BOND ANGLE DEPENDENT LIGAND FIELD MODEL FOR ELECTRONIC CONFIGURATIONS d^2 AND d^3, I

Theoretical Study of the Trigonal Distortion of Tetrahedral Complexes

By

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The energy matrices of the electronic states arising from the symmetry splitting of configurations of d^2 and d^3 systems in trigonally distorted tetrahedral strong ligand fields are given in terms of Coulomb interaction and ligand field parameters and the angle of distortion.

In earlier studies [1—4], the theoretical discussion of the tetragonally distorted tetrahedral case has been presented on the basis of the bond angle-dependent ligand field model. Though this approach proved to be succesful for the interpretation of several properties related with the changes in the electronic energies of a number of transition metal complexes [5—7] of the compositions MA_4, MA_3B and MA_2B_2, nevertheless, later on it proved necessary to adapt the model to the trigonally and rhomboidally distorted tetrahedrons, which take more strictly into account the actual microsymmetries for complexes of MA_3B and MA_2B_2 compositions.

In the present paper, the trigonally distorted tetrahedral case, and in the following one [8] the rhomboidally distorted tetrahedral case for the $d^2(d^8)$ and $d^3(d^7)$ configurations[1], of greatest practical importance, have been treated theoretically. To do this, the procedure outlined in earlier papers has been followed.

In case of four-coordinate tetrahedrally oriented mixed ligand complexes of MA_3B composition three identical (A) ligands are located in three apices of the tetrahedron and one different (B) ligand in the fourth apex. The coordinate system is suitably oriented in such a way that its origin (O) lies in the centre of the tetrahedron and the Z-axis coincides with the O—B straight line. Each of the three identical A ligands encloses the angle α with the +Z-axis[2], so, except the cases $\alpha = 109°28'$ (T_d) and $\alpha = 180°$ ($D_{\infty h}$), the symmetry is C_{3v} for any angle. The coordinates of the ligand positions with respect to the central metal ion are given in Table I.

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[1] The discussion of all the remaining cases: $d^4(d^6)$ and d^5, and further details of the theory can be found in [9].

[2] This Z-axis (the Z-axis of the "trigonally oriented tetrahedron") deviates, of course, by an angle of $\arccos(3)^{-1/2}$ from the Z-axis of the "tetragonally oriented tetrahedron" (comp. with the case described in [1]). Throughout this paper $\frac{\pi}{2} \leq \alpha \leq \pi$.

Table I

Ligand coordinates

Type of complex	Ligand	R_k Metal-ligand distance	ϑ_k Polar angle (from the +Z-axis)	φ_k Azimuthal angle (from the +X-axis)
MA_3B	A^1	R_A	α	0
	A^2	R_A	α	$2\pi/3$
	A^3	R_A	α	$4\pi/3$
	B	R_B	0	0

By using the expression (1) of [1], the actual ligand field operator is of the form:

$$V(C_{3v}) = eq\left\{\left[\frac{3}{2}(3\cos^2\alpha-1)r_2^A(r)+r_2^B(r)\right]P_2^0(\cos\vartheta)+\right.$$
$$+\left[\frac{3}{8}(35\cos^4\alpha-30\cos^2\alpha+3)r_4^A(r)+r_4^B(r)\right]P_4^0(\cos\vartheta)-$$
$$\left.-\frac{1}{16}\sin^3\alpha\cos\alpha\, r_4^A(r)P_4^3(\cos\vartheta)\,(e^{-3i\varphi}+e^{3i\varphi})\right\}. \tag{1}$$

For $\alpha=109°28'$ and $R_A = R_B$, the perturbation potential valid in the regular ("trigonally oriented") tetrahedral ligand field will be effective:

$$V(T_d) = eq\left\{\frac{28}{27}P_4^0(\cos\vartheta)+\frac{\sqrt{2}}{81}P_4^3(\cos\vartheta)\,(e^{-3i\varphi}+e^{3i\varphi})\right\}r_4(r). \tag{2}$$

