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

Robert A. Lang   Riley J. Hickman   Tao Zeng

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.

Contents

1 Vibronic interaction

$(E + A) \otimes (e + a)$ in C_3

2 Vibronic Hamiltonian operator in the complex E basis

$$\hat{H} = \begin{pmatrix} |+\rangle & |-\rangle & |A\rangle \end{pmatrix} \begin{pmatrix} 0 & 0 & H_{+A} \\ 0 & 0 & H_{+A}{}^* \\ H_{+A}{}^* & H_{+A} & 0 \end{pmatrix} \begin{pmatrix} \langle+| \\ \langle-| \\ \langle A| \end{pmatrix}$$

3 Matrix element expansions in the complex E basis

3.1 Order: 0

Number of fitting parameters: H_{+A}: 0.

Polar e-coordinates:

$H^{(0)}_{+A} = 0$

$H^{(0)}_{-A} = 0$

$H^{(0)}_{A+} = 0$

$H^{(0)}_{A-} = 0$

Cartesian e-coordinates:

$H^{(0)}_{+A} = 0$

$H^{(0)}_{-A} = 0$

$H^{(0)}_{A+} = 0$

$H^{(0)}_{A-} = 0$

3.2 Order: 1

Number of fitting parameters: H_{+A}: 2.

Polar e-coordinates:

$$H_{+A}^{(1)} = b_{0,0,-1}^{i}\rho\sin(\phi) + ib_{0,0,-1}^{i}\rho\cos(\phi) - ib_{0,0,-1}^{r}\rho\sin(\phi) + b_{0,0,-1}^{r}\rho\cos(\phi)$$

$$H_{-A}^{(1)} = b_{0,0,-1}^{i}\rho\sin(\phi) - ib_{0,0,-1}^{i}\rho\cos(\phi) + ib_{0,0,-1}^{r}\rho\sin(\phi) + b_{0,0,-1}^{r}\rho\cos(\phi)$$

$$H_{A+}^{(1)} = b_{0,0,-1}^{i}\rho\sin(\phi) - ib_{0,0,-1}^{i}\rho\cos(\phi) + ib_{0,0,-1}^{r}\rho\sin(\phi) + b_{0,0,-1}^{r}\rho\cos(\phi)$$

$$H_{A-}^{(1)} = b_{0,0,-1}^{i}\rho\sin(\phi) + ib_{0,0,-1}^{i}\rho\cos(\phi) - ib_{0,0,-1}^{r}\rho\sin(\phi) + b_{0,0,-1}^{r}\rho\cos(\phi)$$

Cartesian e-coordinates:

$$H_{+A}^{(1)} = ib_{0,0,-1}^{i}x + b_{0,0,-1}^{i}y + b_{0,0,-1}^{r}x - ib_{0,0,-1}^{r}y$$

$$H_{-A}^{(1)} = -ib_{0,0,-1}^{i}x + b_{0,0,-1}^{i}y + b_{0,0,-1}^{r}x + ib_{0,0,-1}^{r}y$$

$$H_{A+}^{(1)} = -ib_{0,0,-1}^{i}x + b_{0,0,-1}^{i}y + b_{0,0,-1}^{r}x + ib_{0,0,-1}^{r}y$$

$$H_{A-}^{(1)} = ib_{0,0,-1}^{i}x + b_{0,0,-1}^{i}y + b_{0,0,-1}^{r}x - ib_{0,0,-1}^{r}y$$

3.3 Order: 2

Number of fitting parameters: H_{+A}: 4.

Polar e-coordinates:

$$\begin{aligned} H_{+A}^{(2)} = {} & -b_{0,0,2}^{i}\rho^2\sin(2\phi) + ib_{0,0,2}^{i}\rho^2\cos(2\phi) + b_{1,0,-1}^{i}\rho z\sin(\phi) + ib_{1,0,-1}^{i}\rho z\cos(\phi) + ib_{0,0,2}^{r}\rho^2\sin(2\phi) + b_{0,0,2}^{r}\rho^2\cos(2\phi) \\ & - ib_{1,0,-1}^{r}\rho z\sin(\phi) + b_{1,0,-1}^{r}\rho z\cos(\phi) \end{aligned}$$

