APPENDIX B. BACKGROUND AND ENERGY LOSS CORRECTIONS

The quantities N_x and N_C in (A-5) represent counting rates *due to scattering* from targets x and C. Then if B represents counting rate due to background when a thick target is in position, $N_x=N_x'-B$, where N_x' is the measured counting rate when x is the scatterer. Letting primes indicate *measured* counting rates generally, we also have $N_{B^{10}}=N_{B^{10}}'-B$ and the left-hand side of (A-5) can be written as

$$\frac{N_x}{N_C}=\frac{N_x'-B}{N_C'-B}=\frac{N_x'-N_{B^{10}}'}{N_C'-N_{B^{10}}'}+\frac{N_{B^{10}}}{N_C'-N_{B^{10}}'}, \qquad \text{(A-6)}$$

where we have neglected $N_{B^{10}}$ in the denominator since $N_{B^{10}}\ll(N_C'-N_{B^{10}}')$. Since the second term on the right-hand side of (A-6) is small for $x=Ni_2B$ or B_2O_3, we can combine (A-5) and (A-6) to give

$$F(\sigma_s/\sigma_t)_{x0}=\frac{N_{x0}'-N_{B^{10}}'}{N_C'-N_{B^{10}}'}\left[1+\frac{(\sigma_s/\sigma_t)_{B^{10}}}{(\sigma_s/\sigma_t)_{x0}}\right]. \qquad \text{(A-7)}$$

The bracketed factor then corrects the background measurement for the small B^{10} scattering contribution. A similar analysis yields for Au

$$F(\sigma_s/\sigma_t)_{Au}=\frac{N_{Au}'-N_{B^{10}}'}{N_C'-N_{B^{10}}'}+F(\sigma_s/\sigma_t)_{B^{10}}. \qquad \text{(A-8)}$$

Since $F(\sigma_s/\sigma_t)$ has been defined as the scattering ratio to carbon for infinitely heavy nuclei, the right-hand sides of (A-7) and (A-8) must further be multiplied by the factors indicated in Secs. III B and III C to correct at least the "singly scattered" counting rate for the finite mass effect. The latter correction arises in the following manner. In writing (A-1) above, the σ_t appearing in the last bracket is more correctly σ_t', the cross section of the target nuclei for neutrons of energy $E'<E$ after collision. Then using the fact that $\langle\cos\theta_0/\cos\theta_1\rangle_{Av}\approx 1$, (σ_s/σ_t) in (A-2) becomes $2\sigma_s/(\sigma_t+\sigma_t')$. Thus, multiplication of the right-hand sides of (A-7) and (A-8) by $(\sigma_t+\sigma_t')/2\sigma_t$ corrects for this effect.

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Configuration Interaction in Mn II

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The theoretical formulas for d^6 and d^5s are compared with the experimental data of Mn II. The relative positions of these configurations in Mn II allow the magnitude of configuration interaction to be determined accurately without the use of a least-squares calculation. Over-all agreement between theory and experiment is improved by the use of separate parameters in the two configurations and by the introduction of the effects of configuration interaction.

The positions of the terms not yet known experimentally are predicted as a help in further analysis of this spectrum. The positions of terms of the d^5s configuration are believed to be predicted with better than usual accuracy by the use of a correction term proportional to $L(L+1)$.

I. TERM VALUES OF Mn II WITHOUT CONFIGURATION INTERACTION

CURTIS[1] has recently extended the experimental analysis[2] of the $3d^54s$ and $3d^6$ configurations of Mn II to include some of the triplet terms, thus making possible a further theoretical analysis of this spectrum.

The term values in Russell-Saunders coupling for the d^5s configuration of Mn II have been calculated by Bowman[3] without allowance for configuration interaction; his results are valid for the terms which are only slightly affected by configuration interaction (i.e., the majority of terms in d^5s), since his least square fit was based on terms that are probably almost free of effects of configuration interaction. We have repeated his least-squares calculation, but have included the additional experimental values[1] for d^5s. The results are given in part (1) of Table I and are essentially in agreement with Bowman's results (the mean deviation of his data is 447 cm^{-1} compared to 412 cm^{-1} for the d^5s terms in Table I). A comparison of the d^6 data with theory, also neglecting effects of configuration interaction, is given in the same column. The mean deviation between theory and experiment, using separate parameters in d^5s and d^6 and neglecting configuration interaction is 678 cm^{-1}.

