

Development of MagSaki(A) Software for the Magnetic Analysis of Dinuclear High-spin Cobalt(II) Complexes Considering Anisotropy in Exchange Interaction

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MagSaki(A) software was developed for the magnetic analysis of dinuclear high-spin cobalt(II) complexes. This software performs magnetic analysis to determine magnetic parameters using five types of theoretical susceptibility equations. A characteristic feature of the software is that the exchange interaction can be treated anisotropically whereas the previous MagSaki software treats the exchange interaction isotropically.

Keywords: Magnetic analysis, Dinuclear high-spin cobalt(II) complex, Anisotropic exchange interaction, MagSaki software series

1 Introduction

The magnetism of transition metal complexes is important to coordination chemistry since magnetic behavior is strongly influenced by the coordination geometry and electronic configuration of metal ions. In general, it is not difficult to analyze the observed magnetic data for most of the first-transition elements because the orbital angular momentum is quenched [1] and only spin angular momentum should be considered. However, in the case of octahedral high-spin cobalt(II) complexes, the contribution of orbital angular momentum is significant [2], and magnetic susceptibility equations, which describe the temperature dependencies of the magnetic susceptibility, are much more complicated for the cobalt(II) complexes than for other first-transition elements.

For mononuclear octahedral high-spin cobalt(II) complexes, Lines and Figgis developed methods for the calculation of the magnetic susceptibility of a high-spin cobalt(II) complex by considering the axial distortion and spin-orbit coupling [3, 4]. For dinuclear complexes containing two equivalent octahedral high-spin cobalt(II) ions, Lines developed a magnetic susceptibility equation for pure octahedral coordination geometries [5], and Sakiyama developed susceptibility equations for distorted octahedral geometries considering the axial dis-

ortion, spin-orbit coupling, and isotropic/anisotropic exchange interaction [6–9].

A first MagSaki software was developed earlier for the purpose of analyzing the observed magnetic data of dinuclear high-spin cobalt(II) complexes [10]; however, the previous MagSaki software always treated the exchange interaction isotropically, which sometimes was not sufficient. Thus, here is a report on the MagSaki(A) software that can treat the exchange interaction anisotropically.

2 Method

The software was developed using REALbasic software [11]. A Macintosh version was developed on a Power Macintosh 7300/180 (OS: J1-7.5.5), and a Windows version was developed on an FMV-BIBLO MG12C (OS: Windows XP Home edition). Magnetic susceptibility equations were taken from references [5–9].

3 Magnetic Parameters

The symbols used in this paper are summarized in Table 1.

Table 1. List of the main symbols [2, 5–9].

Symbol	Unit	Meaning
g	—	g -factor
J	cm^{-1}	Exchange interaction parameter between true spins (3/2)
T	K	Absolute temperature
TIP	$\text{cm}^3 \text{mol}^{-1}$	Temperature-independent paramagnetism
ν	—	Distortion parameter defined as $\Delta/(\kappa \lambda)$
Δ	cm^{-1}	Axial splitting parameter
κ	—	Orbital reduction factor
λ	cm^{-1}	Spin-orbit coupling parameter
μ_{eff}	μ_{B}	Effective magnetic moment
χ_{A}	$\text{cm}^3 \text{mol}^{-1}$	Atomic magnetic susceptibility

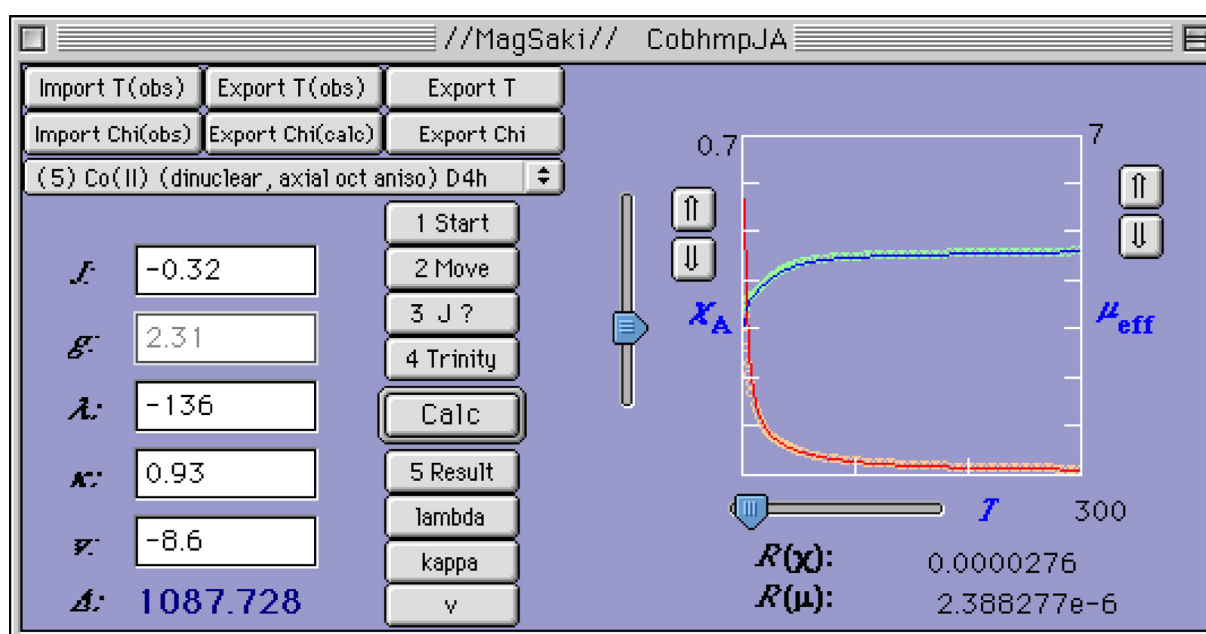


Figure 1. Main window of the MagSaki(A) software.

4 Function of MagSaki(A)

The MagSaki(A) software imports the temperature (T) data and the magnetic susceptibility (χ_{A}) data and displays a χ_{A} versus T graph and an effective magnetic moment (μ_{eff}) versus T graph (Figure 1). The software can calculate theoretical χ_{A} and μ_{eff} values based on five theoretical equations [5–9] and also displays the theoretical curves of χ_{A} and μ_{eff} on the graph. The software can optimize magnetic parameters to fit the theoretical curve to the observed data.

5 Calculation Modes

The MagSaki(A) software has five calculation modes. Mode 1 is for mononuclear octahedral high-spin

cobalt(II) complexes, and modes 2–5 are for dinuclear octahedral high-spin cobalt(II) complexes. The exchange interaction is treated isotropically in modes 2–4 but anisotropically in mode 5. Modes 1–4 already exist in the previous software [10], while mode 5 is an original calculation mode.