$$\begin{aligned} H_{-A}^{(2)} = {} & -b_{0,0,2}^{i}\rho^2\sin(2\phi) - ib_{0,0,2}^{i}\rho^2\cos(2\phi) + b_{1,0,-1}^{i}\rho z\sin(\phi) - ib_{1,0,-1}^{i}\rho z\cos(\phi) - ib_{0,0,2}^{r}\rho^2\sin(2\phi) + b_{0,0,2}^{r}\rho^2\cos(2\phi) \\ & + ib_{1,0,-1}^{r}\rho z\sin(\phi) + b_{1,0,-1}^{r}\rho z\cos(\phi) \end{aligned}$$

$$\begin{aligned} H_{A+}^{(2)} = {} & -b_{0,0,2}^{i}\rho^2\sin(2\phi) - ib_{0,0,2}^{i}\rho^2\cos(2\phi) + b_{1,0,-1}^{i}\rho z\sin(\phi) - ib_{1,0,-1}^{i}\rho z\cos(\phi) - ib_{0,0,2}^{r}\rho^2\sin(2\phi) + b_{0,0,2}^{r}\rho^2\cos(2\phi) \\ & + ib_{1,0,-1}^{r}\rho z\sin(\phi) + b_{1,0,-1}^{r}\rho z\cos(\phi) \end{aligned}$$

$$\begin{aligned} H_{A-}^{(2)} = {} & -b_{0,0,2}^{i}\rho^2\sin(2\phi) + ib_{0,0,2}^{i}\rho^2\cos(2\phi) + b_{1,0,-1}^{i}\rho z\sin(\phi) + ib_{1,0,-1}^{i}\rho z\cos(\phi) + ib_{0,0,2}^{r}\rho^2\sin(2\phi) + b_{0,0,2}^{r}\rho^2\cos(2\phi) \\ & - ib_{1,0,-1}^{r}\rho z\sin(\phi) + b_{1,0,-1}^{r}\rho z\cos(\phi) \end{aligned}$$

Cartesian e-coordinates:

$$H_{+A}^{(2)} = -2b^{i}_{0,0,2}xy + ib^{i}_{0,0,2}\left(x-y\right)\left(x+y\right) + ib^{i}_{1,0,-1}xz + b^{i}_{1,0,-1}yz + 2ib^{r}_{0,0,2}xy + b^{r}_{0,0,2}\left(x-y\right)\left(x+y\right) + b^{r}_{1,0,-1}xz - ib^{r}_{1,0,-1}yz$$

$$H_{-A}^{(2)} = -2b^{i}_{0,0,2}xy - ib^{i}_{0,0,2}\left(x-y\right)\left(x+y\right) - ib^{i}_{1,0,-1}xz + b^{i}_{1,0,-1}yz - 2ib^{r}_{0,0,2}xy + b^{r}_{0,0,2}\left(x-y\right)\left(x+y\right) + b^{r}_{1,0,-1}xz + ib^{r}_{1,0,-1}yz$$

$$H_{A+}^{(2)} = -2b^{i}_{0,0,2}xy - ib^{i}_{0,0,2}\left(x-y\right)\left(x+y\right) - ib^{i}_{1,0,-1}xz + b^{i}_{1,0,-1}yz - 2ib^{r}_{0,0,2}xy + b^{r}_{0,0,2}\left(x-y\right)\left(x+y\right) + b^{r}_{1,0,-1}xz + ib^{r}_{1,0,-1}yz$$

$$H_{A-}^{(2)} = -2b^{i}_{0,0,2}xy + ib^{i}_{0,0,2}\left(x-y\right)\left(x+y\right) + ib^{i}_{1,0,-1}xz + b^{i}_{1,0,-1}yz + 2ib^{r}_{0,0,2}xy + b^{r}_{0,0,2}\left(x-y\right)\left(x+y\right) + b^{r}_{1,0,-1}xz - ib^{r}_{1,0,-1}yz$$

3.4 Order: 3

Number of fitting parameters: H_{+A}: 6.

