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Configurations $3d^n 4p + 3d^{n-1} 4s4p$ in Sc II, Ti II, and V II*

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Experimental levels of the configurations $3d^n4p+3d^{n-1}4s4p$ for Sc II, Ti II, and V II were compared with corresponding calculated values. Electrostatic, spin-orbit interactions, as well as the α, β and T corrections, whenever possible, were considered for $3d^n4p$ and $3d^{n-1}4s4p$. The electrostatic interaction between the configurations $3d^n4p$ and $3d^{n-1}4s4p$ was included explicitly. The rms errors for Sc II, Ti II and V II were 4.6, 75 and 66 cm^{-1}, respectively.

Key words: Configurations $3d^n4p+3d^{n-1}4s4p$; energy levels; interaction between configurations; iron group; second spectra.

1. Introduction

The configurations $(3d+4s)^n$ in the second spectra of the iron group were considered by Racah and Shadmi [1].[2] Individual and general treatments including the α, β, and T corrections were performed for the configurations $3d^n4p$ of the third and second spectra of the iron group by the author [2, 3].[3]

The results for the configurations d^np in the third spectra of the iron group indicate that there the interactions with the configurations $d^{n-1}sp$ are weak [2]. Thus good agreement was obtained between the theoretically predicted levels and experimental levels without taking into consideration the configurations $d^{n-1}sp$. However, the configurations d^np in the second spectra, and especially those on the left side of the periodic table are strongly perturbed by the configurations $d^{n-1}sp$. [3].

The algebraic matrices for the configurations $(d+s)^np$ were put on tape and checked by the author. Unfortunately these matrices could not be used to study systematically the configurations $(3d+4s)^n4p$ here, since the experimental data for the configuration $3d^{n-1}4s4p$ is very scarce and nonexistent for $3d^{n-2}4s^24p$, [4]. Thus it is feasible to consider the configurations $3d^n4p+3d^{n-1}4s4p$ and these only for Sc II, Ti II, V II, and Cu II. In the last case other interaction besides $3d^n4p-3d^{n-1}4s4p$ must be taken into consideration. This problem will be investigated in a future paper.

The parameters A, B, C, F_2, G_1, G_3, α, β, T, ζ_d and ζ_p refer to the configurations d^np. The same parameters primed refer to the configurations $d^{n-1}sp$. The parameters G_{ds} and G_{ps} refer to the interactions d-s and p-s in the configuration $d^{n-1}sp$.

$$G_{ds}=\frac{1}{5}\,G^2(ds)=\frac{R^2(ds,\,sd)}{5}$$

$$G_{ps}=\frac{1}{3}\,G^1(ps)=\frac{R^1(ps,\,sp)}{3}.$$

The parameters of the electrostatic interaction between the configurations d^np and $d^{n-1}sp$ are denoted by H, J, and K

$$H=\frac{R^2(dd,\,ds)}{35}$$

$$J=\frac{R^2(dp,\,sp)}{5}$$

$$K=\frac{R^1(dp,\,ps)}{3}.$$

In Sc II $-3d4p+4s4p$, there are eight terms determined by eight electrostatic parameters, i.e., A, F_2, G_1, G_3, A', G_{ps}, J, and K. Thus the problem is solved mathematically, but the parameters may absorb interactions with other configurations, and thus give a distorted representation of the configuration $3d4p+4s4p$. Hence the parameters of Sc II cannot be considered as being very reliable for use as the starting parameters of Ti II. In Ti II there is an inherent instability if in the core d^2+ds the term $d^2\,{}^1S$ is missing. This is due to the fact that there are then six terms in d^2+ds with the seven electrostatic parameters A, B, C, α, A', G_{ds} and H to determine them. Even if α is held fixed at the value obtained for Ti II from the general least squares of d^np, the values of the other parameters cannot be considered as reliable enough to be used for the next spectrum, V II. On the other hand, in V II $-3d^34p+3d^24s4p$ there are many more terms than electrostatic parameters. It is thus theo-

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[2] Figures in brackets indicate the literature references at the end of this paper.

[3] The reader is referred to the above papers for an explanation of the method used, notation and significance of the various parameters pertaining to d^np.

retically most stable and for this reason it was investigated first.

2. V II $-3d^34p+3d^24s4p$

2.1. Initial Parameters

The starting values of the parameters B, C, F_2, G_1, G_3, α, ζ_d and ζ_p were taken from the configurations d^np of the second spectra, [3]. By making the initial approximation that the values of the above parameters are the same for the configurations d^3p and d^2sp we obtain the following values from the variation of the general least squares where β and T are eliminated:

$$
\begin{aligned}
B&=B'=750\\
C&=C'=2600\\
F_2&=F_2'=310\\
G_1&=G_1'=330\\
G_3&=G_3'=30\\
\alpha&=\alpha'=64\\
\beta&=\beta'=0\\
T&=T'=0\\
\zeta_d&=\zeta_d'=200\\
\zeta_p&=\zeta_p'=260
\end{aligned}
$$

Since G_{ds} represents the interaction of the electrons d and s in the core d^2s, its approximate value can be taken from V III $-d^3+d^2s$. From Shadmi [5], we obtain

$$G_{ds}=1750.$$

A starting value for the parameter G_{ps} is obtained from the interpolation of $G_{ps}(sp)$ and $G_{ps}(d^{10}sp)$. From AEL, Vol. **I**, the center of gravity of $4s(^2S)4py\,^3P$ in Sc II is 39230 cm^{-1} and $4s(^2S)4py\,^1P$ in Sc II is 55716 cm^{-1}. Thus,

$$G_{ps}(sp)=8243.$$

A similar calculation for Ga II $-3d^{10}4s4p$ yields

$$G_{ps}(d^{10}sp)=11212.$$

Thus by interpolation

$$G_{ps}(d^2sp)=8837.$$

Shadmi [5] found that the interaction between the configurations d^n and $d^{n-1}s$ in the third spectra was too weak to determine the value of the parameter H. He thus let H equal to zero for all the spectra of the third row. Furthermore, in the configurations d^np and $d^{n-1}sp$ the relative phase of H with respect to J and K is not known. Thus as a starting point we also let H equal to zero.

The initial values for J and K are obtained from Sc II $-3d4p+4s4p$. The electrostatic interaction matrix for ^1P is given by

$$\begin{pmatrix} X & -\sqrt{2}(K+J) \\ -\sqrt{2}(K+J) & Y \end{pmatrix}.$$

Here X is the unperturbed level $dp\,^1P$. Its value can be taken as the calculated level of $dp\,^1P$, Sc II, in the GLS of d^np. Then from table 12, [3]

$$X=32115.$$

From AEL, [4], the experimental value for the level $dp\,^1P$, Sc II, is 30816. Thus the level $dp\,^1P$ is lowered by 1299 due to the interaction with $sp\,^1P$. Similarly the unperturbed value of the level $sp\,^1P$ is lower by 1299 than the experimental value of $sp\,^1P$, at 55716. Since Y represents the value of the unperturbed level $sp\,^1P$,

$$Y=55716-1299=54417.$$

The eigenvalues λ_1 and λ_2 of the electrostatic interaction matrix of ^1P are simply the experimental levels $dp\,^1P$ and $sp\,^1P$ at 30816 and 55716, respectively.

