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Radiative rates for transitions in Fe XVII⋆

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Abstract. Energies of the lowest 157 levels belonging to the ($1s^2$) $2s^22p^6$, $2s^22p^53\ell$, $2s^22p^54\ell$, $2s^22p^55\ell$, $2s2p^63\ell$, $2s2p^64\ell$ and $2s2p^65\ell$ configurations of Fe XVII have been calculated using the GRASP code of Dyall et al. (1989). Additionally, radiative rates, oscillator strengths, and line strengths are calculated for all electric dipole (E1), magnetic dipole (M1), electric quadrupole (E2), and magnetic quadrupole (M2) transitions among these levels. Comparisons are made with the results already available in the literature, and the accuracy of the data is assessed. Our energy levels are expected to be accurate to better than 1%, whereas results for other parameters are probably accurate to better than 20%.

Key words. atomic data – atomic processes

1. Introduction

Iron is an abundant element, particularly in solar and fusion plasmas, and its emission lines are observed in almost all ionization stages. Emission lines of Ne-like Fe XVII are of special interest, because these have been observed in a variety of plasmas including astrophysical, laser produced, magnetically confined, Z-pinch and EBIT (see, Laming et al. 2000; Bhatia & Doschek 2003; Beiersdorfer et al. 2003 for references). To interpret the vast amount of observational data, atomic parameters such as energy levels, radiative rates, and collision strengths are required. Since there is a paucity of experimental data for these parameters, theoretical results are of vital importance. Therefore, in this work we report our results for energy levels and radiative rates for transitions among the lowest 157 levels of the ($1s^2$) $2s^22p^6$, $2s^22p^53\ell$, $2s^22p^54\ell$, $2s^22p^55\ell$, $2s2p^63\ell$, $2s2p^64\ell$ and $2s2p^65\ell$ configurations of Fe XVII.

Realising the importance of Fe XVII, a number of workers in the past have performed a variety of calculations to compute atomic parameters, particularly energy levels, radiative rates, oscillator strengths, and electron impact excitation collision strengths. The most notable among the available data are the recent calculations of Aggarwal et al. (2003a), Bhatia & Doschek (2003) and Chen et al. (2003). Aggarwal et al. have computed energy levels and radiative rates for transitions among 89 fine-structure levels of the $2s^22p^6$, $2s^22p^53\ell$, $2s^22p^54\ell$, $2s2p^63\ell$, and $2s2p^64\ell$ configurations. Their calculations are fully relativistic, as they have adopted the GRASP (General purpose Relativistic Atomic Structure Program) code of Dyall et al. (1989) for the generation of wavefunctions, and the Dirac Atomic *R*-matrix Code (DARC) of Norrington & Grant (2004) for the computation of collision strengths (Ω). However, their results for Ω are confined to the lowest 55 levels, and are available only at energies above thresholds. Therefore, these results are of limited use because resonances in thresholds region have not been resolved. The closed-channel (Feshbach) resonances are known to contribute significantly to the calculations of effective collision strengths (Υ) or excitation rate coefficients. Therefore, any results of Υ derived from the Ω values of Aggarwal et al. may be seriously underestimated, even at the high temperatures ($T_e \leq 10^7$ K) at which data are required for modelling spectral lines of Fe XVII. Bhatia & Doschek adopted a semi-relativistic approach for the computation of their results. They employed the SuperStructure (SS) code of Eissner et al. (1974) for the computation of wavefunctions, and the *Distorted-Wave* (DW) program of Eissner (1998) for calculating Ω. One-body relativistic operators were included through term coupling coefficients. This semi-relativistic approach does not significantly affect the accuracy of Ω values, as has been shown by a good agreement between the DARC and DW results for a majority of transitions – see Aggarwal et al. for details and comparisons. Furthermore, Bhatia & Doschek included a larger number of levels (73) in their calculations of Ω, and also extended the energy range from the 300 Ryd of Aggarwal et al. to 425 Ryd. However, they too ignored resonances in the thresholds region, and hence their results are again of limited practical use. On the other hand, Chen et al. have not only included all the 89 levels among the configurations listed above, but have also resolved resonances in thresholds region. They have adopted the

