SCIENTIFIC PAPERS
OF THE UNIVERSITY OF PARDUBICE
Series A
Faculty of Chemical Technology
7 (2001)

LIGAND FIELD MODEL FOR (C_{2v}) METALLOCENE COMPLEXES. d^3 AND d^4 STRONG-FIELD ENERGY MATRICES

Josef FIEDLER[a], Ivan PAVLÍK[a,b1] and Martin PAVLIŠTA[b]
[a]Department of General and Inorganic Chemistry,
[b]Research Centre New Inorganic Compounds and Advanced Materials,
The University of Pardubice, CZ–532 10 Pardubice

Received September 19, 2001

Dedicated to Professor Miloslav Frumar on the occasion of his 65th birthday in recognition of his outstanding contribution to the inorganic solid-state chemistry

Strong-field energy matrices expressed in terms of four d-orbital splitting parameters (Ds, Dt, Dq, Dr) and two Racah parameters (B, C) without spin-orbit coupling effects were calculated for the d^3 and d^4 bent (C_{2v}) metallocene derivatives.

Introduction

Very recently, we reported on the ligand field model for bent (C_{2v}) d^1 [1,2] and d^2 [2] metallocene complexes of the type Cp_2ML_n (Cp = η^5-C_5H_5; M = early

[1] To whom correspondence should be addressed.

transition metal; L = ligand, e.g. halide, pseudohalide, CO etc.; n = 1 or 2). It was shown that the one-electron energies of the five split d-orbitals can be expressed in terms of four d-orbital splitting parameters Ds, Dt, Dq, Dr. Also, the strong-field energy matrices for d^2 bent metallocene complexes were calculated [2], containing two additional interelectronic Coulombic interaction (Racah) parameters B and C. In order to complete the many-electron ligand field model for d^N ($n = 2-4$) Cp_2ML_n complexes, we present here the d^3 and d^4 strong-field energy matrices (without spin-orbit coupling).

Theory

In the C_{2v} ligand field, the five-fold degenerate d-orbital set splits into five nondegenerate sublevels. Their one-electron energy terms H_{ii} (i = 1 - 5) and H_{12} have been reported previously [1,2].

Strong-Field Coupling Formalism (Spin-Orbit Coupling Neglected) for d^3 and d^4 Confugurations

As a detailed account of the strong-field coupling scheme applied to metallocenes can be found elsewhere [2,3], this approach will be outlined only briefly here.

The perturbation Hamiltonian $\hat{H}'$ for a d^N electron system without spin-orbit coupling effects reads as follows

$$\hat{H}' = \sum_{i=1}^{N} \hat{V}_{LF}(i) + \sum_{i<j}^{N} \frac{e^2}{4\pi\varepsilon_0 r_{ij}} \qquad (1)$$

where the first term represents the potential of d-electrons of the central metal ion in the ligand field and the second term represents the interelectronic Coulombic repulsion. In the strong-field coupling scheme it holds that

$$\sum_{i=1}^{N} \hat{V}_{LF}(i) > \sum_{i<j}^{N} \frac{e^2}{4\pi\varepsilon_0 r_{ij}} \qquad (2)$$

In matrix elements $\hat{H}'_{mn}$ (Eq. (3)) to be constructed, Ψ_m, Ψ_n (Eq. (4)) are now some of all the possible N-electron strong-field functions constructed from symmetry-adapted linear combinations of antisymmetrized products (Slater

determinants) $|\varphi_u\rangle$ of spinorbitals corresponding to a particular electron orbital configuration $\gamma_1^{n_1}\gamma_2^{n_2}...\gamma_5^{n_5}$ (where $n_1 + n_2 + ... + n_5 = N$).

$$\hat{H}'_{mn} = \langle \Psi_m | \sum_{i=1}^{N} \hat{V}_{LF}(i) + \sum_{i<j}^{N} \frac{e^2}{4\pi\varepsilon_0 r_{ij}} | \Psi_n \rangle \tag{3}$$

$$\Psi_m = \sum_u c_u \varphi_u \tag{4}$$

The three- and four-electron strong-field functions $\Psi_m = |(\gamma_1^{n_1}\gamma_2^{n_2}...\gamma_5^{n_5})^{2S+1}\Gamma, M_s\rangle$ obtained by means of standard procedures [3,4] are listed in the previous paper [2], Table III. Using these three- and four-electron functions, the matrix elements of the operator (1) were calculated as described in [2]. The diagonal elements contain the one-electron energy terms H_{ii} (i = 1 - 5) and H_{12} (see [1,2]) of the occupied d-sublevels (i.e., the splitting parameters Ds, Dt, Dq, Dr) as well as the Racah parameters B and C, while the off-diagonal elements contain the B, C parameters only.

d^3 Bent Metallocenes Cp_2ML_n (n = 1, 2)

The dimension of d^3 representation is 50 × 50. However, the C_{2v} symmetry of the ligand field and zero matrix elements among $^{2S+1}\Gamma$ terms differing both in spin multiplicity and Γ result in reduction to one 1 ×1 spin-quadruplet matrix ($^4A_1$), three 3 × 3 spin-quadruplet matrices ($^4A_2$, $^4B_1$, $^4B_2$) and four 10 × 10 spin-doublet matrices ($^2A_1$, $^2A_2$, $^2B_1$, $^2B_2$. Table I lists the simplified designations of the relevant strong-field terms $|(\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k})^{2S+1}\Gamma, M_S\rangle$. The strong-field energy matrices for the C_{2v} system are presented in Table II.

d^4 Bent Metallocenes Cp_2ML_n (n = 1, 2)

The 100 × 100 dimension of the d^4 representation reduces to three spin-quintuplet matrices ($^5A_2$, $^5B_1$, $^5B_2$), one 2 × 2 spin-quintuplet matrix ($^5A_1$), one 9 × 9 spin-triplet matrix ($^3A_1$), three 11 × 11 spin-singlet matrices ($^1A_2$, $^1B_1$, $^1B_2$), three 12 × 12 spin-triplet matrices ($^3A_2$, $^3B_1$, $^3B_2$), and one 17

× 17 spin-singlet matrix ($^1A_1$). Table III lists the designations of the d^4 strong-field terms $|(\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k}\gamma_l^{n_l})^{2S+1}\Gamma, M_S\rangle$ and Table IV presents the corresponding d^4 strong-field matrices.

The formal correctness of all the d^3 and d^4 strong-field energy matrices was verified by

(i) transforming d^3 functions from $D_{\infty h}$ symmetry [3] to the C_{2v} one and
(ii) comparing results of numerical calculations carried out under zero ligand field strength (Ds = Dt = Dq = Dr = 0) with d^3 and d^4 free ion energies.

Conclusion

The reported d^3 and d^4 strong-field energy matrices may be instrumental in solving various problems of the bent d^3 or d^4 metallocene complexes within the framework of the ligand field model. The representatives of such complexes may be, for example, d^3 $Cp_2V(CO)$ or d^4 $Cp_2M(CO)$ (M = Cr, Mo, W).

Acknowledgements

This work was supported by the Ministry of Education, Youth and Sports of the Czech Republic within the framework of the project LN00A28 (New Inorganic Compounds and Advanced Materials).

References

[1] Pavlík I., Fiedler J., Vinklárek J., Pavlišta M.: Sci. Pap. Univ. Pardubice Ser. A6, 25 (2000).

[2] Pavlík I., Fiedler J., Vinklárek J., Pavlišta M.: Collect. Czech. Chem. Commun. **66**, 228 (2001).

[3] Pavlík I., Černý V., Maxová E.: Collect. Czech. Chem. Commun. **37**, 171 (1972).

[4] Griffith J.S.: *The Theory of Transition-Metal Ions*, Cambridge University Press, Cambridge, 1964.

