

On the Absorption Spectra of Complex Ions. I

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In order to explain the origin of both absorption bands and lines of the octahedral normal complex ions in which the central metal ions belong to iron group elements, the crystalline field approximation interpreted in somewhat generalized sense is adopted. For this purpose the calculation of the energy matrix elements for d^n ($n=1, 2, \dots, 9$) electron configuration in cubic field is performed by means of Racah's method. Comparison of the results with experiments will be made in the following paper.

§ 1. Introduction

Much work, both theoretical and experimental, has been done about the ground states of the normal complex ions of the type $[XY_6]^{3+}$, $[XY_6]^{2+}$, where X represents an iron group element and Y represents a ligand such as H_2O , NH_3 , ethylenediamine, etc.. Especially owing to recent investigations by the method of the paramagnetic resonance absorption, rather detailed knowledge of them has been obtained. As to the excited states, however, little is known of these normal complex ions, and, it seems, there remain many problems to be investigated further from the theoretical point of view.

The optical absorption of both crystals and solutions (aqueous in many cases) containing these complex ions have been studied since the days of Werner by many physicists and chemists, and it is known that the absorption spectra of solutions are quite similar (although the width and the intensity of bands are slightly different) to those of crystals containing the same complex ion as the solutions except for an intense edge absorption ($\log \varepsilon_{\max} \sim 4$) in the ultra violet region which does not appear in the latter, so that they are considered to be due mainly to the absorption of the complex ion as a whole. The absorption spectra of these complex ions are characterized by the presence of several (one to three) bands in the near infrared, visible and ultra violet region (8000 cm^{-1} to 40000 cm^{-1}). Some of them show several sharp absorption lines besides these broad bands (e.g. Chrome Alum).

There have been several explanations of the origin of these spectra, but many of them are only of qualitative nature and it is not yet certain which is the correct one. Only two of them shall be quoted here, because they bear close relation to our calculation. Finkelstein and Van Vleck¹⁾ treated the doublet lines of Chrome Alum at 6700 \AA and obtained quantitative agreement between theory and experiment using the crystalline field approximation, but they left the origin of the broad bands unanswered. Recently, Hartmann and Schlaefer et al.²⁾ treated the problem of broad bands also from the same standing point. They maintained that these absorption bands were due to the transitions between the Stark components of the ground multiplet of the central metal ion, and showed that the number of broad bands (which are observed in the region up to 33000 cm^{-1}) could be reasonably explained on this assumption at least in case the central metal ion has no more than five d-electrons. But they made no mention of the line spectra at all. Though these explanations seem to be reasonable, it is not clear why some of the transitions correspond to the broad bands and the others to the sharp lines. It seems necessary to examine if such an assignment should give the order of magnitude of the observed intensity and the band width theoretically, and if the calculation could predict the position of the absorption maxima satisfactorily.

In order to study to what degree the crystalline field approximation succeeds in explaining the absorption spectra of these complex ions

including both the lines and bands, the energy matrix elements for the electron configuration d^n in cubic field are calculated in this paper.

§ 2. The Crystalline Field Approximation

These complex ions are known to be of the octahedral shape, and the central ion X is considered to be exposed to the cubic electric field (crystalline field) due to the octahedrally coordinated ligands Y.*

In the case of the rare earth salts, the crystalline field is relatively weak because of the screening effect of the electrons in the outer shells, so that, when one wants to study the electronic structure of the rare earth ions it is generally allowed to treat each SL multiplet separately and to consider the splittings of these multiplets due to the crystalline field. In our case of the iron group complex ions, however, the following treatment** will be more adequate, because here d -electrons are exposed directly to the strong crystalline field. In Cubic field the d -level splits into two levels, i.e., triply degenerate $d\varepsilon$ and doubly degenerate $d\gamma$ ($d\varepsilon$ is lower than the original d -level by $-4Dq$, and $d\gamma$ higher by $6Dq$, where Dq is the crystalline field parameter usually used.) and the electrons are accommodated in these two levels. For those complexes where the free $X^{3,2+}$ ion has the electrons configuration d^N , we now take the configurations $d\varepsilon^nd\gamma^{N-n}$ ($n=0$ to N) as the starting point.

If the crystalline field is sufficiently strong, we may neglect the interaction between these configurations. Then the problem is to find the positions of the ST multiplets arising from each configuration mentioned above, but unfortunately the crystalline field is not so strong as to permit us to neglect the configuration interaction entirely and we must take it into account for some of the levels.

As is easily seen, in the calculation under the scheme which we mentioned to be suited for the weak field case, if the interaction between the Stark components of different SL multiplets is fully taken into account as in Finkelstein and Van Vleck's one, the results are of course the same as those calculated in our way, when we construct $d\varepsilon$, $d\gamma$ wave function there by proper linear combinations of the d -wave function.

It is here necessary to consider the meaning

of the "crystalline field." Recently Kleiner⁴⁾ has calculated the strength of the crystalline field Dq of Chrome Alum semi-classically taking the overlapping of the charge cloud of the Cr^{3+} ion and that of H_2O into account, and found that the calculated value was by far smaller (the sign was wrong) than the value estimated from the magnetic susceptibility data, though his model seemed more reasonable than the point-dipole or -charge model^{5),6)} which can give the resonable values of Dq in many cases. This is unfortunate, but this may not be so serious. It seems to us that, as far as Dq is considered as an empirical parameter, the validity of the crystalline field approximation is not so limited as one might suppose from his results, since this approximation can be interpreted in a generalized sense as follows.

That is, we consider $[\text{XY}_6]^{3,2+}$ complex ion as a single molecule whose filled orbitals with lower energies correspond to the inner shells or closed shells of the central ion and ligands in the free states which may be deformed in the complex ion, and whose next higher orbitals are f_2 and e (which correspond to $d\varepsilon$ and $d\gamma$ respectively) belonging to the irreducible representations F_{2g} and E_g of O_h group. This is just the model which corresponds to the crystalline field approximation. f_2 and e orbitals will not have the pure d -character in general, and may be approximated by the linear combinations of d -orbitals and the ligand orbitals. For $d\gamma$ this departure from the atomic d -character will be large, but also for $d\varepsilon$ such deformation would exist as Stevens has recently pointed out⁷⁾. Thus in this generalized crystalline field formalism, Dq is now defined through the relation $\epsilon_e - \epsilon_{f_2} = 10Dq$ where ϵ_e and ϵ_{f_2} denote the orbital energies of e and f_2 orbitals. Furthermore in this molecular treatment, the integrals appearing in the calculation may be different from those in the usual crystalline field approximation, where they are expressed in terms of the Slater integrals for the free ions.

If we go further in this way there is no reason why only two levels f_2 and e should

* Throughout this and the following paper the Jahn-Teller effect is neglected.

** Similar calculations along this line has already been done by Kotani for the case of d^2 and by Kambe and Usui for d^3 ⁸⁾.

be taken into account. But when we include further configurations the calculation would become somewhat tedious and the empirical treatment such as adopted in the following paper would become impossible. Thus we assume with a hope that the generalized crystalline field model will well approximate the reality, and carry out the calculation under this assumption.

In the next section, however, we calculate the energy matrix elements using the atomic $d\varepsilon$ and $d\gamma$, and express them in terms of A , B , C and Dq (A , B , C are the linear combinations of Slater integrals introduced by Racah). Thus, the effect of deformation appears only through the change of B , C from those for the free ions. This was done only to avoid the complexity caused by many unknown parameters which appear when e and

f_2 are considered not to be pure $d\varepsilon$ and $d\gamma$, although the method of calculation is also applicable when the crystalline field approximation is taken in a generalized sense.

