VHEGEN: A vibronic Hamiltonian expansion generator for trigonal and tetragonal polyatomic systems

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Thank you for using `VHEGEN`, the `V`-ibronic `H`-amiltonian `E`-xpansion `GEN`-erator for trigonal and tetragonal polyatomic systems. This is a `VHEGEN` output file compiled by `pdflatex`. If the `VHEGEN` package was used in research resulting in a publication, please reference the article in *Computer Physics Communications* which describes the program ([doi here]). Additional information regarding the matrix element expansion process, including the independent matrix element eigenvalues, their root formulas and constraints, and their transformation to the real basis (if applicable), can be found in the `log` output file. For questions, bugs, or comments, please contact robert.lang@mail.utoronto.ca.

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1 Vibronic interaction

$E'' \otimes (e' + e')$ in D_{3h}

2 Vibronic Hamiltonian operator in the complex E basis

$\hat{H} = \begin{pmatrix} |+\rangle & |-\rangle \end{pmatrix} \begin{pmatrix} H_{++} & H_{+-} \\ H_{-+} & H_{--} \end{pmatrix} \begin{pmatrix} \langle+| \\ \langle-| \end{pmatrix}$

3 Matrix element expansions in the complex E basis

3.1 Order: 0

Number of fitting parameters: H_{++}: 1, H_{+-}: 0.

Polar e-coordinates:

$H_{++}^{(0)} = a_{0,0,0,0}^{r}$

$H_{--}^{(0)} = a_{0,0,0,0}^{r}$

$H_{+-}^{(0)} = 0$

$H_{-+}^{(0)} = 0$

Cartesian e-coordinates:

$H_{++}^{(0)} = a_{0,0,0,0}^{r}$

$H_{--}^{(0)} = a_{0,0,0,0}^{r}$

$H_{+-}^{(0)} = 0$

$H_{-+}^{(0)} = 0$

3.2 Order: 1

Number of fitting parameters: H_{++}: 0, H_{+-}: 2.

Polar e-coordinates:

$$H_{++}^{(1)} = 0$$

$$H_{--}^{(1)} = 0$$

$$H_{+-}^{(1)} = -ib_{0,0,-1,-1}^{r}\rho_{\alpha}\sin\left(\phi_{\alpha}\right) + b_{0,0,-1,-1}^{r}\rho_{\alpha}\cos\left(\phi_{\alpha}\right) - ib_{0,0,0,-1}^{r}\rho_{\beta}\sin\left(\phi_{\beta}\right) + b_{0,0,0,-1}^{r}\rho_{\beta}\cos\left(\phi_{\beta}\right)$$

$$H_{-+}^{(1)} = ib_{0,0,-1,-1}^{r}\rho_{\alpha}\sin\left(\phi_{\alpha}\right) + b_{0,0,-1,-1}^{r}\rho_{\alpha}\cos\left(\phi_{\alpha}\right) + ib_{0,0,0,-1}^{r}\rho_{\beta}\sin\left(\phi_{\beta}\right) + b_{0,0,0,-1}^{r}\rho_{\beta}\cos\left(\phi_{\beta}\right)$$

Cartesian e-coordinates:

$$H_{++}^{(1)} = 0$$

$$H_{--}^{(1)} = 0$$

$$H_{+-}^{(1)} = b_{0,0,-1,-1}^{r}x_{\alpha} - ib_{0,0,-1,-1}^{r}y_{\alpha} + b_{0,0,0,-1}^{r}x_{\beta} - ib_{0,0,0,-1}^{r}y_{\beta}$$

$$H_{-+}^{(1)} = b_{0,0,-1,-1}^{r}x_{\alpha} + ib_{0,0,-1,-1}^{r}y_{\alpha} + b_{0,0,0,-1}^{r}x_{\beta} + ib_{0,0,0,-1}^{r}y_{\beta}$$

3.3 Order: 2

Number of fitting parameters: H_{++}: 3, H_{+-}: 3.

