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その他（別言語等）のタイトル	立方対称場における $dn(n=6-10)$ 電子の波動関数
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Tables of the d^n ($n=6-10$)-electron Wave Functions
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立方対称場における $d^n (n=6-10)$ 電子の波動関数

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概 要

遷移金属イオンを含むイオン結晶の物理的・化学的性質の多くは遷移金属イオンの d 電子を調べることによって理解される。立方対称場では、いくつかの d 電子を持つイオンの電子状態は O 群の既約表現の基底をなし、かつ、パウリ原理に従うように決まる。この論文では $d^n (n=6-10)$ 電子の波動関数を田辺、菅野、上村の方法で求める。なお、 $d^n (n=1-5)$ については、すでに Moritani-Shinada によって発表されている。

Tables of the d^n ($n=6-10$)-electron Wave Functions in the Octahedral Crystalline Field

Many of the interesting physical and chemical properties of the ionic crystals containing transition-metal ions can be understood by examining the behaviors of d -electrons belonging to transition-metal ions. In an octahedral crystalline field, the electronic states of ions with many d -electrons must be formed so that they form the bases of the irreducible representations of the O -group and obey the Pauli principle.

In this note, the wavefunctions of d^n ($n=6, 7, 8, 9, 10$) are constructed according to the method given in Tanabe, Sugano and Kamimura's book. The wavefunctions of d^n ($n=1, 2, 3, 4, 5$) are obtained as Moritani-Shinada Table.

It is well known that the wavefunctions of the electrons in a symmetric field form the bases of the irreducible representations of the group of which elements are the symmetry operations of the field. We now consider the problem of transition-metal ions placed in an octahedral (O_h) symmetric field. The symmetry group we presently concerned with is the O_h -group, but as far as we confine ourselves to d -electrons it is sufficient to consider the O -group. The O -group has five irreducible representations A_1, A_2, E, T_1 and T_2 of which bases are $(e_1), (e_2), (u, v), (\alpha, \beta, \gamma)$ and (ξ, η, ζ) , respectively.

The single d -electron states, which have fivefold degeneracy in a spherical field, split into two classes E and T_2 in an octahedral symmetric field. The basic orbitals can be taken as in the following form

$$E \begin{cases} u = \sqrt{5/16\pi} R(r) (3z^2 - r^2) / r^2, \\ v = \sqrt{5/16\pi} R(r) (x^2 - y^2) / r^2, \end{cases}$$

$$T_2 \begin{cases} \xi = \sqrt{15/4\pi} R(r) yz / r^2 \\ \eta = \sqrt{15/4\pi} R(r) zx / r^2, \\ \zeta = \sqrt{15/4\pi} R(r) xy / r^2, \end{cases}$$

where $R(r)$ is the radial part of the d -wavefunction.

In the case of many electrons, the wavefunctions are also expressed by the bases of the irreducible representations of the O -group, $\Psi(\alpha S \Gamma M \gamma)$, where S and M are the total spin quantum number and that of the z -component, respectively. Γ and γ mean the irreducible representation of the O -group and their base, respectively. The quantum number α denotes the electron configuration $t_2^n e^m$ ($n = 0, 1, 2, 3, 4, 5, 6$; $m = 0, 1, 2, 3, 4$). The many electron wavefunction $\Psi(\alpha S \Gamma M \gamma)$ can be constructed from the wavefunctions of less than electron number states $\Phi(\alpha_1 S_1 \Gamma_1 M_1 \gamma_1)$ and $\Phi(\alpha_2 S_2 \Gamma_2 M_2 \gamma_2)$ in the following way,

$$\Psi(\alpha S \Gamma M \gamma) = \Sigma \Phi(\alpha_1 S_1 \Gamma_1 M_1 \gamma_1) \Phi(\alpha_2 S_2 \Gamma_2 M_2 \gamma_2) \\ \times \langle S_1 M_1 S_2 M_2 | SM \rangle \langle \Gamma_1 \gamma_1 \Gamma_2 \gamma_2 | \Gamma \gamma \rangle$$

where $\langle S_1 M_1 S_2 M_2 | SM \rangle$ and $\langle \Gamma_1 \gamma_1 \Gamma_2 \gamma_2 | \Gamma \gamma \rangle$ are the Wigner coefficient and Clebsch-Gordan coefficient, respectively. Furthermore, the many electron wavefunctions must obey the Pauli principle and therefore the ways of the combinations of S and Γ are restricted. The details of the constructing procedure of the many electron wavefunctions can be found in the references^{11, 21}.

