d^2 and d^8 Trigonal Energy Levels

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The trigonal d^2 and d^8 symmetry adapted eigenvectors and energy determinants have been obtained in two different representations, with and without cubic orientation. Spin-orbit perturbation was applied last in both the representations. The complete theory developed here is necessary in a definitive and a meaningful study of the interpretation of the spectral and magnetic properties of trigonally distorted or substituted cubic systems and of trigonal systems in which the axial part of the ligand field is of such a magnitude that the cubic parentage has no meaning.

1. Introduction

In most transition-metal systems of tetragonal symmetry, axial ligand field seems to don the role of a major perturbation relative to that of spin-orbit interaction. In the case of systems of trigonal symmetry, however, spin-orbital forces seem to dominate while axial ligand field assumes a minor role. With this in mind, the author had recently developed [1] the complete theory of d^2 and d^8 electronic configurations immersed in trigonal ligand field in four different coupling schemes in all of which the axial ligand field was taken to be subservient to the spin-orbit interaction. However, if the axial component of the trigonal ligand field does become large as compared to spin-orbit interaction, which may be the case for the early members of the first transition-metal series, it is necessary to have the energy levels with diagonalization of the total ligand field preceding the diagonalization of spin-orbit perturbation. It is the derivation of the energy levels in this representation that we present in this report. The theory being advanced here is appropriate to trigonal systems (D_{3d}, D_3, C_{3v}) of d^2 and d^8 electronic configurations in which the axial component of the ligand field is of comparable magnitude to spin-orbit interaction or more.

2. Coupling Schemes

We choose to develop the theory in two different coupling schemes. In one formalism, we start with the symmetry adapted two electron cubic wave functions in coordinate space $[X^C(X^C = A_1, A_2, E, T_1, T_2)]$, decompose them properly to correspond to trigonal symmetry $[X^T(X^T = A_1, A_2, E)]$, and then achieve symmetry adaptation in spin-space, Γ_j ($\Gamma_j = \Gamma_1, \Gamma_2, \Gamma_3$). In the alternative formalism, the two electron orbital wave functions are directly constructed in trigonal symmetry (X^T) which will then be spin-adapted. The former representation is useful in the treatment of trigonally substituted or distorted cubic systems whereas the latter is more appropriate to trigonal systems in which the axial part of the ligand field is so large that the cubic parentage loses its significance. These two coupling schemes are designated, respectively, the $\{t_2, e, X^C, X^T, S, \Gamma_j\}$ and $\{a_1(t_2), e_\pm(t_2), e_\pm(e), X^T, S, \Gamma_j\}$ representations.

3. Wave Functions

The trigonally oriented d-orbitals of Eq. (1) are the one-electron basis set in both the representations [2]:

$$\begin{aligned} a_1(t_2) &\equiv t_{2a} = \sigma' = z'^2, \\ e_\pm(t_2) &\equiv t_{2\binom{b}{c}} = \sqrt{\tfrac{1}{3}}\,\pi'_\pm - \sqrt{\tfrac{2}{3}}\,\delta'_{\mp}, \\ e_\pm(e) &\equiv e_{\binom{a}{b}} = \sqrt{\tfrac{2}{3}}\,\pi'_\pm + \sqrt{\tfrac{1}{3}}\,\delta'_{\mp} \end{aligned} \tag{1}$$

where $\pi'_\pm = \sqrt{\tfrac{1}{2}}[(z'x') \pm i(y'z')]$

and $\delta'_\pm = \sqrt{\tfrac{1}{2}}[(x'^2 - y'^2) \pm i(x'y')]$.

The trigonal, or threefold axis, is taken to be the z' axis. The (x', y', z') coordinate system is related to the tetragonal (x, y, z) system by means of the orthonormal transformation defined by the equation,

$$\begin{bmatrix} z' \\ y' \\ x' \end{bmatrix} = \begin{bmatrix} \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} \\ 0 & -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \\ \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} \end{bmatrix} \begin{bmatrix} z \\ y \\ x \end{bmatrix} \tag{2}$$

The procedure of fabricating the symmetry adapted two electron cubic wave functions in coordinate space has been described elsewhere [3,4]. Once they are obtained, they are decomposed to trigonal functions as follows:

$$\mathrm{A}_1^{\mathrm{C}}, \mathrm{T}_{2\mathrm{a}}^{\mathrm{C}} \rightarrow \mathrm{A}_1^{\mathrm{T}}; \mathrm{A}_2^{\mathrm{C}}, \mathrm{T}_{1\mathrm{a}}^{\mathrm{C}} \rightarrow \mathrm{A}_2^{\mathrm{T}};$$
$$\text{and } \mathrm{E}^{\mathrm{C}}_{\binom{\mathrm{a}}{\mathrm{b}}}, \mathrm{T}_{1\binom{\mathrm{b}}{\mathrm{c}}}^{\mathrm{C}}, \mathrm{T}_{2\binom{\mathrm{b}}{\mathrm{c}}}^{\mathrm{C}} \rightarrow \mathrm{E}_{\pm}{}^{\mathrm{T}}.$$

Inclusion of spin space in these functions can then be accomplished with the knowledge of the transformation properties of spin functions $\zeta'(m_s)$ (denoted by α' and β') under $\mathscr{C}_3(z')$, $\mathscr{C}_2(y')$, and $\mathscr{C}_4(z)$ symmetry operations [1]. It should be remembered that the spin functions are also quantized along the (1, 1,1) direction, i. e., along the z' axis. The $\lvert t_2, e, X^{\mathrm{C}}, X^{\mathrm{T}}, S, \Gamma_j \rangle$ wave functions obtained by this procedure are listed in Table 1.

Construction of symmetry adapted wave functions of $\{a_1(t_2), e_{\pm}(t_2), e_{\pm}(e), X^{\mathrm{T}}, S, \Gamma_j\}$ representation in both orbital and spin-space is considerably a simpler procedure. Since octahedral orientation is not maintained in this scheme, suffice it to use the transformation properties of orbital and spin representations under $\mathscr{C}_3(z')$ and $\mathscr{C}_2(y')$ symmetry operations alone. These functions are given in Table 2.

Table 1. The Two-Electron Symmetry Adapted Trigonal Wave Functions, $\lvert t_2, e, X^{\mathrm{C}}, X^{\mathrm{T}}, S, \Gamma_j \rangle$
$[\Psi_0 = (\alpha'\beta' - \beta'\alpha')/\sqrt{2},\ \Psi_0' = (\alpha'\beta' + \beta'\alpha')/\sqrt{2},\ \Psi_+ = -(\alpha'\alpha'),\ \Psi_- = \beta'\beta']$.

