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National Aeronautics and Space Administration
Goddard Space Flight Center
Contract No.NAS-5-12487

ST – SPC – NP – 10819

ON THE RELATIVE INTENSITY OF ION FE XVII LINES
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EFFECTIVE EXCITATION CROSS SECTIONS
OF INTERCOMBINATIONAL TRANSITIONS INTO HELIUM AND FE XVII

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25 MARCH 1969

ST – SPC – NP – 10819

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Preprint No.120
Spectroscopy Laboratory
The Lebedev Institute of Physics
of the USSR Academy of Sciences
Moscow, 1968.

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ABSTRACT

The line intensity ratios $I(2p^5 3s - 2p^6)/\ I(2p^5 3d - 2p^6)$ of Fe XVII in the solar corona are computed with the aid of the Coulomb-Born approximation with exchange included. It is shown that the great intensity of lines from the 3s-configuration is due to cascade radiation processes from levels of 3p and 3d- $(j \neq 1)$ configurations. Exchange excitation and excitation of s-electrons yields a considerable population to these levels. The estimated ratio ~ 1.2 is in accord with the experimental one of ~ 1.3 obtained in [1].

From comparison of theoretical line intensity ratios of transitions $3d - 3p$ with the experimental ones [1], it is found that the 3d-configuration can be described by the scheme of $j - j$-coupling.

The intercombination transitions cross-sections in He and Fe XVII are computed with the aid of the orthogonality functions method [5]. The results are discussed and comparison is made with the experiments of [12 - 13]. The errors and misprints of work [5] are corrected.

* *

1. The intensities of lines corresponding to transitions from configurations $2p^5 3s$ and $2p^5 3d$ into ground state of ion Fe XVII in the solar corona were measured in the work [1]. (The qualitative estimates of these lines' relative intensity for spark spectra [2, 3] agree well with the result of [1]).

The relative intensity of lines (3s −2p) and (3d −2p) then is :

$$\frac{I_{3s}}{I_{3d}} = \frac{I(2p^5 3s - 2p^6)}{I(2p^5 3d - 2p^6)} \simeq 1.$$

This result is quite surprising, for the excitation cross section of transition (2p − 3s) is by two orders smaller than (2p − 3d).

It is shown in the present work that the high intensity of lines with configurations 3s is due to cascade radiation processes through the configuration levels 3p and 3d, optically not connected with the ground state.

The exchange effects and the excitation of electrons from the s-shell play an essential role in the population of these levels.

The de-excitation on account of collision with electrons may be neglected since in conditions of solar corona the probability of such a process is less than the probability of radiation decay.

To begin with, we shall consider the aggregate intensity of transition (3d − 2p). The 3d-configuration includes three levels optically connected with the ground state (total momentum j = 1, see Fig.1). It is evident that the aggregate intensity of these three lines will be:

$$I_{3d-2p} = \hbar\omega \, N_z \, N_e \left[\langle v\sigma^{(j=1)}_{2p-3d} \rangle + \alpha^{(j=1)} \langle v\sigma_{2s-3d} \rangle \right]$$

$$\alpha^{(j=1)} = \frac{A^{(j=1)}}{\sum_j A^{(j)}}$$

where ω is the transition frequency, N_z is the concentration of Fe XVII ions in the ground state, N_e is the density of electrons, $\langle v\sigma^{(j=1)}_{2p-3d} \rangle$ (*) is the aggregate excitation rate of levels with j = 1, $\langle v\sigma_{2s-3d} \rangle$ is the excitation rate of levels with configuration $2s2p^6 3d$ with total momentum j.- $A^{(j)}$ is the probability of radiation decay of configuration $2s2p^6 3d$ to configuration level $2s^2 2p^5 3d$ with total momentum j. The probability of transition ($2s2p^6 3d$ − − $2s2p^6 3p$) is negligibly small by comparison with that of ($2s2p^6 3d - 2s^2 2p^5 3d$).

(*) Here and below we shall consider the distributions by velocities as Maxwellian.

For the considered case the coefficient $\alpha^{(j=1)}$ is simply reduced to the ratio of statistical weights and is equal to 3/20. Thus, the basic mechanism of these levels' population is the excitation of p-electron from the ground state by electron impact.