Table I Simplified designation for d^3 strong-field terms $\left|(\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k})^{2S+1}\Gamma, M_S\right\rangle$

Γ	$\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k}$	Designation		Γ	$\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k}$	Designation	
		$^4\Gamma$	$^2\Gamma$			$^4\Gamma$	$^2\Gamma$
A_1	$a_2^1b_1^1b_2^1$	1	$2^{(a)}$	B_1	$(a_1(z^2))^1(a_1(x^2-y^2))^1b_1^1$	25	$28^{(a)}$
			$3^{(b)}$				$29^{(b)}$
	$(a_1(z^2))^2(a_1(x^2-y^2))^1$		4		$(a_1(z^2))^1a_2^1b_2^1$	26	$30^{(a)}$
	$(a_1(z^2))^1(a_1(x^2-y^2))^2$		5				$31^{(b)}$
	$(a_1(z^2))^1a_2^2$		6		$(a_1(x^2-y^2))^1a_2^1b_2^1$	27	$32^{(a)}$
	$(a_1(z^2))^1b_1^2$		7				$33^{(b)}$
	$(a_1(z^2))^1b_2^2$		8		$(a_1(z^2))^2b_1^1$		34
	$(a_1(x^2-y^2))^1a_2^2$		9		$(a_1(x^2-y^2))^2b_1^1$		35
	$(a_1(x^2-y^2))^1b_1^2$		10		$a_2^2b_1^1$		36
	$(a_1(x^2-y^2))^1b_2^2$		11		$b_1^1b_2^2$		37
A_2	$(a_1(z^2))^1(a_1(x^2-y^2))^1a_2^1$	12	$15^{(a)}$	B_2	$(a_1(z^2))^1(a_1(x^2-y^2))^1b_2^1$	38	$41^{(a)}$
			$16^{(b)}$				$42^{(b)}$
	$(a_1(z^2))^1b_1^1b_2^1$	13	$17^{(a)}$		$(a_1(z^2))^1a_2^1b_1^1$	39	$43^{(a)}$
			$18^{(b)}$				$44^{(b)}$
	$(a_1(x^2-y^2))^1b_1^1b_2^1$	14	$19^{(a)}$		$(a_1(x^2-y^2))^1a_2^1b_1^1$	40	$45^{(a)}$

Table I – Continued

Γ	$\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k}$	Designation		Γ	$\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k}$	Designation	
		$^4\Gamma$	$^2\Gamma$			$^4\Gamma$	$^2\Gamma$
			20[b]				46[b]
	$(a_1(z^2))^2a_2^1$		21		$(a_1(z^2))^2b_2^1$		47
	$(a_1(x^2-y^2))^2a_2^1$		22		$(a_1(x^2-y^2))^2b_2^1$		48
	$a_2^1b_1^2$		23		$a_2^2b_2^1$		49
	$a_2^1b_2^2$		24		$b_1^2b_2^1$		50

Table II Strong-field energy matrices for d^3 bent metallocene complexes

$^4A_1$: $\left|H_{33}+H_{44}+H_{55}-15B\right|\,|1\rangle$

$^2A_1$:

$H_{33}+H_{44}+H_{55}-6B+3C$	0	0	0	0	$(3/2)\cdot 2^{1/2}B$	$-(3/2)\cdot 2^{1/2}B$	$-3\cdot 6^{1/2}B$	$-3(3/2)^{1/2}B$	$-3(3/2)^{1/2}B$	$\|2\rangle$
0	$H_{33}+H_{44}+H_{55}-6B+3C$	0	0	$-6^{1/2}B$	$-5(3/2)^{1/2}B$	$-5(3/2)^{1/2}B$	0	$(3/2)\cdot 2^{1/2}B$	$-(3/2)\cdot 2^{1/2}B$	$\|3\rangle$
0	0	$2H_{11}+H_{22}-8B+4C$	$-H_{12}$	0	$-3^{1/2}B$	$3^{1/2}B$	$4B+C$	$B+C$	$B+C$	$\|4\rangle$
0	0	$-H_{12}$	$H_{11}+2H_{22}-8B+4C$	C	$3B+C$	$3B+C$	0	$-3^{1/2}B$	$3^{1/2}B$	$\|5\rangle$
0	$-6^{1/2}B$	0	C	$H_{11}+2H_{33}-8B+4C$	$3B+C$	$3B+C$	H_{12}	0	0	$\|6\rangle$
$(3/2)\cdot 2^{1/2}B$	$-5(3/2)^{1/2}B$	$-3^{1/2}B$	$3B+C$	$3B+C$	$H_{11}+2H_{44}+7B+4C$	$3B+C$	0	$H_{12}-5\cdot 3^{1/2}B$	0	$\|7\rangle$
$-(3/2)\cdot 2^{1/2}B$	$-5(3/2)^{1/2}B$	$3^{1/2}B$	$3B+C$	$3B+C$	$3B+C$	$H_{11}+2H_{55}+7B+4C$	0	0	$H_{12}+5\cdot 3^{1/2}B$	$\|8\rangle$
$-3\cdot 6^{1/2}B$	0	$4B+C$	0	H_{12}	0	0	$H_{22}+2H_{33}+12B+4C$	$3B+C$	$3B+C$	$\|9\rangle$
$-3(3/2)^{1/2}B$	$(3/2)\cdot 2^{1/2}B$	$B+C$	$-3^{1/2}B$	0	$H_{12}-5\cdot 3^{1/2}B$	0	$3B+C$	$H_{22}+2H_{44}-3B+4C$	$3B+C$	$\|10\rangle$
$-3(3/2)^{1/2}B$	$-3(3/2)^{1/2}B$	$B+C$	$3^{1/2}B$	0	0	$H_{12}+5\cdot 3^{1/2}B$	$3B+C$	$3B+C$	$H_{22}+2H_{55}-3B+4C$	$\|11\rangle$

Table II – continued

$$
{}^4A_2:\begin{vmatrix} H_{11}+H_{22}+H_{33}-12B & 6B & 0 \\ 6B & H_{11}+H_{44}+H_{55}-3B & H_{12} \\ 0 & H_{12} & H_{22}+H_{44}+H_{55}-15B \end{vmatrix}\begin{matrix}|12\rangle\\|13\rangle\\|14\rangle\end{matrix}
$$

$$
{}^2A_2:\begin{vmatrix}
H_{11}+H_{22}+H_{33}+3C & 0 & 6B & 0 & 0 & -3B & (3/2)^{1/2}H_{12} & (3/2)^{1/2}H_{12} & (3/2)\cdot 2^{1/2}B & -(3/2)\cdot 2^{1/2}B \\
0 & H_{11}+H_{22}+H_{33}-8B+3C & 0 & 0 & 0 & -3^{1/2}B & -2^{-1/2}H_{12} & -2^{-1/2}H_{12} & -(3/2)^{1/2}B & (3/2)^{1/2}B \\
6B & 0 & H_{11}+H_{44}+H_{55}+3C & 0 & H_{12} & -3B & 0 & 0 & (3/2)\cdot 2^{1/2}B & -(3/2)\cdot 2^{1/2}B \\
0 & 0 & 0 & H_{11}+H_{44}+H_{55}+4B+3C & -3B & H_{12} & -6^{1/2}B & 0 & -5(3/2)^{1/2}B & -5(3/2)^{1/2}B \\
0 & 0 & H_{12} & -3B & H_{22}+H_{44}+H_{55}-6B+3C & 0 & 0 & 3\cdot 6^{1/2}B & 3(3/2)^{1/2}B & 3(3/2)^{1/2}B \\
-3B & -3^{1/2}B & -3B & H_{12} & 0 & H_{22}+H_{44}+H_{55}-6B+3C & 0 & 0 & -(3/2)\cdot 2^{1/2}B & (3/2)\cdot 2^{1/2}B \\
(3/2)^{1/2}H_{12} & -2^{1/2}H_{12} & 0 & -6^{1/2}B & 0 & 0 & 2H_{11}+H_{33}-8B+4C & 4B+C & B+C & B+C \\
(3/2)^{1/2}H_{12} & -2^{-1/2}H_{12} & 0 & 0 & 3\cdot 6^{1/2} & 0 & 4B+C & 2H_{22}+H_{33}+12B+4C & 3B+C & 3B+C \\
(3/2)\cdot 2^{1/2}B & -(3/2)^{1/2}B & (3/2)\cdot 2^{1/2}B & -5(3/2)^{1/2}B & 3(3/2)^{1/2}B & -(3/2)2^{1/2}B & B+C & 3B+C & H_{33}+2H_{44}-3B+4C & 3B+C \\
-(3/2)\cdot 2^{1/2}B & (3/2)^{1/2}B & -(3/2)\cdot 2^{1/2}B & -5(3/2)^{1/2} & 3(3/2)^{1/2}B & (3/2)\cdot 2^{1/2}B & B+C & 3B+C & 3B+C & H_{33}+2H_{55}-3B+4C
\end{vmatrix}\begin{matrix}|15\rangle\\|16\rangle\\|17\rangle\\|18\rangle\\|19\rangle\\|20\rangle\\|21\rangle\\|22\rangle\\|23\rangle\\|24\rangle\end{matrix}
$$