T. Moritani and M. Shinada gave only the results for the states of d^n ($n = 1, 2, 3, 4, 5$). In this note, we will give the results for d^n ($n = 6, 7, 8, 9, 10$). These states of d^n can be obtained as the complementary states of those of d^{10-n} . The complementary states are obtained by placing holes into the complete shell d^{10} instead of electrons. As to the details of the complementary states we only refer to the book by Tanabe, Sugano and Kamimura.

In the tables, for simplicity, the following notations are used.

(1) Slater determinant

$$\frac{1}{\sqrt{n!}} \begin{vmatrix} \Phi_1(1) & \Phi_2(1) & \cdots & \Phi_n(1) \\ \Phi_1(2) & \Phi_2(2) & \cdots & \Phi_n(2) \\ \cdots & \cdots & \cdots & \cdots \\ \Phi_1(n) & \Phi_2(n) & \cdots & \Phi_n(n) \end{vmatrix} \equiv |\Phi_1 \Phi_2 \cdots \Phi_n|$$

(2) Spin orbitals

Φ implies the wavefunction which has orbital function Φ and up spin function

$\bar{\Phi}$ implies the wavefunction which has orbital function Φ and down spin function.

(3) The numbers on the left shoulder of Γ mean the spin-multiplicity $2S + 1$.

The wavefunctions for the complementary states of those of $\Psi_R(t_2^{6-n}(S_1 \Gamma_1) e^{4-m}(S_2 \Gamma_2) S \Gamma - M \gamma)$ can be obtained as follows.

1) first, we think about 10×10 Slater determinant $\Psi(t_2^6 e^{4 \uparrow} A_1)$.

2) next, we replace the Slater determinant which appears in $\Psi_L(t_2^n(S_1 \Gamma_1) e^m$

$(S_2 \Gamma_2) S \Gamma M \gamma$) with its adjunct Slater determinant (cofactor).

3) we multiply the resulting Slater determinant by phase factor $(-1)^{S-M}$

4) last, we consider the phase relation between L state and R state, that is,

$$\begin{aligned} \Psi_R(t_2^n(S_1 \Gamma_1) e^m(S_2 \Gamma_2) S \Gamma M \gamma) \\ = (-1)^{m n \mu_1 \mu_2} \Psi_L(t_2^n(S_1 \Gamma_1) e^m(S_2 \Gamma_2) S \Gamma M \gamma) \end{aligned}$$

where $\mu_1 = -1$ ($n=3$ and $S_1 \Gamma_1 = {}^4A_2, {}^2E, {}^2T_1$)

$+1$ (otherwise)

$\mu_2 = -1$ ($m=2$ and $S_2 \Gamma_2 = {}^3A_2, {}^1E$)

$+1$ (otherwise)

We tabulate the L states following.

Table 20 $\Psi(t_2^6 S \Gamma M \gamma)$

$S \Gamma$	M	γ	Ψ
1A_1	0	e_1	$ \xi \bar{\xi} \eta \bar{\eta} \zeta \bar{\zeta} $

Table 21 $\Psi(t_2^5 e S \Gamma M \gamma)$

$S \Gamma$	M	γ	Ψ
3T_1	1	r	$- \xi \bar{\xi} \eta \bar{\eta} \zeta v $
3T_2	1	ζ	$- \xi \bar{\xi} \eta \bar{\eta} \zeta u $
1T_1	0	r	$1/\sqrt{2} \{ \xi \bar{\xi} \eta \bar{\eta} \zeta \bar{v} - \xi \bar{\xi} \eta \bar{\eta} \zeta v \}$
1T_2	0	ζ	$1/\sqrt{2} \{ \xi \bar{\xi} \eta \bar{\eta} \zeta \bar{u} - \xi \bar{\xi} \eta \bar{\eta} \zeta u \}$