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⋆ Tables 2–5 are only available in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/420/783

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SS code for the calculations of wavefunctions, and results for Ω have been obtained from the *R*-matrix code of Berrington et al. (1995). Furthermore, their calculations include one-body relativistic operators in the Breit-Pauli approximation. Therefore, the energy levels and radiative rates of Aggarwal et al., and excitation rates of Chen et al. should be the most reliable available to date for transitions among the 89 fine-structure levels noted above.

The motivation for the present work comes from the fact that even the most exhaustive results of Chen et al. (2003) available to date are unable to fully resolve the discrepancy between theory and measurements. Of particular recent interest (beside others) are the six resonance lines of Fe XVII, namely 3C ($2p^6\ ^1S_0$–$2p^5 3d\ ^1P^\circ_1$: 1–17), 3D ($2p^6\ ^1S_0$–$2p^5 3d\ ^3D^\circ_1$: 1–23), 3E ($2p^6\ ^1S_0$–$2p^5 3d\ ^3P^\circ_1$: 1–27), 3F ($2p^6\ ^1S_0$–$2p^5 3s\ ^3P^\circ_1$: 1–5), 3G ($2p^6\ ^1S_0$–$2p^5 3s\ ^1P^\circ_1$: 1–3), and 3H ($2p^6\ ^1S_0$–$2p^5 3s\ ^3P^\circ_2$: 1–2), at respective wavelengths of 15.015 Å, 15.262 Å, 15.450 Å, 16.778 Å, 17.053 Å, and 17.098 Å – see Table 1 below for level indices. These prominent strong lines have been observed in the X-ray spectra of the solar and other stellar coronae, active galactic nuclei, X-ray binaries, and supernovae from the *Chandra* and XMM *Newton* satellites – see Chen et al. for references. Furthermore, line intensity ratios have also been measured on EBIT (electron beam ion trap) machines at the Lawrence Livermore National Laboratory (LLNL: Beiersdorfer et al. 2003 and references therein), and at the National Institute of Standards and Technology (NIST: Laming et al. 2000). There is satisfactory agreement between theory and experiment for the ratio R1 (3C/3D), but the discrepancy is ∼15% for R2 (3E/3C) – see Table 4 of Chen et al. Similarly, the discrepancy is even greater for the ratio R3 (3F/3C), particularly at temperatures below 4×10^6 K, at which Fe XVII has its maximum fractional abundance in ionization equilibrium. Some of the discrepancies between theory and astrophysical observations can perhaps be resolved by the consideration of multi-ion model in stead of the widely used single ion model, as discussed and demonstrated by Doron & Behar (2002). However, there are still serious differences between the LLNL and NIST measurements, while Beiersdorfer et al. (2003) have questioned the accuracy of the atomic data of Chen et al. (2003), suggesting that the contribution of resonances may have been overestimated. Additionally, Beiersdorfer et al. do not observe any appreciable variation in line ratios with energy, whereas Chen et al. do show a significant variation, as expected. To resolve the laboratory measurements, new experiments are planned at NIST (Laming 2003), and we have a fresh look at the theoretical atomic data. This is for several reasons as explained below.

Firstly, in our opinion the most reliable results available to date for effective collision strengths (or excitation rates) are those of Chen et al. (2003), because: (i) they have explicitly resolved the resonances in thresholds region, (ii) have included configuration interaction(CI) and relativistic effects, (iii) have included a large number of levels (89), besides adopting the widely used *R*-matrix method, (iv) have ensured the convergence of Ω with the partial wave expansion, and (v) have taken into account the high energy behaviour of Ω while computing results for Υ. Therefore, we do not see any apparent deficiency in their work. However, the past experience of similar work on other ions of iron has shown that different calculations of comparable complexity and employing the same *R*-matrix method (but in different approximations) often produce strikingly different sets of results. Examples of serious differences are results for Fe XI (Aggarwal & Keenan 2003a,b), Fe XV (Aggarwal et al. 2000, 2001, 2003b), and Fe XXI (Aggarwal & Keenan 2001). Therefore, in the absence of any other results being available for Fe XVII with comparable accuracy, a fresh calculation with an independent approach may be useful in confirming the accuracy of the available atomic data.

