E − 01	3.22E + 00	1.68E + 09
2p64s–2p65p	2Se–2Po	2: 2- 2: 3	117.73	7.45E − 02	5.77E − 02	3.58E + 10
2p64s–2p65p	2Se–2Po	2: 2- 4: 3	117.18	1.38E − 01	1.07E − 01	3.36E + 10
LS	2Se–2Po	2- 6		2.13E − 01	1.65E − 01	3.41E + 10
2p64s–2p66p	2Se–2Po	2: 2- 2: 4	80.73	3.26E − 02	1.73E − 02	3.33E + 10
2p64s–2p66p	2Se–2Po	2: 2- 4: 4	80.57	6.19E − 02	3.28E − 02	3.18E + 10
LS	2Se–2Po	2- 6		9.45E − 02	5.01E − 02	3.24E + 10
2p63p–2p65s	2Po–2Se	2: 1- 2: 3	41.93	1.24E − 02	3.43E − 03	4.71E + 10
2p63p–2p65s	2Po–2Se	4: 1- 2: 3	42.30	1.30E − 02	7.22E − 03	9.66E + 10
LS	2Po–2Se	6- 2		1.28E − 02	1.06E − 02	1.44E + 11
2p64p–2p65s	2Po–2Se	2: 2- 2: 3	146.13	9.76E − 02	9.39E − 02	3.05E + 10
2p64p–2p65s	2Po–2Se	4: 2- 2: 3	147.85	1.03E − 01	2.01E − 01	6.29E + 10
LS	2Po–2Se	6- 2		1.01E − 01	2.95E − 01	9.30E + 10
2p65s–2p65p	2Se–2Po	2: 3- 2: 3	1812.38	2.41E − 01	2.87E + 00	4.89E + 08
2p65s–2p65p	2Se–2Po	2: 3- 4: 3	1690.35	5.18E − 01	5.76E + 00	6.04E + 08
LS	2Se–2Po	2- 6		7.59E − 01	8.63E + 00	5.66E + 08
2p65s–2p66p	2Se–2Po	2: 3- 2: 4	225.02	8.80E − 02	1.30E − 01	1.16E + 10
2p65s–2p66p	2Se–2Po	2: 3- 4: 4	223.76	1.63E − 01	2.40E − 01	1.09E + 10
LS	2Se–2Po	2- 6		2.51E − 01	3.70E − 01	1.11E + 10
……						

where $X\lambda$ represents the electric or magnetic-type operator of multipolarity λ, thus generalizing the electric dipole case $O^{E1} = C^{[1]}r$ of equation (7) to $O^{E\lambda} = C^{[\lambda]}r^\lambda$ (e.g. [15]). Along the line of the E1 case, for which A of equation (8) reads

$$g_j A_{ji}^{E1} = 2.6773 \times 10^9 \text{ s}^{-1} (E_j - E_i)^3 S^{E1}(i, j) \qquad (10)$$

with S of equation (7), higher order transition modes lead to probabilities

$$g_j A_{ji}^{E2} = 2.6733 \times 10^3 \text{ s}^{-1} (E_j - E_i)^5 S^{E2}(i, j), \qquad (11)$$

$$g_j A_{ji}^{M1} = 3.5644 \times 10^4 \text{ s}^{-1} (E_j - E_i)^3 S^{M1}(i, j), \qquad (12)$$

for electric quadrupole (E2) and magnetic dipole (M1) radiation and

$$g_j A_{ji}^{E3} = 1.2050 \times 10^{-3} \text{ s}^{-1} (E_j - E_i)^7 S^{E3}(i, j), \qquad (13)$$

$$g_j A_{ji}^{M2} = 2.3727 \times 10^{-2} \text{ s}^{-1} (E_j - E_i)^5 S^{M2}(i, j), \qquad (14)$$

for electric octopole (E3) and magnetic quadrupole (M2) radiation. Regarding contributions of BP order to M1 see [9].

The lifetime of a level k can be obtained from transition probabilities as

$$\tau_k = \frac{1}{\sum_i A_{ki}}, \qquad (15)$$

where the sum runs over all levels i to which k can decay.

3. Calculations

3.1. BPRM calculations for E1 transitions

With the BPRM code, the CC calculations proceed in several stages. The BPRM package requires orbital wavefunction input for the target or core eigenstates (here provided by SS). From it STG1 computes one- and two-electron radial integrals as specified. STG2 computes angular coefficients for target and collisional channels in *LS*-coupling and target term energies. Stage RECUPD adds the Breit–Pauli algebra, in intermediate coupling computing target levels and with the help of their term coupling coefficients the structure of collisional channel sets of total $J\pi$ on recoupling the *LS* symmetries in a pair-coupling scheme. STGH completes the inner region ($r/a_0 \leqslant$ RA = 4.0) task computing R-matrices for the specified collisional symmetries.

Table 7. Comparison of E1 transitions of Fe XVI line strengths S^{E1} and radiative decay rates A^{E1}: RCC—relativistic coupled cluster, GRASP2—fully relativistic atomic structure [1], BPRM—relativistic Breit–Pauli R-matrix, SS—Breit–Pauli atomic structure.