Polar e-coordinates:

$$\begin{aligned}H_{+A}^{(3)} = {} & b^{i}_{0,2,-1}\rho^{3}\sin\left(\phi\right) + ib^{i}_{0,2,-1}\rho^{3}\cos\left(\phi\right) - b^{i}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) + ib^{i}_{1,0,2}\rho^{2}z\cos\left(2\phi\right) + b^{i}_{2,0,-1}\rho z^{2}\sin\left(\phi\right)\\ & + ib^{i}_{2,0,-1}\rho z^{2}\cos\left(\phi\right) - ib^{r}_{0,2,-1}\rho^{3}\sin\left(\phi\right) + b^{r}_{0,2,-1}\rho^{3}\cos\left(\phi\right) + ib^{r}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) + b^{r}_{1,0,2}\rho^{2}z\cos\left(2\phi\right)\\ & - ib^{r}_{2,0,-1}\rho z^{2}\sin\left(\phi\right) + b^{r}_{2,0,-1}\rho z^{2}\cos\left(\phi\right)\end{aligned}$$

$$\begin{aligned}H_{-A}^{(3)} = {} & b^{i}_{0,2,-1}\rho^{3}\sin\left(\phi\right) - ib^{i}_{0,2,-1}\rho^{3}\cos\left(\phi\right) - b^{i}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) - ib^{i}_{1,0,2}\rho^{2}z\cos\left(2\phi\right) + b^{i}_{2,0,-1}\rho z^{2}\sin\left(\phi\right)\\ & - ib^{i}_{2,0,-1}\rho z^{2}\cos\left(\phi\right) + ib^{r}_{0,2,-1}\rho^{3}\sin\left(\phi\right) + b^{r}_{0,2,-1}\rho^{3}\cos\left(\phi\right) - ib^{r}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) + b^{r}_{1,0,2}\rho^{2}z\cos\left(2\phi\right)\\ & + ib^{r}_{2,0,-1}\rho z^{2}\sin\left(\phi\right) + b^{r}_{2,0,-1}\rho z^{2}\cos\left(\phi\right)\end{aligned}$$

$$\begin{aligned}H_{A+}^{(3)} = {} & b^{i}_{0,2,-1}\rho^{3}\sin\left(\phi\right) - ib^{i}_{0,2,-1}\rho^{3}\cos\left(\phi\right) - b^{i}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) - ib^{i}_{1,0,2}\rho^{2}z\cos\left(2\phi\right) + b^{i}_{2,0,-1}\rho z^{2}\sin\left(\phi\right)\\ & - ib^{i}_{2,0,-1}\rho z^{2}\cos\left(\phi\right) + ib^{r}_{0,2,-1}\rho^{3}\sin\left(\phi\right) + b^{r}_{0,2,-1}\rho^{3}\cos\left(\phi\right) - ib^{r}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) + b^{r}_{1,0,2}\rho^{2}z\cos\left(2\phi\right)\\ & + ib^{r}_{2,0,-1}\rho z^{2}\sin\left(\phi\right) + b^{r}_{2,0,-1}\rho z^{2}\cos\left(\phi\right)\end{aligned}$$

$$\begin{aligned}H_{A-}^{(3)} = {} & b^{i}_{0,2,-1}\rho^{3}\sin\left(\phi\right) + ib^{i}_{0,2,-1}\rho^{3}\cos\left(\phi\right) - b^{i}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) + ib^{i}_{1,0,2}\rho^{2}z\cos\left(2\phi\right) + b^{i}_{2,0,-1}\rho z^{2}\sin\left(\phi\right)\\ & + ib^{i}_{2,0,-1}\rho z^{2}\cos\left(\phi\right) - ib^{r}_{0,2,-1}\rho^{3}\sin\left(\phi\right) + b^{r}_{0,2,-1}\rho^{3}\cos\left(\phi\right) + ib^{r}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) + b^{r}_{1,0,2}\rho^{2}z\cos\left(2\phi\right)\\ & - ib^{r}_{2,0,-1}\rho z^{2}\sin\left(\phi\right) + b^{r}_{2,0,-1}\rho z^{2}\cos\left(\phi\right)\end{aligned}$$