The parameters used in the calculation of Table I are those in the formulas of Racah.[4] The d^6 formulas are in the same form as the d^4 formulas with "$6A$" replaced by "A." In the d^5s formulas, "$10A$" (in Racah's formulas for d^5) was replaced by "D" and the proper multiple of G_2 was subtracted.[5] The parameters were evaluated by least squares.

An effort was made to fit the data using the same B and C parameters in d^5s and d^6, again neglecting configuration interaction, with the result shown in part 2

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[1] C. W. Curtis, Phys. Rev. **78**, 343 (1950).

[2] Other experimental values were taken from C. W. Curtis, Phys. Rev. **53**, 474 (1938). The ^5D of $3d^6$ and the ^7S and ^5S of $3d^54s$ were found previously by M. A. Catalan, Phil. Trans. Roy. Soc. (London), **A223**, 127 (1922); An. Soc. Espan. **26**, 67 (1928); Russell, Astrophys. J. **66**, 233 (1927); and Black and Duffendack, Science **66**, 402 (1927).

[3] D. S. Bowman, Phys. Rev. **59**, 386 (1941). The term values for d^5 configuration were first calculated by M. A. Catalan and M. T. Antunes, Z. Physik **102**, 432 (1936).

[4] G. Racah, Phys. Rev. **62**, 438 (1942); **63**, 367 (1943). These are referred to as II and III, respectively.

[5] J. H. Van Vleck, Phys. Rev. **45**, 405 (1934).

TABLE I. Term values of Mn II (cm^{-1}). (1) No configuration interactions, separate parameters; (2) No configuration interactions, same B and C in both configurations; (3) With configuration interactions, separate parameters; (4) With configuration interaction and a $L(L+1)$-correction (d^5s configuration only). Terms belong to d^5s or d^6 configuration respectively if they are or are not written with a parent term.

Term	Obs.	(1) Calc.	(1) Diff.	(2) Calc.	(2) Diff.	(3) Calc.	(3) Diff.	(4) Calc.	(4) Diff.
$({}^6S){}^7S$	0	99	99	693	693	155	155	10	10
$({}^6S){}^5S$	9473	9732	259	10170	697	9742	269	9578	105
${}^5D$	14584	14928	344	13465	−1119	14844	260		
$({}^4G){}^5G$	27571	26608	−963	26649	−922	26616	−955	27474	−97
$({}^4P){}^5P$	29912	30120	208	30291	379	30215	303	29870	−42
${}^3P$	30277	31347	1070	31253	976	31088	811		
${}^3H$	30650	29598	−1052	29476	−1174	29603	−1047		
${}^3F$	31622	31798	176	31870	248	31753	131		
$({}^4D){}^5D$	32828	33058	230	32757	−71	33000	172	32694	−134
$({}^4G){}^3G$	33215	33030	−185	32967	−248	32447	−768	33232	17
${}^3G$	34874	33412	−1462	33839	−1035	34147	−727		
$({}^4P){}^3P$	36321	36541	220	36609	288	36733	412	36363	42
${}^1I$		36933				36954			
${}^1G$		38178				37984			
${}^3D$	37842	38752	910	39947	2105	38215	373		
$({}^4D){}^3D$	39814	39480	−334	39075	−739	40022	208	39650	164
$({}^2I){}^3I$		38549				38599		40888	
$({}^2I){}^1I$		41760				41815		44091	
${}^1S$		42027				41771			
$({}^4F){}^5F$	43458	43941	483	43380	−78	43814	356	43746	288
$({}^2D){}^3D$						43720		43461	
$({}^2F){}^3F$						43960		44160	
${}^1D$						44055			
$({}^2F){}^1F$						46710		46867	
$({}^2D){}^1D$						46656		46412	
$({}^2H){}^3H$						46737		48100	
${}^1F$						49322			
$({}^2G){}^3G$						48602		49063	
$({}^2H){}^1H$						49927		51283	
$({}^4F){}^3F$						50206		50124	
$({}^2G){}^1G$						51785		52232	
$({}^2F'){}^3F$						52166		51967	
${}^3F'$						55450			
$({}^2F'){}^1F$						55582		55380	
${}^3P'$						55860			
$({}^2S){}^3S$						57638		56438	
${}^1G'$						60602			
$({}^2S){}^1S$						61048		59841	
$({}^2D'){}^3D$						63066		62269	
$({}^2D'){}^1D$						66077		65273	
$({}^2G'){}^3G$						69403		69380	
$({}^2G'){}^1G$						72627		72598	
${}^1D'$						77121			
$({}^2P){}^3P$						84855		83117	
$({}^2P){}^1P$						88005		86258	
$({}^2D''){}^3D$						90853		89401	
${}^1S'$						95127			
$({}^2D''){}^1D$						94071		92613	
$A(d^6)$		30948.3		31789.4		31734.6		—	
$D(d^5s)$		40375.6		39131.2		39876.5		38744.0	
$B(d^6)$		762.85		872.58		802.57		—	
$B(d^5s)$		921.41		872.58		906.63		878.88	
$C(d^6)$		2904.6		3130.0		2879.6		—	
$C(d^5s)$		3137.9		3130.0		3159.4		3139.3	
G_2		1605.4		1579.5		1597.9		1594.6	
H_2		—		—		99		99	
α		—		—		—		69.2	
Mean deviation		$\pm 678\ cm^{-1}$		$\pm 887\ cm^{-1}$		$\pm 551\ cm^{-1}$		$\pm 130\ cm^{-1}$	