Transition		S^{E1}_{ij}				$A^{E1}_{ji} \cdot s$			
i	j	RCCM	GRASP2	BPRM	SS	RCCM	GRASP2	BPRM	SS
$3s\,^2S_{1/2}$	$3p\,^2P_{1/2}$	2.843(−1)	2.965(−1)	2.873(−1)	2.916(−1)	6.134(09)	6.463(09)	6.20(09)	6.29(09)
$3s\,^2S_{1/2}$	$3p\,^2P_{3/2}$	5.731(−1)	5.974(−1)	5.796(−1)	5.853(−1)	7.693(09)	8.087(09)	7.78(09)	7.86(09)
$3s\,^2S_{1/2}$	$4p\,^2P_{1/2}$	2.635(−2)	2.522(−2)	2.612(−2)	2.496(−2)	2.070(11)	1.969(11)	2.05(11)	1.96(11)
$3s\,^2S_{1/2}$	$4p\,^2P_{3/2}$	4.913(−2)	4.700(−2)	4.876(−2)	4.731(−2)	1.950(11)	1.858(11)	1.93(11)	1.88(11)
$3s\,^2S_{1/2}$	$5p\,^2P_{1/2}$	4.543(−3)	5.613(−3)	5.52(−3)	5.125(−3)	9.233(10)	1.137(11)	1.12(11)	1.04(11)
$3s\,^2S_{1/2}$	$5p\,^2P_{3/2}$	8.66(−2)	1.067(−2)	1.05(−2)	1.003(−2)	0.883(11)	1.085(11)	1.07(11)	1.02(11)
$3p\,^2P_{1/2}$	$3d\,^2D_{3/2}$	4.671(−1)	4.859(−1)	4.720(−1)	4.827(−1)	1.495(10)	1.560(10)	1.51(10)	1.54(10)
$3p\,^2P_{1/2}$	$4s\,^2S_{1/2}$	2.682(−2)	2.599(−2)	2.671(−2)	2.536(−2)	1.093(11)	1.052(11)	1.09(11)	1.03(11)
$3p\,^2P_{1/2}$	$4d\,^2D_{3/2}$	1.081(−1)	1.075(−1)	1.079(−1)	1.069(−1)	3.449(11)	3.415(11)	3.45(11)	3.41(11)
$3p\,^2P_{1/2}$	$5s\,^2S_{1/2}$	3.355(−3)	3.438(−3)	3.434(−3)	3.044(−3)	4.605(10)	4.704(10)	4.71(10)	4.18(10)
$3p\,^2P_{1/2}$	$5d\,^2D_{3/2}$	2.214(−2)	2.532(−2)	2.42(−2)	2.402(−2)	1.775(11)	2.020(11)	1.94(11)	1.93(11)
$3p\,^2P_{3/2}$	$3d\,^2D_{3/2}$	9.358(−2)	9.728(−2)	9.499(−2)	9.650(−2)	2.546(09)	2.659(09)	2.59(09)	2.63(09)
$3p\,^2P_{3/2}$	$3d\,^2D_{5/2}$	8.450(−1)	8.774(−1)	8.54(−1)	8.708(−1)	1.569(10)	1.635(10)	1.59(10)	1.62(10)
$3p\,^2P_{3/2}$	$4s\,^2S_{1/2}$	5.768(−2)	5.585(−2)	5.73(−2)	5.506(−2)	2.259(11)	2.173(11)	2.24(11)	2.16(11)
$3p\,^2P_{3/2}$	$4d\,^2D_{3/2}$	2.287(−2)	2.274(−2)	2.274(−2)	2.257(−2)	7.053(10)	6.980(10)	7.02(10)	6.97(10)
$3p\,^2P_{3/2}$	$4d\,^2D_{5/2}$	2.038(−1)	2.030(−1)	2.03(−1)	2.012(−1)	4.199(11)	4.162(11)	4.19(11)	4.15(11)
$3p\,^2P_{3/2}$	$5s\,^2S_{1/2}$	7.089(−3)	7.261(−3)	7.22(−3)	6.910(−3)	9.475(10)	9.676(10)	9.66(10)	9.25(10)
$3p\,^2P_{3/2}$	$5d\,^2D_{5/2}$	4.095(−2)	4.698(−2)	4.45(−2)	4.613(−2)	2.136(11)	2.439(11)	2.32(11)	2.41(11)
$3d\,^2D_{3/2}$	$4p\,^2P_{1/2}$	3.596(−2)	3.460(−2)	3.58(−2)	3.388(−2)	8.051(10)	7.671(10)	8.02(10)	7.58(10)
$3d\,^2D_{3/2}$	$4p\,^2P_{3/2}$	6.771(−3)	6.521(−3)	6.71(−3)	6.389(−3)	7.720(09)	7.366(09)	7.64(09)	7.28(09)
$3d\,^2D_{3/2}$	$4f\,^2F_{5/2}$	7.876(−1)	8.099(−1)	7.95(−1)	8.087(−1)	9.141(11)	9.318(11)	9.23(11)	9.39(11)
$3d\,^2D_{3/2}$	$5p\,^2P_{1/2}$	2.975(−3)	3.526(−3)	3.55(−3)	3.181(−3)	2.565(10)	3.020(10)	3.06(10)	2.74(10)
$3d\,^2D_{3/2}$	$5p\,^2P_{3/2}$	5.700(−4)	6.745(−4)	6.48(−4)	6.114(−4)	2.472(09)	2.905(09)	2.81(09)	2.65(09)
$3d\,^2D_{3/2}$	$5f\,^2F_{5/2}$	1.071(−1)	1.051(−1)	9.98(−2)	1.042(−1)	3.559(11)	3.470(11)	3.32(11)	3.46(11)
$3d\,^2D_{5/2}$	$4p\,^2P_{3/2}$	6.176(−2)	5.936(−2)	6.20(−2)	5.890(−2)	6.995(10)	6.662(10)	7.01(10)	6.66(10)
$3d\,^2D_{5/2}$	$4f\,^2F_{5/2}$	5.648(−2)	5.806(−2)	5.71(−2)	5.810(−2)	6.517(10)	6.642(10)	6.59(10)	6.71(10)
$3d\,^2D_{5/2}$	$5p\,^2P_{3/2}$	5.182(−3)	6.119(−3)	5.93(−3)	5.765(−3)	2.238(10)	2.625(10)	2.56(10)	2.49(10)
$3d\,^2D_{5/2}$	$5f\,^2F_{5/2}$	7.642(−3)	7.509(−3)	7.13(−3)	7.461(−3)	2.529(10)	2.469(10)	2.36(10)	2.47(10)
$4s\,^2S_{1/2}$	$4p\,^2P_{1/2}$	1.073	1.085	1.07	1.095	1.467(09)	1.475(09)	1.44(09)	1.47(09)
$4s\,^2S_{1/2}$	$4p\,^2P_{3/2}$	2.156	2.179	2.15	2.193	1.817(09)	1.833(09)	1.79(09)	1.82(09)
$4s\,^2S_{1/2}$	$5p\,^2P_{1/2}$	5.156(−2)	6.228(−2)	5.80(−2)	5.828(−2)	3.204(10)	3.862(10)	3.60(10)	3.62(10)
$4p\,^2P_{1/2}$	$4d\,^2D_{3/2}$	2.072	2.091	2.07	2.100	3.362(09)	3.351(09)	3.33(09)	3.38(09)
$4p\,^2P_{1/2}$	$5s\,^2S_{1/2}$	9.90(−2)	1.028(−1)	9.49(−2)	9.736(−2)	3.003(10)	3.338(10)	3.08(10)	3.16(10)
$4p\,^2P_{1/2}$	$5d\,^2D_{3/2}$	1.801(−1)	2.090(−1)	1.94(−1)	2.029(−1)	4.848(10)	5.620(10)	5.22(10)	5.47(10)
$4p\,^2P_{3/2}$	$4d\,^2D_{3/2}$	4.153(−1)	4.192(−1)	4.14(−1)	4.202(−1)	5.547(08)	5.660(08)	5.64(08)	5.72(08)
$4p\,^2P_{3/2}$	$4d\,^2D_{5/2}$	3.745	3.778	3.73	3.786	3.421(09)	3.497(09)	3.48(09)	3.53(09)
$4p\,^2P_{3/2}$	$5s\,^2S_{1/2}$	2.118(−1)	2.193(−1)	1.99(−1)	2.106(−1)	6.602(10)	6.872(10)	6.25(10)	6.60(10)
$4p\,^2P_{3/2}$	$5d\,^2D_{3/2}$	3.861(−2)	4.472(−2)	4.08(−2)	4.392(−2)	1.009(10)	1.167(10)	1.07(10)	1.15(10)
$4p\,^2P_{3/2}$	$5d\,^2D_{5/2}$	3.416(−1)	3.979(−1)	3.60(−1)	3.907(−1)	5.964(10)	6.938(10)	6.29(10)	6.83(10)
$4d\,^2D_{3/2}$	$5p\,^2P_{1/2}$	1.491(−1)	1.708(−1)	1.54(−1)	1.665(−1)	3.149(10)	3.590(10)	3.24(10)	3.51(10)

