

Analytical Expressions for Crystal Fields of Hexagonal Symmetry: High Temperature Magnetic Susceptibility Applications*

by

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ABSTRACT

Crystal Field (CF) Theory is a standard tool for analyzing thermal, spectroscopic, magnetic and related properties in solids containing transition ions. In the case of rare earth ions, the CF eigenvalues were the object of a systematic study for cubic and hexagonal symmetry; the results were computed numerically and displayed in table or graphic form. This paper discusses the use of Computer Algebra (CA) to obtain analytical results of interest for the studies of magnetic behavior of rare-earth intermetallic compounds, where the CF has hexagonal symmetry. In the first part, CA techniques are applied to obtain the characteristic polynomials of the CF hamiltonian. A remarkable result is that for most J 's the characteristic polynomials are entirely factored, allowing the analytical derivation of the eigenvalues as a function of the CF parameters. A comparison with the values obtained numerically is made for two cases, showing, as expected, excellent agreement. In the second part, a model hamiltonian containing the CF term and exchange is used, and an expression for the high temperature susceptibility (HTS), suitable for algebraic computation is derived. We compute the HTS expressions using results of the first part plus the partially factored polynomials of the model hamiltonian. In the molecular field approximation, we re-obtain results of the literature for HTS in the parallel and perpendicular directions. This treatment may be extended to other high anisotropy systems, both hexagonal and rhombohedral, as the nitrided R_2Fe_{17} intermetallic compounds.

Key-words: Crystal field eigenvalues; Magnetism; Hexagonal intermetallic compounds.

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1. Introduction

In two recent papers^{1,2} we have used a computer algebra approach to obtain 1) analytical eigenvalues of the Crystal Field Hamiltonian for cubic symmetry; 2) magnetic quantities derived from a model Hamiltonian which includes Crystal Field (CF) and Exchange Interactions. Applications to magnetic properties of some rare-earth intermetallic compounds, which crystallize in the cubic Laves phase structure (C15), of formula RX_2 (R=rare-earth ion, X=non-magnetic ion) were also considered.

The present work is a sequel of the ideas and methods discussed in the above mentioned references^{1,2}, for the case of a CF Hamiltonian with hexagonal symmetry. The paper is divided in the following way: in Section 2 the CF Hamiltonian and the method used to obtain (via Computer Algebra (CA)) the analytical eigenvalues are presented; in Section 3, we list CF analytical eigenvalues for rare-earth ions of $J= 4, 6, 8, 5/2, 7/2, 9/2$ and $15/2$ in hexagonal symmetry. In Section 4 the splitting of the rare-earth ion multiplet due to a combined action of the crystal field and of an effective magnetic field applied in the directions $(0,0,1)$ and $(1,0,0)$ is formulated; the characteristic polynomials are factored into simpler polynomials which are divided into classes. In Section 5, making use of the results obtained in Section 4, we make a direct computation of the inverse susceptibility at high temperature, for directions $(0,0,1)$ and $(1,0,0)$.

2. Crystal Field Hamiltonian

For the case of hexagonal symmetry we have:

$$\mathcal{H}_{CF}^{hex} = B_2^0 O_2^0 + B_4^0 O_4^0 + B_6^0 O_6^0 + B_6^6 O_6^6 \quad (1)$$

where O_m^n are the Stevens operators, expressed in powers of the components of J_z , J_+ and J_- of the angular momentum operator³; B_2^0 , B_4^0 , B_6^0 and B_6^6 are adjustable CF parameters. Eq. 1 applies in a coordinate system (x, y, z) in which the z -axis is parallel to the c -axis of the orthohexagonal cell; z is also assumed as the direction of quantization. Taking $|J, m\rangle$ as eigenfunctions of J_z (J and m are respectively the angular momentum and magnetic quantum numbers), the eigenvalues of \mathcal{H}_{CF} are the roots of the polynomial equation in the variable y

$$\det | \langle n, J | \mathcal{H}_{CF} - y \delta_{n,m} | J, m \rangle | = 0 \quad (2)$$

At this point we make use of REDUCE (a well known computer language) to obtain: 1) the polynomial of degree $2J + 1$; 2) the analytical factors of the corresponding polynomials. It turns out that with the exception of $J= 15/2$ and $J= 8$ the eigenvalues of \mathcal{H}_{CF}^{hex} are analytically expressible in terms of B_n^m . For $J= 15/2$, twelve values are roots of polynomials of the third degree; the remaining four values are roots of second degree polynomials. For $J= 8$, twelve values are again roots of third degree polynomials; two roots of second degree polynomials and three are analytical roots. They are listed in the next section.