The aggregate line intensity of the transition (3s – 3p) (see Fig.1) is:

$$I_{3s-2p} = \hbar\omega \cdot N_z \cdot N_e \left[\langle v\sigma_{2p-3s}\rangle + \langle v\sigma_{2s-3s}\rangle + \right.$$
$$\left. + \langle v\sigma_{2p-3p}\rangle + \alpha^{3p}\langle v\sigma_{2s-3p}\rangle + \langle v\sigma^{(j\neq 1)}_{2p-3d}\rangle + \alpha^{(j=1)}\langle v\sigma_{2s-3d}\rangle\right],$$

$$\alpha^{(3p)} = \frac{A(2s2p^6 3p - 2s^2 2p^5 3p)}{A(2s2p^6 3p - 2s^2 2p^5 3p) + A(2s2p^6 3p - 2s^2 2p^6)} \tag{2}$$

$$\alpha^{(j\neq 1)} = \frac{\sum A^{(j\neq 1)}_{(2s2p^6 3d - 2s^2 2p^5 3d)}}{\sum_j A^{(j)}_{(2s2p^6 3d - 2s^2 2p^5 3d)}}$$

Since the probability of transition $2s2p^6 3p - 2s^2 2p^6$ is much greater than that of transition $2s2p^6 3p - 2s^2 2p^5 3p$, we may neglect the term $\alpha^{(3p)}\langle v\sigma_{2s-3p}\rangle$. The coefficient $\alpha^{(j\neq 1)} = 1 - \alpha^{(j=1)} \simeq 1$ (see above).

2. The excitation cross sections were computed in the Coulomb-Born approximation; the amplitude of exchange scattering was calculated according to the method used in [5]. At the same time, single-electron, semi-empirical wave functions were utilized [6]. The rates of elementary processes, averaged by Maxwellian distribution of electrons by energies, were computed with the help of the obtained cross sections. Following were the approximated formulas for the description of the dependence of $\langle v\sigma\rangle$ on temperature [7]:

$$\langle v\sigma\rangle = 10^{-8}\left(\frac{E_1}{E_0}\cdot\frac{Ry}{\Delta E}\right)^{3/2}\frac{g}{2l_0+1}A\sqrt{\beta}\,\frac{\beta+1}{\beta+\chi}\cdot e^{-\beta} \tag{3}$$

for transitions without spin variation, and

$$\langle v\sigma\rangle = 10^{-8}\left(\frac{E_1}{E_0}\cdot\frac{Ry}{\Delta E}\right)^{3/2}\frac{g}{2l_0+1}\cdot A\cdot\beta^{1/2}\frac{1}{\beta+\chi}e^{-\beta} \tag{3a}$$

for the intercombinational transitions.

Here $\beta = {}^{\Delta E}/_{kT}$, q is the number of equivalent electrons, E_0 and E are respectively the energies of atoms' lower and upper levels, computed from the ionization boundary. Parameters A and χ were determined by the method of least squares by numerical values of $\langle v\sigma \rangle$.

It is easy to see that the aggregate excitation cross section of all levels with the given j is independent of the type of coupling (*). The LS-coupling was practically used in the computations.

The results of calculations are compiled in Table 1 hereafter :

TABLE 1

TRANSITION	A	χ	Formula for the approximation	Levels providing the main contribution	ANNOTATION
2p — 3d (j = 1)	36	0.35	(3)	$^1P_1$ (A = 35.2)	During the computation of partial intercombinational cross sections, considered was the minimum of the possible multipolarities.
2p — 3d (j ≠ 1)	12	0.61	(3a)	^3P, ^3D, ^3F (A = 9.1)	
2p — 3p	21	0.93	(3)	^1S A = 18)	
2p — 3s	1.3	0.4	(3a)	^3S, ^3P, ^3D (A = 0.69)	
2s — 3d	12	0.61	(3)	^1D (A = 9.3)	
2s — 3p	3	0.1	(3)	^1P (A = 2.9)	
2s — 3s	5.2	0.96	(3)	^1S (A = 4.9)	

It may directly be seen from the above Table 1 that the population of levels with configuration $2s^2 2p^5 3d$ and j ≠ 1 is basically determined by exchange effects; they are also responsible for the increase of the cross section of excitation of the $2s^2 2p^5 3p$ - configuration (by ~ 25-30%) and the decrease for the $2s^2 2p^5 3d$ (j = 1) configuration by ~ 10%.

(*) This follows from the unitarity condition of the coefficients of expansion of function Ψ_r by functions Ψ_r/γ and on Γ-assortments of quantum numbers corresponding to pure types of vectorial coupling $\sum_\gamma a_r^\gamma a_{r'}^\gamma = \delta_{rr'}$ and further $\sum_r \sigma_r \sim \sum_\gamma |\sum_r a_r^\gamma f_r|^2 = \sum_\gamma |f_\gamma|^2 \sim \sum_\gamma \sigma_\gamma$ where $\Psi_\gamma = \sum_r a_r^\gamma \Psi_r$, and fr is the amplitude of process' probability.