Table 22 $\Psi(t_2^4 e^2 S \Gamma M \gamma)$

$S \Gamma$	M	γ	Ψ
5T_2	2	ζ	$- \xi \eta \zeta \bar{\zeta} u v $
3T_2	1	ζ	$1/2 \{ \bar{\xi} \eta \zeta \bar{\zeta} u v + \xi \bar{\eta} \zeta \bar{\zeta} u v - \xi \eta \zeta \bar{\zeta} \bar{u} v - \xi \eta \zeta \bar{\zeta} u \bar{v} \}$
3T_2	1	ζ	$1/\sqrt{2} \{ - \xi \eta \zeta \bar{\zeta} \bar{u} v + \xi \eta \zeta \bar{\zeta} u \bar{v} \}$
1T_2	0	ζ	$1/2\sqrt{3} \{ -2 \bar{\xi} \eta \zeta \bar{\zeta} u v + \bar{\xi} \eta \zeta \bar{\zeta} \bar{u} v + \bar{\xi} \eta \zeta \bar{\zeta} u \bar{v} + \xi \bar{\eta} \zeta \bar{\zeta} \bar{u} v + \xi \bar{\eta} \zeta \bar{\zeta} u \bar{v} - 2 \xi \eta \zeta \bar{\zeta} \bar{u} \bar{v} \}$
1T_2	0	ζ	$1/2 \{ \bar{\xi} \eta \zeta \bar{\zeta} v \bar{v} + \bar{\xi} \eta \zeta \bar{\zeta} u \bar{u} - \xi \bar{\eta} \zeta \bar{\zeta} v \bar{v} - \xi \bar{\eta} \zeta \bar{\zeta} u \bar{u} \}$
1T_2	0	ζ	$1/2 \{ \bar{\xi} \eta \zeta \bar{\zeta} v \bar{v} - \bar{\xi} \eta \zeta \bar{\zeta} u \bar{u} - \xi \bar{\eta} \zeta \bar{\zeta} v \bar{v} + \xi \bar{\eta} \zeta \bar{\zeta} u \bar{u} \}$
3T_1	1	r	$1/2 \{ - \xi \eta \zeta \bar{\zeta} v \bar{v} - \xi \eta \zeta \bar{\zeta} u \bar{u} \}$
3T_1	1	r	$1/\sqrt{2} \{ - \xi \eta \zeta \bar{\zeta} v \bar{v} + \xi \eta \zeta \bar{\zeta} u \bar{u} \}$