TABLE II. Intervals of experimentally observed ^3D and ^3G terms (cm^{-1}). The $d^6\,{}^3G$ and the $d^5s\,{}^3D$ are assumed to both have the following percentages of d^6 and d^5s configuration respectively: (*A*) 50 percent–50 percent; (*B*) 64 percent–36 percent; (*C*) 36 percent–64 percent. The $d^5s\,{}^3G$ and the $d^6\,{}^3D$ have percentages of d^6 and d^5s configuration which are complementary.

Interval		Obs.	Calculated *A*	*B*	*C*
d^6	$^3D_3-{}^3D_2$	3.2	−30	−56	−4
d^6	$^3D_2-{}^3D_1$	36.3	46	47	45
d^5s	$^3D_3-{}^3D_2$	−5.2	5	22	−12
d^5s	$^3D_2-{}^3D_1$	−13.2	34	36	31
d^6	$^3G_5-{}^3G_4$	−148.6	−98	−125	−70
d^6	$^3G_4-{}^3G_3$	−94.0	−78	−100	−56
d^5s	$^3G_5-{}^3G_4$	−100.9	−98	−70	−125
d^5s	$^3G_4-{}^3G_3$	−30.1	−78	− 56	−100

of Table I. The mean deviation of 887 cm^{-1} is much larger than the deviation of the preceding calculation, so that the use of separate parameters in the two configurations is desirable.

II. TERM VALUES OF Mn II WITH CONFIGURATION INTERACTION

The ground configuration $3d^54s$ of Mn II interacts with the configurations $3d^6$ and $3d^44s^2$. The matrix elements of these interactions are given in III.[6]

The ^5D of d^4s^2 is the only term of this configuration found experimentally.[2] From the known position of this ^5D, and the values of the parameters already evaluated for d^5s, the effects of configuration interaction of d^4s^2 with either d^6 or d^5s can be estimated. The mean effect on these levels for which experimental data are available is a depression of 40 cm^{-1}; the lowering of any one of these levels is less than 100 cm^{-1}. Since the mean deviation of the final result is 551 cm^{-1}, the effects of interactions with the d^4s^2 configuration might be expected to be unimportant, and the estimate shows that this is so. Interactions with the d^4s^2 configuration have therefore been neglected to simplify the calculation.

Having eliminated the interactions of d^5s and d^6 with d^4s^2, we now turn to consider their interaction with each other. By consideration of those terms which show the effects of configuration interaction most strongly, the radial parameter H_2 for the interaction between d^5s and d^6 configurations has been evaluated in Sec. III as $H_2=99\pm3$ cm^{-1}. The usual procedure is to evaluate this parameter by least squares adjustment of all the data; this is usually an inaccurate procedure, since large changes of this parameter have small effects relative to the mean deviation between theory and experiment.[7]

The improved agreement produced by introducing the effects of configuration interaction between d^5s and d^6 using $H_2=99$ cm^{-1} can be shown by using the parameters already obtained in part (1) of Table I, and calculating the new theoretical values of the energy. The mean deviation is reduced from 678 cm^{-1} to 577 cm^{-1} when this is done. Slightly better agreement can be obtained by carrying out a least squares adjustment to obtain new values of the other parameters, excluding H_2. The results of this calculation are given in part (3) of Table I. The mean deviation is reduced finally to 551 cm^{-1} when effects of configuration interaction are included.