Γ_1 Representation

$\lvert 1\rangle = {}^3A_2[{}^3T_{1g}(t_{2g}{}^2)] = \lvert e_+(t_2)e_-(t_2)\rvert\, \Psi_0'$

$\lvert 2\rangle = {}^3E[{}^3T_{1g}(t_{2g}{}^2)] = 1/\sqrt{2}[-\lvert a_1(t_2)e_+(t_2)\rvert\, \Psi_- + \lvert a_1(t_2)e_-(t_2)\rvert\, \Psi_+]$

$\lvert 3\rangle = {}^3E[{}^3T_{2g}(t_{2g}\,e_g)] = 1/2\,\{[\lvert a_1(t_2)e_+(e)\rvert - \lvert e_-(t_2)e_-(e)\rvert]\, \Psi_- - [\lvert a_1(t_2)e_-(e)\rvert - \lvert e_+(t_2)e_+(e)\rvert]\, \Psi_+\}$

$\lvert 4\rangle = {}^3A_2[{}^3T_{1g}(t_{2g}\,e_g)] = 1/\sqrt{2}[\lvert e_+(t_2)e_-(e)\rvert - \lvert e_-(t_2)e_+(e)\rvert]\, \Psi_0'$

$\lvert 5\rangle = {}^3E[{}^3T_{1g}(t_{2g}\,e_g)] = 1/2\,\{[\lvert a_1(t_2)e_+(e)\rvert + \lvert e_-(t_2)e_-(e)\rvert]\, \Psi_- - [\lvert a_1(t_2)e_-(e)\rvert + e_+(t_2)e_+(e)\rvert]\, \Psi_+\}$

$\lvert 6\rangle = {}^3A_2[{}^3A_{2g}(e_g{}^2)] = \lvert e_+(e)e_-(e)\rvert\, \Psi_0'$

$\lvert 7\rangle = {}^1A_1[{}^1A_{1g}(t_{2g}{}^2)] = 1/\sqrt{3}[\lvert a_1(t_2)a_1(t_2)\rvert + \lvert e_+(t_2)e_-(t_2)\rvert + \lvert e_-(t_2)e_+(t_2)\rvert]\, \Psi_0$

$\lvert 8\rangle = {}^1A_1[{}^1T_{2g}(t_{2g}{}^2)] = 1/\sqrt{6}[-2\,\lvert a_1(t_2)a_1(t_2)\rvert + \lvert e_+(t_2)e_-(t_2)\rvert + \lvert e_-(t_2)e_+(t_2)\rvert]\, \Psi_0$

$\lvert 9\rangle = {}^1A_1[{}^1T_{2g}(t_{2g}\,e_g)] = 1/2[\lvert e_+(t_2)e_-(e)\rvert + \lvert e_-(e)e_+(t_2)\rvert + \lvert e_-(t_2)e_+(e)\rvert + \lvert e_+(e)e_-(t_2)\rvert]\, \Psi_0$

$\lvert 10\rangle = {}^1A_1[{}^1A_{1g}(e_g{}^2)] = 1/\sqrt{2}[\lvert e_+(e)e_-(e)\rvert + \lvert e_-(e)e_+(e)\rvert]\, \Psi_0$

Γ_2 Representation

$\lvert 1\rangle = {}^3E[{}^3T_{1g}(t_{2g}{}^2)] = 1/\sqrt{2}[-\lvert a_1(t_2)e_+(t_2)\rvert\, \Psi_- - \lvert a_1(t_2)e_-(t_2)\rvert\, \Psi_+$

$\lvert 2\rangle = {}^3A_1[{}^3T_{2g}(t_{2g}\,e_g)] = 1/\sqrt{2}[\lvert e_+(t_2)e_-(e)\rvert + \lvert e_-(t_2)e_+(e)\rvert]\, \Psi_0'$

$\lvert 3\rangle = {}^3E[{}^3T_{2g}(t_{2g}\,e_g)] = 1/2\,\{[\lvert a_1(t_2)e_+(e)\rvert - \lvert e_-(t_2)e_-(e)\rvert]\, \Psi_- + [\lvert a_1(t_2)e_-(e)\rvert - \lvert e_+(t_2)e_+(e)\rvert]\, \Psi_+\}$

$\lvert 4\rangle = {}^3E[{}^3T_{1g}(t_{2g}\,e_g)] = 1/2\,\{[\lvert a_1(t_2)e_+(e)\rvert + \lvert e_-(t_2)e_-(e)\rvert]\, \Psi_- + [\lvert a_1(t_2)e_-(e)\rvert + \lvert e_+(t_2)e_+(e)\rvert]\, \Psi_+\}$

$\lvert 5\rangle = {}^1A_2[{}^1T_{1g}(t_{2g}\,e_g)] = 1/2[-\lvert e_+(t_2)e_-(e)\rvert - \lvert e_-(e)e_+(t_2)\rvert + \lvert e_-(t_2)e_+(e)\rvert + \lvert e_+(e)e_-(t_2)\rvert]\, \Psi_0$

$\Gamma_{3(\mathrm{a/b})}$ Representation

$\lvert 1\rangle = {}^3A_2[{}^3T_{1g}(t_{2g}{}^2)] = \lvert e_+(t_2)e_-(t_2)\rvert\, \Psi_{\pm}$

$\lvert 2\rangle = {}^3E[{}^3T_{1g}(t_{2g}{}^2)]^1 = \mp\,\lvert a_1(t_2)e_{\pm}(t_2)\rvert\, \Psi_0'$

$\lvert 3\rangle = {}^3E[{}^3T_{1g}(t_{2g}{}^2)]^2 = \pm\,\lvert a_1(t_2)e_{\mp}(t_2)\rvert]\, \Psi_{\mp}$

$\lvert 4\rangle = {}^3A_1[{}^3T_{2g}(t_{2g}\,e_g)] = \pm 1/\sqrt{2}[\lvert e_+(t_2)e_-(e)\rvert + \lvert e_-(t_2)e_+(e)\rvert]\, \Psi_{\pm}$

$\lvert 5\rangle = {}^3E[{}^3T_{2g}(t_{2g}\,e_g)]^1 = \pm 1/\sqrt{2}[\lvert a_1(t_2)e_{\pm}(e)\rvert - \lvert e_{\mp}(t_2)e_{\mp}(e)\rvert]\, \Psi_0'$

$\lvert 6\rangle = {}^3E[{}^3T_{2g}(t_{2g}\,e_g)]^2 = \mp 1/\sqrt{2}[\lvert a_1(t_2)e_{\mp}(e)\rvert - \lvert e_{\pm}(t_2)e_{\pm}(e)\rvert]\, \Psi_{\mp}$

$\lvert 7\rangle = {}^3A_2[{}^3T_{1g}(t_{2g}\,e_g)] = 1/\sqrt{2}[\lvert e_+(t_2)e_-(e)\rvert - \lvert e_-(t_2)e_+(e)\rvert]\, \Psi_{\pm}$

