JOURNAL OF RESEARCH of the National Bureau of Standards—A. Physics and Chemistry
Vol. 73A, No. 6, November–December 1969

Odd Configurations in Singly-Ionized Copper*

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(August 15, 1969)

Experimental levels of the configurations $3d^94p$, $3d^95p$, $3d^96p$, $3d^84s4p$, $3d^94f$, and $3d^95f$ of Cu II were compared with corresponding calculated values. The electrostatic interactions between the configuration $3d^84s4p$ and the configurations $3d^94p$, $3d^95p$, and $3d^96p$ were considered explicitly. It was shown that the configurations $3d^94f$ and $3d^95f$ of Cu II do not interact strongly with other configurations.

Key words: Copper; energy levels; interaction between configurations; odd configurations; parameters; second spectra.

1. Introduction

The configurations $(3d+4s)^n$ in the second spectra of the iron group were studied by Racah, Shadmi, Oreg, and Stein [1–3].[1] The configurations $3d^n4p$ in the second spectra of the iron group as well as the configurations $3d^n4p+3d^{n-1}4s4p$ for Sc II, Ti II and V II were investigated by the author [4, 5].[2]

An examination of the spectrum of Cu II [6], indicates that the experimental data are very abundant. The configuration d^9p consists of 6 terms splitting into 12 levels. All the predicted levels for the configurations $3d^94p$ and $3d^95p$ are given in AEL [6], whereas for $3d^96p$ only the experimental level $6p\ {}^3P_0$ is missing. The configuration d^8sp comprises 38 terms splitting into 90 levels. In AEL, 29 terms splitting into 65 levels are given for the configuration $3d^84s4p$ with definite term designations. In addition the levels 1^o_1 at 140482? and 3^o_1 at 144241 are assigned to $3d^84s4p$. The configuration d^9f comprises 10 theoretical terms splitting into 20 levels. All the predicted levels for the configurations $3d^94f$ and $3d^95f$ are given in AEL. In addition 5 experimental terms splitting into 8 levels are given for the configuration $3d^96f$. However in the latter configuration 5 levels appear with question marks.

To treat the seven configurations as one problem and consider all the interactions between configurations would involve more electrostatic parameters than the terms available. This method is therefore quite meaningless.

The configuration $3d^94p$ is much lower than the other odd configurations and thus the interaction between configurations is expected to be weak here. This expectation is borne out by treating this configuration individually. The rms error is only 119 cm^{-1} and the 9 experimental g-factors agree well with the calculated values.

Separate treatments of the configurations $3d^84s4p$, $3d^95p$ and $3d^96p$ did not yield favorable results (rms error ~ 250 cm^{-1}). In addition the parameters in these three cases were quite unreasonable. The parameter G_3 even assumed negative values for $3d^84s4p$, $3d^95p$ and $3d^96p$. These results are not surprising since the configurations $3d^95p$ and $3d^96p$ are in the middle of the configuration $3d^84s4p$ and we may expect these three configurations to be strongly interacting. We thus considered the three configurations $3d^84s4p$, $3d^95p$ and $3d^96p$ as one problem, inserting the interactions between configurations $3d^95p-3d^84s4p$ and $3d^96p-3d^84s4p$. The interaction $3d^95p-3d^96p$ was neglected as then there would be too many parameters, causing the subsequent results to become meaningless. In addition, since the configurations $3d^95p$ and $3d^96p$ are separated we do not expect the interaction between these configurations to be very strong. For $3d^95p+3d^84s4p+3d^96p$, the rms error was 136 cm^{-1}.

Separate treatments of the configurations $3d^94f$ and $3d^95f$ yielded excellent results. The rms errors were only 51 and 4.5 cm^{-1}, respectively. We could expect to obtain similar results for $3d^96f$ and can be quite certain that this configuration does not interact strongly with the other configurations. The experimental data for $3d^96f$ is, however, too limited to consider it separately.

Finally, the configurations $3d^94p$, $3d^84s4p$, $3d^95p$, and $3d^96p$ were considered as one problem by inserting the interactions $3d^84s4p-3d^94p$, $3d^84s4p-3d^95p$, and $3d^84s4p-3d^96p$. The purpose here was to obtain approximate values for the parameters of the interaction between the configurations $3d^n4p-3d^{n-1}4s4p$ in the second spectra of the iron group for elements on the right side of the periodic table.

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*An invited paper.

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

[2] The reader is referred to these papers for an explanation of the method used, notation and significance of the various parameters. The numerical values of all levels and parameters are in cm^{-1}.

2. The Configuration $3d^9 4p$—Cu II

The results for Cu II$-3d^9 4p$ in the general treatment of the configurations $d^n p$ of the second spectra of the iron group [4], indicate that the agreement between the observed and calculated values and g-factors of some levels is not very good. In order to ascertain whether these discrepancies are caused by the interaction with $3d^8 4s4p$ or are due to the fact that the parameters were forced to be linear, it is necessary to refer to the individual treatment of Cu II$-3d^9 4p$, [4]. The parameters with their standard errors are given in table 1.

Whereas in the general treatment the highest deviation for Cu II$-3d^9 4p$ is -270, in the individual treatment it is only 167. Furthermore, there is excellent agreement between the observed and calculated g-factors.

As for the general treatment of Cu II $3d^9 4p$, the following changes in designation were made:

$$3d^9(^2\mathrm{D})4p\ ^3\mathrm{D}_2 \longleftrightarrow 3d^9(^2\mathrm{D})4p\ ^1\mathrm{D}_2$$

$${}_{3}d^9(^2\mathrm{D})4p\ ^3\mathrm{D}_3 \longleftrightarrow 3d^9(^2\mathrm{D})4p\ ^1\mathrm{F}_3$$

In both cases there was considerable mixing between the eigenfunctions involved.

TABLE 1. *Parameters for* Cu II$-3\mathrm{d}^9 4\mathrm{p}$

Parameter	Initial value	Final value
A	70,281	69,802 ± 42
F_2	383	344 ± 7
G_1	306	305 ± 7
G_3	45	38 ± 6
α	95	100 (Fix)
ζ_d	821	802 ± 43
ζ_p	536	502 ± 82
rms error		119

3. The Configurations $3d^9 5p + 3d^8 4s4p + 3d^9 6p$—Cu II

3.1. Initial Parameters

The matrix elements of the interactions between configurations $3d^8 4s4p - 3d^9 5p$ and $3d^8 4s4p - 3d^9 6p$ were obtained from Rosenzweig [7]. However, now the interaction matrix elements between the cores $3d^8 4s$ and $3d^9$ vanish. This is due to the fact that since H is the parameter pertaining to the interaction between electrons d and s, the quantum numbers of the electrons p must be the same on both sides of the matrix elements. Thus only the matrices of J and K enter into the electrostatic matrix $d^{n-1}sp-d^n p'$, and with the same coefficients as for $d^{n-1}sp-d^n p$. The matrices of J and K for $d^8 sp - d^9 p'$ and $d^8 sp - d^9 p''$ were added to the previously obtained matrices of $(d+s)^9 p$.