Polar e-coordinates:

$$H_{++}^{(2)} = a_{0,0,1,0}^{r}\rho_{\alpha}\rho_{\beta}\cos\left(\phi_{\alpha} - \phi_{\beta}\right) + a_{0,2,0,0}^{r}\rho_{\beta}^{2} + a_{2,0,0,0}^{r}\rho_{\alpha}^{2}$$

$$H_{--}^{(2)} = a_{0,0,1,0}^{r}\rho_{\alpha}\rho_{\beta}\cos\left(\phi_{\alpha} - \phi_{\beta}\right) + a_{0,2,0,0}^{r}\rho_{\beta}^{2} + a_{2,0,0,0}^{r}\rho_{\alpha}^{2}$$

$$\begin{aligned} H_{+-}^{(2)} = {} & ib_{0,0,0,2}^{r}\rho_{\beta}^{2}\sin\left(2\phi_{\beta}\right) + b_{0,0,0,2}^{r}\rho_{\beta}^{2}\cos\left(2\phi_{\beta}\right) + ib_{0,0,1,2}^{r}\rho_{\alpha}\rho_{\beta}\sin\left(\phi_{\alpha} + \phi_{\beta}\right) + b_{0,0,1,2}^{r}\rho_{\alpha}\rho_{\beta}\cos\left(\phi_{\alpha} + \phi_{\beta}\right) \\ & + ib_{0,0,2,2}^{r}\rho_{\alpha}^{2}\sin\left(2\phi_{\alpha}\right) + b_{0,0,2,2}^{r}\rho_{\alpha}^{2}\cos\left(2\phi_{\alpha}\right) \end{aligned}$$

$$\begin{aligned} H_{-+}^{(2)} = {} & -ib_{0,0,0,2}^{r}\rho_{\beta}^{2}\sin\left(2\phi_{\beta}\right) + b_{0,0,0,2}^{r}\rho_{\beta}^{2}\cos\left(2\phi_{\beta}\right) - ib_{0,0,1,2}^{r}\rho_{\alpha}\rho_{\beta}\sin\left(\phi_{\alpha} + \phi_{\beta}\right) + b_{0,0,1,2}^{r}\rho_{\alpha}\rho_{\beta}\cos\left(\phi_{\alpha} + \phi_{\beta}\right) \\ & - ib_{0,0,2,2}^{r}\rho_{\alpha}^{2}\sin\left(2\phi_{\alpha}\right) + b_{0,0,2,2}^{r}\rho_{\alpha}^{2}\cos\left(2\phi_{\alpha}\right) \end{aligned}$$

Cartesian e-coordinates:

$$H_{++}^{(2)} = a_{0,0,1,0}^{r}\left(x_{\alpha}x_{\beta} + y_{\alpha}y_{\beta}\right) + a_{0,2,0,0}^{r}\left(x_{\beta}^{2} + y_{\beta}^{2}\right) + a_{2,0,0,0}^{r}\left(x_{\alpha}^{2} + y_{\alpha}^{2}\right)$$

$$H_{--}^{(2)} = a_{0,0,1,0}^{r}\left(x_{\alpha}x_{\beta} + y_{\alpha}y_{\beta}\right) + a_{0,2,0,0}^{r}\left(x_{\beta}^{2} + y_{\beta}^{2}\right) + a_{2,0,0,0}^{r}\left(x_{\alpha}^{2} + y_{\alpha}^{2}\right)$$

$$\begin{aligned}H_{+-}^{(2)} = {} & 2ib_{0,0,0,2}^{r}x_{\beta}y_{\beta} + b_{0,0,0,2}^{r}\left(x_{\beta} - y_{\beta}\right)\left(x_{\beta} + y_{\beta}\right) + b_{0,0,1,2}^{r}\left(x_{\alpha}x_{\beta} - y_{\alpha}y_{\beta}\right) + ib_{0,0,1,2}^{r}\left(x_{\alpha}y_{\beta} + x_{\beta}y_{\alpha}\right) \\ & + 2ib_{0,0,2,2}^{r}x_{\alpha}y_{\alpha} + b_{0,0,2,2}^{r}\left(x_{\alpha} - y_{\alpha}\right)\left(x_{\alpha} + y_{\alpha}\right)\end{aligned}$$

$$\begin{aligned}H_{-+}^{(2)} = {} & -2ib_{0,0,0,2}^{r}x_{\beta}y_{\beta} + b_{0,0,0,2}^{r}\left(x_{\beta} - y_{\beta}\right)\left(x_{\beta} + y_{\beta}\right) + b_{0,0,1,2}^{r}\left(x_{\alpha}x_{\beta} - y_{\alpha}y_{\beta}\right) - ib_{0,0,1,2}^{r}\left(x_{\alpha}y_{\beta} + x_{\beta}y_{\alpha}\right) \\ & - 2ib_{0,0,2,2}^{r}x_{\alpha}y_{\alpha} + b_{0,0,2,2}^{r}\left(x_{\alpha} - y_{\alpha}\right)\left(x_{\alpha} + y_{\alpha}\right)\end{aligned}$$

3.4 Order: 3

Number of fitting parameters: H_{++}: 4, H_{+-}: 6.