Secondly, all the resonance lines of Fe XVII, including the prominent ones, exhibit numerous resonances throughout the thresholds region – see Figs. 7–13 of Chen et al. (2003), and hence make a significant contribution to the values of Υ. Since most of the line ratios either measured in the laboratory, or observed in the solar and astrophysical plasmas, are at high energies/temperatures (∼0.8–1.2 keV, 10^6–10^7 K), resonances towards the higher end of the thresholds region may make an appreciable contribution. Therefore, we find that there is scope for improvement in the calculations of Chen et al., because all 50 levels of the $2s^2 2p^5 5\ell$ configurations lie *below* the energy levels of the $2s2p^6 4p$ configuration, and the 18 levels of the $2s2p^6 5\ell$ configurations are just above the levels of the $2s2p^6 4f$ configuration – see Table 1. All the 68 levels of the $2s^2 2p^5 5\ell$ and $2s2p^6 5\ell$ configurations lie in the ∼80–91 Ryd energy range, and interact closely with the levels of the $2s2p^6 4\ell$ configurations. Therefore, the resonances arising from the missing 68 levels *may* make an appreciable contribution. Since calculations for Ω are still in progress the contribution of such resonances cannot be estimated at present. Nevertheless, inclusion of these additional 68 levels in a calculation will be helpful in spectral modelling, because cascading effect from higher levels is important (Chen et al. 2003; Beiersdorfer et al. 2003).

Finally, inclusion of CI with the $2s^2 2p^5 5\ell$ and $2s2p^6 5\ell$ configurations will be helpful in determining the convergence of the expansion of the wavefunction. Therefore, for all the above reasons we are performing a larger calculation with the aim of providing a consistent set of results for energy levels, radiative rates, collision strengths, and effective collision strengths for all transitions among 157 levels of Fe XVII. However, in this paper we are reporting our results for the first two parameters only, because the calculations for Ω are computationally intensive, and hence will take a significant time to complete.

2. Energy levels

The $(1s^2)\ 2s^2 2p^6$, $2s^2 2p^5 3\ell$, $2s^2 2p^5 4\ell$, $2s^2 2p^5 5\ell$, $2s2p^6 3\ell$, $2s2p^6 4\ell$, and $2s2p^6 5\ell$ configurations of Fe XVII give rise to 157 fine-structure levels, listed in Table 1. To generate the wavefunctions, we have used the fully relativistic GRASP code of Dyall et al. (1989) with the option of *extended average level* (EAL), in which a weighted (proportional to $2j + 1$) trace of the Hamiltonian matrix is minimized. This produces a compromise set of orbitals describing closely lying states with moderate accuracy. Also, as in calculations by other workers, we have included CI among the above basic 25 configurations.

Table 1. Target levels of Fe XVII and their threshold energies (in Ryd).