$S \Gamma$	M	r	Ψ
3T_1	1	r	$1/\sqrt{2} \{ - \bar{\xi}\eta\zeta\bar{u}v + \xi\bar{\eta}\zeta\bar{u}v \}$
1T_1	0	r	$1/2 \{ - \bar{\xi}\eta\zeta\bar{u}v + \bar{\xi}\eta\zeta\bar{u}\bar{v} + \xi\bar{\eta}\zeta\bar{u}v - \xi\bar{\eta}\zeta\bar{u}\bar{v} \}$
3E	1	v	$1/\sqrt{6} \{ \eta\bar{\eta}\zeta\bar{u}v + \xi\bar{\xi}\zeta\bar{u}v - 2 \xi\bar{\xi}\eta\bar{\eta}uv \}$
1E	0	v	$1/\sqrt{6} \{ - \eta\bar{\eta}\zeta\bar{u}v + \eta\bar{\eta}\zeta\bar{u}\bar{v} - \xi\bar{\xi}\zeta\bar{u}v + \xi\bar{\xi}\zeta\bar{u}\bar{v} - \xi\bar{\xi}\eta\bar{\eta}uv + \xi\bar{\xi}\eta\bar{\eta}u\bar{v} \}$
1E	0	v	$1/2 \{ \eta\bar{\eta}\zeta\bar{v}v + \eta\bar{\eta}\zeta\bar{u}\bar{u} - \xi\bar{\xi}\zeta\bar{v}v - \xi\bar{\xi}\zeta\bar{u}\bar{u} \}$
1E	0	v	$1/2\sqrt{6} \{ \eta\bar{\eta}\zeta\bar{u}v - \eta\bar{\eta}\zeta\bar{u}\bar{v} + \xi\bar{\xi}\zeta\bar{u}v - \xi\bar{\xi}\zeta\bar{u}\bar{v} - 2 \xi\bar{\xi}\eta\bar{\eta}uv + 2 \xi\bar{\xi}\eta\bar{\eta}u\bar{v} + \sqrt{3} \eta\bar{\eta}\zeta\bar{v}v - \sqrt{3} \eta\bar{\eta}\zeta\bar{u}\bar{u} - \sqrt{3} \xi\bar{\xi}\zeta\bar{v}v + \sqrt{3} \xi\bar{\xi}\zeta\bar{u}\bar{u} \}$
3A_2	1	e_2	$1/\sqrt{3} \{ \eta\bar{\eta}\zeta\bar{u}v + \xi\bar{\xi}\zeta\bar{u}v + \xi\bar{\xi}\eta\bar{\eta}uv \}$
1A_2	0	e_2	$1/2\sqrt{6} \{ \eta\bar{\eta}\zeta\bar{u}v - \eta\bar{\eta}\zeta\bar{u}\bar{v} + \xi\bar{\xi}\zeta\bar{u}v - \xi\bar{\xi}\zeta\bar{u}\bar{v} - 2 \xi\bar{\xi}\eta\bar{\eta}uv + 2 \xi\bar{\xi}\eta\bar{\eta}u\bar{v} - \sqrt{3} \eta\bar{\eta}\zeta\bar{v}v + \sqrt{3} \eta\bar{\eta}\zeta\bar{u}\bar{u} + \sqrt{3} \xi\bar{\xi}\zeta\bar{v}v - \sqrt{3} \xi\bar{\xi}\zeta\bar{u}\bar{u} \}$
1A_1	0	e_1	$1/\sqrt{6} \{ \eta\bar{\eta}\zeta\bar{v}v + \eta\bar{\eta}\zeta\bar{u}\bar{u} + \xi\bar{\xi}\zeta\bar{v}v + \xi\bar{\xi}\zeta\bar{u}\bar{u} + \xi\bar{\xi}\eta\bar{\eta}uv + \xi\bar{\xi}\eta\bar{\eta}u\bar{v} \}$
1A_1	0	e_1	$1/2\sqrt{6} \{ - \eta\bar{\eta}\zeta\bar{v}v + \eta\bar{\eta}\zeta\bar{u}\bar{u} - \xi\bar{\xi}\zeta\bar{v}v + \xi\bar{\xi}\zeta\bar{u}\bar{u} + 2 \xi\bar{\xi}\eta\bar{\eta}uv - 2 \xi\bar{\xi}\eta\bar{\eta}u\bar{v} - \sqrt{3} \eta\bar{\eta}\zeta\bar{u}v + \sqrt{3} \eta\bar{\eta}\zeta\bar{u}\bar{v} + \sqrt{3} \xi\bar{\xi}\zeta\bar{u}v - \sqrt{3} \xi\bar{\xi}\zeta\bar{u}\bar{v} \}$

