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Theory of Complex Spectra. III

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The consideration of the phases of the fractional-parentage coefficients allows the extension of the matrix methods to configurations with more than two equivalent electrons. Tables are given for the parentages of the terms of p^n and d^n. Applications are made to the spin-orbit interaction of the d^n terms and to the electrostatic interaction between the configurations d^n, $d^{n-1}s$, and $d^{n-2}s^2$. Errata in Part II are indicated.

§1. INTRODUCTION

THIS paper deals chiefly with the application of matrix methods to calculations within configurations with more than two equivalent electrons.

It is known that the eigenfunctions built up with the usual vector-coupling formulas[1] are not antisymmetrical as required from the exclusion principle and they must be antisymmetrized afterwards. But if certain of the electrons are equivalent, these antisymmetrized states are no longer normalized and some of them are linearly dependent, so that the calculations become very complicated.

An escape from these difficulties was proposed by Gray and Wills[2] who started from the nlm_sm_l scheme with antisymmetrized eigenfunctions and computed the SL eigenfunctions using angular-momentum operators and orthogonality considerations. This method leads to an orthonormal system of eigenfunctions, but since it gives up the vector-coupling formulas, the matrix of each operator must at first be calculated in the nlm_lm_l scheme and then transformed to the SL scheme, and no use may be made of the powerful matrix methods developed in Chapter III of TAS[1] and also extended in a previous paper of the author.[3]

In order to make full use of the above-mentioned methods, we shall calculate the eigenfunctions of the configuration l^n as linear combinations of the eigenfunctions obtained by the addition of a further electron l to the configuration l^{n-1}. This possibility was already indicated by Goudsmit and Bacher,[4] who introduced the concept of fractional parentage; but they were interested only in the squares of the coefficients of these linear combinations and calculated them with a procedure which, being based on a diagonal-sum method, did not permit them to separate the fractional parentages of duplicated terms.[5] The consideration of the phases of the coefficients of fractional parentage will enable us to calculate them separately also for terms of the same kind occurring in a given configuration and to calculate the matrix elements of every symmetrical operator between configurations containing equivalent electrons.

The fractional parentages of the configurations p^n and d^n are calculated in §3 and §4, whilst §2 contains a lemma on which these calculations are based and §5 deals with the matrices of symmetrical operators. In §6 an analysis is made of the structure of the configurations l^n in connection with the appearance of more terms of the same kind, and §7 contains an application to configuration interactions.

§2. TRANSFORMATIONS BETWEEN THE DIFFERENT COUPLING SCHEMES OF THREE ANGULAR MOMENTA

If we add two angular momenta j_1 and j_2, the magnitude J of the resulting vector and its z-component M characterize completely the states of the system; but if we add three angular momenta, several states may occur with the

[1] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge, 1935) (which we shall denote by TAS), §14[3].
[2] N. M. Gray and L. A. Wills, Phys. Rev. **38**, 248 (1931); TAS §5[8].
[3] G. Racah, Phys. Rev. **62**, 438 (1942) (which we shall denote by II). We refer to this paper and to TAS for definitions, notations, and bibliographical indications.
[4] S. Goudsmit and R. F. Bacher, Phys. Rev. **46**, 948 (1934).
[5] D. H. Menzel and L. Goldberg, Astrophys. J. **84**, 1 (1936).

TABLE I. $(p^3SL\{|p^2(S'L')pSL)$. The different rows are normalized separately, and N is the normalization factor of each linear combination.

p^3	N	p^2 ${}^1S$	${}^3P$	${}^1D$
${}^4S$	1	0	1	0
${}^2P$	$18^{-\frac{1}{2}}$	2	-3	$-5^{\frac{1}{2}}$
${}^2D$	$2^{-\frac{1}{2}}$	0	1	-1

same J and M and a complete characterization of the states needs the specification of the type of coupling of the vectors.

We may for instance couple at first j_1 and j_2 and then add j_3 to their resultant J': In this case the eigenfunctions are

$$\psi({}_1jj_2(J')j_3JM)=\sum_{m_3M'}\psi(j_1j_2J'M')\phi(j_3m_3)\cdot(J'j_3M'm_3|J'j_3JM)$$
$$=\sum_{m_1m_2m_3M'}\phi(j_1m_1)\phi(j_2m_2)\phi(j_3m_3)\cdot(j_1j_2m_1m_2|j_1j_2J'M')\cdot(J'j_3M'm_3|J'j_3JM);\quad(1)$$

but we may also couple at first j_2 and j_3 and then add their resultant J'' to j_1, and in this case the eigenfunctions are

$$\psi(j_1,\,j_2j_3(J''),\,JM)=\sum_{m_1m_2m_3M''}\phi(j_1m_1)\phi(j_2m_2)\phi(j_3m_3)\cdot(j_2j_3m_2m_3|j_2j_3J''M'')\cdot(j_1J''m_1M''|j_1J''JM).\quad(2)$$

The unitary transformation which connects these two representations of the same system is

$$(j_1j_2(J')j_3J|j_1,\,j_2j_3(J''),\,J)=\sum_{m_1m_2m_3M'M''}(J'j_3JM|J'j_3M'm_3)\cdot(j_1j_2J'M'|j_1j_2m_1m_2)\cdot(j_2j_3m_2m_3|j_2j_3J''M'')\cdot(j_1J''m_1M''|j_1J''JM);\quad(3)$$

introducing the expression (16')II for the transformation coefficients for the addition of two angular momenta and using Eqs. (19)II and (37)II we obtain

$$(j_1j_2(J')j_3J|j_1,\,j_2j_3(J''),\,J)=[(2J'+1)(2J''+1)]^{\frac{1}{2}}W(j_1j_2Jj_3;\,J'J''),\quad(4)$$

where W is the function defined by (36')II.

It is sometimes useful to consider the changing of the coupling together with a change in the order of the vectors; the same way as before yields

$$(j_1j_2(J')j_3J|j_1j_3(J'')j_2J)=[(2J'+1)(2J''+1)]^{\frac{1}{2}}W(J'j_3j_2J'';\,Jj_1).\quad(5)$$

If we have three electrons or groups of electrons, the transformations between the different parentages in SL coupling are obvious extensions of (4) and (5): For instance,

$$(s_1l_1s_2l_2(S'L')s_3l_3SL|s_1l_1,\,s_2l_2s_3l_3(S''L''),\,SL)=[(2S'+1)(2S''+1)(2L'+1)(2L''+1)]^{\frac{1}{2}}\cdot W(s_1s_2Ss_3;\,S'S'')W(l_1l_2Ll_3;\,L'L'');\quad(6)$$

a particular case of this transformation was considered in TAS 6[8] 14.

§3. THE EIGENFUNCTIONS OF GROUPS OF EQUIVALENT ELECTRONS

If we couple two equivalent electrons with the usual vector-coupling formulas, we obtain antisymmetric or symmetric eigenfunctions according to whether $S+L$ is even or odd (TAS, p. 231); the eigenfunctions of the states with $S+L$ even are therefore the normalized eigenfunctions of the allowed states of l^2.

If we add in the same way to the allowed states of l^2 a third l electron, the obtained eigenfunctions are in general antisymmetric only with respect to the first two electrons, but not with

TABLE II. $(d^3vSL\{|d^2(v'S'L)dSL)$.

d^3	N	d^2 ${}_0{}^1S$	${}_2{}^3P$	${}_2{}^1D$	${}_2{}^3F$	${}_2{}^1G$
${}_3{}^2P$	$30^{-\frac{1}{2}}$	0	$7^{\frac{1}{2}}$	$15^{\frac{1}{2}}$	$-8^{\frac{1}{2}}$	0
${}_3{}^4P$	$15^{-\frac{1}{2}}$	0	$-8^{\frac{1}{2}}$	0	$-7^{\frac{1}{2}}$	0
${}_1{}^2D$	$60^{-\frac{1}{2}}$	4	-3	$-5^{\frac{1}{2}}$	$-21^{\frac{1}{2}}$	-3
${}_3{}^2D$	$140^{-\frac{1}{2}}$	0	-7	$45^{\frac{1}{2}}$	$21^{\frac{1}{2}}$	-5
${}_3{}^2F$	$70^{-\frac{1}{2}}$	0	$28^{\frac{1}{2}}$	$-10^{\frac{1}{2}}$	$7^{\frac{1}{2}}$	-5
${}_3{}^4F$	$5^{-\frac{1}{2}}$	0	-1	0	2	0
${}_3{}^2G$	$42^{-\frac{1}{2}}$	0	0	$-10^{\frac{1}{2}}$	$21^{\frac{1}{2}}$	$11^{\frac{1}{2}}$
${}_3{}^2H$	$2^{-\frac{1}{2}}$	0	0	0	-1	1

respect to the third. If we apply in effect to $\psi(l^2(S'L')lSL)$ the transformation[6]

$$\psi(l^2(S'L')lSL)=\sum_{S''L''}\psi(l,\,ll(S''L''),\,SL)\cdot(l,\,ll(S''L''),\,SL\,|\,l^2(S'L')lSL),\qquad(7)$$

where the transformation matrix is given by (6), we obtain in general in the sum (7) allowed and forbidden values of $S''L''$ and, therefore, $\psi(l^2(S'L')lSL)$ cannot be an eigenfunction of l^3.

Only such a linear combination

$$\Psi(l^3\alpha SL)=\sum_{S'L'}\psi(l^2(S'L')lSL)\cdot(l^2(S'L')lSL]\!]l^3\alpha SL)\qquad(8)$$

may be the eigenfunction of l^3 for which the coefficients of $\psi(l,\,ll(S''L''),\,SL)$ vanish for every forbidden value of $S''L''$ after the application of the transformation (7); the "coefficients of fractional parentage" $(l^2(S'L')lSL]\!]l^3\alpha SL)$ must therefore satisfy the equation system

$$\sum_{S'L'}(l,\,ll(S''L''),\,SL\,|\,l^2(S'L')lSL)\cdot(l^2(S'L')lSL]\!]l^3\alpha SL)=0\quad(S''+L''\,\text{odd}).\qquad(9)$$

Since a function antisymmetric with respect to the electrons 1 and 2 and also with respect to the electrons 2 and 3 is antisymmetric with respect to all three electrons, the condition (9) is necessary and sufficient for the determination of the coefficients of fractional parentage of the terms of l^3, and the number of independent non-vanishing solutions of (9) for a given SL equals the number of allowed terms of this kind in l^3; if this number is greater than one, the different terms may be distinguished by a parameter α.

As an illustration of this method let us calculate the eigenfunction of the term $p^3\,{}^2D$. It follows from (6) that

$$\psi(p^2(^3P)p\;^2D)=(3/16)^{\frac12}\psi(p,\,pp(^3D),\,^2D)-(3/16)^{\frac12}\psi(p,\,pp(^1P),\,^2D)+(3/4)\psi(p,\,pp(^1D),\,^2D)-(1/4)\psi(p,\,pp(^3P),\,^2D),$$

TABLE III. $(d^4vSL]\!]d^3(v'S'L')dSL)$.

d^4	N	d^3 ${}_3{}^2P$	${}_3{}^4P$	${}_1{}^2D$	${}_3{}^2D$	${}_3{}^2F$	${}_3{}^4F$	${}_3{}^2G$	${}_3{}^2H$
${}_0{}^1S$	1	0	0	1	0	0	0	0	0
${}_4{}^1S$	1	0	0	0	1	0	0	0	0
${}_2{}^3P$	$360^{-\frac12}$	$-14^{\frac12}$	-8	$135^{\frac12}$	$-35^{\frac12}$	$-56^{\frac12}$	$-56^{\frac12}$	0	0
${}_4{}^3P$	$90^{-\frac12}$	5	$-14^{\frac12}$	0	$10^{\frac12}$	-5	4	0	0
${}_2{}^1D$	$280^{-\frac12}$	$-42^{\frac12}$	0	$105^{\frac12}$	$45^{\frac12}$	$28^{\frac12}$	0	$-60^{\frac12}$	0
${}_4{}^1D$	$140^{-\frac12}$	$42^{\frac12}$	0	0	$20^{\frac12}$	$63^{\frac12}$	0	$15^{\frac12}$	0
${}_4{}^3D$	$210^{-\frac12}$	$-14^{\frac12}$	7	0	$60^{\frac12}$	$-21^{\frac12}$	$-21^{\frac12}$	$45^{\frac12}$	0
${}_4{}^5D$	$10^{-\frac12}$	0	$3^{\frac12}$	0	0	0	$7^{\frac12}$	0	0
${}_4{}^1F$	$560^{-\frac12}$	$120^{\frac12}$	0	0	$200^{\frac12}$	$-105^{\frac12}$	0	$-3^{\frac12}$	$-132^{\frac12}$
${}_2{}^3F$	$840^{-\frac12}$	4	$-56^{\frac12}$	$315^{\frac12}$	$15^{\frac12}$	$-14^{\frac12}$	$224^{\frac12}$	$90^{\frac12}$	$110^{\frac12}$
${}_4{}^3F$	$1680^{-\frac12}$	$-200^{\frac12}$	$-448^{\frac12}$	0	$120^{\frac12}$	$-175^{\frac12}$	$-112^{\frac12}$	$-405^{\frac12}$	$220^{\frac12}$
${}_2{}^1G$	$504^{-\frac12}$	0	0	$189^{\frac12}$	-5	$70^{\frac12}$	0	$66^{\frac12}$	$-154^{\frac12}$
${}_4{}^1G$	$1008^{-\frac12}$	0	0	0	$88^{\frac12}$	$385^{\frac12}$	0	$-507^{\frac12}$	$-28^{\frac12}$
${}_4{}^3G$	$1680^{-\frac12}$	0	0	0	$200^{\frac12}$	$315^{\frac12}$	$-560^{\frac12}$	$297^{\frac12}$	$308^{\frac12}$
${}_4{}^3H$	$60^{-\frac12}$	0	0	0	0	$5^{\frac12}$	$20^{\frac12}$	-3	$26^{\frac12}$
${}_4{}^1I$	$10^{-\frac12}$	0	0	0	0	0	0	$3^{\frac12}$	$7^{\frac12}$

$$\psi(p^2(^1D)p\;^2D)=(3/16)^{\frac12}\psi(p,\,pp(^3D),\,^2D)-(3/16)^{\frac12}\psi(p,\,pp(^1P),\,^2D)-(1/4)\psi(p,\,pp(^1D),\,^2D)+(3/4)\psi(p,\,pp(^3P),\,^2D);$$

since in the development of

$$\Psi(p^3\;^2D)=x\psi(p^2(^3P)p\;^2D)+y\psi(p^2(^1D)p\;^2D)$$

the coefficients of

$$\psi(p,\,pp(^3D),\,^2D)\quad\text{and}\quad\psi(p,\,pp(^1P),\,^2D)$$

must vanish, the only possibility, apart from a phase factor, is

$$\Psi(p^3\;^2D)=(1/2)^{\frac12}\psi(p^2(^3P)p\;^2D)-(1/2)^{\frac12}\psi(p^2(^1D)p\;^2D).$$