$\lvert 8\rangle = {}^3E[{}^3T_{1g}(t_{2g}\,e_g)]^1 = \pm 1/\sqrt{2}[\lvert a_1(t_2)e_+(e)\rvert + \lvert e_{\mp}(t_2)e_{\mp}(e)\rvert]\, \Psi_0'$

$\lvert 9\rangle = {}^3E[{}^3T_{1g}(t_{2g}\,e_g)]^2 = \mp 1/\sqrt{2}[\lvert a_1(t_2)e_{\mp}(e)\rvert + \lvert e_{\pm}(t_2)e_{\pm}(e)\rvert]\, \Psi_{\mp}$

$\lvert 10\rangle = {}^3A_2[{}^3A_{2g}(e_g{}^2)] = \lvert e_+(e)e_-(e)\rvert\, \Psi_{\pm}$

$\lvert 11\rangle = {}^1E[{}^1E_g(t_{2g}{}^2)] = 1/\sqrt{3}[-\lvert a_1(t_2)e_{\pm}(t_2)\rvert - \lvert e_{\pm}(t_2)a_1(t_2)\rvert + \lvert e_{\mp}(t_2)e_{\mp}(t_2)\rvert]\, \Psi_0$

$\lvert 12\rangle = {}^1E[{}^1T_{2g}(t_{2g}\,e_g)] = 1/\sqrt{6}[\lvert a_1(t_2)e_{\pm}(t_2)\rvert + \lvert e_{\pm}(t_2)a_1(t_2)\rvert + 2\,\lvert e_{\mp}(t_2)e_{\mp}(t_2)\rvert]\, \Psi_0$

$\lvert 13\rangle = {}^1E[{}^1T_{1g}(t_{2g}\,e_g)] = \tfrac{1}{2}[\lvert a_1(t_2)e_{\pm}(e)\rvert + \lvert e_{\pm}(e)a_1(t_2)\rvert + \lvert e_{\mp}(t_2)e_{\mp}(e)\rvert + \lvert e_{\mp}(e)e_{\mp}(t_2)\rvert]\, \Psi_0$

$\lvert 14\rangle = {}^1E[{}^1T_{2g}(t_{2g}\,e_g)] = \tfrac{1}{2}[\lvert a_1(t_2)e_{\pm}(e)\rvert + \lvert e_{\pm}(e)a_1(t_2)\rvert - \lvert e_{\mp}(t_2)e_{\mp}(e)\rvert - \lvert e_{\mp}(e)e_{\mp}(t_2)\rvert]\, \Psi_0$

$\lvert 15\rangle = {}^1E[{}^1E_g(e_g{}^2)] = \lvert e_{\mp}(e)e_{\mp}(e)\rvert\, \Psi_0$

Table 2. The Two-Electron Symmetry Adapted Trigonal Wave Functions, $|a_1(t_2), e_\pm(t_2), e_\pm(e), X^T, S, \Gamma_j\rangle$ $[\Psi_0=(\alpha'\beta'-\beta'\alpha')/\sqrt{2},\ \Psi_0=(\alpha'\beta'+\beta'\alpha')/\sqrt{2},\ \Psi_+=(\alpha'\alpha'),\ \Psi_-=(\beta'\beta')]$.

Γ_1 Representation

$|1\rangle = {}^3A_2[e(t_2)^2] = |e_+(t_2)e_-(t_2)|\Psi_0'$

$|2\rangle = {}^3E[a_1(t_2)e(t_2)] = -1/\sqrt{2}[|a_1(t_2)e_+(t_2)|\Psi_- + |a_1(t_2)e_-(t_2)|\Psi_+]$

$|3\rangle = {}^3E[a_1(t_2)e(e)] = 1/\sqrt{2}[|a_1(t_2)e_+(e)|\Psi_- + |a_1(t_2)e_-(e)|\Psi_+]$

$|4\rangle = {}^3A_2[e(t_2)e(e)] = 1/\sqrt{2}[|e_+(t_2)e_-(e)| - |e_-(t_2)e_+(e)|]\Psi_0'$

$|5\rangle = {}^3E[e(t_2)e(e)] = 1/\sqrt{2}[|e_-(t_2)e_-(e)|\Psi_- + |e_+(t_2)e_+(e)|\Psi_+]$

$|6\rangle = {}^3A_2[e(e)^2] = |e_+(e)e_-(e)|\Psi_0'$

$|7\rangle = {}^1A_1[a_1(t_2)^2] = |a_1(t_2)a_1(t_2)|\Psi_0$

$|8\rangle = {}^1A_1[e(t_2)^2] = 1/\sqrt{2}[|e_+(t_2)e_-(t_2)| + |e_-(t_2)e_+(t_2)|]\Psi_0$

$|9\rangle = {}^1A_1[e(t_2)e(e)] = \tfrac{1}{2}[|e_+(t_2)e_-(e)| + |e_-(e)e_+(t_2)| + |e_-(t_2)e_+(e)| + |e_+(e)e_-(t_2)|]\Psi_0$

$|10\rangle = {}^1A_1[e(e)^2] = 1/\sqrt{2}[|e_+(e)e_-(e)| + |e_-(e)e_+(e)|]\Psi_0$

Γ_2 Representation

$|1\rangle = {}^3E[a_1(t_2)e(t_2)] = 1/\sqrt{2}[-|a_1(t_2)e_+(t_2)|\Psi_- + |a_1(t_2)e_-(t_2)|\Psi_+]$

$|2\rangle = {}^3A_1[e(t_2)e(e)] = 1/\sqrt{2}[|e_+(t_2)e_-(e)| + |e_-(t_2)e_+(e)|]\Psi_0'$

$|3\rangle = {}^3E[a_1(t_2)e(e)] = 1/\sqrt{2}[|a_1(t_2)e_+(e)|\Psi_- - |a_1(t_2)e_-(e)|\Psi_+]$

$|4\rangle = {}^3E[e(t_2)e(e)] = 1/\sqrt{2}[|e_-(t_2)e_-(e)|\Psi_- - |e_+(t_2)e_+(e)|\Psi_+]$

$|5\rangle = {}^1A_2[e(t_2)e(e)] = \tfrac{1}{2}[-|e_+(t_2)e_-(e)| - |e_-(e)e_+(t_2)| + |e_-(t_2)e_+(e)| + |e_+(e)e_-(t_2)|]\Psi_0$

$\Gamma_{3(a/b)}$ Representation

$|1\rangle = {}^3A_2[e(t_2)^2] = \mp|e_+(t_2)e_-(t_2)|\Psi_\pm$

$|2\rangle = {}^3E[a_1(t_2)e(t_2)]^1 = \mp|a_1(t_2)e_\pm(t_2)|\Psi_0'$

$|3\rangle = {}^3E[a_1(t_2)e(t_2)]^2 = |a_1(t_2)e_\mp(t_2)|\Psi_\mp$

$|4\rangle = {}^3A_1[e(t_2)e(e)] = -1/\sqrt{2}[|e_+(t_2)e_-(e)| + |e_-(t_2)e_+(e)|]\Psi_\pm$