5.1 Mode 1: Mononuclear octahedral high-spin cobalt(II) complex

This mode is useful for mononuclear high-spin cobalt(II) complexes when the coordination geometry is purely octahedral or axially distorted octahedral. Magnetic susceptibility is calculated using a susceptibility equation [6] based on the ideas of Lines [3] and Figgis [4]. The independent parameters are κ , λ , and ν .

Table 2. Magnetic parameters.^a

Complex	κ	λ/cm^{-1}	Δ/cm^{-1}	J/cm^{-1}	g_z^b	g_x^b	$R_\chi^c/10^{-3}$	$R_\mu^d/10^{-4}$	Mode	Reference
1	0.77	-116	572	-0.44	2.11	4.73	0.036	0.036	2	[12]
	0.80	-122	673	-0.30	2.08	4.74	0.033	0.035	5	this work
2	0.96 ^e	-93	616	-0.33	2.09	4.91	0.16	0.59	2	[12]
	0.93	-99	543	-0.33	2.15	4.93	0.22	0.15	2	this work
	0.93	-99	552	-0.21	2.15	4.92	0.20	0.15	5	this work
3	0.98 ^e	-134	749	-0.55	2.18	4.99	0.12	0.89	2	[7]
	0.93	-124	578	-0.54	2.25	4.96	0.16	0.90	2	this work
	0.93	-125	581	-0.38	2.25	4.96	0.11	0.91	5	this work
4	0.84	-138	440	-0.90 ^f	2.45	4.84	1.7	1.6	2	[7]
	0.84	-141	461	-0.67	2.42	4.85	1.6	1.5	5	this work

^a The intermolecular interactions were ignored.

^b These values were calculated using the equations reported in the references.

^c $R_\chi = \sum(\chi_{A,calc} - \chi_{A,obs})^2 / \sum(\chi_{A,obs})^2$.

^d $R_\mu = \sum(\mu_{eff,calc} - \mu_{eff,obs})^2 / \sum(\mu_{eff,obs})^2$.

^e These values were larger than the free ion value (~ 0.93).

^f The reported value was wrong.

5.2 Mode 2: Dinuclear octahedral high-spin cobalt(II) complex ($|\nu| \sim 0$)

This mode is useful for homo-dinuclear high-spin cobalt(II) complexes when the coordination geometry is octahedral and the distortion is small. Magnetic susceptibility is calculated using the susceptibility equation in reference [7]. The independent parameters are J , κ , λ , and ν . It should be emphasized that this mode is useful only when the $|\nu|$ value is small.

5.3 Mode 3: Dinuclear octahedral high-spin cobalt(II) complex ($\nu = 0$)

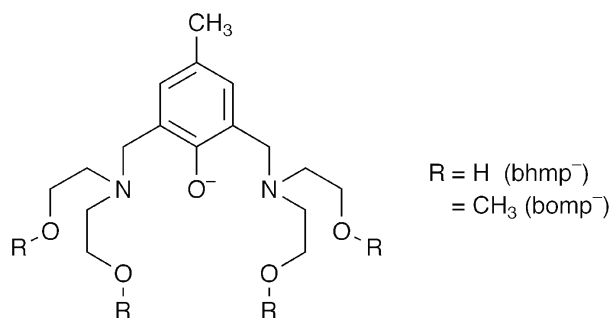
This mode is useful for homo-dinuclear high-spin cobalt(II) complexes when the coordination geometry is purely octahedral. Magnetic susceptibility is calculated using the susceptibility equation in reference [5]. The independent parameters are J and g .

5.4 Mode 4: Dinuclear cobalt(II) complex (spin only)

This mode is useful for homo-dinuclear high-spin cobalt(II) complexes when the orbital angular momentum is perfectly quenched. Magnetic susceptibility is calculated using a general susceptibility equation in the spin-only case [2]. The independent parameters are J , g , θ , and TIP.

5.5 Mode 5: Dinuclear cobalt(II) complex ($\nu = 0$)

This mode is useful for homo-dinuclear high-spin cobalt(II) complexes when the coordination geometry is

Figure 2. Chemical structures of bhmp^- and bomp^- .

axially distorted octahedral. The magnetic susceptibility is calculated using the susceptibility equation (see Appendix) in references [8] and [9]. The independent parameters are J , κ , λ , and ν . It should be noted that the local distortion axes are assumed to be parallel to the molecular principal axis. All the results reported in reference [9] can be obtained using this mode.

6 Examples of magnetic analyses

6.1 Results of parameter optimization

The reported magnetic susceptibility data [7, 12] were analyzed for four dinuclear octahedral high-spin cobalt(II) complexes $[\text{Co}_2(\text{bhmp})(\text{OCOMe})_2]\text{BPh}_4$ (**1**), $[\text{Co}_2(\text{bhmp})(\text{OCOPh})_2]\text{BPh}_4$ (**2**), $[\text{Co}_2(\text{bomp})(\text{OCOMe})_2]\text{BPh}_4$ (**3**), and $[\text{Co}_2(\text{bomp})(\text{OCOPh})_2]\text{BPh}_4$ (**4**) [bhmp^- : 2,6-bis[bis(2-hydroxyethyl)aminomethyl]-4-methylphenolate, bomp^- : 2,6-bis[bis(2-methoxyethyl)aminomethyl]-4-methylphenolate]. The chemical structures of bhmp^- and bomp^- are shown in Figure 2. The reported magnetic parameters and newly obtained parameters are summarized in Table 2.

Table 3. Failed example (example 1b is a failed example).

Example	Complex	κ	λ/cm^{-1}	Δ/cm^{-1}	J/cm^{-1}	g_z	g_x	$R_\chi^a/10^{-3}$	$R_\mu^b/10^{-4}$	Mode	Reference
1a	1	0.80	-122	673	-0.30	2.08	4.74	0.033	0.035	5	this work
1b	1	0.93	-136	1088	-0.32	2.03	4.79	0.028	0.024	5	this work

6.2 Discussion of obtained parameters

The parameters obtained using mode 2 were based on an equation considering the isotropic exchange interaction, whereas the parameters obtained using mode 5 were based on an equation considering the anisotropic exchange interaction. For complexes **2** and **3**, the reported κ values were larger than the free ion value (~ 0.93); thus, the recalculated results using mode 2 are also included in Table 2. Mode 2 is valid only when the distortion is small, but, judging from the Δ values, the distortions are not small. Thus, mode 5 should be used for complexes **1-4**. The J values obtained using mode 2 are 130~160% of the J values obtained using mode 5. This result indicates that an overestimation of the J value occurred when mode 2 was used. In this study, the intermolecular interactions were ignored, and, in mode 5, the local distortion axes were assumed to be parallel to the molecular principal axis.