Polar e-coordinates:

$$H_{++}^{(3)} = a_{0,0,0,3}^{r}\rho_{\beta}^{3}\cos\left(3\phi_{\beta}\right) + a_{0,0,1,3}^{r}\rho_{\alpha}\rho_{\beta}^{2}\cos\left(\phi_{\alpha} + 2\phi_{\beta}\right) + a_{0,0,2,3}^{r}\rho_{\alpha}^{2}\rho_{\beta}\cos\left(2\phi_{\alpha} + \phi_{\beta}\right) + a_{0,0,3,3}^{r}\rho_{\alpha}^{3}\cos\left(3\phi_{\alpha}\right)$$

$$H_{--}^{(3)} = a_{0,0,0,3}^{r}\rho_{\beta}^{3}\cos\left(3\phi_{\beta}\right) + a_{0,0,1,3}^{r}\rho_{\alpha}\rho_{\beta}^{2}\cos\left(\phi_{\alpha} + 2\phi_{\beta}\right) + a_{0,0,2,3}^{r}\rho_{\alpha}^{2}\rho_{\beta}\cos\left(2\phi_{\alpha} + \phi_{\beta}\right) + a_{0,0,3,3}^{r}\rho_{\alpha}^{3}\cos\left(3\phi_{\alpha}\right)$$

$$\begin{aligned}H_{+-}^{(3)} = {} & -ib_{0,0,-2,-1}^{r}\rho_{\alpha}^{2}\rho_{\beta}\sin\left(2\phi_{\alpha} - \phi_{\beta}\right) + b_{0,0,-2,-1}^{r}\rho_{\alpha}^{2}\rho_{\beta}\cos\left(2\phi_{\alpha} - \phi_{\beta}\right) + ib_{0,0,1,-1}^{r}\rho_{\alpha}\rho_{\beta}^{2}\sin\left(\phi_{\alpha} - 2\phi_{\beta}\right) \\ & + b_{0,0,1,-1}^{r}\rho_{\alpha}\rho_{\beta}^{2}\cos\left(\phi_{\alpha} - 2\phi_{\beta}\right) - ib_{0,2,-1,-1}^{r}\rho_{\alpha}\rho_{\beta}^{2}\sin\left(\phi_{\alpha}\right) + b_{0,2,-1,-1}^{r}\rho_{\alpha}\rho_{\beta}^{2}\cos\left(\phi_{\alpha}\right) \\ & - ib_{0,2,0,-1}^{r}\rho_{\beta}^{3}\sin\left(\phi_{\beta}\right) + b_{0,2,0,-1}^{r}\rho_{\beta}^{3}\cos\left(\phi_{\beta}\right) - ib_{2,0,-1,-1}^{r}\rho_{\alpha}^{3}\sin\left(\phi_{\alpha}\right) + b_{2,0,-1,-1}^{r}\rho_{\alpha}^{3}\cos\left(\phi_{\alpha}\right) \\ & - ib_{2,0,0,-1}^{r}\rho_{\alpha}^{2}\rho_{\beta}\sin\left(\phi_{\beta}\right) + b_{2,0,0,-1}^{r}\rho_{\alpha}^{2}\rho_{\beta}\cos\left(\phi_{\beta}\right)\end{aligned}$$

$$\begin{aligned}H_{-+}^{(3)} = {} & ib_{0,0,-2,-1}^{r}\rho_{\alpha}^{2}\rho_{\beta}\sin\left(2\phi_{\alpha} - \phi_{\beta}\right) + b_{0,0,-2,-1}^{r}\rho_{\alpha}^{2}\rho_{\beta}\cos\left(2\phi_{\alpha} - \phi_{\beta}\right) - ib_{0,0,1,-1}^{r}\rho_{\alpha}\rho_{\beta}^{2}\sin\left(\phi_{\alpha} - 2\phi_{\beta}\right) \\ & + b_{0,0,1,-1}^{r}\rho_{\alpha}\rho_{\beta}^{2}\cos\left(\phi_{\alpha} - 2\phi_{\beta}\right) + ib_{0,2,-1,-1}^{r}\rho_{\alpha}\rho_{\beta}^{2}\sin\left(\phi_{\alpha}\right) + b_{0,2,-1,-1}^{r}\rho_{\alpha}\rho_{\beta}^{2}\cos\left(\phi_{\alpha}\right) \\ & + ib_{0,2,0,-1}^{r}\rho_{\beta}^{3}\sin\left(\phi_{\beta}\right) + b_{0,2,0,-1}^{r}\rho_{\beta}^{3}\cos\left(\phi_{\beta}\right) + ib_{2,0,-1,-1}^{r}\rho_{\alpha}^{3}\sin\left(\phi_{\alpha}\right) + b_{2,0,-1,-1}^{r}\rho_{\alpha}^{3}\cos\left(\phi_{\alpha}\right) \\ & + ib_{2,0,0,-1}^{r}\rho_{\alpha}^{2}\rho_{\beta}\sin\left(\phi_{\beta}\right) + b_{2,0,0,-1}^{r}\rho_{\alpha}^{2}\rho_{\beta}\cos\left(\phi_{\beta}\right)\end{aligned}$$

