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ATOMIC STRUCTURE CALCULATION OF  
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STRENGTHS IN Fe ION, I  
(3s-3p and 3p-3d transitions in Fe XV)

January 1984

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Atomic Structure Calculation of Energy Levels  
and Oscillator Strengths in Fe Ion, I  
( 3s - 3p and 3p - 3d transitions in Fe XV )

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Energy levels and oscillator strengths were calculated for 3s-3p and 3p-3d transition arrays in Fe XV, isoelectronic to Mg I. The energy levels are obtained by the Slater-Condon theory of atomic structure, including explicitly the strong configuration interactions. The calculated wavelengths are presented for electric dipole transition with  $gf \geq 0.0001$ . The calculated energy levels are given in diagrams, too. The theoretical spectra are also shown in graphical representation, where the  $gf$  is plotted as a function of the wavelength. The results are compared with experimental data, where available.

Keywords: Fe, Highly Ionized Atom, Wavelength, Energy Level,  
Oscillator Strength, Plasma Diagnostic

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Fe イオンのエネルギー準位と振動子強度の原子構造計算, I  
(Fe XV イオンの  $3s-3p$  及び  $3p-3d$  遷移)

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(1983年12月24日受理)

核融合プラズマにおける不純物問題解明のために必要とされる金属イオンの分光学的データに関する研究の一環として, Fe XV のエネルギー準位及び  $4n=0$ ,  $n=3-3$  遷移の波長と振動子強度の理論計算を行った。計算には Hartree - X R 波動関数と Slater-Condon 理論に基づいた Cowan プログラムを用いた。結果は表及び図としてまとめた。文献調査による実験値は参考として表中に示した。

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## § 1. INTRODUCTION

Knowledge of atomic structure in multiply charged ions of metals is important in the interpretation of spectral data from high temperature plasma. The allowed  $\Delta n=0$ ,  $n=2-2$  transitions of  $2s^2 2p^q - 2s 2p^{q+1}$  and  $2s 2p^{q+1} - 2p^{q+2}$  types in highly ionized atoms have been widely studied. The energy level data have been compiled and published by Fawcett<sup>1)</sup>, and the data for oscillator strengths and the lifetimes are also available<sup>2-5)</sup>. These data are now well established for the ions with  $Z \leq 28$ . The exception is the  $f$ -values for some transitions.

The data, however, on the energy levels of M-shell are not yet established. Little is known for oscillator strengths<sup>2,6)</sup>. The wavelengths for  $\Delta n=0$ ,  $n=3-3$  transitions have been presented by Fawcett<sup>7)</sup> again.

The Fe XV, a member of Mg I isoelectronic sequence, have two electrons outside closed shell, which give rise to singlets and triplets. This spectrum has been studied first by Edlén<sup>8)</sup> in 1936, and then by Fawcett & Peacock<sup>9)</sup>, by Fawcett<sup>10)</sup>. Intercombination line,  $3s^2 \ ^1S_0 - 3s 3p \ ^3P_1$ , was not observed in the above works. Cowan and Widing<sup>11)</sup> identified thirteen Fe XV lines in solar flare spectra by comparison with the calculated wavelengths and the predicted relative intensities. The resonance intersystem line at 417.24 Å was confirmed.

Following the previous work on Ti IX<sup>13)</sup>, Ti X<sup>14)</sup> and Ti XI<sup>15)</sup>, the atomic structure calculation has been extended to Fe XV, using again the program developed by Cowan<sup>16-18)</sup>. The energy levels have been obtained based on the Slater-Condon theory for  $3s^2$ ,  $3s 3p$ ,  $3p^2$ ,  $3s 3d$  and  $3p 3d$  configurations, including explicitly the

configuration interactions. The wavelengths and the weighted oscillator strengths ( $gf$ -values) have been calculated for  $3s-3p$  and  $3p-3d$  transitions. The results are given both in numerical tables and in the graphical representations. The calculated spectra are generated in such that the  $gf$ -value is plotted against wavelength. They will provide a helpful guidance for finding the missing lines, together with the numerical tables.

## § 2. METHOD OF CALCULATION

The method of calculation used in the present work is the same as in the previous ones<sup>13,14,15)</sup>, and it is described in some detail there. The full explanation is given by Bromage<sup>19)</sup> and Cowan<sup>20)</sup>. Therefore only a short description is repeated here. The calculation consists of the following three steps:

- (i) calculation of radial integrals, such as  $E_{av}$ ,  $F^k$ ,  $G^k$ ,  $\zeta_{nl}$  and  $R^k$  by the *ab initio* Hartree-XR wavefunctions,
- (ii) optimization of the above integrals so as to minimize the discrepancy between the observed and calculated energy levels,
- (iii) calculation of wavelengths and oscillator strengths by adopting the scaled radial integrals obtained in the step (ii).

The steps (i) and (ii) were performed separately for the following two configuration groups according to the parity:

1st parity       $3s^2$  (A),  $3p^2$  (B) and  $3s3d$  (C)

2nd parity       $3s3p$  (A) and  $3p3d$  (B)

The electric dipole radial integrals were also computed by the same Hartree-XR wavefunctions, and used in the step (iii)

configuration interactions. The wavelengths and the weighted oscillator strengths ( $gf$ -values) have been calculated for 3s-3p and 3p-3d transitions. The results are given both in numerical tables and in the graphical representations. The calculated spectra are generated in such that the  $gf$ -value is plotted against wavelength. They will provide a helpful guidance for finding the missing lines, together with the numerical tables.

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calculation.

### § 3. RESULTS

The first step calculation gives the *ab initio* values of the single configuration integrals and configuration interaction integrals as shown in the second column "HXR" of Tables 1 and 3. In the second step calculation, the optimization was reduced to manageable size by fixing ratio of  $F^k$ ,  $G^k$ ,  $\zeta$  and  $R^k$  in each integrals<sup>21-23)</sup>, when necessary. The accuracy of the optimization was measured by a root mean square deviation ( $\Delta$ ) and/or a standard deviation ( $\sigma$ ), defined as

$$\Delta = \left[ \sum_i (E_{calc}(i) - E_{obs}(i))^2 / (N_l - N_p) \right]^{1/2}, \quad (1)$$

$$\sigma = \left[ \sum_i (E_{calc}(i) - E_{obs}(i))^2 / N_l \right]^{1/2}, \quad (2)$$

where  $E_{calc}(i)$  and  $E_{obs}(i)$  are  $i$ -th calculated and observed levels, respectively,  $N_l$  is the number of observed energy levels and  $N_p$  is the number of adjustable parameters. The following five kinds of free parameters were used in the optimization:

one average energy	$E_{av}$
one scale factor for	$F^k$
one scale factor for	$G^k$
one scale factor for	$\zeta$
two scale factors for	$R^k$ .

calculation.

### § 3. RESULTS

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one average energy	$E_{\text{av}}$
one scale factor for	$F^k$
one scale factor for	$G^k$
one scale factor for	$\zeta$
two scale factors for	$R^k$ .

The reduced electric dipole radial integrals obtained from the same *ab initio* HXR wavefunctions were utilized in the step (iii) calculation combined with the second step results. In the following Tables and Figures, we closely maintain the format of our previous work on Ti IX<sup>(13)</sup>, Ti X<sup>(14)</sup> and Ti XI<sup>(15)</sup>.

### 3.1 Configurations $3s^2$ (G), $3p^2$ (B) and $3s3d$ (C) of the first parity

All levels of this parity were observed<sup>(11)</sup>. The least-squares optimization, however, cannot be satisfactory, when the above all levels are included simultaneously. Therefore, we have omitted the  $^1S_0$  level, because the isoelectronic regularity for the energy levels of  $^1S_0$  from K VIII to Fe XV is found poorer than for other levels, and because the assignment of this level is tentative as noted in ref. 11. In the least-squares optimization, the single configuration parameters were adjusted first, while  $R^k$  integrals were fixed. Then  $R^k$  integrals were adjusted by keeping the single configuration parameters fixed. This procedure was repeated several times. The fitted parameter values are given in the column "Fitted", and the ratio of "Fitted" to "HXR". The rms deviation  $\Delta$  is  $0.99 \times 10^3 \text{ cm}^{-1}$ , which gives 0.007% of total energy range of the configurations (G+B+C).