For each J the results are labeled using the Γ 's irreducible representation of the hexagonal point group D_{6h} .

3. Eigenvalues of \mathcal{H}_{CF}^{hex}

In the case of semi-integer J, the D_J representation of the rotation group can be reduced to doublets; this can be expressed by irreducible representations of the hexagonal point group D_{6h} : Γ_7 , Γ_8 and or Γ_9 .

Results for J semi-integer

$$J= 5/2 (D_{5/2} = 2\Gamma_7 + \Gamma_8), (Ce^{3+}, Sm^{3+})$$

$$\begin{aligned} E(\Gamma_7^{(1)}) &= -2(2b_{2,0} - b_{4,0}) \\ E(\Gamma_7^{(2)}) &= -b_{2,0} - 3b_{4,0} \\ E(\Gamma_8) &= 5b_{2,0} + b_{4,0} \end{aligned}$$

$$J= 7/2 (D_{7/2} = 2\Gamma_7 + 2\Gamma_8), (Yb^{3+})$$

$$\begin{aligned} E(\Gamma_7^{(1)}) &= -5b_{2,0} + 9b_{4,0} - 5b_{6,0} \\ E(\Gamma_7^{(2)}) &= -3(b_{2,0} + b_{4,0} - 3b_{6,0}) \\ E(\Gamma_8^{(1)}) &= 4b_{2,0} - 3b_{4,0} - 2b_{6,0} - \sqrt{M} \\ E(\Gamma_8^{(2)}) &= 4b_{2,0} - 3b_{4,0} - 2b_{6,0} + \sqrt{M} \end{aligned}$$

$$\begin{aligned} M &= 3b_{2,0}(3b_{2,0} + 20b_{4,0} + 6b_{6,0}) + \\ & 20b_{4,0}(5b_{4,0} + 3b_{6,0}) + (3b_{6,0})^2 + 7(b_{6,6})^2 \end{aligned}$$

$$J= 9/2 (D_{9/2} = \Gamma_7 + 2\Gamma_8 + 2\Gamma_9), (Nd^{3+})$$

$$\begin{aligned} E(\Gamma_7) &= -2(2b_{2,0} - 9b_{4,0} + 4b_{6,0}) \\ E(\Gamma_8^{(1)}) &= (b_{2,0} - 39b_{4,0} - b_{6,0} + \sqrt{N})/2 \\ E(\Gamma_8^{(2)}) &= (b_{2,0} - 39b_{4,0} - b_{6,0} - \sqrt{N})/2 \\ E(\Gamma_9^{(1)}) &= (3b_{2,0} + 21b_{4,0} + 9b_{6,0} + \sqrt{M})/2 \\ E(\Gamma_9^{(2)}) &= (3b_{2,0} + 21b_{4,0} + 9b_{6,0} - \sqrt{M})/2 \end{aligned}$$

$$\begin{aligned} N &= 3b_{2,0}(3b_{2,0} - 10b_{4,0} - 42b_{6,0}) + \\ & 5b_{4,0}(5b_{4,0} + 42b_{6,0}) + (21b_{6,0})^2 + (14b_{6,6})^2 \\ M &= 3[9b_{2,0}(3b_{2,0} + 10b_{4,0} - 2b_{6,0}) + \\ & 15b_{4,0}(5b_{4,0} - 2b_{6,0}) + 3(b_{6,0})^2 + 7(2b_{6,6})^2] \end{aligned}$$

$J= 15/2 (D_{15/2} = 3\Gamma_7 + 2\Gamma_8 + 3\Gamma_9), (Dy^{3+}, Er^{3+})$. The $D_{15/2}$ representation of the rotation group can be reduced to eight doublets:

$$D_{15/2} = 3\Gamma_7 + 2\Gamma_8 + 3\Gamma_9$$

where the Γ'_s are the irreducible representation of the hexagonal point group D_{6h} . The doublets in Γ_7 and Γ_9 are the roots of the third degree polynomials. The two doublets in Γ_8 are

$$\begin{aligned} E(\Gamma_8^{(1)}) &= -12b_{2,0} - 39b_{4,0} + 66b_{6,0} - \sqrt{N} \\ E(\Gamma_8^{(2)}) &= -12b_{2,0} - 39b_{4,0} + 66b_{6,0} + \sqrt{N} \end{aligned}$$

$$\begin{aligned} N &= 3b_{2,0}(3b_{2,0} - 124b_{4,0} + 42b_{6,0}) + 124b_{4,0}(31b_{4,0} - 21b_{6,0}) + \\ &\quad (21b_{6,0})^2 + 55(42b_{6,0})^2 \end{aligned}$$

In the case of integer J, the D_J representation of the rotation group can be reduced to a combination of singlets ($\Gamma_1, \Gamma_2, \Gamma_3$ and Γ_4) and doublets (Γ_5, Γ_6).

