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A REVIEW OF ELECTRON IMPACT EXCITATION OF Fe XV–Fe XVII

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Theoretical electron impact excitation data for Fe XV, Fe XVI, and Fe XVII are critically assessed and recommended data are identified.

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CONTENTS

INTRODUCTION

The ions Fe XV, Fe XVI, and Fe XVII belong to the magnesium-like, sodium-like, and neon-like isoelectronic sequences, respectively. They are each considered in turn.

Fe XV

Early work on this system includes the calculations of Bely and Blaha[1] (Coulomb–Born with some allowances for resonances but neglecting target configuration mixing), Flower and Jordan,[2] Mason,[3] Bhatia and Kastner,[4] and Clark et al.[5] (all distorted-wave calculations). Christensen et al.[6] have calculated intermediate-coupling collision strengths for all 120 transitions between the 16 lowest energy fine-structure levels (Table A) using the University College London (UCL) distorted-wave code, including extensive configuration mixing and Breit–Pauli relativistic corrections. Significant differences with the results of Bhatia and Kastner (who employed a less elaborate form of the same method) were recorded for most transitions, but in general good agreement was found with the distorted-wave results of Mann.[7]

Dufton et al.[8] have carried out an eight-state close-coupling calculation using the R-matrix method to calculate collision strengths for transitions between the 14 lowest energy levels considered in Ref. 6 (see Table A). The R-matrix calculation included the effects of close-coupling and resonances, but employed LS coupling, with the fine-structure transitions being subsequently computed via a unitary transformation of the LS-coupling reactance matrices using the JAJOM code written by Saraph.[9]

Dufton et al.[8] compare their results with those of Christensen et al.[6] for transitions from the four lowest levels $3s^2\ ^1S$ and $3s3p\ ^3P_{0,1,2}$ at their[6] three lowest energies of 15.9, 25.2, and 36.9 Ry. They[8] report agreement to better than 10% in 102 cases, between 10% and 20% in 25 cases, and worse than 20% in 11 cases. A question still remains in this ion over the adequacy of the procedure used to obtain the fine-structure transitions and also over whether enough terms have been included in the eigenstate expansion. A fully relativistic R-matrix calculation including more states in the expansion would be required to settle this question, but such a calculation awaits further developments in the theory and a future generation of computers.

At the present time, the results of Dufton et al.[8] are recommended, together with those of Christensen et al.[6] for transitions involving the $3s4s$ levels. However, collision strengths have not been released so far by Dufton et al.

Pradhan[10] has published distorted-wave results of effective collision strengths as a function of temperature,

TABLE A
Level Designations and Energies for Fe XV (from Ref. 6)

Designation	Energy (cm^{-1})
$3s^2\ ^1S_0$	0
$3s3p\ ^3P_0$	232,600
$3s3p\ ^3P_1$	238,300
$3s3p\ ^3P_2$	252,000
$3s3p\ ^1P_1$	355,400
$3p^2\ ^1D_2$	559,800
$3p^2\ ^3P_0$	556,100
$3p^2\ ^3P_1$	565,600
$3p^2\ ^3P_2$	581,900
$3s3d\ ^3D_1$	681,800
$3s3d\ ^3D_2$	683,100
$3s3d\ ^3D_3$	685,000
$3p^2\ ^1S_0$	664,600
$3s3d\ ^1D_2$	769,600
$3s4s\ ^3S_1$	1,765,200
$3s4s\ ^1S_0$	1,790,900

for all transitions mentioned above for the Mg isoelectronic sequence members S V, Ar VII, Ca IX, Cr XIII, Fe XV, and Ni XVII. Data are available in the form of tabulated values of $\Upsilon_{ij}(T)$ in Ref. 10.

Fe XVI

With the possible exception of the work of Flower and Nussbaumer,[11] all the calculations[5,12–15] for Fe XVI prior to 1989, using variants of the Coulomb–Born or no-exchange distorted-wave methods, may be considered to have been superseded by the results of Mann[7] and Sampson et al.[16] The latter authors present results for the 10 transitions among the $n = 3$ fine-structure levels and for the 80 transitions from these to the excited levels nlj with $n = 4$ and 5, calculated in a relativistic distorted-wave approximation. In all cases where comparison is possible, their results agree with Mann's calculations to within 5% except in the case of one transition, where the difference is about 10%. This is attributed to the inclusion of relativistic effects not considered in Mann's semirelativistic work. The results of Sampson et al. are thus preferred.