The calculated and observed energy levels are listed in Table 2 for the  $3s^2$ ,  $3p^2$  and  $3s3d$ , together with their differences (" $E(C-O)$ "). The agreement is satisfactory. One exception is  $3p^2 \ ^1S$ , which is excluded in the optimization calculation. The level designation and its percentage compositions in LS-basis are also given. The corresponding energy

level diagram is shown in Fig.1 for  $3p^2$  and  $3s3d$  configurations. The percentage compositions are listed from the largest two contributions in the same configuration and one from the other when over about 10%. The average LS-purity is as high as 92%. Hence, the level designation in the column "Term" is given in LS-coupling notation by the most significant component. A pair of levels  $3p^2 \ ^1D_2$  and  $3s3d \ ^1D_2$  are considerably perturbed with strong mutual configuration interaction:  $3p^2 \ ^1D$  has a 16%  $3s3d \ ^1D$  character. One can notice that the appreciable mixing occurs between  $^3P_2$  and  $^1D_2$  levels in  $3p^2$ . This singlet-triplet mixing gives appreciable oscillator strength for some intercombination transitions, which is strictly forbidden in pure LS-coupling.

### 3.2 Configurations $3s3p(\mathcal{A})$ and $3p3d(\mathcal{B})$ of the second parity

The least-squares optimization was performed for the  $3s3p(\mathcal{A})$  and  $3p3d(\mathcal{B})$  configurations, in which one singlet and seven triplet levels were included. The energy of the triplet levels were fixed relative to ground level, based on the observed intercombination<sup>(2)</sup>,  $3s^2 \ ^1S_0 - 3s3p \ ^3P_1$ . The rms deviation  $\Delta$  of  $0.126 \times 10^3 \text{ cm}^{-1}$  was achieved, which yield 0.015% of total energy level spread of configurations  $\mathcal{A}$  and  $\mathcal{B}$ . The Hartree-XR and fitted parameter values are given in Table 3, together with their ratios. The calculated energy levels are given in Table 4, along with the principal percentage compositions in LS-coupling basis. The observed energy levels are also included for comparison, with their difference with the calculated one. The average LS-purity of  $3s3p$  configuration is close to 100%. It should be noted here that the  $^3P_1$  level has only a 0.2%  $^1P_1$  character and consequently

the oscillator strength for  $3s^2 \ ^1S_0 - 3s3p \ ^3P_1$  transition is small as described in 3.3. Energy level diagram for  $3s3p$  configuration is displayed in Fig.2.

In  $3p3d$  configuration, two pairs of energy levels are strongly mixed one another; 995.018 and 981.385 for  $J=2$  and 993.260 and 981.260 for  $J=1$ . The level designation is generally given according to the most significant composition. However, the second pair is the exception, where the second largest composition is adopted as its level designation by considering the smooth connection of energy level diagram as shown in Fig.3. There is a considerable mixing between  $^3F_2$  and  $^1D_2$  levels. This indicates that some spin-forbidden transitions from  $3p3d$  to  $(3s3d + 3p^2)$  gain appreciable oscillator strength, as will be described in 3.3. The calculated energy levels are displayed graphically in Fig.3.

### 3.3 Wavelengths and Oscillator Strengths

The reduced electric dipole radial integrals (Table 10) were obtained from the *ab initio* Hatree-XR wavefunction, and used in the third step calculation without scaling. The calculated wavelengths and the *gf*-values for  $3s^2 - 3s3p$ ,  $3s^2 - 3p3d$ ,  $3s3p - 3p^2$  and  $3s3p - 3s3d$  transition arrays are listed in Table 5, and those for  $3p^2 - 3s3d$  in Table 6, and  $3s3d - 3p3d$  in Table 7, respectively. In Tables 5-7, the observed wavelengths are included for comparison, with the difference between the calculated and observed ones. The agreement of the calculated wavelengths with the observed ones is excellent. In Table 5, the calculated *gf*-values are also given, together with the values

derived by Wiese and Fuhr<sup>6)</sup> for comparison. The agreement is again good. Table 5 shows that the difference between the calculated and observed wavelengths is less than 0.1 Å for all the components of  $^3P - ^3P$  and  $^1P - ^1D$  in  $3s3p - 3p^2$  transition. Therefore, the accuracy of the calculated wavelength for two intercombinations,  $^3P_2 - ^1D_2$  and  $^3P_1 - ^1D_2$ , may be as accurate as for the allowed transitions described above. These two lines have fairly large  $gf$ -value, so that they are likely to be observed at the predicted position within  $\pm 0.1\text{Å}$ . These two lines are indeed observed<sup>11)</sup>. Another intercombination predicted at 435.222Å due to  $^1P_1 - ^3P_2$  is expected to be observed with the same accuracy. For a line of  $^1P_1 - ^1S_0$  in  $3s3p-3p^2$  transition, the calculated wavelength differs from the observed one<sup>7)</sup> by 1.39Å. This is exceptionally large compared with other members. This is solely due to the fact that  $3p^2\ ^1S_0$  was excluded in the least squares optimization of the energy level calculation. As is noted in 3.2, the isoelectronic regularity in energy level of  $3p^2$  is poorer than that of other levels. Therefore, we conclude that there are two ways, whereby the identification is completed in this spectrum. First, this line should be examined again along the isoelectronic sequence. Next, if this transition is confirmed as it is now, the model used in the present calculation has to be modified.

The total number of possible electric dipole transitions among the configurations considered in the present work is shown in Table 8, arranged in decreasing order of wavelength. The listed transitions are limited for  $gf \geq 0.0001$ . The theoretical spectrum was generated from Table 10, and shown in Fig.4, where

the  $gf$ -values are plotted in a logarithmic scale as a function of wavelength. Twelve lines above 420 Å and one line below 180 Å were excluded. Two line rich regions, 226 - 244 Å and 316 - 334 Å are shown in Figures 5 and 6, respectively, with wavelength scale being expanded ten times as large as in Fig. 4. Three Figures 4-6 provide a helpful guidance for identification of missing lines by direct comparison with a recorded spectrogram.

Comparison of the present  $gf$ -value with the NBS work<sup>6)</sup>, listed in Table 5, is graphically displayed in Fig. 7, where  $\log(gf)_{\text{Present}} - \log(gf)_{\text{NBS}}$  is plotted against  $\log(gf)_{\text{Present}}$ . The area between two broken lines shows agreement within  $\pm 20\%$ .

In Table 9, the calculated lifetimes for the excited configurations are tabulated. Most of the levels have lifetimes of the order of 0.01 nsec, while  $3s3p\ ^3P_{0,2}$  are metastable. It should be noted that  $3s3p\ ^3P_1$  level has long lifetime of 19.7 nsec. Therefore, this level is collisionally destroyed before it decays by radiative transition. This indicates that the resonance intercombination is hardly observed from the ordinary light source, where electron density is usually high. In Table 9, the calculated lifetimes are listed, which may provide practical help for the future beam-foil lifetime measurement.

#### § 4. DISCUSSION

The average LS-purity of the first excited configuration of  $3s3p$  is close to 100%, as shown in Table 4. On the other hand, the LS-purity of the levels of  $3p3d$  configuration ranges from 62% to 100%, and the average is 81%. The purity varies from level to

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level in one configuration, and a few level has heavy admixtures from another configuration. In particular,  $^3D_1$  and  $^3P_1$  are labeled by the second components of their eigenvectors for the reason described in 3.2. In  $3p^2$  configuration, the LS-purity of  $^3P_0$  and  $^3P_1$  is almost 100%, while that of  $^3P_2$  is 82%. This gives the reasonable explanation for a difference of the  $gf$ -values between the present intermediate calculation and "LS-multiplet" one<sup>6)</sup>, for  $3s3p\ ^3P_J - 3p^2\ ^3P_J$  transition in Table 5. In Ekberg's<sup>25)</sup> comparison of energy levels in the Mg I sequence (his Fig 3), the curves for  $3s3d\ ^1D_2$  and  $3p^2\ ^1D_2$  plotted from data through Ti XI give a smooth extrapolation to the level values in Fe XV reported here. In Tables 6 and 7, one can notice that several lines with fairly large  $gf$ -value are not yet observed. Some of them are thus expected to be found in the recorded spectrogram. The present calculation, especially the calculated spectra shown in Figures 4-6, may provide helpful guidance for finding these missing lines, although in many cases the apparent line intensity is dependent on conditions of a light source.