Table 8. Comparison of present absorption oscillator strengths f for Fe XVI with those from experiment by Buchet *et al* [4] (a: simulation procedure, b: fit program) and calculation by Weiss [30].

λ	f				$C_i(SL\pi_i)$–$C_j(SL\pi_j)$	g_i–g_j
Å	a	b	Present	Weiss		
251.1	< 0.344	< 0.283	0.286	0.293	$3p\,^2P^o$–$3d\,^2D$	2–4
263.0	0.251	0.188	0.247	0.251	$3p\,^2P^o$–$3d\,^2D$	4–6
360.8	0.126	0.124	0.121	0.124	$3s\,^2S$–$3p\,^2P^o$	2–2
335.4	0.270	0.263	0.262	0.271	$3s\,^2S$–$3p\,^2P^o$	2–4

In a full-scale electron collision calculation for Ne-like iron, i.e. with ground state $1s^2 2s^2 2p^6\,^1S$, one would include levels χ_i of equation (2) arising from L-shell excited configurations, say $2s^2 2p^6(1)$, $2s2p^6 3s(2)$, $2p^5 3p(3)$, $2s^2 2p^5 3d(4)$, $2s^2 2p^5 4s(5)$, $2s^2 2p^5 4p(6)$, $2s^2 2p^5 4d(7)$, $2s^2 2p^5 4f(8)$, $2s2p^6 3s(9)$, $2s2p^6 3p(10)$, $2s2p^6 3d(11)$, $2s2p^6 4s(12)$, $2s2p^6 4p(13)$, $2s2p^6 4d(14)$ and $2s2p^6 4f(15)$; the atomic structure code SS with (roughly optimized)

Thomas–Fermi scaling parameters $\lambda_{nl} = 1.40(1s)$, $1.15(2s)$, $1.10(2p)$, $1.10(3s)$, $1.0(3p)$, $1.0(3d)$, $1.0(4s)$, $1.0(4p)$, $1.0(4d)$ and $1(4f)$ for individual orbitals yields a first-excited state $2p^5 3s\,^3P_2$ at 53.32 Ry.