In getting the eigenvalues of the matrices, we first diagonalized with respect to any pairs of terms that were close together, and then determined the effects of other levels with second-order perturbation theory. The maximum configuration interactions evaluated with perturbation theory were all less than 200 cm^{-1}; the off-diagonal elements of configuration interaction were in all cases less than $\frac{1}{4}$ of the intervals between the levels they connected so that the maximum error in the calculated eigenvalues resulting from the use of perturbation theory is about 15 cm^{-1}.

III. EVALUATION OF THE PARAMETER H_2

The two ^3G terms have an experimentally observed separation of 1659 cm^{-1}, and since the maximum permissible interaction is half of the separation, an upper limit of $H_2\leqslant 102$ cm^{-1} can be established in order that the observed separation will not not be exceeded. The separation of the pair of ^3D terms has an experimental value of 1972 cm^{-1} and this sets a slightly higher limit of $H_2\leqslant 104$ cm^{-1} on the interaction parameter.

In setting the lower limit on the interaction parameter, it is first assumed that Curtis's assignment of the two ^3G and the two ^3D terms to the d^5s or d^6 configurations is correct, and that interactions with other levels

[6] The $d^6-d^4s^2$ interaction is given by Eq. (75) of III; the $d^4s^2-d^5s$ interaction is obtained from Eq. (81) and Table XXII; the d^6-d^5s interaction is obtained from Table XXII by use of the relation,

$$(d^6v'S'L|\Sigma e^2/r_{ij}|d^5(vSL)sS'L)$$
$$=(-1)^{S+S'+\frac{1}{2}v}\left(\frac{2S+1}{2S'+1}\right)^{\frac{1}{2}}(d^5vSL|\Sigma e^2/r_{ij}|d^4(v'S'L)sSL).$$

This may be verified by use of (79) of III.

[7] For convenience the theory was assumed to be exact. This is perhaps misleading, since there is such a large error remaining in the final result after effects of configuration interaction with nearby terms is accounted for (i.e., the mean deviation of 551 cm^{-1} in part 4 of Table I has not been identified in the literature with any specific source of error). We were able to consider the theory exact, because the errors in both ^3G and in both ^3D terms are probably nearly the same, as the results in part 4 of Table I seem to indicate. Since only differences between theoretical formulas were compared with experiment, the errors tended to cancel. This line of reasoning is justified generally for Mn II only by the over-all consistency obtained in the results.

Usually one cannot find interacting terms which are sufficiently close together to set an upper limit on the interaction parameters which is small enough to be of any use. It seems rather important to decide how far in error a least-squares determination of the parameters may be, and whether it might not be more accurate to estimate values from neighboring spectra if no better method is available. We might point out, that the separation of a pair of ^2H terms of Cr II sets an upper limit $H_2\leqslant 121$ cm^{-1} on the interaction parameter in that spectrum. Since A. A. Schweizer [Phys. Rev. **80**, 1080 (1950)] obtains a value $H_2=150$ cm^{-1} by least squares, the least-squares evaluation would seem to be too high.

not experimentally known will have negligible effect in establishing these assignments. It is then possible to show that the parameter "B" must have a larger value in the d^5s configuration than in the d^6 configuration, since one would otherwise be obliged to interchange the assignments of one or the other pairs of terms. The larger the magnitude of the difference of B-values, the less configuration interaction is needed to account for the observed separations, so that the largest reasonable difference in B-values sets a lower limit on the magnitude of configuration interaction. This lower limit is not very sensitive to the magnitude of the assumed difference in B-values, as long as this difference is not unreasonably large. Using the difference of 160 cm^{-1} from part (1) of Table I, the maximum possible separation of the ^3D and ^3G terms without configuration interaction is about 550 cm^{-1}. In order that configuration interaction cause the remaining part of the observed separation, the parameter H_2 must have a value of about 96 cm^{-1}.

We take the value $H_2=99\pm3$ cm^{-1} which is the mean of the upper and lower limits.