Cartesian e-coordinates:

$$\begin{aligned}H_{++}^{(3)} = {} & a_{0,0,0,3}^{r}x_{\beta}\left(x_{\beta}^{2} - 3y_{\beta}^{2}\right) + a_{0,0,1,3}^{r}\left(x_{\alpha}\left(x_{\beta}^{2} - y_{\beta}^{2}\right) - 2x_{\beta}y_{\alpha}y_{\beta}\right) \\ & + a_{0,0,2,3}^{r}\left(-2x_{\alpha}y_{\alpha}y_{\beta} + x_{\beta}\left(x_{\alpha}^{2} - y_{\alpha}^{2}\right)\right) + a_{0,0,3,3}^{r}x_{\alpha}\left(x_{\alpha}^{2} - 3y_{\alpha}^{2}\right)\end{aligned}$$

$$\begin{aligned}H_{--}^{(3)} = {} & a_{0,0,0,3}^{r}x_{\beta}\left(x_{\beta}^{2} - 3y_{\beta}^{2}\right) + a_{0,0,1,3}^{r}\left(x_{\alpha}\left(x_{\beta}^{2} - y_{\beta}^{2}\right) - 2x_{\beta}y_{\alpha}y_{\beta}\right) \\ & + a_{0,0,2,3}^{r}\left(-2x_{\alpha}y_{\alpha}y_{\beta} + x_{\beta}\left(x_{\alpha}^{2} - y_{\alpha}^{2}\right)\right) + a_{0,0,3,3}^{r}x_{\alpha}\left(x_{\alpha}^{2} - 3y_{\alpha}^{2}\right)\end{aligned}$$

$$
\begin{aligned}
H_{+-}^{(3)} = &\; ib^r_{0,0,-2,-1}\left(-2x_\alpha x_\beta y_\alpha + y_\beta\left(x_\alpha^2 - y_\alpha^2\right)\right) + b^r_{0,0,-2,-1}\left(2x_\alpha y_\alpha y_\beta + x_\beta\left(x_\alpha^2 - y_\alpha^2\right)\right) \\
&+ b^r_{0,0,1,-1}\left(x_\alpha\left(x_\beta^2 - y_\beta^2\right) + 2x_\beta y_\alpha y_\beta\right) - ib^r_{0,0,1,-1}\left(2x_\alpha x_\beta y_\beta + y_\alpha\left(-x_\beta^2 + y_\beta^2\right)\right) \\
&+ b^r_{0,2,-1,-1}x_\alpha\left(x_\beta^2 + y_\beta^2\right) - ib^r_{0,2,-1,-1}y_\alpha\left(x_\beta^2 + y_\beta^2\right) + b^r_{0,2,0,-1}x_\beta\left(x_\beta^2 + y_\beta^2\right) - ib^r_{0,2,0,-1}y_\beta\left(x_\beta^2 + y_\beta^2\right) \\
&+ b^r_{2,0,-1,-1}x_\alpha\left(x_\alpha^2 + y_\alpha^2\right) - ib^r_{2,0,-1,-1}y_\alpha\left(x_\alpha^2 + y_\alpha^2\right) + b^r_{2,0,0,-1}x_\beta\left(x_\alpha^2 + y_\alpha^2\right) - ib^r_{2,0,0,-1}y_\beta\left(x_\alpha^2 + y_\alpha^2\right)
\end{aligned}
$$