The values of the parameters F_2, G_1, G_3, α, ζ_d, and ζ_p obtained from $3d^9 4p$ in the variation of the GLS (general least-squares) with β and T eliminated [4], were used as initial values for the configuration $3d^8 4s4p$. The parameters B and C were obtained from the same GLS by adding to the values of $3d^8 4p$ the linear intervals of 65 and 310 respectively. Thus, initially,

$$\begin{aligned} B' &= 1140\ \text{[3]}\\ C' &= 4460\\ F_2' &= 370\\ G_1' &= 300\\ G_3' &= 40\\ \alpha' &= 97\\ \zeta_d' &= 770\\ \zeta_p' &= 460 \end{aligned} \tag{1}$$

Since G_{ds}' is the parameter of the $d-s$ interaction for the core $d^8 s$ its approximate value can be taken *from* Cu III$=3d^9+3d^8 4s$. From Shadmi [8], we obtain

$$G_{ds}' = 1890. \tag{2}$$

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, the center of gravity of $4s(^2\mathrm{S})4p\ y^3\mathrm{P}$ in Sc II is 39230 and $4s(^2\mathrm{S})4p\ y^1\mathrm{P}$ in Sc II is 55716. Thus,

$$G_{ps}'(sp) = 8243. \tag{3}$$

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

$$G_{ps}'(d^{10}sp) = 11212. \tag{4}$$

Hence by interpolation,

$$G_{ps}'(d^8 sp) = 10620. \tag{5}$$

In order to obtain an approximate value for the height of the configuration $d^8 sp$, it is most reasonable to consider the quintets as they have, of course, no interaction with $d^9 p$. From an examination of the experimental data it would seem most appropriate to consider the electrostatic interaction matrix of ^{5}F as there the Lande interval rule is satisfied well, and unlike ^{5}D, in ^{5}F there is no level given with a question mark. Then, approximately,

$$^5\mathrm{F}_{\mathrm{C.G.}} = A' - 8B' - 2G_{ds}' + 3F_2' - G_{ps}' + 12\alpha' = 113700. \tag{6}$$

Using values for the parameters obtained previously we get

$$A' = 134{,}950. \tag{7}$$

For the configurations $3d^9 5p$ and $3d^9 6p$ initial values of the parameters were obtained by using the electro-

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[3] Unprimed quantities refer to the configuration $3d^9 4p$, primed quantities to $3d^8 4s4p$, doubly-primed to $3d^9 5p$ and triply-primed to $3d^9 6p$.

static matrices of d^9p (p. 299, TAS [9]), and taking the centers of gravity of the experimental terms [6]. Then

$$\begin{aligned} A'' &= 121360 \\ F_2'' &= 114 \\ G_1'' &= 115 \\ G_3'' &= 61 \\ A''' &= 139950 \\ F_2''' &= 11 \\ G_1''' &= 56 \\ G_3''' &= 43. \end{aligned} \tag{8}$$

Unlike the electrostatic parameters, the spin-orbit interaction parameters obtained in the individual treatments of $3d^95p$ and $3d^96p$ were quite reasonable. Thus they were adopted as starting values here:

$$\begin{aligned} \zeta_d'' &= 856 \\ \zeta_p'' &= 142 \\ \zeta_d''' &= 740 \\ \zeta_p''' &= 27. \end{aligned} \tag{9}$$

In the initial diagonalization the parameters of the interaction between configurations were not inserted. From the results of $3d^n4p+3d^{n-1}4s4p$ for Sc II, Ti II, and V II [5], we note that both J and K are positive and K is almost three times J. However, here the interactions are between $3d^84s4p-3d^95p$ and $3d^84s4p-3d^96p$, and thus we would expect the parameters to be considerably smaller than for

$$3d^n4p-3d^{n-1}4s4p, \qquad n \leqslant 3.$$

Thus, in the second iteration the following values for the parameters of the interactions between configurations were inserted:

$$\begin{aligned} J(3d^84s4p-3d^95p) &= J(3d^84s4p-3d^96p) = 200 \\ K(3d^84s4p-3d^95p) &= K(3d^84s4p-3d^96p) = 600. \end{aligned} \tag{10}$$

3.2. Results and Discussion

Of the 90 levels assigned to $3d^95p+3d^84s4p+3d^96p$ in AEL we found it necessary to omit the following five levels:

1. $3d^84s(^2\mathrm{D})4p''' \; ^1\mathrm{P}$ at 125400
2. $3d^84s(^4\mathrm{P})4p^{\mathrm{iv}} \; ^5\mathrm{S}$ at 128366
3. $3d^84s(^2\mathrm{D})4p''' \; ^1\mathrm{D}$ at 130632
4. $3d^84s(^4\mathrm{P})4p^{\mathrm{iv}} \; 1_1^0$ at 140482 ?
5. $3d^84s(^4\mathrm{P})4p^{\mathrm{iv}} \; 3_1^0$ at 144241.

The following changes in designation were found necessary:

1. AEL $d^8s(^2\mathrm{F})p'' \; ^3\mathrm{F}_3 \longleftrightarrow$ AEL $d^8s(^2\mathrm{F})p'' \; ^3\mathrm{G}_3$
2. AEL $d^8s(^2\mathrm{D})p'' \; ^3\mathrm{D}_{2,3} \longleftrightarrow$ AEL $d^8s(^4\mathrm{P})p^{\mathrm{iv}\,5}\mathrm{P}_{2,3}$
3. AEL $d^8s(^2\mathrm{D})p'' \; ^3\mathrm{D}_1 \longrightarrow \; ^3\mathrm{P}(^3\mathrm{P}) \; ^5\mathrm{P}_1$
4. AEL $d^8s(^4\mathrm{P})p^{\mathrm{iv}} \; ^5\mathrm{P}_1 \longrightarrow \; ^1\mathrm{D}(^3\mathrm{P}) \; ^3\mathrm{P}_1$
5. AEL $d^8s(^2\mathrm{D})p''' \; ^1\mathrm{F} \longrightarrow \; ^3\mathrm{P}(^3\mathrm{P}) \; ^5\mathrm{D}_3$
6. AEL $d^8s(^4\mathrm{P})p^{\mathrm{iv}} \; ^5\mathrm{D}_3 \longrightarrow \; ^3\mathrm{P}(^3\mathrm{P}) \; ^5\mathrm{D}_4$
7. AEL $d^8s(^2\mathrm{P})p^{\mathrm{v}} \; ^3\mathrm{P}_1 \longleftrightarrow$ AEL $d^8s(^2\mathrm{P})p^{\mathrm{v}} \; ^3\mathrm{D}_1$
8. AEL $d^8s(^2\mathrm{P})p^{\mathrm{v}} \; ^1\mathrm{D} \longrightarrow \; ^3\mathrm{P}(^3\mathrm{P}) \; ^5\mathrm{S}$
9. AEL $d^8s(^2\mathrm{G})p^{\mathrm{vi}} \; ^1\mathrm{H} \longrightarrow \; ^1\mathrm{G}(^3\mathrm{P}) \; ^3\mathrm{H}_5$
10. AEL $d^8s(^2\mathrm{G})p^{\mathrm{vi}} \; ^3\mathrm{F}_2 \longrightarrow (^2\mathrm{D})6p \; ^3\mathrm{P}_2$
11. AEL $d^8s(^2\mathrm{G})p^{\mathrm{vi}} \; ^3\mathrm{F}_3 \longrightarrow (^2\mathrm{D})6p \; ^1\mathrm{F}$
12. AEL $d^8s(^2\mathrm{G})p^{\mathrm{vi}} \; ^3\mathrm{F}_4 \longrightarrow \; ^3\mathrm{F}(^1\mathrm{P})^3\mathrm{F}_4$
13. AEL $(^2\mathrm{D})6p \; ^3\mathrm{D}_{2,3} \longrightarrow \; ^3\mathrm{F}(^1\mathrm{P})^3\mathrm{F}_{2,3}$
14. AEL $(^2\mathrm{D})6p \; ^3\mathrm{P}_2 \longrightarrow (^2\mathrm{D})6p \; ^1\mathrm{D}$
15. AEL $(^2\mathrm{D})6p \; ^1\mathrm{D} \longrightarrow (^2\mathrm{D})6p \; ^3\mathrm{D}_2$
16. AEL $(^2\mathrm{D})6p \; ^3\mathrm{F}_3 \longrightarrow (^2\mathrm{D})6p \; ^3\mathrm{D}_3$
17. AEL $(^2\mathrm{D})6p \; ^1\mathrm{F} \longrightarrow (^2\mathrm{D})6p \; ^3\mathrm{F}_3$.