The same method may also be extended to the configurations l^n, if the fractional parentages of l^{n-1} are known. In this case

$$\Psi(l^n\alpha SL)=\sum_{\alpha'S'L'}\psi(l^{n-1}(\alpha'S'L')lSL)\cdot(l^{n-1}(\alpha'S'L')lSL]\!]l^n\alpha SL)$$
$$=\sum_{\alpha'S'L'\alpha''S''L''}\psi(l^{n-2}(\alpha''S''L'')l(S'L')lSL)\cdot(l^{n-2}(\alpha''S''L'')lS'L']\!]l^{n-1}\alpha'S'L')\cdot(l^{n-1}(\alpha'S'L')lSL]\!]l^n\alpha SL),\qquad(10)$$

and the coefficients of fractional parentage $(l^{n-1}(\alpha'S'L')lSL]\!]l^n\alpha SL)$ must satisfy the equa-

[6] Since we shall mostly consider transformations and operators which are diagonal with respect to M_S and M_L and independent of them, we shall in general neglect these quantum numbers.

TABLE IV. $(d^5vSL[\![d^4(v'S'L')dSL)$.

d^5	N	d^4: ${}_0{}^1S$	${}_4{}^1S$	${}_2{}^3P$	${}_4{}^3P$	${}_2{}^1D$	${}_4{}^1D$	${}_4{}^3D$	${}_4{}^5D$	${}_4{}^1F$	${}_2{}^3F$	${}_4{}^3F$	${}_2{}^1G$	${}_4{}^1G$	${}_4{}^3G$	${}_4{}^3H$	${}_4{}^1I$
${}_5{}^2S$	$5^{-1/2}$	0	0	0	0	0	$-2^{1/2}$	$3^{1/2}$	0	0	0	0	0	0	0	0	0
${}_5{}^6S$	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
${}_3{}^2P$	$150^{-1/2}$	0	0	$14^{1/2}$	5	$30^{1/2}$	$15^{1/2}$	$10^{1/2}$	0	$-15^{1/2}$	-4	-5	0	0	0	0	0
${}_3{}^4P$	$300^{-1/2}$	0	0	-8	$14^{1/2}$	0	0	$35^{1/2}$	$-75^{1/2}$	0	$-56^{1/2}$	$56^{1/2}$	0	0	0	0	0
${}_1{}^2D$	$50^{-1/2}$	$6^{1/2}$	0	-3	0	$-5^{1/2}$	0	0	0	0	$-21^{1/2}$	0	-3	0	0	0	0
${}_3{}^2D$	$350^{-1/2}$	0	$-14^{1/2}$	-7	$-14^{1/2}$	$45^{1/2}$	$-10^{1/2}$	$60^{1/2}$	0	$35^{1/2}$	$21^{1/2}$	$-21^{1/2}$	-5	$-11^{1/2}$	$45^{1/2}$	0	0
${}_5{}^2D$	$700^{-1/2}$	0	$-56^{1/2}$	0	$126^{1/2}$	0	$90^{1/2}$	$60^{1/2}$	0	$35^{1/2}$	0	$189^{1/2}$	0	$99^{1/2}$	$45^{1/2}$	0	0
${}_5{}^4D$	$700^{-1/2}$	0	0	0	$126^{1/2}$	0	0	$-135^{1/2}$	$-175^{1/2}$	0	0	$-84^{1/2}$	0	0	$180^{1/2}$	0	0
${}_3{}^2F$	$2800^{-1/2}$	0	0	$448^{1/2}$	$-200^{1/2}$	$-160^{1/2}$	$180^{1/2}$	$120^{1/2}$	0	$105^{1/2}$	$112^{1/2}$	$-175^{1/2}$	-20	$275^{1/2}$	$-405^{1/2}$	$220^{1/2}$	0
${}_5{}^2F$	$2800^{-1/2}$	0	0	0	$360^{1/2}$	0	-10	$600^{1/2}$	0	$-525^{1/2}$	0	$-315^{1/2}$	0	$495^{1/2}$	-3	$-396^{1/2}$	0
${}_3{}^4F$	$700^{-1/2}$	0	0	$-56^{1/2}$	-4	0	0	$-15^{1/2}$	$-175^{1/2}$	0	$224^{1/2}$	$14^{1/2}$	0	0	$-90^{1/2}$	$-110^{1/2}$	0
${}_3{}^2G$	$8400^{-1/2}$	0	0	0	0	$-800^{1/2}$	-10	$600^{1/2}$	0	$-7^{1/2}$	$1680^{1/2}$	$945^{1/2}$	$880^{1/2}$	$845^{1/2}$	$891^{1/2}$	$924^{1/2}$	$-728^{1/2}$
${}_5{}^2G$	$18480^{-1/2}$	0	0	0	0	0	$1452^{1/2}$	$968^{1/2}$	0	$-2541^{1/2}$	0	$4235^{1/2}$	0	$-1215^{1/2}$	$-5577^{1/2}$	$-308^{1/2}$	$-2184^{1/2}$
${}_5{}^4G$	$420^{-1/2}$	0	0	0	0	0	0	5	$-105^{1/2}$	0	0	$-70^{1/2}$	0	0	$-66^{1/2}$	$154^{1/2}$	0
${}_3{}^2H$	$1100^{-1/2}$	0	0	0	0	0	0	0	0	$33^{1/2}$	$-220^{1/2}$	$55^{1/2}$	$220^{1/2}$	$-5^{1/2}$	$-99^{1/2}$	$286^{1/2}$	$182^{1/2}$
${}_5{}^2I$	$550^{-1/2}$	0	0	0	0	0	0	0	0	0	0	0	0	$-45^{1/2}$	$99^{1/2}$	$231^{1/2}$	$-175^{1/2}$

tion system

$$\sum_{\alpha'S'L'} (S''L'', ll(S'''L'''), SL\,|\,S''L''l(S'L')lSL) \cdot (l^{n-2}(\alpha''S''L'')lS'L'[\![l^{n-1}\alpha'S'L') \cdot (l^{n-1}(\alpha'S'L')lSL[\![l^n\alpha SL) = 0 \quad (S'''+L''' \text{ odd}). \quad (11)$$

The systems (9) and (11) do not fix the phases of the eigenfunctions of the different terms, nor the scheme in the case of more terms of the same kind, but give the fractional parentages in any arbitrary orthonormal scheme; the convenience of a particular choice of the scheme will be considered in §6.

The fractional parentages of the terms of p^3, d^3, d^4, and d^5 calculated with this method are given in Tables I–IV. The phases of the eigenfunctions of p^3 and d^3 are in agreement with those of TAS $4^8\,6j$ and $5^8\,6$ with the exception of $p^3\,{}^2P$; it must however be remarked that these phases differ from those of Ufford[7] for the terms ${}^4P$, ${}^2F$, ${}^4F$, and ${}^2G$ of d^3.

The coefficients of fractional parentage considered by Goudsmit and Bacher and by Menzel and Goldberg are n times the squares of our coefficients.

It must be pointed out that the matrix $(l^{n-1}(\alpha'S'L')lSL[\![l^n\alpha SL)$ is not an ordinary unitary matrix, but only a rectangular matrix which is a part of a unitary one, since its columns do not exhaust all states of $l^{n-1}l$, but only those which are allowed in l^n; the hermitian conjugate

$$(l^n\alpha SL[\![l^{n-1}(\alpha'S'L')lSL) = [l^{n-1}(\alpha'S'L')lSL[\![l^n\alpha SL]^* \quad (12)$$

does therefore satisfy the relation

$$\sum_{\alpha'S'L'} (l^n\alpha SL[\![l^{n-1}(\alpha'S'L')lSL) \cdot (l^{n-1}(\alpha'S'L')lSL[\![l^n\alpha''SL) = \delta(\alpha\alpha''); \quad (13)$$

but a matrix multiplication in the opposite order has no sense, if the sum is limited to the antisymmetric states of l^n. In calculations with only symmetrical operators we may however, treat formally the matrix $(l^{n-1}(\alpha'S'L')lSL[\![l^n\alpha SL)$ as a common unitary matrix without weakening the general laws of matrix calculations, since symmetrical operators do not connect states of different symmetry and, therefore, the sum over the neglected states vanishes.

§4. FRACTIONAL PARENTAGES IN ALMOST CLOSED SHELLS

We shall determine in this section a relation between the fractional parentages of the terms of an almost closed shell l^{4l+2-n} and those of the terms of l^{n+1}. This relation will not only avoid long numerical calculations, but will also give us the eigenfunctions of the terms of l^{4l+2-n} with the phases fixed by the convention of §6 of II.

[7] C. W. Ufford, Phys. Rev. 44, 732 (1933).

According to §6 of II two terms of l^n and of l^{4l+2-n} will be called conjugated[8] if their eigenfunctions appear multiplied with each other in the relation

$$\Psi(l^{4l+2}\,{}^1S)=\binom{4l+2}{n}^{-\frac12}\sum_{\alpha SLM_SM_L}[(2S+1)\cdot(2L+1)]^{\frac12}\Psi_{\mathfrak{L}}(l^n\alpha SLM_SM_L)\cdot\Psi_{\mathfrak{R}}(l^{4l+2-n}\alpha SL-M_S-M_L)\cdot(SSM_S-M_S|SS00)\cdot(LLM_L-M_L|LL00),\quad(14)$$

where $\mathfrak{L}$ denotes the group of the first n electrons of the shell and $\mathfrak{R}$ the group of the remaining $4l+2-n$; owing to (16′)II we have

$$\Psi(l^{4l+2}\,{}^1S)=\binom{4l+2}{n}^{-\frac12}\sum_{\alpha SLM_SM_L}(-1)^{S+L-M_S-M_L}\Psi_{\mathfrak{L}}(l^n\alpha SLM_SM_L)\cdot\Psi_{\mathfrak{R}}(l^{4l+2-n}\alpha SL-M_S-M_L).\quad(15a)$$

In the same way, if we consider the group $\mathfrak{L}'$ of the first $n+1$ electrons of the shell and the group $\mathfrak{R}'$ of the remaining $4l+1-n$, we may also write

$$\Psi(l^{4l+2}\,{}^1S)=\binom{4l+2}{n+1}^{-\frac12}\cdot\sum_{\alpha'S'L'M_S'M_L'}(-1)^{S'+L'-M_S'-M_L'}\cdot\Psi_{\mathfrak{L}'}(l^{n+1}\alpha'S'L'M_S'M_L')\cdot\Psi_{\mathfrak{R}'}(l^{4l+1-n}\alpha'S'L'-M_S'-M_L').\quad(15b)$$

It follows from (10) that

$$\Psi_{\mathfrak{L}'}(l^{n+1}\alpha'S'L'M_S'M_L')=\sum_{\alpha SLM_SM_Lm_sm_l}\Psi_{\mathfrak{L}}(l^n\alpha SLM_SM_L)\cdot\phi_{n+1}(m_sm_l)(S\tfrac12M_Sm_s|S\tfrac12S'M_S')\cdot(LlM_Lm_l|LlL'M_L')\cdot(l^n(\alpha SL)lS'L'\rrbracket l^{n+1}\alpha'S'L'),\quad(16)$$

and

$$\Psi_{\mathfrak{R}}(l^{4l+2-n}\alpha SL-M_S-M_L)=\sum_{\alpha'S'L'M_S'M_L'm_sm_l}\cdot\Psi_{\mathfrak{R}''}(l^{4l+1-n}\alpha'S'L'-M_S'-M_L')\phi_{4l+2}(m_sm_l)\cdot(S'\tfrac12-M_S'm_s|S'\tfrac12S-M_S)\cdot(L'l-M_L'm_l|L'lL-M_L)\cdot(l^{4l+1-n}(\alpha'S'L')lSL\rrbracket l^{4l+2-n}\alpha SL);$$

here $\mathfrak{R}''$ is the group of the electrons $n+1$, $n+2,\cdots 4l+1$. Since $\Psi_{\mathfrak{R}}$ is antisymmetric, the substitution of the electron $4l+2$ by the electron $n+1$ and of the group $\mathfrak{R}''$ by the group $\mathfrak{R}'$ mulplies $\Psi_{\mathfrak{R}}$ by $(-1)^{n+1}$, and then

$$\Psi_{\mathfrak{R}}(l^{4l+2-n}\alpha SL-M_S-M_L)=\sum_{\alpha'S'L'M_S'M_L'm_sm_l}(-1)^{n+1}\phi_{n+1}(m_sm_l)\cdot\Psi_{\mathfrak{R}'}(l^{4l+1-n}\alpha'S'L'-M_S'-M_L')\,{}^{m}(S'\tfrac12-M_S'm_s|S'\tfrac12S-M_S)\cdot(L'l-M_L'm_l|L'lL-M_L)\cdot(l^{4l+1-n}(\alpha'S'L')lSL\rrbracket l^{4l+2-n}\alpha SL).\quad(17)$$