The radial energy integrals were adjusted from their *ab initio* Hartree-XR values, while the radial electric dipole integrals were not. Therefore, the  $gf$ -values of transition between levels, of which at least one is subject to strong configuration interaction, are less accurate. However, the relative  $gf$ -values are fairly reliable, because the dipole integrals have a very little influence on them. Fuhr *et al.*<sup>6)</sup> noted that the  $gf$ -values in their table need to be replaced by intermediate coupling data. The present calculation meets to this need. The transition probability situation in Fe XV is thus

improved. The absolute  $gf$ -values can be determined only after the lifetimes are measured. In this context, Table 9 may be helpful for practical purpose of lifetime measurement.

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## ADDENDA

Present calculation of Fe XV was carried out as an extension of the previous work on Ti IX, Ti X and Ti XI. After the completion of the present work, Fawcett [1,2] published the same calculation on Fe XV. While we were concentrated on Ti and Fe, he presented systematic calculation of Al-like ions from Cl V to Ni XVI and Mg-like ions from S V to Ni XVII. The present results are in agreement with ref. [2]. However, when compared with the observed data, the present results show better agreement. We present here the wavelengths and *gf*-values for forbidden lines in addition to that for allowed ones. The graphical representations are also displayed.

- [1] B.C. Fawcett : "Calculated oscillator strengths and wavelengths for allowed transitions within the third shell for ions in the Al-like isoelectronic sequence between Cl V and Ni XVI", Atomic Data and Nuclear Data Tables 28 (1983) 557-578.
- [2] B.C. Fawcett : "Calculated oscillator strengths and wavelengths for allowed transitions within the third shell for ions in the Mg-like isoelectronic sequence between S V and Ni XVII", Atomic Data and Nuclear Data Tables 28 (1983) 579-596.

Table 1 Parameter values (in  $10^3 \text{ cm}^{-1}$ ) for  $3s^2$ ,  $3p^2$  and  $3s3d$  configurations in Fe XV. Ratio is defined as Fitted/HXR.

Parameters	Hartree-XR	Fitted	Ratio	C.I.
$E_{av}(3s^2)$	0.000	5.804	-----	
$E_{av}(3p^2)$	575.314	587.083	1.020	
$F^2(3p,3p)$	147.419	131.947	0.895	
$\zeta(3p)$	14.328	13.303	.928	
$E_{av}(3s,3d)$	679.212	690.929	1.017	
$\zeta(3d)$	1.497	1.040	0.695	
$G^2(3s,3d)$	126.421	105.606	0.835	
$R^1(ss,pp)$	190.176	106.393	0.599	$3s^2 * 3p^2$
$R^1(pp,sd)$	172.202	153.350	0.891	$3p^2 * 3s3d$
$\Delta$		0.99 *		
$\sigma$		0.44		

\* Number of free parameter is 7.

Table 2 Calculated and observed energy levels (in  $10^3 \text{ cm}^{-1}$ ) for  $3s^2$ ,  $3p^2$  and  $3s3d$  configurations in Fe XV.

Conf	Term	J	E(calc)	E(obs)	E(C-O)*	Percentage Composition
$3s^2$	$^1S$	0	0.00	0.000	0.00	99%
$3p^2$	$^3P$	2	581.700	581.701 <sup>a</sup>	-0.001	82%, 13% $^1D$
	$^3P$	1	564.598	564.597 <sup>a</sup>	0.001	100%
	$^3P$	0	554.503	544.505 <sup>a</sup>	-0.002	97%
	$^1D$	2	559.606	559.606 <sup>a</sup>	0.000	67%, 18% $^3P$ , 16% $3s3d$ $^1D$
	$^1S$	0	659.667	660.984 <sup>b</sup>	-1.317 <sup>†</sup>	96%
$3s3d$	$^3D$	3	681.408	681.432 <sup>a</sup>	-0.024	100%
	$^3D$	2	679.835	679.775 <sup>a</sup>	0.060	100%
	$^3D$	1	678.808	678.844 <sup>a</sup>	-0.036	100%
	$^1D$	2	762.135	762.135 <sup>a</sup>	0.000	80%, 19% $3p^2$ $^1D$

<sup>a</sup>Cowan and Widing (1973), ref.11).

<sup>b</sup>Fawcett (1971), ref.7).

<sup>†</sup>See text for detail.



Table 3. Parameter values (in  $10^3 \text{ cm}^{-1}$ ) for 3s3p and 3p3d configurations in Fe XV. Ratio is defined as Fitted/HXR.

Parameters	Hartree-XR	Fitted	Ratio	C.I.
$E_{av}(3s3p)$	261.225	277.614	1.063	
$\zeta(3p)$	14.393	13.328	0.926	
$G^1(3s, 3p)$	190.685	172.501	0.905	
$E_{av}(3p3d)$	970.011	981.148	1.011	
$\zeta(3p)$	14.321	13.261	0.926	
$\zeta(3d)$	1.494	1.271	0.851	
$F^2(3p, 3d)$	147.977	125.403	0.847	
$G^1(3p, 3d)$	164.355	148.682	0.905	
$G^3(3p, 3d)$	108.538	98.188	0.905	
$R^1(sp, pd)$	172.490	137.992	0.800	3s3p * 3p3d
$R^2(sp, pd)$	130.904	104.723	0.800	3s3p * 3p3d
$\Delta$		0.126*		
$\sigma$		0.048		

\* Number of free parameter is 6.

Table 4. Calculated and observed energy levels (in  $10^3 \text{ cm}^{-1}$ ) for 3s3p and 3p3d configurations in Fe XV.

Conf	Term	J	E(calc)	E(obs)	E(C-O)*	% Composition
3s3p	$^3P$	2	253.809	253.826 <sup>a</sup>	-0.017	100%
	$^3P$	1	239.733	239.663 <sup>a</sup>	0.070	100%
	$^3P$	0	233.875	233.928 <sup>a</sup>	-0.103	100%
	$^1P$	1	351.932	351.932 <sup>a</sup>	0.000	98%
3p3d	$^3F$	4	949.660	949.660 <sup>b</sup>	0.000	100%
	$^3F$	3	938.190	938.190 <sup>b</sup>	0.000	99%
	$^3F$	2	928.451	928.450 <sup>b</sup>	0.001	89%, 11% $^1D$
	$^3D$	3	994.940			98%
	$^3D$	2	995.018			66%, 33% $^3P$
	$^3D$	1	993.260			37%, 63% $^3P$
	$^3P$	2	981.385			63%, 32% $^3D$
	$^3P$	1	981.260			36%, 62% $^3D$
	$^3P$	0	991.572			100%
	$^1F$	3	1063.879			99%
	$^1D$	2	949.657			84%, 10% $^3F$
	$^1P$	1	1069.544			97%

<sup>a, b</sup> See footnote in Table 3.

Table 5 Calculated and observed wavelengths for  $3s^2 - 3s3p$ ,  $3s^2 - 3p3d$ ,  $3s3p - 3p^2$  and  $3s3p - 3s3d$  transition arrays in Fe XV, with calculated weighted oscillator strengths.