We thus obtain

$$J+K=\pm 3915.$$

For the case of ^3P the electrostatic interaction matrix is

$$\begin{pmatrix} x & \sqrt{2}(K-J) \\ \sqrt{2}(K-J) & y \end{pmatrix}.$$

Performing a similar calculation as for ^1P and using values for the center of gravity yields

$$K-J=\pm 1660.$$

From the above values for the sum and difference of K and J it is not possible to solve for these parameters uniquely. All four possibilities were considered by performing four different diagonalizations with all the parameters except J and K having the same values in all diagonalizations. From the least squares calculations it was evident that both J and K must be positive and that $K>J$. This result is in agreement with the values of J and K obtained by Z. B. Goldschmidt in the rare-earth spectra [6].

Thus the following values of J and K were taken for the first diagonalization of V II,

$$J=1100, \qquad K=2800.$$

In order to obtain starting values for the parameters A and A' those terms whose electrostatic interaction matrix elements are of order two, here ^5F and ^5G, are considered. Since all the levels of $3d^24s(b^4F)4py\,^5G$ are given as uncertain in AEL, [4], ^5G is neglected.

The electrostatic interaction matrix of ^{5}F is given by

$$\begin{pmatrix} A-15B+3F_2-6G_1-26G_3+12\alpha & \frac{-3\sqrt{5}}{5}(K-J) \\ \frac{-3\sqrt{5}}{5}(K-J) & A'-8B'-2G_{ds}-3F_2'-G_1'-16G_3'-G_{ps}+12\alpha' \end{pmatrix}$$

Using the values of the parameters already found the above matrix becomes

$$\begin{pmatrix} A-12312 & \frac{-3\sqrt{5}}{5}(1700) \\ \frac{-3\sqrt{5}}{5}(1700) & A'-19309 \end{pmatrix}$$

From AEL [4], the centers of gravity of $3d^3(a\,^4F)4pz\,^5F$ and $3d^24s(b\,^4F)4py\,^5F$ are 37042 and 63972 cm^{-1} respectively. By evaluating the sum and difference of the eigenvalues of the above matrix we obtain

$$A=49550 \quad \text{and} \quad A'=83090$$

2.2. Results

The configuration d^3p comprises 48 theoretical terms splitting into 110 levels. In d^2sp there are 38 terms splitting into 90 levels. In AEL, 41 terms splitting into 101 levels are assigned to the configuration V II $-d^3p$ and 9 terms splitting into 27 levels are assigned to V II $-d^2sp$. In addition, there are 7 odd experimental levels without definite configuration assignments. Of the 135 experimental levels which may be fitted to d^3p+d^2sp the following 12 levels were neglected:

1. The level 1_4° at 62762.
2. The five levels of $3d^24s\ (b\,^4F)\ 4py\,^5G$.
3. The level $3d^24s\ (b\,^2G)\ 4p\ x\,^1H$.
4. The level $3d^24s\ (b\,^2G)\ 4p\ w\,^1G$.
5. The level $3d^24s\ (b\,^2G)\ 4p\ w\,^1F$.
6. The level $u\,^3F_4$ at 76644.
7. The level 2_3° at 76405.
8. The level $w\,^1D$ at 78791.

Of the 123 levels fitted it was necessary to make the following changes in assignment:

1. $3d^3\ (a\,^2P)4px\,^3D \leftrightarrow 3d^3(a\,^4P)4py\,^3D$.
2. $3d^3\ (a\,^2D)4py\,^1P \leftrightarrow 3d^3\ (a\,^2P)4pz\,^1P$.
3. AEL $3d^3\ (c\,^2D)\ 4pt\,^3D_{1,2,3}? \rightarrow 3d^2(^1D)4s4p(^3P)^3D$.
4. AEL $u\,^3F_{2,3} \rightarrow 3d^2(^3P)4s4p\ (^3P)\ ^5P$.

In addition, the following pairs of terms were strongly mixed:

1. $3d^3(a\,^4F)4pz\,^5F_{1,2,3}$ and $3d^3(a\,^4F)4pz\,^3D_{1,2,3}$.
2. $3d^3(a\,^4P)4pz\,^3P_{0,1,2}$ and $3d^3(a\,^4P)4py\,^5D_{0,1,2}$.
3. $3d^3(^2H)4px\,^3G_3$ and $3d^3(a\,^2D)4py\,^1F_3$.

The 123 levels were fitted by means of 16 free electrostatic parameters and 3 free spin-orbit parameters to yield a rms error of only 66. The following parameters were obtained in the least squares of the final iteration:

$$\begin{aligned}
A&=51096\pm74\\
A'&=82727\pm119\\
B=B'&=792\pm2\\
C=C'&=2746\pm12\\
G_{ds}&=1820\pm25\\
F_2&=339\pm2\\
F_2'&=392\pm10\\
G_1=G_1'&=360\pm2\\
G_3=G_3'&=30\pm1\\
G_{ps}&=7900\ (\text{fix})\\
\alpha&=32\pm2\\
\alpha'&=77\pm10\\
\beta=\beta'&=-179\pm66\\
T=T'&=-3.8\pm0.3\\
H&=86\pm7\\
J&=1011\pm72\\
K&=3288\pm58\\
\zeta_d&=171\pm10\\
\zeta_d'&=197\pm15\\
\zeta_p=\zeta_p'&=262\pm20\\
\Delta&=66.
\end{aligned}$$

As G_{ps} is much larger than G_{ds} the interaction p–s is stronger than the interaction d–s. Thus, the levels of the configuration d^2sp are coupled as $d^2\ (v_1S_1L_1)\ sp\ (^{1,3}P)\ SL$ and not $d^2s\ (S_2L_1)p\ SL$, as given in AEL.

In the variation of the least squares from which the above parameters were taken the sum of the squares of the deviations dropped only from 483, 520 to 454, 850. Thus, no further iteration was required.

2.3. Discussion

Of the 12 levels neglected, 3 could be fitted with deviations much larger than the rms error of 66, whereas the other 9 levels definitely have no place in the configurations d^3p+d^2sp.

All the five levels of the term $3d^24s(b\,^4F)4py\,^5G$ are given as uncertain in AEL. In addition all the combinations of $y\,^5G$ with even levels are given with a question mark in the original paper of Meggers and Moore [7]. In the initial diagonalization the mean difference between the experimental and theoretical levels of $d^2s(^4F)y\,^5G$ was over 4000. This value is much higher than for the other levels and so immediately the levels of $y\,^5G$ were neglected.

The level 1_4° at 62762 could be fitted to $d^3(^2F)p\,^3F_4$ with a deviation of 310. However, as this deviation is almost five times the rms error and there is no experimental g value, it was decided not to include this level.

The levels $3d^24s(^2G)4p$ [^1H, ^1G, and ^1F] are theoretically at 98370, 96020, and 102680, respectively. Thus, the assignments given in AEL are definitely not correct for these levels. The level $w\,^1H$ at 70936 cannot be assigned to any level of J equal to 5. The closest calculated level to $w\,^1G$ for J equal to 4 is $d^2s(^2F)p\,^1G$ at 73563. Therefore, the level $w\,^1G$ must also be neglected. The level $w\,^1F$ at 74664 could be assigned to $d^2s(^2G)p\,^3F_3$ with a deviation of around-350. For the same reasons as for the level 1°_4, the level $w\,^1F$ was not included. These three levels could conceivably belong to $3d^35p$.