If we introduce (17) in (15a) and (16) in (15b), we may equate the coefficients of each product $\Psi_{\mathfrak{L}}\phi_{n+1}\Psi_{\mathfrak{R}'}$ separately, since for different quantum numbers these products are orthogonal, and obtain

$$\binom{4l+2}{n}^{-\frac12}(-1)^{S+L-M_S-M_L+n+1}\cdot(S'\tfrac12-M_S'm_s|S'\tfrac12S-M_S)\cdot(L'l-M_L'm_l|L'lL-M_L)\cdot(l^{4l+1-n}(\alpha'S'L')lSL\rrbracket l^{4l+2-n}\alpha SL)=\binom{4l+2}{n+1}^{-\frac12}(-1)^{S'+L'-M_S'-M_L'}\cdot(S\tfrac12M_Sm_s|S\tfrac12S'M_S')(LlM_Lm_l|LlL'M_L')\cdot(l^n(\alpha SL)lS'L'\rrbracket l^{n+1}\alpha'S'L').\quad(18)$$

Owing to (16′)II and (19a)II, and to the fact that $n+1$ has the same parity as $2(S'+L')$, we get

$$(l^{4l+1-n}(\alpha'S'L')lSL\rrbracket l^{4l+2-n}\alpha SL)=(-1)^{S+S'+L+L'-l-\frac12}\cdot\left[\frac{(n+1)(2S'+1)(2L'+1)}{(4l+2-n)(2S+1)(2L+1)}\right]^{\frac12}\cdot(l^n(\alpha SL)lS'L'\rrbracket l^{n+1}\alpha'S'L'),\quad(19)$$

which is the requested relation.

[8] To the correlation defined in §6 of II we shall reserve the word "conjugation," since other types of correlations between terms of different configurations will be found in §6 of this paper.

TABLE V. $(p^2SL\|U^{(2)}\|p^2S'L')$.

	^1S	^3P	^1D
^1S	0	0	$\frac{2}{3}(3)^{1/2}$
^3P	0	-1	0
^1D	$\frac{2}{3}(3)^{1/2}$	0	$\frac{1}{3}(21)^{1/2}$

TABLE VI. $(p^3SL\|U^{(2)}\|p^3SL')$.

	^4S	^2P	^2D
^4S	0	0	0
^2P	0	0	$-(3)^{1/2}$
^2D	0	$(3)^{1/2}$	0

From (19) and (13) we obtain also

$$\sum_{\alpha SL}(2S+1)(2L+1)(l^{n-1}(\alpha'S'L')lSL]\!]l^n\alpha SL)\cdot(l^n\alpha SL[\![l^{n-1}(\alpha''S'L')lSL)$$
$$=[(4l+3-n)/n](2S'+1)(2L'+1)\delta(\alpha'\alpha''). \quad (20)$$

For the determination of the fractional parentages of the terms of l^{2l+2} it must, however, be observed that (19) gives the parentages of $\Psi_{\mathfrak{R}}(l^{2l+2})$ with respect to $\Psi_{\mathfrak{R}}(l^{2l+1})$, and that the eigenfunctions of l^{2l+1} determined by the methods of the preceding section are $\Psi_{\mathfrak{L}}(l^{2l+1})$; since it was shown in §6 of II that the terms of l^{2l+1} split in two classes, according to the two possibilities of (76)II, we must change the sign in the relation (19) if $\Psi_{\mathfrak{R}}(l^{2l+1}\alpha'S'L')$ belongs to the class for which the minus sign holds in (76)II. The classification of the terms from this point of view will be considered in subsection (5) of §6.

§5. MATRIX COMPONENTS OF SYMMETRIC OPERATORS

We are at first interested in the matrix components $(\lambda^{\rm I}|F|\lambda^{\rm II})$ of the quantity

$$F=\sum_1^n {}_i f_i, \quad (21)$$

where f_i is an operator which operates on the

TABLE VII. $(d^3vSL\|35\,U^{(2)}\|d^3v'S'L')$.

	${}_3{}^2P$	${}_3{}^4P$	${}_1{}^2D$	${}_3{}^2D$	${}_3{}^2F$	${}_3{}^4F$	${}_3{}^2G$	${}_3{}^2H$
${}_3{}^2P$	$-2(21)^{1/2}$	0	$-\frac{21}{2}(10)^{1/2}$	$\frac{1}{2}(210)^{1/2}$	$-4(21)^{1/2}$	0	0	0
${}_3{}^4P$	0	$7(21)^{1/2}$	0	0	0	$-14(6)^{1/2}$	0	0
${}_1{}^2D$	$\frac{21}{2}(10)^{1/2}$	0	$\frac{35}{2}$	$\frac{15}{2}(21)^{1/2}$	$-7(15)^{1/2}$	0	$-15(7)^{1/2}$	0
${}_3{}^2D$	$-\frac{1}{2}(210)^{1/2}$	0	$\frac{15}{2}(21)^{1/2}$	$\frac{15}{2}$	$-9(35)^{1/2}$	0	$-5(3)^{1/2}$	0
${}_3{}^2F$	$-4(21)^{1/2}$	0	$7(15)^{1/2}$	$9(35)^{1/2}$	$7(6)^{1/2}$	0	$2(210)^{1/2}$	$-(2310)^{1/2}$
${}_3{}^4F$	0	$-14(6)^{1/2}$	0	0	0	$-7(6)^{1/2}$	0	0
${}_3{}^2G$	0	0	$-15(7)^{1/2}$	$-5(3)^{1/2}$	$-2(210)^{1/2}$	0	$3(22)^{1/2}$	$-(462)^{1/2}$
${}_3{}^2H$	0	0	0	0	$-(2310)^{1/2}$	0	$(462)^{1/2}$	$(3003)^{1/2}$

TABLE VIIIa. $(d^4\ {}_v{}^1L\|35\,U^{(2)}\|d^4\ {}_{v'}{}^1L')$.

	${}_0{}^1S$	${}_4{}^1S$	${}_2{}^1D$	${}_4{}^1D$	${}_4{}^1F$	${}_2{}^1G$	${}_4{}^1G$	${}_4{}^1I$
${}_0{}^1S$	0	0	$7(30)^{1/2}$	0	0	0	0	0
${}_4{}^1S$	0	0	$3(70)^{1/2}$	$4(35)^{1/2}$	0	0	0	0
${}_2{}^1D$	$7(30)^{1/2}$	$3(70)^{1/2}$	-5	$-30(2)^{1/2}$	0	$4(5)^{1/2}$	$8(55)^{1/2}$	0
${}_4{}^1D$	0	$4(35)^{1/2}$	$-30(2)^{1/2}$	-15	$10(14)^{1/2}$	$10(10)^{1/2}$	$2(110)^{1/2}$	0
${}_4{}^1F$	0	0	0	$-10(14)^{1/2}$	$\frac{35}{2}(6)^{1/2}$	$-7(70)^{1/2}$	$-\frac{1}{2}(770)^{1/2}$	0
${}_2{}^1G$	0	0	$4(5)^{1/2}$	$10(10)^{1/2}$	$7(70)^{1/2}$	$5(22)^{1/2}$	$5(2)^{1/2}$	$-2(455)^{1/2}$
${}_4{}^1G$	0	0	$8(55)^{1/2}$	$2(110)^{1/2}$	$\frac{1}{2}(770)^{1/2}$	$5(2)^{1/2}$	$-\frac{125}{22}(22)^{1/2}$	$-\frac{8}{11}(5005)^{1/2}$
${}_4{}^1I$	0	0	0	0	0	$-2(455)^{1/2}$	$-\frac{8}{11}(5005)^{1/2}$	$\frac{35}{11}(143)^{1/2}$

TABLE VIIIb. $(d^4vSL\|35\,U^{(2)}\|d^4v'S'L')$ for $S=1,\ 2$.

	${}_2{}^3P$	${}_4{}^3P$	${}_4{}^3D$	${}_4{}^5D$	${}_2{}^3F$	${}_4{}^3F$	${}_4{}^3G$	${}_4{}^3H$
${}_2{}^3P$	$-\frac{7}{3}(21)^{1/2}$	$\frac{14}{3}(6)^{1/2}$	$-\frac{28}{3}(15)^{1/2}$	0	$\frac{14}{3}(6)^{1/2}$	$\frac{28}{3}(6)^{1/2}$	0	0
${}_4{}^3P$	$\frac{14}{3}(6)^{1/2}$	$\frac{19}{3}(21)^{1/2}$	$-\frac{4}{3}(210)^{1/2}$	0	$\frac{22}{3}(21)^{1/2}$	$\frac{8}{3}(21)^{1/2}$	0	0
${}_4{}^3D$	$\frac{28}{3}(15)^{1/2}$	$\frac{4}{3}(210)^{1/2}$	5	0	$-4(35)^{1/2}$	$4(35)^{1/2}$	$20(3)^{1/2}$	0
${}_4{}^5D$	0	0	0	-35	0	0	0	0
${}_2{}^3F$	$\frac{14}{3}(6)^{1/2}$	$\frac{22}{3}(21)^{1/2}$	$4(35)^{1/2}$	0	$\frac{7}{3}(6)^{1/2}$	$\frac{49}{3}(6)^{1/2}$	$-3(210)^{1/2}$	$\frac{2}{3}(2310)^{1/2}$
${}_4{}^3F$	$\frac{28}{3}(6)^{1/2}$	$\frac{8}{3}(21)^{1/2}$	$-4(35)^{1/2}$	0	$\frac{49}{3}(6)^{1/2}$	$\frac{77}{6}(6)^{1/2}$	$-\frac{1}{2}(210)^{1/2}$	$\frac{2}{3}(2310)^{1/2}$
${}_4{}^3G$	0	0	$20(3)^{1/2}$	0	$3(210)^{1/2}$	$\frac{1}{2}(210)^{1/2}$	$-\frac{3}{2}(22)^{1/2}$	$-2(462)^{1/2}$
${}_4{}^3H$	0	0	0	0	$\frac{2}{3}(2310)^{1/2}$	$\frac{2}{3}(2310)^{1/2}$	$2(462)^{1/2}$	$\frac{1}{3}(3003)^{1/2}$

TABLE IXa. $(d^5\, {}_v{}^2L \| 35\, U^{(2)} \| d^5\, {}_{v'}{}^2L')$.

	${}_5{}^2S$	${}_3{}^2P$	${}_1{}^2D$	${}_3{}^2D$	${}_5{}^2D$	${}_3{}^2F$	${}_5{}^2F$	${}_3{}^2G$	${}_5{}^2G$	${}_3{}^2H$	${}_5{}^2I$
${}_5{}^2S$	0	0	0	$4(70)^{\frac{1}{2}}$	0	0	0	0	0	0	0
${}_3{}^2P$	0	0	$-7(30)^{\frac{1}{2}}$	0	$5(105)^{\frac{1}{2}}$	0	$4(105)^{\frac{1}{2}}$	0	0	0	0
${}_1{}^2D$	0	$7(30)^{\frac{1}{2}}$	0	$15(7)^{\frac{1}{2}}$	0	$-14(5)^{\frac{1}{2}}$	0	$-10(21)^{\frac{1}{2}}$	0	0	0
${}_3{}^2D$	$4(70)^{\frac{1}{2}}$	0	$15(7)^{\frac{1}{2}}$	0	$5(2)^{\frac{1}{2}}$	0	$10(7)^{\frac{1}{2}}$	0	$-6(55)^{\frac{1}{2}}$	0	0
${}_5{}^2D$	0	$-5(105)^{\frac{1}{2}}$	0	$5(2)^{\frac{1}{2}}$	0	0	0	$20(6)^{\frac{1}{2}}$	0	0	0
${}_3{}^2F$	0	0	$14(5)^{\frac{1}{2}}$	0	0	0	$-7(30)^{\frac{1}{2}}$	0	0	0	0
${}_5{}^2F$	0	$4(105)^{\frac{1}{2}}$	0	$-10(7)^{\frac{1}{2}}$	0	$-7(30)^{\frac{1}{2}}$	0	$4(42)^{\frac{1}{2}}$	0	$-2(462)^{\frac{1}{2}}$	0
${}_3{}^2G$	0	0	$-10(21)^{\frac{1}{2}}$	0	$20(6)^{\frac{1}{2}}$	0	$-4(42)^{\frac{1}{2}}$	0	$9(30)^{\frac{1}{2}}$	0	$4(273)^{\frac{1}{2}}$
${}_5{}^2G$	0	0	0	$-6(55)^{\frac{1}{2}}$	0	0	0	$9(30)^{\frac{1}{2}}$	0	$6(70)^{\frac{1}{2}}$	0
${}_3{}^2H$	0	0	0	0	0	0	$-2(462)^{\frac{1}{2}}$	0	$-6(70)^{\frac{1}{2}}$	0	$7(13)^{\frac{1}{2}}$
${}_5{}^2I$	0	0	0	0	0	0	0	$4(273)^{\frac{1}{2}}$	0	$-7(13)^{\frac{1}{2}}$	0

TABLE IXb. $(d^5\, {}_v{}^4L \| 35\, U^{(2)} \| d^5\, {}_{v'}{}^4L')$.