Transition			Wavelength (in Å)					
Conf	Term	J-J	Calc	Obs	C-O	gf	gf*	
3s <sup>2</sup> -3s3p	<sup>1</sup> S- <sup>1</sup> P	0-1	284.146	284.146 <sup>a</sup>	0.000	0.8611	0.80	
	<sup>1</sup> S- <sup>3</sup> P	0-1	417.130	417.24 <sup>a</sup>	-0.11	0.0040	0.0044	
3s <sup>2</sup> -3p3d	<sup>1</sup> S- <sup>1</sup> P	0-1	93.498			0.0093		
3s3p-3p <sup>2</sup>	<sup>3</sup> P- <sup>3</sup> P	2-2	304.979	305.00 <sup>b</sup>	-0.02	0.8762	0.885	
	<sup>3</sup> P- <sup>3</sup> P	1-2	292.426	292.36 <sup>b</sup>	0.07	0.2796	0.286	
	<sup>3</sup> P- <sup>3</sup> P	2-1	321.762	321.79 <sup>a</sup>	-0.03	0.3363	0.332	
				321.761 <sup>b</sup>	0.001			
	<sup>3</sup> P- <sup>3</sup> P	1-1	307.821	307.74 <sup>a</sup>	0.08	0.2103	0.209	
				307.78 <sup>b</sup>	0.04			
	<sup>3</sup> P- <sup>3</sup> P	1-0	317.693	317.62 <sup>b</sup>	0.07	0.2709	0.268	
	<sup>3</sup> P- <sup>3</sup> P	0-1	302.368	302.45 <sup>b</sup>	-0.08	0.2874	0.285	
	<sup>1</sup> P- <sup>1</sup> D	1-2	481.524	481.53 <sup>a</sup>	0.01	0.2692	0.269	
				481.52 <sup>b</sup>	0.00			
	<sup>1</sup> P- <sup>1</sup> S	1-0	324.955	323.57 <sup>a</sup>	1.39	0.2693	0.315	
	<sup>1</sup> P- <sup>3</sup> P	1-2	435.222			0.0745	0.066	
	<sup>1</sup> P- <sup>3</sup> P	1-1	470.221			0.0009	0.0008	
	<sup>1</sup> P- <sup>3</sup> P	1-0	493.655			0.0018	0.0023	
	<sup>3</sup> P- <sup>1</sup> D	2-2	327.014	327.03 <sup>a</sup>	-0.02	0.1763	0.160	
	<sup>3</sup> P- <sup>1</sup> D	1-2	312.624	312.55 <sup>a</sup>	0.07	0.0896	0.081	
	<sup>3</sup> P- <sup>1</sup> S	1-0	238.133			0.0033		
3s3p-3s3d	<sup>3</sup> P- <sup>3</sup> D	2-3	233.864	233.86 <sup>a</sup>	0.00	1.2619	1.370	
				233.865 <sup>b</sup>	-0.01			
	<sup>3</sup> P- <sup>3</sup> D	2-2	234.727			0.2260	0.225	
	<sup>3</sup> P- <sup>3</sup> D	1-2	227.220	227.22 <sup>a</sup>	0.00	0.6943	0.690	
	<sup>3</sup> P- <sup>3</sup> D	2-1	235.295			0.0150	0.016	
	<sup>3</sup> P- <sup>3</sup> D	1-1	227.752	227.70 <sup>b</sup>	0.05	0.2306	0.231	
	<sup>3</sup> P- <sup>3</sup> D	0-1	224.753	224.76 <sup>a</sup>	-0.01	0.3137	0.314	
				224.745 <sup>b</sup>	0.008			
	<sup>1</sup> P- <sup>1</sup> D	1-2	243.782	243.782 <sup>a</sup>	0.000	1.8612	1.869	
				243.783 <sup>b</sup>	-0.001			
	<sup>1</sup> P- <sup>3</sup> D	1-2	304.968			0.0017	0.0010	
	<sup>1</sup> P- <sup>3</sup> D	1-1	305.926			0.0012	0.0010	
	<sup>3</sup> P- <sup>1</sup> D	2-2	196.724			0.0005	0.0003	
<sup>3</sup> P- <sup>1</sup> D	1-2	191.423			0.0102	0.0084		

<sup>a</sup>Cowan *et al.*, (1973), ref.11).

<sup>b</sup>Fawcett (1971), ref.7).

\*Fuhr *et al.*, (1981), ref.6).

†See text for detail.

Table 6 Calculated and observed wavelengths for  $3p^2 - 3p3d$  transition in Fe XV, with calculated weighted oscillator strengths.

Transition		Wavelength (in Å)			gf	gf*
Term	J-J	Calc	Obs	C-O		
$3p-3F$	2-3	280.512			0.0108	
$3p-3F$	2-2	288.391			0.0073	
$3p-3F$	1-2	274.836			0.0020	
$3p-3D$	2-3	241.990			1.5437	
$3p-3D$	2-2	241.945			0.7982	
$3p-3D$	1-2	232.331			0.3337	
$3p-3D$	2-1	242.978			0.1831	
$3p-3D$	1-1	233.284			0.4456	
$3p-3D$	0-1	227.916			0.0068	
$3p-3P$	2-2	250.197			0.1416	
$3p-3P$	1-2	239.930			0.9375	
$3p-3P$	2-1	250.275			0.0244	
$3p-3P$	1-1	240.003			0.0611	
$3p-3P$	0-1	234.325	234.79 <sup>a</sup>	-0.46	0.6708	
$3p-3P$	1-0	234.206			0.1874	
$1D-1F$	2-3	198.305			0.8169	1.16
$1D-1D$	2-2	256.376			0.7924	
$1D-1P$	2-1	196.102			0.0047	
$1S-1P$	0-1	243.976			0.7620	
$1D-3F$	2-2	271.116			0.1048	
$1D-3F$	2-3	264.142			0.0118	
$1D-3D$	2-3	229.709			0.4467	
$1D-3D$	2-2	229.668			0.1342	
$1D-3D$	2-1	230.598			0.0406	
$1D-3P$	2-2	237.091			0.0046	
$1D-3P$	2-1	237.161			0.0039	
$1S-3P$	0-1	310.952			0.0011	
$3p-1F$	2-3	207.392			0.2484	
$3p-1D$	2-2	271.770			0.0918	
$3p-1D$	1-2	259.700			0.0393	
$3p-1P$	2-1	204.983			0.0013	
$3p-1P$	1-1	198.041			0.0015	
$3p-1P$	0-1	194.159			0.0046	

\* Fuhr *et al.*, (1981), ref.6).

Source of observed data: see footnote in Table 5.

Table 7 Calculated and observed wavelengths for 3s3d - 3p3d transition in Fe XV, with calculated weighted oscillator strengths.

Transition		Wavelength (in Å )				
Term	J-J	Calc	Obs	C-O	gf	gf*
$^3D-^3F$					2.467 <sup>†</sup>	2.265 <sup>†</sup>
$^3D-^3F$	3-4	372.784	372.78 <sup>b</sup>	0.00	1.1187	
$^3D-^3F$	3-3	389.435			0.1539	
$^3D-^3F$	2-3	387.064	387.00 <sup>b</sup>	0.06	0.6787	
$^3D-^3F$	3-2	404.788			0.0017	
$^3D-^3F$	2-2	402.227			0.1099	
$^3D-^3F$	1-2	400.572	400.65 <sup>b</sup>	-0.08	0.4037	
$^3D-^3D$	3-3	318.947			0.8204	
$^3D-^3D$	2-3	317.354			0.1922	
$^3D-^3D$	3-2	318.868			0.0425	
$^3D-^3D$	2-2	317.276			0.5837	
$^3D-^3D$	1-2	316.246			0.1332	
$^3D-^3D$	2-1	319.055			0.0781	
$^3D-^3D$	1-1	318.013			0.3921	
$^3D-^3P$	3-2	333.358			0.6790	
$^3D-^3P$	2-2	331.619			0.0093	
$^3D-^3P$	1-2	330.494			0.0315	
$^3D-^3P$	2-1	331.758			0.3783	
$^3D-^3P$	1-1	330.631			0.0550	
$^3D-^3P$	1-0	319.729			0.1625	
$^1D-^1F$	2-3	331.407			2.2544	1.89
$^1D-^1D$	2-2	533.270			0.1256	
$^1D-^1P$	2-1	325.300			0.6612	
$^1D-^3F$	2-3	568.005			0.0048	
$^1D-^3F$	2-2	601.266			0.0135	
$^1D-^3D$	2-3	429.544			0.0052	
$^1D-^3D$	2-1	432.666			0.0003	
$^1D-^3P$	2-2	456.100			0.0065	
$^1D-^3P$	2-2	429.401			0.0002	
$^1D-^3P$	2-1	456.362			0.0058	
$^3D-^1F$	3-3	261.458			0.0106	
$^3D-^1F$	2-3	260.387			0.0021	
$^3D-^1D$	3-2	372.787			0.0421	
$^3D-^1D$	2-2	370.614			0.0104	
$^3D-^1D$	1-2	369.209			0.0480	
$^3D-^1P$	2-1	256.602			0.0052	
$^3D-^1P$	1-1	255.927			0.0014	

\*Fuhr et al., (1981), ref.6).