6.3 Failed example and caution

The MagSaki(A) software has several automatic optimization functions to determine a magnetic parameter set; however, the obtained parameter set is not always the true one. A failed example is included in Table 3. Both examples 1a and 1b were obtained for complex **1** using mode 5 of the software. Judging from the discrepancy factors R_χ and R_μ , example 1b seems to be better and is the best-fitting parameter. However, the Δ value of example 1b (1088 cm^{-1}) is much larger than the Δ values of the other related complexes **2-4**, listed in Table 2. Thus, example 1b is concluded to be a wrong parameter set. When software users access the automatic optimization functions, they should carefully ascertain that the obtained parameter set is a true set.

7 Requirements

The software will run on Power Macintosh computers with Systems 7-9, on emulation mode with Macintosh OS X, and on Windows computers with Windows XP system.

8 Distribution

The author will distribute the MagSaki(A) software free of charge to anyone who requests it. Information about MagSaki(A) software is available on the Sakiyama Laboratory Home Page (<http://www-kschem0.kj.yamagata-u.ac.jp/~sakiyama/>).

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Appendix

Magnetic susceptibility equation for Mode 5

$$\chi_A = \frac{\chi_z + 2\chi_x}{3}$$

$$\chi_z = N \frac{F_1}{F_2}$$

$$\chi_x = N \frac{F_3}{F_2}$$

$$F_1 = \sum_{n=\pm 1} \left(\frac{E_{z,n}^{(1)^2}}{kT} \right) \exp \left[\frac{-E_n^{(0)} + \frac{J_{eff}}{4} - \frac{D_{tri}}{3}}{kT} \right] + \sum_{n=\pm 1} (-2E_{z,n}^{(2)}) \exp \left[\frac{-E_n^{(0)}}{kT} \right] + \sum_{n \neq \pm 1} \left(\frac{E_{z,n}^{(1)^2}}{kT} - 2E_{z,n}^{(2)} \right) \exp \left[\frac{-E_n^{(0)}}{kT} \right]$$

$$F_2 = \frac{1}{4} \sum_{n=\pm 1} \exp \left[\frac{-E_n^{(0)} - \frac{3J_{eff}}{4}}{kT} \right] + \frac{1}{2} \sum_{n=\pm 1} \exp \left[\frac{-E_n^{(0)} + \frac{J_{eff}}{4} - \frac{D_{tri}}{3}}{kT} \right] + \frac{1}{4} \sum_{n=\pm 1} \exp \left[\frac{-E_n^{(0)} + \frac{J_{eff}}{4} + \frac{2D_{tri}}{3}}{kT} \right] + \sum_{n \neq \pm 1} \exp \left[\frac{-E_n^{(0)}}{kT} \right]$$

$$F_3 = \sum_{n=\pm 1} \left(\frac{E_{x,n}^{(1)^2}}{D_{tri}} \right) \left\{ \exp \left[\frac{-E_n^{(0)} + \frac{J_{eff}}{4} + \frac{2D_{tri}}{3}}{kT} \right] - \exp \left[\frac{-E_n^{(0)} + \frac{J_{eff}}{4} - \frac{D_{tri}}{3}}{kT} \right] \right\} + \sum_{n=\pm 1} (-2E_{x,n}^{(2)}) \exp \left[\frac{-E_n^{(0)}}{kT} \right] + \sum_{n \neq \pm 1} \left(\frac{E_{x,n}^{(1)^2}}{kT} - 2E_{x,n}^{(2)} \right) \exp \left[\frac{-E_n^{(0)}}{kT} \right] \quad (D_{tri} \neq 0)$$

$$F_3 = \sum_{n=\pm 1} \left(\frac{E_{x,n}^{(1)^2}}{kT} \right) \exp \left[\frac{-E_n^{(0)} + \frac{J_{eff}}{4}}{kT} \right] + \sum_{n \neq \pm 1} (-2E_{x,n}^{(2)}) \exp \left[\frac{-E_n^{(0)}}{kT} \right] + \sum_{n \neq \pm 1} \left(\frac{E_{x,n}^{(1)^2}}{kT} - 2E_{x,n}^{(2)} \right) \exp \left[\frac{-E_n^{(0)}}{kT} \right] \quad (D_{tri} = 0)$$

$$(n = \pm 1 \dots \pm 6)$$

$$\Delta = v\kappa\lambda$$

$$E_{\pm 1}^{(0)} = -\frac{2c_2^2\Delta}{3} - 3\sqrt{\frac{3}{2}}c_1c_2\kappa\lambda - 3\sqrt{2}c_2c_3\kappa\lambda + c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) + c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right)$$

$$E_{\pm 2}^{(0)} = -\frac{2c_4^2\Delta}{3} - 3\sqrt{\frac{3}{2}}c_4c_5\kappa\lambda + c_5^2 \left(\frac{\Delta}{3} - \frac{3\kappa\lambda}{4} \right)$$

$$E_{\pm 3}^{(0)} = -\frac{2c_7^2\Delta}{3} - 3\sqrt{\frac{3}{2}}c_6c_7\kappa\lambda - 3\sqrt{2}c_7c_8\kappa\lambda + c_8^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) + c_6^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right)$$

$$E_{\pm 4}^{(0)} = -\frac{2c_{10}^2\Delta}{3} - 3\sqrt{\frac{3}{2}}c_9c_{10}\kappa\lambda - 3\sqrt{2}c_{10}c_{11}\kappa\lambda + c_{11}^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) + c_9^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right)$$

$$E_{\pm 5}^{(0)} = -\frac{2c_{12}^2\Delta}{3} - 3\sqrt{\frac{3}{2}}c_{12}c_{13}\kappa\lambda + c_{13}^2 \left(\frac{\Delta}{3} - \frac{3\kappa\lambda}{4} \right)$$