	${}_3{}^4P$	${}_5{}^4D$	${}_3{}^4F$	${}_5{}^4G$
${}_3{}^4P$	0	$7(15)^{\frac{1}{2}}$	0	0
${}_5{}^4D$	$-7(15)^{\frac{1}{2}}$	0	$8(35)^{\frac{1}{2}}$	0
${}_3{}^4F$	0	$-8(35)^{\frac{1}{2}}$	0	$15(14)^{\frac{1}{2}}$
${}_5{}^4G$	0	0	$-15(14)^{\frac{1}{2}}$	0

TABLE X. $(p^2SL \| 6^{\frac{1}{2}} V^{(11)} \| p^2S'L')$.

	${}^1S$	${}^3P$	${}^1D$
${}^1S$	0	$-\frac{1}{2}(30)^{\frac{1}{2}}$	0
${}^3P$	$-\frac{1}{2}(30)^{\frac{1}{2}}$	3	$(6)^{\frac{1}{2}}$
${}^1D$	0	$(6)^{\frac{1}{2}}$	0

TABLE XI. $(p^3SL \| 6^{\frac{1}{2}} V^{(11)} \| p^3S'L')$.

	${}^4S$	${}^2P$	${}^2D$
${}^4S$	0	$2(3)^{\frac{1}{2}}$	0
${}^2P$	$2(3)^{\frac{1}{2}}$	0	$(15)^{\frac{1}{2}}$
${}^2D$	0	$-(15)^{\frac{1}{2}}$	0

electron i, and λ^{I} and λ^{II} are states of the configurations I and II; owing to the antisymmetry of $\Psi(\lambda^{\mathrm{I}})$ and $\Psi(\lambda^{\mathrm{II}})$ we have

$$(\lambda^{\mathrm{I}}|F|\lambda^{\mathrm{II}}) = \sum_1^n {}_i \int \bar{\Psi}(\lambda^{\mathrm{I}}) f_i \Psi(\lambda^{\mathrm{II}}) d\tau$$

$$= n \int \bar{\Psi}(\lambda^{\mathrm{I}}) f_i \Psi(\lambda^{\mathrm{II}}) d\tau. \quad (22)$$

If $\mathrm{I} = \mathrm{II} = l^n$, putting $i = n$ and assuming for Ψ the expression (10), we obtain

$$(l^n\alpha SLM_SM_L|F|l^n\alpha'S'L'M_S'M_L')$$

$$= n \sum_{\alpha_1S_1L_1} (l^n\alpha SL\{\!|l^{n-1}(\alpha_1S_1L_1)lSL)$$

$$\cdot (S_1L_1l_nSLM_SM_L|f_n|S_1L_1l_nS'L'M_S'M_L')$$

$$\cdot (l^{n-1}(\alpha_1S_1L_1)lS'L'|\!\}l^n\alpha'S'L'), \quad (23)$$

where $(S_1L_1l_nSLM_SM_L|f_n|S_1L_1l_nS'L'M_S'M_L')$ may now be calculated with the ordinary matrix methods of Chapter III of TAS and of II.

As application of this formula we calculated the matrix components of the tensors $\boldsymbol{U}^{(2)}$ and $\boldsymbol{V}^{(11)}$, defined by (102)II, for the configurations p^2, p^3, d^3, d^4, and d^5; the results are given in Tables V–XIV. For d^2 the matrices were already given by (103)II; it must, however, be noted that an error occurred in the final form of the manuscript, and all the elements of (103c)II and (103d)II must be multiplied by $(3/2)^{\frac{1}{2}}$.

From the elements of $\boldsymbol{V}^{(11)}$ the matrix components of the spin-orbit interaction may easily be obtained: it follows in effect from the relation

$$\boldsymbol{l} = [l(l+1)(2l+1)]^{\frac{1}{2}} \boldsymbol{u}^{(1)} \quad (24)$$

and from (38)II and (102)II that

$$(l^n\alpha SLJM|\textstyle\sum_i (\boldsymbol{s}_i \cdot \boldsymbol{l}_i)|l^n\alpha'S'L'JM)$$

$$= (-1)^{S+L'-J}[l(l+1)(2l+1)]^{\frac{1}{2}}$$

$$\cdot (l^n\alpha SL\|V^{(11)}\|l^n\alpha'S'L')W(SLS'L';J1). \quad (25)$$

If in (22) $\mathrm{I} = l^n$ and $\mathrm{II} = l^{n-1}l'$, the terms of II are characterized by S and L and by the quantum numbers of the parent ion l^{n-1}; $\Psi(\lambda^{\mathrm{II}})$ has in this case the expression

$$\Psi(l^{n-1}(\alpha_1S_1L_1)l'S'L'M_S'M_L')$$

$$= (1/n)^{\frac{1}{2}} \sum_1^n {}_i (-1)^{P_i}$$

$$\cdot \psi(l^{n-1}(\alpha_1S_1L_1)l_i'S'L'M_S'M_L'), \quad (26)$$

where in the right side we consider the group l^{n-1} as composed by the electrons $1, 2, \cdots, i-1, i+1, \cdots, n$, and P_i is the parity of the permutation which exchanges i with n. Introducing

TABLE XII. $(d^3vSL\|30^{\frac12}V^{(11)}\|d^3v'S'L')$.

	$_3{}^2P$	$_3{}^4P$	$_1{}^2D$	$_3{}^2D$	$_3{}^2F$	$_3{}^4F$	$_3{}^2G$	$_3{}^2H$
$_3{}^2P$	2	$-2(14)^{\frac12}$	$-\frac12(42)^{\frac12}$	$\frac92(2)^{\frac12}$	0	0	0	0
$_3{}^4P$	$2(14)^{\frac12}$	$(10)^{\frac12}$	$-4(3)^{\frac12}$	0	0	0	0	0
$_1{}^2D$	$\frac12(42)^{\frac12}$	$-4(3)^{\frac12}$	$\frac32(5)^{\frac12}$	$-\frac12(105)^{\frac12}$	$(42)^{\frac12}$	$-(42)^{\frac12}$	0	0
$_3{}^2D$	$-\frac92(2)^{\frac12}$	0	$-\frac12(105)^{\frac12}$	$-\frac12(5)^{\frac12}$	$(2)^{\frac12}$	$5(2)^{\frac12}$	0	0
$_3{}^2F$	0	0	$-(42)^{\frac12}$	$-(2)^{\frac12}$	$-\frac12(14)^{\frac12}$	$-(14)^{\frac12}$	$\frac32-(10)^{\frac12}$	0
$_3{}^4F$	0	0	$-(42)^{\frac12}$	$5(2)^{\frac12}$	$(14)^{\frac12}$	$2(35)^{\frac12}$	$-3(10)^{\frac12}$	0
$_3{}^2G$	0	0	0	0	$\frac32(10)^{\frac12}$	$-3(10)^{\frac12}$	$\frac{9}{10}(30)^{\frac12}$	$\frac65(55)^{\frac12}$
$_3{}^2H$	0	0	0	0	0	0	$-\frac65(55)^{\frac12}$	$\frac35(55)^{\frac12}$

TABLE XIII. $(d^4vSL\|30^{\frac12}V^{(11)}\|d^4v'S'L')$.

	$_0{}^1S$	$_4{}^1S$	$_2{}^3P$	$_4{}^3P$	$_2{}^1D$	$_4{}^1D$	$_4{}^3D$	$_4{}^5D$	$_4{}^1F$	$_2{}^3F$	$_4{}^3F$	$_2{}^1G$	$_4{}^1G$	$_4{}^3G$	$_4{}^3H$	$_4{}^1I$
$_0{}^1S$	0	0	$3(3)^{\frac12}$	0	0	0	0	0	0	0	0	0	0	0	0	0
$_4{}^1S$	0	0	$-(7)^{\frac12}$	$2(2)^{\frac12}$	0	0	0	0	0	0	0	0	0	0	0	0
$_2{}^3P$	$3(3)^{\frac12}$	$-(7)^{\frac12}$	1	$-2(14)^{\frac12}$	$-\frac12(14)^{\frac12}$	$2(7)^{\frac12}$	0	$-4(5)^{\frac12}$	0	0	0	0	0	0	0	0
$_4{}^3P$	0	$2(2)^{\frac12}$	$-2(14)^{\frac12}$	2	2	$\frac12(2)^{\frac12}$	$\frac92(2)^{\frac12}$	$\frac12(70)^{\frac12}$	0	0	0	0	0	0	0	0
$_2{}^1D$	0	0	$-\frac12(14)^{\frac12}$	2	0	0	$2(10)^{\frac12}$	0	0	2	4	0	0	0	0	0
$_4{}^1D$	0	0	$2(7)^{\frac12}$	$\frac12(2)^{\frac12}$	0	0	$-(5)^{\frac12}$	0	0	$(2)^{\frac12}$	$-4(2)^{\frac12}$	0	0	0	0	0
$_4{}^3D$	0	0	0	$-\frac92(2)^{\frac12}$	$-2(10)^{\frac12}$	$(5)^{\frac12}$	$-1\frac12(5)^{\frac12}$	$\frac52(7)^{\frac12}$	$-2(5)^{\frac12}$	$5(2)^{\frac12}$	$(2)^{\frac12}$	0	0	0	0	0
$_4{}^5D$	0	0	$-4(5)^{\frac12}$	$\frac12(70)^{\frac12}$	0	0	$-\frac52(7)^{\frac12}$	$1\frac52$	0	$-(70)^{\frac12}$	$(70)^{\frac12}$	0	0	0	0	0
$_4{}^1F$	0	0	0	0	0	0	$-2(5)^{\frac12}$	0	0	$(35)^{\frac12}$	$\frac12(35)^{\frac12}$	0	0	$-\frac92$	0	0
$_2{}^3F$	0	0	0	0	2	$(2)^{\frac12}$	$-5(2)^{\frac12}$	$-(70)^{\frac12}$	$-(35)^{\frac12}$	$(14)^{\frac12}$	$-(14)^{\frac12}$	$-(3)^{\frac12}$	$(33)^{\frac12}$	$3(10)^{\frac12}$	0	0
$_4{}^3F$	0	0	0	0	4	$-4(2)^{\frac12}$	$-(2)^{\frac12}$	$(70)^{\frac12}$	$-\frac12(35)^{\frac12}$	$-(14)^{\frac12}$	$-\frac12(14)^{\frac12}$	$5(3)^{\frac12}$	$-\frac12(33)^{\frac12}$	$-\frac32(10)^{\frac12}$	0	0
$_2{}^1G$	0	0	0	0	0	0	0	0	0	$-(3)^{\frac12}$	$5(3)^{\frac12}$	0	0	3	$-(66)^{\frac12}$	0
$_4{}^1G$	0	0	0	0	0	0	0	0	0	$(33)^{\frac12}$	$-\frac12(33)^{\frac12}$	0	0	$\frac32(11)^{\frac12}$	$2(6)^{\frac12}$	0
$_4{}^3G$	0	0	0	0	0	0	0	0	$-\frac92$	$-3(10)^{\frac12}$	$\frac32(10)^{\frac12}$	-3	$-\frac32(11)^{\frac12}$	$\frac{9}{10}(30)^{\frac12}$	$\frac65(55)^{\frac12}$	0
$_4{}^3H$	0	0	0	0	0	0	0	0	0	0	0	$-(66)^{\frac12}$	$2(6)^{\frac12}$	$-\frac65(55)^{\frac12}$	$\frac35(55)^{\frac12}$	$-\frac32(26)$
$_4{}^1I$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	$-\frac32(26)^{\frac12}$	0

(10) and (26) in (22) and putting $i=n$, we have

$$(l^n\alpha SLM_SM_L|F|l^{n-1}(\alpha_1S_1L_1)l'S'L'M_S'M_L')$$
$$=n^{\frac12}(l^n\alpha SL\{\!|l^{n-1}(\alpha_1S_1L_1)lSL)$$
$$\cdot(S_1L_1l_nSLM_SM_L|f_n|S_1L_1l_n'S'L'M_S'M_L'). \quad (27)$$

This formula, which is the extension of TAS $6^8$17, gives a rigorous demonstration to the method of Menzel and Goldberg[9] and also fixes for such transitions the phases of the matrix components, which are necessary for transformations to other types of vector coupling (TAS, p. 252).