$$
\begin{aligned}
H_{-+}^{(3)} = &\; -ib^r_{0,0,-2,-1}\left(-2x_\alpha x_\beta y_\alpha + y_\beta\left(x_\alpha^2 - y_\alpha^2\right)\right) + b^r_{0,0,-2,-1}\left(2x_\alpha y_\alpha y_\beta + x_\beta\left(x_\alpha^2 - y_\alpha^2\right)\right) \\
&+ b^r_{0,0,1,-1}\left(x_\alpha\left(x_\beta^2 - y_\beta^2\right) + 2x_\beta y_\alpha y_\beta\right) + ib^r_{0,0,1,-1}\left(2x_\alpha x_\beta y_\beta + y_\alpha\left(-x_\beta^2 + y_\beta^2\right)\right) \\
&+ b^r_{0,2,-1,-1}x_\alpha\left(x_\beta^2 + y_\beta^2\right) + ib^r_{0,2,-1,-1}y_\alpha\left(x_\beta^2 + y_\beta^2\right) + b^r_{0,2,0,-1}x_\beta\left(x_\beta^2 + y_\beta^2\right) + ib^r_{0,2,0,-1}y_\beta\left(x_\beta^2 + y_\beta^2\right) \\
&+ b^r_{2,0,-1,-1}x_\alpha\left(x_\alpha^2 + y_\alpha^2\right) + ib^r_{2,0,-1,-1}y_\alpha\left(x_\alpha^2 + y_\alpha^2\right) + b^r_{2,0,0,-1}x_\beta\left(x_\alpha^2 + y_\alpha^2\right) + ib^r_{2,0,0,-1}y_\beta\left(x_\alpha^2 + y_\alpha^2\right)
\end{aligned}
$$

4 Vibronic Hamiltonian operator in the real E basis

$$\hat{H} = \begin{pmatrix} |X\rangle & |Y\rangle \end{pmatrix} \begin{pmatrix} H_{XX} & H_{XY} \\ H_{YX} & H_{YY} \end{pmatrix} \begin{pmatrix} \langle X| \\ \langle Y| \end{pmatrix}$$

5 Matrix element expansions in the real E basis

5.1 Order: 0

Number of fitting parameters: H_{XX}: 1 (all from H_{++}), H_{XY}: 0.

Polar e-coordinates:

$$H_{XX}^{(0)} = a^r_{0,0,0,0}$$

$$H_{XY}^{(0)} = 0$$

$$H_{YX}^{(0)} = 0$$

$$H_{YY}^{(0)} = a^r_{0,0,0,0}$$

Cartesian e-coordinates:

$$H_{XX}^{(0)} = a^r_{0,0,0,0}$$

$$H_{XY}^{(0)} = 0$$

$$H_{YX}^{(0)} = 0$$

$$H_{YY}^{(0)} = a^r_{0,0,0,0}$$

5.2 Order: 1

Number of fitting parameters: H_{XX}: 2 (all from H_{+-}), H_{XY}: 2 (all from H_{+-}).

Polar e-coordinates:

$$H_{XX}^{(1)} = b_{0,0,-1,-1}^{r}\rho_{\alpha}\cos(\phi_{\alpha}) + b_{0,0,0,-1}^{r}\rho_{\beta}\cos(\phi_{\beta})$$

$$H_{XY}^{(1)} = b_{0,0,-1,-1}^{r}\rho_{\alpha}\sin(\phi_{\alpha}) + b_{0,0,0,-1}^{r}\rho_{\beta}\sin(\phi_{\beta})$$

$$H_{YX}^{(1)} = b_{0,0,-1,-1}^{r}\rho_{\alpha}\sin(\phi_{\alpha}) + b_{0,0,0,-1}^{r}\rho_{\beta}\sin(\phi_{\beta})$$

$$H_{YY}^{(1)} = -b_{0,0,-1,-1}^{r}\rho_{\alpha}\cos(\phi_{\alpha}) - b_{0,0,0,-1}^{r}\rho_{\beta}\cos(\phi_{\beta})$$

Cartesian e-coordinates:

$$H_{XX}^{(1)} = b_{0,0,-1,-1}^{r}x_{\alpha} + b_{0,0,0,-1}^{r}x_{\beta}$$

$$H_{XY}^{(1)} = b_{0,0,-1,-1}^{r}y_{\alpha} + b_{0,0,0,-1}^{r}y_{\beta}$$

$$H_{YX}^{(1)} = b_{0,0,-1,-1}^{r}y_{\alpha} + b_{0,0,0,-1}^{r}y_{\beta}$$

$$H_{YY}^{(1)} = -b_{0,0,-1,-1}^{r}x_{\alpha} - b_{0,0,0,-1}^{r}x_{\beta}$$

5.3 Order: 2

Number of fitting parameters: H_{XX}: 6 (3 from H_{++}, 3 from H_{+-}), H_{XY}: 3 (all from H_{+-}).