The two levels $u\,^3F_{2,3}$ at 76220 and 76386 fit with deviations of 47 and -37 to the calculated levels $d^2s(^4P)p\,^5P_{2,3}$. However, the level $u\,^3F_4$ at 76644 could not be assigned to any theoretical level of J equal to 4. The level $w\,^1D$ at 78791 would fit with a deviation of only about 210 to the level $d^3(B^2D)p\,^3P_2$. However, as $w\,^1D$ is given as uncertain in AEL, we were reluctant to insert it and make the subsequent change in assignment. If, on the other hand, the level $w\,^1D$ is assigned to $d^3(B^2D)p\,^1D$, then the deviation is 700, which is definitely too high.

The term $3d^3$ $(c^2D)4pt\,^3D$, whose assignment is questioned in AEL, fits very well to the theoretical term $d^2s(^2D)p\,^3D$, both in the values and g-factors of the levels. In one variation the levels $t\,^3D$ were fitted with the same theoretical assignments. However, then the deviations were much larger and in addition, a value of β equal to -700 was obtained, which seems definitely too high when compared with the values of β in the GLS of d^np [3].

The level 3°_3 at 79040 has a deviation of only -48 when assigned to $d^2s(^3G)p\,^3G_3$.

It is evident from the theoretical compositions that the parents of the terms $z\,^1P$ and $y\,^1P$ should be exchanged, as indicated by the second change.

The final parameters seem very reasonable. It is impossible to have both A' and G_{ps} free since all the terms of d^2sp inserted have nearly the same derivative of -1 with respect to G_{ps}. Nevertheless, it was found that with G_{ps} equal to 7900 instead of the original value of 8837, the results are improved. This is due to the fact that a few of the levels of d^2sp inserted, have corresponding eigenvalues, whose derivatives with respect to G_{ps} are positive. Thus, G_{ps} is not completely undefined, but since if it is left free the deviation in G_{ps} is greater than 1000, it is more meaningful to have this parameter fixed. Variations were performed in which all or a few of the parameters, B', C', G_1', G_3', and ζ_p' were allowed to be free. Although the values of the parameters were reasonable, they were not well defined. This follows from the fact that there are only 9 experimental terms in d^2sp which split into 28 levels and thus it is more reasonable to have

$$B' = B$$
$$C' = C$$
$$G_1' = G_1$$
$$G_3' = G_3$$
$$\zeta_p' = \zeta_p.$$

However, the parameters F_2', α', and ζ_d' should be free as not only do they have well-defined reasonable values, but they also lower the rms error. If α' is forced to equal α, and no other changes are made, the rms error rises from 66 to 74. If, in addition ζ_d' equals ζ_d, the rms error increases to 81. If, furthermore, F_2' equals F_2 the rms error rises to 98.

The parameters β and T are significant. We are not able to compare the effect of β and T in the last iteration because β and T already differed from zero in the diagonalization of that iteration. In the previous iteration, the rms error with β and T fixed at zero was 121, whereas with β and T free, the rms error dropped to 79. The values of β and T for that iteration were

$$\beta = -190 \pm 71$$
$$T = -3.9 \pm 0.4.$$

The values of the parameters J and K are also very reasonable and do not differ greatly from the initial values. As expected, H is small but well defined.

The agreement between the experimental and calculated g values is very good except for the case of $(^4P)y\,^5D_4$. The eigenfunction of this level comprises 97 per cent $(^4P)\,^5D$, and the remaining 3 per cent are also ^5D. Thus, the calculated g value exactly equals the theoretical g value of 1.500. The value of 2.28 in AEL seems definitely not correct as 1.5 is the highest theoretical g value for any level of J equal to 4 in the configurations $d^3p + d^2sp$.

By considering the interaction with the configuration d^2sp, not only is there a great improvement in the fitting of the experimental levels (rms error of 66 versus 269 for V II $- d^3p$), but also the g values fit much better now. As a particular example we can consider the two levels $d^3(^4F)pz\,^5F_1$ and $d^3(^4F)pz\,^3D_1$, whose experimental g factors are 0.35 and 0.24, respectively. In the treatment of V II $- d^3p$ the calculated g factors for these two levels are 0.166 and 0.596, whereas the present calculated values are 0.300 and 0.238, respectively.

3. Ti II $-3d^24p + 3d4p4s$

3.1. Initial Parameters

As for V II, the initial parameters B, C, F_2, G_1, G_3, α, ζ_d, and ζ_p were taken from the GLS of the configurations d^np of the second spectra, [3]. From the variation with β and T eliminated and with the same approximation as for V II,

$$B = 685$$
$$C = 2290$$
$$F_2 = F_2' = 300$$
$$G_1 = G_1' = 335$$
$$G_3 = G_3' = 29$$
$$\alpha = 58$$
$$\zeta_d = \zeta_d' = 130$$
$$\zeta_p = \zeta_p' = 230.$$

The initial values of G_{ds}, H, J, and K for Ti II can be taken from the final results of V II. Then

$$G_{ds}=1820$$
$$H=86$$
$$J=1011$$
$$K=3288.$$

As for V II the initial value of G_{ps} is obtained by interpolating the values of G_{ps} from Sc II and Ga II. Then,

$$G_{ps}=8540.$$

The initial values of A and A' were obtained from the electrostatic interaction matrix of ^{4}P, which is of order 2 one term assigned to d^2p and the other to dsp. Performing a calculation similar to that of ^{5}F for V II yields

$$A=38435$$
$$A'=64775.$$

From the GLS of d^np [3], the value of A for Ti II $-d^2p$ equals 37607. This value is, as expected, lower than the present value since the configuration $3d^24p$ is lower than $3d4s4p$ and thus each term of $3d^24p$ which feels an interaction with $3d4s4p$ tends to be lowered by this interaction. In the diagonalization of Ti II$-d^2p+dsp$, the matrices of $(d+s)^2p$ were used with all the parameters pertaining to the configuration s^2p having a value equal to zero.

3.2. Discussion and Results

The configuration d^2p comprises 19 theoretical terms splitting into 45 levels. In dsp there are 12 theoretical terms splitting into 23 levels. In AEL, 18 terms splitting into 43 levels are assigned to d^2p and 7 terms splitting into 17 levels are assigned to dsp.

As in V II, the interaction s-p is much stronger than the interaction d-s and so the levels of dsp are coupled as d(^{2}D)sp(^{1,3}P)SL.