Results for J integer

$$J=4 \ (D_4 = \Gamma_1 + \Gamma_3 + \Gamma_4 + 2\Gamma_5 + \Gamma_6), \ (\text{Pr}^{3+}, \text{Pm}^{3+})$$

$$\begin{aligned} E(\Gamma_1) &= -2(10b_{2,0} - 9b_{4,0} + 10b_{6,0}) \\ E(\Gamma_3) &= 7b_{2,0} - 21b_{4,0} - 17b_{6,0} + 7b_{6,6} \\ E(\Gamma_4) &= 7b_{2,0} - 21b_{4,0} - 17b_{6,0} - 7b_{6,6} \\ E(\Gamma_5^{(1)}) &= (20b_{2,0} + 3b_{4,0} + 26b_{6,0} + \sqrt{M})/2 \\ E(\Gamma_5^{(2)}) &= (20b_{2,0} + 3b_{4,0} + 26b_{6,0} - \sqrt{M})/2 \\ E(\Gamma_6) &= -17b_{2,0} + 9b_{4,0} + b_{6,0} \end{aligned}$$

$$\begin{aligned} M &= 72b_{2,0}(18b_{2,0} + 25b_{4,0} - 18b_{6,0}) + \\ &\quad 25b_{4,0}(25b_{4,0} - 36b_{6,0}) + (18b_{6,0})^2 + 7(4b_{6,6})^2 \end{aligned}$$

$$J=6 \ (D_6 = 2\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + 2\Gamma_5 + 2\Gamma_6), \ (\text{Tb}^{3+}, \text{Tm}^{3+})$$

$$\begin{aligned} E(\Gamma_1^{(1)}) &= (8b_{2,0} + 183b_{4,0} - 18b_{6,0} - \sqrt{M})/2 \\ E(\Gamma_1^{(2)}) &= (8b_{2,0} + 183b_{4,0} - 18b_{6,0} + \sqrt{M})/2 \\ E(\Gamma_2) &= 11(2b_{2,0} + 9b_{4,0} + 2b_{6,0}) \\ E(\Gamma_3) &= -5b_{2,0} - 54b_{4,0} + 43b_{6,0} - 84b_{6,6} \\ E(\Gamma_4) &= -5b_{2,0} - 54b_{4,0} + 43b_{6,0} + 84b_{6,6} \\ E(\Gamma_5^{(1)}) &= -(8b_{2,0} + 85b_{4,0} - 30b_{6,0} + \sqrt{N})/2 \\ E(\Gamma_5^{(2)}) &= -(8b_{2,0} + 85b_{4,0} - 30b_{6,0} - \sqrt{N})/2 \\ E(\Gamma_6^{(1)}) &= -(2b_{2,0} + 2b_{4,0} + 75b_{6,0} + \sqrt{G})/2 \\ E(\Gamma_6^{(2)}) &= -(2b_{2,0} + 2b_{4,0} + 75b_{6,0} - \sqrt{G})/2 \end{aligned}$$

$$\begin{aligned}
 M &= 72b_{2,0}(18b_{2,0} + 15b_{4,0} + 62b_{6,0}) + \\
 &\quad 15b_{4,0}(15b_{4,0} + 124b_{6,0}) + \\
 &\quad (62b_{6,0})^2 + 462(4b_{6,6})^2 \\
 N &= 24b_{2,0}(6b_{2,0} - 107b_{4,0} - 14b_{6,0}) + \\
 &\quad 107b_{4,0}(107b_{4,0} + 28b_{6,0}) + \\
 &\quad (14b_{6,0})^2 + 30(28b_{6,6})^2 \\
 G &= 48b_{2,0}(12b_{2,0} - 130b_{4,0} - 35b_{6,0}) + \\
 &\quad 25b_{4,0}(676b_{4,0} + 364b_{6,0}) + \\
 &\quad (35b_{6,0})^2 + 66(14b_{6,6})^2
 \end{aligned}$$