The following levels showed very strong mixing and the main contribution in each case was not the same as that given in AEL:

1. $(^2\mathrm{D})5p \; ^1\mathrm{F}$ and $(^2\mathrm{D})5p \; ^3\mathrm{F}_3$
2. $(^2\mathrm{D})5p \; ^1\mathrm{D}$, $d^8s(^2\mathrm{F})p'' \; ^1\mathrm{D}$, and $(^2\mathrm{D})5p \; ^3\mathrm{D}_2$
3. $^3\mathrm{F}(^1\mathrm{P})^3\mathrm{F}_{2,3,4}$ and $^1\mathrm{G}(^3\mathrm{P})^3\mathrm{F}_{2,3,4}$
4. $(^2\mathrm{D})6p \; ^3\mathrm{P}_2$ and $(^2\mathrm{D})6p \; ^1\mathrm{P}$.

The 85 experimental levels were fitted by means of 26 final parameters with an rms error of 136. The parameters with their standard errors are given in table 2. The final value of 1430 ± 66 for G'_{ds} seems too low when compared with the initial value of 1890. Martin and Sugar [10] resolved a similar problem for Cu I by introducing the Sack correction

$$E_s[S(S+1)-S_c(S_c+1)],$$

where S is the net spin of d^8sp and S_c is the spin of d^8s, which absorbed the distortion in the $d-s$ interaction.

Since G'_{ps} is much larger than G'_{ds}, the $p-s$ interaction is stronger than the $d-s$ interaction. Thus the levels of the configuration d^8sp are coupled as $d^8\,(S_1L_1)_{sp}(^{1,3}\mathrm{P})SL$ and not $d^8s(S_2L_1)p\,SL$ as given in AEL.

For each of the rejected levels there is no *corresponding* theoretical level predicted in the vicinity of the experimental level given for that particular J.

The closest theoretical level of J equal to 1 for $4p''' \; ^1\mathrm{P}$ given at 125,400, is the level $^1\mathrm{D}(^3\mathrm{P})^3\mathrm{D}_1$ at around 129,000. An examination of the original paper by Shenstone [11], reveals that this level has only the three combinations with $3d^{10}a \; ^1\mathrm{S}$, $3d^94s \; ^1\mathrm{D}$ and $3d^95s \; ^1\mathrm{D}$. We omitted this level from the calculations on the basis of not being relevant to the interactions considered.

The level $4p^{\mathrm{iv}} \; ^5\mathrm{S}$ at 128,366 has altogether five combinations with even levels, the J values of which are 1, 2, and 3. Thus, the J value of this level should be 2. Since the nearest theoretically predicted level for J equal to 2 is at 137,190, the level $4p^{\mathrm{iv}} \; ^5\mathrm{S}$ was neglected.

The level $4p''' \; ^1\mathrm{D}$ only has the two combinations with $3d^94s \; ^1\mathrm{D}$ and $3d^95s \; ^1\mathrm{D}$. Thus, conceivably, this

TABLE 2. *Parameters for* Cu II $-3d^95p+3d^84s4p+3d^96p$

Parameter	Initial value	Final value
A'	134,950	134,252 ± 44
A''	121,360	121,591 ± 88
A'''	139,950	139,725 ± 117
B'	1,140	1,210 ± 5
C'	4,460	4,777 ± 34
G'_{ds}	1,890	1,430 ± 66
F'_2	370	486 ± 6
F''_2	114	88 ± 12
F'''_2	11	10 ± 9
G'_1	300	428 ± 13
G''_1	115	73 ± 13
G'''_1	56	10 ± 14
G'_3	40	74 ± 6
G''_3	61	15 ± 8
G'''_3	43	0 (Fix)
G'_{ps}	10,620	10,836 ± 40
α'	97	72 ± 6
$J(3d^84s4p-3d^95p)$	200	291 ± 110
$K(3d^84s4p-3d^95p)$	600	761 ± 56
$J(3d^84s4p-3d^96p)$	200	150 ± 114
$K(3d^84s4p-3d^96p)$	600	674 ± 351
ζ'_d	770	933 ± 25
ζ''_d	856	811 ± 46
ζ'''_d	740	843 ± 47
ζ'_p	460	686 ± 62
ζ''_p	142	184 ± 111
ζ'''_p	27	48 ± 51
rms error		136

level could be given a J assignment of either 1, 2, or 3. However, even then the smallest deviation would be almost 2000, and hence we also neglected this level.

The level $3d^84s(^4P)4p^{iv}1^o_1$, given at 140482, with a question mark, has only the combinations with $3d^84s^2\,{}^3F_2$ and $3d^94s\,{}^3D_1$. Thus the value of J for this level should be either 1 or 2. However, the nearest level of J equal to 1 is ${}^3P({}^3P){}^3S$ at 138720. Had there been several combinations of this level with even levels of J equal to 0 and 1, then perhaps the level 1^o_1, could have been assigned to either ${}^3P({}^3P){}^1S$ or $({}^2D)6p\,{}^3P_0$. However, with only the two combinations given by Shenstone [11], the level 1^o_1 has to be rejected. Similarly the level $3d^84s({}^4P)4p^{iv}3^o_1$, has only two combinations, i.e., with $3d^84s^2\,{}^3P_0$ and $3d^94s\,{}^3D_2$, both given with question marks by Shenstone [11]. As there are no theoretically predicted levels for J equal to either 0, 1, or 2 in that vicinity, this level had to be rejected as well.

It should be noted that the predicted level $4p'''\,{}^1P$, i.e., ${}^1D({}^1P){}^1P$ is at 153778, whereas the predicted level $4p^{iv}\,{}^5S$, i.e., ${}^3P({}^3P){}^5S$ is at 136223. The theoretically predicted level $p'''\,{}^1D$, i.e., ${}^1D({}^1P){}^1D$ is at 150054.