The experimental value for the center of gravity of the term $d(^2\mathrm{D})sp\,^3\mathrm{P}x\,^2\mathrm{P}$ in AEL is 53126. Theoretically, this term was calculated initially at 59900. Thus, the experimental levels of the terms $x\,^2$P cannot be fitted to the calculated levels of this term. Now, in the region 52000–54000 there are the theoretical terms $d(^2\mathrm{D})sp(^3\mathrm{P})y\,^4\mathrm{F}$, $d(^2\mathrm{D})sp(^3\mathrm{P})x\,^4\mathrm{D}$ and $d(^2\mathrm{D})sp(^3\mathrm{P})w\,^2\mathrm{D}$. Thus, it is possible to fit only one of the two experimental levels, $x^4\mathrm{D}_{1/2}$ at 52330 and $x\,^2\mathrm{P}_{1/2}$ at 53121. On the other hand, we can attempt to fit the level $x\,^2\mathrm{P}_{3/2}$ at 53128 to the theoretical level $y\,^4\mathrm{F}_{3/2}$, as the term $^2\mathrm{D}(^3\mathrm{P})^4\mathrm{F}$ predicted in this region, is not found experimentally. With these assignments the rms error in the least squares of the first diagonalization was 162. We also considered the variation in which the following changes were made:

AEL $\quad 3d4s\,(a\,^2\mathrm{D})4px\,^2\mathrm{P}_{1/2,3/2}\rightarrow d(^2\mathrm{D})sp(^3\mathrm{P})x\,^4\mathrm{D}_{1/2,3/2}$

AEL $\quad 3d4s\,(a\,^2\mathrm{D})4px\,^4\mathrm{D}_{3/2,5/2,7/2}\rightarrow d(^2\mathrm{D})sp(^3\mathrm{P})y\,^4\mathrm{F}_{3/2,5/2,7/2}$

and then the level $x\,^4\mathrm{D}_{1/2}$ at 52330 was neglected. In this variation the rms error was 121. In addition, from a consideration of the combinations of $x\,^2\mathrm{P}_{3/2}$ and $x\,^4\mathrm{D}_{3/2}$, [8], it is more reasonable to fit the level $x\,^4\mathrm{D}_{3/2}$ to $y\,^4\mathrm{F}_{3/2}$ than to fit $x\,^2\mathrm{P}_{3/2}$ to $y\,^4\mathrm{F}_{3/2}$. Thus, the latter variation was considered for parameters of the next iteration and subsequently the above changes were adopted.

Since the experimental term $d^2(^1\mathrm{S})p\,^2\mathrm{P}$ is missing, it is necessary to hold α fixed at the initial value of 58.

Using the initial approximation that the parameters F_2, G_1, G_3, ζ_d, and ζ_p of d^2p and dsp are equal in the least squares, we found that H tended to change its sign from the value given in the diagonalization. This instability in H was overcome by giving the parameter F_2' freedom. It then became apparent that also G_1' and G_3' should be free in order to improve the results. However, the parameters ζ_d' and ζ_p' are not well defined by the experimental data available. Thus, we set

$$\zeta_d'=\zeta_d \quad \text{and} \quad \zeta_p'=\zeta_p$$

In the final variation of the least squares, 30 experimental terms splitting into 59 levels were fitted by 15 free electrostatic parameters and 2 free spin-orbit interaction parameters to yield a rms error of only 75. In the least squares of the last iteration the sum of the squares of the deviations dropped only from 237,680 to 236,621. The final values for the parameters were

$$A=38036\pm23$$
$$A'=63372\pm56$$
$$B=704\pm2$$
$$C=2391\pm11$$
$$G_{ds}=1379\pm39$$
$$F_2=335\pm3$$
$$F_2'=419\pm7$$
$$G_1=364\pm3$$
$$G_1'=485\pm14$$
$$G_3=34\pm2$$
$$G_3'=60\pm4$$
$$G_{ps}=7326\pm63$$
$$\alpha=58\ (\mathrm{Fix})$$
$$H=29\pm16$$
$$J=1363\pm102$$
$$K=3240\pm56$$
$$\zeta_d=\zeta_d'=117\pm9$$
$$\zeta_p=\zeta_p'=243\pm24$$
$$\Delta=75.$$

In Ti II the interaction with the configuration dsp is very important. In Ti II$-d^2p$ the rms error was 319, whereas here for d^2p+dsp, it is reduced to only 75.

4. Sc II $-3d4p+4s4p$

4.1. Initial Parameters

The initial values of the parameters F_2, G_1, G_3, ζ_d, and ζ_p were taken from the GLS of the configurations d^np of the second spectra with β and T eliminated [3]. For G_{ps} the approximate value of 8243 needed for interpolating the initial value of G_{ps} for V II, was used here. The initial values of J and K were taken from the final values of Ti II$-3d^24p+4s4p$. Thus for Sc II initially,

$$F_2=290$$
$$G_1=340$$
$$G_3=27$$
$$G_{ps}=8243$$
$$J=1363$$
$$K=3240$$
$$\zeta_d=68$$
$$\zeta_p=\zeta_p'=200.$$

The initial values of A and A' were obtained by using the electrostatic matrices of ^{3}P and ^{1}P and averaging. Then,

$$A=29595$$
$$A'=46148.$$

4.2. Discussion and Results

The configuration dp comprises 6 terms splitting into 12 levels and the configuration sp has 2 theoretical terms splitting into 4 levels. All 16 experimental levels are given for Sc II in AEL.

The 8 terms splitting into 16 levels were determined in the least squares calculations by 8 electrostatic parameters and 3 spin-orbit interaction parameters. The rms error obtained was only 4.6. There were no changes in assignment and the 10 experimental g factors fitted very well to the calculated values. The following values for the parameters were obtained in the final least-squares:

$$A=29357\pm2$$
$$A'=46130\pm7$$
$$F_2=325\pm0.4$$
$$G_1=386\pm0.4$$
$$G_3=25\pm0.4$$
$$G_{ps}=7835\pm9$$
$$J=1254\pm10$$
$$K=3248\pm6$$
$$\zeta_d=81\pm2$$
$$\zeta_p=181\pm5$$
$$\zeta_p'=251\pm5$$
$$\Delta=4.6.$$

Although there are 8 electrostatic parameters to determine the 8 terms, we note that the above parameters are very reasonable when compared with those of V II and Ti II. We thus conclude that there is a strong interaction between the configurations dp and sp, but neither dp nor sp feels any strong interaction(s) from other configuration(s). Otherwise, this interaction(s) would be noticed from the values of the above parameters.

5. Tables of the Observed and Calculated Levels and *g*-Factors

In the column "NAME" the calculated designation of the term is given. Whenever the terms of the parent d^n have different seniorities these are denoted by the letters A and B, the lower calculated term being designated by A. Whenever a calculated term has a corresponding experimental term, the small letters $z, y, x, \ldots$ are used as in AEL. The terms of $d^{n-1}sp$ are denoted by $d^{n-1}v_1S_1L_1\ (sp\ ^{1,3}\mathrm{P})SL$.

The entries in the columns "J", "OBS. LEVEL cm^{-1}" "CALC. LEVEL cm^{-1}" are self-evident. In the column "PERCENTAGE", for each calculated level either the three highest contributions or all those contributions exceeding 5 percent are given.

Whenever the experimental and calculated term designations differ, the experimental designation is entered in the column "AEL" using the notation of C. E. Moore [4]. In many instances the exchanges involve complete terms rather than isolated levels. Unless specified otherwise the entries in the column "AEL" pertain to exchanges in terms.

The column "O−C" gives the difference between the observed and calculated values of the levels.

The columns "OBS. g-FACTOR" and "CALC. g-FACTOR" give the observed and calculated values of the Lande g-factors respectively.