$J=8$ ($D_8 = 2\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + 3\Gamma_5 + 3\Gamma_6$), (Ho^{3+}). Six of the roots are on two third degree polynomials. Where

$$\begin{aligned}
 b_{2,0} &= F_2^0 B_2^0 = W(1 - |y|) \\
 b_{4,0} &= F_4^0 B_4^0 = Wyx \\
 b_{6,0} &= F_6^0 B_6^0 = Wy(1 - |x|)(1 - |z|) \\
 b_{6,6} &= F_6^6 B_6^6 = Wyz(1 - |x|)
 \end{aligned}$$

and W , x , y and z are an extension of the Lea et al.⁴ notation to hexagonal symmetry (see Andres et al.⁵ and Wallace and Segal⁶); the F_m^n are given elsewhere⁷.

One should emphasize that the algebraic diagonalization presented here provides analytical values for the energy levels, valid for any set of B_m^n parameters, whereas the numerical diagonalization has to be repeated for each set of parameters. In other words, to obtain the energy levels in the usual procedure, one has to run a computer program using standard library routines which calculate eigenvalues and eigenvectors (for details see books on numerical methods). In our case, starting from the analytical results (Section 3), given a set of B 's, all one needs is a pocket calculator. In addition the analytical results are also important in obtaining the HTS's (high-temperature susceptibilities), dealt with in Section 5.

To illustrate the effectiveness of our eigenvalue expressions we have given in Table 1 and Table 2 a comparison of eigenvalues computed from our expressions and from references (5) and (11). For each rare earth ion, the calculations used the same set of B_m^n parameters (given in Ref. (5) for Pr and in Ref. (11) for Nd).

Table 1

Comparison of results obtained from the analytical methods of Computer Algebra (present work) and numerical procedures for $J = 4$ applied to PrNi_5 (Ref. (5)). Both calculations used the same set of B_m^n parameters given in Ref. (5).

Representation	Eigenvalues for $J = 4$	
Γ_i	Computer Algebra E_i/k (K)	Numerical E_i/k (K)
Γ_5^1	331.0	332.0
Γ_3	156.5	156.8
Γ_5^2	48.0	48.2
Γ_6	39.2	39.4
Γ_1	22.8	22.9
Γ_4	0	0

Table 2

Comparison of results obtained from the analytical methods of Computer Algebra (present work) and numerical procedures for $J = 9/2$, applied to NdNi_5 (Ref. (11)). Both calculations used the same set of B_m^n parameters given in Ref. (11).

Representation	Eigenvalues for $J = 9/2$	
Γ_i	Computer Algebra E_i/k (K)	Numerical E_i/k (K)
Γ_9^1	241.26	241.3
Γ_8^1	163.84	163.8
Γ_7	50.38	50.4
Γ_9^2	18.23	18.2
Γ_8^2	0	0

4. Splitting by CF and Magnetic Interaction

In what follows we make the assumption that magnetic quantities can be deduced from the following model Hamiltonian

$$\mathcal{H} = \mathcal{H}_{CF} + \mathcal{H}_{mag} \quad (3)$$

where

$$\mathcal{H}_{mag} = -g\mu_B \mathbf{h} \cdot \mathbf{J} \quad (4)$$

and

$$g\mu_B \mathbf{h} = g\mu_B \mathbf{h}_0 + \lambda_0(g-1)^2 \langle \mathbf{J} \rangle \quad (5)$$

In (4) g is the Landé factor, μ_B the Bohr magneton, λ_0 the exchange parameter and \mathbf{h}_0 is the applied field; $\langle \mathbf{J} \rangle$ is the thermal average of the angular momentum operator \mathbf{J} .

If the eigenvalues of \mathcal{H} are given in explicit form, the magnetic moments in the \mathbf{n} direction (\mathbf{n} is a unit vector), are given by

$$g\mu_B \langle i | \mathbf{J} \cdot \mathbf{n} | i \rangle \equiv -\frac{dy_i}{dh} = -g\mu_B \frac{dy_i}{d\alpha} \quad (6)$$

where $h = \mathbf{h} \cdot \mathbf{n}$ and $\alpha = g\mu_B h$.

In what follows we take $\mathbf{n} = (1, 0, 0)$ and $(0, 0, 1)$.