$|5\rangle = {}^3E[a_1(t_2)e(e)]^1 = \pm|a_1(t_2)e_\pm(e)|\Psi_0'$

$|6\rangle = {}^3E[a_1(t_2)e(e)]^2 = -|a_1(t_2)e_\mp(e)|\Psi_\mp$

$|7\rangle = {}^3A_2[e(t_2)e(e)] = \mp 1/\sqrt{2}[|e_+(t_2)e_-(e)| - |e_-(t_2)e_+(e)|]\Psi_\pm$

$|8\rangle = {}^3E[e(t_2)e(e)]^1 = \pm|e_\mp(t_2)e_\mp(e)|\Psi_0'$

$|9\rangle = {}^3E[e(t_2)e(e)]^2 = |e_\pm(t_2)e_\pm(e)|\Psi_\mp$

$|10\rangle = {}^3A_2[e(e)^2] = \mp|e_+(e)e_-(e)|\Psi_\pm$

$|11\rangle = {}^1E[a_1(t_2)e(t_2)] = 1/\sqrt{2}[|a_1(t_2)e_\pm(t_2)| + |e_\pm(t_2)a_1(t_2)|]\Psi_0$

$|12\rangle = {}^1E[e(t_2)^2] = |e_\mp(t_2)e_\mp(t_2)|\Psi_0$

$|13\rangle = {}^1E[a_1(t_2)e(e)] = 1/\sqrt{2}[|a_1(t_2)e_\pm(e)| + |e_\pm(e)a_1(t_2)|]\Psi_0$

$|14\rangle = {}^1E[e(t_2)e(e)] = 1/\sqrt{2}[|e_\mp(t_2)e_\mp(e)| + |e_\mp(e)e_\mp(t_2)|]\Psi_0$

$|15\rangle = {}^1E[e(e)^2] = |e_\mp(e)e_\mp(c)|\Psi_0$

The unitary transformation matrices of Table 3 connect the wave functions in the two representations. The corresponding eight electron wave functions of both representations can be easily obtained, if needed, from those listed by considering the two electrons as holes.

4. Energy Matrices

The parametrization of various perturbations is well-known. We shall use the $D\,q$, $D\,\sigma$, $D\,\tau$ parameters [5] for the trigonal ligand field perturbation. The electron correlation perturbation gives rise to the A, B, C parameters. The one-electron spin-orbit coupling constant, ζ, is the parameter of spin-orbit perturbation. The complete list of nonvanishing electron correlation integrals of trigonally oriented d-orbitals [Eq. (1)] [1] facilitates the calculation of electron correlation matrix elements.

The perturbation matrices of $\{t_2, e, X^C, X^T, S, \Gamma_j\}$ representation are included in Tables 4 a, b, c, and those of $\{a_1(t_2), e_\pm(t_2), e_\pm(e), X^T, S, \Gamma_j\}$ representation in Table 5 a, b, c. The parameter A, being a common additive term in the diagonal elements, has been omitted from these matrices. The

Table 3. $\{t_2, e, X^C, X^T, S, \Gamma_j \mid a_1(t_2), e_\pm(t_2), e_\pm(e), X^T, S, \Gamma_j\}$ Transformation Matrices.

Γ_1, Γ_3: $^3A_2$	$[e(t_2)^2]$	$[e(t_2)e(e)]$	$[e(e)^2]$
$[^3T_{1g}(t_{2g}^2)]$	1	0	0
$[^3T_{1g}(t_{2g}e_g)]$	0	1	0
$[^3A_{2g}(e_g^2)]$	0	0	1

$\Gamma_1, \Gamma_2, \Gamma_3^\nu$: ^3E	$[a_1(t_2)e(t_2)]$	$[a_1(t_2)e(e)]$	$[e(t_2)e(e)]$	$\nu=1$ or 2
$[^3T_{1g}(t_{2g}^2)]$	1	0	0	
$[^3T_{2g}(t_{2g}e_g)]$	0	$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$	
$[^3T_{1g}(t_{2g}e_g)]$	0	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	

Γ_3: ^3E	$[a_1(t_2)e(t_2)]^1$	$[a_1(t_2)e(t_2)]^2$	$[a_1(t_2)e(e)]^1$	$[a_1(t_2)e(e)]^2$	$[e(t_2)e(e)]^1$	$[e(t_2)e(e)]^2$
$[^3T_{1g}(t_{2g}^2)]^1$	1	0	0	0	0	0
$[^3T_{1g}(t_{2g}^2)]^2$	0	1	0	0	0	0
$[^3T_{2g}(t_{2g}e_g)]^1$	0	0	$\sqrt{\frac{1}{2}}$	0	$-\sqrt{\frac{1}{2}}$	0
$[^3T_{2g}(t_{2g}e_g)]^2$	0	0	0	$-\sqrt{\frac{1}{2}}$	0	$\sqrt{\frac{1}{2}}$
$[^3T_{1g}(t_{2g}e_g)]^1$	0	0	$\sqrt{\frac{1}{2}}$	0	$\sqrt{\frac{1}{2}}$	0
$[^3T_{1g}(t_{2g}e_g)]^2$	0	0	0	$-\sqrt{\frac{1}{2}}$	0	$-\sqrt{\frac{1}{2}}$

Γ_2, Γ_3: $^3A_1$	$[e(t_2)e(e)]$	Γ_2: $^1A_2$	$[e(t_2)e(e)]$
$[^3T_{2g}(t_{2g}e_g)]$	1	$[^1T_{1g}(t_{2g}e_g)]$	1

Γ_1: $^1A_1$	$[a_1(t_2)^2]$	$[e(t_2)^2]$	$[e(t_2)e(e)]$	$[e(e)^2]$
$[^1A_{1g}(t_{2g}^2)]$	$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{2}{3}}$	0	0
$[^1T_{2g}(t_{2g}^2)]$	$-\sqrt{\frac{2}{3}}$	$\sqrt{\frac{1}{3}}$	0	0
$[^1T_{2g}(t_{2g}e_g)]$	0	0	1	0
$[^1A_{1g}(e_g^2)]$	0	0	0	1

Γ_3: ^1E	$[a_1(t_2)e(t_2)]$	$[e(t_2)^2]$	$[a_1(t_2)e(e)]$	$[e(t_2)e(e)]$	$[e(e)^2]$
$[^1E_g(t_{2g}^2)]$	$-\sqrt{\frac{2}{3}}$	$\sqrt{\frac{1}{3}}$	0	0	0
$[^1T_{2g}(t_{2g}^2)]$	$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{2}{3}}$	0	0	0
$[^1T_{1g}(t_{2g}e_g)]$	0	0	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	0
$[^1T_{2g}(t_{2g}e_g)]$	0	0	$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$	0
$[^1E_g(e_g^2)]$	0	0	0	0	1

Dq parameter is diagonal, as expected, in the secular determinants of both the coupling schemes. The $D\sigma$ and $D\tau$ parameters are not completely diagonal even in the $\{a_1(t_2), e_\pm(t_2), e_\pm(\mathrm{e}), X^T, S, \Gamma_j\}$ scheme because of the nonvanishing one-electron off-diagonal matrix element $\langle e_\pm(t_2) | V | e_\pm(e) \rangle = \frac{\sqrt{2}}{3}(3D\sigma - 5D\tau)$. The total ligand field is completely diagonalized in this latter scheme, however, in the limit $3D\sigma = 5D\tau$. The electron correlation is diagonalized in the quantum numbers $\{X^C\}$ and $\{X^T\}$, respectively, in the coupling schemes with and without cubic orientation. The ζ parameter, of course, is diagonal only in the $\{\Gamma_j\}$ quantum number in both the representations.