Index	Configuration	Level	Expt.[a]	GRASP[b]	GRASP[c]
1	$2s^22p^6$	$^1S_0$	00.0000	00.0000	0.0000
2	$2s^22p^53s$	$^3P^o_2$	53.2966	53.1622	53.1706
3	.....	$^1P^o_1$	53.4367	53.3059	53.3143
4	.....	$^3P^o_0$	54.2269	54.0917	54.0986
5	.....	$^3P^o_1$	54.3140	54.1813	54.1897
6	$2s^22p^53p$	$^3S_1$	55.5218	55.3881	55.3951
7	.....	$^3D_2$	55.7788	55.6551	55.6636
8	.....	$^3D_3$	55.8974	55.7720	55.7804
9	.....	$^1P_1$	55.9804	55.8596	55.8682
10	.....	$^3P_2$	56.1137	55.9902	55.9989
11	.....	$^3P_0$	56.5155	56.4021	56.4098
12	.....	$^3D_1$	56.6672	56.5441	56.5526
13	.....	$^3P_1$	56.9061	56.7801	56.7885
14	.....	$^1D_2$	56.9337	56.8086	56.8171
15	.....	$^1S_0$	57.8894	57.9529	57.9419
16	$2s^22p^53d$	$^3P^o_0$	58.8983	58.7676	58.7755
17	.....	$^3P^o_1$	58.9818	58.8392	58.8470
18	.....	$^3P^o_2$	59.0977	58.9758	58.9838
19	.....	$^3F^o_4$	59.1042	58.9842	58.9913
20	.....	$^3F^o_3$	59.1612	59.0447	59.0521
21	.....	$^1D^o_2$	59.2876	59.1739	59.1821
22	.....	$^3D^o_3$	59.3666	59.2541	59.2625
23	.....	$^3D^o_1$	59.7080	59.6062	59.6131
24	.....	$^3F^o_2$	60.0877	59.9701	59.9778
25	.....	$^3D^o_2$	60.1618	60.0286	60.0370
26	.....	$^1F^o_3$	60.1974	60.0705	60.0784
27	.....	$^1P^o_1$	60.6004	60.6356	60.6368
28	$2s2p^63s$	$^3S_1$	.....	63.2048	63.2124
29	.....	$^1S_0$	.....	63.6956	63.6988
30	$2s2p^63p$	$^3P^o_0$	.....	65.6263	65.6342
31	.....	$^3P^o_1$	65.6012	65.6594	65.6674
32	.....	$^3P^o_2$	.....	65.8295	65.8373
33	.....	$^1P^o_1$	65.9238	65.9717	65.9800
34	$2s2p^63d$	$^3D_1$	.....	68.9168	68.9199
35	.....	$^3D_2$	.....	68.9268	68.9299
36	.....	$^3D_3$	.....	68.9459	68.9492
37	.....	$^1D_2$	.....	69.3192	69.3246
38	$2s^22p^54s$	$^3P^o_2$	.....	71.6515	71.6597
39	.....	$^1P^o_1$	71.8607	71.6987	71.7069
40	.....	$^3S_1$	.....	72.5806	72.5874
41	$2s^22p^54p$	$^3P^o_0$	.....	72.5829	72.5911
42	$2s^22p^54s$	$^3P^o_1$	72.7465	72.6071	72.6153
43	$2s^22p^54p$	$^3D_2$	.....	72.6448	72.6530
44	.....	$^3D_3$	.....	72.6937	72.7022
45	.....	$^1P_1$	.....	72.7239	72.7323
46	$2s^22p^54p$	$^3P_2$	.....	72.7669	72.7756
47	.....	$^3P_0$	.....	73.0629	73.0634
48	.....	$^3D_1$	.....	73.5564	73.5649

Table 1. continued.