The single-electron trigonal ligand field matrix elements then are

$$\langle d_0|\,V(C_{3v})\,|d_0\rangle = 2D_2^0(3)+6D_4^0(3), \tag{3.1}$$
$$\langle d_{\pm 1}|\,V(C_{3v})\,|d_{\pm 1}\rangle = D_2^0(3)-4D_4^0(3), \tag{3.2}$$
$$\langle d_{\pm 2}|\,V(C_{3v})\,|d_{\pm 2}\rangle = -2D_2^0(3)+D_4^0(3), \tag{3.3}$$
$$\langle d_{\mp 1}|V(C_{3v})\,|d_{\pm 2}\rangle = \pm D_4^3(3), \tag{3.4}$$

or, considering the splitting,

$$d(C_{3v}) = a+2e \tag{4}$$

of the fivefold d-orbital and the forms

$$a = d_{z^2}, \tag{5.1}$$
$$e_1^1 = \sqrt{\frac{1}{3}}\left(\sqrt{2}\,d_{x^2-y^2}+d_{xz}\right), \tag{5.2}$$
$$e_1^2 = \sqrt{\frac{1}{3}}\left(\sqrt{2}\,d_{xy}+d_{yz}\right), \tag{5.3}$$
$$e_2^1 = \sqrt{\frac{1}{3}}\left(d_{x^2-y^2}-\sqrt{2}\,d_{xz}\right). \tag{5.4}$$
$$e_2^2 = \sqrt{\frac{1}{3}}\left(d_{xy}-\sqrt{2}\,d_{yz}\right), \tag{5.5}$$

of the real d-orbitals[3] in trigonal field, the energy matrix elements[4] of the real d-functions are

$$\langle a|\, V(C_{3v})\,|a\rangle = 2D_2^0(3) + 6D_4^0(3), \tag{6.1}$$

$$\langle e_1^1|\, V(C_{3v})\,|e_1^1\rangle = \langle e_1^2|\, V(C_{3v})\,|e_1^2\rangle = -D_2^0(3) - \frac{2}{3}D_4^0(3) - \frac{2\sqrt{2}}{3}D_4^3(3), \tag{6.2}$$

$$\langle e_2^1|\, V(C_{3v})\,|e_2^1\rangle = \langle e_2^2|\, V(C_{3v})\,|e_2^2\rangle = -\frac{7}{3}D_4^0(3) + \frac{2\sqrt{2}}{3}D_4^3(3), \tag{6.3}$$

$$\langle e_1^1|\, V(C_{3v})\,|e_2^1\rangle = \langle e_1^2|\, V(C_{3v})\,|e_2^2\rangle = -\sqrt{2}\,D_2^0(3) + \frac{5\sqrt{2}}{3}D_4^0(3) + \frac{1}{3}D_4^3(3). \tag{6.4}$$

The meaning of the quantities[5] occurring in the expressions (3) and (6) are as follows (for simplicity R_A taken equal to R_B):

$$D_2^0(3) = \frac{6}{7}\varrho\left[1 + \frac{3}{2}(3\cos^2\alpha - 1)\right]Dq, \tag{7.1}$$

$$D_4^0(3) = \frac{2}{7}\left[1 + \frac{3}{8}(35\cos^4\alpha - 30\cos^2\alpha + 3)\right]Dq, \tag{7.2}$$

$$D_4^3(3) = \frac{15}{2}\sin^3\alpha\cos\alpha\, Dq, \tag{7.3}$$

where

$$Dq = \frac{1}{6}R_4(r), \tag{8}$$

and

$$\varrho = \frac{R_2(r)}{R_4(r)}. \tag{9}$$

The explanations of other symbols are given in former papers (see [1—4, 7, 9, 10, 13]). Applying the strong field approximation to the $d^2(d^8)$ and $d^3(d^7)$ congurations appearing most frequently in practice, according to the general procedure [10] of the ligand field method [11], the energy matrix elements of the multi-electron states can be obtained as the sums of integrals composed of the operator (1) and of either wave functions of types described in [12] or the product eigenfunctions of a recursion method [13] and of integrals of the same functions and the operator (8) of [1]. Thus the energy matrices for d^2 are:

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[3] The subscripts of e in the suffix of the functions indicate the two e-orbitals in (4) and the superscripts of e distinguish one function from the other of the degenerate pairs of functions.