The entries are in ascending order of magnitude of the calculated terms.

TABLE 1. *Observed and calculated levels of* Sc II, 3d4p + 4s4p

NAME	J	PERCENTAGE	AEL	OBS. LEVEL (cm^{-1})	CALC. LEVEL (cm^{-1})	O–C	OBS. g-FACTOR	CALC. g-FACTOR
$(^2D)z\,^1D$	2	$99+1(^2D)^3F$		26081.32	26081.18	0.14	1.00	0.998
$(^2D)z\,^3F$	2	$99+1(^2D)^1D$		27443.65	27446.31	−2.66	0.65	0.672
	3	$99+1(^2D)^3D$		27602.32	27604.11	−1.79	1.10	1.085
	4	100		27841.17	27836.83	4.34	1.25	1.250
$(^2D)z\,^3D$	1	100		27917.69	27912.04	5.65	0.51	0.502
	2	99		28021.21	28020.89	0.32	1.16	1.165
	3	99		28161.03	28167.08	−6.05	1.33	1.331
$(^2D)z\,^3P$	0	$90+10(^2S)^3P$		29736.22	29736.98	−0.76		
	1	$88+10(^2S)^3P$		29742.12	29743.62	−1.50		1.489
	2	$90+10(^2S)^3P$		29823.92	29821.63	2.29	1.50	1.499
$(^2D)z\,^1P$	1	$91+7(^2D)^1P$		30815.65	30815.64	0.01	1.00	1.008
$(^2D)z\,^1F$	3	100		32349.98	32349.98	0.00	1.00	1.000
$(^2S)y\,^3P$	0	$90+10(^2D)^3P$		39001.59	39001.63	−0.04		
	1	$90+10(^2D)^3P$		39114.44	39114.06	0.38		1.500
	2	$90+10(^2D)^3P$		39344.90	39345.23	−0.33		1.500
$(^2S)y\,^1P$	1	$93+7(^2D)^1P$		55715.52	55715.52	0.00		1.000

TABLE 2. *Observed and calculated levels of* Ti II – 3d²4p + 3d4s4p

NAME	J	PERCENTAGE	AEL	OBS. LEVEL (cm^{-1})	CALC. LEVEL (cm^{-1})	O–C	OBS. g-FACTOR	CALC. g-FACTOR
$(^3F)z\,^4G$	5/2	98		29544	29592	−48	0.57:	0.577
	7/2	99		29734	29780	−46	0.98:	0.986
	9/2	100		29968	30013	−45		1.172
	11/2	100		30241	30287	−46		1.273
$(^3F)z\,^4F$	3/2	96		30837	30760	77	0.40:	0.412
	5/2	98		30959	30886	73	1.03:	1.031
	7/2	98		31114	31045	69	1.24:	1.238
	9/2	99		31301	31234	67		1.333
$(^3F)z\,^2F$	5/2	$85+7(^1D)^2F$		31207	31237	−30	0.86:	0.867
	7/2	$89+7(^1D)^2F$		31491	31499	−8	1.14:	1.147
$(^3F)z\,^2D$	3/2	$83+9(^3P)^2D$		31756	31742	14	0.92	0.797
	5/2	$78+8(^3P)^2D+5(^3F)^4D$		32026	32019	7	1.20	1.191
$(^3F)z\,^4D$	1/2	96		32532	32577	−45	0.00	0.000
	3/2	94		32603	32643	−40	1.20	1.188
	5/2	91		32698	32733	−35	1.37	1.362
	7/2	95		32767	32793	−26	1.43:	1.426
$(^3F)z\,^2G$	7/2	95		34543	34517	26	0.89:	0.889
	9/2	95		34748	34705	43	1.11:	1.113
$(^3P)z\,^2S$	1/2	99		37431	37448	−17	2.09	1.997
$(^1D)z\,^2P$	1/2	97		39675	39563	112	0.67:	0.672
	3/2	$73+19(^1D)^2D$		39603	39424	179	1.21	1.220
$(^1D)y\,^2D$	3/2	$61+21(^1D)^2P+8(^3P)^2D$		39233	39498	−265	0.80:	0.932
	5/2	$42+40(^1D)^2F+6(^3P)^2D$		39477	39603	−126	1.20:	1.048
$(^1D)y\,^2F$	5/2	$49+37(^1D)^2D+4(^3P)^2D$		39927	39907	−20	0.86:	1.016
	7/2	$87+8(^3F)^2F$		40075	39988	87	1.14:	1.152

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TABLE 2. *Observed and calculated levels of* Ti II – 3d²4p + 3d4s4p – *Continued*

NAME	J	PERCENTAGE	AEL	OBS. LEVEL (cm⁻¹)	CALC. LEVEL (cm⁻¹)	O–C	OBS. g-FACTOR	CALC. g-FACTOR
$(^3P)z\ ^4S$	3/2	96		40027	40109	−82		1.972
$(^3P)y\ ^4D$	1/2	97		40330	40287	43		0.002
	3/2	96		40426	40387	39		1.197
	5/2	95		40582	40547	35		1.368
	7/2	93		40798	40767	31		1.418
$(^3P)z\ ^4P$	1/2	96		41997	41988	9		2.664
	3/2	96		42069	42070	−1		1.731
	5/2	96		42209	42255	−16		1.598
$(^1G)y\ ^2G$	7/2	95		43741	43746	−5	0.89:	0.891
	9/2	95		43781	43787	−6	1.11:	1.110
$(^3P)x\ ^2D$	3/2	$74+12(^1D)^2D+5(^3P)^2P$		44915	44990	−75	0.80:	0.828
	5/2	$79+12(^1D)^2D$		44902	44976	−74	1.20:	1.200
$(^3P)y\ ^2P$	1/2	94		45473	45419	54	0.66:	0.667
	3/2	89		45549	45499	50	1.33:	1.304
$(^1G)z\ ^2H$	9/2	99		45674	45667	7		0.910
	11/2	100		45909	45922	−13		1.092
$(^1G)x\ ^2F$	5/2	$90+7\,^2D(^3P)^2F$		47625	47631	−6	0.86:	0.856
	7/2	$90+7\,^2D(^3P)^2F$		47467	47453	14	1.14:	1.142
$^2D(^3P)^4F$	3/2	98	$ds(a\ ^3D)px\ ^4D$	52459	52342	117		0.407
	5/2	98		52471	52478	−7		1.031
	7/2	99		52631	52672	−41		1.239
	9/2	99			52916			1.333
$^2D(^3P)^4D$	1/2	97	$ds(a\ ^3D)px\ ^2P$	53121	53088	33		0.001
	3/2	95		53128	53150	−22		1.188
	5/2	91			53257			1.361
	7/2	96			53436			1.427
$^2D(^3P)w\ ^2D$	3/2	92	$ds(a\ ^3D)pw\ ^2D$	53597	53628	−31		0.802
	5/2	89		53555	53601	−46		1.211
$^2D(^3P)y\ ^4P$	1/2	97	$ds(a\ ^3D)py\ ^4P$	56223	56241	−18		2.666
	3/2	96		56249	56267	−18		1.733
	5/2	96		56326	56329	−3		1.599
$^2D(^3P)w\ ^2F$	5/2	96	$ds(a\ ^3D)pw\ ^2F$	59322	59300	22		0.856
	7/2	96		59468	59453	15		1.144
$^2D(^3P)^2P$	1/2	$80+20(^1S)^2P$			60059			0.667
	3/2	$84+16(^1S)^2P$			59969			1.333
$(^1S)^2P$	1/2	$74+20\,^2D(^3P)^2P$			64325			0.667
	3/2	$78+16\,^2D(^3P)^2P$			64500			1.333
$^2D(^1P)v\ ^2D$	3/2	95	$ds(b\ ^1D)pv\ ^2D$	69327	69322	5		0.801
	5/2	94		69622	69573	49		1.197
$^2D(^1P)v\ ^2F$	5/2	94	$ds(b\ ^1D)pv\ ^2F$	70606	70680	−74		0.859
	7/2	95		70893	70875	18		1.143
$^2D(^1P)^2P$	1/2	92			73597			0.667
	3/2	92			73879			1.333