$$E_{\pm 6}^{(0)} = \frac{\Delta}{3} - \frac{9\kappa\lambda}{4}$$

$$\begin{aligned}
c_1 &= \frac{d_1}{|d_1|} \sqrt{d_1^2 / (d_1^2 + d_2^2 + d_3^2)} \\
c_2 &= \frac{d_2}{|d_2|} \sqrt{d_2^2 / (d_1^2 + d_2^2 + d_3^2)} \\
c_3 &= \frac{d_3}{|d_3|} \sqrt{d_3^2 / (d_1^2 + d_2^2 + d_3^2)} \\
c_4 &= \frac{d_4}{|d_4|} \sqrt{d_4^2 / (d_4^2 + d_5^2)} \\
c_5 &= \frac{d_5}{|d_5|} \sqrt{d_5^2 / (d_4^2 + d_5^2)} \\
c_6 &= \frac{d_6}{|d_6|} \sqrt{d_6^2 / (d_6^2 + d_7^2 + d_8^2)} \\
c_7 &= \frac{d_7}{|d_7|} \sqrt{d_7^2 / (d_6^2 + d_7^2 + d_8^2)} \\
c_8 &= \frac{d_8}{|d_8|} \sqrt{d_8^2 / (d_6^2 + d_7^2 + d_8^2)} \\
c_9 &= \frac{d_9}{|d_9|} \sqrt{d_9^2 / (d_9^2 + d_{10}^2 + d_{11}^2)} \\
c_{10} &= \frac{d_{10}}{|d_{10}|} \sqrt{d_{10}^2 / (d_9^2 + d_{10}^2 + d_{11}^2)} \\
c_{11} &= \frac{d_{11}}{|d_{11}|} \sqrt{d_{11}^2 / (d_9^2 + d_{10}^2 + d_{11}^2)} \\
c_{12} &= \frac{d_{12}}{|d_{12}|} \sqrt{d_{12}^2 / (d_{12}^2 + d_{13}^2)} \\
c_{13} &= \frac{d_{13}}{|d_{13}|} \sqrt{d_{13}^2 / (d_{12}^2 + d_{13}^2)} \\
d_1 &= \sqrt{6}/V_1 \\
d_2 &= -1 \\
d_3 &= \sqrt{8}/(V_1 + 2) \\
d_4 &= 1 \\
d_5 &= \frac{3 - 4v - \sqrt{225 - 24v + 16v^2}}{6\sqrt{6}} \\
d_6 &= \sqrt{6}/V_2 \\
d_7 &= -1 \\
d_8 &= \sqrt{8}/(V_2 + 2) \\
d_9 &= \sqrt{6}/V_3 \\
d_{10} &= -1 \\
d_{11} &= \sqrt{8}/(V_3 + 2) \\
d_{12} &= 1 \\
d_{13} &= \frac{3 - 4v + \sqrt{225 - 24v + 16v^2}}{6\sqrt{6}}
\end{aligned}$$

$$\begin{aligned}
V_1 &= \frac{-15 - 4v}{9} - \frac{-441 - 48v - 16v^2}{9 \sqrt[3]{-3861 - 2376v - 288v^2 - 64v^3 + 36\sqrt{3}\sqrt{-18225 - 2484v - 1161v^2 - 72v^3 - 16v^4}}} + \\
&\quad \frac{\sqrt[3]{-3861 - 2376v - 288v^2 - 64v^3 + 36\sqrt{3}\sqrt{-18225 - 2484v - 1161v^2 - 72v^3 - 16v^4}}}{9} \\
V_2 &= \frac{-15 - 4v}{9} + \frac{(1 - \sqrt{3}i)(-441 - 48v - 16v^2)}{18 \sqrt[3]{-3861 - 2376v - 288v^2 - 64v^3 + 36\sqrt{3}\sqrt{-18225 - 2484v - 1161v^2 - 72v^3 - 16v^4}}} - \\
&\quad \frac{(1 + \sqrt{3}i) \sqrt[3]{-3861 - 2376v - 288v^2 - 64v^3 + 36\sqrt{3}\sqrt{-18225 - 2484v - 1161v^2 - 72v^3 - 16v^4}}}{18} \\
V_3 &= \frac{-15 - 4v}{9} + \frac{(1 + \sqrt{3}i)(-441 - 48v - 16v^2)}{18 \sqrt[3]{-3861 - 2376v - 288v^2 - 64v^3 + 36\sqrt{3}\sqrt{-18225 - 2484v - 1161v^2 - 72v^3 - 16v^4}}} - \\
&\quad \frac{(1 - \sqrt{3}i) \sqrt[3]{-3861 - 2376v - 288v^2 - 64v^3 + 36\sqrt{3}\sqrt{-18225 - 2484v - 1161v^2 - 72v^3 - 16v^4}}}{18} \\
E_{z,1}^{(1)} &= -E_{z,-1}^{(1)} = \frac{1}{2}c_2^2g_e\beta + c_3^2\beta \left(-\frac{g_e}{2} - \frac{3\kappa}{2}\right) + c_1^2\beta \left(\frac{3g_e}{2} + \frac{3\kappa}{2}\right) \\
E_{z,2}^{(1)} &= -E_{z,-2}^{(1)} = \frac{3}{2}c_4^2g_e\beta + c_5^2\beta \left(-\frac{g_e}{2} - \frac{3\kappa}{2}\right) \\
E_{z,3}^{(1)} &= -E_{z,-3}^{(1)} = \frac{1}{2}c_7^2g_e\beta + c_8^2\beta \left(-\frac{g_e}{2} - \frac{3\kappa}{2}\right) + c_6^2\beta \left(\frac{3g_e}{2} + \frac{3\kappa}{2}\right) \\
E_{z,4}^{(1)} &= -E_{z,-4}^{(1)} = \frac{1}{2}c_{10}^2g_e\beta + c_{11}^2\beta \left(-\frac{g_e}{2} - \frac{3\kappa}{2}\right) + c_9^2\beta \left(\frac{3g_e}{2} + \frac{3\kappa}{2}\right) \\
E_{z,5}^{(1)} &= -E_{z,-5}^{(1)} = \frac{3}{2}c_{12}^2g_e\beta + c_{13}^2\beta \left(\frac{g_e}{2} - \frac{3\kappa}{2}\right) \\
E_{z,6}^{(1)} &= -E_{z,-6}^{(1)} = \beta \left(\frac{3g_e}{2} - \frac{3\kappa}{2}\right) \\
E_{z,\pm 1}^{(2)} &= \left[\frac{1}{2}c_2c_7g_e\beta + c_3c_8\beta \left(-\frac{g_e}{2} - \frac{3\kappa}{2}\right) + c_1c_6\beta \left(\frac{3g_e}{2} + \frac{3\kappa}{2}\right) \right]^2 / \\
&\quad \left[-\frac{2c_2^2\Delta}{3} + \frac{2c_7^2\Delta}{3} - 3\sqrt{\frac{3}{2}}c_1c_2\kappa\lambda - 3\sqrt{2}c_2c_3\kappa\lambda + 3\sqrt{\frac{3}{2}}c_6c_7\kappa\lambda + 3\sqrt{2}c_7c_8\kappa\lambda + \right. \\
&\quad \left. c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4}\right) - c_8^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4}\right) + c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4}\right) - c_6^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4}\right) \right] + \\
&\quad \left[\frac{1}{2}c_2c_{10}g_e\beta + c_3c_{11}\beta \left(-\frac{g_e}{2} - \frac{3\kappa}{2}\right) + c_1c_9\beta \left(\frac{3g_e}{2} + \frac{3\kappa}{2}\right) \right]^2 / \\
&\quad \left[-\frac{2c_2^2\Delta}{3} + \frac{2c_{10}^2\Delta}{3} - 3\sqrt{\frac{3}{2}}c_1c_2\kappa\lambda - 3\sqrt{2}c_2c_3\kappa\lambda + 3\sqrt{\frac{3}{2}}c_9c_{10}\kappa\lambda + 3\sqrt{2}c_{10}c_{11}\kappa\lambda + \right. \\
&\quad \left. c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4}\right) - c_{11}^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4}\right) + c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4}\right) - c_9^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4}\right) \right]
\end{aligned}$$