We now make use of Eq. 2, substituting \mathcal{H} for \mathcal{H}_{CF} and obtain, using REDUCE, polynomials of degree $2J + 1$, which are however very complicated. Fortunately, REDUCE can factor most of the polynomials into simpler factors. For instance, for $J = 5/2$, we have 6 first degree factor polynomials, for \mathbf{h} along (001), and 2 third degree factor polynomials for the direction (100).

Typical polynomial factors are presented in Appendix A for $J = 5/2$. All relevant magnetic information is contained in these factor polynomials. Let $P(y, B_m^n, \alpha)$ be one of the above mentioned factors, whose roots y_i are the energy eigenvalues. In Section 5 we will need the roots y_i^0 of the pure crystal field hamiltonian, the limits $\lim_{\alpha \rightarrow 0} \frac{dy}{d\alpha}$ and $\lim_{\alpha \rightarrow 0} \frac{d^2y}{d\alpha^2}$, in order to obtain the magnetic susceptibilities at high temperature. These limits are obtained from the following relations

$$P(y, B_m^n, \alpha) = 0 \quad (7)$$

$$\frac{\partial P}{\partial y} \left(\frac{dy}{d\alpha} \right) + \frac{\partial P}{\partial \alpha} = 0 \quad (8)$$

$$P_y \frac{d^2y}{d\alpha^2} + [P_{yy} \frac{dy}{d\alpha} + 2P_{\alpha y}] \frac{dy}{d\alpha} + P_{\alpha\alpha} = 0 \quad (9)$$

$$P_y \frac{d^3y}{d\alpha^3} + 3[P_{yy} \frac{dy}{d\alpha} + P_{\alpha y}] \frac{d^2y}{d\alpha^2} + P_{yyy} \left(\frac{dy}{d\alpha} \right)^3 + 3[P_{yy\alpha} \frac{dy}{d\alpha} + P_{\alpha\alpha y}] \frac{dy}{d\alpha} + P_{\alpha\alpha\alpha} = 0$$

5. High temperature susceptibilities

With W. G. Penney and R. Schlapp⁸ we begin with the basic definition of magnetization (per magnetic ion)

$$m = -\frac{\sum_{i=1}^{2J+1} (dy_i/dh) \exp(-y_i/k_B T)}{\sum_{i=1}^{2J+1} \exp(-y_i/k_B T)} \quad (10)$$

For high temperature and up to $(\frac{y_i}{k_B T})^2$

$$m = g\mu_B \left[\frac{\sum_{i=1}^{2J+1} \frac{\partial(y_i^2)}{\partial\alpha}}{2k_B T(2J+1)} - \frac{\sum_{i=1}^{2J+1} \frac{\partial(y_i^3)}{\partial\alpha}}{6k_B^2 T^2(2J+1)} \right] \quad (11)$$

This is the results of Penney and Schlapp⁸ adapted for our notation. Using (5), from (12) we obtain

$$\chi^{-1} \cong \frac{1}{C} [T - (\frac{C_1}{C} + C\lambda)] (g\mu_B)^{-2} \quad (12)$$

where χ is the magnetic susceptibility and

$$C = \frac{1}{(2J+1)2k_B} \sum_{i=1}^{2J+1} \lim_{\alpha \rightarrow 0} \frac{1}{\alpha} \frac{\partial(y_i^2)}{\partial\alpha} \quad (13)$$

and

$$C_1 = \frac{1}{(2J+1)6k_B^2} \sum_{i=1}^{2J+1} \lim_{\alpha \rightarrow 0} \frac{1}{\alpha} \frac{\partial(y_i^3)}{\partial\alpha} \quad (14)$$

Therefore, in order to obtain the susceptibilities in different directions we will need to compute the limits as $\alpha \rightarrow 0$ in (14) and (15). We obtain

$$C = \frac{1}{(2J+1)k_B} \sum_{i=1}^{2J+1} [y_i^0 (\frac{d^2 y_i}{d\alpha^2})_0 + (\frac{dy_i}{d\alpha})_0^2] \quad (15)$$

$$C_1 = \frac{1}{(2J+1)2k_B^2} \sum_{i=1}^{2J+1} y_i^0 [y_i^0 (\frac{d^2 y_i}{d\alpha^2})_0 + 2(\frac{dy_i}{d\alpha})_0^2] \quad (16)$$

In what follows we compute C and C₁ for the case in which the magnetic interaction is described in the molecular field approximation (Eqs. 4 and 5).