The necessity for the changes 1, 2, and 3 was already clearly evident from the initial diagonalization. Later it became apparent that in order to improve the agreement, the level $p^{iv}\,{}^5P_1$ should be assigned to the vacant level ${}^1D({}^3P){}^3P_1$.

Also from the initial diagonalization it was found that for J equal to 3 there is only one level in the neighborhood of 131000. As the theoretical level $d^8s({}^2D)p'''\,{}^1F$, i.e., ${}^1D({}^1P){}^1F$ is predicted at around 150500, it would seem that the experimental level $p'''\,{}^1F$ should be neglected. However, an examination of the combinations for the levels $p'''\,{}^1F$ and $p^{iv}\,{}^5D_3$ [11], permits an alternate more satisfying possibility. The level $p^{iv}\,{}^5D_3$ has combinations only with J equal to 3 and 4. The level $p'''\,{}^1F$ has ten combinations with even levels. Eight of these ten combinations are with triplets and seven of the ten are with J equal to 2. From the above considerations the level $p'''\,{}^1F$ must be a valid level and assigned to J equal to 3, but the level $p^{iv}\,{}^5D_3$ could conceivably be assigned to J equal to 4, i.e., to the level ${}^3P({}^3P){}^5D_4$. The level $p'''\,{}^1F$ is then assigned to $p^{iv}\,{}^5D_3$.

The exchange 7 was performed in a later iteration. After the exchange, the theoretical splittings of the terms $p^v\,{}^3P$ and $p^v\,{}^3D$ correspond more closely to the experimental splittings. It should be noted that there is considerable mixing between the eigenfunctions of the two levels $p^v\,{}^3P_2$ and $p^v\,{}^3D_2$.

Attempts to fit the level $d^8s({}^2P)p^v\,{}^1D$ at 135953 to the theoretical level ${}^3P({}^3P){}^1D$ gave deviations of the order of 1000. As this level has ten combinations with even levels, it is definitely a valid level. Since eight of the ten combinations are with triplets and since this level fits very nicely to ${}^3P({}^3P){}^5S$, we adopted the change 8.

The changes 9 to 16 were performed after numerous attempts to fit as many levels as possible with the same assignments as given in AEL. These changes are mainly due to the fact that the coupling for the configuration $3d^96p$ is far from LS – probably much closer to jl – and in addition this configuration is very strongly mixed with the terms ${}^3F({}^1P){}^3D$, ${}^3F$ and ${}^1G({}^3P){}^3F$ of $3d^84s4p$. The above facts are vividly illustrated in the "PERCENTAGE" column of table 7.

Finally, the predicted level ${}^1S({}^3P){}^3P_2$ is at around 175000 and thus the experimental level $d^8s({}^2S)p^{vii}\,{}^3P_2$ must be fitted with different assignment. The agreement is very good if this level is assigned to ${}^1D({}^1P){}^1D$, which is mixed with ${}^3P({}^1P){}^3P_2$.

The final parameters seem very reasonable, although most of the parameters pertaining to the configuration $3d^96p$ are not well defined. This is especially true for the parameter G'''_3, which had a value 1 ± 9, and thus was fixed at 0 in the final variation. The parameters β and T were eliminated as they have no significance here because no levels based on $d^8\,{}^1S$ are known experimentally.

4. The Configurations

$3d^94p+3d^95p+3d^84s4p+3d^96p$ – Cu II

Initially the parameters for the configurations $3d^95p+3d^84s4p+3d^96p$ were taken from table 2. The starting values for the parameters of $3d^94p$ were obtained from table 1. Initial values for the parameters of the interaction between the configurations $3d^9 4p$ and $3d^8 4s4p$ were estimated by considering the values obtained for the interaction $3d^n 4p - 3d^{n-1} 4s4p$ in Sc II, Ti II, and V II, as well as the results of table 2 for the interactions $3d^9 5p - 3d^8 4s4p$ and $3d^9 6p - 3d^8 4s4p$. The following starting values were used for the parameters of the interaction $3d^9 4p - 3d^8 4s4p$:

$$\begin{aligned} H(3d^9 4p - 3d^8 4s4p) &= 50 \\ J(3d^9 4p - 3d^8 4s4p) &= 500 \\ K(3d^9 4p - 3d^8 4s4p) &= 1500. \end{aligned} \tag{11}$$

In AEL, 102 levels are assigned to the four configurations $3d^9 4p$, $3d^9 5p$, $3d^8 4s4p$, and $3d^9 6p$. Omitting the same levels as in the previous section and performing the same changes in designation as well as the changes

$$({}^2\mathrm{D})4p\ {}^3\mathrm{D}_2 \longleftrightarrow ({}^2\mathrm{D})4p\ {}^1\mathrm{D}$$

$$({}^2\mathrm{D})4p\ {}^3\mathrm{D}_3 \longleftrightarrow ({}^2\mathrm{D})4p\ {}^1\mathrm{F}$$

we fitted 97 experimental levels with an rms error of 117. The final parameters are given in table 3.

The final parameters seem very reasonable. Although the standard errors especially for the parameters of the interactions between configurations are very high, a fair estimate is obtained for them. When left free, the parameter G_3''' had a value of 0.5 ± 8, and thus in the final variation we considered it fixed at zero.

Whereas the rms error for $3d^9 5p + 3d^8 4s4p + 3d^9 6p$ is 136 and the rms error for $3d^9 4p$ is 119, here the rms error is reduced to 117. Thus, the interaction between the configurations $3d^9 4p$ and $3d^8 4s4p$ improves the agreement by only a very small amount especially when compared with the large improvements in Sc II, Ti II and V II, due to the insertion of the interactions between the configurations $3d^n 4p - 3d^{n-1} 4s4p$, $n \leqslant 3$, [5].

TABLE 3. *Parameters for* Cu II$-3d^9 4p + 3d^9 5p + 3d^8 4s4p + 3d^9 6p$

Parameter	Initial value	Final value
A	69,802	$70,333 \pm 173$
A'	134,252	$134,295 \pm 110$
A''	121,591	$121,679 \pm 176$
A'''	139,725	$139,739 \pm 129$
B'	1,210	$1,210 \pm 10$
C'	4,777	$4,760 \pm 107$
G'_{ds}	1,430	$1,503 \pm 63$
F_2	344	347 ± 11
F'_2	486	484 ± 5
F''_2	88	91 ± 12
F'''_2	10	11 ± 12
G_1	305	291 ± 18
G'_1	428	393 ± 20
G''_1	73	73 ± 12
G'''_1	10	23 ± 16
G_3	38	30 ± 8
G'_3	74	69 ± 5
G''_3	15	12 ± 7
G'''_3	0	0 (Fix)
G'_{ps}	10,836	$10,799 \pm 44$
α'	72	77 ± 14
$H(3d^8 4s4p - 3d^9 4p)$	50	183 ± 74
$J(3d^8 4s4p - 3d^9 4p)$	500	795 ± 301
$K(3d^8 4s4p - 3d^9 4p)$	1,500	$3,007 \pm 542$
$J(3d^8 4s4p - 3d^9 5p)$	291	427 ± 253
$K(3d^8 4s4p - 3d^9 5p)$	761	$1,013 \pm 307$
$J(3d^8 4s4p - 3d^9 6p)$	150	398 ± 143
$K(3d^8 4s4p - 3d^9 6p)$	674	776 ± 163
ζ_d	802	816 ± 48
ζ'_d	933	938 ± 22
ζ''_d	811	817 ± 34
ζ'''_d	843	829 ± 41
ζ_p	502	525 ± 87
ζ'_p	686	630 ± 53
ζ''_p	184	152 ± 88
ζ'''_p	48	34 ± 41
rms error		117

5. The Configuration $3d^9 4f$ Cu II

The electrostatic matrices of $d^9 f$ are given on p. 299 TAS [9]. The spin-orbit matrices can be obtained from those of df by changing the sign of the matrix of ζ_d. These matrices are given on p. 206, TAS.