§ 3. The Calculation of Energy Matrices and the Results

When we adopt the scheme stated in § 2 and confine ourselves to the states which come from the configurations $d\varepsilon^n d\gamma^{N-n}$ ($n=0, \dots, N$), the orthonormal basic functions to construct the energy matrix of symmetry species ST' are $\Psi(d\varepsilon^n(S_1\Gamma_1)d\gamma^{N-n}(S_2\Gamma_2)ST')$. The matrix elements of the scalar (cubic scalar in this case) operator $G_N = \sum_{i>j}^N g_{ij}$ between these states can be calculated by means of the following recurrence formula, which is a generalization of the formula (1) of R IV⁸⁾:

$$\begin{aligned}
 & (\gamma_1^n(S_1\Gamma_1)\gamma_2^{N-n}(S_2\Gamma_2)SI'|G_N|\gamma_1^{n'}(S_3\Gamma_3)\gamma_2^{N-n'}(S_4\Gamma_4)SI') \\
 & = \sqrt{nn'}/(N-2) \sum_{S'S''\bar{S}T'T''\bar{T}} (\gamma_1^n S_1\Gamma_1\{|r_1, r_1^{n-1}(S'T')S_1\Gamma_1\rangle (r_1 S'T'(S_1\Gamma_1)S_2\Gamma_2 SI'| \\
 & \quad r_1, S'T'S_2\Gamma_2(\bar{S}\bar{T})SI'\rangle (\gamma_1^{n-1}(S'T')\gamma_2^{N-n}(S_2\Gamma_2)\bar{S}\bar{T}|G_{N-1}|\gamma_1^{n'-1}(S''T'')\gamma_2^{N-n'}(S_4\Gamma_4)\bar{S}\bar{T}) \\
 & \quad \times (r_1, S''T''S_4\Gamma_4(\bar{S}\bar{T})SI'|r_1 S''T''(S_3\Gamma_3)S_4\Gamma_4 SI') (r_1 r_1^{n'-1}(S''T'')S_3\Gamma_3|) \gamma_1^{n''} S_3\Gamma_3) \\
 & + \sqrt{(N-n)(N-n')/(N-2)} \sum_{S'S''\bar{S}T'T''\bar{T}} (\gamma_2^{N-n} S_2\Gamma_2\{|r_2^{N-n-1}(S'T')r_2 S_2\Gamma_2\rangle \\
 & \quad \times (S_1\Gamma_1, S'T' r_2(S_2\Gamma_2)SI'|S_1\Gamma_1 S'T'(\bar{S}\bar{T})r_2 SI') \\
 & \quad \times (r_1^n(S_1\Gamma_1)\gamma_2^{N-n-1}(S'T')\bar{S}\bar{T}|G_{N-1}|\gamma_1^{n''}(S_3\Gamma_3)\gamma_2^{N-n'-1}(S''T'')\bar{S}\bar{T}) \\
 & \quad \times (S_3\Gamma_3 S''T''(\bar{S}\bar{T})r_2 SI'|S_3\Gamma_3, S''T''r_2(S_4\Gamma_4)SI') \\
 & \quad \times (r_2^{N-n'-1}(S''T'')r_2 S_4\Gamma_4|) \gamma_2^{N-n'} S_4\Gamma_4) . \tag{3.1}
 \end{aligned}$$

Although r_1 , r_2 and T' 's here are the symbols for the irreducible representations of the octahedral group (r_1 , r_2 being E and F_2 respectively), this formula is generally valid for any other group.

In order to calculate this matrix element for the N electron system, it is necessary to know the transformation matrices $(S'T'S''T''(\bar{S}\bar{T}), S''T'''SI'|S'T', S'T''S''T'''(\bar{S}\bar{T})SI')$ and the coefficients of the fractional parentage ($r^n SI'\{|r^{n-1}(S'T')r SI'\}$ (c.f.p.) besides the matrix elements for the $N-1$ electron system.

The transformation matrices were simply calculated according to the definition (3) of R III⁸⁾, and the Clebsch-Gordan coefficients thereby used are given in Table I.

The c.f.p. for n -electrons are obtained solv-

ing the following linear equations which are (11) of R III, assuming that we know those for $n-1$ electrons and the transformation matrices of the type $(S''T'', rr(S''T''))SI'|S'T''r(S'T')r SI')$:

$$\begin{aligned}
 & \sum_{S'T'} (S''T'', rr(S''T''))SI'|S''T''r(S'T')r SI') \\
 & \quad \times (r^{n-2}(S''T'')r SI'|) r^{n-1} S'T' \\
 & \quad \times (r^{n-1}(S'T')r SI'|) r^n SI' = 0 . \tag{3.2}
 \end{aligned}$$

Here $S''T'''$'s denote the "forbidden states" for the configuration r^2 . For instance, in the case of $r=d\varepsilon$ they are 3A_1 , 3E , 1F_1 and 3F_2 . c.f.p. calculated in this way are given at the end of this paper (Table II), together with the c.f.p. of the type $(r^{n-2}(S'T')r^2(S'T'')SI'|) r^n SI'$ which were calculated according to (32) of R III and useful in some cases (see below).

Further relation analogous to Eq. (29) of R III was also used:

$$\begin{aligned} & (\gamma, \gamma^{n-1}(S'T')SI'| \} \gamma^n SI') \\ & = (-)^{s'+1/2-s+f(\gamma T' T')+n+1} \\ & \quad \times (\gamma^{n-1}(S'T')\gamma SI'| \} \gamma^n SI') , \end{aligned} \quad (3.3)$$

where

$$\begin{aligned} f(\gamma T' T) &= 1 \quad \text{for} \quad (\gamma T' T) = (EEA_2), \\ & \quad (F_1 F_1 F_1), \\ & \quad (F_2 F_2 F_1), \\ &= 0 \quad \text{otherwise.} \end{aligned}$$

The formula (3.1) is rather complicated and the calculation becomes somewhat tedious when one uses this formula as it is. But it is often not necessary to carry out both summations and the labor is greatly reduced especially when one of the two sums becomes simple owing to the restriction on the summation parameters.

This fact applies to the calculation of the non-diagonal elements.

Without loss of generality we may assume $n'+3>n\geq n'$. When $n-n'=2$, applying (3.1) successively we see that this type of matrix elements has a single ancestor of the type $(\gamma_1^2 SI'|g|\gamma_2^2 SI')$, and in this case, it can be shown (Appendix) that the ratio of two sums is a constant which depends only N , n , n' , and therefore it is sufficient to calculate the simpler sum. When $n-n'=1$, we have two ancestors for this type of elements, i.e.,

$(\gamma_1 \gamma_2 SI'|g|\gamma_2^2 SI')$ and $(\gamma_1^2 SI'|g|\gamma_1 \gamma_2 SI')$ so that no simplification can be obtained. But in our case fortunately there is no ancestor of the type $(d\delta d\gamma SI'|g|d\gamma^2 SI')$, because configurations $d\delta d\gamma$ and $d\gamma^2$ have no common state SI' , and we can simplify the formula (3.1) in a similar way as was made in the case $n-n'=2$. In the last case, i.e., when $n=n'$, there are three ancestors, namely $(\gamma_1^2 SI'|g|\gamma_1^2 SI')$, $(\gamma_2^2 SI'|g|\gamma_2^2 SI')$ and $(\gamma_1 \gamma_2 SI'|g|\gamma_1 \gamma_2 SI')$. The non-diagonal elements in this case are, however, seen to originate only from the last type of the three ancestors mentioned above, i.e., $(\gamma_1 \gamma_2 SI'|g|\gamma_1 \gamma_2 SI')$, so also in this case the same simplification is achieved in the calculation of these elements.

In some of the last cases the matrix elements of G_N are calculated more easily from those of G_{N-2} or from an ancestor directly by making use of the c.f.p. of the type

$$(\gamma^{n-2}(S'T')\gamma^2(S''T'')SI'| \} \gamma^n SI')$$

than from those of G_{N-1} . The recurrence formulae of this type are easily obtained in a way analogous to (3.1) and some of these are already given in (33) of R III.