Bound states of Fe XVI with $\frac{1}{2} \leqslant J \leqslant \frac{19}{2}$ of even and odd parities, $n \leqslant 10$, $l \leqslant 9$, $0 \leqslant L \leqslant 10$ are computed from the R-matrices in STGB [24], which solves θ_i and c_j in (2) as an eigenvalue problem (6), scanning through the poles in the

Table 9. Sample set of fine structure levels of Fe XVI for which forbidden transitions have been obtained. The indices (cf) correspond to configurations $2p^63s(1)$, $2p^63p(2)$, $2p^63d(3)$, $2p^64s(4)$, $2p^64p(5)$, $2p^64d(6)$, $2p^64f(7)$, $2p^65s(8)$, $2p^65p(9)$, $2p^65d(10)$, $2p^65f(11)$, $2p^65g(12)$, $2p^53s^2(13)$, $2p^53s3p(14)$, $2p^53s3d(15)$, $2p^53s4s(16)$, $2p^53s4p(17)$, $2p^53s4d(18)$, $2p^53s4f(19)$, $2p^53p^2(20)$, $2p^53p3d(21)$ and $2s2p^63p^2(22)$.

i.e.	SLp(cf)	$2J$	E/Ry
1	2Se(1)	1	0.00000E+00
2	2Po(2)	1	2.52600E+00
3	2Po(2)	3	2.71690E+00
4	2De(3)	3	6.15560E+00
5	2De(3)	5	6.18210E+00
6	2Se(4)	1	1.70200E+01
7	2Po(5)	1	1.80220E+01
8	2Po(5)	3	1.80950E+01
9	2De(6)	3	1.93620E+01
10	2De(6)	5	1.93730E+01
11	2Fo(7)	5	1.99110E+01
12	2Fo(7)	7	1.99150E+01
13	2Se(8)	1	2.42580E+01
14	2Po(9)	1	2.47610E+01
15	2Po(9)	3	2.47970E+01
16	2De(10)	3	2.54070E+01
17	2De(10)	5	2.54120E+01
18	2Fo(11)	5	2.56850E+01
19	2Fo(11)	7	2.56880E+01
20	2Ge(12)	7	2.57220E+01
21	2Ge(12)	9	2.57230E+01
22	2Po(13)	3	5.26932E+01
23	2Po(13)	1	5.36060E+01
24	4Se(14)	3	5.44566E+01
25	4De(14)	5	5.47036E+01
26	4De(14)	7	5.47528E+01
27	4De(14)	3	5.47636E+01
28	4De(14)	1	5.48771E+01
29	4Pe(14)	5	5.49676E+01
30	4Pe(14)	3	5.49789E+01
			......

(e + ion) Hamiltonian with a suitably fine mesh in the effective quantum number ν.

A demanding step in the calculations is the theoretical level identification, since the computed bound levels are initially known only by their negative eigenvalues or effective quantum numbers. The spectroscopic designations of the fine structure energy levels are obtained by analyzing quantum defects, matching components of the relevant LS terms and channel percentage contributions corresponding to the integrated wavefunctions in the outer region. These criteria are built into the level identification code PRCBPID [17]. A level may be assigned to one or more LS terms based on its dominant channel, which also provides information on the configuration, and the J value of the core and outer electrons. Hund's rule for total spin multiplicity and orbital angular momemtum is also invoked for levels from the same configuration. Finally, a level is assigned to the full designation $C_t(S_tL_t\pi_t)J_tnlJ(SL)\pi$, as the configuration, LS term, 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 and parity of the $(N+1)$-electron system.

Bound–bound transition data are computed with code STGBB [25] exploiting partial wave output on θ (in equation (2)) from STGB. All transitions are processed

for proper energies and transition wavelengths using code PBPRAD. The calculated energies have been replaced by measured energies for improved accuracy where available. A subset of transitions employing only these observed levels has been processed with complete spectroscopic notation for direct comparison with experiments and diagnostic applications.

3.2. Atomic structure calculations for forbidden transitions

Radiative transition probabilities for forbidden transitions in Fe XVI were obtained from configuration mixing atomic structure calculations using SS, which computes multipole transitions in Breit–Pauli approximation. A total of 22 configurations with orbitals up to 5g are included (table 9). The scaling parameters for the Thomas–Fermi–Dirac–Amaldi potential λ_{nl} for the orbitals are 1.38(1s), 1.15(2s), 1.08(2p), 1.05(3s), 1.01(3p), 1.0(3d), 1.0(4s), 1.0(4p), 1.0(4d), 1.0(4f), 1.0(5s), 1.0(5p), 1.0(5d), 1.0(5f) and 1.0(5g). The forbidden transitions considered are electric quadrupole (E2) and octupole (E3), and magnetic dipole (M1) and quadrupole (M2). The computed data have been processed by replacing the calculated energies by the limited number of observed energies available, using the code PRCSS.

4. Results and discussion

Oscillator strengths (f-values), line strengths S and radiative transition probabilities A of Fe XVI are presented for allowed electric dipole and intercombination transitions E1, and for forbidden E2, E3, M1 and M2 transitions. The large set of atomic parameters should comprise a reasonably complete set for all practical applications. The results for energy levels and radiative transition rates are discussed separately.

4.1. Energy levels

A total of 96 bound fine structure levels of Fe XVI are obtained from BPRM calculations. They correspond to total angular momenta $1/2 \leqslant J \leqslant 19/2$ of even and odd parities with $n \leqslant 10$, $0 \leqslant l \leqslant 12$, total orbital angular momenta $0 \leqslant L \leqslant 12$ and spin multiplicity $(2S+1) = 2$. Table 1 presents a partial set of binding energies and comparison with available observed energy levels compiled by NIST. Spectroscopic identifications of calculated energy levels are assigned according to the most probable designation based on the criteria described in the computations section. Comparison between the calculated BPRM energies and the measured values in table 1 shows that most of the calculated levels are well within 1% accuracy. The level index I_J in the table is the relative position of the calculated level in the given $J\pi$ symmetry. The index establishes the correspondence between calculated and observed levels.