TABLE 3. *Observed and calculated levels of* V II $3d^34p+3d^24s4p$

NAME	J	PERCENTAGE	AEL	OBS. LEVEL (cm^{-1})	CALC. LEVEL (cm^{-1})	O–C	OBS. g-FACTOR	CALC. g-FACTOR
$(^4F)z\,^5G$	2	100		34593	34590	3	0.31	0.334
	3	100		34746	34740	6	0.93	0.917
	4	100		34947	34939	8	1.14	1.150
	5	100		35193	35184	9	1.16	1.267
	6	100		35483	35473	10		1.333
$(^4F)z\,^3D$	1	$51+42(^4F)^5F$	$d^3(a\,^4F)pz\,^5F$	36489	36470	19	0.35	0.300
	2	$44+44(^4F)^5F$	$d^3(a\,^4F)pz\,^3D$	37041	37020	21	1.08	1.117
	3	$55+21(^4F)^5D+17(^4F)^5F$		37205	37207	-2	1.32	1.354
$(^4F)z\,^5F$	1	$56+37(^4F)^3D$	$d^3(a\,^4F)pz\,^3D$	36955	36925	30	0.24	0.238
	2	$54+38(^4F)^3D$	$d^3(a\,^4F)pz\,^5F$	36674	36654	20	1.08	1.086
	3	$81+13(^4F)^3D$		36919	36897	22	1.24	1.269
	4	98		37151	37126	25		1.350
	5	98		37352	37338	14	1.40:	1.398
$(^4F)z\,^5D$	0	97		37201	37254	-53		
	1	94		37259	37311	-52	1.39	1.464
	2	$87+10(^4F)^3D$		37369	37421	-52	1.39	1.462
	3	$73+23(^4F)^3D$		37521	37572	-51	1.47	1.458
	4	97		37531	37603	-72	1.44	1.498
$(^4F)z\,^3G$	3	$91+7(^2G)^3G$		39234	39268	-34	0.84	0.752
	4	$91+7(^2G)^3G$		39404	39437	-33	1.03	1.052
	5	$91+7(^2G)^3G$		39613	39652	-39	1.19	1.202
$(^4F)z\,^3F$	2	94		40002	40007	-5	0.65	0.667
	3	94		40196	40203	-7	1.02	1.083
	4	94		40430	40444	-14	1.22	1.250
$(^4P)z\,^5P$	1	94		46755	46669	86	2.28	2.446
	2	$62+20(^4P)^5D+14(^4P)^3P$		46880	46809	71	1.65	1.705
	3	98		47052	46957	95	1.58	1.663
$(^4P)z\,^3P$	0	$39+48(^4P)^5D$	$d^3(a\,^4P)py\,^5D$	47028	47047	-19		
	1	$48+41(^4P)^5D$		47108	47113	-5	1.43	1.511
	2	$44+34(^4P)^5P+13(^4P)^5D$	$d^3(a\,^4P)pz\,^3P$	46740	46754	-14	1.48	1.614
$(^4P)z\,^5D$	0	$48+40(^4P)^3P$	$d^3(a\,^4P)pz\,^3P$	46586	46627	-41		
	1	$55+33(^4P)^3P$		46690	46717	-27	1.44	1.537
	2	$63+26(^4P)^3P$	$d^3(a\,^4P)py\,^5D$	47102	47092	10	1.47	1.511
	3	95		47181	47152	29	1.48:	1.502
	4	97		47420	47380	40	(2.28)	1.500
$(^2G)z\,^3H$	4	$88+12(^2H)^3H$		47056	47047	9	0.78	0.801
	5	$87+12(^2H)^3H$		47297	47281	16	1.01	1.034
	6	$87+12(^2H)^3H$		47608	47578	30	1.13	1.166
$(^2P)z\,^1S$	0	$90+7(^4P)^3P$		48258	48473	-215		
$(^2G)y\,^3G$	3	$80+7(^4F)^3G+7(^2G)^1F$		48580	48654	-74	0.67	0.784
	4	$87+7(^4F)^3G$		48731	48815	-84	1.02	1.054
	5	$84+7(^4F)^3G$		48853	48940	-87	1.22	1.187
$(^2G)y\,^3F$	2	$78+15(A\,^2D)^3F$		49202	49254	-52	0.63	0.680
	3	$46+29(^2G)^1F+10(^2G)^3G$		49211	49215	-4	0.99	1.017
	4	$60+28(^2G)^1G$		49269	49265	4	1.18	1.174
$(^2G)z\,^1F$	3	$49+34(^2G)^3G+7(A\,^2D)^1F$		49568	49518	50	0.97	1.033
$(^2G)z\,^1H$	5	$72+21(^2H)^1H$		49593	49545	48	0.95	1.011
$(^2G)z\,^1G$	4	$69+23(^2G)^3F$		49724	49678	46	0.96	1.068
$(^4P)z\,^5S$	2	96		49731	49738	-7		1.992
$(^2P)z\,^1D$	2	$50+36(A\,^2D)^1D$		49898	49920	-22	0.93	0.999