The matrix elements of the electrostatic interaction for two electron system are easily calculated and the results are given below. Here (u, v) and (ξ, η, ζ) denote the real orbitals which belong to the irreducible representations E_g and F_{2g} respectively of the octahedral group.

$$\left. \begin{aligned} n-n' &= 0 \quad (d\delta^2 SI'|g|d\delta^2 SI') \\ SI' &= {}^1A_1: (\xi\xi|g|\xi\xi) + 2K(\zeta\eta) = (A+10B+5C), \\ & {}^1E: (\xi\xi|g|\xi\xi) - K(\zeta\eta) = (A+B+2C), \\ & {}^3F_1: J(\xi\eta) - K(\zeta\eta) = (A-5B), \\ & {}^1F_2: J(\xi\eta) + K(\zeta\eta) = (A+B+2C), \\ & (d\delta d\gamma SI'|g|d\delta d\gamma SI') \\ SI' &= {}^1F_1: J(\zeta v) + K(\zeta v) = (A+4B+2C), \\ & {}^3F_1: J(\zeta v) - K(\zeta v) = (A+4B), \\ & {}^1F_2: J(\zeta u) + K(\zeta u) = (A+2C), \\ & {}^3F_2: J(\zeta u) - K(\zeta u) = (A-8B), \\ & (d\gamma^2 SI'|g|d\gamma^2 SI') \\ SI' &= {}^1A_1: 2(uu|g|uu) - J(uv) - K(uv) = (A+8B+4C), \\ & {}^3A_2: J(uv) - K(uv) = (A-8B), \\ & {}^1E: J(uv) + K(uv) = (A+2C), \\ n-n' &= 1 \quad (d\delta^2 SI'|g|d\delta d\gamma SI') \\ SI' &= {}^3F_1: 2(\eta\xi|g|v\zeta) = (6B), \\ & {}^1F_2: 2(\eta\xi|g|u\zeta) = (2\sqrt{3}B), \\ n-n' &= 2 \quad (d\delta^2 SI'|g|d\gamma^2 SI') \\ SI' &= {}^1A_1: \sqrt{3/2} \{ K(\xi u) + K(\xi v) \} = (\sqrt{6}(2B+C)), \end{aligned} \right\} \quad (3.4)$$

$$^1E : \sqrt{3} \quad \{K(\xi u) - K(\xi v)\} = (-2\sqrt{3}B),$$

where

$$J(ab) = (ab|g|ab), \quad K(ab) = (ab|g|ba).$$

To obtain these results the following relations were used, which come from the transformation properties of the basic orbitals;

$$\left. \begin{aligned} (\xi\xi|g|\xi\xi) &= (\eta\eta|g|\eta\eta) = (\zeta\zeta|g|\zeta\zeta), \\ (\xi\xi|g|\eta\eta) &= (\eta\eta|g|\zeta\zeta) = (\zeta\zeta|g|\xi\xi), \\ (\bar{u}u|g|\bar{u}u) &= (v\bar{v}|g|\bar{v}\bar{v}), \\ (\bar{u}u|g|\bar{v}v) &= (\bar{u}u|g|\bar{u}u) - J(uv) - K(uv), \\ (\eta\xi|g|\bar{v}\zeta) &= -(\eta\xi|g|\zeta v), \\ (\eta\xi|g|\bar{u}\zeta) &= (\eta\xi|g|\zeta u), \\ (\xi\xi|g|\bar{u}u) &= (\eta\eta|g|\bar{u}u), \\ (\xi\xi|g|\bar{v}v) &= (\eta\eta|g|\bar{v}v), \\ (\xi\xi|g|\bar{u}u) - (\xi\xi|g|\bar{v}v) &= 2/\sqrt{3} (\xi\xi|g|uv), \\ (\zeta\zeta|g|\bar{u}u) &= -1/2(\eta\eta|g|\bar{u}u) + 3/2(\eta\eta|g|\bar{v}v), \\ (\zeta\zeta|g|\bar{v}v) &= 3/2(\eta\eta|g|\bar{u}u) - 1/2(\eta\eta|g|\bar{v}v), \end{aligned} \right\} \quad (3.5)$$

and from their reality;

$$\left. \begin{aligned} (\zeta\zeta|g|\eta\eta) &= K(\zeta\eta), & (\bar{u}u|g|\bar{v}v) &= K(uv), \\ (\zeta\zeta|g|\bar{u}u) &= K(\zeta u), & (\zeta\zeta|g|\bar{v}v) &= K(\zeta v), \\ (\xi\xi|g|\bar{u}u) &= K(\xi u), & (\xi\xi|g|\bar{v}v) &= K(\xi v). \end{aligned} \right\} \quad (3.6)$$

Using these matrix elements of $G_2 = 1/r_{12}$, we can now proceed to calculate the matrix elements of $G_N = \sum_{i>j}^N 1/r_{ij}$. The complete energy matrix is obtained adding the orbital (crystalline field) energies to its diagonal elements.

As was mentioned at the end of § 2, we now return to the crystalline field approxi-

mation in normal sense, and assume the orbitals (u, v) and (ξ, η, ζ) are pure d_r and d_s respectively, namely, of the form;

$$\left. \begin{aligned} u &= R(r)Y_{20}(\theta\varphi), \\ v &= 1/\sqrt{2} R(r)\{Y_{22}(\theta\varphi) + Y_{2-2}(\theta\varphi)\}, \\ \xi &= -i/\sqrt{2} R(r)\{Y_{21}(\theta\varphi) + Y_{2-1}(\theta\varphi)\}, \\ \eta &= -1/\sqrt{2} R(r)\{Y_{21}(\theta\varphi) - Y_{2-1}(\theta\varphi)\}, \\ \zeta &= i/\sqrt{2} R(r)\{Y_{22}(\theta\varphi) - Y_{2-2}(\theta\varphi)\}. \end{aligned} \right\} \quad (3.7)$$

The matrix elements (3.4) are accordingly expressed in terms of Racah's parameters A , B , C as are shown at the right hand side of (3.4) in parenthesis.

The orbital energy for the configuration $d\bar{\epsilon}^n d\gamma^{N-n}$ is given by $(6N-10n)Dq$.

The results thus obtained are given in Table III, where the term $N(N-1)/2 \cdot A$ in the diagonal elements is omitted. They were checked by examining whether they gave the energies of the free state when Dq was set equal to zero, or not.

Conjugation is simple in this case, that is, we can obtain the energy matrices for d^{10-N} from those for d^N merely changing the sign of Dq^1 . Conjugate states are given at the top of the columns of each matrix in Table III.

Table I. Tables of the clebsch-gordan coefficients. $(\Gamma_1\gamma_1\Gamma_2\gamma_2|\Gamma_1\Gamma_2\Gamma\gamma)$

$A_2 \times A_2$		$A_2 \times E$		$A_2 \times F_1$	
Γ	A_1	Γ	E	Γ	F_2
γ_1	γ_2	γ_1	γ	γ_1	ξ
e_1		u	v	α	η
e_2	e_2	v		β	ζ
				γ	
					1
					1
					1

$A_2 \times F_2$		$E \times E$	
Γ	F_1	Γ	A_1
γ_1	α	γ	e_1
ξ	β		e_2
e_2	γ		u
ζ			v

$E \times E$	
Γ	A_1
γ_1	e_1
u	$1/\sqrt{2}$
v	$1/\sqrt{2}$
u	$-1/\sqrt{2}$
v	$1/\sqrt{2}$
v	$1/\sqrt{2}$

Table I. (continued)

 $E \times F_1$

		Γ	F_1			F_2		
γ_1	γ_2	γ	α	β	γ	ξ	η	ζ
u	α		-1/2		$\sqrt{3}/2$			
u	β			-1/2	$-\sqrt{3}/2$			
u	γ				1			
v	α		$\sqrt{3}/2$		1/2			
v	β			- $\sqrt{3}/2$	1/2			-1
v	γ				1			