The corresponding energy matrices of d^8 electronic configuration can be obtained, within a constant additive electron correlation term in the diagonal elements, simply by reversing the sign of Dq, $D\sigma$, $D\tau$, and ζ. It is interesting to note that the similarity of d^8 and d^3 configurations in cubic and quadrate ligand fields in the limit of zero spin-orbit interaction [6] extends to trigonal symmetry also. Thus, the

Table 5 a. d^2 Trigonal $\{a_1(t_2), e_\pm(t_2), e_\pm(e), X^T, S, \Gamma_j\}$ Energy Matrices, Γ_1 Representation.

Γ_1	${}^3A_2[e(t_2)^2]$	${}^3E[a_1(t_2)e(t_2)]$	${}^3E[a_1(t_2)e(e)]$	${}^3A_2[e(t_2)e(e)]$	${}^3E[e(t_2)e(e)]$	${}^3A_2[e(e)^2]$	${}^1A_1[a_1(t_2)^2]$	${}^1A_1[e(t_2)^2]$	${}^1A_1[e(t_2)e(e)]$	${}^1A_1[e(e)^2]$
${}^3A_2[e(t_2)^2]$	$-8Dq -2D\sigma -(4/3)D\tau -5B$	$(\sqrt{2}/2)\zeta$	0	$(2/3)(3D\sigma -5D\tau) -6B$	ζ	0	0	$-\zeta$	ζ	0
${}^3E[a_1(t_2)e(t_2)]$		$-8Dq +D\sigma +(16/3)D\tau -5B +(1/2)\zeta$	$-(\sqrt{2}/3)(3D\sigma -5D\tau) -3\sqrt{2}B +(\sqrt{2}/2)\zeta$	$(\sqrt{2}/2)\zeta$	$-3\sqrt{2}B$	0	$-\zeta$	$-(\sqrt{2}/2)\zeta$	$-(\sqrt{2}/2)\zeta$	0
${}^3E[a_1(t_2)e(e)]$			$2Dq +2D\sigma +(11/3)D\tau -2B$	$-(1/2)\zeta$	$6B$	$-\zeta$	$\sqrt{2}\zeta$	0	$(1/2)\zeta$	ζ
${}^3A_2[e(t_2)e(e)]$				$2Dq -D\sigma -3D\tau +4B$	0	$(2/3)(3D\sigma -5D\tau)$	0	ζ	$-(1/2)\zeta$	ζ
${}^3E[e(t_2)e(e)]$					$2Dq -D\sigma -3D\tau -2B -(1/2)\zeta$	ζ	0	ζ	0	ζ
${}^3A_2[e(e)^2]$						$12Dq -(14/3)D\tau -8B$	0	0	ζ	0
${}^1A_1[a_1(t_2)^2]$							$-8Dq +4D\sigma +12D\tau +4B+3C$	$\sqrt{2}(3B +C)$	$-2\sqrt{2}B$	$\sqrt{2}(2B+C)$
${}^1A_1[e(t_2)^2]$								$-8Dq -2D\sigma -(4/3)D\tau +7B+4C$	$(2/3)(3D\sigma -5D\tau) +2B$	$4B+2C$
${}^1A_1[e(t_2)e(e)]$									$2Dq-D\sigma -3D\tau +2C$	$(2/3)(3D\sigma -5D\tau)$
${}^1A_1[e(e)^2]$										$12Dq -(14/3)D\tau +8B+4C$

Table 4 a. d^2 Trigonal $\{t_2, e, X^C, X^T, S, \Gamma_j\}$ Energy Matrices, Γ_1 Representation (left part).

Γ_1	$^3A_2[^3T_{1g}(t_{2g}^2)]$	$^3E[^3T_{1g}(t_{2g}^2)]$	$^3E[^3T_{2g}(t_{2g}\,e_g)]$	$^3A_2[^3T_{1g}(t_{2g}\,e_g)]$	$^3E[^3T_{1g}(t_{2g}\,e_g)]$
$^3A_2[^3T_{1g}(t_{2g}^2)]$	$-8\,Dq-2\,D\sigma-(4/3)\,D\tau-5\,B$	$(\sqrt{2}/2)\,\zeta$	$-(\sqrt{2}/2)\,\zeta$	$(2/3)\,(3\,D\sigma-5\,D\tau)-6\,B$	$(\sqrt{2}/2)\,\zeta$
$^3E[^3T_{1g}(t_{2g}^2)]$		$-8\,Dq+D\sigma+(16/3)\,D\tau-5\,B+(1/2)\,\zeta$	$-(1/3)\,(3\,D\sigma-5\,D\tau)+(1/2)\,\zeta$	$(\sqrt{2}/2)\,\zeta$	$-(1/3)\,(3\,D\sigma-5\,D\tau)-6\,B+(1/2)\,\zeta$
$^3E[^3T_{2g}(t_{2g}\,e_g)]$			$2\,Dq+(1/2)\,D\sigma+(1/3)\,D\tau-8\,B-(1/4)\,\zeta$	$-(\sqrt{2}/4)\,\zeta$	$(1/6)\,(9\,D\sigma+20\,D\tau)+(1/4)\,\zeta$
$^3A_2[^3T_{1g}(t_{2g}\,e_g)]$				$2\,Dq-D\sigma-3\,D\tau+4\,B$	$-(\sqrt{2}/4)\,\zeta$
$^3E[^3T_{1g}(t_{2g}\,e_g)]$					$2\,Dq+(1/2)\,D\sigma+(1/3)\,D\tau+4\,B-(1/4)\,\zeta$
$^3A_2[^3A_{2g}(e_g^2)]$					
$^1A_1[^1A_{1g}(t_{2g}^2)]$					
$^1A_1[^1T_{2g}(t_{2g}^2)]$					
$^1A_1[^1T_{2g}(t_{2g}\,e_g)]$					
$^1A_1[^1A_{1g}(e_g^2)]$					

Table 4 b. d^2 Trigonal $\{t_2, e, X^C, X^T, S, \Gamma_j\}$ Energy Matrices, Γ_2 Representation.