Polar e-coordinates:

$$\begin{aligned} H_{XX}^{(2)} = {} & a_{0,0,1,0}^{r}\rho_{\alpha}\rho_{\beta}\cos(\phi_{\alpha}-\phi_{\beta}) + a_{0,2,0,0}^{r}\rho_{\beta}^{2} + a_{2,0,0,0}^{r}\rho_{\alpha}^{2} + b_{0,0,0,2}^{r}\rho_{\beta}^{2}\cos(2\phi_{\beta}) \\ & + b_{0,0,1,2}^{r}\rho_{\alpha}\rho_{\beta}\cos(\phi_{\alpha}+\phi_{\beta}) + b_{0,0,2,2}^{r}\rho_{\alpha}^{2}\cos(2\phi_{\alpha}) \end{aligned}$$

$$H_{XY}^{(2)} = -b_{0,0,0,2}^{r}\rho_{\beta}^{2}\sin(2\phi_{\beta}) - b_{0,0,1,2}^{r}\rho_{\alpha}\rho_{\beta}\sin(\phi_{\alpha}+\phi_{\beta}) - b_{0,0,2,2}^{r}\rho_{\alpha}^{2}\sin(2\phi_{\alpha})$$

$$H_{YX}^{(2)} = -b_{0,0,0,2}^{r}\rho_{\beta}^{2}\sin(2\phi_{\beta}) - b_{0,0,1,2}^{r}\rho_{\alpha}\rho_{\beta}\sin(\phi_{\alpha}+\phi_{\beta}) - b_{0,0,2,2}^{r}\rho_{\alpha}^{2}\sin(2\phi_{\alpha})$$

$$\begin{aligned} H_{YY}^{(2)} = {} & a_{0,0,1,0}^{r}\rho_{\alpha}\rho_{\beta}\cos(\phi_{\alpha}-\phi_{\beta}) + a_{0,2,0,0}^{r}\rho_{\beta}^{2} + a_{2,0,0,0}^{r}\rho_{\alpha}^{2} - b_{0,0,0,2}^{r}\rho_{\beta}^{2}\cos(2\phi_{\beta}) \\ & - b_{0,0,1,2}^{r}\rho_{\alpha}\rho_{\beta}\cos(\phi_{\alpha}+\phi_{\beta}) - b_{0,0,2,2}^{r}\rho_{\alpha}^{2}\cos(2\phi_{\alpha}) \end{aligned}$$

Cartesian e-coordinates:

$$H_{XX}^{(2)} = a_{0,0,1,0}^{r}\left(x_\alpha x_\beta + y_\alpha y_\beta\right) + a_{0,2,0,0}^{r}\left(x_\beta^2 + y_\beta^2\right) + a_{2,0,0,0}^{r}\left(x_\alpha^2 + y_\alpha^2\right) + b_{0,0,0,2}^{r}\left(x_\beta - y_\beta\right)\left(x_\beta + y_\beta\right)$$
$$+ b_{0,0,1,2}^{r}\left(x_\alpha x_\beta - y_\alpha y_\beta\right) + b_{0,0,2,2}^{r}\left(x_\alpha - y_\alpha\right)\left(x_\alpha + y_\alpha\right)$$

$$H_{XY}^{(2)} = -2b_{0,0,0,2}^{r} x_\beta y_\beta - b_{0,0,1,2}^{r}\left(x_\alpha y_\beta + x_\beta y_\alpha\right) - 2b_{0,0,2,2}^{r} x_\alpha y_\alpha$$

$$H_{YX}^{(2)} = -2b_{0,0,0,2}^{r} x_\beta y_\beta - b_{0,0,1,2}^{r}\left(x_\alpha y_\beta + x_\beta y_\alpha\right) - 2b_{0,0,2,2}^{r} x_\alpha y_\alpha$$

$$H_{YY}^{(2)} = a_{0,0,1,0}^{r}\left(x_\alpha x_\beta + y_\alpha y_\beta\right) + a_{0,2,0,0}^{r}\left(x_\beta^2 + y_\beta^2\right) + a_{2,0,0,0}^{r}\left(x_\alpha^2 + y_\alpha^2\right) - b_{0,0,0,2}^{r}\left(x_\beta - y_\beta\right)\left(x_\beta + y_\beta\right)$$
$$- b_{0,0,1,2}^{r}\left(x_\alpha x_\beta - y_\alpha y_\beta\right) - b_{0,0,2,2}^{r}\left(x_\alpha - y_\alpha\right)\left(x_\alpha + y_\alpha\right)$$

5.4 Order: 3

Number of fitting parameters: H_{XX}: 10 (4 from H_{++}, 6 from H_{+-}), H_{XY}: 6 (all from H_{+-}).