None of the calculations includes the effects of close coupling or resonances. The magnitude of these contributions is unknown. A close-coupling calculation for this ion is required to settle this question. Until this is forthcoming, the Sampson et al.[16] results are recommended.

It should be noted that Sampson et al. present results for the entire Na-like isoelectronic sequence, $22 \leqslant Z \leqslant 92$. Data are available in the form of tabulated values of collision strengths Ω in Table III of Ref. 16.

Fe XVII

Energy levels for Fe XVII are given in Table B. These are from the work of Bhatia and Doschek[17] who indicate that they were derived from experimental observations.[18,19] A comparison of the energy levels given by Bhatia and Doschek with those from Ref. 18 indicates that in naming the levels, these authors used only the eigenvector components from Ref. 18 to establish level identifications, but did not adopt the designations given there; rather, they choose to maintain the term designations of the lower-Z ions of the Ne I sequence. Moreover, there are small differences (up to 1300 cm^{-1}) between the energies quoted in Ref. 17 and Ref. 18, while Ref. 19 does not contain energy levels explicitly. Early nonrelativistic distorted-wave results (Refs. 20–23) were superseded by the relativistic distorted-wave results of Mann[7] who calculated level-to-level collision strengths for all $n = 2$–3 and 2–4 excitations, but his published results were summed over fine-structure levels. A nonrelativistic distorted-wave plus term-coupling calculation was carried out by Bhatia et al.[24] and Bhatia and Doschek[17] and they presented level-to-level collision strengths and rate coefficients for all 2–3 and 3–3 excitations. A similar calculation has been carried out by Cornille et al.[25] for all possible transitions with active $2p$, $3l$, and $4l$ orbitals. Relativistic distorted-wave level-to-level cross sections and rate coefficients have been tabulated by Hagelstein and Jung[26] for all 2–3 and 3–3 excitations. Zhang et al. have presented Coulomb–Born-exchange[27] and fully relativistic distorted-wave[28] level-to-level collision strengths for all 2–3 and 2–4 excitations.

All of these preceding works neglect the contribution from resonances, which have been shown to be important for most nondipole transitions.[29,30] Early work by Smith et al.[29] was shown by Chen and Reed[30] to overestimate the resonant contribution and so the results in Ref. 30 are to be preferred. Reference 30 contains tabulations of level-to-level excitation rate coefficients for $2p$–$3s$ and $2p$–$3p$ excitations, calculated using a relativistic distorted-wave approximation that included the effect of the $3ln'l'$ (all $n'l'$), $4l4l'$, and $4l5l'$ resonances. The resonant

TABLE B
Level Designations and Energies for Fe XVII (from Ref. 17)

Designation	Energy (cm^{-1})
$2p^6\ ^1S_0$	0
$2p^5 3s\ ^3P_2$	5,849,320
$2p^5 3s\ ^1P_1$	5,864,590
$2p^5 3s\ ^3P_0$	5,951,212
$2p^5 3s\ ^3P_1$	5,960,870
$2p^5 3p\ ^3S_1$	6,093,407
$2p^5 3p\ ^3D_2$	6,121,606
$2p^5 3p\ ^3D_3$	6,134,630
$2p^5 3p\ ^3P_1$	6,143,730
$2p^5 3p\ ^3P_2$	6,158,360
$2p^5 3p\ ^3P_0$	6,202,450
$2p^5 3p\ ^1P_1$	6,219,114
$2p^5 3p\ ^3D_1$	6,245,225
$2p^5 3p\ ^1D_2$	6,248,350
$2p^5 3p\ ^1S_0$	6,353,230
$2p^5 3d\ ^3P_0$	6,463,942
$2p^5 3d\ ^3P_1$	6,472,500
$2p^5 3d\ ^3P_2$	6,486,288
$2p^5 3d\ ^3F_4$	6,486,530
$2p^5 3d\ ^3F_3$	6,492,788
$2p^5 3d\ ^3D_2$	6,506,650
$2p^5 3d\ ^3D_3$	6,515,320
$2p^5 3d\ ^3D_1$	6,552,200
$2p^5 3d\ ^3F_2$	6,594,461
$2p^5 3d\ ^1D_2$	6,606,500
$2p^5 3d\ ^1F_3$	6,606,500
$2p^5 3d\ ^1P_1$	6,660,000

and nonresonant contributions to the total rate coefficient were tabulated separately. A further calculation for Fe XVII is in progress using the Breit–Pauli *R*-matrix method.[31]

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