Index	Configuration	Level	Expt.[a]	GRASP[b]	GRASP[c]
49	.....	$^3P_1$	.....	73.6435	73.6515
50	.....	$^1D_2$	.....	73.6597	73.6682
51	$2s^22p^54d$	$^3P^o_0$	.....	73.8051	73.8125
52	.....	$^3P^o_1$	73.9584	73.8374	73.8449
53	.....	$^3F^o_4$	.....	73.8771	73.8853
54	.....	$^3P^o_2$	.....	73.8903	73.8982
55	.....	$^3F^o_3$	.....	73.8992	73.9075
56	$2s^22p^54p$	$^1S_0$	.....	73.9250	73.9148
57	$2s^22p^54d$	$^1D^o_2$	.....	73.9453	73.9538
58	.....	$^3D^o_3$	.....	73.9733	73.9819
59	.....	$^3D^o_1$	74.3047	74.1736	74.1765
60	$2s^22p^54f$	$^3D_1$	.....	74.4536	74.4623
61	.....	$^1G_4$	.....	74.4546	74.4625
62	.....	$^3G_5$	.....	74.4559	74.4638
63	.....	$^3D_2$	.....	74.4639	74.4726
64	.....	$^3F_3$	.....	74.4888	74.4975
65	.....	$^1D_2$	.....	74.4929	74.5015
66	.....	$^1F_3$	.....	74.4955	74.5040
67	.....	$^3F_4$	.....	74.5012	74.5096
68	$2s^22p^54d$	$^3F^o_2$	.....	74.8209	74.8292
69	.....	$^3D^o_2$	.....	74.8396	74.8476
70	.....	$^1F^o_3$	.....	74.8622	74.8705
71	.....	$^1P^o_1$	75.1704	75.0349	75.0358
72	$2s^22p^54f$	$^3G_3$	.....	75.4005	75.4086
73	.....	$^3G_4$	.....	75.4087	75.4168
74	.....	$^3D_3$	.....	75.4171	75.4258
75	.....	$^3F_2$	.....	75.4180	75.4267
76	$2s^22p^5\ 5s$	$^3P^o_2$	.....	.....	79.6047
77	.....	$^1P^o_1$	79.79	.....	79.6289
78	$2s^22p^55p$	$^3S_1$	.....	.....	80.0630
79	.....	$^3D_2$	.....	.....	80.0985
80	.....	$^3D_3$	.....	.....	80.1230
81	.....	$^1P_1$	.....	.....	80.1382
82	.....	$^3P_2$	.....	.....	80.1593
83	.....	$^1S_0$	.....	.....	80.3254
84	$2s^22p^5\ 5s$	$^3P^o_0$	.....	.....	80.5357
85	.....	$^3P^o_1$	80.70	.....	80.5468
86	$2s^22p^5\ 5d$	$^3P^o_0$	.....	.....	80.6646
87	.....	$^3P^o_1$	80.70	.....	80.6813
88	.....	$^3F^o_4$	.....	.....	80.6989
89	.....	$^3P^o_2$	.....	.....	80.7066
90	.....	$^3F^o_3$	.....	.....	80.7092
91	.....	$^1D^o_2$	.....	.....	80.7310
92	.....	$^3D^o_3$	.....	.....	80.7445
93	.....	$^1P^o_1$	81.85	.....	80.8554
94	$2s^22p^5\ 5f$	$^3D_1$	.....	.....	80.9757
95	.....	$^3D_2$	.....	.....	80.9842
96	.....	$^3G_5$	.....	.....	80.9868

Table 1. continued.