$$E_{z,\pm 2}^{(2)} = \left[\frac{3}{2}c_4c_{12}g_e\beta + c_5c_{13}\beta \left(\frac{g_e}{2} - \frac{3\kappa}{2} \right) \right]^2 /$$

$$\left[-\frac{2c_4^2\Delta}{3} + \frac{2c_{12}^2\Delta}{3} - 3\sqrt{\frac{3}{2}}c_4c_5\kappa\lambda + 3\sqrt{\frac{3}{2}}c_{12}c_{13} + c_5^2 \left(\frac{\Delta}{3} - \frac{3\kappa\lambda}{4} \right) - c_{13}^2 \left(\frac{\Delta}{3} - \frac{3\kappa\lambda}{4} \right) \right]$$

$$E_{z,\pm 3}^{(2)} = \left[\frac{1}{2}c_2c_7g_e\beta + c_3c_8\beta \left(-\frac{g_e}{2} - \frac{3\kappa}{2} \right) + c_1c_6\beta \left(\frac{3g_e}{2} + \frac{3\kappa}{2} \right) \right]^2 /$$

$$\left[\frac{2c_2^2\Delta}{3} - \frac{2c_7^2\Delta}{3} + 3\sqrt{\frac{3}{2}}c_1c_2\kappa\lambda + 3\sqrt{2}c_2c_3\kappa\lambda - 3\sqrt{\frac{3}{2}}c_6c_7\kappa\lambda - 3\sqrt{2}c_7c_8\kappa\lambda - \right.$$

$$c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) + c_8^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) - c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right) + c_6^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right) \left. \right] +$$

$$\left[\frac{1}{2}c_7c_{10}g_e\beta + c_8c_{11}\beta \left(-\frac{g_e}{2} - \frac{3\kappa}{2} \right) + c_6c_9\beta \left(\frac{3g_e}{2} + \frac{3\kappa}{2} \right) \right]^2 /$$

$$\left[-\frac{2c_7^2\Delta}{3} + \frac{2c_{10}\Delta}{3} + 3\sqrt{\frac{3}{2}}c_6c_7\kappa\lambda - 3\sqrt{2}c_7c_8\kappa\lambda + 3\sqrt{\frac{3}{2}}c_9c_{10}\kappa\lambda - 3\sqrt{2}c_{10}c_{11}\kappa\lambda + \right.$$

$$c_8^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) - c_{11}^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) + c_6^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right) - c_9^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right) \left. \right]$$

$$E_{z,\pm 4}^{(2)} = \left[\frac{1}{2}c_2c_{10}g_e\beta + c_3c_{11}\beta \left(-\frac{g_e}{2} - \frac{3\kappa}{2} \right) + c_1c_9\beta \left(\frac{3g_e}{2} + \frac{3\kappa}{2} \right) \right]^2 /$$

$$\left[\frac{2c_2^2\Delta}{3} - \frac{2c_{10}\Delta}{3} - 3\sqrt{\frac{3}{2}}c_1c_2\kappa\lambda + 3\sqrt{2}c_2c_3\kappa\lambda - 3\sqrt{\frac{3}{2}}c_9c_{10}\kappa\lambda + 3\sqrt{2}c_{10}c_{11}\kappa\lambda - \right.$$

$$c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) + c_{11}^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) - c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right) + c_9^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right) \left. \right] +$$

$$\left[\frac{1}{2}c_7c_{10}g_e\beta + c_8c_{11}\beta \left(-\frac{g_e}{2} - \frac{3\kappa}{2} \right) + c_6c_9\beta \left(\frac{3g_e}{2} + \frac{3\kappa}{2} \right) \right]^2 /$$

$$\left[\frac{2c_7^2\Delta}{3} - \frac{2c_{10}^2\Delta}{3} + 3\sqrt{\frac{3}{2}}c_6c_7\kappa\lambda + 3\sqrt{2}c_7c_8\kappa\lambda - 3\sqrt{\frac{3}{2}}c_9c_{10}\kappa\lambda - 3\sqrt{2}c_{10}c_{11}\kappa\lambda - \right.$$

$$c_8^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) + c_{11}^2 \left(\frac{\Delta}{3} + \frac{3\kappa\lambda}{4} \right) - c_6^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right) + c_9^2 \left(\frac{\Delta}{3} + \frac{9\kappa\lambda}{4} \right) \left. \right]$$

$$E_{z,\pm 5}^{(2)} = \left[\frac{3}{2}c_4c_{12}g_e\beta + c_5c_{13}\beta \left(\frac{g_e}{2} - \frac{3\kappa}{2} \right) \right]^2 /$$

$$\left[\frac{2c_4^2\Delta}{3} - \frac{2c_{12}^2\Delta}{3} + 3\sqrt{\frac{3}{2}}c_4c_5\kappa\lambda - 3\sqrt{\frac{3}{2}}c_{12}c_{13}\kappa\lambda - c_5^2 \left(\frac{\Delta}{3} - \frac{3\kappa\lambda}{4} \right) + c_{13}^2 \left(\frac{\Delta}{3} - \frac{3\kappa\lambda}{4} \right) \right]$$

$$E_{z,\pm 6}^{(2)} = 0$$

$$E_{x,1}^{(1)} = -E_{x,-1}^{(1)} = c_2^2g_e\beta + \sqrt{3}c_1c_3g_e\beta - \frac{3c_2c_3\beta\kappa}{\sqrt{2}}$$

$$E_{x,\pm 2}^{(1)} = 0$$

$$E_{x,3}^{(1)} = -E_{x,-3}^{(1)} = c_7^2g_e\beta + \sqrt{3}c_6c_8g_e\beta - \frac{3c_7c_8\beta\kappa}{\sqrt{2}}$$

$$E_{x,4}^{(1)} = -E_{x,-4}^{(1)} = c_{10}^2g_e\beta + \sqrt{3}c_9c_{11}g_e\beta - \frac{3c_{10}c_{11}\beta\kappa}{\sqrt{2}}$$