Table II – continued

$^4B_1$:

$$\begin{vmatrix} H_{11}+H_{22}+H_{44}-12B & 3B & 3\cdot 3^{1/2}B \\ 3B & H_{11}+H_{33}+H_{55}-12B & H_{12}+3\cdot 3^{1/2}B \\ 3\cdot 3^{1/2}B & H_{12}+3\cdot 3^{1/2}B & H_{22}+H_{33}+H_{55}-6B \end{vmatrix}$$

$|25\rangle$ $|26\rangle$ $|27\rangle$

$^2B_1$:

$$\begin{vmatrix} H_{11}+H_{22}+H_{44}-9/2B+3C & -(3/2)\cdot 3^{1/2}B & 3B & 0 & -(3/2)\cdot 3^{1/2}B & (3/2)B & (3/2)^{1/2}H_{12}-(9/2)\cdot 2^{1/2}B & -(3/2)^{1/2}H_{12}-3\cdot 2^{1/2}B & 0 & -(3/2)\cdot 2^{1/2}B \\ -(3/2)\cdot 3^{1/2}B & H_{11}+H_{22}+H_{44}-7/2B+3C & 0 & -3B & (9/2)B & (1/2)\cdot 3^{1/2}B & -2^{-1/2}H_{12}+(3/2)^{1/2}B & -2^{-1/2}H12_B+2\cdot 6^{1/2} & 0 & (3/2)^{1/2}B \\ 3B & 0 & H_{11}+H_{33}+H_{55}-9/2B+3C & -(3/2)\cdot 3^{1/2}B & H_{12}+(3/2)\cdot 3^{1/2}B & -(3/2)B & -(9/2)\cdot 2^{1/2}B & 0 & -3\cdot 2^{1/2}B & -(3/2)2^{1/2}B \\ 0 & -3B & -(3/2)\cdot 3^{1/2}B & H_{11}+H_{33}+H_{55}-(7/2)B+3C & -(3/2)B & H_{12}+(5/2)\cdot 3^{1/2}B & (3/2)^{1/2}B & 0 & 2\cdot 6^{1/2}B & (3/2)^{1/2}B \\ -(3/2)\cdot 3^{1/2}B & (9/2)B & H_{12}+(3/2)\cdot 3^{1/2}B & -(3/2)B & H_{22}+H_{33}+H_{55}-(3/2)B+3C & (3/2)\cdot 3^{1/2}B & 0 & 3(3/2)^{1/2}B & 0 & 3(3/2)^{1/2}B \\ (3/2)B & (1/2)\cdot 3^{1/2}B & -(3/2)B & H_{12}+(5/2)\cdot 3^{1/2}B & (3/2)\cdot 3^{1/2}B & H_{22}+H_{33}+H_{55}+(3/2)B+C & 0 & (3/2)\cdot 2^{1/2}B & 3\cdot 2^{1/2}B & (9/2)\cdot 2^{1/2}B \\ (3/2)^{1/2}H_{12}-(9/2)\cdot 2^{1/2}B & -2^{-1/2}H_{12}+(3/2)^{1/2}B & -(9/2)\cdot 2^{1/2}B & (3/2)^{1/2}B & 0 & 0 & 2H_{11}+H_{44}+7B+4C & 4B+C & 4B+C & B+C \\ -(3/2)^{1/2}H_{12}-3\cdot 2^{1/2}B & -2^{-1/2}H_{12}+2\cdot 6^{1/2}B & 0 & 0 & 3(3/2)^{1/2}B & (3/2)\cdot 2^{1/2}B & 4B+C & 2H_{22}+H_{44}-3B+4C & C & 3B+C \\ 0 & 0 & -3\cdot 2^{1/2}B & 2\cdot 6^{1/2}B & 0 & 3\cdot 2^{1/2}B & 4B+C & C & 2H_{33}+H_{44}-3B+4C & 3B+C \\ -(3/2)2^{1/2}B & (3/2)^{1/2}B & -(3/2)2^{1/2}B & (3/2)^{1/2}B & 3(3/2)^{1/2}B & (9/2)\cdot 2^{1/2} & B+C & 3B+C & 3B+C & H_{44}+2H_{55}-3B+4C \end{vmatrix}$$

$|28\rangle$ $|29\rangle$ $|30\rangle$ $|31\rangle$ $|32\rangle$ $|33\rangle$ $|34\rangle$ $|35\rangle$ $|36\rangle$ $|37\rangle$

Table II – continued

$^4B_2$:

$$\begin{vmatrix} H_{11}+H_{22}+H_{55}-12B & -3B & 3\cdot3^{1/2}B \\ -3B & H_{11}+H_{33}+H_{44}-12B & H_{12}-3\cdot3^{1/2}B \\ 3\cdot3^{1/2}B & H_{12}-3\cdot3^{1/2}B & H_{22}+H_{33}+H_{44}-6B \end{vmatrix} \begin{matrix} |38\rangle \\ |39\rangle \\ |40\rangle \end{matrix}$$

$^2B_2$:

$$\begin{vmatrix} H_{11}+H_{22}+H_{55}-(9/2)B+3C & -(3/2)\cdot3^{1/2}B & -3B & 0 & -(3/2)\cdot3^{1/2}B & (3/2)B & (3/2)^{1/2}H_{12}+(9/2)\cdot2^{1/2}B & (3/2)^{1/2}H_{12}+3\cdot2^{1/2}B & 0 & (3/2)\cdot2^{1/2}B \\ -(3/2)\cdot3^{1/2}B & H_{11}+H_{22}+H_{55}-(7/2)B+3C & 0 & 3B & (9/2)B & (1/2)\cdot3^{1/2}B & -2^{-1/2}H_{12}-(3/2)^{1/2}B & -2^{-1/2}H_{12}-2\cdot6^{1/2}B & 0 & -(3/2)^{1/2}B \\ -3B & 0 & H_{11}+H_{33}+H_{44}-(9/2)B+3C & -(3/2)\cdot3^{1/2}B & H_{12}-(3/2)\cdot3^{1/2}B & (3/2)B & -(9/2)\cdot2^{1/2}B & 0 & -3\cdot2^{1/2}B & -(3/2)\cdot2^{1/2}B \\ 0 & 3B & -(3/2)\cdot3^{1/2}B & H_{11}+H_{33}+H_{44}-(7/2)B+3C & (3/2)B & H_{12}-(5/2)\cdot3^{1/2}B & (3/2)^{1/2}B & 0 & 2\cdot6^{1/2}B & (3/2)^{1/2}B \\ -(3/2)\cdot3^{1/2}B & (9/2)B & H_{12}-(3/2)\cdot3^{1/2}B & (3/2)B & H_{22}+H_{33}+H_{44}-(3/2)B+3C & (3/2)\cdot3^{1/2}B & 0 & -3(3/2)^{1/2}B & 0 & -3(3/2)^{1/2}B \\ (3/2)B & (1/2)\cdot3^{1/2}B & (3/2)B & H_{12}-(5/2)\cdot3^{1/2}B & (3/2)\cdot3^{1/2}B & H_{22}+H_{33}+H_{44}+(3/2)B+3C & 0 & -(3/2)\cdot2^{1/2}B & -3\cdot2^{1/2}B & -(9/2)\cdot2^{1/2}B \\ (3/2)^{1/2}H_{12}+(9/2)\cdot2^{1/2}B & -2^{-1/2}H_{12}-(3/2)^{1/2}B & -(9/2)\cdot2^{1/2}B & (3/2)^{1/2}B & 0 & 0 & 2H_{11}+H_{55}+7B+4C & 4B+C & 4B+C & B+C \\ (3/2)^{1/2}H_{12}+3\cdot2^{1/2}B & -2^{1/2}H_{12}-2\cdot6^{1/2}B & 0 & 0 & -3(3/2)^{1/2}B & -(3/2)\cdot2^{1/2}B & 4B+C & 2H_{22}+H_{55}-3B+4C & C & 3B+C \\ 0 & 0 & -3\cdot2^{1/2}B & 2\cdot6^{1/2}B & 0 & -3\cdot2^{1/2}B & 4B+C & C & 2H_{33}+H_{55}-3B+4C & 3B+C \\ (3/2)\cdot2^{1/2}B & -(3/2)^{1/2}B & -(3/2)\cdot2^{1/2}B & (3/2)^{1/2}B & -3(3/2)^{1/2}B & -(9/2)\cdot2^{1/2}B & B+C & 3B+C & 3B+C & 2H_{44}+H_{55}-3B+4C \end{vmatrix} \begin{matrix} |41\rangle \\ |42\rangle \\ |43\rangle \\ |44\rangle \\ |45\rangle \\ |46\rangle \\ |47\rangle \\ |48\rangle \\ |49\rangle \\ |50\rangle \end{matrix}$$