[4] Throughout this paper the interaction between the states e_1 and e_2 has been neglected. This has no serious effect on the energies, especially at angles close to that of the regular tetrahedron and $\varrho = 1$. For a more precise treatment, the solutions of the one-electron energy matrix containing the off-diagonal elements $\langle e_1|V(C_{3v})|e_2\rangle$ should be used to calculate the matrix elements of multi-electron states at given angles.

[5] The subscripts 2 and 4 of D refer to the degree l, the superscripts 0 and 3 to the order m of the associated Legendre polynomial $P_l^m(\cos\vartheta)$ involved in the operator (1) and the adjoining number 3 in parentheses refers to the (trigonal) symmetry. In the expressions (10) and (11) the latter are omitted.

$$\begin{array}{c|ccc}
{}^3E & (a)(e_1) & (a)(e_2) & (e_1)(e_2) \\
\hline
(a)(e_1) & 3B+D_2^0+\frac{16}{3}D_4^0-\frac{2\sqrt{2}}{3}D_4^3 & 3\sqrt{2}B & 3\sqrt{2}B \\
(a)(e_2) & & 6B+2D_2^0+\frac{11}{3}D_4^0+\frac{2\sqrt{2}}{3}D_4^3 & 6B \\
(e_1)(e_2) & & & 6B-D_2^0-3D_4^0
\end{array} \tag{10.1}$$

$$\begin{array}{c|c}
{}^3A_1 & (e_1)(e_2) \\
\hline
(e_1)(e_2) & -D_2^0-3D_4^0
\end{array} \tag{10.2}$$

$$\begin{array}{c|ccc}
{}^3A_2 & (e_1)^2 & (e_2)^2 & (e_1)(e_2) \\
\hline
(e_1)^2 & 3B-2D_2^0-\frac{4}{3}D_4^0-\frac{4\sqrt{2}}{3}D_4^3 & 0 & -6B \\
(e_2)^2 & & -\frac{14}{3}D_4^0+\frac{4\sqrt{2}}{3}D_4^3 & 0 \\
(e_1)(e_2) & & & 12B-D_2^0-3D_4^0
\end{array} \tag{10.3}$$

$$\begin{array}{c|cccc}
{}^1A_1 & (a)^2 & (e_1)^2 & (e_2)^2 & (e_1)(e_2) \\
\hline
(a)^2 & \begin{array}{c}12B+3C+4D_2^0+\\+12D_4^0\end{array} & \sqrt{2}(3B+C) & \sqrt{2}(2B+C) & -2\sqrt{2}B \\
(e_1)^2 & & \begin{array}{c}15B+4C-2D_2^0-\\-\frac{4}{3}D_4^0-\frac{4\sqrt{2}}{3}D_4^3\end{array} & 4B+2C & 2B \\
(e_2)^2 & & & \begin{array}{c}12B+2C-\\-\frac{14}{3}D_4^0+\frac{4\sqrt{2}}{3}D_4^3\end{array} & 0 \\
(e_1)(e_2) & & & & 8B+2C-D_2^0-3D_4^0
\end{array} \tag{10.4}$$

$$\begin{array}{c|c}
{}^1A_2 & (e_1)(e_2) \\
\hline
(e_1)(e_2) & 12B+2C-D_2^0-3D_4^0
\end{array} \tag{10.5}$$