If in (22) $\mathrm{I}=l^{n-p}l'^p$ and $\mathrm{II}=l^{n-p-1}l'^{p+1}$, the terms of each configuration are characterized by S and L and by the quantum numbers of the groups of equivalent electrons; in the same way as for the precedent case we obtain

$$(l^{n-p}(\alpha_1S_1L_1),\ l'^p(\alpha_2S_2L_2),$$
$$SLM_SM_L|F|l^{n-p-1}(\alpha_1'S_1'L_1'),$$
$$l'^{p+1}(\alpha_2'S_2'L_2'),\ S'L'M_S'M_L')$$

^{9} D. H. Menzel and L. Goldberg, Phys. Rev. **47**, 424 (1935) and reference 5.

$$=[(n-p)(p+1)]^{\frac12}\sum_{S_3L_3}$$
$$(l^{n-p}\alpha_1S_1L_1\cdot\{\!|l^{n-p-1}(\alpha_1'S_1'L_1')lS_1L_1)$$
$$\cdot(S_1'L_1'l_{n-p}(S_1L_1),\ S_2L_2,$$
$$SLM_SM_L|f_{n-p}|S_1'L_1'l'_{n-p}(S_3L_3),$$
$$S_2L_2,\ S'L'M_S'M_L')$$
$$\cdot(S_1'L_1'l'(S_3L_3),$$
$$S_2L_2,\ S'L'|S_1'L_1',\ l'S_2L_2(S_2'L_2'),\ S'L')$$
$$\cdot(l',l'^p(\alpha_2S_2l_2),S_2'L_2'|\!\}l'^{p+1}\alpha_2'S_2'L_2'). \quad (28)$$

In connection with this result it must be observed that $(l,\ l^{n-1}(\alpha'S'L'),\ SL|\!\}l^n\alpha SL)$ is not $(l^{n-1}(\alpha'S'L')lSL|\!\}l^n\alpha SL)$, but it is easy to see that the two coefficients are connected by the relation

$$(l,\ l^{n-1}(\alpha'S'L'),\ SL|\!\}l^n\alpha SL)$$
$$=(-)^{S+L+S'+L'-l-\frac12}$$
$$\cdot(l^{n-1}(\alpha'S'L')lSL|\!\}l^n\alpha SL). \quad (29)$$

It is unnecessary to consider the matrix elements of F for transitions between more com-

TABLE XIV. $(d^5vSL\|30^{\frac{1}{2}}V^{(11)}\|d^5v'S'L')$.

	${}_5{}^2S$	${}_5{}^6S$	${}_3{}^2P$	${}_3{}^4P$	${}_1{}^2D$	${}_3{}^2D$	${}_5{}^2D$	${}_5{}^4D$	${}_3{}^2F$	${}_5{}^2F$	${}_3{}^4F$	${}_3{}^2G$	${}_5{}^2G$	${}_5{}^4G$	${}_3{}^2H$	${}_5{}^2I$
${}_5{}^2S$	0	0	-4	$(14)^{\frac{1}{2}}$	0	0	0	0	0	0	0	0	0	0	0	0
${}_5{}^6S$	0	0	0	$3(10)^{\frac{1}{2}}$	0	0	0	0	0	0	0	0	0	0	0	0
${}_3{}^2P$	4	0	0	0	$-(14)^{\frac{1}{2}}$	0	1	$2(2)^{\frac{1}{2}}$	0	0	0	0	0	0	0	0
${}_3{}^4P$	$(14)^{\frac{1}{2}}$	$3(10)^{\frac{1}{2}}$	0	0	-8	0	$-2(14)^{\frac{1}{2}}$	$-(70)^{\frac{1}{2}}$	0	0	0	0	0	0	0	0
${}_1{}^2D$	0	0	$(14)^{\frac{1}{2}}$	-8	0	$-(35)^{\frac{1}{2}}$	0	0	$2(14)^{\frac{1}{2}}$	0	$-2(14)^{\frac{1}{2}}$	0	0	0	0	0
${}_3{}^2D$	0	0	0	0	$-(35)^{\frac{1}{2}}$	0	$(10)^{\frac{1}{2}}$	$-4(5)^{\frac{1}{2}}$	0	$-2(10)^{\frac{1}{2}}$	0	0	0	0	0	0
${}_5{}^2D$	0	0	-1	$-2(14)^{\frac{1}{2}}$	0	$(10)^{\frac{1}{2}}$	0	0	8	0	-2	0	0	0	0	0
${}_5{}^4D$	0	0	$2(2)^{\frac{1}{2}}$	$(70)^{\frac{1}{2}}$	0	$4(5)^{\frac{1}{2}}$	0	0	$4(2)^{\frac{1}{2}}$	0	$-4(5)^{\frac{1}{2}}$	0	0	0	0	0
${}_3{}^2F$	0	0	0	0	$-2(14)^{\frac{1}{2}}$	0	-8	$4(2)^{\frac{1}{2}}$	0	$-\frac{1}{2}(70)^{\frac{1}{2}}$	0	0	$-\frac{1}{2}(66)^{\frac{1}{2}}$	$5(6)^{\frac{1}{2}}$	0	0
${}_5{}^2F$	0	0	0	0	0	$2(10)^{\frac{1}{2}}$	0	0	$-\frac{1}{2}(70)^{\frac{1}{2}}$	0	$-(70)^{\frac{1}{2}}$	$\frac{9}{2}(2)^{\frac{1}{2}}$	0	0	0	0
${}_3{}^4F$	0	0	0	0	$-2(14)^{\frac{1}{2}}$	0	-2	$4(5)^{\frac{1}{2}}$	0	$(70)^{\frac{1}{2}}$	0	0	$-(66)^{\frac{1}{2}}$	$(15)^{\frac{1}{2}}$	0	0
${}_3{}^2G$	0	0	0	0	0	0	0	0	0	$-\frac{3}{2}(2)^{\frac{1}{2}}$	0	0	$-\frac{3}{2}(22)^{\frac{1}{2}}$	$-3(2)^{\frac{1}{2}}$	0	0
${}_5{}^2G$	0	0	0	0	0	0	0	0	$\frac{1}{2}(66)^{\frac{1}{2}}$	0	$-(66)^{\frac{1}{2}}$	$-\frac{3}{2}(22)^{\frac{1}{2}}$	0	0	$-4(3)^{\frac{1}{2}}$	0
${}_5{}^4G$	0	0	0	0	0	0	0	0	$5(6)^{\frac{1}{2}}$	0	$2(15)^{\frac{1}{2}}$	$3(2)^{\frac{1}{2}}$	0	0	$-2(33)^{\frac{1}{2}}$	0
${}_3{}^2H$	0	0	0	0	0	0	0	0	0	0	0	0	$4(3)^{\frac{1}{2}}$	$-2(33)^{\frac{1}{2}}$	0	$-3(13)^{\frac{1}{2}}$
${}_5{}^2I$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	$3(13)^{\frac{1}{2}}$	0

plicated configurations, since all other cases may be reduced to these three by means of TAS I[8]16.

The calculation by the same method of the matrix components of the scalar operator

$$G=\sum_{i<j} g_{ij} \tag{30}$$

needs in some cases the knowledge of $\Psi(l^n\alpha SL)$ as linear combination of the eigenfunctions of $l^{n-2}l^2$:

$$\Psi(l^n\alpha SL)=\sum_{\alpha_1S_1L_1S_2L_2}\psi(l^{n-2}(\alpha_1S_1L_1),\; l^2(S_2L_2),\,SL)(l^{n-2}(\alpha_1S_1L_1),\; l^2(S_2L_2),\,SL]\!]l^n\alpha SL); \tag{31}$$

the coefficients of this expression are given by the formula

$$\begin{aligned}(l^{n-2}(\alpha_1S_1L_1),\,l^2(S_2L_2),\,SL]\!]l^nSL) &=\sum_{\alpha'S'L'}(S_1L_1,\,l^2(S_2L_2),\\ &\quad SL]\!]S_1L_1l(S'L')lSL)\\ &\quad\cdot(l^{n-2}(\alpha_1S_1L_1)lS'L']\!]l^{n-1}\alpha'S'L')\\ &\quad\cdot(l^{n-1}(\alpha'S'L')lSL]\!]l^n\alpha SL).\end{aligned} \tag{32}$$

The following results are easily derived:

$$\begin{aligned}(l^n\alpha SL|G|l^n\alpha' SL) &=\tfrac{1}{2}n(n-1)\sum_{\alpha_1S_1L_1S_2L_2}(l^n\alpha SL[\![l^{n-2}(\alpha_1S_1L_1),\\ &\quad\cdot l^2(S_2L_2),\,SL)(l^2S_2L_2|g|l^2S_2L_2)\\ &\quad\cdot(l^{n-2}(\alpha_1S_1L_1),\,l^2(S_2L_2),\,SL]\!]l^n\alpha' SL),\end{aligned} \tag{33a}$$

$$\begin{aligned}(l^n\alpha SL|G|l^{n-1}(\alpha'S'L')l'SL) &=(n-1)n^{\frac{1}{2}}\sum_{\alpha_1S_1L_1S_2L_2}(l^n\alpha SL[\![l^{n-2}(\alpha_1S_1L_1),\\ &\quad l^2(S_2L_2),\,SL)(l_il_jS_2L_2|g_{ij}|l_il_j'S_2L_2)\\ &\quad\cdot(S_1L_1,\,ll'(S_2L_2),\,SL|S_1L_1l(S'L')l'SL)\\ &\quad\cdot(l^{n-2}(\alpha_1S_1L_1)lS'L']\!]l^{n-1}\alpha'S'L'),\end{aligned} \tag{33b}$$

$$\begin{aligned}(l^n\alpha SL|G|l^{n-2}(\alpha_1S_1L_1),\,l'^2(S_2L_2),\,SL) &=[n(n-1)/2]^{\frac{1}{2}}(l^n\alpha SL[\![l^{n-2}(\alpha_1S_1L_1),\\ &\quad l^2(S_2L_2),\,SL)(l^2S_2L_2|g|l'^2S_2L_2).\end{aligned} \tag{33c}$$

Since the actual application of (32) needs generally very long calculations, the formulas (33) are of practical use only in a few particular cases; in other cases it is simpler to express g_{ij} as a sum of scalar products of tensors and to reduce the problem to the calculation of tensors of the type F. Applications of both methods will be shown in the next sections.

§6. THE STRUCTURE OF THE CONFIGUATIONS l^n

In this section we shall classify the terms of the configuration l^n according to the eigenvalues of

$$Q=\sum_{i<j} q_{ij}, \tag{34}$$

where q_{ij} is a scalar operator which operates on the two equivalent electrons i and j and is defined by the relation

$$(l^2LM|q_{ij}|l^2LM)=(2l+1)\delta(L,0). \tag{35}$$

It will be shown that to every term of l^n with non-vanishing Q a term of the same kind corresponds in l^{n-2}, and this fact will allow us to assign to each term a "seniority number" according to the value of n for which the term appeared for the first time. Some useful relation between the fractional parentages of corresponding terms will be obtained and it will also be shown that the classification of the terms of l^{2l+1} according to the two possibilities of (76)II depends only on the seniority of the term.

(1) The Eigenvalues of Q

It follows from (42)II and (40a)II that

$$\sum_{0}^{2l}{}_r (2r+1)W(llll;0r)W(llll;Lr)=\delta(L,0); \quad (36)$$

expressing $W(llll;0r)$ by (36′)II and using also (38)II and (58)II we get for q_{ij} the expression

$$q_{ij}=\sum_{0}^{2l}{}_r (-1)^r(2r+1)(\boldsymbol{u}_i^{(r)}\cdot\boldsymbol{u}_j^{(r)}). \quad (37)$$

Since $\boldsymbol{u}^{(0)}$ is a scalar and, owing to (33)II,

$$\boldsymbol{u}^{(r)2}=(2l+1)^{-1}, \quad (38)$$

we have also

$$q_{ij}=(2l+1)^{-1}+\sum_{1}^{2l}{}_r (-1)^r(2r+1)(\boldsymbol{u}_i^{(r)}\cdot\boldsymbol{u}_j^{(r)}) \quad (37')$$

and

$$Q=\tfrac{1}{2}n(n-2l-1)(2l+1)^{-1}+\tfrac{1}{2}\sum_{1}^{2l}{}_r (-1)^r(2r+1)U^{(r)2}. \quad (39)$$

We shall henceforth consider only schemes for which also Q is diagonal, i.e., schemes for which

$$(l^n\alpha SL|Q|l^n\alpha' SL)=Q(l^n\alpha SL)\delta(\alpha\alpha'). \quad (40)$$

It follows from (39) and (74)II that if Q is diagonal in a given scheme of l^n, it is also diagonal in the conjugate scheme of l^{4l+2-n}, and that

$$Q(l^{4l+2-n}\alpha SL)=Q(l^n\alpha SL)+2l+1-n. \quad (41)$$

In order to calculate the possible values of $Q(l^n\alpha SL)$, we express it by means of (33a) and (35):

$$Q(l^n\alpha SL)\delta(\alpha\alpha')=\tfrac{1}{2}n(n-1)(2l+1)\cdot\sum_{\beta'}(l^n\alpha SL[\![l^{n-2}(\beta' SL),l^2(^1S),SL)\cdot(l^{n-2}(\beta' SL),l^2(^1S),SL]\!]l^n\alpha' SL). \quad (42)$$

Multiplying the two sides by

$$(l^n\alpha' SL[\![l^{n-2}(\beta SL),l^2(^1S),SL)$$

and adding with respect to α' we have

$$Q(l^n\alpha SL)(l^n\alpha SL[\![l^{n-2}(\beta SL),l^2(^1S),SL)=\sum_{\alpha'\beta'}(l^n\alpha SL[\![l^{n-2}(\beta' SL),l^2(^1S),SL)\cdot(l^{n-2}(\beta' SL),l^2(^1S),SL]\!]l^n\alpha' SL)\cdot(l^n\alpha' SL[\![l^{n-2}(\beta SL),l^2(^1S),SL);$$

the summation with respect to α' may be made by means of (42) after transforming the last two factors by the relation

$$(l^{n-2}(\beta SL),l^2(^1S),SL]\!]l^n\alpha SL)=\left[\frac{(4l+3-n)(4l+4-n)}{n(n-1)}\right]^{\frac{1}{2}}\cdot(l^{4l+2-n}(\alpha SL),l^2(^1S),SL]\!]l^{4l+4-n}\beta SL), \quad (43)$$

which is analogous to (19) and may be obtained in the same way; we get

$$Q(l^n\alpha SL)(l^n\alpha SL[\![L^{n-2}(\beta SL),l^2(^1S),SL)=(l^n\alpha SL[\![l^{n-2}(\beta SL),l^2(^1S),SL)Q(l^{4l+4-n}\beta SL). \quad (44)$$

Owing to (41) $(l^n\alpha SL[\![l^{n-2}(\beta SL),l^2(^1S),SL)$ may be different from zero only if

$$Q(l^n\alpha SL)=Q(l^{n-2}\beta SL)+2l+3-n, \quad (45)$$

and according to (42) the only non-vanishing values of $Q(l^n\alpha SL)$ are those which are connected to a $Q(l^{n-2}\beta SL)$ by (45).