However, we noted some interesting polarization effects. It is typical of such closed shells that Rydberg series of a collisional electron bound to the ground state are rarely perturbed up to fairly high values of n; below this limit radiative data can be computed with a one-state target—which implies no term coupling! In our case excited target levels start at about 35 Ry above (Fe XVII) ^{1}S, and from there bound

Table 10. Sample sets of radiative decay rates A $= A*$s for the forbidden electric quadrupole (AE2), electric octupole (AE3), magnetic dipole (AM1) and magnetic quadrupole (AM3) of Fe XVI. The level numbers (i, j) and configurations indices (Ci, Cj) correspond to those in table 9, that is $2p^63s(1)$, $2p^63p(2)$, $2p^63d(3)$, $2p^64s(4)$, $2p^64p(5)$, $2p^64d(6)$, $2p^64f(7)$, $2p^65s(8)$, $2p^65p(9)$, $2p^65d(10)$, $2p^65f(11)$, $2p^65g(12)$, $2p^53s^2(13)$, $2p^53s3p(14)$, $2p^53s3d(15)$, $2p^53s4s(16)$, $2p^53s4p(17)$, $2p^53s4d(18)$, $2p^53s4f(19)$, $2p^53p^2(20)$, $2p^53p3d(21)$ and $2s2p^63p^2(22)$. T denotes the LS term $SL\pi$ and N_{tr} is the number of transitions.

$i-j$	$T_iC_i-T_jC_j$	g_i-g_j	λ/Å	E_i/Ry	E_j/Ry	AE2	AM1
			E2 and M1, $N_{tr} = 20005$				
2–3	2Po 2–2Po 2	2–4	4773	2.53E+0	2.72E+0	2.36E−02	8.26E+01
1–4	2Se 1–2De 3	2–4	148.04	0.00E+0	6.16E+0	6.61E+05	9.18E−01
1–5	2Se 1–2De 3	2–6	147.40	0.00E+0	6.18E+0	6.78E+05	0.00E+00
4–5	2De 3–2De 3	4–6	34387	6.16E+0	6.18E+0	2.49E−07	2.65E−01
1–6	2Se 1–2Se 4	2–2	53.54	0.00E+0	1.70E+1	0.00E+00	7.24E+01
4–6	2De 3–2Se 4	4–2	83.88	6.16E+0	1.70E+1	9.00E+06	1.38E−01
5–6	2De 3–2Se 4	6–2	84.08	6.18E+0	1.70E+1	1.36E+07	0.00E+00
2–7	2Po 2–2Po 5	2–2	58.81	2.53E+0	1.80E+1	0.00E+00	3.76E+01
3–7	2Po 2–2Po 5	4–2	59.54	2.72E+0	1.80E+1	6.84E+07	4.83E+03
2–8	2Po 2–2Po 5	2–4	58.53	2.53E+0	1.81E+1	3.42E+07	2.06E+03
3–8	2Po 2–2Po 5	4–4	59.26	2.72E+0	1.81E+1	3.41E+07	1.38E+02
7–8	2Po 5–2Po 5	2–4	12483	1.80E+1	1.81E+1	2.60E−03	4.62E+00
1–9	2Se 1–2De 6	2–4	47.06	0.00E+0	1.94E+1	1.36E+08	1.76E+00
4–9	2De 3–2De 6	4–4	69.00	6.16E+0	1.94E+1	1.55E+07	4.83E+01
5–9	2De 3–2De 6	6–4	69.14	6.18E+0	1.94E+1	6.68E+06	2.26E+02
6–9	2Se 4–2De 6	2–4	89.10	1.70E+1	1.94E+1	8.22E+04	2.15E−02
1–10	2Se 1–2De 6	2–6	47.04	0.00E+0	1.94E+1	1.36E+08	0.00E+00
4–10	2De 3–2De 6	4–6	68.94	6.16E+0	1.94E+1	4.42E+06	9.21E+01
			E3 and M2, $N_{tr} = 7078$				
$i-j$	$T_iC_i-T_jC_j$	g_i-g_j	λ/Å	E_i/Ry	E_j/Ry	AE3	AM2
2–5	2Po 2–2De 3	2–6	249.25	2.53E+0	6.18E+0	1.69E−01	3.22E+01
5–7	2De 3–2Po 5	6–2	76.97	6.18E+0	1.80E+1	2.38E+03	2.45E+03
2–10	2Po 2–2De 6	2–6	54.09	2.53E+0	1.94E+1	1.30E+04	1.45E+04
7–10	2Po 5–2De 6	2–6	674.51	1.80E+1	1.94E+1	9.07E−03	9.58E−01
1–11	2Se 1–2Fo 7	2–6	45.77	0.00E+0	1.99E+1	4.04E+04	7.29E−07
6–11	2Se 4–2Fo 7	2–6	315.21	1.70E+1	1.99E+1	6.94E−01	3.19E−15
1–12	2Se 1–2Fo 7	2–8	45.76	0.00E+0	1.99E+1	4.05E+04	0.00E+00
4–12	2De 3–2Fo 7	4–8	66.23	6.16E+0	1.99E+1	1.93E+03	2.88E+04
6–12	2Se 4–2Fo 7	2–8	314.77	1.70E+1	1.99E+1	7.02E−01	0.00E+00
9–12	2De 6–2Fo 7	4–8	1647	1.94E+1	1.99E+1	5.05E−06	9.23E−03
11–13	2Fo 7–2Se 8	6–2	209.63	1.99E+1	2.43E+1	2.18E+01	2.70E−15
12–13	2Fo 7–2Se 8	8–2	209.82	1.99E+1	2.43E+1	2.92E+01	0.00E+00
5–14	2De 3–2Po 9	6–2	49.05	6.18E+0	2.48E+1	2.68E+02	2.24E+03
10–14	2De 6–2Po 9	6–2	169.13	1.94E+1	2.48E+1	3.77E+02	2.35E+02
12–16	2Fo 7–2De 10	8–4	165.93	1.99E+1	2.54E+1	5.39E+01	4.24E+01
2–17	2Po 2–2De 10	2–6	39.82	2.53E+0	2.54E+1	1.47E+03	1.53E+04
7–17	2Po 5–2De 10	2–6	123.31	1.80E+1	2.54E+1	1.06E+03	4.47E+02
14–17	2Po 9–2De 10	2–6	1399	2.48E+1	2.54E+1	1.04E−03	6.88E−02

Table 11. Comparison of the present radiative decay rates A and line strengths S for E2 transitions in Fe XVI with those from previous calculations. The capital letter in the second column indicates accuracy rating by NIST.