Cartesian e-coordinates:

$$\begin{aligned}H_{+A}^{(3)} = {} & ib^{i}_{0,2,-1}x\left(x^{2}+y^{2}\right) + b^{i}_{0,2,-1}y\left(x^{2}+y^{2}\right) - 2b^{i}_{1,0,2}xyz + ib^{i}_{1,0,2}z\left(x-y\right)\left(x+y\right) + ib^{i}_{2,0,-1}xz^{2} + b^{i}_{2,0,-1}yz^{2}\\ & + b^{r}_{0,2,-1}x\left(x^{2}+y^{2}\right) - ib^{r}_{0,2,-1}y\left(x^{2}+y^{2}\right) + 2ib^{r}_{1,0,2}xyz + b^{r}_{1,0,2}z\left(x-y\right)\left(x+y\right) + b^{r}_{2,0,-1}xz^{2} - ib^{r}_{2,0,-1}yz^{2}\end{aligned}$$

$$\begin{aligned}H_{-A}^{(3)} = {} & -ib^{i}_{0,2,-1}x\left(x^{2}+y^{2}\right) + b^{i}_{0,2,-1}y\left(x^{2}+y^{2}\right) - 2b^{i}_{1,0,2}xyz - ib^{i}_{1,0,2}z\left(x-y\right)\left(x+y\right) - ib^{i}_{2,0,-1}xz^{2} + b^{i}_{2,0,-1}yz^{2}\\ & + b^{r}_{0,2,-1}x\left(x^{2}+y^{2}\right) + ib^{r}_{0,2,-1}y\left(x^{2}+y^{2}\right) - 2ib^{r}_{1,0,2}xyz + b^{r}_{1,0,2}z\left(x-y\right)\left(x+y\right) + b^{r}_{2,0,-1}xz^{2} + ib^{r}_{2,0,-1}yz^{2}\end{aligned}$$

$$H^{(3)}_{A+} = -ib^i_{0,2,-1}x\left(x^2+y^2\right) + b^i_{0,2,-1}y\left(x^2+y^2\right) - 2b^i_{1,0,2}xyz - ib^i_{1,0,2}z\left(x-y\right)\left(x+y\right) - ib^i_{2,0,-1}xz^2 + b^i_{2,0,-1}yz^2 + b^r_{0,2,-1}x\left(x^2+y^2\right) + ib^r_{0,2,-1}y\left(x^2+y^2\right) - 2ib^r_{1,0,2}xyz + b^r_{1,0,2}z\left(x-y\right)\left(x+y\right) + b^r_{2,0,-1}xz^2 + ib^r_{2,0,-1}yz^2$$

$$H^{(3)}_{A-} = ib^i_{0,2,-1}x\left(x^2+y^2\right) + b^i_{0,2,-1}y\left(x^2+y^2\right) - 2b^i_{1,0,2}xyz + ib^i_{1,0,2}z\left(x-y\right)\left(x+y\right) + ib^i_{2,0,-1}xz^2 + b^i_{2,0,-1}yz^2 + b^r_{0,2,-1}x\left(x^2+y^2\right) - ib^r_{0,2,-1}y\left(x^2+y^2\right) + 2ib^r_{1,0,2}xyz + b^r_{1,0,2}z\left(x-y\right)\left(x+y\right) + b^r_{2,0,-1}xz^2 - ib^r_{2,0,-1}yz^2$$

4 Vibronic Hamiltonian operator in the real E basis

$$\hat{H} = \begin{pmatrix} |X\rangle & |Y\rangle \end{pmatrix} \begin{pmatrix} H_0 & H_0 & H_{re(XA)X1.0*I*im(XA)} \\ H_0 & H_0 & H_{re(XA)Y1.0*I*im(XA)} \\ H_{re(XA)Y1.0*I*im(XA)} & H_{re(XA)X1.0*I*im(XA)} & H_0 \end{pmatrix} \begin{pmatrix} \langle X| \\ \langle Y| \end{pmatrix}$$

5 Matrix element expansions in the real E basis

5.1 Order: 0

Number of fitting parameters:

Polar e-coordinates:

$$H^{(0)}_{XA} = 0$$

$$H^{(0)}_{YA} = 0$$

$$H^{(0)}_{AX} = 0$$

$$H^{(0)}_{AY} = 0$$

Cartesian e-coordinates:

$$H^{(0)}_{XA} = 0$$

$$H^{(0)}_{YA} = 0$$

$$H^{(0)}_{AX} = 0$$

$$H^{(0)}_{AY} = 0$$

5.2 Order: 1

Number of fitting parameters:

Polar e-coordinates:

$$H_{XA}^{(1)} = \sqrt{2}\left(b_{0,0,-1}^{i}\rho\sin\left(\phi\right) + b_{0,0,-1}^{r}\rho\cos\left(\phi\right)\right)$$

$$H_{YA}^{(1)} = -\sqrt{2}\left(b_{0,0,-1}^{i}\rho\cos\left(\phi\right) - b_{0,0,-1}^{r}\rho\sin\left(\phi\right)\right)$$

$$H_{AX}^{(1)} = \sqrt{2}\left(b_{0,0,-1}^{i}\rho\sin\left(\phi\right) + b_{0,0,-1}^{r}\rho\cos\left(\phi\right)\right)$$

$$H_{AY}^{(1)} = -\sqrt{2}\left(b_{0,0,-1}^{i}\rho\cos\left(\phi\right) - b_{0,0,-1}^{r}\rho\sin\left(\phi\right)\right)$$

Cartesian e-coordinates:

$$H_{XA}^{(1)} = \sqrt{2}\left(b_{0,0,-1}^{i}y + b_{0,0,-1}^{r}x\right)$$

$$H_{YA}^{(1)} = -\sqrt{2}\left(b_{0,0,-1}^{i}x - b_{0,0,-1}^{r}y\right)$$

$$H_{AX}^{(1)} = \sqrt{2}\left(b_{0,0,-1}^{i}y + b_{0,0,-1}^{r}x\right)$$

$$H_{AY}^{(1)} = -\sqrt{2}\left(b_{0,0,-1}^{i}x - b_{0,0,-1}^{r}y\right)$$

5.3 Order: 2

Number of fitting parameters:

Polar e-coordinates:

$$H_{XA}^{(2)} = \sqrt{2}\left(-b_{0,0,2}^{i}\rho^{2}\sin\left(2\phi\right) + b_{1,0,-1}^{i}\rho z\sin\left(\phi\right) + b_{0,0,2}^{r}\rho^{2}\cos\left(2\phi\right) + b_{1,0,-1}^{r}\rho z\cos\left(\phi\right)\right)$$

$$H_{YA}^{(2)} = -\sqrt{2}\left(b_{0,0,2}^{i}\rho^{2}\cos\left(2\phi\right) + b_{1,0,-1}^{i}\rho z\cos\left(\phi\right) + b_{0,0,2}^{r}\rho^{2}\sin\left(2\phi\right) - b_{1,0,-1}^{r}\rho z\sin\left(\phi\right)\right)$$

$$H_{AX}^{(2)} = \sqrt{2}\left(-b_{0,0,2}^{i}\rho^{2}\sin\left(2\phi\right) + b_{1,0,-1}^{i}\rho z\sin\left(\phi\right) + b_{0,0,2}^{r}\rho^{2}\cos\left(2\phi\right) + b_{1,0,-1}^{r}\rho z\cos\left(\phi\right)\right)$$

$$H_{AY}^{(2)} = -\sqrt{2}\left(b_{0,0,2}^{i}\rho^{2}\cos\left(2\phi\right) + b_{1,0,-1}^{i}\rho z\cos\left(\phi\right) + b_{0,0,2}^{r}\rho^{2}\sin\left(2\phi\right) - b_{1,0,-1}^{r}\rho z\sin\left(\phi\right)\right)$$

Cartesian e-coordinates:

$$H^{(2)}_{XA} = \sqrt{2}\left(-2b^{i}_{0,0,2}xy + b^{i}_{1,0,-1}yz + b^{r}_{0,0,2}\left(x - y\right)\left(x + y\right) + b^{r}_{1,0,-1}xz\right)$$

$$H^{(2)}_{YA} = -\sqrt{2}\left(b^{i}_{0,0,2}\left(x - y\right)\left(x + y\right) + b^{i}_{1,0,-1}xz + 2b^{r}_{0,0,2}xy - b^{r}_{1,0,-1}yz\right)$$

$$H^{(2)}_{AX} = \sqrt{2}\left(-2b^{i}_{0,0,2}xy + b^{i}_{1,0,-1}yz + b^{r}_{0,0,2}\left(x - y\right)\left(x + y\right) + b^{r}_{1,0,-1}xz\right)$$

$$H^{(2)}_{AY} = -\sqrt{2}\left(b^{i}_{0,0,2}\left(x - y\right)\left(x + y\right) + b^{i}_{1,0,-1}xz + 2b^{r}_{0,0,2}xy - b^{r}_{1,0,-1}yz\right)$$