Since the coupling here is definitely not Russell-Saunders, we try to find initial parameters by writing down the separate matrices of $d^9 f$ for each of the seven J values. By making use of the fact that the trace of a matrix equals the sum of its eigenvalues, we obtain seven equations for the eight parameters A, $F_2(df)$, $F_4(df)$, $G_1(df)$, $G_3(df)$, $G_5(df)$, ζ_d, and ζ_f. We further make the initial approximation that $G_5(df)$ equals zero.

By solving the resulting seven equations we obtained for F_4 and G_3 very small negative values. Thus, approximately,

$$\begin{aligned} A &= 136{,}850 \\ F_2 &= 6 \\ F_4 &= 0 \\ G_1 &= 2 \\ G_3 &= 0 \\ G_5 &= 0 \\ \zeta_f &= 10 \\ \zeta_d &= 860. \end{aligned} \tag{12}$$

From an energy diagram of $3d^9 4f$ it is evident that the coupling is close to $j-l$. As explained by Racah [12], it is possible, by means of the diagonalization routine, to obtain the $j-l$ assignment of each level by taking $\zeta_d \gg F_2 > 0$, and all other parameters equal to zero.

The $j-l$ notation used in table 8 of the observed and calculated levels of $3d^9 4f$ is that of Racah as illustrated on p. 116 AEL, Vol. **II,** [6]. The final parameters obtained are given in table 4.

TABLE 4. *Parameters for* Cu II – 3d⁹4f

Parameter	Initial value	Final value
A	136,850	136,870 ± 12
$F_2\,(fd)$	6	8.3 ± 1.0
$F_4\,(fd)$	0	0.6 ± 0.4
$G_1\,(fd)$	2	1.7 ± 1.3
$G_3\,(fd)$	0	0 (Fix)
$G_5\,(fd)$	0	0 (Fix)
ζ_f	10	5.0 ± 8.3
ζ_d	860	837 ± 9
rms error		51

As the parameters G_3 and G_5, when left to vary freely, assume small negative values with standard errors larger than their actual values, the meaningful variation to consider in the least-squares is the one with G_3 and G_5 fixed at their initial values of zero.

6. The Configuration $3d^95f$ – Cu II

An energy diagram of $3d^95f$ indicates that the coupling here is almost pure $j-l$. By performing similar calculations as for $3d^94f$ for the initial parameters with G_5 equal to zero, it is found that F_4, G_3, and ζ_f have very small negative values. Then letting F_4, G_3, and ζ_f equal zero, and using the traces of J equal to 0, 1, 5, and 6, we obtain the following equations:

$$\begin{aligned} A-24F_2-\zeta_d &= 145{,}890 \\ 3A-54F_2+70G_1-\zeta_d/2 &= 439{,}873 \\ 3A-5F_2-\zeta_d/2 &= 440{,}007 \\ A-10F_2-\zeta_d &= 145{,}952. \end{aligned} \tag{13}$$

Solving (13) yields:

$$\begin{aligned} A &= 146{,}812 \\ F_2 &= 4.4 \\ G_1 &= 1.2 \\ \zeta_d &= 816. \end{aligned} \tag{14}$$

As for $3d^94f$ the $j-l$ assignments were obtained for each level, as indicated in table 9. The final parameters are given in table 5.

The parameters F_4, G_3, G_5, and ζ_f are not significant here. When left free, the standard errors in these parameters are much larger than their actual values. The latter never exceed 0.2.

TABLE 5. *Parameters for* Cu II – 3d⁹5f

Parameter	Initial value	Final value
A	146,812	146,810 ± 1
$F_2(fd)$	4.4	3.7 ± 0.1
$F_4(fd)$	0	0 (Fix)
$G_1(fd)$	1.2	0.9 ± 0.1
$G_3(fd)$	0	0 (Fix)
$G_5(fd)$	0	0 (Fix)
ζ_f	0	0 (Fix)
ζ_d	816	828 ± 1
rms error		4.5

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

In the column "NAME" the calculated designation of the term is given. The terms of d^8sp are denoted by $d^8S_1L_1$ $(sp^{1,\,3}P)$SL. For the configuration $3d^94f$ and

TABLE 6. *Observed and calculated levels of* Cu II 3d⁹4p, *individual treatment*

Name	J	Percentage	AEL		Obs. Level (cm⁻¹)	Calc. Level (cm⁻¹)	O–C	Obs. g	Calc. g
			Config.	Desig.					
$(^2D)^3P$	0	100			68,850	68,852	−2		
	1	97			67,917	67,976	−59	1.49	1.480
	2	98			66,419	66,572	−153	1.49	1.493
$(^2D)^3F$	2	$94+4(^2D)^3D$			69,868	69,718	150	0.67	0.694
	3	$69+29(^2D)^1F$			68,448	68,412	36	1.06	1.065
	4	100			68,731	68,564	167	1.23	1.250
$(^2D)^1F$	3	$62+19(^2D)^3D+18(^2D)^3F$	$3d^9(^2D_{5/2})4p$	$4p\ ^3D$	70,842	70,858	−16		1.079
$(^2D)^1D$	2	$61+33(^2D)^3D+5(^2D)^3F$	$3d^9(^2D_{5/2})4p$	$4p\ ^3D$	71,494	71,555	−61	1.08	1.044
$(^2D)^3D$	1	98			73,102	73,137	−35	0.47	0.517
	2	$61+37(^2D)^1D$	$3d^9(^2D_{3/2})4p$	$4p\ ^1D$	73,353	73,381	−28	0.99	1.103
	3	$78+12(^2D)^3F+9(^2D)^1F$	$3d^9(^2D_{3/2})4p$	$4p\ ^1F$	71,920	71,919	1		1.272
$(^2D)^1P$	1	98			73,596	73,595	1	1.04	1.002

$3d^95f$ the $j-l$ notation of Racah is used (see p. 116 AEL, Vol. II).

The entries in the columns "*J*", "OBS. LEVEL cm^{-1}" and "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, [6].