Polar e-coordinates:

$$H_{XX}^{(3)} = a_{0,0,0,3}^{r}\rho_\beta^3\cos\left(3\phi_\beta\right) + a_{0,0,1,3}^{r}\rho_\alpha\rho_\beta^2\cos\left(\phi_\alpha + 2\phi_\beta\right) + a_{0,0,2,3}^{r}\rho_\alpha^2\rho_\beta\cos\left(2\phi_\alpha + \phi_\beta\right) + a_{0,0,3,3}^{r}\rho_\alpha^3\cos\left(3\phi_\alpha\right)$$
$$+ b_{0,0,-2,-1}^{r}\rho_\alpha^2\rho_\beta\cos\left(2\phi_\alpha - \phi_\beta\right) + b_{0,0,1,-1}^{r}\rho_\alpha\rho_\beta^2\cos\left(\phi_\alpha - 2\phi_\beta\right) + b_{0,2,-1,-1}^{r}\rho_\alpha\rho_\beta^2\cos\left(\phi_\alpha\right) + b_{0,2,0,-1}^{r}\rho_\beta^3\cos\left(\phi_\beta\right)$$
$$+ b_{2,0,-1,-1}^{r}\rho_\alpha^3\cos\left(\phi_\alpha\right) + b_{2,0,0,-1}^{r}\rho_\alpha^2\rho_\beta\cos\left(\phi_\beta\right)$$

$$H_{XY}^{(3)} = b_{0,0,-2,-1}^{r}\rho_\alpha^2\rho_\beta\sin\left(2\phi_\alpha - \phi_\beta\right) - b_{0,0,1,-1}^{r}\rho_\alpha\rho_\beta^2\sin\left(\phi_\alpha - 2\phi_\beta\right) + b_{0,2,-1,-1}^{r}\rho_\alpha\rho_\beta^2\sin\left(\phi_\alpha\right) + b_{0,2,0,-1}^{r}\rho_\beta^3\sin\left(\phi_\beta\right)$$
$$+ b_{2,0,-1,-1}^{r}\rho_\alpha^3\sin\left(\phi_\alpha\right) + b_{2,0,0,-1}^{r}\rho_\alpha^2\rho_\beta\sin\left(\phi_\beta\right)$$

$$H_{YX}^{(3)} = b_{0,0,-2,-1}^{r}\rho_\alpha^2\rho_\beta\sin\left(2\phi_\alpha - \phi_\beta\right) - b_{0,0,1,-1}^{r}\rho_\alpha\rho_\beta^2\sin\left(\phi_\alpha - 2\phi_\beta\right) + b_{0,2,-1,-1}^{r}\rho_\alpha\rho_\beta^2\sin\left(\phi_\alpha\right) + b_{0,2,0,-1}^{r}\rho_\beta^3\sin\left(\phi_\beta\right)$$
$$+ b_{2,0,-1,-1}^{r}\rho_\alpha^3\sin\left(\phi_\alpha\right) + b_{2,0,0,-1}^{r}\rho_\alpha^2\rho_\beta\sin\left(\phi_\beta\right)$$

$$H_{YY}^{(3)} = a_{0,0,0,3}^{r}\rho_\beta^3\cos\left(3\phi_\beta\right) + a_{0,0,1,3}^{r}\rho_\alpha\rho_\beta^2\cos\left(\phi_\alpha + 2\phi_\beta\right) + a_{0,0,2,3}^{r}\rho_\alpha^2\rho_\beta\cos\left(2\phi_\alpha + \phi_\beta\right) + a_{0,0,3,3}^{r}\rho_\alpha^3\cos\left(3\phi_\alpha\right)$$
$$- b_{0,0,-2,-1}^{r}\rho_\alpha^2\rho_\beta\cos\left(2\phi_\alpha - \phi_\beta\right) - b_{0,0,1,-1}^{r}\rho_\alpha\rho_\beta^2\cos\left(\phi_\alpha - 2\phi_\beta\right) - b_{0,2,-1,-1}^{r}\rho_\alpha\rho_\beta^2\cos\left(\phi_\alpha\right) - b_{0,2,0,-1}^{r}\rho_\beta^3\cos\left(\phi_\beta\right)$$
$$- b_{2,0,-1,-1}^{r}\rho_\alpha^3\cos\left(\phi_\alpha\right) - b_{2,0,0,-1}^{r}\rho_\alpha^2\rho_\beta\cos\left(\phi_\beta\right)$$