TABLE 3. *Observed and calculated levels of* V II $3d^34p+3d^24s4p$—*Continued*

NAME	J	PERCENTAGE	AEL	OBS. LEVEL (cm^{-1})	CALC. LEVEL (cm^{-1})	O−C	OBS. g-FACTOR	CALC. g-FACTOR
$(^2P)y\ ^3P$	0	$63+36(A^2D)^3P$		50662	50545	117		
	1	$50+29(A^2D)^3P+10(^2P)^3D$		50739	50647	92	1.39	1.328
	2	$58+38(A^2D)^3P$		51123	51030	93	1.51	1.493
$(^2P)y\ ^3D$	1	$52+21(^4P)^3D+9(^2P)^3P$	$d^3(a\ ^4P)py\ ^3D$	50474	50539	−65	0.49	0.675
	2	$58+27(^4P)^3D$		50775	50843	−68	1.11	1.157
	3	$55+32(^4P)^3D$		51086	51155	−69	1.27	1.327
$(^2P)z\ ^3S$	1	$82+11(^4P)^3S$		52181	52099	82	1.85	1.974
$(^2H)y\ ^3H$	4	$86+12(^2G)^3H$		52083	52046	37	0.70	0.804
	5	$87+12(^2G)^3H$		52154	52123	31	0.98	1.034
	6	$87+12(^2G)^3H$		52253	52229	24	1.04:	1.166
$(A^2D)x\ ^3F$	2	$74+12(^2G)^3F$		52246	52299	−53	0.68	0.710
	3	$58+22(^4P)^3D+9(^2G)^3F$		52392	52436	−44	1.07	1.157
	4	$85+10(^2G)^3F$		52658	52718	−60	1.18:	1.250
$(^4P)x\ ^3D$	1	$52+16(^2P)^3D+13(A^2D)^3D$	$d^3(a\ ^2P)px\ ^3D$	52604	52562	42	0.63	0.577
	2	$51+25(^2P)^3D+13(A^2D)^3D$		52700	52624	76	1.10	1.137
	3	$34+29(^2P)^3D+23(A^2D)^3F$		52767	52680	87	1.26	1.266
$(A^2D)z\ ^1P$	1	$73+11(^2P)^1P$	$d^3(a\ ^2P)pz\ ^1P$	52804	52833	−29	0.92	0.951
$(^2H)z\ ^3I$	5	99		52878	52848	30	0.84:	0.835
	6	100		53077	53047	30	0.98	1.024
	7	100		53320	53290	30	1.11:	1.143
$(A^2D)w\ ^3D$	1	$76+12(^2P)^3D$		53751	53722	29	0.49:	0.522
	2	$80+11(^2P)^3D$		53869	53852	17	1.10	1.169
	3	$84+7(^2P)^3D$		53927	53914	13	1.37	1.325
$(^2H)y\ ^1G$	4	$82+11(^2F)^1G$		54144	54131	13	1.00	1.001
$(A^2D)x\ ^3P$	0	$52+30(^2P)^3P+14(^4P)^3P$		54813	54817	−4		
	1	$48+28(^2P)^3P+13(^4P)^3P$		54718	54723	−5		1.499
	2	$48+32(^2P)^3P+15(^4P)^3P$		54716	54696	20		1.496
$(A^2D)y\ ^1F$	3	$53+34(^2H)^3G$		55142	55156	−14	0.94	0.912
$(^2H)x\ ^3G$	3	$57+33(A^2D)^1F$		55350	55344	6	0.82	0.848
	4	$88+6\ ^3F(^3P)^3G$		55304	55255	49	1.02	1.049
	5	$79+10(^2H)^1H$		55207	55160	47	1.15	1.174
$(^2H)z\ ^1I$	6	100		55403	55428	−25	1.01:	1.001
$(^2H)y\ ^1H$	5	$66+20(^2G)^1H+12(^2H)^3G$		55499	55546	−47	1.03:	1.026
$(^4P)y\ ^3S$	1	$55+22(^2P)^1P+10(^2P)^3S$		55663	55809	−146	1.92	1.708
$(^2P)y\ ^1P$	1	$60+25(^4P)^3S+8(A^2D)^1P$	$d^3(a\ ^2D)y\ ^1P$	56171	55996	175	1.05:	1.273
$(A^2D)y\ ^1D$	2	$54+40(^2P)^1D$		57343	57292	51	0.98	1.002
$^3F(^3P)^5G$	2	96			62055			0.347
	3	$90+8(^2F)^3F$			62211			0.933
	4	$88+10(^2F)^3F$			62452			1.161
	5	100			62722			1.267
	6	100			63043			1.333
$(^2F)w\ ^3F$	2	$85+7\ ^3F(^1P)^3F$		62085	62255	−170	0.58:	0.656
	3	$80+9\ ^3F(^3P)^5G$		62133	62286	−153	1.00	1.067
	4	$78+11\ ^3F(^3P)^5G$		62176	62299	−123	1.36:	1.237

TABLE 3. *Observed and calculated levels of* V II $3d^34p + 3d^24s4p$ – Continued

NAME	J	PERCENTAGE	AEL	OBS. LEVEL (cm^{-1})	CALC. LEVEL (cm^{-1})	O–C	OBS. g-FACTOR	CALC. g-FACTOR
$^3F(^3P)y\,^5F$	1	98	$d^2s(b\,^4F)$ $py\,^5F$	63548:	63472	76		0.001
	2	98		63657	63576	81		1.000
	3	98		63817	63731	86		1.249
	4	98		64027	63934	93		1.348
	5	$91 + 7(^2F)^3G$		64287	64181	106		1.385
$(^2F)w\,^3G$	3	95		64057	64037	20	0.72:	0.753
	4	94		64131	64116	15	1.02	1.052
	5	$89 + 7\,^3F(^3P)^5F$		64229	64228	1		1.215
$(^2F)x\,^1D$	2	$67 + 16(^2F)^3D + 9(B\,^2D)^1D$		64586	64777	−191	1.03:	1.028
$(^2F)v\,^3D$	1	$88 + 6\,^3P(^3P)^3D$		64931	64921	10	0.46:	0.500
	2	$72 + 15(^2F)^1D + 6\,^3P(^3P)^3D$		64804	64822	−18	1.02:	1.137
	3	$88 + 6\,^3P(^3P)^3D$		64604	64629	−25	1.22:	1.331
$(^2F)x\,^1G$	4	$87 + 10(^2H)^1G$		65790	65855	−65	0.94	1.001
$^3F(^3P)x\,^5D$	0	94	$d^2s(b\,^4F)$ $px\,^5D$	65783	65817	−34		
	1	94		65816	65857	−41		1.497
	2	93		65885	65940	−55		1.497
	3	93		65997	66071	−74		1.495
	4	94		66159	66260	−101		1.499
$(^2F)x\,^1F$	3	$74 + 22\,^3F(^3P)^1F$		66304	66122	182	0.95	1.004
$^3F(^3P)v\,^3F$	2	$77 + 11\,^1D(^3P)^3F$	$d^2s(b\,^4F)$ $pv\,^3F$	67738	67779	−41		0.669
	3	$77 + 11\,^1D(^3P)^3F$		67905	67938	−33		1.084
	4	$78 + 11\,^1D(^3P)^3F$		68147	68169	−22		1.250
$^3F(^3P)u\,^3D$	1	$81 + 4\,^1D(^3P)^3D$	$d^2s(b\,^4F)$ $pu\,^3D$	68759	68764	−5		0.502
	2	$80 + 4\,^1D(^3P)^3D$		68798	68831	−33		1.166
	3	$80 + 4\,^1D(^3P)^3D$		68945	68994	−49		1.331
$^3F(^3P)v\,^3G$	3	92	$d^2s(b\,^4F)$ $pv\,^3G$	69644	69649	−5		0.753
	4	92		69912	69869	43		1.051
	5	93		70228	70149	79		1.200
$^3F(^3P)^1F$	3	$73 + 19(^2F)^1F$			71348			1.000
$^3F(^3P)^1D$	2	$82 + 9\,^3P(^3P)^1D$			71376			1.001
$^3F(^3P)^1G$	4	93			73563			1.005
$^3P(^3P)^5S$	2	95			73059			1.993
$^3P(^3P)^5D$	0	96			73664			
	1	96			73721			1.499
	2	95			73830			1.495
	3	94			73986			1.490
	4	90			74181			1.483
$^3P(^3P)^3S$	1	92			74039			1.986
$^1D(^3P)^3F$	2	$80 + 12\,^3F(^1P)^3F$			74792			0.674
	3	$79 + 12\,^3F(^1P)^3F$			74912			1.095
	4	$76 + 10\,^3F(^1P)^3F$			75121			1.263
$^1D(^3P)^3P$	0	$89 + 6\,^3P(^3P)^1S$			75249			
	1	$77 + 9\,^1D(^3P)^3D$			75252			1.433
	2	$84 + 6\,^1D(^3P)^3D$			75104			1.490