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

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

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

TABLE 7.—*Observed and calculated levels of* Cu II $3d^95p+3d^84s4p+3d^96p$

Name	*J*	Percentage	AEL		Obs. Level (cm^{-1})	Calc. Level (cm^{-1})	O–C	Calc. *g*
			Config.	Desig.				
^{3}F(^{3}P)^{5}D	0	94				111,640		
	1	93	$3d^84s(^4F)4p$	$4p'\ ^5D$	111,124?	111,249	−125	1.482
	2	92	$3d^84s(^4F)4p$	$4p'\ ^5D$	110,363	110,481	−118	1.484
	3	91	$3d^84s(^4F)4p$	$4p'\ ^5D$	109,276	109,392	−116	1.490
	4	94	$3d^84s(^4F)4p$	$4p'\ ^5D$	107,942	108,072	−130	1.496
^{3}F(^{3}P)^{5}G	2	96	$3d^84s(^4F)4p$	$4p'\ ^5G$	112,424	112,383	41	0.362
	3	89 + 7^{3}F(^{3}P)^{5}F	$3d^84s(^4F)4p$	$4p'\ ^5G$	111,877	111,811	66	0.940
	4	84 + 10^{3}F(^{3}P)^{5}F	$3d^84s(^4F)4p$	$4p'\ ^5G$	111,219	111,122	97	1.167
	5	83 + 13^{3}F(^{3}P)^{5}F	$3d^84s(^4F)4p$	$4p'\ ^5G$	110,632	110,489	143	1.281
	6	100				110,168		1.333
^{3}F(^{3}P)^{5}F	1	98	$3d^84s(^4F)4p$	$4p'\ ^5F$	114,756	114,672	84	0.021
	2	92	$3d^84s(^4F)4p$	$4p'\ ^5F$	114,482	114,373	109	0.981
	3	86 + 7^{3}F(^{3}P)^{5}G	$3d^84s(^4F)4p$	$4p'\ ^5F$	114,000	113,859	141	1.223
	4	84 + 9^{3}F(^{3}P)^{5}G	$3d^84s(^4F)4p$	$4p'\ ^5F$	113,303	113,125	178	1.324
	5	86 + 11^{3}F(^{3}P)^{5}G				112,189		1.380
^{3}F(^{3}P)^{3}G	3	74 + 22^{3}F(^{3}P)^{3}D	$3d^84s(^2F)4p$	$4p''\ ^3F$	116,644	116,690	−46	0.893
	4	81 + 21^{3}F(^{3}P)^{1}G	$3d^84s(^2F)4p$	$4p''\ ^3G$	115,360	115,402	−42	1.050
	5	94	$3d^84s(^2F)4p$	$4p''\ ^3G$	115,546	115,611	−65	1.205
^{3}F(^{3}P)^{3}D	1	88 + 6^{1}D(^{3}P)^{3}D	$3d^84s(^2F)4p$	$4p''\ ^3D$	118,071	118,069	2	0.500
	2	76 + 10^{3}F(^{3}P)^{3}F + 7^{1}D(^{3}P)^{3}D	$3d^84s(^2F)4p$	$4p''\ ^3D$	117,130	117,091	39	1.109
	3	60 + 19^{3}F(^{3}P)^{3}G + 9^{1}D(^{3}P)^{3}D	$3d^84s(^2F)4p$	$4p''\ ^3D$	116,375	116,376	−1	1.183
^{3}F(^{3}P)^{3}F	2	83 + 9^{3}F(^{3}P)^{3}D	$3d^84s(^2F)4p$	$4p''\ ^3F$	119,040	119,081	−41	0.725
	3	63 + 16^{3}F(^{3}P)^{1}F + 8^{3}F(^{3}P)^{3}D	$3d^84s(^2F)4p$	$4p''\ ^3G$	118,143	118,114	29	1.088
	4	89	$3d^84s(^2F)4p$	$4p''\ ^3F$	117,667	117,674	−7	1.242
^{3}F(^{3}P)^{1}G	4	74 + 21^{3}F(^{3}P)^{3}G	$3d^84s(^2F)4p$	$4p''\ ^1G$	118,992	119,063	−71	1.020
(^{2}D)5*p* ^{1}F	3	47 + 39(^{2}D)5*p* ^{3}F	$3d^9(^2D_{5/2})5p$	$5p\ ^3F$	120,685	120,670	15	1.003
(^{2}D)5*p* ^{1}D	2	43 + 33^{3}F(^{3}P)^{1}D + 12(^{2}D)5*p* ^{3}D	$3d^84s(^2F)4p$	$4p''\ ^1D$	120,876	120,878	−2	1.041
^{3}F(^{3}P)^{1}F	3	42 + 35(^{2}D)5*p*^{3}D + 16(^{2}D)5*p* ^{3}F	$3d^84s(^2F)4p$	$4p''\ ^1F$	121,079	121,068	11	1.134
^{3}F(^{3}P)^{1}D	2	40 + 28(^{2}D)5*p*^{3}D + 24(^{2}D)5*p* ^{3}F	$3d^9(^2D_{5/2})5p$	$5p\ ^3D$	121,982	121,974	8	0.991
(^{2}D)5*p* ^{3}P	0	99			122,224	122,231	−7	
	1	66 + 28(^{2}D)5*p* ^{1}P			120,920	120,947	−27	1.352
	2	94			120,092	120,125	−33	1.492
(^{2}D)5*p* ^{3}F	2	69 + 16(^{2}D)5*p*^{3}D + 7(^{2}D)5*p* ^{1}D			122,746	122,667	79	0.810
	3	40 + 45(^{2}D)5*p*^{1}F + 8(^{2}D)5*p* ^{3}D	$3d^9(^2D_{3/2})5p$	$5p\ ^1F$	123,017	123,033	−16	1.090
	4	97			120,790	120,718	72	1.246
(^{2}D)5*p* ^{1}P	1	60 + 33(^{2}D)5*p* ^{3}P			122,868	122,848	20	1.172
(^{2}D)5*p* ^{3}D	1	85 + 12(^{2}D)5*p* ^{1}P			123,305	123,343	−38	0.575
	2	36 + 45(^{2}D)5*p* ^{1}D + 12^{3}F(^{3}P)^{1}D	$3d^9(^2D_{3/2})5p$	$5p\ ^1D$	123,557	123,557	0	1.067
	3	53 + 30^{3}F(^{3}P)^{1}F			121,525	121,664	−139	1.204

TABLE 7.—*Observed and calculated levels of* Cu II $3d^95p+3d^84s4p+3d^96p$—Continued