$$\begin{array}{l|ccccc}
{}^1E & (e_1)^2 & (e_2)^2 & (a)(e_1) & (a)(e_2) & (e_1)(e_2) \\
\hline
(e_1)^2 & 9B+2C-2D_2^0-\frac{4}{3}D_4^0-\frac{4\sqrt{2}}{3}D_4^3 & 2B & 0 & -2B & -2B \\
(e_2)^2 & & 8B+2C-\frac{14}{3}D_4^0+\frac{4\sqrt{2}}{3}D_4^3 & 2\sqrt{2}B & 0 & 2B \\
(a)(e_1) & & & 9B+2C+D_2^0+\frac{16}{3}D_4^0-\frac{2\sqrt{2}}{3}D_4^3 & \sqrt{2}B & \sqrt{2}B \\
(a)(e_2) & & & & 10B+2C+2D_2^0+\frac{11}{3}D_4^0+\frac{2\sqrt{2}}{3}D_4^3 & -2B \\
(e_1)(e_2) & & & & & 10B+2C-D_2^0-3D_4^0
\end{array} \qquad (10.6)$$

and for d^3:

$$\begin{array}{l|c}
{}^4A_1 & (e_1)(e_2)(a) \\
\hline
(e_1)(e_2)(a) & D_2^0+3D_4^0
\end{array} \qquad (11.1)$$

$$\begin{array}{l|ccc}
{}^4A_2 & (e_1)^2(a) & (e_2)^2(a) & (e_1)(e_2)(a) \\
\hline
(e_1)^2(a) & \frac{14}{3}D_4^0-\frac{4\sqrt{2}}{3}D_4^3 & 0 & 0 \\
(e_2)^2(a) & & 3B+2D_2^0+\frac{4}{3}D_4^0+\frac{4\sqrt{2}}{3}D_4^3 & -6B \\
(e_1)(e_2)(a) & & & 12B+D_2^0+3D_4^0
\end{array} \qquad (11.2)$$

$$\begin{array}{l|ccc}
{}^4E & (e_1)^2(e_2) & (e_2)^2(e_1) & (e_1)(e_2)(a) \\
\hline
(e_1)^2(e_2) & 6B-2D_2^0-\frac{11}{3}D_4^0-\frac{2\sqrt{2}}{3}D_4^3 & 3\sqrt{2}B & 6B \\
(e_2)^2(e_1) & & 3B-D_2^0-\frac{16}{3}D_4^0+\frac{2\sqrt{2}}{3}D_4^3 & 3\sqrt{2}B \\
(e_1)(e_2)(a) & & & 6B+D_2^0+3D_4^3
\end{array} \qquad (11.3)$$

$^2A_1$	$(e_1)^2(a)$	$(e_2)^2(a)$	$(e_1)^2(e_2)$	$(e_2)^2(e_1)$	$(e_1)(e_2)(a)$	$(e_1)(e_2)(a)$
$(e_1)^2(a)$	$15B+5C+\frac{14}{3}D_4^0-$ $-\frac{4\sqrt{2}}{3}D_4^3$	$2(2B+C)$	$5\sqrt{2}B$	$-2B$	0	$\sqrt{3}B$
$(e_2)^2(a)$		$21B+5C+2D_2^0+$ $+\frac{4}{3}D_4^0+\frac{4\sqrt{2}}{3}D_4^3$	$\sqrt{2}B$	$-10B$	0	$-\sqrt{3}B$
$(e_1)^2(e_2)$			$14B+3C-2D_2^0-$ $-\frac{11}{3}D_4^0-\frac{2\sqrt{2}}{3}D_4^3$	$\sqrt{2}B$	0	$-2\sqrt{3}B$
$(e_2)^2(e_1)$				$13B+3C-D_2^0-$ $-\frac{16}{3}D_4^0+\frac{2\sqrt{2}}{3}D_4^3$	0	$\sqrt{6}B$
$(e_1)(e_2)(a)$					$\frac{21}{2}B+3C+D_2^0+3D_4^0$	0
$(e_1)(e_2)(a)$						$\frac{15}{2}B+3C+D_2^0+3D_4^0$

(11.4)