λ	$A*$s		S		C_i-C_j	$SL\pi_i-SL\pi_j$	g_i-g_j
Å	[29]	Present	[5]	Present			
147.407	6.80E+05 : C	6.78E+05	0.177	0.169	2p63s–2p63d	2S–2D	2–6
148.043	6.70E+05 : C	6.61E+05	0.118	0.112	2p63s–2p63d	2S–2D	2–4
47.050	1.44E+08 : C	1.36E+08	0.108	0.112	2p63s–2p64d	2S–2D	2–6
47.077	1.50E+08 : D	1.36E+08	0.0721	0.0748	2p63s–2p64d	2S–2D	2–4
35.860	7.6eE+07 : D	6.42E+07			2p63s–2p65d	2S–2D	2–6
35.860	7.8eE+07 : D	6.38E+07			2p63s–2p65d	2S–2D	2–4
39.348	3.6eE+07 : D	3.25E+07			2p63p–2p65f	2Po–2Fo	2–6
39.671	4.5eE+07 : D	4.33E+07			2p63p–2p65f	2Po–2Fo	4–8

collisional electrons with $n \geqslant 3$ never drop below the target ground state (and a few allowed electrons associated with Rydberg $n = 2$ remain). In table 1, violent series perturbation, moreover inverting the nd doublet, starts setting in at $n = 9$, hence the ν_o column added to follow the development of this series: see quantum defect jump in the order of

0.05! Up to $n = 8$, one can expect adequate radiative results from our single target state expansion. We shall retain core polarization effects from those four among the 14 configurations that correlate with the ground state symmetry ^{1}S (lowering the ground state by 54.5 mRy). Their successive eigenvector components are 0.99956, −0.02707, −0.01226,

−0.00235 and −0.00072. Similarly, we include all $(N+1)$-electron-bound channel functions Φ_j in equation (2) from single holes in 2s, 2p, 3s to maximum occupancies of $2s^2$, $2p^6$, $3s^2$, $3p^2$, $3d^2$, $4s^2$, $4p^2$, $4d^2$ and 4f. So much about H^{NR} or interacting *electric* charges.

There remain tricky choices on *magnetic* interaction. Starting with

$$H_N^{so} = \sum_{i=1}^{N} f_i^{so}, \quad f^{so} = \frac{\alpha^2 Z}{r^3} \vec{l} \cdot \vec{s}, \quad \zeta_{\kappa l, \kappa' l}^0 = \left\langle \kappa l \left| \frac{\alpha^2 Z}{r^3} \right| \kappa' l \right\rangle, \tag{16}$$

the one-body radial integrals appearing as spin–orbit parameters ζ^0, we exploit a facility of the standard BPRM code absorbing the two-body magnetic interactions $g(so + so') + g(ss')$ for closed shells nl into ζ à la Blume and Watson, but we have to modify it ad hoc. Standard BPRM naturally assumes a closed shell target to be accompanied by excited states. In our case, the L-shell is therefore treated as open and the valence electrons up to `NRANG2` continuum basis functions $u(r)$ for each partial-wave-ℓ interact magnetically only with the two K-shell electrons. Such effective spin–orbit parameters $\zeta_{nl}^{[K]}$ clearly lead to significantly overestimated FS splittings because of neglected magnetic shielding by L-shell electrons. Short of a full-scale explicit expansion of the L-shell magnetic effects g_{ij} in terms of an elaborate angular algebra and two-body integrals N_λ and V_λ, the equivalent of Slater's two-body Coulomb integrals R_λ, there is the obvious shortcut to our particular case: the ad hoc shielding by $2s^2 2p^6$ as well in effective spin–orbit parameters $\zeta_{nl}^{[K+L]}$. Then, the only matrix elements that misjudge FS splitting are from correlation contributions, hence energetically remote from the considered energies and therefore with not much weight while adequately serving their Coulomb task, namely providing for polarization correlation. This is borne out in table 1. Gratifying is the improvement at low values of n, before the onset of diluting effects: see table 2.

The complete set of calculated energy levels of Fe XVI is available electronically. Following previous work, e.g. [12], the energies are presented in two formats for applications: (i) LSJ component format where fine structure levels are grouped as components of the LS term, showing spectroscopic completeness of the set, and (ii) $J\pi$ set where levels of a given symmetry are listed in ascending order of energies as described below.

4.1.1. LSJ energies: The LSJ format arranges levels according to the same configuration $CLSJ$, useful for spectroscopic identification and diagnostics. It provides a check for completeness of the set of energy levels that belong to a term LS and detects any missing level. Table 3 presents a sample set of Fe XVI levels, in successive columns denoting the parent core $C_t(SL\pi J)_t$, the outer electron nl, total angular momentum J, energy E in Rydbergs, the effective quantum number v of the valence electron expressed by equation (3), where E_t is the next immediate target threshold energy and LS the most likely term designation for the level. The top line in each set is the expected number (Nlv) of fine structure levels for a possible term $^{(2S+1)}L^\pi$ at given configurations. Within each set, the spin multiplicity $(2S+1)$ and parity π are fixed, but L varies. Specified in parentheses

next to each L are all possible J-values associated with the given LS term. This line is followed by energy levels of the same configurations; $Nlv(c)$ at the end specifies total number of calculated J-levels found for the set. If $Nlv = Nlv(c)$ then the calculated energy set for the given term is complete. It may be noted that levels in the table are grouped consistently in energies and effective quantum numbers, also confirming consistent level identification.