Name	J	Percentage	AEL		Obs. Level (cm^{-1})	Calc. Level (cm^{-1})	O–C	Calc. g
			Config.	Desig.				
$^3P(^3P)^5P$	1	95	$3d^84s(^2D)4p$	$4p'''\,^3D$	125,569	125,659	−90	2.440
	2	89	$3d^84s(^2D)4p$	$4p'''\,^3D$	125,248	125,335	−87	1.784
	3	$89+8\,^1D(^3P)^3D$	$3d^84s(^2D)4p$	$4p'''\,^3D$	125,231	125,261	−30	1.628
$^1D(^3P)^3F$	2	$70+14\,^1D(^3P)^3D$	$3d^84s(^2D)4p$	$4p'''\,^3F$	128,570	128,480	90	0.822
	3	$69+12\,^3P(^3P)^5D+8\,^1D(^3P)^3D$	$3d^84s(^2D)4p$	$4p'''\,^3F$	128,559	128,585	−36	1.178
	4	$63+30\,^3P(^3P)^5D$	$3d^84s(^2D)4p$	$4p'''\,^3F$	128,778	128,731	47	1.327
$^1D(^3P)^3D$	1	$62+10\,^1D(^3P)^3P+10\,^3F(^3P)^3D$				128,751		0.790
	2	$59+18\,^1D(^3P)^3F+8\,^3F(^3P)^3D$	$3d^84s(^4P)4p$	$4p^{iv}\,^5P$	128,853	128,890	−37	1.113
	3	$65+9\,^1D(^3P)^3F+8\,^3P(^3P)^5P$	$3d^84s(^4P)4p$	$4p^{iv}\,^5P$	129,117	129,082	35	1.331
$^1D(^3P)^3P$	0	$63+33\,^3P(^3P)^3P$				129,001		
	1	$54+21\,^1D(^3P)^3D+18\,^3P(^3P)^3P$	$3d^84s(^4P)4p$	$4p^{iv}\,^5P$	129,760	129,721	39	1.290
	2	$73+14\,^3P(^3P)^3P+7\,^1D(^3P)^3D$	$3d^84s(^2D)4p$	$4p'''\,^3P$	130,386	130,375	11	1.490
$^3P(^3P)^5D$	0	91	$3d^84s(^4P)4p$	$4p^{iv}\,^5D$	131,206	131,045	161	
	1	91	$3d^84s(^4P)4p$	$4p^{iv}\,^5D$	130,945	131,021	−76	1.486
	2	88	$3d^84s(^4P)4p$	$4p^{iv}\,^5D$	130,945	131,012	−67	1.465
	3	$80+12\,^1D(^3P)^3F$	$3d^84s(^2D)4p$	$4p'''\,^1F$	131,044	131,106	38	1.438
	4	$65+27\,^1D(^3P)^3F$	$3d^84s(^4P)4p$	$4p^{iv}\,^5D_3$	131,313	131,377	−64	1.417
$^3P(^3P)^3D$	1	$59+18\,^3P(^3P)^3P+7\,^1D(^3P)^3P$	$3d^84s(^2P)4p$	$4p^{v}\,^3P$	134,360	134,277	83	0.765
	2	$42+28\,^3P(^3P)^3P$	$3d^84s(^2P)4p$	$4p^{v}\,^3D$	134,676	134,714	−38	1.288
	3	$56+27\,^3F(^1P)^3D$	$3d^84s(^2P)4p$	$4p^{v}\,^3D$	133,985	134,013	−28	1.323
$^3P(^3P)^3P$	0	$63+33\,^1D(^3P)^3P$	$3d^84s(^2P)4p$	$4p^{v}\,^3P$	135,484	135,440	44	
	1	$52+18\,^1D(^3P)^3P+15\,^3P(^3P)^3D$	$3d^84s(^2P)4p$	$4p^{v}\,^3D$	135,136	135,087	49	1.184
	2	$50+26\,^3P(^3P)^3D+9\,^1D(^3P)^3D$	$3d^84s(^2P)4p$	$4p^{v}\,^3P$	133,826	133,710	116	1.378
$^3F(^1P)^3G$	3	$68+15\,^1G(^3P)^3F$	$3d^84s(^4F)4p$	$4p'\,^3G$	137,078	137,061	17	0.857
	4	$67+22\,^3F(^1P)^3F$	$3d^84s(^4F)4p$	$4p'\,^3G$	135,835	135,925	−90	1.115
	5	100	$3d^84s(^4F)4p$	$4p'\,^3G$	134,111	133,887	224	1.200
$^3P(^3P)^5S$	2	92	$3d^84s(^2P)4p$	$4p^{v}\,^1D$	135,953	136,223	−270	1.958
$^1G(^3P)^3H$	4	99	$3d^84s(^2G)4p$	$4p^{vi}\,^3H$	136,694	136,594	100	0.802
	5	100	$3d^84s(^2G)4p$	$4p^{vi}\,^1H$	137,082	136,925	157	1.034
	6	100				137,359		1.167
$^3P(^3P)^1P$	1	$86+7\,^3P(^3P)^3P$	$3d^84s(^2P)4p$	$4p^{v}\,^1P$	137,213	137,118	95	1.039
$^1G(^3P)^3F$	2	$44+34\,^3F(^1P)^3F+14\,^3P(^3P)^1D$	$3d^84s(^4F)4p$	$4p'\,^3F$	137,649	137,493	156	0.744
	3	$26+27\,^3F(^1P)^3F+22(^2D)6p\,^3D$	$3d^84s(^4F)4p$	$4p'\,^3F$	136,442	136,446	−4	1.158
	4	$39+49(^2D)6p\,^3F+10\,^3F(^1P)^3F$	$3d^84s(^4F)4p$	$4p'\,^3F$	134,743	135,017	−274	1.243
$^3P(^3P)^1D$	2	$59+7\,^1G(^3P)^3F+6(^2D)6p\,^3D$				137,701		0.985
$^3F(^1P)^3D$	1	$52+21(^2D)6p\,^3D+15\,^3P(^3P)^3D$	$3d^84s(^4F)4p$	$4p'\,^3D$	137,914	137,851	63	0.546
	2	$44+21\,^3P(^3P)^1D+14(^2D)6p\,^3D$	$3d^84s(^4F)4p$	$4p'\,^3D$	136,799	136,751	48	1.119
	3	$43+36\,^3P(^3P)^3D+11\,^1D(^3P)^3D$	$3d^84s(^4F)4p$	$4p'\,^3D$	135,734	135,791	−57	1.320
$(^2D)6p\,^1F$	3	$34+43(^2D)6p\,^3F+14\,^1G(^3P)^3F$	$3d^84s(^2G)4p$	$4p^{vi}\,^3F$	138,402	138,467	−65	1.048
$^3P(^3P)^3S$	1	99				138,723		1.992
$(^2D)6p\,^1P$	1	$47+39(^2D)6p\,^3P+9\,^3F(^1P)^3D$	$3d^9(^2D_{5/2})6p$	$6p\,^3P$	139,242	139,199	43	1.138
$^3F(^1P)^3F$	2	$31+22(^2D)6p\,^3F+20\,^1G(^3P)^3F$	$3d^9(^2D_{5/2})6p$	$6p\,^3D$	139,710	139,949	−239	0.661
	3	$39+28\,^3F(^1P)^3G+22\,^1G(^3P)^3F$	$3d^9(^2D_{5/2})6p$	$6p\,^3D$	139,741	139,861	−120	0.998
	4	$53+31\,^3F(^1P)^3G+11\,^1G(^3P)^3F$	$3d^84s(^2G)4p$	$4p^{vi}\,^3F$	137,939	138,088	−149	1.187
$^3P(^3P)^1S$	0	97				140,345		
$(^2D)6p\,^3P$	0	97				140,977		
	1	$54+44(^2D)6p\,^1P$	$3d^9(^2D_{3/2})6p$	$6p\,^1P$	140,948	141,028	−44	1.276
	2	$76+19(^2D)6p\,^1D$	$3d^84s(^2G)4p$	$4p^{vi}\,^3F$	139,028	138,861	167	1.398

TABLE 7.—*Observed and calculated levels of* Cu II $3d^95p+3d^84s4p+3d^96p$—Continued