Γ_2	$^3E[^3T_{1g}(t_{2g}^2)]$	$^3A_1[^3T_{2g}(t_{2g}\,e_g)]$	$^3E[^3T_{2g}(t_{2g}\,e_g)]$	$^3E[^3T_{1g}(t_{2g}\,e_g)]$	$^1A_2[^1T_{1g}(t_{2g}\,e_g)]$
$^3E[^3T_{1g}(t_{2g}^2)]$	$-8\,Dq+D\sigma+(16/3)\,D\tau-5\,B+(1/2)\,\zeta$	$(\sqrt{2}/2)\,\zeta$	$-(1/3)\,(3\,D\sigma-5\,D\tau)+(1/2)\,\zeta$	$-(1/3)\,(3\,D\sigma-5\,D\tau)-6\,B+(1/2)\,\zeta$	$(\sqrt{2}/2)\,\zeta$
$^3A_1[^3T_{2g}(t_{2g}\,e_g)]$		$2\,Dq-D\sigma-3\,D\tau-8\,B$	$(\sqrt{2}/4)\,\zeta$	$(\sqrt{2}/4)\,\zeta$	$(1/2)\,\zeta$
$^3E[^3T_{2g}(t_{2g}\,e_g)]$			$2\,Dq+(1/2)\,D\sigma+(1/3)\,D\tau-8\,B-(1/4)\,\zeta$	$(1/6)\,(9\,D\sigma+20\,D\tau)+(1/4)\,\zeta$	$(\sqrt{2}/4)\,\zeta$
$^3E[^3T_{1g}(t_{2g}\,e_g)]$				$2\,Dq+(1/2)\,D\sigma+(1/3)\,D\tau+4\,B-(1/4)\,\zeta$	$(\sqrt{2}/4)\,\zeta$
$^1A_2[^1T_{1g}(t_{2g}\,e_g)]$					$2\,Dq-D\sigma-3\,D\tau+4\,B+2\,C$

Table 4 a. (Right part).

$^3A_2[^3A_{2g}(e_g^2)]$	$^1A_1[^1A_{1g}(t_{2g}^2)]$	$^1A_1[^1T_{2g}(t_{2g}^2)]$	$^1A_1[^1T_{2g}(t_{2g}\,e_g)]$	$^1A_1[^1A_{1g}(e_g^2)]$
0	$-(\sqrt{6}/3)\zeta$	$-(\sqrt{3}/3)\zeta$	ζ	0
0	$-(2\sqrt{3}/3)\zeta$	$(\sqrt{6}/6)\zeta$	$-(\sqrt{2}/2)\zeta$	0
$-\sqrt{2}\,\zeta$	0	$-(\sqrt{6}/2)\zeta$	$(\sqrt{2}/4)\zeta$	0
$(2/3)(3\,D\sigma-5\,D\tau)$	$(\sqrt{6}/3)\zeta$	$(\sqrt{3}/3)\zeta$	$-(1/2)\zeta$	ζ
0	$(2\sqrt{3}/3)\zeta$	$-(\sqrt{6}/6)\zeta$	$(\sqrt{2}/4)\zeta$	$\sqrt{2}\,\zeta$
$12\,Dq-(14/3)D\tau$ $-8\,B$	0	0	ζ	0
	$-8\,Dq+(28/9)D\tau$ $+10\,B+5\,C$	$-(2\sqrt{2}/9)(9\,D\sigma$ $+20\,D\tau)$	$(2\sqrt{6}/9)(3\,D\sigma-5\,D\tau)$	$\sqrt{6}(2\,B+C)$
		$-8\,Dq+2\,D\sigma$ $+(68/9)D\tau$ $+B+2\,C$	$(2\sqrt{3}/9)(3\,D\sigma-5\,D\tau)$ $+2\sqrt{3}\,B$	0
			$2\,Dq-D\sigma-3\,D\tau$ $+2\,C$	$(2/3)(3\,D\sigma-5\,D\tau)$
				$12\,Dq-(14/3)D\tau$ $+8\,B+4\,C$

trigonal splittings of the d^8 cubic triplet levels in this limit (and neglecting configuration interaction) can be seen to be (cf. Tables 4 a, b, c):

$$(^3A_1-{}^3E)\,[^3T_{2g}(t_{2g}^5\,e_g^3)] = (3/2)D\sigma+(10/3)D\tau\,,$$
$$(^3A_2-{}^3E)\,[^3T_{1g}(t_{2g}^5\,e_g^3)] = (3/2)D\sigma+(10/3)D\tau\,,$$

and

$$(^3A_2-{}^3E)\,[^3T_{1g}(t_{2g}^4\,e_g^4)] = 3\,D\sigma+(20/3)D\tau\,,$$

which are exactly same as the trigonal splittings of the corresponding quartet levels of cubic d^3 (cf. Ref. 4). In fact, just as in the cubic and quadrate cases, the trigonal energy determinants of the triplet levels of d^8 are identical with those of the quartet levels of d^3 except for a constant additive energy term of $(25\,A-35\,B+21\,C)$ in the diagonal elements and for phases.

Table 5 b. d^2 Trigonal $\{a_1(t_2), e_\pm(t_2), e_\pm(e), X^{\mathrm{T}}, S, \Gamma_j\}$ Energy Matrices, Γ_2 Representation.

Γ_2	$^3E[a_1(t_2)e(t_2)]$	$^3A_1[e(t_2)e(e)]$	$^3E[a_1(t_2)e(e)]$	$^3E[e(t_2)e(e)]$	$^1A_2[e(t_2)e(e)]$
$^3E[a_1(t_2)e(t_2)]$	$-8\,Dq+D\sigma$ $+(16/3)D\tau-5\,B$ $+(1/2)\zeta$	$(\sqrt{2}/2)\zeta$	$-(\sqrt{2}/3)(3\,D\sigma$ $-5\,D\tau)$ $-3\sqrt{2}\,B$ $+(\sqrt{2}/2)\zeta$	$-3\sqrt{2}\,B$	$(\sqrt{2}/2)\zeta$
$^3A_1[e(t_2)e(e)]$		$2\,Dq-D\sigma$ $-3\,D\tau-8\,B$	$(1/2)\zeta$	0	$(1/2)\zeta$
$^3E[a_1(t_2)e(e)]$			$2\,Dq+2\,D\sigma$ $+(11/3)D\tau-2\,B$	$6\,B$	$(1/2)\zeta$
$^3E[e(t_2)e(e)]$				$2\,Dq-D\sigma$ $-3\,D\tau-2\,B$ $-(1/2)\zeta$	0
$^1A_2[e(t_2)e(e)]$					$2\,Dq-D\sigma$ $-3\,D\tau+4\,B$ $+2\,C$

Table 4 c. d^2 Trigonal $\{t_2, e, X^C, X^T, S, \Gamma_j\}$ Energy Matrices, Γ_3 Representation (left part).