For the first case, we illustrate the computation of C and C₁ for J=5/2. The polynomial factors, the derivatives $(\frac{dy_i}{d\alpha})_0$ and $(\frac{d^2 y_i}{d\alpha^2})_0$ are given in Appendix A and y_i^0 are given at the beginning of Section 3. For this case $C^\perp = \frac{35}{12k_B}$; $C_1^\perp = \frac{-28B_0^2}{3k_B^2}$; $C^\parallel = C^\perp$ and $C_1^\parallel = \frac{C_1^\perp}{2}$. The procedure can be repeated for other values of J. The results are:

$$C^\parallel = J(J+1)/3k_B \quad C_1^\parallel = b_{2,0} C(2J-1)(2J+3)/5(k_B)^2 \quad (17)$$

$$C^\perp = C^\parallel \quad C_1^\perp = -C_1^\parallel/2 \quad (18)$$

These confirm the formulae given by Boutron^{9,10}, obtained through an analysis of $\sum_i y_i^n = \text{Tr}(\mathcal{H}^n)$ and its derivatives (with respect to the magnetic field) using the tools of group theory (e.g. summation rules).

One advantage of the CA approach is that, not only it is more direct, but also it is an easier one. Experimental studies of high temperature susceptibilities use the results^{9,10} to determine the B_2^0 and exchange parameters, as was done by Barthem et al.^{11,12} in analyzing the high temperature susceptibilities of NdNi₅ and PrNi₅.

The examples given here show the potentiality of CA in solving difficult problems involving crystal field and magnetic interactions.

Appendix A

Factor polynomials of the characteristic polynomial for $J = 5/2$

$$\begin{aligned}
 P(y, B_m^n, \alpha)^\pm &= -y^3 \pm 3y^2\alpha/2 + y[21b_{2,0}^2 \mp 6b_{2,0}\alpha + 7b_{4,0}^2 \pm 3b_{4,0}\alpha + 13(\alpha/2)^2] + \\
 &20b_{2,0}^3 + 54b_{2,0}^2b_{4,0} \mp 15b_{2,0}^2\alpha/2 - 20b_{2,0}b_{4,0}^2 \mp 24b_{2,0}b_{4,0}\alpha - \\
 &5b_{2,0}\alpha^2 - 6b_{4,0}^3 \mp 9b_{4,0}^2\alpha/2 - 9b_{4,0}\alpha^2/2 \mp 15(\alpha/2)^3
 \end{aligned}$$

First and second derivatives of y_i (in relation to α), for $\alpha = 0$

$$\begin{aligned}
 \left(\frac{dy_1}{d\alpha}\right)_0 &= 0 & \left(\frac{dy_2}{d\alpha}\right)_0 &= 0 & \left(\frac{dy_3}{d\alpha}\right)_0 &= 3/2 \\
 \left(\frac{dy_4}{d\alpha}\right)_0 &= 0 & \left(\frac{dy_5}{d\alpha}\right)_0 &= 0 & \left(\frac{dy_6}{d\alpha}\right)_0 &= -3/2
 \end{aligned}$$

$$\begin{aligned}
 \left(\frac{d^2y_1}{d\alpha^2}\right)_0 &= \frac{3(11b_{2,0} + 19b_{4,0})}{4(9b_{2,0}^2 - 9b_{2,0}b_{4,0} - 10b_{4,0}^2)} \\
 \left(\frac{d^2y_2}{d\alpha^2}\right)_0 &= \frac{5}{4(3b_{2,0} + 2b_{4,0})} \\
 \left(\frac{d^2y_3}{d\alpha^2}\right)_0 &= \frac{-4}{3b_{2,0} - 5b_{4,0}} \\
 \left(\frac{d^2y_4}{d\alpha^2}\right)_0 &= \frac{3(11b_{2,0} + 19b_{4,0})}{4(9b_{2,0}^2 - 9b_{2,0}b_{4,0} - 10b_{4,0}^2)} \\
 \left(\frac{d^2y_5}{d\alpha^2}\right)_0 &= \frac{5}{4(3b_{2,0} + 2b_{4,0})} \\
 \left(\frac{d^2y_6}{d\alpha^2}\right)_0 &= \frac{-4}{3b_{2,0} - 5b_{4,0}}
 \end{aligned}$$

$$C = \frac{35}{12} \quad C_1^\perp = -\frac{14b_{2,0}}{3} = -\frac{28B_2^0}{3}$$

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