IV. VERIFICATION OF ASSIGNMENTS FROM INTERVALS

The assignments of the pair of ^3G and the pair of ^3D terms of d^5s and d^6 are the least certain of Curtis's assignments owing to the strong configuration interaction. In this section we obtain additional confirmation of these assignments by consideration of the intervals, and in Sec. V from a consideration of the triplet-quintet separation. The analysis of both these sections also confirms the conclusions of Sec. III in regard to the separation of these pairs of terms in the absence of configuration interaction.

In Table II we have calculated the intervals of the pair of ^3D and the pair of ^3G terms for three possible cases; (A) the terms are a 50–50 mixture of d^5s and d^6 configurations, (B) the term of higher energy (i.e., the d^5s ^3D and the d^6 ^3G according to Curtis's assignments) contains 64 percent of d^6 configuration and 36 percent of d^5s configuration, and (C) the term of higher energy contains 64 percent of d^5s configuration and 36 percent of d^6 configuration. The term of lower energy contains the complementary composition, e.g., 36 percent of d^6 and 64 percent of d^5s in case B. The parameter, ζ_d, which defines the elements of spin-orbit interaction in the d^6 configuration was assumed to have a value 260 cm^{-1} which is the value found in the $3d^6$ ^5D; the corresponding parameter in the $3d^54s$ configuration was taken as 300 cm^{-1}, midway between the value in the $3d^6$ ^5D and the $3d^44s^2$ ^5D. A more accurate interpolation[8] was not considered necessary for these calculations. The matrix elements of spin-orbit interaction were taken from III.[9]

In carrying out the calculations for the pair of ^3G terms it was assumed that the splitting was due solely to the diagonal spin-orbit interaction of the d^6 component of the eigenfunction. Comparison of the calculated results with experiment shows that case B, the choice which agrees with Curtis's assignments, is strongly favored. More extended calculations that include the effects of nondiagonal spin-orbit interaction with other terms, largely explain the remaining deviation between case B and experiment so that there is little doubt about the assignments of the ^3G terms being correct.

For the calculation of the intervals of the pair of ^3D terms it was necessary to include the large effects of nondiagonal spin-orbit interaction with the $d^5(^4P)s\,^3P$ along with the splitting due to the diagonal spin-orbit interaction of the d^6 component of the eigenfunction. The calculated intervals agree best with experiment for case C, which is the case in agreement with Curtis's assignments. The large error in explaining the d^5s $^3D_2-{}^3D_1$ interval may be partly due to the neglect of effects of configuration interaction with other ^3D terms, since nondiagonal spin-orbit interaction with other levels seems to explain only about half the error.

It would require overly elaborate calculations to explain fully the observed intervals. However, the best ratio of d^6 to d^5s eigenfunction is moderately well defined by the approximate calculation of Table II; i.e., the two ^3G and the two ^3D terms have approximately a 64 percent/36 percent composition, with the dominating configuration the one required by Curtis's assignments. The separation of the terms in the absence of configuration interaction is 7/25 of the experimentally observed separation for this ratio of components, or 464 cm^{-1} for the pair of ^3G terms and 552 cm^{-1} for the pair of ^3D terms. Within the accuracy of the calculations, this is consistent with the upper limit of 550 cm^{-1} placed on the separation in Sec. III.

V. VERIFICATION OF ASSIGNMENTS FROM QUINTET-TRIPLET SEPARATION

We have found[10] that in the d^5s configuration of Fe III the parameter G_2 has very consistent values when determined by subtraction of the experimental values of terms based on the same parent. If this is assumed to be true for all d^5s terms that are free from effects of configuration interaction, then from the experimentally determined positions of the d^5s ^5G and the d^5s ^5D the positions of the corresponding triplets of d^5s, which are based on the same parent, can be determined

[8] H. A. Robinson and G. H. Shortley, Phys. Rev. **52**, 713 (1937).

[9] For the d^6 configuration relation (25) and Table XIII of III are used. For the d^5s configuration, Table XIV is used with the following relation which is derived from II, Eq. (44);

$$(d^n(vSL)sS_1LJ|\Sigma\xi(r_i)\mathbf{l}_i\cdot\mathbf{s}_i|d^n(v'S'L')sS_1'L'J)$$
$$=(-)^{L'-S'-J-\frac{1}{2}}W(S_1LS_1'L';J1)W(SS_1S'S_1';\tfrac{1}{2}1)$$
$$\times[(2S_1+1)(2S_1'+1)]^{\frac{1}{2}}(d^nvSL\|30^{\frac{1}{2}}V^{(11)}\|d^nv'S'L')\zeta_d.$$

The nondiagonal elements of the $d^5(^4D)s\,^3D-d^5(^4P)s\,^3P$ spin-orbit interaction are found to be $\frac{1}{4}(35)^{\frac{1}{2}}\zeta_d$ and $5/12(7)^{\frac{1}{2}}\zeta_d$ for the elements with $J=2$ and $J=1$ respectively.