The obtained data allow us to estimate the ratio of line intensities with configurations $2s^2 2p^5 3s$ to $2s^2 2p^5 3d$. Inasmuch as the distance between levels 3s and 3d is much less than kT, this ratio is practically independent of the temperature:

$$\frac{I_{3s}}{I_{3d}} \simeq 1.2. \tag{4}$$

Taking into account the experimental error and also the fact that the influence of levels with $n \geqslant 4$ was omitted in the calculations ($\underline{n}$ being the main quantum number), the agreement with experiment must be considered as satisfactory. The contribution to line intensity from photorecombination and dielectron recombination processes is negligibly small, as was shown by numerical estimates.

3. The intensities of three lines of transition 3d - 2p are also brought out in work [1]. This allows us to derive certain conclusions on the type of coupling in configuration 3d.

Compiled in Table 2 are the calculation for the relative intensity of these lines in different types of coupling for the excited state (the ground state is described by the LS-coupling).

TABLE 2

Type of coupling	Exp. [1]	L – S	j – l	j – j	Intermediate couplings [10]
15.012 A	0.62	$^1S \leftarrow {}^3D_1$ 0.02	$^1S \leftarrow {}^2P_{3/2}[3/2]$ 0.33	$^1S \leftarrow (3/2, 5/2)$ 0.6	0.76
15.26 A	0.38	$^1S \leftarrow {}^1P_1$ 1	$^1S \leftarrow P_{3/2}[3/2]$ 0.33	$^1S \leftarrow (1/2, 3/2)$ 0.33	0.23
15.45 A	0.1	$^1S \leftarrow {}^3P_1$ 0.01	$^1S \leftarrow P_{3/2}[3/2]$ 0.33	$^1S \leftarrow (3/2, 3/2)$ 0.07	0.01

It may be seen from Table 2 that the configuration 3d is described by the j - j coupling with good precision.

***

Effective Excitation Cross Sections of Intercombinational Transitions into He and Fe XVII

According to work [5], the effective excitation cross section for intercombinational transitions has the form (subscripts 0 and 1 denote respectively the initial and final states) (*) :

$$\sigma = \pi a_0^2 \frac{16}{K_0^2} \sum_{\lambda_0 \lambda_1 L_T}' \Big| \sum_{\varkappa}' b_\varkappa B_{\varkappa L_T} R_\varkappa \Big|^2 ;$$

$$b_\varkappa = \left[\frac{(2\ell_1+1)(2\ell_0+1)(2\lambda_1+1)}{(2\varkappa+1)} \right]^{1/2} \begin{pmatrix} \ell_0 & \varkappa & \ell_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0 & \varkappa & \ell_1 \\ 0 & 0 & 0 \end{pmatrix} ;$$

$$B_{\varkappa L_T} = \sqrt{N}\, G^{S_0 L_0}_{S_p L_p} \left[\frac{(2S_1+1)(2L_1+1)(2\varkappa+1)(2L_T+1)(2\ell_0+1)}{2(2S_p+1)} \right]^{1/2} \times \begin{Bmatrix} \lambda_0 & \ell_1 & \varkappa \\ L_0 & L_p & \ell_0 \\ L_T & L_1 & \lambda_1 \end{Bmatrix} ; \qquad (5)$$

$$R_\varkappa = \iint dr_1\, dr_2\, P_0(r_1)\, g_{\lambda_0}(r_2) \frac{r_<^\varkappa}{r_>^{\varkappa+1}} P_1(r_2)\, g_{\lambda_1}(r_1) ;$$

$$g_{\lambda_0} = F_{\lambda_0} - \langle F_{\lambda_0} | P_1 \rangle P_1 \, \delta_{\lambda_0 \ell_1} ;$$

$$g_{\lambda_1} = F_{\lambda_1} - \langle F_{\lambda_1} | P_0 \rangle P_0 \, \delta_{\lambda_1 \lambda_0} ;$$

where $G^{S_0 L_0}_{S_p L_p}$ is a genealogical coefficient, K and λ denote the impulse and the momentum of the outer electron, P(r) is a radial function of optical electron ion, N is the number of equivalent electrons, $F_\lambda(r)$ is a Coulomb radial function, whereupon

$$F_\lambda(r) \xrightarrow[r \to \infty]{} 1/\sqrt{K}\, \sin\!\left(Kr + \frac{Z}{K} \ln 2ZKr + \delta\right).$$

For the cross-section summed up along L_1 , formulas (5) admit substantial simplifications and may be written in the form:

$$\sigma = N \frac{2S_1+1}{2(2S_p+1)} \sum_{\lambda_0 \lambda_1}' \sigma_{\lambda_0 \lambda_1} ;$$

$$\sigma_{\lambda_0 \lambda_1} = \pi a_0^2 \frac{16}{K_0^2} \sum_{\varkappa}' | b_\varkappa R_\varkappa |^2 . \qquad (6)$$

(*) Correction for work [5]: In formula (8) $\frac{2\pi^3}{K_1 K_0}$ should be substituted for $\frac{2\pi^3 K_0}{K_1}$.