5.4 Order: 3

Number of fitting parameters:

Polar e-coordinates:

$$H^{(3)}_{XA} = \sqrt{2}\left(b^{i}_{0,2,-1}\rho^{3}\sin\left(\phi\right) - b^{i}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) + b^{i}_{2,0,-1}\rho z^{2}\sin\left(\phi\right) + b^{r}_{0,2,-1}\rho^{3}\cos\left(\phi\right) + b^{r}_{1,0,2}\rho^{2}z\cos\left(2\phi\right) + b^{r}_{2,0,-1}\rho z^{2}\cos\left(\phi\right)\right)$$

$$H^{(3)}_{YA} = -\sqrt{2}\left(b^{i}_{0,2,-1}\rho^{3}\cos\left(\phi\right) + b^{i}_{1,0,2}\rho^{2}z\cos\left(2\phi\right) + b^{i}_{2,0,-1}\rho z^{2}\cos\left(\phi\right) - b^{r}_{0,2,-1}\rho^{3}\sin\left(\phi\right) + b^{r}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) - b^{r}_{2,0,-1}\rho z^{2}\sin\left(\phi\right)\right)$$

$$H^{(3)}_{AX} = \sqrt{2}\left(b^{i}_{0,2,-1}\rho^{3}\sin\left(\phi\right) - b^{i}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) + b^{i}_{2,0,-1}\rho z^{2}\sin\left(\phi\right) + b^{r}_{0,2,-1}\rho^{3}\cos\left(\phi\right) + b^{r}_{1,0,2}\rho^{2}z\cos\left(2\phi\right) + b^{r}_{2,0,-1}\rho z^{2}\cos\left(\phi\right)\right)$$

$$H^{(3)}_{AY} = -\sqrt{2}\left(b^{i}_{0,2,-1}\rho^{3}\cos\left(\phi\right) + b^{i}_{1,0,2}\rho^{2}z\cos\left(2\phi\right) + b^{i}_{2,0,-1}\rho z^{2}\cos\left(\phi\right) - b^{r}_{0,2,-1}\rho^{3}\sin\left(\phi\right) + b^{r}_{1,0,2}\rho^{2}z\sin\left(2\phi\right) - b^{r}_{2,0,-1}\rho z^{2}\sin\left(\phi\right)\right)$$

Cartesian e-coordinates:

$$H^{(3)}_{XA} = \sqrt{2}\left(b^{i}_{0,2,-1}y\left(x^{2} + y^{2}\right) - 2b^{i}_{1,0,2}xyz + b^{i}_{2,0,-1}yz^{2} + b^{r}_{0,2,-1}x\left(x^{2} + y^{2}\right) + b^{r}_{1,0,2}z\left(x - y\right)\left(x + y\right) + b^{r}_{2,0,-1}xz^{2}\right)$$

$$H^{(3)}_{YA} = -\sqrt{2}\left(b^{i}_{0,2,-1}x\left(x^{2} + y^{2}\right) + b^{i}_{1,0,2}z\left(x - y\right)\left(x + y\right) + b^{i}_{2,0,-1}xz^{2} - b^{r}_{0,2,-1}y\left(x^{2} + y^{2}\right) + 2b^{r}_{1,0,2}xyz - b^{r}_{2,0,-1}yz^{2}\right)$$

$$H^{(3)}_{AX} = \sqrt{2}\left(b^{i}_{0,2,-1}y\left(x^{2} + y^{2}\right) - 2b^{i}_{1,0,2}xyz + b^{i}_{2,0,-1}yz^{2} + b^{r}_{0,2,-1}x\left(x^{2} + y^{2}\right) + b^{r}_{1,0,2}z\left(x - y\right)\left(x + y\right) + b^{r}_{2,0,-1}xz^{2}\right)$$

$$H^{(3)}_{AY} = -\sqrt{2}\left(b^{i}_{0,2,-1}x\left(x^{2} + y^{2}\right) + b^{i}_{1,0,2}z\left(x - y\right)\left(x + y\right) + b^{i}_{2,0,-1}xz^{2} - b^{r}_{0,2,-1}y\left(x^{2} + y^{2}\right) + 2b^{r}_{1,0,2}xyz - b^{r}_{2,0,-1}yz^{2}\right)$$