$^2A_2$	$(e_1)^2(a)$	$(e_2)^2(a)$	$(e_1)^2(e_2)$	$(e_2)^2(e_1)$	$(e_1)(e_2)(a)$	$(e_1)(e_2)(a)$
$(e_1)^2(a)$	$9B+3C+\frac{14}{3}D_4^0-$ $-\frac{4\sqrt{2}}{3}D_4^3$	0	$-\sqrt{6}\,B$	$2\sqrt{3}\,B$	$\sqrt{3}\,B$	B
$(e_2)^2(a)$		$9B+3C+2D_2^0+$ $+\frac{4}{3}D_4^0+\frac{4\sqrt{2}}{3}D_4^3$	$-\sqrt{6}\,B$	$2\sqrt{3}\,B$	$-\sqrt{3}\,B$	B
$(e_1)^2(e_2)$			$14B+3C-2D_2^0-$ $-\frac{11}{3}D_4^0-\frac{2\sqrt{2}}{3}D_4^3$	$-\sqrt{2}\,B$	$-4B$	$2\sqrt{3}\,B$
$(e_2)^2(e_1)$				$13B+3C-D_2^0-$ $-\frac{16}{3}D_4^0+\frac{2\sqrt{2}}{3}D_4^3$	$2\sqrt{2}\,B$	$\sqrt{6}\,B$
$(e_1)(e_2)(a)$					$\frac{29}{2}B+3C+D_2^0+3D_4^0$	$-\frac{\sqrt{3}}{2}B$
$(e_1)(e_2)(a)$						$\frac{39}{2}B+3C+D_2^0+D_4^0$

(11.5)

^2E	$(e_1)^3$	$(e_2)^3$	$(a)^2(e_1)$	$(a)^2(e_2)$	$(e_1)^2(a)$	$(e_2)^2(a)$	$(e_1)^2(e_2)$	$(e_1)^2(e_2)$ ...
$(e_1)^3$	$12B+4C-$ $-3D_2^0-2D_4^0-$ $-2\sqrt{2}D_4^3$	0	$3B+C$	0	0	0	$-6B$	$-2\sqrt{3}B$
$(e_2)^3$		$7B+4C-$ $-7D_4^0+$ $+2\sqrt{2}D_4^3$	0	$2B+C$	0	0	$\sqrt{2}(2B+C)$	0
$(a)^2(e_1)$			$12B+4C+3D_2^0+$ $+\frac{21}{2}D_4^0-\frac{2\sqrt{2}}{3}D_4^3$	$5\sqrt{2}B$	0	$-2B$	B	$-\sqrt{3}B$
$(a)^2(e_2)$				$17B+4C+4D_2^0+$ $+\frac{29}{3}D_4^0+\frac{2\sqrt{2}}{3}D_4^3$	$\sqrt{2}B$	0	$\sqrt{2}(3B+C)$	0
$(e_1)^2(a)$					$9B+3C+$ $+\frac{14}{3}D_4^0-\frac{4\sqrt{2}}{3}D_4^3$	$2B$	$5B$	$-\sqrt{3}B$
$(e_2)^2(a)$						$13B+3C+2D_2^0+$ $+\frac{4}{3}D_4^0+\frac{4\sqrt{2}}{3}D_4^3$	0	0
$(e_1)^2(e_2)$							$20B+5C-2D_2^0-$ $-\frac{11}{3}D_4^0-\frac{2\sqrt{2}}{3}D_4^3$	0
$(e_1)^2(e_2)$								$12B+3C-2D_2^0-$ $-\frac{11}{3}D_4^0-\frac{2\sqrt{2}}{3}D_4^3$
$\vdots$								

(11.6a)