Index	Configuration	Level	Expt.[a]	GRASP[b]	GRASP[c]
97	.....	$^1G_4$	.....	.....	80.9869
98	.....	$^3F_3$	.....	.....	80.9997
99	.....	$^1D_2$	.....	.....	81.0059
100	.....	$^1F_3$	.....	.....	81.0067
101	.....	$^3G_4$	.....	.....	81.0099
102	$2s^22p^5$ 5g	$^3F^o_2$	.....	.....	81.0102
103	.....	$^3F^o_3$	.....	.....	81.0121
104	.....	$^1H^o_5$	.....	.....	81.0189
105	.....	$^3H^o_6$	.....	.....	81.0206
106	.....	$^3G^o_3$	.....	.....	81.0243
107	.....	$^3G^o_4$	.....	.....	81.0256
108	.....	$^1G^o_4$	.....	.....	81.0301
109	.....	$^3G^o_5$	.....	.....	81.0317
110	$2s^22p^5$ 5p	$^3D_1$	.....	.....	81.0215
111	.....	$^3P_1$	.....	.....	81.0539
112	.....	$^1D_2$	.....	.....	81.0729
113	.....	$^3P_0$	.....	.....	81.1638
114	$2s2p^64s$	$^3S_1$	.....	81.5593	81.5934
115	$2s^22p^5$ 5d	$^3F^o_2$	.....	.....	81.6362
116	.....	$^3D^o_2$	.....	.....	81.6441
117	.....	$^1F^o_3$	.....	.....	81.6568
118	.....	$^3D^o_1$	80.98	.....	81.7289
119	$2s2p^64s$	$^1S_0$	.....	81.7322	81.7463
120	$2s^22p^5$ 5f	$^3G_3$	.....	.....	81.9260
121	.....	$^3D_3$	.....	.....	81.9298
122	.....	$^3G_4$	.....	.....	81.9307
123	.....	$^3F_2$	.....	.....	81.9337
124	$2s^22p^5$ 5g	$^1F^o_3$	.....	.....	81.9537
125	.....	$^3F^o_4$	.....	.....	81.9551
126	.....	$^3H^o_4$	.....	.....	81.9574
127	.....	$^3H^o_5$	.....	.....	81.9592
128	$2s2p^64p$	$^3P^o_0$	.....	82.5375	82.5523
129	.....	$^3P^o_1$	82.5244	82.5493	82.5635
130	.....	$^3P^o_2$	.....	82.6183	82.6321
131	.....	$^1P^o_1$	82.6702	82.6654	82.6771
132	$2s2p^64d$	$^3D_1$	.....	83.7747	83.7876
133	.....	$^3D_2$	.....	83.7793	83.7923
134	.....	$^3D_3$	.....	83.7880	83.8011
135	.....	$^1D_2$	.....	83.9205	83.9300
136	$2s2p^64f$	$^3F^o_2$	.....	84.3381	84.3522
137	.....	$^3F^o_3$	.....	84.3394	84.3541
138	.....	$^3F^o_4$	.....	84.3430	84.3581
139	.....	$^1F^o_3$	.....	84.3538	84.3681
140	$2s2p^65s$	$^3S_1$	.....	.....	89.4930
141	.....	$^1S_0$	.....	.....	89.5737
142	$2s2p^65p$	$^3P^o_0$	.....	.....	89.9790
143	.....	$^3P^o_1$	90.01	.....	89.9847
144	.....	$^3P^o_2$	.....	.....	90.0191
145	.....	$^1P^o_1$	90.01	.....	90.0413
146	$2s2p^65d$	$^3D_1$	.....	.....	90.5803
147	.....	$^3D_2$	.....	.....	90.5827
148	.....	$^3D_3$	.....	.....	90.5873
149	.....	$^1D_2$	.....	.....	90.6501
150	$2s2p^65f$	$^3F^o_2$	.....	.....	90.8618
151	.....	$^3F^o_3$	.....	.....	90.8625
152	.....	$^3F^o_4$	.....	.....	90.8642
153	.....	$^1F^o_3$	.....	.....	90.8719
154	$2s2p^65g$	$^3G_3$	.....	.....	90.8915
155	.....	$^3G_4$	.....	.....	90.8914
156	.....	$^3G_5$	.....	.....	90.8931
157	.....	$^1G_4$	.....	.....	90.8934

[a] NIST (`http://www.physics.nist.gov/PhysRefData`).
[b] GRASP results of Aggarwal et al. (2003a) for 89 levels.
[c] Present results from GRASP for 157 levels.