 $E \times F_2$

		Γ	F_1			F_2		
γ_1	γ_2	γ	α	β	γ	ξ	η	ζ
u	ξ		- $\sqrt{3}/2$		-1/2			
u	η		$\sqrt{3}/2$		-1/2			
u	ζ				1			
v	ξ		-1/2		$\sqrt{3}/2$			
v	η			-1/2	$-\sqrt{3}/2$			
v	ζ				1			

 $F_1 \times F_1$

		Γ	A_1	E			F_1	F_2			
γ_1	γ_2	γ	e_1	u	v	α	β	γ	ξ	η	ζ
α	α			-1/ $\sqrt{3}$	1/ $\sqrt{6}$	-1/ $\sqrt{2}$					
α	β							-1/ $\sqrt{2}$		-1/ $\sqrt{2}$	
α	γ						1/ $\sqrt{2}$			-1/ $\sqrt{2}$	
α	α							1/ $\sqrt{2}$			-1/ $\sqrt{2}$
β	β			-1/ $\sqrt{3}$	1/ $\sqrt{6}$	1/ $\sqrt{1}$					
β	γ						-1/ $\sqrt{2}$		-1/ $\sqrt{2}$		-1/ $\sqrt{2}$
γ	α						-1/ $\sqrt{2}$			-1/ $\sqrt{2}$	
γ	β					1/ $\sqrt{2}$			-1/ $\sqrt{2}$		-1/ $\sqrt{2}$
γ	γ			-1/ $\sqrt{3}$	-2/ $\sqrt{6}$						

 $F_1 \times F_2$

		Γ	A_2	E			F_1	F_2			
γ_1	γ_2	γ	e_2	u	v	α	β	γ	ξ	η	ζ
ξ	ξ			-1/ $\sqrt{3}$	-1/ $\sqrt{2}$	-1/ $\sqrt{6}$					
α	η							1/ $\sqrt{2}$		-1/ $\sqrt{2}$	
ζ	ξ						1/ $\sqrt{2}$			1/ $\sqrt{2}$	
ξ	ξ							1/ $\sqrt{2}$			1/ $\sqrt{2}$
β	η			-1/ $\sqrt{3}$	1/ $\sqrt{2}$	-1/ $\sqrt{6}$					
ζ	ξ					1/ $\sqrt{2}$			-1/ $\sqrt{2}$		
ξ	ξ						1/ $\sqrt{2}$			-1/ $\sqrt{2}$	
β	η			-1/ $\sqrt{3}$	1/ $\sqrt{2}$	-1/ $\sqrt{6}$					
ζ	ξ					1/ $\sqrt{2}$			-1/ $\sqrt{2}$		
ξ	ξ						1/ $\sqrt{2}$			-1/ $\sqrt{2}$	
γ	η					1/ $\sqrt{2}$			1/ $\sqrt{2}$		
ζ	ξ			-1/ $\sqrt{3}$	2/ $\sqrt{6}$						

Table I. (continued)

$F_2 \times F_2$		Γ	A_1	E			F_1	F_2			
γ_1	γ_2	γ	e_1	u	v	α	β	γ	ξ	η	ζ
ξ				$1/\sqrt{3}$	$-1/\sqrt{6}$	$1/\sqrt{2}$					
ξ	η						$1/\sqrt{2}$			$1/\sqrt{2}$	
ζ							$-1/\sqrt{2}$			$1/\sqrt{2}$	
ξ							$-1/\sqrt{2}$			$1/\sqrt{2}$	
η	η			$1/\sqrt{3}$	$-1/\sqrt{6}$	$-1/\sqrt{2}$					
ζ							$1/\sqrt{2}$			$1/\sqrt{2}$	
ξ							$1/\sqrt{2}$			$1/\sqrt{2}$	
ζ	η						$-1/\sqrt{2}$			$1/\sqrt{2}$	
ξ				$1/\sqrt{3}$	$2/\sqrt{6}$						

Table II.

Tables of the C. F. P. ($\gamma^{n-1}(S'\Gamma')\gamma S\Gamma| \} \gamma^n S\Gamma$). $(d\varepsilon^{n-1}(S'\Gamma')d\varepsilon S\Gamma| \} d\varepsilon^n S\Gamma)$ $n=3$

$S'\Gamma'$		1A_1	3F_1	1E	1F_2
$S\Gamma$					
4A_2			1		
2F_1			$1/\sqrt{2}$	$1/\sqrt{3}$	$1/\sqrt{6}$
2E			$1/\sqrt{2}$		$1/\sqrt{2}$
2F_2		$\sqrt{2}/3$	$1/\sqrt{2}$	$-1/3$	$-1/\sqrt{6}$

 $n=4$

$S'\Gamma'$		4A_2	2F_1	2E	2F_2
$S\Gamma$					
1A_1					1
3F_1			$1/\sqrt{3}$	$-1/2$	$-1/\sqrt{6}$
1E				$\sqrt{3}/2$	1/2
1F_2				$1/2$	$1/\sqrt{2}$

 $n=5$

$S'\Gamma'$		1A_1	3F_1	1E	1F_2
$S\Gamma$					
2F_2			$1/\sqrt{15}$	$\sqrt{3}/\sqrt{5}$	$-\sqrt{2}/\sqrt{15}$

 $(d\gamma^2(S'\Gamma')d\gamma^2 E| \} d\gamma^3 E)$

$S'\Gamma'$		1A_1	1E	3A_2
$S\Gamma$				
2E			$1/\sqrt{6}$	$-1/\sqrt{3}$

Tables of the C. F. P. ($\gamma^{n-2}(S_1\Gamma_1)\gamma^2(S_2\Gamma_2)S\Gamma| \} \gamma^n S\Gamma$) $(d\varepsilon^{n-2}(S_1\Gamma_1)d\varepsilon^2(S_2\Gamma_2)S\Gamma| \} d\varepsilon^n S\Gamma)$ $n=4$

$S\Gamma = ^1A_1$		$S_2\Gamma_2$	1A_1	3F_1	1E	1F_2
$S_1\Gamma_1$						
1A_1			$\sqrt{2}/3$			
3F_1				$1/\sqrt{2}$		
1E					$-1/3$	
1F_2						$-1/\sqrt{6}$

$S\Gamma = ^3F_1$		$S_2\Gamma_2$	1A_1	3F_1	1E	1F_2
$S_1\Gamma_1$						
1A_1					$1/3\sqrt{2}$	
3F_1					$1/3\sqrt{2}$	$1/\sqrt{3}$
1E						$1/3$
1F_2						$1/\sqrt{6}$

 $n=5$

$S\Gamma = ^1E$		$S_2\Gamma_2$	1A_1	3F_1	1E	1F_2
$S_1\Gamma_1$						
1A_1					$1/3\sqrt{2}$	
3F_1					$-1/\sqrt{2}$	
1E						$1/3$
1F_2						$1/\sqrt{6}$

$S\Gamma = ^1F_2$		$S_2\Gamma_2$	1A_1	3F_1	1E	1F_2
$S_1\Gamma_1$						
1A_1						$1/3\sqrt{2}$
3F_1						$-1/\sqrt{2}$
1E						
1F_2						

Table II. (continued)

$n=5$				$(d\gamma^2(S_1F_1)d\gamma^2(S_2F_2)^1A_1])d\gamma^4{}^1A_1)$			
$SF={}^2F_2$				S_2F_2			
S_1F_1	1A_1	3F_1	1E	1F_2	1A_1	1E	3A_2
4A_2		$1/\sqrt{5}$				$1/\sqrt{6}$	
2F_1		$\sqrt{3}/2\sqrt{5}$	$1/\sqrt{10}$	$1/2\sqrt{5}$			$-1/\sqrt{3}$
2E		$1/\sqrt{10}$		$-1/\sqrt{10}$			
2F_2	$1/\sqrt{15}$	$-\sqrt{3}/2\sqrt{5}$	$-1/\sqrt{30}$	$-1/2\sqrt{5}$			$1/\sqrt{2}$

Table III.