Compiled in Table 3 are the cross sections of transitions $1s^{2\,1}S - 1s2s\,^3S$ and $1s^{2\,1}S - 1s2p\,^3P$ in the Helium atom (*), computed according to (5) and the Ochkur method [11]. For great energies the quantity $\sigma\cdot(E/\Delta E)^3$ must approach a constant limit. According to the experiment of [12], for the transition $1s - 2s\ ^3S$, this constant must be equal to 0.1, and for 1s - 2p [13] to ~ 0.3.

It should be noted that the quantity $\sigma\cdot(E/\Delta E)^3$, computed by formulas (5) for transitions 1s - 2s and 1s - 2p, has a maximum for $E/\Delta E \sim 3$. This should apparently be related to method's [5] shortcoming.

The effective intercombinational transitions in the ion Fe XVII are compiled in Table 4.

The authors acknowledge L. A. Vaynshteyn's discussion of the work.

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CONTRACT No.NAS-5-12487
VOLT INFORMATION SCIENCES, INC.
1145 - 19th St.NW
WASHINGTON D.C. 20036.
Telephone: (202) 223-6700 (X-36).

Translated by ANDRE L. BRICHANT
on 24 - 25 March 1969

(*) The numerical calculations by orthogonalized functions' method in [5] are beset with errors.

TABLE 3

$\sqrt{\frac{E-\Delta E}{\Delta E}}$	$1s-2s$				$1s-2p$			
	σ		$\sigma\cdot(E/\Delta E)^3$		σ		$\sigma\cdot(E/\Delta E)^3$	
	Ort.	[11]	Ort.	[11]	Ort.	[11]	Ort.	[11]
0,1	−2 34	−2 89	−2 34	−2 99	−1 32	−1 31	−1 32	−1 31
0,2	−2 72	−1 17	−2 38	−2 98	−1 54	−1 55	−1 60	−1 62
0,4	−1 13	−1 30	−1 20	−1 47	−1 69	−1 73	0 10	0 11
0,8	−2 60	−1 27	−1 27	0 12	−1 48	−1 40	0 21	0 18
1,6	−2 16	−2 50	0 72	0 22	−2 98	−2 48	0 44	0 21
3.2	−3 24	−3 18	0 34	0 25	−3 25	−3 15	0 35	0 21
6,4	−5 46	−5 38	0 35	0 27	−5 49	−5 38	0 35	0 27

TABLE 4

$\sqrt{\frac{E-\Delta E}{\Delta E}}$	$2p-3s$	$2p-3p$	$2p-3d$
0,1	1 69	2 26	2 63
0,2	1 64	2 24	2 60
0,4	1 53	2 20	2 46
0,8	1 27	2 10	2 19
1,6	0 43	1 17	1 22
3,2	−1 18	−1 59	−1 78
	0 92	1 42	2 13
	0 39	0 37	0 61

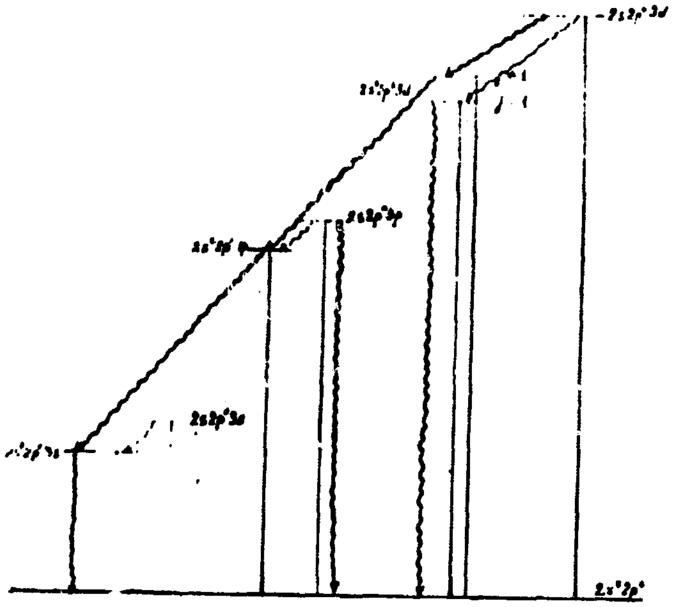

Fig.1 (*)

(*) [Fig.1, just as most of formulas in the text had to be reproduced as such, since they are just as difficult to read in the original preprint].