In Table 1 we list our energies for the 157 fine-structure levels of Fe XVII. Also included in the table are the experimentally compiled energies of NIST (`http://www.physics.nist.gov/PhysRefData`), and energies of 89 levels reported in our previous work (Aggarwal et al. 2003a) using the same GRASP code. Other available experimental and theoretical results have already been compared and discussed in our previous work, and are therefore not included in Table 1. Experimental energies for all levels are not available, but the agreement is better than 1% for the common levels. Furthermore, the level orderings are the same in both theoretical and experimental results, which is highly satisfying. Similarly, apart from the additional 68 levels included in the present work, the agreement with the previous results is better than 1%. In fact, the discrepancy is less than 0.02 Ryd, except for level 114 ($2s2p^64s\ ^3S_1$) for which the present results are higher by 0.034 Ryd, amounting to less than 0.05%. Therefore, we may state with confidence that the energy levels listed in Table 1 are accurate to better than 1%.

While computing our energy levels (and radiative rates), we also explored the impact of including larger CI. Configurations such as $2p^63\ell^2$, $2p^64\ell^2$, $2p^65\ell^2$, $2p^63\ell4\ell$, and $2p^63\ell5\ell$ do not have any appreciable effect either on energy levels or radiative rates, because levels arising from the above configurations lie in the 118–175 Ryd energy range, well above that of the 157 levels in Table 1, i.e. below 91 Ryd. Similarly, levels of the $2s2p^53\ell^2$, $2s2p^54\ell^2$ etc. configurations have energies above 118 Ryd, and have no noticeable effect on the energies of the lower levels. Therefore, inclusion of these higher levels in a calculation may affect the calculations of Ω (and particularly of Υ at very high temperatures), but is non-contributory to the determination of energy levels and radiative rates among the lower levels. To conclude, inclusion of 68 levels of the $2s^22p^55\ell$ and $2s2p^65\ell$ configurations will be beneficial for the subsequent computation of Υ, whereas the higher levels are too distant to make any significant contribution.

3. Radiative rates

The absorption oscillator strength (f_{ij}) and radiative rate A_{ji} (in s^{-1}) for a transition $i \rightarrow j$ are related by the following expression:

$$f_{ij} = \frac{mc}{8\pi^2 e^2} {\lambda_{ji}}^2 \frac{\omega_j}{\omega_i} A_{ji} = 1.49 \times 10^{-16} \lambda_{ji}^2 (\omega_j/\omega_i) A_{ji} \quad (1)$$

where m and e are the electron mass and charge, respectively, c is the velocity of light, λ_{ji} is the transition energy/wavelength in Å, and ω_i and ω_j are the statistical weights of the lower i and upper j levels, respectively. Similarly, the oscillator strength f_{ij} (dimensionless) and the line strength S (in atomic unit, 1 au = 6.460×10^{-36} cm^2 esu^2) are related by the following standard equations:
for the electric dipole (E1) transitions:

$$A_{ji} = \frac{2.0261 \times 10^{18}}{\omega_j \lambda_{ji}^3} S \quad \text{and} \quad f_{ij} = \frac{303.75}{\lambda_{ji} \omega_i} S, \quad (2)$$

for the magnetic dipole (M1) transitions:

$$A_{ji} = \frac{2.6974 \times 10^{13}}{\omega_j \lambda_{ji}^3} S \quad \text{and} \quad f_{ij} = \frac{4.044 \times 10^{-3}}{\lambda_{ji} \omega_i} S, \quad (3)$$

for the electric quadrupole (E2) transitions:

$$A_{ji} = \frac{1.1199 \times 10^{18}}{\omega_j \lambda_{ji}^5} S \quad \text{and} \quad f_{ij} = \frac{167.89}{\lambda_{ji}^3 \omega_i} S, \quad (4)$$

and
for the magnetic quadrupole (M2) transitions:

$$A_{ji} = \frac{1.4910 \times 10^{13}}{\omega_j \lambda_{ji}^5} S \quad \text{and} \quad f_{ij} = \frac{2.236 \times 10^{-3}}{\lambda_{ji}^3 \omega_i} S. \quad (5)$$

In Tables 2–5 we present transition energies (ΔE_{ij} in Å), radiative rates (A_{ji} in s^{-1}), oscillator strengths (f_{ij}, dimensionless), and line strengths (S in au), in length form only, for all 3401 electric dipole (E1), 3334 magnetic dipole (M1), 4439 electric quadrupole (E2), and 4503 magnetic quadrupole (M2) transitions, respectively, among the 157 levels of Fe XVII. The indices used to represent the lower and upper levels of a transition have already been defined in Table 1. Also, in calculating the above parameters we have used the Breit and QED corrected theoretical energies/wavelengths as listed in Table 1. It may be noted that E1 (allowed and intercombination) transitions are the most important for applications, but data for other transitions are also required for modelling calculations, and that is why we have presented here a complete set of results for all types of transitions.