Energy Matrices

 d^3 2F_2 ($a {}^2D$, $b {}^2D$, 2F , 2G , 2H) $d\varepsilon^3({}^2F_2)d\gamma^4 \quad d\varepsilon^4({}^3F_1)d\gamma^3 \quad d\varepsilon^4({}^1F_2)d\gamma^3 \quad d\varepsilon^5d\gamma^2({}^1A_1) \quad d\varepsilon^5d\gamma^2({}^1E)$

$d\varepsilon^3$	$-12Dq$ $+5C$	$-3\sqrt{3}B$	$-5\sqrt{3}B$	$4B+2C$	$2B$
$d\varepsilon^2({}^3F_1)d\gamma$	$-2Dq$ $-6B+3C$	$3B$		$-3\sqrt{3}B$	$-3\sqrt{3}B$
$d\varepsilon^2({}^1F_2)d\gamma$	$-2Dq$ $+4B+3C$		$-\sqrt{3}B$	$\sqrt{3}B$	
$d\varepsilon d\gamma^2({}^1A_1)$	$8Dq$ $+6B+5C$			$10B$	
$d\varepsilon d\gamma^2({}^1E)$	$8Dq$ $-2B+3C$				

 2F_1 (2P , 2F , 2G , 2H) $d\varepsilon^3({}^2F_1)d\gamma^4 \quad d\varepsilon^4({}^3F_1)d\gamma^3 \quad d\varepsilon^4({}^1F_2)d\gamma^3 \quad d\varepsilon^5d\gamma^2({}^3A_2) \quad d\varepsilon^5d\gamma^2({}^1E)$

$d\varepsilon^3$	$-12Dq$ $-6B+3C$	$-3B$	$3B$	0	$-2\sqrt{3}B$
$d\varepsilon^2({}^3F_1)d\gamma$	$-2Dq$ $+3C$	$-3B$		$3B$	$3\sqrt{3}B$
$d\varepsilon^2({}^1F_2)d\gamma$	$-2Dq$ $-6B+3C$		$-3B$	$-\sqrt{3}B$	
$d\varepsilon d\gamma^2({}^3A_2)$	$8Dq$ $-6B+3C$			$2\sqrt{3}B$	
$d\varepsilon d\gamma^2({}^1E)$	$8Dq$ $-2B+3C$				

 2E ($a {}^2D$, $b {}^2D$, 2G , 2H) $d\varepsilon^3({}^2E)d\gamma^4 \quad d\varepsilon^4({}^1A_1)d\gamma^3 \quad d\varepsilon^4({}^1E)d\gamma^3 \quad d\varepsilon^6d\gamma$

$d\varepsilon^3$	$-12Dq$ $-6B+3B$	$-6\sqrt{2}B$	$-3\sqrt{2}B$	0	
$d\varepsilon^2({}^1A_1)d\gamma$	$-2Dq$ $+8B+6C$	$10B$		$\sqrt{3}(2B+C)$	
$d\varepsilon^2({}^1E)d\gamma$	$-2Dq$ $-B+3C$		$2\sqrt{3}B$		
$d\gamma^3$	$18Dq$ $-8B+4C$				

Table III. (continued)

4F_4	$(^4P, ^4F)$		4A_2	$(^4F) d\gamma^3$	$-12Dq - 15B$	$d\varepsilon^3(^4A_2)d\gamma^4$
	$d\varepsilon^4(^3F_1)d\gamma^3$	$d\varepsilon^5d\gamma^2(^3A_2)$	4F_2	$(^4F) d\varepsilon^2(^3F_1)d\gamma$	$-2Dq - 15B$	$d\varepsilon^4(^3F_1)d\gamma^3$
$d\varepsilon^2(^3F_1)d\gamma$	$-2Dq$	$6B$	2A_1	$(^2G) d\varepsilon^2(^1E)d\gamma^3$	$-2Dq - 11B + 3C$	$d\varepsilon^4(^1E)d\gamma^3$
	$-3B$		2A_2	$(^2F) d\varepsilon^2(^1E)d\gamma$	$-2Dq + 9B + 3C$	$d\varepsilon^4(^1E)d\gamma^3$
		$8Dq$				
		$-12B$				
d^4						
3F_1	$(a^3P, b^3P, a^3F, b^3F, ^3G, ^3H)$					
	$d\varepsilon^2(^3F_1)d\gamma^4$	$d\varepsilon^3(^2F_1)d\gamma^3$	$d\varepsilon^3(^2F_2)d\gamma^3$	$d\varepsilon^4(^3F_1)d\gamma^2(^1A_1)$	$d\varepsilon^4(^3F_1)d\gamma^2(^1E)$	$d\varepsilon^4(^1F_2)d\gamma^2(^3A_2)$
$d\varepsilon^4$	$-16Dq$	$-V\sqrt{6}B$	$-3V\sqrt{2}B$	$V\sqrt{2}(2B+C)$	$-2V\sqrt{2}B$	0
	$-15B+5C$					0
$d\varepsilon^3(^2F_1)d\gamma$	$-6Dq$	$-11B+4C$	$5V\sqrt{3}B$	$V\sqrt{3}B$	$-V\sqrt{3}B$	$3B$
						$V\sqrt{6}B$
$d\varepsilon^3(^2F_2)d\gamma$	$-6Dq$	$-3B+6C$	$-3B$	$-3B$	$5V\sqrt{3}B$	$V\sqrt{2}(B+C)$
$d\varepsilon^2(^3F_1)d\gamma^2(^1A_1)$	$4Dq$	$-B+6C$	$-10B$	0	$3V\sqrt{2}B$	
$d\varepsilon^2(^3F_1)d\gamma^2(^1E)$	$4Dq$	$-9B+4C$	$-2V\sqrt{3}B$	$-3V\sqrt{2}B$	$-3V\sqrt{2}B$	
$d\varepsilon^2(^1F_2)d\gamma^2(^3A_2)$	$4Dq$	$-11B+4C$	$V\sqrt{6}B$			
$d\varepsilon d\gamma^3$	$14Dq$	$-16B+5C$				
1F_2						
	$(a^1D, b^1D, a^1G, b^1G, ^1F, ^1I)$					
	$d\varepsilon^2(^1F_2)d\gamma^4$	$d\varepsilon^3(^2F_1)d\gamma^3$	$d\varepsilon^3(^2F_2)d\gamma^3$	$d\varepsilon^4(^3F_1)d\gamma^2(^3A_2)$	$d\varepsilon^4(^1F_2)d\gamma^2(^1E)$	$d\varepsilon^4(^1F_2)d\gamma^2(^1A_1)$
$d\varepsilon^4$	$-16Dq$	$3V\sqrt{2}B$	$-5V\sqrt{6}B$	0	$-2V\sqrt{2}B$	$V\sqrt{2}(2B+C)$
	$-9B+7C$					0
$d\varepsilon^3(^2F_1)d\gamma$	$-6Dq$	$-9B+6C$	$-5V\sqrt{3}B$	$3B$	$-3B$	$-V\sqrt{6}B$
$d\varepsilon^3(^2F_2)d\gamma$	$-6Dq$	$+3B+8C$	$-3V\sqrt{3}B$	$5V\sqrt{3}B$	$-5V\sqrt{3}B$	$V\sqrt{2}(3B+C)$
$d\varepsilon^2(^3F_1)d\gamma^2(^3A_2)$	$4Dq$	$-9B+6C$	$-6B$	0	$-3V\sqrt{6}B$	
$d\varepsilon^2(^1F_2)d\gamma^2(^1E)$	$4Dq$	$-3B+6C$	$-10B$	$V\sqrt{6}B$		
$d\varepsilon^2(^1F_2)d\gamma^2(^1A_1)$	$4Dq$	$+5B+8C$	$+5B+8C$	$V\sqrt{6}B$		
$d\varepsilon d\gamma^3$	$14Dq$	$+7C$				
1A_1						
	$(a^1S, b^1S, a^1G, b^1G, ^1I)$					
	$d\varepsilon^2(^1A_1)d\gamma^4$	$d\varepsilon^3(^2E)d\gamma^3$	$d\varepsilon^4(^1A_1)d\gamma^2(^1A_1)$	$d\varepsilon^4(^1E)d\gamma^2(^1E)$	$d\varepsilon^6$	
$d\varepsilon^4$	$-16Dq$	$-12V\sqrt{2}B$	$V\sqrt{2}(4B+2C)$	$2V\sqrt{2}B$	0	
	$+10C$					
$d\varepsilon^3(^2E)d\gamma$	$-6Dq$	$+6C$	$-12B$	$-6B$	0	
$d\varepsilon^2(^1A_1)d\gamma^2(^1A_1)$	$4Dq$	$+14B+11C$	$20B$	$V\sqrt{6}(2B+C)$		
$d\varepsilon^2(^1E)d\gamma^2(^1E)$	$4Dq$	$-3B+6C$	$2V\sqrt{6}B$			
$d\gamma^4$	$24Dq$	$-16B+8C$				