<sup>†</sup>Multilet sum.

Source of observed data: see footnote in Table 5.

Table 8 Calculated and observed wavelengths for transitions between  $(3s^2 + 3p^2 + 3s3d)$  and  $(3s3p + 3p3d)$  configurations with calculated  $gf$ -value in Fe XV. Arranged in order of decreasing wavelength.

No	Transitin				Wavelength( Å )		gf
	Energy (10 <sup>3</sup> cm <sup>-1</sup> )	Conf	Term	J-J	Calc	Obs	
1	762.135- 928.451	3s3d-3p3d	<sup>1</sup> D- <sup>3</sup> F	2-2	601.266		0.0135
2	762.135- 938.190	3s3d-3p3d	<sup>1</sup> D- <sup>3</sup> F	2-3	568.005		0.0048
3	762.135- 949.657	3s3d-3p3d	<sup>1</sup> D- <sup>1</sup> D	2-2	533.270		0.1256
4	351.932- 554.502	3s3p-3p <sup>2</sup>	<sup>1</sup> P- <sup>3</sup> P	1-0	493.655		0.0018
5	351.932- 559.605	3s3p-3p <sup>2</sup>	<sup>1</sup> P- <sup>1</sup> D	1-2	481.524	481.53 <sup>a</sup>	0.2692
6	351.932- 564.597	3s3p-3p <sup>2</sup>	<sup>1</sup> P- <sup>3</sup> P	1-1	470.221		0.0009
7	762.135- 981.259	3s3d-3p3d	<sup>1</sup> D- <sup>3</sup> P	2-1	456.362		0.0058
8	762.135- 981.385	3s3d-3p3d	<sup>1</sup> D- <sup>3</sup> P	2-2	456.100		0.0065
9	351.932- 581.699	3s3p-3p <sup>2</sup>	<sup>1</sup> P- <sup>3</sup> P	1-2	435.222		0.0745
10	762.135- 993.260	3s3d-3p3d	<sup>1</sup> D- <sup>3</sup> D	2-1	432.666		0.0003
11	762.135- 994.940	3s3d-3p3d	<sup>1</sup> D- <sup>3</sup> D	2-3	429.544		0.0052
12	762.135- 995.017	3s3d-3p3d	<sup>1</sup> D- <sup>3</sup> P	2-2	429.401		0.0002
13	0.000- 239.733	3s <sup>2</sup> -3s3p	<sup>1</sup> S- <sup>3</sup> P	0-1	417.130	417.24 <sup>a</sup>	0.0040
14	681.408- 928.451	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> F	3-2	404.788		0.0017
15	679.835- 928.451	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> F	2-2	402.227		0.1099
16	678.808- 928.451	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> F	1-2	400.572	400.65 <sup>b</sup>	0.4037
17	681.408- 938.190	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> F	3-3	389.435		0.1539
18	679.835- 938.190	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> F	2-3	387.064	387.00 <sup>b</sup>	0.6787
19	681.408- 949.657	3s3d-3p3d	<sup>3</sup> D- <sup>1</sup> D	3-2	372.787		0.0421
20	681.408- 949.660	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> F	3-4	372.784	372.78 <sup>b</sup>	1.1187
21	679.835- 949.657	3s3d-3p3d	<sup>3</sup> D- <sup>1</sup> D	2-2	370.614		0.0104
22	678.808- 949.657	3s3d-3p3d	<sup>3</sup> D- <sup>1</sup> D	1-2	369.209		0.0480
23	681.408- 981.385	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> P	3-2	333.358		0.6790
24	679.835- 981.259	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> P	2-1	331.758		0.3783
25	679.835- 981.385	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> P	2-2	331.619		0.0093
26	762.135-1063.879	3s3d-3p3d	<sup>1</sup> D- <sup>1</sup> F	2-3	331.407		2.2544
27	678.808- 981.259	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> P	1-1	330.631		0.0550
28	678.808- 981.385	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> P	1-2	330.494		0.0315
29	253.809- 559.605	3s3p-3p <sup>2</sup>	<sup>3</sup> P- <sup>1</sup> D	2-2	327.014	327.03 <sup>a</sup>	0.1763
30	762.135-1069.544	3s3d-3p3d	<sup>1</sup> D- <sup>1</sup> P	2-1	325.300		0.6612
31	351.932- 659.667	3s3p-3p <sup>2</sup>	<sup>1</sup> P- <sup>1</sup> S	1-0	324.955	323.57 <sup>a</sup>	0.2693
32	253.809- 564.597	3s3p-3p <sup>2</sup>	<sup>3</sup> P- <sup>3</sup> P	2-1	321.762	321.79 <sup>a</sup>	0.3363
33	678.808- 991.572	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> P	1-0	319.729		0.1625
34	679.835- 993.260	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> D	2-1	319.055		0.0781
35	681.408- 994.940	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> D	3-3	318.947		0.8204
36	681.408- 995.017	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> D	3-2	318.868		0.0425
37	678.808- 993.260	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> D	1-1	318.013		0.3921
38	239.733- 554.502	3s3p-3p <sup>2</sup>	<sup>3</sup> P- <sup>3</sup> P	1-0	317.693	317.62 <sup>b</sup>	0.2709
39	679.835- 994.940	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> D	2-3	317.354		0.1922
40	679.835- 995.017	3s3d-3p3d	<sup>3</sup> D- <sup>3</sup> D	2-2	317.276		0.5837