$$E_{x,\pm 5}^{(1)} = 0$$

$$E_{x,\pm 6}^{(1)} = 0$$

$$\begin{aligned}
E_{x,\pm 1}^{(2)} = & \left(\frac{1}{2} \sqrt{3} c_2 c_4 g_e \beta + c_3 c_5 g_e \beta - \frac{3c_1 c_4 \beta \kappa}{2\sqrt{2}} - \frac{3c_2 c_5 \beta \kappa}{2\sqrt{2}} \right)^2 / \\
& \left[-\frac{2c_2^2 \Delta}{2} + \frac{2c_4^2 \Delta}{3} - 3\sqrt{\frac{3}{2}} c_1 c_2 \kappa \lambda - 3\sqrt{2} c_2 c_3 \kappa \lambda + 3\sqrt{\frac{3}{2}} c_4 c_5 \kappa \lambda - \right. \\
& \left. c_5^2 \left(\frac{\Delta}{3} - \frac{3\kappa \lambda}{4} \right) + c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) + c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] + \\
& \left(\frac{1}{2} \sqrt{3} c_2 c_{12} g_e \beta + c_3 c_{13} g_e \beta - \frac{3c_1 c_{13} \beta \kappa}{2\sqrt{2}} - \frac{3c_2 c_{13} \beta \kappa}{2\sqrt{2}} \right)^2 / \\
& \left[-\frac{2c_2^2 \Delta}{3} + \frac{2c_{12}^2 \Delta}{3} - 3\sqrt{\frac{3}{2}} c_1 c_2 \kappa \lambda - 3\sqrt{2} c_2 c_3 \kappa \lambda + 3\sqrt{\frac{3}{2}} c_{12} c_{13} \kappa \lambda - \right. \\
& \left. c_{13}^2 \left(\frac{\Delta}{3} - \frac{3\kappa \lambda}{4} \right) + c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) + c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] + \\
& \left[c_2 c_7 g_e \beta + \frac{1}{2} \sqrt{3} (c_3 c_6 + c_1 c_8) g_e \beta - \frac{3(c_3 c_7 + c_2 c_8) \beta \kappa}{2\sqrt{2}} \right]^2 / \\
& \left[-\frac{2c_2^2 \Delta}{3} + \frac{2c_7^2 \Delta}{3} - 3\sqrt{\frac{3}{2}} c_1 c_2 \kappa \lambda - 3\sqrt{2} c_2 c_3 \kappa \lambda + 3\sqrt{\frac{3}{2}} c_6 c_7 \kappa \lambda + 3\sqrt{2} c_7 c_8 \kappa \lambda + \right. \\
& \left. c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) - c_8^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) + c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) - c_6^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] + \\
& \left[c_2 c_{10} g_e \beta + \frac{1}{2} \sqrt{3} (c_3 c_9 + c_1 c_{11}) g_e \beta - \frac{3(c_3 c_{10} + c_2 c_{11}) \beta \kappa}{2\sqrt{2}} \right]^2 / \\
& \left[-\frac{2c_2^2 \Delta}{3} + \frac{2c_{10}^2 \Delta}{3} - 3\sqrt{\frac{3}{2}} c_1 c_2 \kappa \lambda - 3\sqrt{2} c_2 c_3 \kappa \lambda + 3\sqrt{\frac{3}{2}} c_9 c_{10} \kappa \lambda + 3\sqrt{2} c_{10} c_{11} \kappa \lambda + \right. \\
& \left. c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) - c_{11}^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) + c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) - c_9^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] \\
E_{x,\pm 2}^{(2)} = & \left(\frac{1}{2} \sqrt{3} c_5 g_e \beta - \frac{3c_4 \beta \kappa}{2\sqrt{2}} \right)^2 / \\
& \left[-\frac{\Delta}{3} - \frac{2c_4^2 \Delta}{3} + \frac{9\kappa \lambda}{4} - 3\sqrt{\frac{3}{2}} c_4 c_5 \kappa \lambda + c_5^2 \left(\frac{\Delta}{3} - \frac{3\kappa \lambda}{4} \right) \right] + \\
& \left(\frac{1}{2} \sqrt{3} c_2 c_4 g_e \beta + c_3 c_5 g_e \beta - \frac{3c_1 c_4 \beta \kappa}{2\sqrt{2}} - \frac{3c_2 c_5 \beta \kappa}{2\sqrt{2}} \right)^2 / \\
& \left[\frac{2c_2^2 \Delta}{3} - \frac{2c_4^2 \Delta}{3} + 3\sqrt{\frac{3}{2}} c_1 c_2 \kappa \lambda + 3\sqrt{2} c_2 c_3 \kappa \lambda - 3\sqrt{\frac{3}{2}} c_4 c_5 \kappa \lambda + \right. \\
& \left. c_5^2 \left(\frac{\Delta}{3} - \frac{3\kappa \lambda}{4} \right) - c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) - c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] + \\
& \left(\frac{1}{2} \sqrt{3} c_4 c_7 g_e \beta + c_5 c_8 g_e \beta - \frac{3c_4 c_6 \beta \kappa}{2\sqrt{2}} - \frac{3c_5 c_7 \beta \kappa}{2\sqrt{2}} \right)^2 / \\
& \left[-\frac{2c_4^2 \Delta}{3} + \frac{2c_7^2 \Delta}{3} - 3\sqrt{\frac{3}{2}} c_4 c_5 \kappa \lambda + 3\sqrt{\frac{3}{2}} c_6 c_7 \kappa \lambda + 3\sqrt{2} c_7 c_8 \kappa \lambda + \right. \\
& \left. c_5^2 \left(\frac{\Delta}{3} - \frac{3\kappa \lambda}{4} \right) - c_8^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) - c_6^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] +
\end{aligned}$$