(2) The "Seniority Number"

Putting for $Q\neq 0$

$$v_{\alpha\beta}(QSL)=(l^n\alpha SL[\![l^{n-2}(\beta SL),l^2(^1S),SL), \quad (46)$$

where α may assume all values for which $Q(l^n\alpha SL)=Q$, and β all values which satisfy (45), we have from (42) that

$$\tfrac{1}{2}n(n-1)(2l+1)\cdot\sum_\beta v_{\alpha\beta}(QSL)\overset{\dagger}{v}_{\beta\alpha'}(QSL)=Q\delta(\alpha\alpha'), \quad (47)$$

and also from (43) and again (42) that

$$\tfrac{1}{2}n(n-1)(2l+1)\cdot\sum_\alpha \overset{\dagger}{v}_{\beta\alpha}(QSL)v_{\alpha\beta'}(QSL)=Q\delta(\beta\beta'); \quad (47')$$

it follows that for two given values of Q which are connected by (45) the number of independent states of given S and L is the same in l^n and l^{n-2}, and that the matrix

$$u_{\alpha\beta}(QSL)=[\tfrac{1}{2}n(n-1)(2l+1)/Q]^{\frac{1}{2}}v_{\alpha\beta}(QSL) \quad (48)$$

is a unitary one. If we apply to the eigenfunctions of l^n the transformation u, and consider the states with eigenfunctions

$$\Psi(l^n\beta SL)=\sum_\alpha \Psi(l^n\alpha SL)u_{\alpha\beta},$$

we obtain

$$(l^{n-2}(\beta' SL),\, l^2(^1S),\, SL]\!]l^n\beta SL) =[Q(l^n\beta SL)]^{\frac{1}{2}}[\tfrac{1}{2}n(n-1)(2l+1)]^{-\frac{1}{2}}\delta(\beta\beta'); \quad (49)$$

i.e., it is possible to find a scheme of l^n in which not only Q is diagonal, but also each term of l^n with $Q\neq 0$ corresponds to a well-defined term of l^{n-2} whose Q is connected to $Q(l^n\beta SL)$ by (45). If also $Q(l^{n-2}\beta SL)\neq 0$, this term corresponds to a term of l^{n-4} and so forth; each chain of corresponding terms begins with a term $l^v\beta SL$ which has $Q=0$.

We may thus assign to each term in the QSL scheme a "seniority number" v, which indicates the number of electrons of the first member of its chain; it follows immediately from (45) that Q depends only on n and v and that its values are given by

$$Q(n,v)=\tfrac{1}{4}(n-v)(4l+4-n-v). \quad (50)$$

Confronting (41) and (50) we see that conjugate terms have the same seniority.

The seniority number suffices for distinguishing the different terms of the same kind in the configurations d^n but not in f^n, since there are in f^n terms of the same kind which have also the same seniority. For such configurations an unspecified parameter α must be maintained besides v; terms corresponding according to (49) will have the same values of v and of α.

With this convention Eq. (49) which defines the correspondence between terms of the same chain becomes

$$(l^{n-2}(\alpha' v' SL),\, l^2(^1S),\, SL]\!]l^n\alpha v SL) =[Q(n,v)]^{\frac{1}{2}}[\tfrac{1}{2}n(n-1) \cdot(2l+1)]^{-\frac{1}{2}}\delta(vv')\delta(\alpha\alpha'). \quad (49')$$

In this paper all tables of matrix elements are given in the QSL scheme and the seniority number is indicated by a prefix under the multiplicity number of each term: for instance the two ^2D terms of d^3, which were indicated in TAS (p. 228) by a^2D and b^2D, are therefore, respectively, denoted by ${}_1^2D$ and ${}_3^2D$.

(3) The High Degeneracies

Majorana's operator of position exchange may be defined for equivalent electrons by the relation

$$(l^2LM|M_{ij}|l^2LM)=(-1)^L \quad (51)$$

and may also be expressed, according to Dirac's vector model, by

$$M_{ij}=-[\tfrac{1}{2}+2(\mathbf{s}_i\cdot\mathbf{s}_j)]. \quad (52)$$

From (43)II we have

$$\sum_{0}^{2l}{}_r\,(-1)^r(2r+1)W(llll;0r)W(llll;Lr) =(-1)^LW(llll;L0); \quad (53)$$

expressing $W(llll;0r)$ and $W(llll;L0)$ by (36)II and using also (38)II and (58)II we get for M_{ij} the expression

$$M_{ij}=\sum_{0}^{2l}{}_r\,(2r+1)(\mathbf{u}_i^{(r)}\cdot\mathbf{u}_j^{(r)}). \quad (54)$$

Adding this equation to (37) and introducing (52) we have

$$2\sum_{0}^{l}{}_t\,(4t+1)(\mathbf{u}_i^{(2t)}\cdot\mathbf{u}_j^{(2t)}) =q_{ij}-[\tfrac{1}{2}+2(\mathbf{s}_i\cdot\mathbf{s}_j)]. \quad (55)$$

It follows therefore from §4 of II and particularly from (51)II that if Slater's integrals F^k are proportional to $(2k+1)/C_{llk}$, the electrostatic interaction between two equivalent electrons is proportional to (55) and then the electrostatic-energy matrix is diagonal in the QSL scheme and its eigenvalues are only functions of n, v, and S. This fact explains the high degeneracies observed by Laporte and Platt[10] for these particular ratios of the parameters; unfortunately these ratios are only hypothetical, since they are excluded by the property of F^k of being a decreasing function of k (TAS, p. 177).

[10] O. Laporte and J. R. Platt, Phys. Rev. 61, 305 (1942).

(4) Relations Between Parentages of Corresponding Terms

If we express $\Psi(l^n)$ as linear combination of $\psi(l^{n-1}l)$ with $\Psi(l^{n-1})$ as linear combination of $\psi(l^{n-3}l^2)$, express on the other hand $\Psi(l^n)$ as combination of $\psi(l^{n-2}l^2)$ with $\Psi(l^{n-2})$ as combination of $\psi(l^{n-3}l)$, and compare the two developments, we obtain

$$\sum_{\alpha''v''}(l^{n-3}(\alpha'v'S'L'),l^2(^1S),S'L'\rrbracket l^{n-1}\alpha''v''S'L')\cdot(l^{n-1}(\alpha''v''S'L')lSL\rrbracket l^n\alpha vSL)$$
$$=\sum_{\alpha'''v'''}(l^{n-3}(\alpha'v'S'L')lSL\rrbracket l^{n-2}\alpha'''v'''SL)\cdot(l^{n-2}(\alpha'''v'''SL),l^2(^1S),SL\rrbracket l^n\alpha vSL),\quad(56)$$

and owing to (49′) and (50)

$$[(n-v'-1)(4l+5-n-v')/(n-2)]^{\frac{1}{2}}\cdot(l^{n-1}(\alpha'v'S'L')lSL\rrbracket l^n\alpha vSL)$$
$$=(l^{n-3}(\alpha'v'S'L')lSL\rrbracket l^{n-2}\alpha vSL)\cdot[(n-v)(4l+4-n-v)/n]^{\frac{1}{2}}.\quad(57)$$

It is easy to deduce from this recursion formula that

$$(l^{n-1}(\alpha'v'S'L')lSL\rrbracket l^n\alpha vSL)=0\qquad(v'\neq v\pm1),\quad(58a)$$

$$(l^{n-1}(\alpha'v-1S'L')lSL\rrbracket l^n\alpha vSL)=[(4l+4-n-v)v/2n(2l+2-v)]^{\frac{1}{2}}\cdot(l^{v-1}(\alpha'v-1S'L')lSL\rrbracket l^v\alpha vSL),\quad(58b)$$

$$(l^{n-1}(\alpha'v+1S'L')lSL\rrbracket l^n\alpha vSL)=[(n-v)(v+2)/2n]^{\frac{1}{2}}\cdot(l^{v+1}(\alpha'v+1S'L')lSL\rrbracket l^{v+2}\alpha vSL).\quad(58c)$$

Comparing (58b) with (13) we obtain the more accurate orthogonality relations

$$\sum_{\alpha'S'L'}(l^n\alpha vSL\llbracket l^{n-1}(\alpha'v-1S'L')lSL)\cdot(l^{n-1}(\alpha'v-1S'L')lSL\rrbracket l^n\alpha''vSL)$$
$$=[(4l+4-n-v)v/2n(2l+2-v)]\delta(\alpha\alpha'')\quad(59a)$$

and

$$\sum_{\alpha'S'L'}(l^n\alpha vSL\llbracket l^{n-1}(\alpha'v+1S'L')lSL)\cdot(l^{n-1}(\alpha'v+1S'L')lSL\rrbracket l^n\alpha''vSL)$$
$$=[(n-v)(4l+4-v)/2n(2l+2-v)]\delta(\alpha\alpha'');\quad(59b)$$

comparing (58c) with (20) we obtain also

$$\sum_{\alpha SL}(2S+1)(2L+1)\cdot(l^{n-1}(\alpha'v+1S'L')lSL\rrbracket l^n\alpha vSL)\cdot(l^n\alpha vSL\llbracket l^{n-1}(\alpha''v+1S'L')lSL)$$
$$=(2S'+1)(2L'+1)\cdot[(n-v)(v+1)/2n(2l+1-v)]\delta(\alpha'\alpha'')\quad(60a)$$

and

$$\sum_{\alpha SL}(2S+1)(2L+1)\cdot(l^{n-1}(\alpha'v-1S'L')lSL\rrbracket l^n\alpha vSL)\cdot(l^n\alpha vSL\llbracket l^{n-1}(\alpha''v-1S'L')lSL)$$
$$=(2S'+1)(2L'+1)[(4l+4-n-v)\cdot(4l+5-v)/2n(2l+3-v)]\delta(\alpha'\alpha'').\quad(60b)$$

Another useful relation is the following:

$$(l^{v+1}(\alpha'v+1S'L')lSL\rrbracket l^{v+2}\alpha vSL)=(-1)^{S+L+l+\frac{1}{2}-S'-L'}\cdot\left[\frac{(2S'+1)(2L'+1)(v+1)}{(2S+1)(2L+1)(v+2)(2l+1-v)}\right]^{\frac{1}{2}}\cdot(l^v(\alpha vSL)lS'L'\rrbracket l^{v+1}\alpha'v+1S'L');\quad(61)$$

since this relation is verified for $v=0$ ($S=L=0$, $S'=\frac{1}{2}$, $L'=l$), it suffices to prove that if it holds for $v=v'-1$ it holds also for $v=v'$.

We use for this purpose the expressions (32) and (49′) of $(l^{v'}(\alpha v'SL),\ l^2(^1S),\ SL\rrbracket l^{v'+2}\alpha v'SL)$: owing to (6), (58), and (50) we have

$$\sum_{\alpha_1S_1L_1}(-1)^{S+L+l+\frac{1}{2}-S_1-L_1}\cdot\left[\frac{(2S_1+1)(2L_1+1)}{2(2l+1)(2S+1)(2L+1)}\right]^{\frac{1}{2}}\cdot(l^{v'}(\alpha v'SL)lS_1L_1\rrbracket l^{v'+1}\alpha_1v'-1S_1L_1)\cdot\left[\frac{(2l+1-v')v'}{(v'+2)(2l+2-v')}\right]^{\frac{1}{2}}\cdot(l^{v'-1}(\alpha_1v'-1S_1L_1)lSL\rrbracket l^{v'}\alpha v'SL)$$
$$+\sum_{\alpha_2S_2L_2}(-1)^{S+L+l+\frac{1}{2}-S_2-L_2}\cdot\left[\frac{(2S_2+1)(2L_2+1)}{2(2l+1)(2S+1)(2L+1)}\right]^{\frac{1}{2}}\cdot(l^{v'}(\alpha v'SL)lS_2L_2\rrbracket l^{v'+1}\alpha_2v'+1S_2L_2)\cdot(l^{v'+1}(\alpha_2v'+1S_2L_2)lSL\rrbracket l^{v'+2}\alpha v'SL)$$
$$=\left[\frac{2(2l+1-v')}{(v'+1)(v'+2)(2l+1)}\right]^{\frac{1}{2}}.\quad(62)$$

If (61) holds for $v=v'-1$ we may calculate the first sum with the aid of (59a) and obtain

$$-\frac{v'}{2l+2-v'}\left[\frac{2l+1-v'}{2(v'+1)(v'+2)(2l+1)}\right]^{\frac{1}{2}};$$

the second sum must then have the value

$$\frac{4l+4-v'}{2l+2-v'}\left[\frac{2l+1-v'}{2(v'+1)(v'+2)(2l+1)}\right]^{\frac{1}{2}},$$

and owing to (59b), to (60b) and to the well-known corollary of Schwarz's inequality, this fact is possible only if (61) holds also for $v=v'$.

By the use of the formulas (58) and (61) the calculation of the fractional parentages is considerably simplified: Only the parentages of the "new" terms ($v=n$) must really be calculated by the methods of §3; all others may be quickly deduced from them.