Table 8 Continued

41	678.808-	995.017	3s3d-3p3d	$^3D-^3D$	1-2	316.246		0.1332
42	239.733-	559.605	3s3p-3p <sup>2</sup>	$^3P-^1D$	1-2	312.624	312.55 <sup>a</sup>	0.0896
43	659.667-	981.259	3p <sup>2</sup> -3p3d	$^1S-^3P$	0-1	310.952		0.0011
44	239.733-	564.597	3s3p-3p <sup>2</sup>	$^3P-^3P$	1-1	307.821	307.74 <sup>a</sup>	0.2103
45	351.932-	678.808	3s3p-3s3d	$^1P-^3D$	1-1	305.926		0.0012
46	253.809-	581.699	3s3p-3p <sup>2</sup>	$^3P-^3P$	2-2	304.979	305.00 <sup>b</sup>	0.8762
47	351.932-	679.835	3s3p-3s3d	$^1P-^3D$	1-2	304.968		0.0017
48	233.875-	564.597	3s3p-3p <sup>2</sup>	$^3P-^3P$	0-1	302.368	302.45 <sup>b</sup>	0.2874
49	239.733-	581.699	3s3p-3p <sup>2</sup>	$^3P-^3P$	1-2	292.426	292.36 <sup>b</sup>	0.2796
50	581.699-	928.451	3p <sup>2</sup> -3p3d	$^3P-^3F$	2-2	288.391		0.0073
51	0.000-	351.932	3s <sup>2</sup> -3s3p	$^1S-^1P$	0-1	284.146	284.146 <sup>a</sup>	0.8611
52	581.699-	938.190	3p <sup>2</sup> -3p3d	$^3P-^3F$	2-3	280.512		0.0108
53	564.597-	928.451	3p <sup>2</sup> -3p3d	$^3P-^3F$	1-2	274.836		0.0020
54	581.699-	949.657	3p <sup>2</sup> -3p3d	$^3P-^1D$	2-2	271.770		0.0918
55	559.605-	928.451	3p <sup>2</sup> -3p3d	$^1D-^3F$	2-2	271.116		0.1048
56	559.605-	938.190	3p <sup>2</sup> -3p3d	$^1D-^3F$	2-3	264.142		0.0118
57	681.408-	1063.879	3s3d-3p3d	$^3D-^1F$	3-3	261.458		0.0106
58	679.835-	1063.879	3s3d-3p3d	$^3D-^1F$	2-3	260.387		0.0021
59	564.597-	949.657	3p <sup>2</sup> -3p3d	$^3P-^1D$	1-2	259.700		0.0393
60	679.835-	1069.544	3s3d-3p3d	$^3D-^1P$	2-1	256.602		0.0052
61	559.605-	949.657	3p <sup>2</sup> -3p3d	$^1D-^1D$	2-2	256.376		0.7924
62	678.808-	1069.544	3s3d-3p3d	$^3D-^1P$	1-1	255.927		0.0014
63	581.699-	981.259	3p <sup>2</sup> -3p3d	$^3P-^3P$	2-1	250.275		0.0244
64	581.699-	981.385	3p <sup>2</sup> -3p3d	$^3P-^3P$	2-2	250.197		0.1416
65	659.667-	1069.544	3p <sup>2</sup> -3p3d	$^1S-^1P$	0-1	243.976		0.7620
66	351.932-	762.135	3s3p-3s3d	$^1P-^1D$	1-2	243.782	243.782 <sup>a</sup>	1.8612
67	581.699-	993.260	3p <sup>2</sup> -3p3d	$^3P-^3D$	2-1	242.978		0.1831
68	581.699-	994.940	3p <sup>2</sup> -3p3d	$^3P-^3D$	2-3	241.990		1.5437
69	581.699-	995.017	3p <sup>2</sup> -3p3d	$^3P-^3D$	2-2	241.945		0.7982
70	564.597-	981.259	3p <sup>2</sup> -3p3d	$^3P-^3P$	1-1	240.003		0.0611
71	564.597-	981.385	3p <sup>2</sup> -3p3d	$^3P-^3P$	1-2	239.930		0.9375
72	239.733-	659.667	3s3p-3p <sup>2</sup>	$^3P-^1S$	1-0	238.133		0.0033
73	559.605-	981.259	3p <sup>2</sup> -3p3d	$^1D-^3P$	2-1	237.161		0.0039
74	559.605-	981.385	3p <sup>2</sup> -3p3d	$^1D-^3P$	2-2	237.091		0.0046
75	253.809-	678.808	3s3p-3s3d	$^3P-^3D$	2-1	235.295		0.0150
76	253.809-	679.835	3s3p-3s3d	$^3P-^3D$	2-2	234.727		0.2260
77	554.502-	981.259	3p <sup>2</sup> -3p3d	$^3P-^3P$	0-1	234.325	234.79 <sup>a</sup>	0.6708
78	564.597-	991.572	3p <sup>2</sup> -3p3d	$^3P-^3P$	1-0	234.206		0.1874
79	253.809-	681.408	3s3p-3s3d	$^3P-^3D$	2-3	233.864	233.86 <sup>a</sup>	1.2619
80	564.597-	993.260	3p <sup>2</sup> -3p3d	$^3P-^3D$	1-1	233.284		0.4456
81	564.597-	995.017	3p <sup>2</sup> -3p3d	$^3P-^3D$	1-2	232.331		0.3337
82	559.605-	993.260	3p <sup>2</sup> -3p3d	$^1D-^3D$	2-1	230.598		0.0406
83	559.605-	994.940	3p <sup>2</sup> -3p3d	$^1D-^3D$	2-3	229.709		0.4467
84	559.605-	995.017	3p <sup>2</sup> -3p3d	$^1D-^3D$	2-2	229.668		0.1342
85	554.502-	993.260	3p <sup>2</sup> -3p3d	$^3P-^3D$	0-1	227.916		0.0068
86	239.733-	678.808	3s3p-3s3d	$^3P-^3D$	1-1	227.752	227.70 <sup>b</sup>	0.2306
87	239.733-	679.835	3s3p-3s3d	$^3P-^3D$	1-2	227.220	227.22 <sup>a</sup>	0.6943
88	233.875-	678.808	3s3p-3s3d	$^3P-^3D$	0-1	224.753	224.76 <sup>a</sup>	0.3137
89	581.699-	1063.879	3p <sup>2</sup> -3p3d	$^3P-^1F$	2-3	207.392		0.2484
90	581.699-	1069.544	3p <sup>2</sup> -3p3d	$^3P-^1P$	2-1	204.983		0.0013

Table 8. Continued

91	559.605-1063.879	$3p^2 - 3p3d$	$^1D-^1F$	2-3	198.305	0.8169
92	564.597-1069.544	$3p^2 - 3p3d$	$^3P-^1P$	1-1	198.041	0.0015
93	253.809- 762.135	$3s3p-3s3d$	$^3P-^1D$	2-2	196.724	0.0005
94	559.605-1069.544	$3p^2 - 3p3d$	$^1D-^1P$	2-1	196.102	0.0047
95	554.502-1069.544	$3p^2 - 3p3d$	$^3P-^1P$	0-1	194.159	0.0046
96	239.733- 762.135	$3s3p-3s3d$	$^3P-^1D$	1-2	191.423	0.0102
97	0.000-1069.544	$3s^2 - 3p3d$	$^1S-^1P$	0-1	93.498	0.0093

<sup>a</sup>Cowan *et al.*, (1973), ref.11).

<sup>b</sup>Fawcett (1971), ref.7).

<sup>†</sup>See text for detail.

Table 9 Calculated lifetimes (in nsec) for levels of the excited configurations in Fe XV.

Conf	Term	J	Energy	Lifetime*
3p <sup>2</sup>	<sup>3</sup> P	2	581.70	5.73(-2)
	<sup>3</sup> P	1	564.60	5.22(-2)
	<sup>3</sup> P	0	554.50	5.57(-2)
	<sup>1</sup> D	2	559.61	2.01(-1)
	<sup>1</sup> S	0	659.67	5.75(-2)
3s3d	<sup>3</sup> D	3	681.41	4.55(-2)
	<sup>3</sup> D	2	679.84	4.27(-2)
	<sup>3</sup> D	1	678.81	4.11(-2)
	<sup>1</sup> D	2	762.14	2.37(-2)
3s3p	<sup>3</sup> P	2	253.81	----
	<sup>3</sup> P	1	239.73	1.97(+1)
	<sup>3</sup> P	0	233.88	----
	<sup>1</sup> P	1	351.93	4.22(-2)
3p3d	<sup>3</sup> F	4	949.66	1.68(-1)
	<sup>3</sup> F	3	938.19	1.79(-1)
	<sup>3</sup> F	2	928.45	1.57(-1)
	<sup>3</sup> D	3	994.94	2.34(-2)
	<sup>3</sup> D	2	995.02	2.51(-2)
	<sup>3</sup> D	1	981.26	2.54(-2)
	<sup>3</sup> P	2	981.39	2.98(-2)
	<sup>3</sup> P	1	993.26	2.67(-2)
	<sup>3</sup> P	0	991.57	3.00(-2)
	<sup>1</sup> F	3	1063.88	2.22(-2)
	<sup>1</sup> D	2	949.66	4.98(-2)
	<sup>1</sup> P	1	1069.54	2.19(-2)

\*Figures in parentheses are the power of 10 by which the preceding number should be multiplied.