Table III Simplified designation for d^4 strong-field terms $\left|(\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k}\gamma_l^{n_l})^{2S+1}\Gamma, M_S\right\rangle$

Γ	$\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k}\gamma_l^{n_l}$	Designation			Γ	$\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k}\gamma_l^{n_l}$	Designation		
		$^5\Gamma$	$^3\Gamma$	$^1\Gamma$			$^5\Gamma$	$^3\Gamma$	$^1\Gamma$
A_1	$(a_1(z^2))^1a_2^1b_1^1b_2^1$	1	$3^{(a)}$	$12^{(a)}$	B_1	$(a_1(z^2))^1(a_1(x^2-y^2))^1a_2^1b_2^1$	53	$54^{(a)}$	$66^{(a)}$
			$4^{(b)}$	$13^{(b)}$				$55^{(b)}$	$67^{(b)}$
			$5^{(c)}$					$56^{(c)}$	
	$(a_1(x^2-y^2))^1a_2^1b_1^1b_2^1$	2	$6^{(a)}$	$14^{(a)}$		$(a_1(z^2))^2(a_1(x^2-y^2))^1b_1^1$		57	68
			$7^{(b)}$	$15^{(b)}$		$(a_1(z^2))^2a_2^1b_2^1$		58	69
			$8^{(c)}$			$(a_1(z^2))^1(a_1(x^2-y^2))^2b_1^1$		59	70
	$(a_1(z^2))^1(a_1(x^2-y^2))^1a_2^2$		9	16		$(a_1(x^2-y^2))^2a_2^1b_2^1$		60	71
	$(a_1(z^2))^1(a_1(x^2-y^2))^1b_1^2$		10	17		$(a_1(z^2))^1a_2^2b_1^1$		61	72
	$(a_1(z^2))^1(a_1(x^2-y^2))^1b_2^2$		11	18		$(a_1(x^2-y^2))^1a_2^2b_1^1$		62	73
	$(a_1(z^2))^2(a_1(x^2-y^2))^2$			19		$a_2^1b_1^2b_2^1$		63	74
	$(a_1(z^2))^2a_2^2$			20		$(a_1(z^2))^1b_1^1b_2^2$		64	75
	$(a_1(z^2))^2b_1^2$			21		$(a_1(x^2-y^2))^1b_1^1b_2^2$		65	76
	$(a_1(z^2))^2b_2^2$			22					
	$(a_1(x^2-y^2))^2a_2^2$			23	B_2	$(a_1(z^2))^1(a_1(x^2-y^2))^1a_2^1b_1^1$	77	$78^{(a)}$	$90^{(a)}$
	$(a_1(x^2-y^2))^2b_1^2$			24				$79^{(b)}$	$91^{(b)}$
	$(a_1(x^2-y^2))^2b_2^2$			25				$80^{(c)}$	

Table III – Continued

Γ	$\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k}\gamma_l^{n_l}$	Designation			Γ	$\gamma_i^{n_i}\gamma_j^{n_j}\gamma_k^{n_k}\gamma_l^{n_l}$	Designation		
		$^5\Gamma$	$^3\Gamma$	$^1\Gamma$			$^5\Gamma$	$^3\Gamma$	$^1\Gamma$
	$a_2^2b_1^2$			26		$(a_1(z^2))^2(a_1(x^2-y^2))^1b_2^1$		81	92
	$a_2^2b_2^2$			27		$(a_1(z^2))^2a_2^1b_1^1$		82	93
	$b_1^2b_2^2$			28		$(a_1(z^2))^1(a_1(x^2-y^2))^2b_2^1$		83	94
						$(a_1(x^2-y^2))^2a_2^1b_1^1$		84	95
A_2	$(a_1(z^2))^1(a_1(x^2-y^2))^1b_1^1b_2^1$	29	30[a]	42[a]		$(a_1(z^2))^1a_2^2b_2^1$		85	96
			31[b]	43[b]		$(a_1(x^2-y^2))^1a_2^2b_2^1$		86	97
			32[c]			$(a_1(z^2))^1b_1^2b_2^1$		87	98
	$(a_1(z^2))^2(a_1(x^2-y^2))^1a_2^1$		33	44		$(a_1(x^2-y^2))^1b_1^2b_2^1$		88	99
	$(a_1(z^2))^2b_1^1b_2^1$		34	45		$a_2^1b_1^1b_2^2$		89	100
	$(a_1(z^2))^1(a_1(x^2-y^2))^2a_2^1$		35	46					
	$(a_1(x^2-y^2))^2b_1^1b_2^1$		36	47					
	$a_2^2b_1^1b_2^2$		37	48					
	$(a_1(z^2))^1a_2^1b_1^2$		38	49					
	$(a_1(x^2-y^2))^1a_2^1b_1^2$		39	50					
	$(a_1(z^2))^1a_2^1b_2^2$		40	51					
	$(a_1(x^2-y^2))^1a_2^1b_2^2$		41	52					

Table IV Strong-field energy matrices for d^4 bent metallocene complexes

$^5A_1$:

$$\begin{vmatrix} H_{11}+H_{33}+H_{44}+H_{55}-21B & H_{12} \\ H_{12} & H_{22}+H_{33}+H_{44}+H_{55}-21B \end{vmatrix} \begin{matrix} |1\rangle \\ |2\rangle \end{matrix}$$

$^3A_1$:

$$\begin{vmatrix} H_{11}+H_{33}+H_{44}+H_{55}-13B+4C & -2\cdot 2^{1/2}B & 0 & H_{12} & 0 & -2(3/2)^{1/2}B & -6B & -3B & -3B \\ -2\cdot 2^{1/2}B & H_{11}+H_{33}+H_{44}+H_{55}-9B+4C & 0 & 0 & H_{12} & -3^{1/2}B & 3\cdot 2^{1/2}B & (3/2)\cdot 2^{1/2}B & (3/2)\cdot 2^{1/2}B \\ 0 & 0 & H_{11}+H_{33}+H_{44}+H_{55}-11B+4C & -2(3/2)^{1/2}B & -3^{1/2}B & H_{12} & 0 & (3/2)\cdot 2^{1/2}B & -(3/2)\cdot 2^{1/2}B \\ H_{12} & 0 & -2(3/2)^{1/2}B & H_{22}+H_{33}+H_{44}+H_{55}-9B+4C & 0 & 0 & 0 & -3^{1/2}B & 3^{1/2}B \\ 0 & H_{12} & -3^{1/2}B & 0 & H_{22}+H_{33}+H_{44}+H_{55}-15B+4C & 0 & 0 & (3/2)^{1/2}B & -(3/2)^{1/2}B \\ -2(3/2)^{1/2}B & -3^{1/2}B & H_{12} & 0 & 0 & H_{22}+H_{33}+H_{44}+H_{55}-9B+4C & 2(3/2)^{1/2}B & 5(3/2)^{1/2}B & 5(3/2)^{1/2}B \\ -6B & 3\cdot 2^{1/2} & 0 & 0 & 0 & 2(3/2)^{1/2}B & H_{11}+H_{22}+2H_{33}-8B+5C & 3B+C & 3B+C \\ -3B & (3/2)\cdot 2^{1/2}B & (3/2)\cdot 2^{1/2}B & -3^{1/2}B & (3/2)^{1/2}B & 5(3/2)^{1/2}B & 3B+C & H_{11}+H_{22}+2H_{44}-8B+5C & 3B+C \\ -3B & (3/2)\cdot 2^{1/2}B & -(3/2)\cdot 2^{1/2}B & 3^{1/2}B & -(3/2)^{1/2}B & 5(3/2)^{1/2}B & 3B+C & 3B+C & H_{11}+H_{22}+2H_{55}-8B+5C \end{vmatrix} \begin{matrix} |3\rangle \\ |4\rangle \\ |5\rangle \\ |6\rangle \\ |7\rangle \\ |8\rangle \\ |9\rangle \\ |10\rangle \\ |11\rangle \end{matrix}$$