[10] (To be published.)

as they would be in the absence of effects of configuration interaction. The relationship of the hypothetical position to the center of gravity of the pair of terms then determines the assignments and the separation in the absence of configuration interaction.

The theoretical separation of quintets and triplets is found to be $4G_2=6310\pm100$ cm^{-1} from the G_2 value of the $^5S-^7S$ separation. To be on the safe side, an error has been assumed which is over three times that needed to include the results of five such determinations in Fe III.[10] In Mn II the $^5P-^3P$ separation leads to a value $4G_2=6409$ cm^{-1}, or if the effects of configuration interaction on the ^3P level are allowed for, $4G_2=6299$ cm^{-1}. This is in close agreement with the value determined from the $^5S-^7S$ separation.

The position of the ^3G of d^5s should be 33881 ± 100 cm^{-1} in the absence of configuration interaction. The center of gravity of the pair of ^3G terms is at 34045 cm^{-1} so that the ^3G of lower energy should be assigned to d^5s in agreement with Curtis's assignments. The separation of the pair of ^3G terms would be 328 ± 200 cm^{-1} in the absence of configuration interaction, which is in agreement with an upper limit of 550 cm^{-1} given in Sec. III and Sec. IV.

The position of the ^3D of d^5s should be 39138 ± 100 cm^{-1} in the absence of configuration interaction. The center of gravity of the pair of ^3D terms is at 38828 cm^{-1} so that the ^3D of higher energy should be assigned to d^5s in agreement with Curtis's assignments. The separation of the pair of ^3D terms would be 620 ± 200 cm^{-1} in the absence of configuration interaction, which is somewhat above the upper limit of 550 cm^{-1}. If a correction is made to account for the effect of the configuration interaction of a ^3D level which is theoretically located at 43720 cm^{-1}, then the separation in the absence of configuration interaction between the two observed ^3D terms is reduced from 620 ± 200 cm^{-1} to 390 ± 200 cm^{-1}.[11]

VI. "CORRECTED" TERM VALUES FOR THE d^5s CONFIGURATION

We have found[10] that a correction of the form

$$\Delta E=\alpha L(L+1)$$

added to the theoretical term values for the d^5s configuration of Fe III reduces the mean deviation (for 21 experimental values) from 857 cm^{-1} to 105 cm^{-1}. We are trying to find a theoretical basis for this correction, but at present it must be accepted on an empirical basis and assumed applicable to all d^5s configurations.

In Mn II, uncertainty in the location of d^6 terms leads to errors in the calculation of the positions of d^5s terms which are important when mean deviations of 100 cm^{-1} are being considered; this is due to the large effects of configuration interaction on the positions of d^5s terms in Mn II. This error was partly overcome by correcting the experimental values of d^6 terms (whenever these values were available) for the effects of configuration interaction to get the diagonal elements of electrostatic interaction for d^6. The error in doing this is considerably less than the error in the theoretically calculated diagonal elements of d^6. The effect of configuration interaction due to d^4s^2 was again neglected, chiefly because it was felt that there was too little experimental data to justify the assumptions necessary for its inclusion; this also could lead to appreciable errors.

The least-squares calculation is carried out for d^5s in a way similar to that used in Sec. I, except that the correction ΔE is first added to each term and the experimental data is corrected for effects of configuration interaction. Using the parameters obtained in this way, the eigenvalues with configuration interaction are then calculated. The result does not depend on the fact that the d^5s experimental data were corrected, as this was only an intermediate step carried out to obtain the best choice of d^5s parameters. The dependence on effects of configuration interaction with d^6 is defined in such a way that the eigenvalues of the matrices for the d^6 terms are required to equal the experimental values for the d^6 terms where such values are available; for other d^6 terms, the diagonal elements for the d^6 parts of the matrix are evaluated with the parameters of part (3) of Table I. The results of this calculation are given in part (4) of Table I; the mean deviation is 130 cm^{-1}.

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[11] A small effect of configuration interaction on the ^5D is included.