Name	J	Percentage	AEL		Obs. Level (cm^{-1})	Calc. Level (cm^{-1})	O–C	Calc. g
			Config.	Desig.				
$(^2D)6p\ ^1D$	2	$36+14(^2D)6p\,^3P+13(^2D)6p\,^3D$	$3d^9(^2D_{5/2})6p$	$6p\ ^3P$	139,217	139,053	164	1.183
$(^2D)6p\ ^3D$	1	$78+14\,^3F(^1P)^3D$			141,245	141,484	−239	0.539
	2	$53+23\,^1D(^1P)^1D+6(^2D)6p\,^3P$	$3d^9(^2D_{5/2})6p$	$6p\ ^1D$	141,542	141,240	302	1.104
	3	$56+24(^2D)6p\,^1F+8\,^3F(^1P)^3F$	$3d^9(^2D_{5/2})6p$	$6p\ ^3F$	139,331	139,295	36	1.227
$(^2D)6p\ ^3F$	2	$58+19\,^3F(^1P)^3F+11\,^1G(^3P)^3F$			141,734	141,579	155	0.723
	3	$55+23(^2D)6p\,^1F+13\,^3F(^1P)^3F$	$3d^9(^2D_{3/2})6p$	$6p\ ^1F$	141,204	141,260	−56	1.077
	4	$49+30\,^1G(^3P)^3F+18\,^3F(^1P)^3F$			139,396	139,736	−340	1.249
$^1G(^3P)^3G$	3	99				143,346		0.752
	4	99				143,435		1.050
	5	99				143,500		1.200
$^1D(^1P)^1D$	2	$52+43\,^3P(^1P)^3P$	$3d^84s(^2S)4p$	$4p^{\text{vii}}\ ^3P$	150,250	150,054	196	1.220
$^1D(^1P)^1F$	3	$83+11\,^3P(^1P)^3D$				150,521		1.036
$^3P(^1P)^3P$	0	98				152,190		
	1	$75+19\,^1D(^1P)^1P$				151,298		1.391
	2	$55+43\,^1D(^1P)^1D$				152,383		1.278
$^1D(^1P)^1P$	1	$71+22\,^3P(^1P)^3P$				153,778		1.110
$^3P(^1P)^3D$	1	93				155,336		0.518
	2	95				154,968		1.165
	3	$86+9\,^1D(^1P)^1F$				154,568		1.293
$^1G(^1P)^1H$	5	100				158,704		1.000
$^3P(^1P)^3S$	1	98				159,422		1.978
$^1G(^1P)^1F$	3	$92+6\,^1D(^1P)^1F$				159,919		1.004
$^1G(^1P)^1G$	4	100				165,078		1.000
$^1S(^3P)^3P$	0	99				173,635		
	1	99				173,934		1.500
	2	99				174,559		1.500
$^1S(^1P)^1P$	1	99				195,915		1.000

TABLE 8. *Observed and calculated levels of* Cu II $3d^9 4f$

Name $j-l$		J	AEL	Obs. level (cm^{-1})	Calc. level (cm^{-1})	O−C	Calc. g
Config.	Desig.						
$3d^9(^2D_{5/2})4f$	$4f$ [0½]	0	^3P	135,902	135,838	64	
		1	^1P	135,958	135,962	−4	0.756
$3d^9(^2D_{5/2})4f$	$4f$ [1½]	1	^3P	135,864	135,864	0	1.362
		2	^3P	135,911	135,929	−18	1.279
$3d^9(^2D_{5/2})4f$	$4f$ [2½]	2	^3D	136,014	136,037	−23	0.914
		3	^3D	135,990	136,042	−52	1.230
$3d^9(^2D_{5/2})4f$	$4f$ [3½]	3	^3F	136,036	136,128	−92	0.964
		4	^3G	136,270	136,135	135	1.168
$3d^9(^2D_{5/2})4f$	$4f$ [4½]	4	^3F	136,133	136,125	8	1.018
		5	^3G	136,161	136,133	28	1.174
$3d^9(^2D_{5/2})4f$	$4f$ [5½]	5	^3H	135,934	135,951	−17	1.016
		6	^3H	135,931	135,959	−28	1.167
$3d^9(^2D_{3/2})4f$	$4f$ [1½]	1	^3D	138,029	138,024	5	0.882
		2	^1D	138,003	137,997	6	1.324
$3d^9(^2D_{3/2})4f$	$4f$ [2½]	2	^3F	138,177	138,157	20	0.816
		3	^1F	138,131	138,165	−34	1.149
$3d^9(^2D_{3/2})4f$	$4f$ [3½]	3	^3G	138,262	138,234	28	0.824
		4	^1G	138,220	138,242	−22	1.082
$3d^9(^2D_{3/2})4f$	$4f$ [4½]	4	^3H	138,074	138,067	7	0.832
		5	^1H	138,064	138,076	−12	1.044

TABLE 9. *Observed and calculated levels of* Cu II $3d^9 5f$

Name		J	AEL	Obs. level (cm^{-1})	Calc. level (cm^{-1})	O−C	Calc. g
Config.	Desig.						
$3d^9(^2D_{5/2})5f$	$5f$ [0½]	0	^3P	145,889.6	145,891.3	−1.7	
		1	^3P	145,901.1	145,904.0	−2.9	1.360
$3d^9(^2D_{5/2})5f$	$5f$ [1½]	1	^1P	145,955.7	145,956.5	−0.8	0.749
		2	^3D	145,985.4	145,983.8	1.6	0.913
$3d^9(^2D_{5/2})5f$	$5f$ [2½]	2	^3P	145,927.5	145,931.3	−3.8	1.267
		3	^3D	145,978.4	145,983.8	−5.4	1.224
$3d^9(^2D_{5/2})5f$	$5f$ [3½]	3	^3F	146,021.5	146,026.3	−4.8	0.965
		4	^3G	146,029.5	146,026.3	3.2	1.195
$3d^9(^2D_{5/2})5f$	$5f$ [4½]	4	^3F	146,024.0	146,025.8	−1.8	0.993
		5	^3G	146,032.5	146,025.8	6.7	1.176
$3d^9(^2D_{5/2})5f$	$5f$ [5½]	5	^3H	145,945.8	145,943.8	2.0	1.015
		6	^3H	145,951.7	145,943.8	7.9	1.167
$3d^9(^2D_{3/2})5f$	$5f$ [1½]	1	^3D	148,016.3	148,014.6	1.7	0.892
		2	^1D	147,987.7	147,989.7	−2.0	1.333
$3d^9(^2D_{3/2})5f$	$5f$ [2½]	2	^3F	148,066.3	148,068.4	−2.1	0.820
		3	^1F	148,061.7	148,068.4	−6.7	1.157
$3d^9(^2D_{3/2})5f$	$5f$ [3½]	3	^3G	148,103.2	148,104.7	−1.5	0.821
		4	^1G	148,105.6	148,104.7	0.9	1.083
$3d^9(^2D_{3/2})5f$	$5f$ [4½]	4	^3H	148,033.7	148,026.4	7.3	0.829
		5	^1H	148,028.8	148,026.4	2.4	1.042

The work described in this paper was supported in part by the National Bureau of Standards, Washington, D.C.

The author wishes to acknowledge with everlasting gratitude and appreciation the unremitting kind interest in this work by the late Professor Giulio Racah.

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(Paper 73A6–573)