4.1.2. In Jπ energies: In the $J\pi$ format the fine structure levels are presented according to various $J\pi$ symmetries and listed in descending energy order. Table 4 exemplifies the format. It is convenient for easy implementation in astrophysical and plasma models requiring a large number of energy levels up to a pre-specified energy, say in the Boltzmann–Saha equation and all corresponding transitions.

The top of each set specifies the total number of energy levels Nlv followed by the level information. The levels are identified with configuration and term designation of the parent core, the outer electron quantum numbers (nl), absolute energy in Rydberg, the effective quantum number (v) and the final LS term designation assigned.

4.2. Oscillator strengths for allowed E1 transitions

The dipole allowed electric E1 $(\Delta J = 0 \pm 1)$ transitions are obtained from BPRM calculations. The 92 bound levels of Fe XVI yield 822 dipole allowed E1 (same-spin multiplet) and intercombination (spin-change multiplet) transitions. The table of oscillator strengths for complete sets of fine structure transitions is available electronically. It contains the level energies (table 4), oscillator strengths f, line strengths S and the radiative decay rates A. Although these three quantities are related, each one may be useful in different applications depending on the specific needs of users. Whereas they differ only in factors of energies and dynamical constants, we provide all three not only for easy usage but also for self-consistency in converting one form to the other.

Table 5 shows a partial set of transitions in Fe XVI. The top-most line specifies the nuclear charge $(Z = 26)$ and number of electrons in an ion $(N_{ion} = 8)$. This is followed by sets of oscillator strengths belonging to various pairs of symmetries $J_i \pi_i - J_k \pi_k$. The transition symmetries are expressed in the form of the statistical weight factors, $g = 2J + 1$ and parity π. Thus table 5 presents transitions in levels of symmetries $J = 1/2^e - J = 1/2^o$, each with eight levels, altogether 64 transitions. The first two columns are level indices I_i and I_k whose identification can be found from the energy table 4; the third column is the transition wavelength λ. The wavelengths are approximate since computed with $1 \, \text{Ry}/(\hbar c) = 109\,737.32 \, \text{cm}^{-1}$ for an infinitely heavy nucleus, hence $\hbar c/\text{Ry} = 911.2671 \, \text{Å}$; the NIST database www.nist.gov does offer wavelengths in a center of mass frame for Na. The fourth and fifth columns provide the energies E_i and E_k in Rydbergs for the initial and final levels. The sixth column is f, the absorption oscillator strength in length formulation. The sign of f indicates the upper and lower levels in transitions, such that a negative value means that i is the lower level while a positive value means k is the lower level. Column seven is the line strength S, and the last

column of the transition probability or the radiative decay rate A_{ki}. Spectroscopic notation of the transition can be obtained from table 4 by referrring to the values of $J_i\pi_i$, I_i, $J_k\pi_k$ and I_k. Calculated energies have been replaced by the observed energies wherever available.

Table 6 presents part of a subset of 325 E1 transition probabilities for Fe XVI where all levels are observed ones and are labeled spectroscopically with the same designation as in the NIST database. They are obtained from the calculated line strengths S, the energy-independent quantity, but using observed energies. The procedure improves accuracy and is commonly used in NIST tabulations. The purpose of this table is to identify a transition through its observed wavelength. Astrophysical models also usually observed transition energies when available. The *LS* multiplets in the table are useful for various comparisons with other calculations, and experiments where fine-structure transitions cannot be resolved. The level indices I and K next to the statistical weight factors are the calculated energy positions of the symmetries involved in transitions.

The present work also aims at benchmarking the BPRM method for radiative excitation with other methods and approximations. Table 7 compares BPRM line strengths S and transition probabilities A with those from three different atomic structure calculations, RCC, GRASP2 and SS. The RCC and SS values were calculated by us independently, while those from GRASP2 were taken from [1]. All approximations show very good agreement amongst one another in general, although some differences are found. For example, the line strength for the $3s\,^2S_{1/2}$–$3p\,^2P_{1/2}$ transition from BPRM and RCC agree better with each other, while that from GRASP2 agrees better with SS. For the $3s\,^2S_{1/2}$–$5p\,^2P_{3/2}$ transition BPRM is in better agreement with GRASP2 and SS, while RCC is lower. The differences are due to the approximations made in the calculations and choice of configurations to represent a state. On balance, the very good agreement benchmarks the high accuracy of the large-scale BPRM results.

The present E1 oscillator strengths are also compared with observation in table 8: Buchet *et al* [4] used the beam-foil technique to measure lifetimes of the upper levels of four transitions given in the table and thereby obtained the oscillator strengths. They determined the lifetimes in two ways: (a) from a simulation procedure and (b) with a fitting program. For each transition the f-values from BPRM agree very well with experiment and an early calculation by Weiss [30].

4.3. Radiative decay rates for forbidden transitions

Forbidden transitions are relatively weak and are observed mostly among low-lying levels. However, they provide important diagnostics for ambient conditions in many plasma sources. Forbidden E2, E3, M1 and M2 transitions are presented for levels with orbitals up to 5g. The set of 22 configurations has yielded 102 *LS* terms and 230 fine structure levels. However, only 21 levels lie below the ionization threshold. A total of 27083 transitions are obtained among the 230 fine structure levels. Table 9 presents a subset of the fine structure energy levels in ascending order.