Table III. (continued)

 d^4

$$^1E (a^1D, b^1D, a^1G, b^1G, ^1I)$$

$$d\varepsilon^2(1E)d\gamma^4 \quad d\varepsilon^3(2E)d\gamma^3 \quad d\varepsilon^4(1E)d\gamma^2(^1A_1) \quad d\varepsilon^4(1A_1)d\gamma^2(1E) \quad d\varepsilon^4(1E)d\gamma^2(1E)$$

$d\varepsilon^4$	$\frac{-16Dq}{-9B+7C}$	$6B$	$\sqrt{2}(2B+C)$	$-2B$	$-4B$
$d\varepsilon^3(2E)d\gamma$	$\frac{-6Dq}{-6B+6C}$	$-3\sqrt{2}B$	$-12B$	0	
$d\varepsilon^2(1E)d\gamma^2(^1A_1)$	$\frac{4Dq}{+5B+8C}$	$10\sqrt{2}B$	$-10\sqrt{2}B$		
$d\varepsilon^2(1A_1)d\gamma^2(1E)$	$\frac{4Dq}{+6B+9C}$	0			
$d\varepsilon^2(1E)d\gamma^2(1E)$	$\frac{4Dq}{-3B+6C}$				

$^3F_2 ({}^3D, a^3F, b^3F, {}^3G, {}^3H)$

$d\varepsilon^3(2F_1)d\gamma^3 \quad d\varepsilon^3(2F_2)d\gamma^3 \quad d\varepsilon^4(3F_1)d\gamma^2({}^3A_2) \quad d\varepsilon^4(3F_1)d\gamma^2(1E) \quad d\varepsilon^5d\gamma$

$d\varepsilon^3(2F_1)d\gamma$	$\frac{-6Dq}{-9B+4C}$	$-5\sqrt{3}B$	$\sqrt{6}B$	$\sqrt{3}B$	$-\sqrt{6}B$
$d\varepsilon^3(2F_2)d\gamma$	$\frac{-6Dq}{-5B+6C}$	$-3\sqrt{2}B$	$3B$	$\sqrt{2}(3B+C)$	
$d\varepsilon^2(3F_1)d\gamma^2({}^3A_2)$	$\frac{4Dq}{-13B+4C}$	$-2\sqrt{2}B$	$-6B$		
$d\varepsilon^2(3F_1)d\gamma^2(1E)$	$\frac{4Dq}{-9B+4C}$	$3\sqrt{2}B$			
$d\varepsilon d\gamma^3$	$\frac{14Dq}{-8B+5C}$				

$^1F_1 ({}^1F, a^1G, b^1G, {}^1I)$

$d\varepsilon^3(2F_1)d\gamma^3 \quad d\varepsilon^3(2F_2)d\gamma^3 \quad d\varepsilon^4(1F_2)d\gamma^2(1E) \quad d\varepsilon^5d\gamma$

$d\varepsilon^3(2F_1)d\gamma$	$\frac{-6Dq}{-3B+6C}$	$5\sqrt{3}B$	$3B$	$\sqrt{6}B$	
$d\varepsilon^3(2F_2)d\gamma$	$\frac{-6Dq}{-3B+8C}$	$-5\sqrt{3}B$	$\sqrt{2}(B+C)$		
$d\varepsilon^2(1F_2)d\gamma^2(1E)$	$\frac{4Dq}{-3B+6C}$	$-V\sqrt{6}B$			
$d\varepsilon d\gamma^3$	$\frac{14Dq}{-16B+7C}$				

$^3E ({}^3D, {}^3G, {}^3H)$

$d\varepsilon^3(4A_2)d\gamma^3 \quad d\varepsilon^3(2E)d\gamma^3 \quad d\varepsilon^4(1E)d\gamma^2({}^3A_2) \quad d\varepsilon^3(2E)d\gamma^3 \quad d\varepsilon^4(1A_1)d\gamma^2({}^3A_2)$

$d\varepsilon^3(4A_2)d\gamma$	$\frac{-6Dq}{-13B+4C}$	$-4B$	0	$d\varepsilon^3(2E)d\gamma$	$\frac{-6Dq}{-8B+4C}$	$-12B$
$d\varepsilon^3(2E)d\gamma$	$\frac{-6Dq}{-10B+4C}$	$-3\sqrt{2}B$		$d\varepsilon^2(1A_1)d\gamma^2({}^3A_2)$	$\frac{4Dq}{-2B+7C}$	
$d\varepsilon^2(1E)d\gamma^2({}^3A_2)$	$\frac{4Dq}{-11B+4C}$					

$^1A_2 ({}^1F, {}^1I)$

$d\varepsilon^3(2E)d\gamma^3 \quad d\varepsilon^4(1E)d\gamma^2(1E)$

$d\varepsilon^3(2E)d\gamma$	$\frac{-6Dq}{-12B+6C}$	$6B$	${}^5E ({}^5D) \quad d\varepsilon^3(4A_2)d\gamma$	$-6Dq-21B$	$d\varepsilon^3(4A_2)d\gamma^3$
$d\varepsilon^2(1E)d\gamma^2(1E)$	$\frac{4Dq}{-3B+6C}$		${}^5F_2 ({}^5D) \quad d\varepsilon^2(3F_1)d\gamma^2({}^3A_2)$	$4Dq-21B$	$d\varepsilon^4(3F_1)d\gamma^2({}^3A_2)$
			${}^3A_1 ({}^3G) \quad d\varepsilon^3(2E)d\gamma$	$-6Dq-12B+4C$	$d\varepsilon^3(2E)d\gamma^3$

Table III. (continued)