The most complete and accurate set of A-values available in the literature to compare with are our earlier results (Aggarwal et al. 2003a) for E1 transitions among the 89 levels up to the $n = 4$ configurations. Results of earlier workers, limited to a lesser number of transitions, have already been compared and discussed in our previous work, and therefore here we focus on the comparison between our present and earlier results alone. As seen in Table 1, the lowest 75 levels are common between the two calculations. A comparison made between our earlier and present results for transitions among these 75 levels, shows an agreement of better than 20% for all strong transitions with $f \geq 0.01$, and the only exception is the 47–71 ($2s^2 2p^5 4p\ ^3P_2$–$2s^2 2p^5 4d\ ^1P^\circ_1$) intercombination transition, for which the present results are lower by 30%. This highly satisfactory agreement between the two sets of results confirms that A-values have converged within the $n = 5$ configurations, and the results presented in Tables 2–5 are accurate to better than 20% for a majority of strong transitions. However, for weaker transitions the results may be comparatively less accurate.

In a recent paper, Nahar et al. (2003) have reported radiative rates for a large number of transitions. They included 490 levels for the calculations of E1 transitions, but only 89 for other types of transitions. For the E1 transitions they adopted the R-matrix code of Berrington et al. (1995), and included one-body relativistic operators in a Breit-Pauli approximation. This method generates results for a large number of transitions with comparatively less effort than required in a standard atomic structure code such as GRASP, but the accuracy achieved is generally not high mainly because of the exclusion of two-body relativistic operators. The level orderings of their R-matrix calculations are also slightly different than those of NIST or obtained from GRASP – see, for example, levels 9–13 in Table 7 of Nahar et al. The inadequacy of this method to produce accurate results for radiative rates has already been commented on by Nahar et al. (and see their Table 6 for comparisons with other results), and has recently been discussed in detail by Hibbert (2003). For the remaining E2, M1 and M2 transitions, Nahar et al. have adopted the GRASP program as by us, and hence the results are expected to be similar. However, as stated earlier they have included only 89 levels in their calculations, whereas 157 levels are included in the present work. Furthermore, for the E2 transitions a factor of 2/3 is associated in the relationship between A and S. Nahar et al. have absorbed it in the calculations of S, whereas we have kept it in the multiplying coefficient in Eq. (4), which is in agreement with others, such as NIST (`http://physics.nist.gov/Pubs/AtSpec/node17.html`). As a result of this, our listed values of S for E2 transitions are higher by 50% than those reported by Nahar et al., whereas the A-values are comparable. To conclude, for the included 157 levels of Fe XVII, the present work reports a consistent set of radiative rates for all types of transitions, and the accuracy achieved is higher than available to date.

4. Conclusions

In this work, energy levels, radiative rates, oscillator strengths, and line strengths for transitions among the lowest 157 fine-structure levels of Fe XVII are computed using the fully relativistic GRASP code of Dyall et al. (1989), and results are reported for electric and magnetic dipole and quadrupole transitions. Energy levels agree in magnitude and orderings with the listings of NIST, and are assessed to be accurate to better than 1%. However, the accuracy of other parameters for a majority of strong transitions is better than 20%. Our calculations for other required atomic parameters (Ω and Υ) are still in progress, and will take a considerably long time to complete.

We hope with the availability of those results (along with the present ones) some of the discrepancies between theory and observations will be resolved.

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