Table 10 Calculated reduced electric dipole radial integrals (in atomic units) in Fe XV.

Transition		Reduced E1 integral
3s <sup>2</sup>	- 3s3p	(3s:R1:3p)= 0.6759
3s3p	- 3p <sup>2</sup>	(3s:R1:3p)=-0.6762
	- 3s3d	(3p:R1:3d)=-0.8671
3p <sup>2</sup>	- 3p3d	(3p:R1:3d)= 0.8688
3s3d	- 3p3d	(3s:R1:3p)= 0.6765



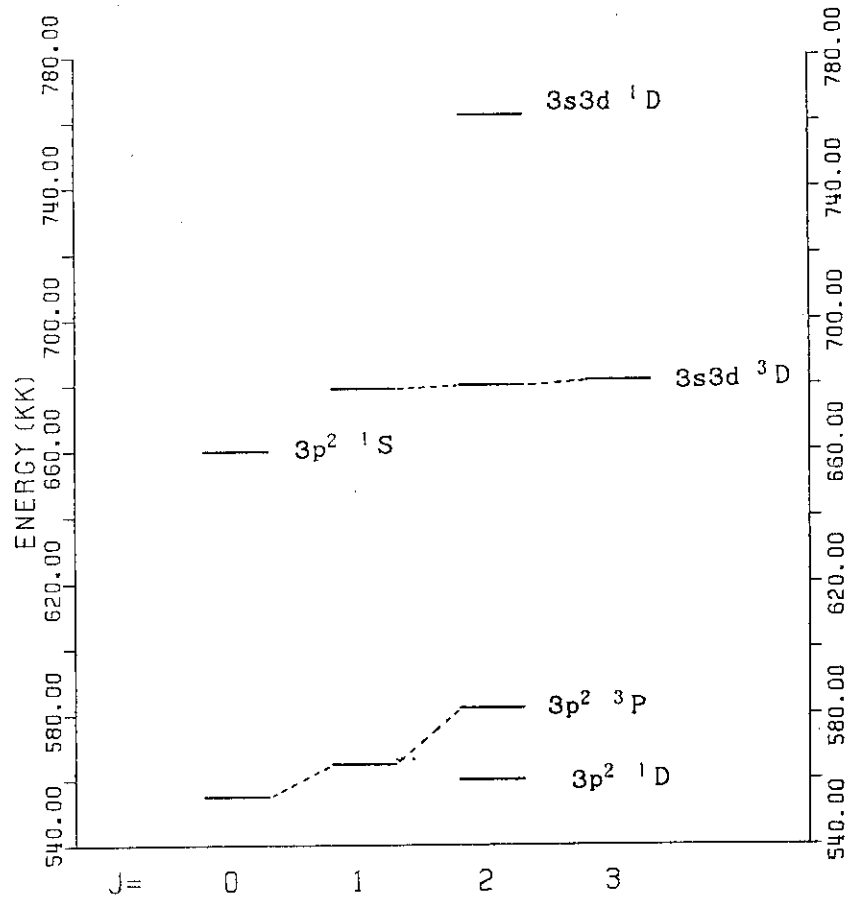


Fig.1 Calculated energy level diagram of  $3p^2$  (B) and  $3s3d$  (C) configurations of the first parity in Fe XV. Energy is in  $10^3 \text{ cm}^{-1}$ .

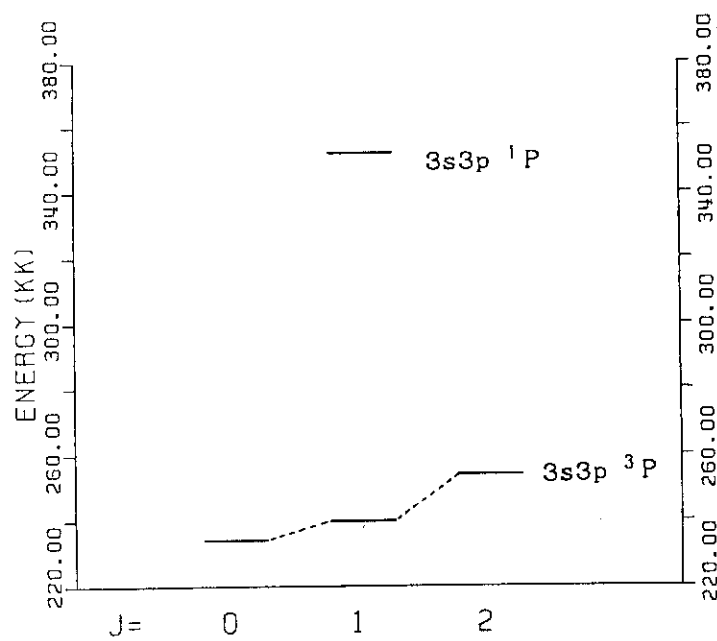


Fig.2 Calculated energy level diagram of  $3s3p$  configuration of the second parity in Fe XV. Energy in  $10^3 \text{ cm}^{-1}$ .

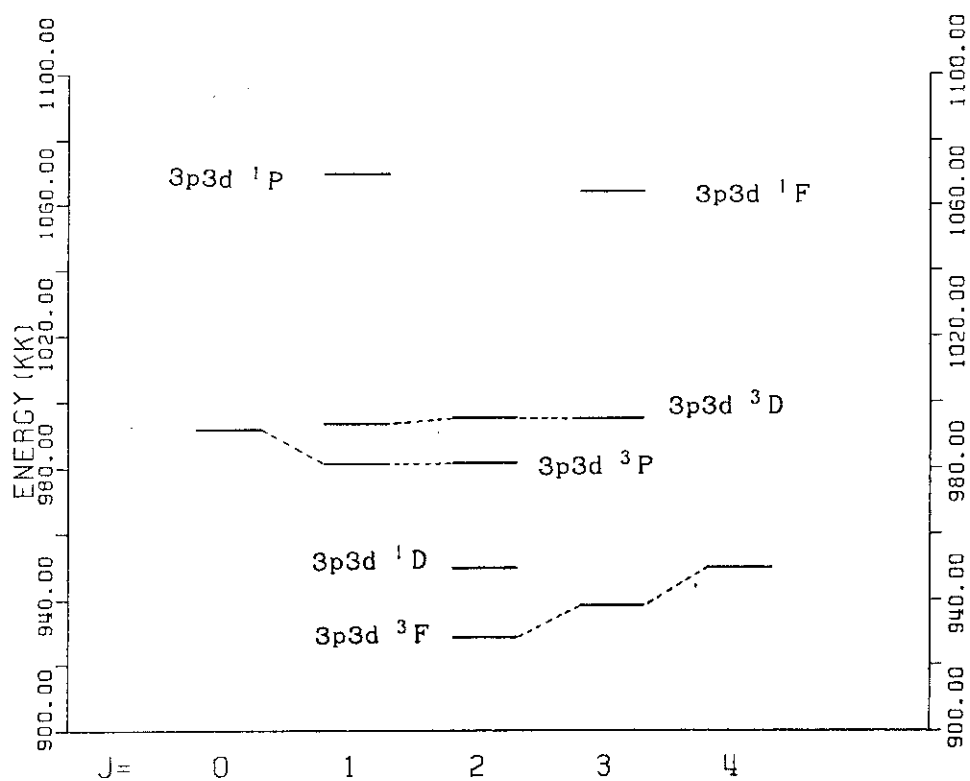


Fig.3 Calculated energy level diagram of 3p3d configuration of the the second parity in Fe XV. Energy in  $10^3 \text{ cm}^{-1}$ .