Table 23 $\Psi(t_2^3 e^3 S \Gamma M r)$

$S \Gamma$	M	r	Ψ
5E	2	v	$ \xi\eta\zeta uv\bar{v} $
3E	1	v	$1/2\sqrt{3} \{ - \bar{\xi}\eta\zeta uv\bar{v} - \xi\bar{\eta}\zeta uv\bar{v} - \xi\eta\zeta uv\bar{v} + 3 \xi\eta\zeta uv\bar{v} \}$
3E	1	v	$1/2\sqrt{3} \{ -\sqrt{3} \bar{\xi}\eta\zeta uv\bar{v} + \sqrt{3} \xi\bar{\eta}\zeta uv\bar{v} - \xi\bar{\eta}\zeta uv\bar{v} - \bar{\xi}\eta\zeta uv\bar{v} + 2 \xi\eta\zeta uv\bar{v} \}$
1E	0	v	$1/2\sqrt{6} \{ \sqrt{3} \bar{\xi}\eta\zeta uv\bar{v} - \sqrt{3} \xi\bar{\eta}\zeta uv\bar{v} - \sqrt{3} \bar{\xi}\eta\zeta uv\bar{v} + \sqrt{3} \xi\bar{\eta}\zeta uv\bar{v} + 2 \bar{\xi}\eta\zeta uv\bar{v} + 2 \xi\bar{\eta}\zeta uv\bar{v} - \bar{\xi}\eta\zeta uv\bar{v} - \xi\bar{\eta}\zeta uv\bar{v} - \bar{\xi}\eta\zeta uv\bar{v} - \bar{\xi}\eta\zeta uv\bar{v} \}$
3T_1	1	r	$1/\sqrt{2} \{ - \eta\bar{\eta}\zeta uv\bar{v} + \xi\bar{\xi}\zeta uv\bar{v} \}$
3T_1	1	r	$1/\sqrt{2} \{ \eta\bar{\eta}\zeta uv\bar{v} + \xi\bar{\xi}\zeta uv\bar{v} \}$
1T_1	0	r	$1/2 \{ \eta\bar{\eta}\zeta uv\bar{v} - \xi\bar{\xi}\zeta uv\bar{v} - \eta\bar{\eta}\zeta uv\bar{v} + \xi\bar{\xi}\zeta uv\bar{v} \}$
1T_1	0	r	$1/2 \{ - \eta\bar{\eta}\zeta uv\bar{v} - \xi\bar{\xi}\zeta uv\bar{v} + \eta\bar{\eta}\zeta uv\bar{v} + \xi\bar{\xi}\zeta uv\bar{v} \}$
3T_2	1	ζ	$1/\sqrt{2} \{ \eta\bar{\eta}\zeta uv\bar{v} - \xi\bar{\xi}\zeta uv\bar{v} \}$

$S \Gamma$	M	r	ψ
3T_2	1	ζ	$1/\sqrt{2}(\eta\bar{\eta}\zeta u\bar{v} + \xi\bar{\xi}\zeta u\bar{v})$
1T_2	0	ζ	$1/2\{- \eta\bar{\eta}\zeta u\bar{v} + \xi\bar{\xi}\zeta u\bar{v} + \eta\bar{\eta}\zeta u\bar{v} - \xi\bar{\xi}\zeta u\bar{v} \}$
1T_2	0	ζ	$1/2\{- \eta\bar{\eta}\zeta u\bar{v} - \xi\bar{\xi}\zeta u\bar{v} + \eta\bar{\eta}\zeta u\bar{v} + \xi\bar{\xi}\zeta u\bar{v} \}$
3A_1	1	e_1	$1/2\sqrt{3}\{-\sqrt{3} \bar{\xi}\eta\zeta u\bar{v} + \sqrt{3} \xi\bar{\eta}\zeta u\bar{v} - \xi\bar{\eta}\zeta u\bar{v} - \bar{\xi}\eta\zeta u\bar{v} + 2 \xi\bar{\eta}\zeta u\bar{v} \}$
1A_1	0	e_1	$1/2\sqrt{6}\{\sqrt{3} \bar{\xi}\eta\zeta u\bar{v} - \sqrt{3} \xi\bar{\eta}\zeta u\bar{v} + 2 \bar{\xi}\eta\zeta u\bar{v} - \xi\bar{\eta}\zeta u\bar{v} - \xi\bar{\eta}\zeta u\bar{v} - \sqrt{3} \bar{\xi}\eta\zeta u\bar{v} + \sqrt{3} \xi\bar{\eta}\zeta u\bar{v} - \xi\bar{\eta}\zeta u\bar{v} - \bar{\xi}\eta\zeta u\bar{v} + 2 \xi\bar{\eta}\zeta u\bar{v} \}$
3A_2	1	e_2	$1/2\sqrt{3}\{-\sqrt{3} \bar{\xi}\eta\zeta u\bar{v} + \sqrt{3} \xi\bar{\eta}\zeta u\bar{v} + \xi\bar{\eta}\zeta u\bar{v} + \bar{\xi}\eta\zeta u\bar{v} - 2 \xi\bar{\eta}\zeta u\bar{v} \}$
1A_2	0	e_2	$1/2\sqrt{6}\{\sqrt{3} \bar{\xi}\eta\zeta u\bar{v} - \sqrt{3} \xi\bar{\eta}\zeta u\bar{v} - 2 \bar{\xi}\eta\zeta u\bar{v} + \xi\bar{\eta}\zeta u\bar{v} + \bar{\xi}\eta\zeta u\bar{v} - \sqrt{3} \xi\bar{\eta}\zeta u\bar{v} + \sqrt{3} \xi\bar{\eta}\zeta u\bar{v} + \xi\bar{\eta}\zeta u\bar{v} - \bar{\xi}\eta\zeta u\bar{v} - 2 \xi\bar{\eta}\zeta u\bar{v} \}$