Table IV – continued

^{1}A:

$H_{11}+H_{33}+H_{44}+H_{55}-(15/2)B+6C$	$-(3/2)\cdot3^{1/2}B$	$H_{12}-(3/2)\cdot3^{1/2}B$	$(3/2)B$	$-(9/2)\cdot2^{1/2}B$	$-3\cdot2^{1/2}B$	$-(3/2)\cdot2^{1/2}B$	0	$3^{1/2}B$	$4\cdot3^{1/2}B$	$3^{1/2}B$	0	0	0	$3^{1/2}B$	$4\cdot3^{1/2}B$	$3^{1/2}B$	|12)
$-(3/2)\cdot3^{1/2}B$	$H_{11}+H_{33}+H_{44}+H_{55}-(9/2)B+6C$	$(3/2)B$	$H_{12}+(3/2)\cdot3^{1/2}B$	$-3(3/2)^{1/2}B$	0	$-3(3/2)^{1/2}B$	0	$-3B$	$-6B$	$-9B$	0	0	0	$-9B$	$-6B$	$-3B$	|13)
$H_{12}-(3/2)\cdot3^{1/2}B$	$(3/2)B$	$H_{22}+H_{33}+H_{44}+H_{55}-(9/2)B+6C$	$(3/2)\cdot3^{1/2}B$	$(3/2)^{1/2}B$	$2\cdot6^{1/2}B$	$(3/2)^{1/2}B$	0	0	0	0	$-9B$	$-6B$	$-3B$	$-3B$	$-6B$	$-9B$	|14)
$(3/2)B$	$H_{12}+(3/2)\cdot3^{1/2}B$	$(3/2)\cdot3^{1/2}B$	$H_{22}+H_{33}+H_{44}+H_{55}-(15/2)B+6C$	$-(3/2)\cdot2^{1/2}B$	$-3\cdot2^{1/2}B$	$-(9/2)\cdot2^{1/2}B$	0	0	0	0	$-3\cdot3^{1/2}B$	0	$-3\cdot3^{1/2}B$	$-3\cdot3^{1/2}B$	0	$-3\cdot3^{1/2}B$	|15)
$-(9/2)\cdot2^{1/2}B$	$-3(3/2)^{1/2}B$	$(3/2)^{1/2}B$	$-(3/2)\cdot2^{1/2}B$	$H_{11}+H_{22}+2H_{33}+7C$	$3B+C$	$3B+C$	0	$2^{1/2}H_{12}$	0	0	$2^{1/2}H_{12}$	0	0	$6^{1/2}B$	$-6^{1/2}B$	0	|16)
$-3\cdot2^{1/2}B$	0	$2\cdot6^{1/2}B$	$-3\cdot2^{1/2}B$	$3B+C$	$H_{11}+H_{22}+2H_{44}+7C$	$3B+C$	$-6^{1/2}B$	0	$2^{1/2}H_{12}-5\cdot6^{1/2}B$	0	0	$2^{1/2}H_{12}-5\cdot6^{1/2}B$	0	0	0	$-6^{1/2}B$	|17)
$-(3/2)\cdot2^{1/2}B$	$-3(3/2)^{1/2}B$	$(3/2)^{1/2}$	$-(9/2)\cdot2^{1/2}B$	$3B+C$	$3B+C$	$H_{11}+H_{22}$ $2H_{55}+7C$	$6^{1/2}B$	0	0	$2^{1/2}H_{12}+5\cdot6^{1/2}B$	0	0	$2^{1/2}H_{12}+5\cdot6^{1/2}B$	0	0	$6^{1/2}B$	|18)
0	0	0	0	0	$-6^{1/2}B$	$6^{1/2}B$	$2H_{11}+2H_{22}-16B+8C$	C	$3B+C$	$3B+C$	$4B+C$	$B+C$	$B+C$	0	0	0	|19)
$3^{1/2}B$	$-3B$	0	0	$2^{1/2}H_{12}$	0	0	C	$2H_{11}+2H_{33}-16B+8C$	$3B+C$	$3B+C$	$4B+C$	0	0	$B+C$	$B+C$	0	|20)
$4\cdot3^{1/2}B$	$-6B$	0	0	0	$2^{1/2}H_{12}-5\cdot6^{1/2}B$	0	$3B+C$	$3B+C$	$2H_{11}+2H_{44}+14B+8C$	$3B+C$	0	$4B+C$	0	$4B+C$	0	$B+C$	|21)
$3^{1/2}B$	$-9B$	0	0	0	0	$2^{1/2}H_{12}+5\cdot6^{1/2}B$	$3B+C$	$3B+C$	$3B+C$	$2H_{11}+2H_{55}+14B+8C$	0	0	$4B+C$	0	$4B+C$	$B+C$	|22)
0	0	$-9B$	$-3\cdot3^{1/2}$	$2^{1/2}H_{12}$	0	0	$4B+C$	$4B+C$	0	0	$2H_{22}+2H_{33}+24B+8C$	$3B+C$	$3B+C$	$3B+C$	$3B+C$	0	|23)
0	0	$-6B$	0	0	$2^{1/2}H_{12}-5\cdot6^{1/2}B$	0	$B+C$	0	$4B+C$	0	$3B+C$	$2H_{22}+2H_{44}-6B+8C$	$3B+C$	C	0	$3B+C$	|24)
0	0	$-3B$	$-3\cdot3^{1/2}B$	0	0	$2^{1/2}H_{12}+5\cdot6^{1/2}B$	$B+C$	0	0	$4B+C$	$3B+C$	$3B+C$	$2H_{22}+2H_{55}-6B+8C$	0	C	$3B+C$	|25)
$3^{1/2}B$	$-9B$	$-3B$	$-3\cdot3^{1/2}B$	$6^{1/2}B$	0	0	0	$B+C$	$4B+C$	0	$3B+C$	C	0	$2H_{33}+2H_{44}-6B+8C$	$3B+C$	$3B+C$	|26)
$4\cdot3^{1/2}B$	$-6B$	$-6B$	0	$-6^{1/2}B$	0	0	0	$B+C$	0	$4B+C$	$3B+C$	0	C	$3B+C$	$2H_{33}+2H_{55}-6B+8C$	$3B+C$	|27)
$3^{1/2}B$	$-3B$	$-9B$	$-3\cdot3^{1/2}B$	0	$-6^{1/2}B$	$6^{1/2}B$	0	0	$B+C$	$B+C$	0	$3B+C$	$3B+C$	$3B+C$	$3B+C$	$2H_{44}+2H_{55}-6B+8C$	|28)

Table IV – Continued

$^1A_2$: $\begin{vmatrix} H_{11}+H_{22}+H_{44} \\ +H_{55}-21B \end{vmatrix}$ |29⟩