^2E	…	$(e_1)^2(e_2)$	$(e_2)^2(e_1)$	$(e_2)^2(e_1)$	$(e_2)^2(e_1)$	$(e_1)(e_2)(a)$	$(e_1)(e_2)(a)$
$(e_1)^3$		$4\sqrt{2}B$	$\sqrt{2}(2B+C)$	0	$-2B$	0	0
$(e_2)^3$		$-2B$	0	0	0	$-\sqrt{2}B$	$\sqrt{6}B$
$(a)^2(e_1)$		$\sqrt{2}B$	$\sqrt{2}(2B+C)$	0	0	$-B$	$-3\sqrt{3}B$
$(a)^2(e_2)$		0	B	$\sqrt{3}B$	$\sqrt{2}B$	$-B$	$3\sqrt{3}B$
$(e_1)^2(a)$		0	0	0	$-2B$	$3B$	$\sqrt{3}B$
$(e_2)^2(a)$		$\sqrt{2}B$	$-5\sqrt{2}B$	$\sqrt{6}B$	0	B	$-\sqrt{3}B$
$(e_1)^2(e_2)$		$-5\sqrt{2}B$	$-\frac{\sqrt{2}}{2}B$	$-\frac{\sqrt{6}}{2}B$	$-B$	$\frac{\sqrt{2}}{2}B$	$-\sqrt{6}B$
$(e_1)^2(e_2)$		$-\sqrt{6}B$	$-\frac{3\sqrt{6}}{2}B$	$\frac{3\sqrt{2}}{2}B$	$3\sqrt{2}B$	$2\sqrt{3}B$	$-4B$
⋮							

(11.6b) (cont.)

^2E	…	$(e_1)^2(e_2)$	$(e_2)^2(e_1)$	$(e_2)^2(e_1)$	$(e_2)^2(e_1)$	$(e_1)(e_2)(a)$	$(e_1)(e_2)(a)$
⋮							
$(e_1)^2(e_2)$		$14B+3C-2D_2^0-$ $-\frac{11}{3}D_4^0-\frac{2\sqrt{2}}{3}D_4^3$	B	$-\sqrt{3}B$	0	0	0
$(e_2)^2(e_1)$			$21B+5C-D_2^0-$ $-\frac{16}{3}D_4^0+\frac{2\sqrt{2}}{3}D_4^3$	0	$-5\sqrt{2}B$	$-\frac{3\sqrt{2}B}{2}$	$-\frac{\sqrt{6}}{2}B$
$(e_2)^2(e_1)$				$9B+3C-D_2^0-$ $-\frac{16}{3}D_4^0+\frac{2\sqrt{2}}{3}D_4^3$	$\sqrt{6}B$	0	0
$(e_2)^2(e_1)$					$13B+3C-D_2^0-$ $-\frac{16}{3}D_4^0+\frac{2\sqrt{2}}{3}D_4^3$	0	0
$(e_1)(e_2)(a)$						$\frac{25}{2}B+3C+D_2^0+3D_4^0$	$-\sqrt{3}B$
$(e_1)(e_2)(a)$							$\frac{27}{2}B+3C+D_2^0+3D_4^0$

(11.6c) (cont.)

The expressions (10) and (11) can easily be adapted to the cases of d^8 and d^7 by leaving the matrix elements of the Coulomb interactions (containing the linear combinations of Racah's B and C parameters) unchanged and by reversing the signs of the ligand field energies given by linear combinations of D_2^0, D_4^0 and D_4^3 with respect to the cases d^2 and d^3. The theoretical results obtained can be used for the explanation of the physico-chemical properties connected with the electronic energies and with their changes in trigonally distorted tetrahedral complexes of MA_3B composition.

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МОДЕЛЬ УГЛОВОЙ ЗАВИСИМОСТИ ЛИГАНДНЫХ ПОЛЕЙ d^2 И d^3 ЭЛЭКТРОННЫХ КОНФИГУРАЦИЙ, I

Теоретическое рассмотрение тригональной деформации тетраэдрических комплексов

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Используя приближение сильного поля в тригонально деформированной тетраэдрической системе, рассчитали энергетические состояния матриксов энергии, происходящих из расщепления d^2 и d^3 электронных конфигураций, как функции кулоновских взаимодействий, параметров лигандных полей и угла деформации.