2F_2 (a^2F , b^2F , a^2G , b^2G , 2H , 2I , a^2D , b^2D , c^2D)

 d^5

$d\varepsilon^5$	$-20B+10C$	$3V\sqrt{6}B$	$V\sqrt{6}B$	0	$-2V\sqrt{3}B$	$4B+2C$	$2B$	0	0	0	0
$d\varepsilon^4(^3F_1)d\gamma$	$-8B+9C$	$-10Dq$	$3B$	$\sqrt{6}/2B$	$-3V\sqrt{2}/2B$	$3V\sqrt{6}/2B$	0	0	$4B+C$	0	0
$d\varepsilon^4(^1F_2)d\gamma$	$-18B+9C$	$-10Dq$	$3V\sqrt{6}/2B$	$-3V\sqrt{2}/2B$	$5V\sqrt{6}/2B$	$-5V\sqrt{6}/2B$	C	0	0	0	0
$d\varepsilon^3(^2F_1)d\gamma^2(^3A_2)$	$-16B+8C$	$2V\sqrt{3}B$	0	$2V\sqrt{3}B$	0	0	$-3V\sqrt{6}/2B$	$-V\sqrt{6}/2B$	0	0	0
$d\varepsilon^3(^2F_1)d\gamma^2(^1E)$	$-12B+8C$	$-10V\sqrt{3}B$	$-12B+8C$	$-10V\sqrt{3}B$	0	$3V\sqrt{2}/2B$	$3V\sqrt{2}/2B$	$3V\sqrt{2}/2B$	$-2V\sqrt{3}B$	$-5V\sqrt{6}/2B$	$4B+2C$
$d\varepsilon^3(^2F_2)d\gamma^2(^1A_1)$	$d\varepsilon^3(^2F_2)d\gamma^2(^1E)$	$2B+12C$	$d\varepsilon^3(^2F_2)d\gamma^2(^1A_1)$	$2B+12C$	0	$-6B+10C$	$-6B+10C$	$-5V\sqrt{6}/2B$	$3V\sqrt{6}/2B$	$-2B$	$10Dq$
$d\varepsilon^2(^1F_2)d\gamma^3(^2E)$	$d\varepsilon^2(^1F_2)d\gamma^3(^2E)$	$-18B+9C$	$d\varepsilon^2(^1F_2)d\gamma^3(^2E)$	$-18B+9C$	$-18B+9C$	$10Dq$	$3B$	$-V\sqrt{6}B$	$-8B+9C$	$-3V\sqrt{6}B$	$20Dq$
$d\varepsilon^2(^3F_1)d\gamma^3(^2E)$	$d\varepsilon^2(^3F_1)d\gamma^3(^2E)$	$-10Dq$	$d\varepsilon^2(^3F_1)d\gamma^4$	$d\varepsilon^2(^3F_1)d\gamma^4$	$d\varepsilon^2(^3F_1)d\gamma^4$	$-8B+9C$	$-20B+10C$	$-20B+10C$	$-8B+9C$	$-3V\sqrt{6}B$	$-20Dq$
$d\varepsilon^4(^3F_1)d\gamma$	$-22B+9C$	$-10Dq$	$-3B$	$-3V\sqrt{2}/2B$	$3V\sqrt{2}/2B$	$-3V\sqrt{2}/2B$	$-3V\sqrt{6}/2B$	0	0	C	C
$d\varepsilon^4(^1F_2)d\gamma$	$-8B+9C$	$-10Dq$	$3V\sqrt{2}/2B$	$3V\sqrt{2}/2B$	$15V\sqrt{2}/2B$	$5V\sqrt{6}/2B$	$10V\sqrt{3}B$	$4B+C$	0	$-3V\sqrt{2}/2B$	$-3V\sqrt{2}/2B$
$d\varepsilon^3(^2F_1)d\gamma^2(^1A_1)$	$-4B+10C$	0	0	0	0	0	0	$3V\sqrt{2}/2B$	$-3V\sqrt{2}/2B$	$-3V\sqrt{2}/2B$	$-3V\sqrt{2}/2B$
$d\varepsilon^3(^2F_1)d\gamma^2(^1E)$	$-12B+8C$	$-12B+8C$	$d\varepsilon^3(^2F_2)d\gamma^2(^1A_2)$	$-10B+10C$	$d\varepsilon^3(^2F_2)d\gamma^2(^1E)$	$2V\sqrt{3}B$	$15V\sqrt{2}/2B$	$15V\sqrt{2}/2B$	$-3V\sqrt{2}/2B$	$-3V\sqrt{2}/2B$	$-3V\sqrt{2}/2B$
$d\varepsilon^2(^1F_2)d\gamma^3$	$d\varepsilon^2(^1F_2)d\gamma^3$	$10Dq$	$-8B+9C$	$-8B+9C$	$-8B+9C$	$-3B$	$-3B$	$-3B$	$-22B+9C$	$-22B+9C$	$10Dq$

Table III. (continued)

 d^5 2E (a^2D , b^2D , c^2D , a^2G , b^2G , 2H , 2I)

$d\varepsilon^4(1A_1)d\gamma$	$\frac{-10Dq}{-4B+12C}$	$10B$	$6B$	$6V\sqrt{3}B$	$6V\sqrt{2}B$	$-2B$	$4B+2C$
$d\varepsilon^4(1E)d\gamma$	$\frac{-10Dq}{-13B+9C}$	$-3B$	$3V\sqrt{3}B$	0	$2B+C$	$2B$	
$d\varepsilon^3(2E)d\gamma^2(1A_1)$	$\frac{-10Dq}{-4B+10C}$	0	0	$-3B$	$-6B$		
$d\varepsilon^3(2E)d\gamma^2(3A_2)$	$\frac{-16B+8C}{-12B+8C}$	$2V\sqrt{6}B$	$-3V\sqrt{3}B$	$6V\sqrt{3}B$			
$d\varepsilon^3(2E)d\gamma^2(1E)$	$\frac{10Dq}{-12B+8C}$	0	$6V\sqrt{2}B$				
$d\varepsilon^2(1E)d\gamma^3$	$\frac{10Dq}{-13B+9C}$						
$d\varepsilon^2(1A_1)d\gamma^3$	$\frac{10Dq}{-4B+12C}$						

 2A_1 (2S , a^2G , b^2G , 2I)

$d\varepsilon^4(1E)d\gamma$	$\frac{-10Dq}{-3B+9C}$	$-3V\sqrt{2}B$	0	$6B+C$
$d\varepsilon^3(2E)d\gamma^2(1E)$	$\frac{-12B+8C}{-19B+8C}$	$-4V\sqrt{3}B$	$3V\sqrt{2}B$	
$d\varepsilon^3(4A_2)d\gamma^2(3A_2)$		$-19B+8C$	0	
$d\varepsilon^2(1E)d\gamma^3$			$10Dq$	$-3B+9C$

 2A_2 (a^2F , b^2F , 2I) 4F_1 (4P , 4F , 4G)

$d\varepsilon^4(1E)d\gamma$	$\frac{-10Dq}{-23B+9C}$	$3V\sqrt{2}B$	$-2B+C$	$d\varepsilon^4(3F_1)d\gamma$	$\frac{-10Dq}{-25B+6C}$	$-3V\sqrt{2}B$	C
$d\varepsilon^3(2E)d\gamma^2(1E)$	$\frac{-12B+8C}{-23B+9C}$	$-3V\sqrt{2}B$		$d\varepsilon^3(2F_2)d\gamma^2(3A_2)$	$\frac{-16B+7C}{-21B+5C}$	$-3V\sqrt{2}B$	
$d\varepsilon^2(1E)d\gamma^3$				$d\varepsilon^2(3F_1)d\gamma^3$	$\frac{10Dq}{-25B+6C}$		

 4F_2 (4F , 4G , 4D) 4E (4D , 4G)

$d\varepsilon^4(3F_1)d\gamma$	$\frac{-10Dq}{-17B+6C}$	$V\sqrt{6}B$	$4B+C$	$d\varepsilon^3(2E)d\gamma^2(3A_2)$	$\frac{-22B+5C}{-21B+5C}$	$-2V\sqrt{3}B$
$d\varepsilon^3(2F_1)d\gamma^2(3A_2)$	$\frac{-22B+5C}{-17B+6C}$	$-V\sqrt{6}B$		$d\varepsilon^3(4A_2)d\gamma^2(1E)$	$\frac{10Dq}{-21B+5C}$	
$d\varepsilon^2(3F_1)d\gamma^3$						

 6A_1 (6S) $d\varepsilon^3(4A_2)d\gamma^2(3A_2)$ $-35B$ 4A_1 (4G) $d\varepsilon^3(4A_2)d\gamma^2(3A_2)$ $-25B+5C$ 4A_2 (4F) $d\varepsilon^3(4A_2)d\gamma^2(1A_1)$ $-13B+7C$

Appendix

Here we will show by induction that the following relation holds between the first and second sum in (3.1) in certain cases:

$$(\text{the first sum in (3.1)} \text{ for } N \text{ electron system}) = A(N:mn') (\text{the second sum in (3.1)} \text{ for } N \text{ electron system}), \quad (\text{A.1})$$

with

$$A(N:nn') = \{1 + A(N-1:n-1, n'-1)\} / \{1 + A^{-1}(N-1:n, n')\}. \quad (\text{A.2})$$

$A(N:nn')$ is a constant (including zero) depending only on N , n and n' . (When the sum on the right hand side of (A.1) is zero, we consider A^{-1} to be zero.)