Γ_3	${}^3A_2[{}^3T_{1g}(t_{2g}{}^2)]$	${}^3E[{}^3T_{1g}(t_{2g}{}^2)]^1$	${}^3E[{}^3T_{1g}(t_{2g}{}^2)]^2$	${}^3A_1[{}^3T_{2g}(t_{2g}e_g)]$	${}^3E[{}^3T_{2g}(t_{2g}e_g)]^1$	${}^3E[{}^3T_{2g}(t_{2g}e_g)]^2$	${}^3A_2[{}^3T_{1g}(t_{2g}e_g)]$
${}^3A_2[{}^3T_{1g}\, t_{2g}{}^2)]$	$-8Dq -2D\sigma -(4/3)D\tau -5B$	$-(1/2)\zeta$	0	$-\zeta$	$(1/2)\zeta$	0	$(2/3)(3D\sigma -5D\tau) -6B$
${}^3E[{}^3T_{1g}(t_{2g}{}^2)]^1$		$-8Dq +D\sigma +(16/3)D\tau -5B$	0	$-(1/2)\zeta$	$-(1/3)(3D\sigma -5D\tau)$	$-\zeta$	$-(1/2)\zeta$
${}^3E[{}^3T_{1g}(t_{2g}{}^2)]^2$			$-8Dq +D\sigma +(16/3)D\tau -5B -(1/2)\zeta$	0	ζ	$-(1/3)(3D\sigma -5D\tau) -(1/2)\zeta$	0
${}^3A_1[{}^3T_{2g}(t_{2g}e_g)]$				$2Dq - D\sigma -3D\tau -8B$	$-(1/4)\zeta$	0	$-(1/2)\zeta$
${}^3E[{}^3T_{2g}(t_{2g}e_g)]^1$					$2Dq +(1/2)D\sigma +(1/3)D\tau -8B$	0	$(1/4)\zeta$
${}^3E[{}^3T_{2g}(t_{2g}e_g)]^2$						$2Dq +(1/2)D\sigma +(1/3)D\tau -8B +(1/4)\zeta$	0
${}^3A_2[{}^3T_{1g}(t_{2g}e_g)]$							$2Dq - D\sigma -3D\tau +4B$
${}^3E[{}^3T_{1g}(t_{2g}e_g)]^1$							
${}^3E[{}^3T_{1g}(t_{2g}e_g)]^2$							
${}^3A_2[{}^3A_{2g}(e_g{}^2)]$							
${}^1E[{}^1E_g(t_{2g}{}^2)]$							
${}^1E[{}^1T_{2g}(t_{2g}{}^2)]$							
${}^1E[{}^1T_{1g}(t_{2g}e_g)]$							
${}^1E[{}^1T_{2g}(t_{2g}e_g)]$							
${}^1E[{}^1E_g(e_g{}^2)]$							

Table 4 c. (Right part).

${}^3E[{}^3T_{1g}$ $(t_{2g}\,e_g)]^1$	${}^3E[{}^3T_{1g}$ $(t_{2g}\,e_g)]^2$	${}^3A_2[{}^3A_{2g}$ $(e_g^2)]$	${}^1E[{}^1E_{1g}$ $(t_{2g}^2)]$	${}^1E[{}^1T_{2g}$ $(t_{2g}^2)]$	${}^1E[{}^1T_{1g}$ $(t_{2g}\,e_g)]$	${}^1E[{}^1T_{2g}$ $(t_{2g}\,e_g)]$	${}^1E({}^1E_g$ $(e_g^2)]$
$-(1/2)\zeta$	0	0	$(\sqrt{6}/6)\zeta$	$-(\sqrt{3}/6)\zeta$	$-(1/2)\zeta$	$(1/2)\zeta$	0
$-(1/3)(3D\sigma-5D\tau)-6B$	0	0	$(\sqrt{6}/6)\zeta$	$-(\sqrt{3}/6)\zeta$	$(1/2)\zeta$	$(1/2)\zeta$	0
0	$-(1/3)(3D\sigma-5D\tau)-6B-(1/2)\zeta$	0	$(\sqrt{6}/6)\zeta$	$(\sqrt{3}/3)\zeta$	0	$-\zeta$	0
$-(1/4)\zeta$	0	ζ	0	$-(\sqrt{3}/2)\zeta$	$(1/4)\zeta$	$(1/4)\zeta$	$-(\sqrt{2}/2)\zeta$
$(1/6)(9D\sigma+20D\tau)$	$(1/2)\zeta$	ζ	0	$-(\sqrt{3}/2)\zeta$	$-(1/4)\zeta$	$(1/4)\zeta$	$(\sqrt{2}/2)\zeta$
$-(1/2)\zeta$	$(1/6)(9D\sigma+20D\tau)-(1/4)\zeta$	0	0	0	$-(1/2)\zeta$	0	$-(\sqrt{2}/2)\zeta$
$(1/4)\zeta$	0	$(2/3)(3D\sigma-5D\tau)$	$(\sqrt{6}/3)\zeta$	$(\sqrt{3}/6)\zeta$	$-(1/4)\zeta$	$-(1/4)\zeta$	$-(\sqrt{2}/2)\zeta$
$2Dq+(1/2)D\sigma+(1/3)D\tau+4B$	0	0	$(\sqrt{6}/3)\zeta$	$(\sqrt{3}/6)\zeta$	$(1/4)\zeta$	$-(1/4)\zeta$	$-(\sqrt{2}/2)\zeta$
	$2Dq+(1/2)D\sigma+(1/3)D\tau+4B+(1/4)\zeta$	0	$(\sqrt{6}/3)\zeta$	$-(\sqrt{3}/3)\zeta$	0	$(1/2)\zeta$	$-(\sqrt{2}/2)\zeta$
		$12Dq-(14/3)D\tau-8B$	0	0	0	$-\zeta$	0
			$-8Dq+(28/9)D\tau)+B+2C$	$-(\sqrt{2}/9)(9D\sigma+20D\tau)$	0	$-(2\sqrt{6}/9)(3D\sigma-5D\tau)$	$2\sqrt{3}B$
				$-8Dq-D\sigma+(8/9)D\tau+B+2C$	$(\sqrt{3}/3)(3D\sigma-5D\tau)$	$-(\sqrt{3}/9)(3D\sigma-5D\tau)+2\sqrt{3}B$	0
					$2Dq+(1/2)D\sigma+(1/3)D\tau+4B+2C$	$(1/6)(9D\sigma+20D\tau)$	$(\sqrt{2}/3)(3D\sigma-5D\tau)$
						$2Dq+(1/2)D\sigma+(1/3)D\tau+2C$	$-(\sqrt{2}/3)(3D\sigma-5D\tau)$
							$12Dq-(14/3)D\tau+2C$

Table 5 c. d^2 Trigonal $\{a_1(t_2), e_\pm(t_2), e_\pm(e), X^T, S, \Gamma_j\}$ Energy Matrices, Γ_3 Representation (left part).