Table 24 $\Psi (t_2^2 e^4 S \Gamma M_T)$

$S \Gamma$	M	r	ψ
3T_1	1	r	$ \xi\eta u\bar{v} $
1A_1	0	e_1	$1/\sqrt{3}(\xi\bar{\xi}u\bar{v} + \eta\bar{\eta}u\bar{v} + \zeta\bar{\zeta}u\bar{v})$
1E	0	v	$1/\sqrt{2}(\xi\bar{\xi}u\bar{v} - \eta\bar{\eta}u\bar{v})$
1T_2	0	ζ	$1/\sqrt{2}(\xi\bar{\xi}u\bar{v} - \eta\bar{\eta}u\bar{v})$

Table 25 $\Psi (t_2^6 e S \Gamma M_T)$

$S \Gamma$	M	r	ψ
2E	1/2	v	$ \xi\bar{\xi}\eta\bar{\eta}\zeta\bar{v} $

Table 26 $\Psi (t_2^5 e^2 S \Gamma M_T)$

$S \Gamma$	M	r	ψ
4T_1	3/2	r	$- \xi\bar{\xi}\eta\bar{\eta}\zeta u\bar{v} $
2T_1	1/2	r	$1/\sqrt{2}(- \xi\bar{\xi}\eta\bar{\eta}\zeta u\bar{v} + \xi\bar{\xi}\eta\bar{\eta}\zeta u\bar{v})$
2T_1	1/2	r	$1/\sqrt{6}(2 \xi\bar{\xi}\eta\bar{\eta}\zeta u\bar{v} - \xi\bar{\xi}\eta\bar{\eta}\zeta u\bar{v} - \xi\bar{\xi}\eta\bar{\eta}\zeta u\bar{v})$
2T_2	1/2	ζ	$1/\sqrt{2}(\xi\bar{\xi}\eta\bar{\eta}\zeta u\bar{v} + \xi\bar{\xi}\eta\bar{\eta}\zeta u\bar{v})$

$S \Gamma$	M	r	
2T_2	1/2	ζ	$1/\sqrt{2} (\xi\bar{\xi}\eta\bar{\eta}\zeta v\bar{v} - \xi\bar{\xi}\eta\bar{\eta}\zeta u\bar{u})$