(5) Relations Between Correspondence and Conjugation

It follows from (43) that if two eigenfunctions $\Psi_{\mathfrak{L}}(l^n\alpha vSL)$ and $\Psi_{\mathfrak{L}}(l^{n+2}\alpha vSL)$ correspond according to (49′), also the eigenfunctions of their conjugate states $\Psi_{\mathfrak{R}}(l^{4l+2-n}\alpha vSL)$ and $\Psi_{\mathfrak{R}}(l^{4l-n}\alpha vSL)$ correspond in the same way. But if, in order to make full use of (74)II, we assume as standard scheme the scheme of the $\Psi_{\mathfrak{L}}$ for $n\leqslant 2l+1$ and that of the $\Psi_{\mathfrak{R}}$ for $n\geqslant 2l+2$, we cannot use (49′) for the determination of $(l^{2l}(\alpha' vSL),\ l^2({}^1S),\ SL]\!]l^{2l+2}\alpha vSL)$, nor can we use (19) for $n=2l$ without knowing which of the two possibilities of (76)II holds for each term of l^{2l+1}.

In order to solve these questions we consider provisorily the system of functions $\Psi_{\mathfrak{L}}(l^{2l+2}\alpha vSL)$ defined by means of (49′) and the system of functions $\Psi_{\mathfrak{R}}(l^{2l+1}\alpha' v'S'L')$ defined by means of (14), and seek the relation between the parentages of $\Psi_{\mathfrak{L}}(l^{2l+2}\alpha vSL)$ with respect to $\Psi_{\mathfrak{L}}(l^{2l+1}\alpha' v'S'L')$ and the parentages of $\Psi_{\mathfrak{R}}(l^{2l+2}\alpha vSL)$ with respect to $\Psi_{\mathfrak{R}}(l^{2l+1}\alpha' v'S'L')$. Using (19), (58), and (61), and owing to the fact that $2S$ is even and $2S'$ is odd, we get

$$(l^{2l+1}(\alpha' v+1S'L')lSL]\!]l^{2l+2}\alpha vSL)_{\mathfrak{R}} = (l^{2l+1}(\alpha' v+1S'L')lSL]\!]l^{2l+2}\alpha vSL)_{\mathfrak{L}} \quad (63a)$$

and

$$(l^{2l+1}(\alpha' v-1S'L')lSL]\!]l^{2l+2}\alpha vSL)_{\mathfrak{R}} = -(l^{2l+1}(\alpha' v-1S'L')lSL]\!]l^{2l+2}\alpha vSL). \quad (63b)$$

If we assume

$$\Psi_{\mathfrak{R}}(l^{2l+1}\ {}_1{}^2L) = \Psi_{\mathfrak{L}}(l^{2l+1}\ {}_1{}^2L), \quad (64)$$

it follows by the alternate use of (63a) and (63b) that

$$\begin{aligned}\Psi_{\mathfrak{R}}(l^{2l+1}\alpha vSL) &= (-1)^{v-1/2}\Psi_{\mathfrak{L}}(l^{2l+1}\alpha vSL),\\ \Psi_{\mathfrak{R}}(l^{2l+2}\alpha vSL) &= (-1)^{v/2}\Psi_{\mathfrak{L}}(l^{2l+2}\alpha vSL).\end{aligned} \quad (65)$$

If we had assumed a minus sign in (64), the relations (65) would have also the opposite sign; the choice between these two possibilities depends on the phase of $\Psi(l^{4l+2}\ {}^1{}_0S)$, and it may be shown that (64) is in agreement with the convention of §5 of TAS for the eigenfunctions of closed shells.

The relations (65) must be taken in account if we use (19) for $n=21$ or (49′) for $n=2l+2$ and $n=2l+3$, and also if we calculate the coefficients of fractional parentage for $n\geqslant 2l+2$ by means of (58) instead of (19).

(6) Relations Between Matrix Components of Tensors

It follows immediately from (23) and (58) that the matrix components of every operator F between two states of l^n may be different from zero only if

$$\Delta v=0,\quad \pm 2, \quad (66)$$

and that

$$\begin{aligned}&(l^n\alpha vSLM_SM_L|F|l^n\alpha' v-2S'L'M_S'M_L')\\ &=\tfrac{1}{2}[(n+2-v)(4l+4-n-v)/(2l+2-v)]^{\frac{1}{2}}\\ &\cdot(l^v\alpha vSLM_SM_L|F|l^v\alpha' v-2S'L'M_S'M_L');\end{aligned} \quad (67)$$

owing to (65) a minus sign, however, must be introduced in this formula for $n\geqslant 2l+2$.

If $\Delta v=0$ the sum (23) splits in two sums according to the two possibilities $v-1$ and $v+1$ of the seniority numbers of l^{n-1}, but only the first sum may be immediately expressed as in the preceding case by means of the matrix components for l^v; the second sum is to be expressed by means of the matrix components for l^v and those for another arbitrary configuration $l^{n'}$. If we assume $n'=4l+2-v$, the final result is found to be

$$(l^n\alpha vSLM_SM_L|F|l^n\alpha' vS'L'M_S'M_L')$$
$$=[(4l+2-n-v)/2(2l+1-v)]$$
$$\cdot(l^v\alpha vSLM_SM_L|F|l^v\alpha' vS'L'M_S'M_L')$$
$$+[(n-v)/2(2l+1-v)]$$
$$\cdot(l^{4l+2-v}\alpha vSLM_SM_L|F|l^{4l+2-v}$$
$$\cdot\alpha' vS'L'M_S'M_L'). \quad (68)$$

If F is an irreducible tensor, it follows from (68) and (74)II that

$$(l^n\alpha vSL\|T^{(\kappa k)}\|l^n\alpha' vS'L')$$
$$=(l^v\alpha vSL\|T^{(\kappa k)}\|l^v\alpha' vS'L') \quad (\kappa+k \text{ odd}), \quad (69\text{a})$$

$$(l^n\alpha vSL\|T^{(\kappa k)}\|l^n\alpha' vS'L')$$
$$=\frac{2l+1-n}{2l+1-v}(l^v\alpha vSL\|T^{(\kappa k)}\|l^v\alpha' vS'L')$$
$$(\kappa+k \text{ even}). \quad (69\text{b})$$

From (67), (65), and (74)II we get also

$$(l^n\alpha vSL\|T^{(\kappa k)}\|l^n\alpha' v-2S'L')=0$$
$$(\kappa+k \text{ odd}). \quad (70)$$

The remarkable result that a tensor of odd degree is diagonal with respect to v and that its submatrices are independent of n may be obtained also in a more direct way. It follows from the triangular conditions and from the fact that in l^2 only states with even $S+L$ are allowed, that for $\kappa+k$ odd

$$(l^2\,{}^1S|\boldsymbol{t}_1^{(\kappa k)}+\boldsymbol{t}_2^{(\kappa k)}|l^2SLM_SM_L)$$
$$=(l^2SLM_SM_L|\boldsymbol{t}_1^{(\kappa k)}+\boldsymbol{t}_2^{(\kappa k)}|l^2\,{}^1S)=0$$

and, therefore,

$$q_{ij}(\boldsymbol{t}_i^{(\kappa k)}+\boldsymbol{t}_j^{(\kappa k)})=(\boldsymbol{t}_i^{(\kappa k)}+\boldsymbol{t}_j^{(\kappa k)})q_{ij}=0$$
$$(\kappa+k \text{ odd}); \quad (71)$$

since all other $\boldsymbol{t}_h^{(\kappa k)}$ commute with q_{ij}, $\boldsymbol{T}^{(\kappa k)}$ commutes with q_{ij} and also with Q, and is therefore diagonal with respect to v. From (71) we have also

$$Q\boldsymbol{T}=\boldsymbol{T}Q=\sum_{\substack{i<j\\ i\neq h\neq j}} \boldsymbol{t}_h q_{ij};$$

calculating the matrix of this operator with the methods of §5 and owing to (49′) we obtain

$$(l^n\alpha vSL\|T^{(\kappa k)}\|l^n\alpha' vS'L')$$
$$=(l^{n-2}\alpha vSL\|T^{(\kappa k)}\|l^{n-2}\alpha' vS'L'),$$

which is equivalent to (69a).

The matrices of the tensor $\boldsymbol{V}^{(12)}$ defined by (102)II were calculated for the configurations p^2, p^3, d^3, d^4 and d^5 using also (69a); the results are given in Tables XV–XIX. The matrices given in Tables V and XIX are sufficient for the calculation of the spectra of the configurations p^nl and d^np with the methods of §8 of II.

TABLE XV. $(p^2SL\|2V^{(12)}\|p^2S'L')$.

	^1S	^3P	^1D
^1S	0	0	0
^3P	0	$-(6)^{\frac{1}{2}}$	-3
^1D	0	-3	0

TABLE XVI. $(p^3SL\|2V^{(12)}\|p^3S'L')$.

	^4S	^2P	^2D
^4S	0	0	$-2(2)^{\frac{1}{2}}$
^2P	0	$(6)^{\frac{1}{2}}$	0
^2D	$2(2)^{\frac{1}{2}}$	0	$-(14)^{\frac{1}{2}}$

§7. THE ELECTROSTATIC INTERACTION BETWEEN d^n, $d^{n-1}s$ AND $d^{n-2}s^2$

The electrostatic interaction between $d^2\,{}^1S$ and $s^2\,{}^1S$ is given by

$$(d^2\,{}^1S|e^2/r|s^2\,{}^1S)$$
$$=R^2(dd,ss)(d^2\,{}^1S|P_2(\cos\omega)|s^2\,{}^1S), \quad (72)$$

where R^2 is defined by TAS 8^68 and ω is the angle between the radii vectors of the two electrons. From (51)II we have

$$(2\|C^{(2)}\|0)=1, \quad (73)$$

and hence from (45)II and (38)II we get

$$(d^2\,{}^1S|P_2(\cos\omega)|s^2\,{}^1S)=1/5^{\frac{1}{2}};$$

since

$$R^2(dd,ss)=R^2(ds,sd)=G^2(ds)=5G_2(ds),$$

(72) becomes

$$(d^2\,{}^1S|e^2/r|s^2\,{}^1S)=5^{\frac{1}{2}}G_2. \quad (74)$$

Introducing this result in (33c) and owing to

TABLE XVII. $(d^3vSL\|70\,V^{(12)}\|d^3v'S'L')$.

	$_3{}^2P$	$_3{}^4P$	$_1{}^2D$	$_3{}^2D$	$_3{}^2F$	$_3{}^4F$	$_3{}^2G$	$_3{}^2H$
$_3{}^2P$	$-19(14)^{1/2}$	-28	0	$8(35)^{1/2}$	$-8(14)^{1/2}$	$-22(14)^{1/2}$	0	0
$_3{}^4P$	28	$14(35)^{1/2}$	0	$-28(10)^{1/2}$	56	$-28(10)^{1/2}$	0	0
$_1{}^2D$	0	0	$35(6)^{1/2}$	0	0	0	0	0
$_3{}^2D$	$-8(35)^{1/2}$	$-28(10)^{1/2}$	0	$-5(6)^{1/2}$	$-4(210)^{1/2}$	$4(210)^{1/2}$	$-60(2)^{1/2}$	0
$_3{}^2F$	$-8(14)^{1/2}$	-56	0	$4(210)^{1/2}$	-77	-98	$3(35)^{1/2}$	$-4(385)^{1/2}$
$_3{}^4F$	$22(14)^{1/2}$	$-28(10)^{1/2}$	0	$4(210)^{1/2}$	98	$-14(10)^{1/2}$	$-18(35)^{1/2}$	$4(385)^{1/2}$
$_3{}^2G$	0	0	0	$-60(2)^{1/2}$	$-3(35)^{1/2}$	$-18(35)^{1/2}$	$3(33)^{1/2}$	$12(77)^{1/2}$
$_3{}^2H$	0	0	0	0	$-4(385)^{1/2}$	$-4(385)^{1/2}$	$-12(77)^{1/2}$	$-(2002)^{1/2}$

TABLE XVIII. $(d^44SL\|70\,V^{(12)}\|d^44S'L')$.

	$_4{}^1S$	$_4{}^3P$	$_4{}^1D$	$_4{}^3D$	$_4{}^5D$	$_4{}^1F$	$_4{}^3F$	$_4{}^1G$	$_4{}^3G$	$_4{}^3H$	$_4{}^1I$
$_4{}^1S$	0	0	0	$4(210)^{1/2}$	0	0	0	0	0	0	0
$_4{}^3P$	0	$6(14)^{1/2}$	$-15(35)^{1/2}$	$-3(35)^{1/2}$	-105	$-12(35)^{1/2}$	$12(14)^{1/2}$	0	0	0	0
$_4{}^1D$	0	$-15(35)^{1/2}$	0	$5(6)^{1/2}$	0	0	0	0	$60(2)^{1/2}$	0	0
$_4{}^3D$	$-4(210)^{1/2}$	$3(35)^{1/2}$	$-5(6)^{1/2}$	$-15/2(6)^{1/2}$	$15/2(210)^{1/2}$	$-10(21)^{1/2}$	$9(210)^{1/2}$	$6(165)^{1/2}$	$15(2)^{1/2}$	0	0
$_4{}^5D$	0	-105	0	$-15/2(210)^{1/2}$	$-35/2(30)^{1/2}$	0	$35(6)^{1/2}$	0	$15(70)^{1/2}$	0	0
$_4{}^1F$	0	$12(35)^{1/2}$	0	$-10(21)^{1/2}$	0	0	$-21(10)^{1/2}$	0	$12(14)^{1/2}$	$-6(154)^{1/2}$	0
$_4{}^3F$	0	$12(14)^{1/2}$	0	$-9(210)^{1/2}$	$35(6)^{1/2}$	$21(10)^{1/2}$	-42	0	$-12(35)^{1/2}$	$6(385)^{1/2}$	0
$_4{}^1G$	0	0	0	$-6(165)^{1/2}$	0	0	0	0	$27(10)^{1/2}$	$6(210)^{1/2}$	0
$_4{}^3G$	0	0	$-60(2)^{1/2}$	$15(2)^{1/2}$	$-15(70)^{1/2}$	$12(14)^{1/2}$	$12(35)^{1/2}$	$-27(10)^{1/2}$	$-6(33)^{1/2}$	$-6(77)^{1/2}$	$-12(91)^{1/2}$
$_4{}^3H$	0	0	0	0	0	$6(154)^{1/2}$	$6(385)^{1/2}$	$6(210)^{1/2}$	$6(77)^{1/2}$	$-3(2002)^{1/2}$	$-7(39)^{1/2}$
$_4{}^1I$	0	0	0	0	0	0	0	0	$12(91)^{1/2}$	$-7(39)^{1/2}$	0

TABLE XIX. $(d^55SL\|70\,V^{(12)}\|d^55S'L')$.