Comparison of these levels with the measured values (NIST compilation) shows agreement within 1%. Nevertheless, the transition rates are reprocessed with the available observed energies for improved accuracy.

Sample sets of radiative decay rates for the forbidden transitions in Fe XVI are given in table 10. The parity remains unchanged for the E2 and M1 transitions and hence they are presented together. On the other hand, parity changes for E3 and M2 transitions which are also grouped together. The complete sets of energies and the transitions processed from SS output with standard spectroscopic notation are available electronically.

The present *A*-coefficients for forbidden transitions for Fe XVI are compared with those by Tull *et al* [29], available in the tabulation by NIST, and by Charro *et al* [5] in table 11. The NIST data for the coefficients *A* are from multiplet values by Tull *et al* [29] assuming a pure LS-coupling scheme; [5] obtains the line strengths for E2 transitions using a relativistic quantum defect orbital (RQDO) formalism. The present results for both *A* and *S* agree very well with those from NIST and by Charro *et al* [5].

5. Conclusion

An extensive set of parameters for radiative transitions is presented for both allowed and forbidden transitions in Fe XVI. Large-scale allowed transition calculations employ the R-matrix Breit–Pauli code, those for forbidden transitions the Breit–Pauli atomic structure code SS. Very good agreement, within 1%, is found between calculated and measured results.

One main objective of the present work was to benchmark the BPRM method for radiative decay rates. The BPRM results have been compared with three other approximations: the RCC method, the relativistic Dirac–Fock results from GRASP2 and the relativistic Breit–Pauli calculations using SS. All four methods show very good agreement among one another. The BPRM oscillator strengths are also in very good agreement with a few available measured values.

The present results are expected to be accurate and complete enough for most astrophysical and laboratory applications. Results for Fe XVI transitions have been published by a number of authors using various approximations. However, multipole forbidden transitions have not heretofore been studied extensively with adequate precision. Rates *A* for forbidden transitions are largely in agreement with those available at NIST and [5].

All data are available electronically at the website (labeled NORAD) www.astronomy.ohio-state.edu/~nahar/ nahar_ radiativeatomicdata/index.html

References

[1] Aggarwal K M and Keenan F P 2007 *Astron. Astrophys.* **463** 399

[2] Berrington K A, Burke P G, Butler K, Seaton M J, Storey P J, Taylor K T and Yan Yu 1987 *J. Phys.* B **20** 6379–97

[3] Berrington K A, Eissner W B and Norrington P H 1995 *Comput. Phys. Commun.* **92** 290–420

[4] Buchet J P, Buchet-Poulizac M C, Denis A, Désesquelles A and Druetta M 1980 *Phys. Rev.* A **22** 2061–8

[5] Charro E, Bielińska-Wąz D and Martín I 2000 *J. Phys.* B **33** 1855–67

[6] Cornille M, Dubau J, Faucher P, Bély-Dubau F and Blancard C 1994 *Astron. Astrophys. Suppl. Ser.* **105** 77

[7] Cornille M, Dubau J, Mason H E, Blancard C and Brown W A 1997 *Astron. Astrophys.* **320** 333

[8] Eissner W, Jones M and Nussbaumer H 1974 *Comput. Phys. Commun.* **8** 270–306

[9] Eissner W and Zeippen C J 1981 *J. Phys.* B **14** 2125–37

[10] Grupe D, Komossa S, Gallo LC, Fabian AC, Larsson J, Pradhan AK, Xu D and Miniutti G 2008 *Astrophys. J.* **681** 982

[11] Hummer D G, Berrington K A, Eissner W, Pradhan A K, Saraph H E and Tully J A 1993 *Astron. Astrophys.* **279** 298–309 (IP)

[12] Nahar S N 2000 *Astron. Astrophys. Suppl. Ser.* **127** 253

[13] Nahar S N 2003 *Astron. Astrophys.* **413** 779

[14] Nahar S N, Delahaye F, Pradhan A K and Zeippen C J 2000 *Astron. Astrophys. Suppl. Ser.* **144** 141

[15] Nahar S N, Eissner W, Chen G X and Pradhan A K 2003 *Astron. Astrophys.* **408** 789

[16] Nahar S N and Pradhan A K 1999 *Astron. Astrophys. Suppl. Ser.* **135** 347

[17] Nahar S N and Pradhan A K 2000 *Phys. Scr.* **61** 675

[18] Oelgoetz J 2006 *PhD Thesis* OSU Ohio State University

[19] Oelgoetz J, Fontes CJ, Zhang HL and Pradhan AK 2007 *Phys. Rev.* A **76** 062504

[20] Oelgoetz J, Fontes C J, Zhang H L, Montenegro M, Nahar S N and Pradhan A K 2007 *Mon. Not. R. Astron. Soc.* **382** 761

[21] Parpia F A, Froese Fischer C and Grant I P 1996 *Comput. Phys. Commun.* **94** 249–71

[22] Scott N S and Burke P G 1980 *J. Phys.* B **13** 4299–314

[23] Scott N S and Taylor K T 1982 *Comput. Phys. Commun.* **25** 347

[24] Seaton M J 1985 *J. Phys.* B **18** 2111–31

[25] Seaton M J 1986 *J. Phys.* B **19** 2601–10

[26] Seaton M J 1987 *J. Phys.* B **20** 6363–6

[27] Sur C and Chaudhuri R K 2004 *J. Phys.* B **37** 4127

[28] Sur C and Chaudhuri R K 2007 *Phys. Rev.* A **76** 032503

[29] Tull C E, Jackson M, McEachran R P and Cohen M 1972 *J. Quant. Spectrosc. Radiat. Transfer* **12** 893–900

[30] Weiss A W 1977 *J. Quant. Spectrosc. Radiat. Transfer* **18** 481–90