$$\begin{aligned}
& \left(\frac{1}{2} \sqrt{3} c_4 c_{10} g_e \beta + c_5 c_{11} g_e \beta - \frac{3 c_4 c_9 \beta \kappa}{2 \sqrt{2}} - \frac{3 c_5 c_{10} \beta \kappa}{2 \sqrt{2}} \right)^2 / \\
& \left[-\frac{2 c_4^2 \Delta}{3} + \frac{2 c_{10} \Delta}{3} - 3 \sqrt{\frac{3}{2}} c_4 c_5 \kappa \lambda + 3 \sqrt{\frac{3}{2}} c_9 c_{10} \kappa \lambda + 3 \sqrt{2} c_{10} c_{11} \kappa \lambda + \right. \\
& \left. c_5^2 \left(\frac{\Delta}{3} - \frac{3 \kappa \lambda}{4} \right) - c_{11}^2 \left(\frac{\Delta}{3} + \frac{3 \kappa \lambda}{4} \right) - c_9^2 \left(\frac{\Delta}{3} + \frac{9 \kappa \lambda}{4} \right) \right] \\
E_{x, \pm 3}^{(2)} = & \left(\frac{1}{2} \sqrt{3} c_4 c_7 g_e \beta + c_5 c_8 g_e \beta - \frac{3 c_4 c_6 \beta \kappa}{2 \sqrt{2}} - \frac{3 c_5 c_7 \beta \kappa}{2 \sqrt{2}} \right)^2 / \\
& \left[\frac{2 c_4^2 \Delta}{3} - \frac{2 c_7^2 \Delta}{3} + 3 \sqrt{\frac{3}{2}} c_4 c_5 \kappa \lambda - 3 \sqrt{\frac{3}{2}} c_6 c_7 \kappa \lambda - 3 \sqrt{2} c_7 c_8 \kappa \lambda - \right. \\
& \left. c_5^2 \left(\frac{\Delta}{3} - \frac{3 \kappa \lambda}{4} \right) + c_8^2 \left(\frac{\Delta}{3} + \frac{3 \kappa \lambda}{4} \right) + c_6^2 \left(\frac{\Delta}{3} + \frac{9 \kappa \lambda}{4} \right) \right] + \\
& \left(\frac{1}{2} \sqrt{3} c_7 c_{12} g_e \beta + c_8 c_{13} g_e \beta - \frac{3 c_6 c_{12} \beta \kappa}{2 \sqrt{2}} - \frac{3 c_7 c_{13} \beta \kappa}{2 \sqrt{2}} \right)^2 / \\
& \left[-\frac{2 c_7^2 \Delta}{3} + \frac{2 c_{12}^2 \Delta}{3} - 3 \sqrt{\frac{3}{2}} c_6 c_7 \kappa \lambda - 3 \sqrt{2} c_7 c_8 \kappa \lambda + 3 \sqrt{\frac{3}{2}} c_{12} c_{13} \kappa \lambda - \right. \\
& \left. c_{13}^2 \left(\frac{\Delta}{3} - \frac{3 \kappa \lambda}{4} \right) + c_8^2 \left(\frac{\Delta}{3} + \frac{3 \kappa \lambda}{4} \right) + c_6^2 \left(\frac{\Delta}{3} + \frac{9 \kappa \lambda}{4} \right) \right] + \\
& \left[c_2 c_7 g_e \beta + \frac{1}{2} \sqrt{3} (c_3 c_6 + c_1 c_8) g_e \beta - \frac{3 (c_3 c_7 + c_2 c_8) \beta \kappa}{2 \sqrt{2}} \right]^2 / \\
& \left[\frac{2 c_2^2 \Delta}{3} - \frac{2 c_7^2 \Delta}{3} + 3 \sqrt{\frac{3}{2}} c_1 c_2 \kappa \lambda + 3 \sqrt{2} c_2 c_3 \kappa \lambda - 3 \sqrt{\frac{3}{2}} c_6 c_7 \kappa \lambda - 3 \sqrt{2} c_7 c_8 \kappa \lambda - \right. \\
& \left. c_3^2 \left(\frac{\Delta}{3} + \frac{3 \kappa \lambda}{4} \right) + c_8^2 \left(\frac{\Delta}{3} + \frac{3 \kappa \lambda}{4} \right) - c_1^2 \left(\frac{\Delta}{3} + \frac{9 \kappa \lambda}{4} \right) + c_6^2 \left(\frac{\Delta}{3} + \frac{9 \kappa \lambda}{4} \right) \right] + \\
& \left[c_7 c_{10} g_e \beta + \frac{1}{2} \sqrt{3} (c_8 c_9 + c_6 c_{11}) g_e \beta - \frac{3 (c_8 c_{10} + c_7 c_{11}) \beta \kappa}{2 \sqrt{2}} \right]^2 / \\
& \left[-\frac{2 c_7^2 \Delta}{3} + \frac{2 c_{10}^2 \Delta}{3} - 3 \sqrt{\frac{3}{2}} c_6 c_7 \kappa \lambda - 3 \sqrt{2} c_7 c_8 \kappa \lambda + 3 \sqrt{\frac{3}{2}} c_9 c_{10} \kappa \lambda + 3 \sqrt{2} c_{10} c_{11} \kappa \lambda + \right. \\
& \left. c_8^2 \left(\frac{\Delta}{3} + \frac{3 \kappa \lambda}{4} \right) - c_{11}^2 \left(\frac{\Delta}{3} + \frac{3 \kappa \lambda}{4} \right) + c_6^2 \left(\frac{\Delta}{3} + \frac{9 \kappa \lambda}{4} \right) - c_9^2 \left(\frac{\Delta}{3} + \frac{9 \kappa \lambda}{4} \right) \right] \\
E_{x, \pm 4}^{(2)} = & \left(\frac{1}{2} \sqrt{3} c_4 c_{10} g_e \beta + c_5 c_{11} g_e \beta - \frac{3 c_4 c_9 \beta \kappa}{2 \sqrt{2}} - \frac{3 c_5 c_{10} \beta \kappa}{2 \sqrt{2}} \right)^2 / \\
& \left[\frac{2 c_4^2 \Delta}{3} - \frac{2 c_{10}^2 \Delta}{3} + 3 \sqrt{\frac{3}{2}} c_4 c_5 \kappa \lambda - 3 \sqrt{\frac{3}{2}} c_9 c_{10} \kappa \lambda - 3 \sqrt{2} c_{10} c_{11} \kappa \lambda - \right. \\
& \left. c_5^2 \left(\frac{\Delta}{3} - \frac{3 \kappa \lambda}{4} \right) + c_{11}^2 \left(\frac{\Delta}{3} + \frac{3 \kappa \lambda}{4} \right) + c_9^2 \left(\frac{\Delta}{3} + \frac{9 \kappa \lambda}{4} \right) \right] +
\end{aligned}$$