Cartesian e-coordinates:

$$H_{XX}^{(3)} = a_{0,0,0,3}^{r} x_\beta\left(x_\beta^2 - 3y_\beta^2\right) + a_{0,0,1,3}^{r}\left(x_\alpha\left(x_\beta^2 - y_\beta^2\right) - 2x_\beta y_\alpha y_\beta\right) + a_{0,0,2,3}^{r}\left(-2x_\alpha y_\alpha y_\beta + x_\beta\left(x_\alpha^2 - y_\alpha^2\right)\right)$$
$$+ a_{0,0,3,3}^{r} x_\alpha\left(x_\alpha^2 - 3y_\alpha^2\right) + b_{0,0,-2,-1}^{r}\left(2x_\alpha y_\alpha y_\beta + x_\beta\left(x_\alpha^2 - y_\alpha^2\right)\right) + b_{0,0,1,-1}^{r}\left(x_\alpha\left(x_\beta^2 - y_\beta^2\right) + 2x_\beta y_\alpha y_\beta\right)$$
$$+ b_{0,2,-1,-1}^{r} x_\alpha\left(x_\beta^2 + y_\beta^2\right) + b_{0,2,0,-1}^{r} x_\beta\left(x_\beta^2 + y_\beta^2\right) + b_{2,0,-1,-1}^{r} x_\alpha\left(x_\alpha^2 + y_\alpha^2\right) + b_{2,0,0,-1}^{r} x_\beta\left(x_\alpha^2 + y_\alpha^2\right)$$

$$H_{XY}^{(3)} = -b_{0,0,-2,-1}^{r}\left(-2x_\alpha x_\beta y_\alpha + y_\beta\left(x_\alpha^2 - y_\alpha^2\right)\right) + b_{0,0,1,-1}^{r}\left(2x_\alpha x_\beta y_\beta + y_\alpha\left(-x_\beta^2 + y_\beta^2\right)\right)$$
$$+ b_{0,2,-1,-1}^{r} y_\alpha\left(x_\beta^2 + y_\beta^2\right) + b_{0,2,0,-1}^{r} y_\beta\left(x_\beta^2 + y_\beta^2\right) + b_{2,0,-1,-1}^{r} y_\alpha\left(x_\alpha^2 + y_\alpha^2\right) + b_{2,0,0,-1}^{r} y_\beta\left(x_\alpha^2 + y_\alpha^2\right)$$

$$
\begin{aligned}
H_{YX}^{(3)} = &-b_{0,0,-2,-1}^{r}\left(-2x_{\alpha}x_{\beta}y_{\alpha}+y_{\beta}\left(x_{\alpha}^{2}-y_{\alpha}^{2}\right)\right)+b_{0,0,1,-1}^{r}\left(2x_{\alpha}x_{\beta}y_{\beta}+y_{\alpha}\left(-x_{\beta}^{2}+y_{\beta}^{2}\right)\right)\\
&+b_{0,2,-1,-1}^{r}y_{\alpha}\left(x_{\beta}^{2}+y_{\beta}^{2}\right)+b_{0,2,0,-1}^{r}y_{\beta}\left(x_{\beta}^{2}+y_{\beta}^{2}\right)+b_{2,0,-1,-1}^{r}y_{\alpha}\left(x_{\alpha}^{2}+y_{\alpha}^{2}\right)+b_{2,0,0,-1}^{r}y_{\beta}\left(x_{\alpha}^{2}+y_{\alpha}^{2}\right)
\end{aligned}
$$

$$
\begin{aligned}
H_{YY}^{(3)} = &\, a_{0,0,0,3}^{r}x_{\beta}\left(x_{\beta}^{2}-3y_{\beta}^{2}\right)+a_{0,0,1,3}^{r}\left(x_{\alpha}\left(x_{\beta}^{2}-y_{\beta}^{2}\right)-2x_{\beta}y_{\alpha}y_{\beta}\right)+a_{0,0,2,3}^{r}\left(-2x_{\alpha}y_{\alpha}y_{\beta}+x_{\beta}\left(x_{\alpha}^{2}-y_{\alpha}^{2}\right)\right)\\
&+a_{0,0,3,3}^{r}x_{\alpha}\left(x_{\alpha}^{2}-3y_{\alpha}^{2}\right)-b_{0,0,-2,-1}^{r}\left(2x_{\alpha}y_{\alpha}y_{\beta}+x_{\beta}\left(x_{\alpha}^{2}-y_{\alpha}^{2}\right)\right)-b_{0,0,1,-1}^{r}\left(x_{\alpha}\left(x_{\beta}^{2}-y_{\beta}^{2}\right)+2x_{\beta}y_{\alpha}y_{\beta}\right)\\
&-b_{0,2,-1,-1}^{r}x_{\alpha}\left(x_{\beta}^{2}+y_{\beta}^{2}\right)-b_{0,2,0,-1}^{r}x_{\beta}\left(x_{\beta}^{2}+y_{\beta}^{2}\right)-b_{2,0,-1,-1}^{r}x_{\alpha}\left(x_{\alpha}^{2}+y_{\alpha}^{2}\right)-b_{2,0,0,-1}^{r}x_{\beta}\left(x_{\alpha}^{2}+y_{\alpha}^{2}\right)
\end{aligned}
$$