For this purpose we assume similar relation for $N-1$ electron system, namely

$$\begin{array}{l} \text{(the first sum in (3.1)} \\ \text{for } N-1 \text{ electron system) } = \end{array} \frac{A(N-1:nn')}{\text{(the second sum in (3.1)}} \begin{array}{l} \text{for } N-1 \text{ electron system).} \\ \end{array} \quad (\text{A.3})$$

To verify the relation (A.1), we express

$$(\gamma_1^{n-1}(S'\Gamma')\gamma_2^{N-n}(S_2\Gamma_2)\overline{S}\overline{\Gamma}|G_{N-1}|\gamma_1^{n'-1}(S'\Gamma'')\gamma_2^{N-n'}(S_4\Gamma_4)\overline{S}\overline{\Gamma})$$

and

$$(\gamma_1^n(S_1\Gamma_1)\gamma_2^{N-n-1}(S'\Gamma')\overline{S}\overline{\Gamma}|G_{N-1}|\gamma_1^{n''}(S_3\Gamma_3)\gamma_2^{N-n'-1}(S'\Gamma'')\overline{S}\overline{\Gamma})$$

in (A.1) by

$$(\gamma_1^{n-1}(S'\Gamma')\gamma_2^{N-n-1}(S_0'\Gamma_0')\overline{S_0}\overline{\Gamma_0}|G_{N-2}|\gamma_1^{n'-1}(S''\Gamma'')\gamma_2^{N-n'-1}(S_0''\Gamma_0'')\overline{S_0}\overline{\Gamma_0})$$

using both the recurrence formula and the assumed relation (A.3), and apply the following relation for the transformation matrices;

$$\begin{array}{ccc} \sum_{\overline{\Gamma}} (\Gamma^1, \Gamma_3\Gamma_4(\Gamma^2)\Gamma | \Gamma^1\Gamma_3(\overline{\Gamma}), \Gamma_4\Gamma) & & \sum_{\overline{\Gamma}} (\Gamma_1\Gamma_2(\Gamma^1), \Gamma^2\Gamma | \Gamma_1, \Gamma_2\Gamma^2(\overline{\Gamma})\Gamma) \\ (\Gamma_1\Gamma_2(\Gamma^1), \Gamma_3\overline{\Gamma} | \Gamma_1, \Gamma_2\Gamma_3(\Gamma'')\overline{\Gamma}) & & (\Gamma_2, \Gamma_3\Gamma_4(\Gamma^2)\overline{\Gamma} | \Gamma_2\Gamma_3(\Gamma''), \Gamma_4\overline{\Gamma}) \\ (\Gamma_1, \overline{\Gamma}_2\overline{\Gamma}_3(\Gamma'')\overline{\Gamma} | \Gamma_1\overline{\Gamma}_2(\Gamma^3), \overline{\Gamma}_3\overline{\Gamma}) & = & (\overline{\Gamma}_2\overline{\Gamma}_3(\Gamma''), \Gamma_4\overline{\Gamma} | \overline{\Gamma}_2, \overline{\Gamma}_3\Gamma_4(\Gamma^4)\overline{\Gamma}) \\ (\Gamma^3\overline{\Gamma}_3(\overline{\Gamma}), \Gamma_4\Gamma | \Gamma^3, \overline{\Gamma}_3\Gamma_4(\Gamma^4)\Gamma) & & (\Gamma_1, \overline{\Gamma}_2\Gamma^4(\overline{\Gamma})\Gamma | \Gamma_1\overline{\Gamma}_2(\Gamma^3), \Gamma^4\Gamma). \end{array} \quad (\text{A.4})$$

(A.4) can be proved in the following way:

the left hand side

$$\begin{aligned} &= \sum_{\overline{\Gamma}} (\Gamma_1\Gamma_2(\Gamma^1), \Gamma_3\Gamma_4(\Gamma^2)\Gamma | \Gamma_1, \Gamma_2\Gamma_3(\Gamma'')\overline{\Gamma})\Gamma_4\Gamma \\ &\quad (\Gamma_1, \overline{\Gamma}_2\overline{\Gamma}_3(\Gamma'')\overline{\Gamma})\Gamma_4\Gamma | \Gamma_1\overline{\Gamma}_2(\Gamma^3)\overline{\Gamma}_3\Gamma_4(\Gamma^4)\Gamma \\ &= \sum_{\overline{\Gamma}} (\Gamma_1\Gamma_2(\Gamma^1), \Gamma_3\Gamma_4(\Gamma^2)\Gamma | \Gamma_1, \Gamma_2\Gamma_3(\Gamma'')\Gamma_4(\overline{\Gamma})\Gamma) \\ &\quad (\Gamma_1, \overline{\Gamma}_2\overline{\Gamma}_3(\Gamma'')\Gamma_4(\overline{\Gamma})\Gamma | \Gamma_1\overline{\Gamma}_2(\Gamma^3)\overline{\Gamma}_3\Gamma_4(\Gamma^4)\Gamma) \\ &= \text{the right hand side,} \end{aligned}$$

because

$$\sum_{\overline{\Gamma}} (\Gamma_1\Gamma''(\overline{\Gamma})\Gamma_4\Gamma | \Gamma_1, \Gamma''\Gamma_4(\underline{\Gamma})\Gamma)(\Gamma_1, \Gamma''\Gamma_4(\underline{\Gamma})\Gamma | \Gamma_1\Gamma''(\overline{\Gamma}')\Gamma_4\Gamma) = \delta(\overline{\Gamma}, \overline{\Gamma}').$$

To complete the proof for the simplification of the recurrence formula for non-diagonal elements described in § 3, it is necessary to show that the relation (A.3) holds for 4 electron system. This is possible only when a single ancestor exists and so the value of $A(3:nn')$ or $A^{-1}(3:nn')$ is equal to zero.

For the case of $n-n'=2$, where the ancestor of the type $(\gamma_1^2S\Gamma|g|\gamma_2^2S\Gamma)$ and the constants $A(3:2, 0)$ and $A(3:3, 1)$ are zero, we obtain the value of $A(4:3, 1)$ as unity and so on, using the relation (A.2). $A(N:N, N-2)$ and $A(N:2, 0)$ are always zero, because we have only one sum in the recurrence formula for these configurations. The general expression

for $A(N:nn')$ in this case is

$$A(N:n, n-2) = (n-2)/(N-n). \quad (\text{A.7})$$

As was mentioned in § 3, there is only one ancestor of the type $(\gamma_1^2S\Gamma|g|\gamma_2^2S\Gamma)$ for the case of $n-n'=1$ in our special problem of the octahedral group, and the constant A is given by

$$A(N:n, n-1) = (n-2)/(N-n). \quad (\text{A.8})$$

For the non-diagonal elements in the case of $n-n'=0$, we see that A takes the following values:

$$A(N:n, n) = (n-1)/(N-n-1). \quad (\text{A.9})$$

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