Table 27 $\Psi (t_2^4 e^3 S \Gamma M r)$

$S \Gamma$	M	r	Ψ
4T_1	3/2	r	$- \xi\eta\zeta\bar{\zeta}u\bar{v}\bar{v} $
4T_2	3/2	ζ	$ \xi\eta\zeta\bar{\zeta}u\bar{u}\bar{v} $
2A_1	1/2	e_1	$1/2\sqrt{3} \{ - \eta\bar{\eta}\zeta\bar{\zeta}u\bar{v}\bar{v} - \xi\bar{\xi}\zeta\bar{\zeta}u\bar{v}\bar{v} + 2 \xi\bar{\xi}\eta\bar{\eta}u\bar{v}\bar{v} + \sqrt{3} \eta\bar{\eta}\zeta\bar{\zeta}u\bar{u}\bar{v} - \sqrt{3} \xi\bar{\xi}\zeta\bar{\zeta}u\bar{u}\bar{v} \}$
2A_2	1/2	e_2	$1/2\sqrt{3} \{ - \eta\bar{\eta}\zeta\bar{\zeta}u\bar{u}\bar{v} - \xi\bar{\xi}\zeta\bar{\zeta}u\bar{u}\bar{v} + 2 \xi\bar{\xi}\eta\bar{\eta}u\bar{u}\bar{v} - \sqrt{3} \eta\bar{\eta}\zeta\bar{\zeta}u\bar{v}\bar{v} + \sqrt{3} \xi\bar{\xi}\zeta\bar{\zeta}u\bar{v}\bar{v} \}$
2E	1/2	v	$1/2\sqrt{3} \{ - \eta\bar{\eta}\zeta\bar{\zeta}u\bar{u}\bar{v} - \xi\bar{\xi}\zeta\bar{\zeta}u\bar{u}\bar{v} + 2 \xi\bar{\xi}\eta\bar{\eta}u\bar{u}\bar{v} + \sqrt{3} \eta\bar{\eta}\zeta\bar{\zeta}u\bar{v}\bar{v} - \sqrt{3} \xi\bar{\xi}\zeta\bar{\zeta}u\bar{v}\bar{v} \}$
2E	1/2	v	$1/\sqrt{3} \{ \eta\bar{\eta}\zeta\bar{\zeta}u\bar{u}\bar{v} + \xi\bar{\xi}\zeta\bar{\zeta}u\bar{u}\bar{v} + \xi\bar{\xi}\eta\bar{\eta}u\bar{u}\bar{v} \}$
2T_1	1/2	r	$1/\sqrt{6} \{ -2 \xi\eta\zeta\bar{\zeta}u\bar{v}\bar{v} + \xi\eta\zeta\bar{\zeta}u\bar{v}\bar{v} + \bar{\xi}\eta\zeta\bar{\zeta}u\bar{v}\bar{v} \}$
2T_1	1/2	r	$1/\sqrt{2} \{ \bar{\xi}\eta\zeta\bar{\zeta}u\bar{u}\bar{v} - \xi\eta\zeta\bar{\zeta}u\bar{u}\bar{v} \}$
2T_2	1/2	ζ	$1/\sqrt{6} \{ 2 \xi\eta\zeta\bar{\zeta}u\bar{u}\bar{v} - \xi\eta\zeta\bar{\zeta}u\bar{u}\bar{v} - \bar{\xi}\eta\zeta\bar{\zeta}u\bar{u}\bar{v} \}$
2T_2	1/2	ζ	$1/\sqrt{2} \{ \bar{\xi}\eta\zeta\bar{\zeta}u\bar{v}\bar{v} - \xi\eta\zeta\bar{\zeta}u\bar{v}\bar{v} \}$

Table 28 $\Psi (t_2^3 e^4 S \Gamma M r)$

$S \Gamma$	M	r	Ψ
4A_2	3/2	e_2	$- \xi\eta\zeta u\bar{u}\bar{v}\bar{v} $
2E	1/2	v	$1/\sqrt{6} \{ 2 \xi\eta\zeta u\bar{u}\bar{v}\bar{v} - \xi\eta\zeta u\bar{u}\bar{v}\bar{v} - \bar{\xi}\eta\zeta u\bar{u}\bar{v}\bar{v} \}$
2T_1	1/2	r	$1/\sqrt{2} \{ \zeta\bar{\xi}\eta\bar{u}\bar{u}\bar{v}\bar{v} - \zeta\eta\bar{u}\bar{u}\bar{v}\bar{v} \}$
2T_2	1/2	ζ	$1/\sqrt{2} \{ \zeta\bar{\xi}\eta\bar{u}\bar{u}\bar{v}\bar{v} + \zeta\eta\bar{u}\bar{u}\bar{v}\bar{v} \}$