	$_5{}^2S$	$_5{}^6S$	$_5{}^2D$	$_5{}^4D$	$_5{}^2F$	$_5{}^2G$	$_5{}^4G$	$_5{}^2I$
$_5{}^2S$	0	0	$-4(210)^{1/2}$	$-6(105)^{1/2}$	0	0	0	0
$_5{}^6S$	0	0	0	$70(3)^{1/2}$	0	0	0	0
$_5{}^2D$	$-4(210)^{1/2}$	0	$15(6)^{1/2}$	$60(3)^{1/2}$	$-20(21)^{1/2}$	-4	$-20(15)^{1/2}$	0
$_5{}^4D$	$6(105)^{1/2}$	$-70(3)^{1/2}$	$-60(3)^{1/2}$	$10(15)^{1/2}$	0	$8(330)^{1/2}$	$-40(3)^{1/2}$	0
$_5{}^2F$	0	0	$20(21)^{1/2}$	0	-105	$(1155)^{1/2}$	$14(105)^{1/2}$	0
$_5{}^2G$	0	0	$-4(165)^{1/2}$	$-8(330)^{1/2}$	$-(1155)^{1/2}$	$125/11(33)^{1/2}$	$-10(3)^{1/2}$	$8/11(30030)^{1/2}$
$_5{}^4G$	0	0	$20(15)^{1/2}$	$-40(3)^{1/2}$	$14(105)^{1/2}$	$10(3)^{1/2}$	$-10(330)^{1/2}$	$-2(2730)^{1/2}$
$_5{}^2I$	0	0	0	0	0	$8/11(30030)^{1/2}$	$2(2730)^{1/2}$	$-35/11(858)^{1/2}$

(49′) we obtain

$$(d^nvSL|\sum e^2/r_{ij}|d^{n-2}s^2v'SL)=[Q(n,v)]^{\frac{1}{2}}\delta(vv')G_2;\quad (75)$$

owing to the conventions of subsection (5) of §6, a minus sign must be introduced for $n=6$, $v=2$ and for $n=7$, $v=3$.

The calculation of the interaction between the configurations d^n and $d^{n-1}s$ by means of (33b) is easy only for $n=3$, since in this case

$$(d,\,d^2(^1D),\,SL]\!]d^3vSL)$$

may be obtained from Table II by means of (29); but, as it was already mentioned at the end of §5, the calculations for $n\geqslant 4$ become very long, and it appears more convenient to use the following method.

The interaction in question is given by

$$(d^nvSL|\sum e^2/r_{ij}|d^{n-1}(v'S'L)sSL)=R^2(dd,\,ds)\cdot(d^nvSL|\sum P_2(\cos\omega_{ij})|d^{n-1}(v'S'L)sSL);\quad (76)$$

owing to (45)II and to the fact that $\sum_i \mathbf{C}_i{}^{(2)2}$ is a scalar and its non-diagonal matrix components vanish, we have

$$(d^nvSL|\sum_{i<j} P_2(\cos\omega_{ij})|d^{n-1}(v'S'L)sSL)=\tfrac{1}{2}(d^nvSL|[\sum_i \mathbf{C}_i{}^{(2)}]^2|d^{n-1}(v'S'L)sSL),\quad (77)$$

TABLE XX. $(d^3vSL|\Sigma e^2/r_{ij}|d^2(v'S'L')sSL)$.

d^3	d^2s	H_2
${}_3{}^2P$	$({}_2{}^3P)^2P$	$3(35)^{\frac{1}{2}}$
${}_3{}^4P$	$({}_2{}^3P)^4P$	0
${}_1{}^2D$	$({}_2{}^1D)^2D$	$-\frac{1}{2}(70)^{\frac{1}{2}}$
${}_3{}^2D$	$({}_2{}^1D)^2D$	$\frac{3}{2}(30)^{\frac{1}{2}}$
${}_3{}^2F$	$({}_2{}^3F)^2F$	$-3(10)^{\frac{1}{2}}$
${}_3{}^4F$	$({}_2{}^3F)^4F$	0
${}_3{}^2G$	$({}_2{}^1G)^2G$	$-5(2)^{\frac{1}{2}}$

and using (33)II we obtain

$$2(2L+1)(d^nvSL|\sum_{i<j} P_2(\cos\,\omega_{ij})|d^{n-1}(v'S'L)sSL)$$
$$=\sum_{v''L''}(-1)^{L-L''}$$
$$\cdot(d^nvSL\|\sum_i C_i^{(2)}\|d^nv''SL'')$$
$$\cdot(d^nv''SL''\|\sum_i C_i^{(2)}\|d^{n-1}(v'S'L)sSL)$$
$$+\sum_{v''L''}(-1)^{L-L''}$$
$$\cdot(d^nvSL\|\sum_i C_i^{(2)}\|d^{n-1}(v''S'L'')sSL'')$$
$$\cdot(d^{n-1}(v''S'L'')sSL''\|\sum_i C_i^{(2)}\|d^{n-1}(v'S'L)sSL). \quad (78)$$

From (27), (44)II, (80)II, and (73) we obtain finally

$$(d^nvSL|\sum e^2/r_{ij}|d^{n-1}(v'S'L)sSL)$$
$$=(n/14)^{\frac{1}{2}}[\sum_{v''L''}(-1)^{L-L''}$$
$$\cdot(d^nvSL\|U^{(2)}\|d^nv''SL'')$$
$$\cdot(d^nv''SL''[\![d^{n-1}(v'S'L)dSL)$$
$$\cdot(2L''+1)^{\frac{1}{2}}/(2L+1)+\sum_{v''L''}(-1)^{L-L''}$$
$$\cdot(d^nvSL[\![d^{n-1}(v''S'L'')dSL)$$
$$\cdot(d^{n-1}v''S'L''\|U^{(2)}\|d^{n-1}v'S'L)/$$
$$(2L+1)^{\frac{1}{2}}]R^2(dd,ds). \quad (79)$$

By means of this formula the interaction between the configurations d^n and $d^{n-1}s$ was calculated for $n=3$, 4, 5; the results are different from zero only if $v'=v\pm1$ and are given in Tables XX–XXII, where the quantity

$$H_2=R^2(dd,ds)/35 \quad (80)$$

was assumed as parameter. For $n=3$ our results agree with those given by Marvin.[11]

TABLE XXI. $(d^4vSL|\Sigma e^2/r_{ij}|d^3(v'S'L')sSL)$.

d^4	d^3s	H_2	d^4	d^3s	H_2
${}_2{}^3P$	$({}_3{}^2P)^3P$	$(70)^{\frac{1}{2}}$	${}_4{}^1F$	$({}_3{}^2F)^1F$	-15
${}_2{}^3P$	$({}_3{}^4P)^3P$	0	${}_2{}^3F$	$({}_3{}^2F)^3F$	$-2(5)^{\frac{1}{2}}$
${}_4{}^3P$	$({}_3{}^2P)^3P$	$-2(5)^{\frac{1}{2}}$	${}_2{}^3F$	$({}_3{}^4F)^3F$	0
${}_4{}^3P$	$({}_3{}^4P)^3P$	$2(70)^{\frac{1}{2}}$	${}_4{}^3F$	$({}_3{}^2F)^3F$	$3(5)^{\frac{1}{2}}$
${}_2{}^1D$	$({}_1{}^2D)^1D$	$-(105)^{\frac{1}{2}}$	${}_4{}^3F$	$({}_3{}^4F)^3F$	$-4(5)^{\frac{1}{2}}$
${}_2{}^1D$	$({}_3{}^2D)^1D$	$-3(5)^{\frac{1}{2}}$	${}_2{}^1G$	$({}_3{}^2G)^1G$	$\frac{10}{3}(3)^{\frac{1}{2}}$
${}_4{}^1D$	$({}_3{}^2D)^1D$	$6(10)^{\frac{1}{2}}$	${}_4{}^1G$	$({}_3{}^2G)^1G$	$\frac{5}{3}(33)^{\frac{1}{2}}$
${}_4{}^3D$	$({}_3{}^2D)^3D$	$-4(5)^{\frac{1}{2}}$	${}_4{}^3G$	$({}_3{}^2G)^3G$	$3(5)^{\frac{1}{2}}$
			${}_4{}^3H$	$({}_3{}^2H)^3H$	$-2(5)^{\frac{1}{2}}$

TABLE XXII. $(d^5vSL|\Sigma e^2/r_{ij}|d^4(v'S'L')sSL)$.

d^5	d^4s	H_2	d^5	d^4s	H_2
${}_5{}^2S$	$({}_4{}^1S)^2S$	$8(5)^{\frac{1}{2}}$	${}_3{}^2F$	$({}_2{}^3F)^2F$	$-2(15)^{\frac{1}{2}}$
${}_3{}^2P$	$({}_2{}^3P)^2P$	$(210)^{\frac{1}{2}}$	${}_3{}^2F$	$({}_4{}^3F)^2F$	$-\frac{3}{2}(15)^{\frac{1}{2}}$
${}_3{}^2P$	$({}_4{}^3P)^2P$	$(15)^{\frac{1}{2}}$	${}_5{}^2F$	$({}_4{}^1F)^2F$	$\frac{7}{2}(5)^{\frac{1}{2}}$
${}_3{}^4P$	$({}_2{}^3P)^4P$	0	${}_5{}^2F$	$({}_4{}^3F)^2F$	$\frac{15}{2}(3)^{\frac{1}{2}}$
${}_3{}^4P$	$({}_4{}^3P)^4P$	$(105)^{\frac{1}{2}}$	${}_3{}^4F$	$({}_2{}^3F)^4F$	0
${}_1{}^2D$	$({}_2{}^1D)^2D$	$-(35)^{\frac{1}{2}}$	${}_3{}^4F$	$({}_4{}^3F)^4F$	$-(30)^{\frac{1}{2}}$
${}_3{}^2D$	$({}_2{}^1D)^2D$	$3(5)^{\frac{1}{2}}$	${}_3{}^2G$	$({}_2{}^1G)^2G$	$-\frac{10}{3}(3)^{\frac{1}{2}}$
${}_3{}^2D$	$({}_4{}^1D)^2D$	$3(10)^{\frac{1}{2}}$	${}_3{}^2G$	$({}_4{}^1G)^2G$	$\frac{5}{6}(33)^{\frac{1}{2}}$
${}_3{}^2D$	$({}_4{}^3D)^2D$	$2(15)^{\frac{1}{2}}$	${}_3{}^2G$	$({}_4{}^3G)^2G$	$-\frac{3}{2}(15)^{\frac{1}{2}}$
${}_5{}^2D$	$({}_4{}^1D)^2D$	$-(5)^{\frac{1}{2}}$	${}_5{}^2G$	$({}_4{}^1G)^2G$	$-\frac{9}{2}(5)^{\frac{1}{2}}$
${}_5{}^2D$	$({}_4{}^3D)^2D$	$-3(30)^{\frac{1}{2}}$	${}_5{}^2G$	$({}_4{}^3G)^2G$	$-\frac{5}{2}(11)^{\frac{1}{2}}$
${}_5{}^4D$	$({}_4{}^3D)^4D$	$-\frac{3}{2}(30)^{\frac{1}{2}}$	${}_5{}^4G$	$({}_4{}^3G)^4G$	$5(2)^{\frac{1}{2}}$
${}_5{}^4D$	$({}_4{}^5D)^4D$	$-\frac{5}{2}(14)^{\frac{1}{2}}$	${}_3{}^2H$	$({}_4{}^3H)^2H$	$(15)^{\frac{1}{2}}$
${}_3{}^2F$	$({}_4{}^1F)^2F$	$-\frac{15}{2}$	${}_5{}^2I$	$({}_4{}^1I)^2I$	$(5)^{\frac{1}{2}}$

The interaction between the configurations $d^{n-1}s$ and $d^{n-2}s^2$ may be calculated in the same way; the result is

$$(d^{n-1}(v'S'L)sSL|\sum e^2/r_{ij}|d^{n-2}s^2vSL)$$
$$=(-1)^{S+\frac{1}{2}-S'}\left[\frac{2S'+1}{2S+1}\right]^{\frac{1}{2}}$$
$$\cdot(d^{n-1}v'S'L|\sum e^2/r_{ij}|d^{n-2}(vSL)sS'L). \quad (81)$$

[11] H. H. Marvin, Phys. Rev. 47, 521 (1935).