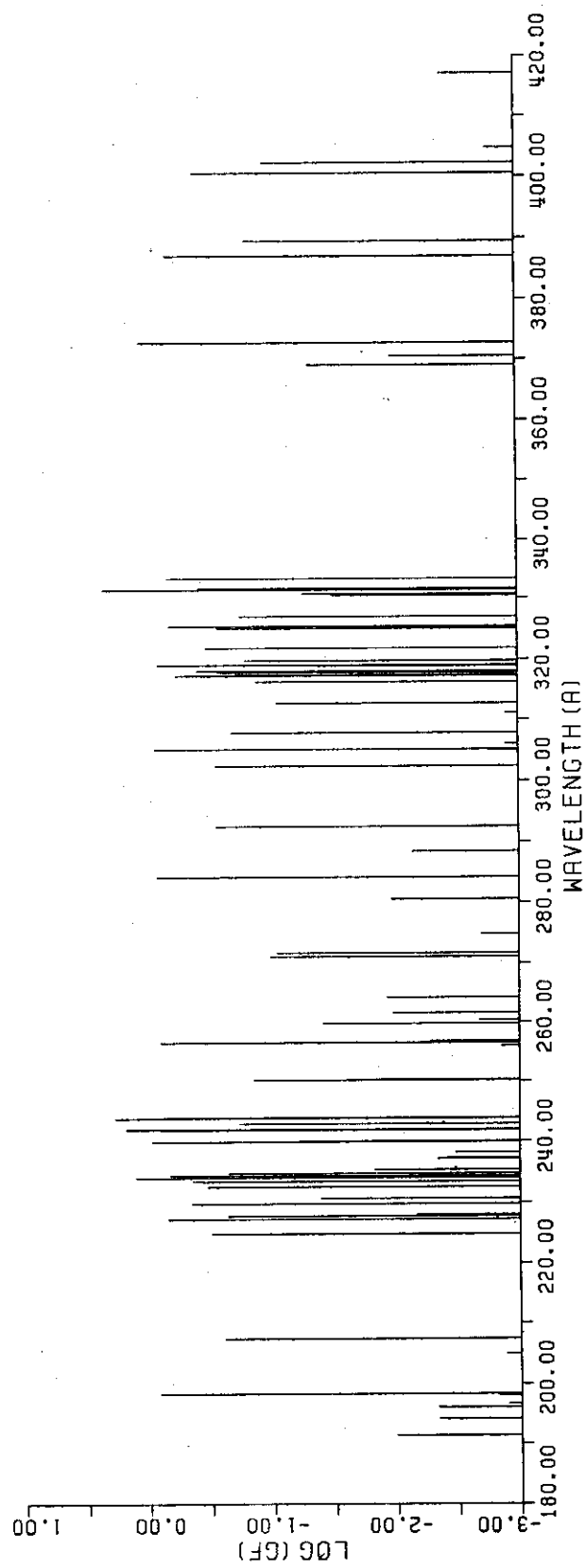


Fig.4. Calculated line pattern for the transitions in Fe XV, reproduced from Table 8.

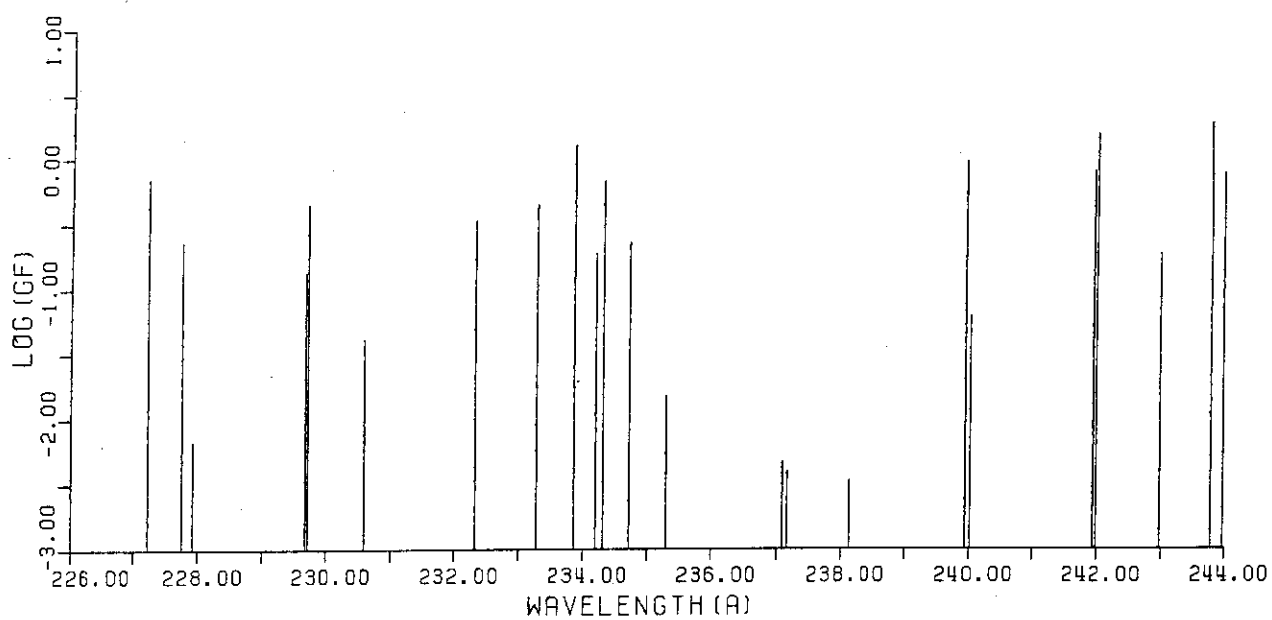


Fig.5 Enlarged partial line pattern in the wavelength range 226 to 244 Å .

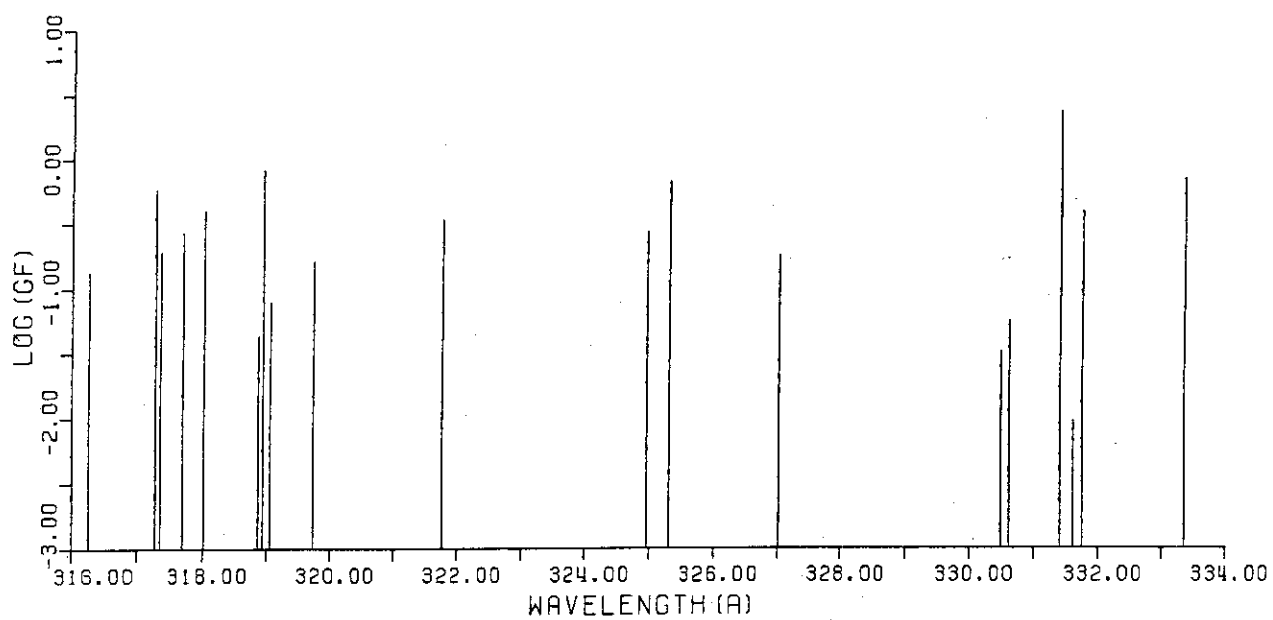


Fig.6 Enlarged partial line pattern in the wavelength range 316 to 334 Å .