TABLE 3. *Observed and calculated levels of* V II $3d^34p + 3d^24s4p$—*Continued*

NAME	J	PERCENTAGE	AEL	OBS. LEVEL (cm^{-1})	CALC. LEVEL (cm^{-1})	O–C	OBS. g-FACTOR	CALC. g-FACTOR
^{1}D(^{3}P)t ^{3}D	1	58 + 12(B^{2}D)^{3}D + 11 ^{1}D(^{3}P)^{3}D	d^3(c ^{2}D) pt ^{3}D	75715:	75695	20	0.50:	0.624
	2	56 + 13(B^{2}D)^{3}D + 8 ^{1}D(^{3}P)^{3}D		75758	75796	−38	1.14:	1.224
	3	54 + 19 ^{3}P(^{3}P)^{5}P + 10(B^{2}D)^{3}D		75848	75840	8	1.27:	1.396
^{3}P(^{3}P)^{1}S	0	92			75927			
^{3}P(^{3}P)^{5}P	1	94			76052			2.456
	2	92	u ^{3}F	76220	76173	47		1.787
	3	80 + 10 ^{1}D(^{3}P)^{3}D	u ^{3}F	76386	76422	−36		1.599
(B^{2}D)^{3}D	1	73 + 18 ^{1}D(^{3}P)^{3}D			77278			0.510
	2	70 + 19 ^{1}D(^{3}P)^{3}D			77277			1.172
	3	69 + 22 ^{1}D(^{3}P)^{3}D			77322			1.334
(B^{2}D)^{1}D	2	74 + 14 ^{3}P(^{3}P)^{1}D			78093			0.982
(B^{2}D)^{3}F	2	66 + 12(B^{2}D)^{3}P + 6 ^{1}G(^{3}P)^{3}F			78566			0.834
	3	85 + 8 ^{1}G(^{3}P)^{3}F			78594			1.084
	4	86 + 8 ^{1}G(^{3}P)^{3}F			78689			1.250
(B^{2}D)^{3}P	0	66 + 33 ^{3}P(^{3}P)^{3}P			78753			
	1	66 + 23 ^{3}P(^{3}P)^{3}P			78694			1.492
	2	55 + 24 ^{3}P(^{3}P)^{3}P + 15(B^{2}D)^{3}F			78578			1.347
^{1}G(^{3}P)^{3}G	3	77 + 21 ^{3}F(^{1}P)^{3}G	3°	79040	79089	−49		0.750
	4	79 + 19 ^{3}F(^{1}P)^{3}G			79166			1.050
	5	81 + 17 ^{3}F(^{1}P)^{3}G			79259			1.200
(B^{2}D)^{1}F	3	93			80596			1.001
^{3}P(^{3}P)^{3}D	1	64 + 14 ^{3}F(^{1}P)^{3}D + 8 ^{1}D(^{3}P)^{3}D			81585			0.513
	2	66 + 14 ^{3}F(^{1}P)^{3}D + 7 ^{1}D(^{3}P)^{3}D			81658			1.166
	3	67 + 15 ^{3}F(^{1}P)^{3}D + 7 ^{1}D(^{3}P)^{3}D			81737			1.333
^{1}G(^{3}P)^{3}H	4	99			82179			0.800
	5	99			82309			1.034
	6	100			82465			1.167
(B^{2}D)^{1}P	1	55 + 42 ^{3}P(^{3}P)^{1}P			82512			0.988
^{3}F(^{1}P)^{3}F	2	91			82636			0.669
	3	48 + 38 ^{3}F(^{1}P)^{3}G + 9 ^{1}G(^{3}P)^{3}G			82865			0.924
	4	72 + 17 ^{3}F(^{1}P)^{3}G			83305			1.209
^{3}F(^{1}P)^{3}G	3	42 + 43 ^{3}F(^{1}P)^{3}F + 8 ^{1}G(^{3}P)^{3}G			83004			0.910
	4	64 + 19 ^{3}F(^{1}P)^{3}F + 12 ^{1}G(^{3}P)^{3}G			83152			1.091
	5	83 + 13 ^{1}G(^{3}P)^{3}G			83495			1.200
^{3}P(^{3}P)^{3}P	0	70 + 28(B^{2}D)^{3}P			83859			
	1	71 + 27(B^{2}D)^{3}P			83909			1.499
	2	71 + 25(B^{2}D)^{3}P			84010			1.487
^{3}P(^{3}P)^{1}D	2	64 + 10 ^{3}F(^{3}P)^{1}D + 10(B^{2}D)^{1}D			84561			1.017
^{3}F(^{1}P)^{3}D	1	80 + 13 ^{3}P(^{3}P)^{3}D			84591			0.502
	2	79 + 12 ^{3}P(^{3}P)^{3}D			84854			1.160
	3	82 + 13 ^{3}P(^{3}P)^{3}D			85203			1.333
^{1}G(^{3}P)^{3}F	2	86 + 9(B^{2}D)^{3}F			86594			0.668
	3	86 + 10(B^{2}D)^{3}F			86516			1.083
	4	85 + 10(B^{2}D)^{3}F			86414			1.250
^{3}P(^{3}P)^{1}P	1	55 + 41(B^{2}D)^{1}P			88072			1.000
^{1}D(^{1}P)^{1}F	3	93			91023			1.002
^{1}D(^{1}P)^{1}P	1	67 + 27 ^{3}P(^{1}P)^{3}S			91172			1.282
^{3}P(^{1}P)^{3}S	1	69 + 26 ^{1}D(^{1}P)^{1}P			91547			1.717

TABLE 3. *Observed and calculated levels of* V II $3d^3 4p + 3d^2 4s4p$ — *Continued*

NAME	J	PERCENTAGE	AEL	OBS. LEVEL (cm^{-1})	CALC. LEVEL (cm^{-1})	O–C	OBS. g-FACTOR	CALC. g-FACTOR
$^1D(^1P)^1D$	2	$83 + 6\ ^3P(^1P)^3D$			93563			1.014
$^3P(^1P)^3D$	1	$89 + 7\ ^3F(^1P)^3D$			93810			0.501
	2	$83 + 6\ ^1D(^1P)^1D$			93961			1.157
	3	$89 + 6\ ^3F(^1P)^3D$			94104			1.331
$^3P(^1P)^3P$	0	92			94873			
	1	92			95927			1.499
	2	91			96041			1.496
$^1G(^1P)^1G$	4	96			96025			1.000
$^1G(^1P)^1H$	5	99			98373			1.000
$^1S(^3P)^3P$	0	93			102293			
	1	93			102392			1.500
	2	94			102594			1.500
$^1G(^1P)^1F$	3	94			102676			1.000
$^1S(^1P)^1P$	1	96			118520			1.000

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