Table 29 $\Psi (t_2^6 e^2 S \Gamma M r)$

$S \Gamma$	M	r	Ψ
3A_2	1	e_2	$ \xi\bar{\xi}\eta\bar{\eta}\zeta\bar{\zeta}u\bar{v} $
1A_1	0	e_1	$1/\sqrt{2} \{ \xi\bar{\xi}\eta\bar{\eta}\zeta\bar{\zeta}u\bar{u} + \xi\bar{\xi}\eta\bar{\eta}\zeta\bar{\zeta}v\bar{v} \}$
1E	0	v	$1/\sqrt{2} \{ \xi\bar{\xi}\eta\bar{\eta}\zeta\bar{\zeta}u\bar{v} + \xi\bar{\xi}\eta\bar{\eta}\zeta\bar{\zeta}v\bar{u} \}$

Table 30 $\Psi (t_2^5 e^3 S \Gamma M \gamma)$

$S \Gamma$	M	γ	Ψ
3T_1	1	γ	$ \xi \bar{\xi} \eta \bar{\eta} \zeta u \bar{u} v $
3T_2	1	ζ	$ \xi \bar{\xi} \eta \bar{\eta} \zeta u \bar{v} $
1T_1	0	γ	$1/\sqrt{2} \{ - \xi \bar{\xi} \eta \bar{\eta} \zeta u \bar{u} v + \xi \bar{\xi} \eta \bar{\eta} \zeta u \bar{v} v \}$
1T_2	0	ζ	$1/\sqrt{2} \{ - \xi \bar{\xi} \eta \bar{\eta} \zeta u \bar{v} v + \xi \bar{\xi} \eta \bar{\eta} \zeta u \bar{u} v \}$

Table 31 $\Psi (t_2^4 e^4 S \Gamma M \gamma)$

$S \Gamma$	M	γ	Ψ
3T_1	1	γ	$- \xi \eta \zeta \bar{\zeta} u \bar{u} v $
1A_1	0	e_1	$1/\sqrt{3} \{ \xi \bar{\xi} \eta \bar{\eta} u \bar{u} v + \eta \bar{\eta} \zeta \bar{\zeta} u \bar{u} v + \zeta \bar{\zeta} \xi \bar{\xi} u \bar{u} v \}$
1E	0	v	$1/\sqrt{2} \{ - \zeta \bar{\zeta} \xi \bar{\xi} u \bar{u} v + \eta \bar{\eta} \zeta \bar{\zeta} u \bar{u} v \}$
1T_2	0	ζ	$1/\sqrt{2} \{ - \xi \eta \zeta \bar{\zeta} u \bar{u} v + \bar{\xi} \eta \zeta \bar{\zeta} u \bar{u} v \}$

Table 32 $\Psi (t_2^6 e^3 S \Gamma M \gamma)$

$S \Gamma$	M	γ	Ψ
2E	$1/2$	v	$ \xi \bar{\xi} \eta \bar{\eta} \zeta \bar{\zeta} u \bar{u} v $

Table 33 $\Psi (t_2^5 e^4 S \Gamma M \gamma)$

$S \Gamma$	M	γ	Ψ
2T_2	$1/2$	ζ	$ \xi \bar{\xi} \eta \bar{\eta} \zeta u \bar{u} v $

Table 34 $\Psi (t_2^6 e^4 S \Gamma M \gamma)$

$S \Gamma$	M	γ	Ψ
1A_1	0	e_1	$ \xi \bar{\xi} \eta \bar{\eta} \zeta \bar{\zeta} u \bar{u} v $

References

- 1) H. Kamimura, S. Sugano and Y. Tanabe, Ligand Field Theory and Its Applications (in Japanese), (Shokabo, Tokyo, 1970).
- 2) S. Sugano, Y. Tanabe and H. Kamimura, Multiplets of Transition-Metal Ions in Crystals, (Academic Press, N. Y., 1970).
- 3) T. Moritani and M. Shinada, Rep. Univ. Electro-Comm, 24-1, (Sci. and Tech. Sect.), 79 24(1), 1973.