$$\begin{aligned}
& \left(\frac{1}{2} \sqrt{3} c_{10} c_{12} g_e \beta + c_{11} c_{13} g_e \beta - \frac{3c_9 c_{12} \beta \kappa}{2\sqrt{2}} - \frac{3c_{10} c_{13} \beta \kappa}{2\sqrt{2}} \right)^2 / \\
& \left[-\frac{2c_{10}^2 \Delta}{3} + \frac{2c_{12}^2 \Delta}{3} - 3\sqrt{\frac{3}{2}} c_9 c_{10} \kappa \lambda - 3\sqrt{2} c_{10} c_{11} \kappa \lambda + 3\sqrt{\frac{3}{2}} c_{12} c_{13} \kappa \lambda - \right. \\
& \left. c_{13}^2 \left(\frac{\Delta}{3} - \frac{3\kappa \lambda}{4} \right) + c_{11}^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) + c_9^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] + \\
& \left[c_2 c_{10} g_e \beta + \frac{1}{2} \sqrt{3} (c_3 c_9 + c_1 c_{11}) g_e \beta - \frac{3(c_3 c_{10} + c_2 c_{11}) \beta \kappa}{2\sqrt{2}} \right]^2 / \\
& \left[\frac{2c_2^2 \Delta}{3} - \frac{2c_{10}^2 \Delta}{3} + 3\sqrt{\frac{3}{2}} c_1 c_2 \kappa \lambda + 3\sqrt{2} c_2 c_3 \kappa \lambda - 3\sqrt{\frac{3}{2}} c_9 c_{10} \kappa \lambda - 3\sqrt{2} c_{10} c_{11} \kappa \lambda - \right. \\
& \left. c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) + c_{12}^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) - c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) + c_9^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] + \\
& \left[c_7 c_{10} g_e \beta + \frac{1}{2} \sqrt{3} (c_8 c_9 + c_6 c_{11}) g_e \beta - \frac{3(c_8 c_{10} + c_7 c_{11}) \beta \kappa}{2\sqrt{2}} \right]^2 / \\
& \left[\frac{2c_7^2 \Delta}{3} - \frac{2c_{10}^2 \Delta}{3} + 3\sqrt{\frac{3}{2}} c_6 c_7 \kappa \lambda + 3\sqrt{2} c_7 c_8 \kappa \lambda - 3\sqrt{\frac{3}{2}} c_9 c_{10} \kappa \lambda - 3\sqrt{2} c_{10} c_{11} \kappa \lambda - \right. \\
& \left. c_8^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) + c_{11}^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) - c_6^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) + c_9^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] \\
E_{x,\pm 5}^{(2)} &= \left(\frac{1}{2} \sqrt{3} c_{13} g_e \beta - \frac{2c_{12} \beta \kappa}{2\sqrt{2}} \right)^2 / \\
& \left[-\frac{\Delta}{3} - \frac{2c_{12}^2 \Delta}{3} + \frac{9\kappa \lambda}{4} - 3\sqrt{\frac{3}{2}} c_{12} c_{13} \kappa \lambda + c_{13}^2 \left(\frac{\Delta}{3} - \frac{3\kappa \lambda}{4} \right) \right] + \\
& \left(\frac{1}{2} \sqrt{3} c_2 c_{12} g_e \beta + c_3 c_{13} g_e \beta - \frac{3c_1 c_{12} \beta \kappa}{2\sqrt{2}} - \frac{3c_2 c_{13} \beta \kappa}{2\sqrt{2}} \right)^2 / \\
& \left[\frac{2c_2^2 \Delta}{3} - \frac{2c_{12}^2 \Delta}{3} + 3\sqrt{\frac{3}{2}} c_1 c_2 \kappa \lambda + 3\sqrt{2} c_2 c_3 \kappa \lambda - 3\sqrt{\frac{3}{2}} c_{12} c_{13} \kappa \lambda + \right. \\
& \left. c_{13}^2 \left(\frac{\Delta}{3} - \frac{3\kappa \lambda}{4} \right) - c_3^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) - c_1^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] + \\
& \left(\frac{1}{2} \sqrt{3} c_7 c_{12} g_e \beta + c_8 c_{13} g_e \beta - \frac{3c_6 c_{12} \beta \kappa}{2\sqrt{2}} - \frac{3c_7 c_{13} \beta \kappa}{2\sqrt{2}} \right)^2 / \\
& \left[\frac{2c_7^2 \Delta}{3} - \frac{2c_{12}^2 \Delta}{3} + 3\sqrt{\frac{3}{2}} c_6 c_7 \kappa \lambda + 3\sqrt{2} c_7 c_8 \kappa \lambda - 3\sqrt{\frac{3}{2}} c_{12} c_{13} \kappa \lambda + \right. \\
& \left. c_{13}^2 \left(\frac{\Delta}{3} - \frac{3\kappa \lambda}{4} \right) - c_8^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) - c_6^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right] + \\
& \left(\frac{1}{2} \sqrt{3} c_{10} c_{12} g_e \beta + c_{11} c_{13} g_e \beta - \frac{3c_9 c_{12} \beta \kappa}{2\sqrt{2}} - \frac{3c_{10} c_{13} \beta \kappa}{2\sqrt{2}} \right)^2 / \\
& \left[\frac{2c_{10}^2 \Delta}{3} - \frac{2c_{12}^2 \Delta}{3} + 3\sqrt{\frac{3}{2}} c_9 c_{10} \kappa \lambda + 3\sqrt{2} c_{10} c_{11} \kappa \lambda - 3\sqrt{\frac{3}{2}} c_{12} c_{13} \kappa \lambda + \right. \\
& \left. c_{13}^2 \left(\frac{\Delta}{3} - \frac{3\kappa \lambda}{4} \right) - c_{11}^2 \left(\frac{\Delta}{3} + \frac{3\kappa \lambda}{4} \right) - c_9^2 \left(\frac{\Delta}{3} + \frac{9\kappa \lambda}{4} \right) \right]
\end{aligned}$$

$$E_{x,\pm 6}^{(2)} = \left(\frac{1}{2} \sqrt{3} c_5 g_e \beta - \frac{3c_4 \beta \kappa}{2\sqrt{2}} \right)^2 / \left[\frac{\Delta}{3} + \frac{2c_4^2 \Delta}{3} - \frac{9\kappa\lambda}{4} + 3\sqrt{\frac{3}{2}} c_4 c_5 \kappa \lambda - c_5^2 \left(\frac{\Delta}{3} - \frac{3\kappa\lambda}{4} \right) \right] + \left(\frac{1}{2} \sqrt{3} c_{13} g_e \beta - \frac{3c_{12} \beta \kappa}{2\sqrt{2}} \right)^2 / \left[\frac{\Delta}{3} + \frac{2c_{12}^2 \Delta}{3} - \frac{9\kappa\lambda}{4} + 3\sqrt{\frac{3}{2}} c_{12} c_{13} \kappa \lambda - c_{13}^2 \left(\frac{\Delta}{3} - \frac{3\kappa\lambda}{4} \right) \right]$$

$$J_{eff} = \alpha_x^2 J,$$

$$D_{eff} = [\alpha_x^2 - \alpha_z^2] J.$$

$$D_{tri} = D_{eff} / 2$$

$$\alpha_z = 3c_1^2 + c_2^2 - c_3^2,$$

$$\alpha_x = 2c_2^2 + 2\sqrt{3} c_1 c_3.$$