$^3A_2$:

$$\begin{vmatrix}
H_{11}+H_{22}+H_{44} \\ +H_{55}-13B+4C & -2\cdot 2^{1/2}B & 0 & 0 & 0 & 6B & 0 & 0 & 3B & -3^{1/2}B & 3B & 3^{1/2}B \\
-2\cdot 2^{1/2}B & H_{11}+H_{22}+H_{44} \\ +H_{55}-9B+4C & 0 & 0 & 2^{1/2}H_{12} & -3\cdot 2^{1/2}B & 2^{1/2}H_{12} & 0 & -(3/2)\cdot 2^{1/2}B & -(3/2)^{1/2}B & -(3/2)\cdot 2^{1/2}B & (3/2)^{1/2}B \\
0 & 0 & H_{11}+H_{22}+H_{44} \\ +H_{55}-11B+4C & 6^{1/2}B & 6^{1/2}B & 0 & -6^{1/2}B & 0 & -(3/2)\cdot 2^{1/2}B & 5\cdot(3/2)^{1/2}B & (3/2)\cdot 2^{1/2}B & 5\cdot(3/2)^{1/2}B \\
0 & 0 & 6^{1/2}B & 2H_{11}+H_{22} \\ +H_{33}-16B+5C & 6B & -H_{12} & 0 & 0 & -3^{1/2}B & B+C & 3^{1/2}B & B+C \\
0 & 2^{1/2}H_{12} & 6^{1/2}B & 6B & 2H_{11}+H_{44} \\ +H_{55}+5B+5C & 0 & 4B+C & 4B+C & -3^{1/2}B & 0 & 3^{1/2}B & 0 \\
6B & -3\cdot 2^{1/2}B & 0 & -H_{12} & 0 & H_{11}+2H_{22} \\ +H_{33}-8B+5C & 0 & 0 & 3B+C & -3^{1/2}B & 3B+C & 3^{1/2}B \\
0 & 2^{1/2}H_{12} & -6^{1/2}B & 0 & 4B+C & 0 & 2H_{22}+H_{44} \\ +H_{55}-15B+5C & C & 0 & -3B & 0 & -3B \\
0 & 0 & 0 & 0 & 4B+C & 0 & C & 2H_{33}+H_{44} \\ +H_{55}-15B+5C & 3^{1/2}B & -3B & -3^{1/2}B & -3B \\
3B & -(3/2)\cdot 2^{1/2}B & -(3/2)\cdot 2^{1/2}B & -3^{1/2}B & -3^{1/2}B & 3B+C & 0 & 3^{1/2}B & H_{11}+H_{33} \\ +2H_{44}-8B+5C & H_{12}-5\cdot 3^{1/2}B & 3B+C & 0 \\
-3^{1/2}B & -(3/2)^{1/2}B & 5\cdot(3/2)^{1/2}B & B+C & 0 & -3^{1/2}B & -3B & -3B & H_{12}-5\cdot 3^{1/2}B & H_{22}+H_{33} \\ +2H_{44}-6B+5C & 0 & 3B+C \\
3B & -(3/2)\cdot 2^{1/2}B & (3/2)\cdot 2^{1/2}B & 3^{1/2}B & 3^{1/2}B & 3B+C & 0 & -3^{1/2}B & 3B+C & 0 & H_{11}+H_{33} \\ +2H_{55}-8B+5C & H_{12}+5\cdot 3^{1/2}B \\
3^{1/2}B & (3/2)^{1/2}B & 5\cdot(3/2)^{1/2}B & B+C & 0 & 3^{1/2}B & -3B & -3B & 0 & 3B+C & H_{12}+5\cdot 3^{1/2}B & H_{22}+H_{33} \\ +2H_{55}-6B+5C
\end{vmatrix}$$

|30⟩ |31⟩ |32⟩ |33⟩ |34⟩ |35⟩ |36⟩ |37⟩ |38⟩ |39⟩ |40⟩ |41⟩

Table IV – Continued

$$
{}^{1}A_2:\quad
\begin{vmatrix}
H_{11}+H_{22}+H_{44}+H_{55}-(15/2)B+6C & -(3/2)\cdot 3^{1/2}B & (3/2)^{1/2}B & -2^{-1/2}H_{12}-3\cdot(3/2)^{1/2}B & 9\cdot 2^{-1/2}B & -2^{-1/2}H_{12}+3\cdot(3/2)^{1/2}B & 0 & 3\cdot 2^{1/2}B & (3/2)^{1/2}B & 3\cdot 2^{-1/2}B & 2\cdot 6^{1/2}B \\
-(3/2)\cdot 3^{1/2}B & H_{11}+H_{22}+H_{44}+H_{55}-(9/2)B+6C & -3\cdot 2^{-1/2}B & (3/2)^{1/2}H_{12}-3\cdot 2^{-1/2}B & 3\cdot(3/2)^{1/2}B & (3/2)^{1/2}H_{12}+3\cdot 2^{-1/2}B & 0 & 0 & -9\cdot 2^{-1/2}B & 3\cdot(3/2)^{1/2}B & -3\cdot 2^{1/2}B \\
(3/2)^{1/2}B & -3\cdot 2^{-1/2}B & 2H_{11}+H_{22}\ H_{33}-16B+7C & 0 & -H_{12} & 0 & 0 & -3^{1/2}B & B+C & 3^{1/2}B & B+C \\
-2^{-1/2}H_{12}-3\cdot(3/2)^{1/2}B & (3/2)^{1/2}H_{12}-3\cdot 2^{-1/2}B & 0 & 2H_{11}+H_{44}+H_{55}+11B+7C & 0 & 4B+C & 4B+C & -5\cdot 3^{1/2}B & 0 & -5\cdot 3^{1/2}B & 0 \\
9\cdot 2^{-1/2}B & 3\cdot(3/2)^{1/2}B & -H_{12} & 0 & H_{11}+2H_{22}+H_{33}+7C & 2\cdot 3^{1/2}B & 0 & 3B+C & -3^{1/2}B & 3B+C & 3^{1/2}B \\
-2^{-1/2}H_{12}+3\cdot(3/2)^{1/2}B & (3/2)^{1/2}H_{12}+3\cdot 2^{-1/2}B & 0 & 4B+C & 2\cdot 3^{1/2}B & 2H_{22}+H_{44}+H_{55}-9B+7C & C & 0 & -3B & 0 & 3B \\
0 & 0 & 0 & 4B+C & 0 & C & 2H_{33}+H_{44}+H_{55}-9B+7C & -5\cdot 3^{1/2}B & 3B & -5\cdot 3^{1/2}B & -3B \\
3\cdot 2^{1/2}B & 0 & -3^{1/2}B & -5\cdot 3^{1/2}B & 3B+C & 0 & -5\cdot 3^{1/2}B & H_{11}+H_{33}\ 2H_{44}+7C & H_{12}-5\cdot 3^{1/2}B & 3B+C & 0 \\
(3/2)^{1/2}B & -9\cdot 2^{-1/2}B & B+C & 0 & -3^{1/2}B & -3B & 3B & H_{12}-5\cdot 3^{1/2}B & H_{22}+H_{33}+2H_{44}-6B+7C & 0 & 3B+C \\
3\cdot 2^{-1/2}B & 3\cdot(3/2)^{1/2}B & 3^{1/2}B & -5\cdot 3^{1/2}B & 3B+C & 0 & -5\cdot 3^{1/2}B & 3B+C & 0 & H_{11}+H_{33}+2H_{55}+7C & H_{12}+5\cdot 3^{1/2}B \\
2\cdot 6^{1/2}B & -3\cdot 2^{1/2}B & B+C & 0 & 3^{1/2}B & 3B & -3B & 0 & 3B+C & H_{12}+5\cdot 3^{1/2}B & H_{22}+H_{33}+2H_{55}-6B+7C
\end{vmatrix}
\quad \begin{matrix} |42\rangle \\ |43\rangle \\ |44\rangle \\ |45\rangle \\ |46\rangle \\ |47\rangle \\ |48\rangle \\ |49\rangle \\ |50\rangle \\ |51\rangle \\ |52\rangle \end{matrix}
$$

$$
{}^{5}B_1:\quad \begin{vmatrix} H_{11}+H_{22}+H_{33}+H_{55}-21B \end{vmatrix} \quad |53\rangle
$$

Table IV – Continued

$^3B_1$:

$H_{11}+H_{22}+H_{33}+H_{55}-13B+4C$	$2^{1/2}B$	0	$3\cdot3^{1/2}B$	$3^{1/2}B$	$3B$	$-3^{1/2}B$	0	$2\cdot3^{1/2}B$	0	$3B$	$3^{1/2}B$	|54⟩
$2^{1/2}B$	$H_{11}+H_{22}+H_{33}+H_{55}-9B+4C$	$-3B$	$3\cdot(3/2)^{1/2}B$	$2^{1/2}H_{12}+5\cdot(3/2)^{1/2}B$	$-3\cdot2^{-1/2}B$	$2^{1/2}H_{12}+5\cdot(3/2)^{1/2}B$	0	$6^{1/2}B$	$6^{1/2}B$	$-3\cdot2^{-1/2}B$	$(3/2)^{1/2}B$	|55⟩
0	$-3B$	$H_{11}+H_{22}+H_{33}+H_{55}-11B+4C$	$-(3/2)^{1/2}B$	$(3/2)^{1/2}B$	$3\cdot2^{-1/2}B$	$-(3/2)^{1/2}B$	$3\cdot2^{1/2}B$	$-2\cdot6^{1/2}B$	0	$9\cdot2^{-1/2}B$	$-(3/2)^{1/2}B$	|56⟩
$3\cdot3^{1/2}B$	$3\cdot(3/2)^{1/2}B$	$-(3/2)^{1/2}B$	$2H_{11}+H_{22}+H_{44}-10B+5C$	$3B$	$-H_{12}+2\cdot3^{1/2}B$	0	0	$4B+C$	0	$3^{1/2}B$	$B+C$	|57⟩
$3^{1/2}B$	$2^{1/2}H_{12}+5\cdot(3/2)^{1/2}B$	$(3/2)^{1/2}B$	$3B$	$2H_{11}+H_{33}+H_{55}-10B+5C$	0	$4B+C$	$2\cdot3^{1/2}B$	0	$B+C$	$3^{1/2}B$	0	|58⟩
$3B$	$-3\cdot2^{-1/2}B$	$3\cdot2^{-1/2}B$	$-H_{12}+2\cdot3^{1/2}B$	0	$H_{11}+2H_{22}+H_{44}-14B+5C$	$-3\cdot3^{1/2}B$	C	0	0	$3B+C$	$3^{1/2}B$	|59⟩
$-3^{1/2}B$	$2^{1/2}H_{12}+5\cdot(3/2)^{1/2}B$	$-(3/2)^{1/2}B$	0	$4B+C$	$-3\cdot3^{1/2}B$	$2H_{22}+H_{33}+H_{55}+5C$	0	0	$3B+C$	0	$-3B$	|60⟩
0	0	$3\cdot2^{1/2}$	0	$2\cdot3^{1/2}B$	C	0	$H_{11}+2H_{33}H_{44}-14B+5C$	$H_{12}-3\cdot3^{1/2}B$	$3^{1/2}B$	$3B+C$	0	|61⟩
$2\cdot3^{1/2}B$	$6^{1/2}B$	$-2\cdot6^{1/2}B$	$4B+C$	0	0	0	$H_{12}-3\cdot3^{1/2}B$	$H_{22}+2H_{33}+H_{44}+5C$	$-3B$	0	$3B+C$	|62⟩
0	$6^{1/2}B$	0	0	$B+C$	0	$3B+C$	$3^{1/2}B$	$-3B$	$H_{33}+2H_{44}+H_{55}-15B+5C$	$2\cdot3^{1/2}B$	0	|63⟩
$3B$	$-3\cdot2^{-1/2}B$	$9\cdot2^{-1/2}B$	$3^{1/2}B$	$3^{1/2}B$	$3B+C$	0	$3B+C$	0	$2\cdot3^{1/2}B$	$H_{11}+H_{44}+2H_{55}+B+5C$	$H_{12}+2\cdot3^{1/2}B$	|64⟩
$3^{1/2}B$	$(3/2)^{1/2}B$	$-(3/2)^{1/2}B$	$B+C$	0	$3^{1/2}B$	$-3B$	0	$3B+C$	0	$H_{12}+2\cdot3^{1/2}B$	$H_{22}+H_{44}+2H_{55}-15B+5C$	|65⟩

Table IV – Continued

$$
{}^{1}B_{1}:\begin{vmatrix}
H_{11}+H_{22}+H_{33}+H_{55}-12B+6C & 0 & 2\cdot6^{1/2}B & -2^{-1/2}H_{12}-2\cdot6^{1/2}B & 3\cdot2^{-1/2}B & -2^{-1/2}H_{12}-(3/2)^{1/2}B & -3\cdot2^{-1/2}B & (3/2)^{1/2}B & -(3/2)^{1/2}B & 0 & (3/2)^{1/2}B \\
0 & H_{11}+H_{22}+H_{33}+H_{55}+6C & 3\cdot2^{1/2}B & (3/2)^{1/2}H_{12}+3\cdot2^{1/2}B & 3\cdot(3/2)^{1/2}B & (3/2)^{1/2}H_{12}+9\cdot2^{-1/2}B & 3\cdot(3/2)^{1/2}B & 9\cdot2^{-1/2}B & 3\cdot2^{-1/2}B & 3\cdot6^{1/2}B & 3\cdot2^{-1/2}B \\
2\cdot6^{1/2}B & 3\cdot2^{1/2}B & 2H_{11}+H_{22}+H_{44}-4B+7C & -3B & -H_{12}+4\cdot3^{1/2}B & 0 & 0 & 4B+C & 0 & 3^{1/2}B & B+C \\
-2^{-1/2}H_{12}-2\cdot6^{1/2}B & (3/2)^{1/2}H_{12}+3\cdot2^{1/2}B & -3B & 2H_{11}+H_{33}+H_{55}-4B+7C & 0 & 4B+C & 4\cdot3^{1/2}B & 0 & B+C & 3^{1/2}B & 0 \\
3\cdot2^{-1/2}B & 3\cdot(3/2)^{1/2}B & -H_{12}+4\cdot3^{1/2}B & 0 & H_{11}+2H_{22}+H_{44}-12B+7C & -3^{1/2}B & C & 0 & 0 & 3B+C & 3^{1/2}B \\
-2^{-1/2}H_{12}-(3/2)^{1/2}B & (3/2)^{1/2}H_{12}+9\cdot2^{-1/2}B & 0 & 4B+C & -3^{1/2}B & 2H_{22}+H_{33}+H_{55}+6B+7C & 0 & 6B & 3B+C & 0 & 9B \\
-3\cdot2^{-1/2}B & 3\cdot(3/2)^{1/2}B & 0 & 4\cdot3^{1/2}B & C & 0 & H_{11}+2H_{33}+H_{44}-12B+7C & H_{12}-3^{1/2}B & 3^{1/2}B & 3B+C & 0 \\
(3/2)^{1/2}B & 9\cdot2^{-1/2}B & 4B+C & 0 & 0 & 6B & H_{12}-3^{1/2}B & H_{22}+2H_{33}+H_{44}+6B+7C & 9B & 0 & 3B+C \\
-(3/2)^{1/2}B & 3\cdot2^{-1/2}B & 0 & B+C & 0 & 3B+C & 3^{1/2}B & 9B & H_{33}+2H_{44}+H_{55}-9B+7C & 4\cdot3^{1/2}B & 6B \\
0 & 3\cdot6^{1/2}B & 3^{1/2}B & 3^{1/2}B & 3B+C & 0 & 3B+C & 0 & 4\cdot3^{1/2}B & H_{11}+H_{44}+2H_{55}+3B+7C & H_{12}+4\cdot3^{1/2}B \\
(3/2)^{1/2}B & 3\cdot2^{-1/2}B & B+C & 0 & 3^{1/2}B & 9B & 0 & 3B+C & 6B & H_{12}+4\cdot3^{1/2}B & H_{22}+H_{44}+2H_{55}-9B+7C
\end{vmatrix}
\begin{matrix}|66\rangle\\|67\rangle\\|68\rangle\\|69\rangle\\|70\rangle\\|71\rangle\\|72\rangle\\|73\rangle\\|74\rangle\\|75\rangle\\|76\rangle\end{matrix}
$$

$$
{}^{5}B_{2}:\begin{vmatrix} H_{11}+H_{22}+H_{33}+H_{44}-21B \end{vmatrix}|77\rangle
$$

Table IV – Continued

$^3B_2$:

$H_{11}+H_{22}+H_{33}+H_{44}-13B+4C$	$2^{1/2}B$	0	$3\cdot3^{1/2}B$	$-3^{1/2}B$	$-3B$	$3^{1/2}B$	0	$2\cdot3^{1/2}B$	$-3B$	$3^{1/2}B$	0	|78⟩
$2^{1/2}B$	$H_{11}+H_{22}+H_{33}+H_{44}-9B+4C$	$-3B$	$3\cdot(3/2)^{1/2}B$	$2^{1/2}H_{12}-5\cdot(3/2)^{1/2}B$	$3\cdot2^{-1/2}B$	$2^{1/2}H_{12}-5\cdot(3/2)^{1/2}B$	0	$6^{1/2}B$	$3\cdot2^{-1/2}B$	$(3/2)^{1/2}B$	$-6^{1/2}B$	|79⟩
0	$-3B$	$H_{11}+H_{22}+H_{33}+H_{44}-11B+4C$	$-(3/2)^{1/2}B$	$-(3/2)^{1/2}B$	$-3\cdot2^{-1/2}B$	$(3/2)^{1/2}B$	$-3\cdot2^{1/2}B$	$-2\cdot6^{1/2}B$	$-9\cdot2^{-1/2}B$	$-(3/2)^{1/2}B$	0	|80⟩
$3\cdot3^{1/2}B$	$3\cdot(3/2)^{1/2}B$	$-(3/2)^{1/2}B$	$2H_{11}+H_{22}+H_{55}-10B+5C$	$-3B$	$-H_{12}-2\cdot3^{1/2}B$	0	0	$4B+C$	$-3^{1/2}B$	$B+C$	0	|81⟩
$-3^{1/2}B$	$2^{1/2}H_{12}-5\cdot(3/2)^{1/2}B$	$-(3/2)^{1/2}B$	$-3B$	$2H_{11}+H_{33}+H_{44}-10B+5C$	0	$4B+C$	$2\cdot3^{1/2}B$	0	$3^{1/2}B$	0	$B+C$	|82⟩
$-3B$	$3\cdot2^{-1/2}B$	$-3\cdot2^{-1/2}B$	$-H_{12}-2\cdot3^{1/2}B$	0	$H_{11}+2H_{22}+H_{55}-14B+5C$	$-3\cdot3^{1/2}B$	C	0	$3B+C$	$-3^{1/2}B$	0	|83⟩
$3^{1/2}B$	$2^{1/2}H_{12}-5\cdot(3/2)^{1/2}B$	$(3/2)^{1/2}B$	0	$4B+C$	$-3\cdot3^{1/2}B$	$2H_{22}+H_{33}+H_{44}+5C$	0	0	0	$3B$	$3B+C$	|84⟩
0	0	$-3\cdot2^{1/2}B$	0	$2\cdot3^{1/2}B$	C	0	$H_{11}+2H_{33}+H_{55}-14B+5C$	$H_{12}+3\cdot3^{1/2}B$	$3B+C$	0	$3^{1/2}B$	|85⟩
$2\cdot3^{1/2}B$	$6^{1/2}B$	$-2\cdot6^{1/2}B$	$4B+C$	0	0	0	$H_{12}+3\cdot3^{1/2}B$	$H_{22}+2H_{33}+H_{55}+5C$	0	$3B+C$	$3B$	|86⟩
$-3B$	$3\cdot2^{-1/2}B$	$-9\cdot2^{-1/2}B$	$-3^{1/2}B$	$3^{1/2}B$	$3B+C$	0	$3B+C$	0	$H_{11}+2H_{44}+H_{55}+B+5C$	$H_{12}-2\cdot3^{1/2}B$	$2\cdot3^{1/2}B$	|87⟩
$3^{1/2}B$	$(3/2)^{1/2}B$	$-(3/2)^{1/2}B$	$B+C$	0	$-3^{1/2}B$	$3B$	0	$3B+C$	$H_{12}-2\cdot3^{1/2}B$	$H_{22}+2H_{44}+H_{55}-15B+5C$	0	|88⟩
0	$-6^{1/2}B$	0	0	$B+C$	0	$3B+C$	$3^{1/2}B$	$3B$	$2\cdot3^{1/2}B$	0	$H_{33}+H_{44}+2H_{55}-15B+5C$	|89⟩

Table IV – Continued

	$H_{11}+H_{22}+H_{33}+H_{44}-12B+6C$	0	$2\cdot6^{1/2}B$	$-2^{-1/2}H_{12}+2\cdot6^{1/2}B$	$-3\cdot2^{-1/2}B$	$-2^{-1/2}H_{12}+(3/2)^{1/2}B$	$3\cdot2^{-1/2}B$	$(3/2)^{1/2}B$	0	$(3/2)^{1/2}B$	$(3/2)^{1/2}B$	|90⟩
	0	$H_{11}+H_{22}+H_{33}+H_{44}+6C$	$3\cdot2^{1/2}B$	$(3/2)^{1/2}H_{12}-3\cdot2^{1/2}B$	$-3\cdot(3/2)^{1/2}B$	$(3/2)^{1/2}H_{12}-9\cdot2^{-1/2}B$	$-3\cdot(3/2)^{1/2}B$	$9\cdot2^{-1/2}B$	$-3\cdot6^{1/2}B$	$3\cdot2^{-1/2}B$	$-3\cdot2^{-1/2}B$	|91⟩
	$2\cdot6^{1/2}B$	$3\cdot2^{1/2}B$	$2H_{11}+H_{22}+H_{55}-4B+7C$	$3B$	$-H_{12}-4\cdot3^{1/2}B$	0	0	$4B+C$	$-3^{1/2}B$	$B+C$	0	|92⟩
	$-2^{-1/2}H_{12}+2\cdot6^{1/2}B$	$(3/2)^{1/2}H_{12}-3\cdot2^{1/2}B$	$3B$	$2H_{11}+H_{33}+H_{44}-4B+7C$	0	$4B+C$	$4\cdot3^{1/2}$	0	$3^{1/2}B$	0	$B+C$	|93⟩
	$-3\cdot2^{-1/2}B$	$-3\cdot(3/2)^{1/2}B$	$-H_{12}-4\cdot3^{1/2}B$	0	$H_{11}+2H_{22}+H_{55}-12B+7C$	$-3^{1/2}B$	C	0	$3B+C$	$-3^{1/2}B$	0	|94⟩
$^1B_1$:	$-2^{-1/2}H_{12}+(3/2)^{1/2}B$	$(3/2)^{1/2}H_{12}-9\cdot2^{-1/2}B$	0	$4B+C$	$-3^{1/2}B$	$2H_{22}+H_{33}+H_{44}+6B+7C$	0	$-6B$	0	$-9B$	$3B+C$	|95⟩
	$3\cdot2^{-1/2}B$	$-3\cdot(3/2)^{1/2}B$	0	$4\cdot3^{1/2}B$	C	0	$H_{11}+2H_{33}+H_{55}-12B+7C$	$H_{12}+3^{1/2}B$	$3B+C$	0	$3^{1/2}B$	|96⟩
	$(3/2)^{1/2}B$	$9\cdot2^{-1/2}B$	$4B+C$	0	0	$-6B$	$H_{12}+3^{1/2}B$	$H_{22}+2H_{33}+H_{55}+6B+7C$	0	$3B+C$	$-9B$	|97⟩
	0	$-3\cdot6^{1/2}B$	$-3^{1/2}B$	$3^{1/2}B$	$3B+C$	0	$3B+C$	0	$H_{11}+2H_{44}+H_{55}+3B+7C$	$H_{12}-4\cdot3^{1/2}B$	$4\cdot3^{1/2}B$	|98⟩
	$(3/2)^{1/2}B$	$3\cdot2^{-1/2}B$	$B+C$	0	$-3^{1/2}B$	$-9B$	0	$3B+C$	$H_{12}-4\cdot3^{1/2}B$	$H_{22}+2H_{44}+H_{55}-9B+7C$	$-6B$	|99⟩
	$(3/2)^{1/2}B$	$-3\cdot2^{-1/2}B$	0	$B+C$	0	$3B+C$	$3^{1/2}B$	$-9B$	$4\cdot3^{1/2}B$	$-6B$	$H_{33}+H_{44}+2H_{55}-9B+7C$	|100⟩