Γ_3	$^3A_2[e(t_2)^2]$	$^3E[a_1(t_2)$ $e(t_2)]^1$	$^3E[a_1(t_2)$ $e(t_2)]^2$	$^3A_1[e(t_2)$ $e(e)]$	$^3E[a_1(t_2)$ $e(e)]^1$	$^3E[a_1(t_2)$ $e(e)]^2$
$^3A_2[e(t_2)^2]$	$-8\,Dq$ $-2\,D\sigma$ $-(4/3)\,D\tau$ $-5\,B$	$-(1/2)\,\zeta$	0	$-\zeta$	0	0
$^3E[a_1(t_2)$ $e(t_2)]^1$		$-8\,Dq$ $+D\sigma$ $+(16/3)\,D\tau$ $-5\,B$	0	$-(1/2)\,\zeta$	$-(\sqrt{2}/3)$ $(3\,D\sigma$ $-5\,D\tau)$ $-3\sqrt{2}\,B$	$-(\sqrt{2}/2)\,\zeta$
$^3E[a_1(t_2)$ $e(t_2)]^2$			$-8\,Dq$ $+D\sigma$ $+(16/3)\,D\tau$ $-5\,B$ $-(1/2)\,\zeta$	0	$(\sqrt{2}/2)\,\zeta$	$-(\sqrt{2}/3)$ $(3\,D\sigma$ $-5\,D\tau)$ $-+3\sqrt{2}\,B$ $-(\sqrt{2}/2)\,\zeta$
$^3A_1[e(t_2)$ $e(e)]$				$2\,Dq-D\sigma$ $-3\,D\tau-8\,B$	$-(\sqrt{2}/4)\,\zeta$	0
$^3E[a_1(t_2)$ $e(e)]^1$					$2\,Dq+2\,D\sigma$ $+(11/3)\,D\tau$ $-2\,B$	0
$^3E[a_1(t_2)$ $e(e)]^2$						$2\,Dq+2\,D\sigma$ $+(11/3)\,D\tau$ $-2\,B$
$^3A_2[e(t_2)$ $e(e)]$						
$^3E[e(t_2)$ $e(e)]^1$						
$^3E[e(t_2)$ $e(e)]^2$						
$^3A_2[e(e)^2]$						
$^1E[a_1(t_2)$ $e(t_2)]$						
$^1E[e(t_2)^2]$						
$^1E[a_1(t_2)$ $e(e)]$						
$^1E[e(t_2)$ $e(e)]$						
$^1E[e(e)^2]$						

5. Summary

The development of the complete theory of electronic energy levels of d^2 and d^8 transition-metal systems in trigonal symmetry is presented by obtaining the symmetry adapted eigenvectors and energy determinants in two different coupling schemes, one diagonalizing only the cubic portion of the ligand field and the other almost diagonalizing the total ligand field except for a few nonzero off-diagonal matrix elements containing the axial component of the ligand field resulting because of a nonvanishing one-electron matrix element

$$\langle e_\pm(e_2)|V|e_\pm(e)\rangle = (\sqrt{2}/3)(3\,D\sigma - D\tau).$$

Table 5 c. (Right part).

$^3A_2[e(t_2)\,e(e)]$	$^3E[e(t_2)\,e(e)]^1$	$^3E[e(t_2)\,e(e)]^2$	$^3A_2[e(e)^2]$	$^1E[a_1(t_2)\,e(t_2)]$	$^1E[e(t_2)^2]$	$^1E[a_1(t_2)\,e(e)]$	$^1E[e(t_2)\,e(e)]$	$^1E[e(e)^2]$
$(2/3)(3D\sigma-5D\tau)-6B$	$-(\sqrt{2}/2)\zeta$	0	0	$-(1/2)\zeta$	0	0	$-(\sqrt{2}/2)\zeta$	0
$-(1/2)\zeta$	$-3\sqrt{2}B$	$(\sqrt{2}/2)\zeta$	0	$-(1/2)\zeta$	0	$(\sqrt{2}/2)\zeta$	0	0
0	$-(\sqrt{2}/2)\zeta$	$3\sqrt{2}B$	0	0	$(\sqrt{2}/2)\zeta$	$-(\sqrt{2}/2)\zeta$	$(\sqrt{2}/2)\zeta$	0
$-(1/2)\zeta$	0	0	ζ	$-(1/2)\zeta$	$-(\sqrt{2}/2)\zeta$	$(\sqrt{2}/4)\zeta$	0	$-(\sqrt{2}/2)\zeta$
$(\sqrt{2}/4)\zeta$	$6B$	$(1/2)\zeta$	$(\sqrt{2}/2)\zeta$	$-(\sqrt{2}/2)\zeta$	0	0	0	0
0	$-(1/2)\zeta$	$6B$	0	$-(\sqrt{2}/2)\zeta$	0	0	$-(1/2)\zeta$	$-\zeta$
$2Dq-D\sigma-3D\tau+4B$	0	0	$(2/3)(3D\sigma-5D\tau)$	$-(1/2)\zeta$	$(\sqrt{2}/2)\zeta$	$-(\sqrt{2}/4)\zeta$	0	$-(\sqrt{2}/2)\zeta$
	$2Dq-D\sigma-3D\tau--2B$	0	$-(\sqrt{2}/2)\zeta$	0	ζ	0	$(1/2)\zeta$	$-\zeta$
		$2Dq-D\sigma-3D\tau-2B+(1/2)\zeta$	0	$-(\sqrt{2}/2)\zeta$	0	$(1/2)\zeta$	0	0
			$12Dq-(14/3)D\tau-8B$	0	0	$-(\sqrt{2}/2)\zeta$	$(\sqrt{2}/2)\zeta$	0
				$-8Dq+D\sigma+(16/3)D\tau+B+2C$	0	$(\sqrt{2}/3)(3D\sigma-5D\tau)+\sqrt{2}B$	$-\sqrt{2}B$	$-2\sqrt{2}B$
					$-8Dq-2D\sigma-4/3D\tau+B+2C$	$2B$	$(2/3)(3D\sigma-5D\tau)-2B$	$2B$
						$2Dq+2D\sigma+(11/3)D\tau+2B+2C$	$2B$	0
							$2Dq-D\sigma-3D\tau+2B+2C$	$(2/3)(3D\sigma-5D\tau)$
								$12Dq-(14/3)D\tau+2C$

Spin-orbital forces are included as a final perturbation in both the representations. The trigonally distorted or substituted cubic systems as well as the trigonal systems for which cubic parentage designation of the energy levels has no meaning can be studied by the theory developed.

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