

# Karplus dependence of spin-spin coupling constants revisited theoretically. Part 1: Second-order double perturbation theory

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## Supplementary Information

### Derivation of Eq. (64).

The general resulting equation for the FC contribution to vicinal spin-spin coupling constant in MO LCAO approximation reads as follows:

$$J_{H_1 H_2}^{FC} [H_I^0] = \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \sum_{\substack{AB \\ CD}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \sum_{\substack{n_3 l_3 m_3 \\ n_4 l_4 m_4}} C_{in_1 l_1 m_1}^A C_{an_2 l_2 m_2}^B C_{an_3 l_3 m_3}^C C_{in_4 l_4 m_4}^D \cdot \\ \cdot \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_1}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_1}) \varphi_{n_3 l_3 m_3}^C(\mathbf{r}_{CH_2}) \varphi_{n_4 l_4 m_4}^D(\mathbf{r}_{DH_2}) \quad (1)$$

Here,  $A, B, C,$  and  $D$  run over all atoms  $Q = \{H_1, H_2, C_1, C_2\}$ . Indexes  $a, b, c, \dots$  and  $i, j, k, \dots$  are assigned to unoccupied and occupied molecular orbitals, respectively;  $\varphi_{n_i l_i m_i}^Q(\mathbf{r}_{QH_{1,2}})$  is the spatial atomic orbital localized on atom  $Q$  characterized with a set of three quantum numbers  $\{n_i, l_i, m_i\}$ : principal, azimuthal and magnetic;  $\varepsilon_a - \varepsilon_i$  appearing in Eq. (1) denotes the energy differences between Hartree-Fock unoccupied and occupied molecular orbitals;  $\mathbf{r}_{QH_{1,2}}$  is a short notation of the vector difference:  $\mathbf{r}_{QH_{1,2}} = \mathbf{r}_{H_{1,2}} - \mathbf{r}_Q$ . Based on Eq. (1), it is easy to evaluate the number of atomic sums to be equal to  $4^4$ , which thus can be separated into 16 general types:

$$J_{H_1 H_2}^{FC} [H_I^0] = \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \sum_{\substack{n_3 l_3 m_3 \\ n_4 l_4 m_4}} \\ \left\{ C_{in_1 l_1 m_1}^{H_1} C_{an_2 l_2 m_2}^{H_1} C_{an_3 l_3 m_3}^{H_2} C_{in_4 l_4 m_4}^{H_2} \varphi_{n_1 l_1 m_1}^{H_1}(\mathbf{0}) \varphi_{n_2 l_2 m_2}^{H_1}(\mathbf{0}) \varphi_{n_3 l_3 m_3}^{H_2}(\mathbf{0}) \varphi_{n_4 l_4 m_4}^{H_2}(\mathbf{0}) + \right. \\ \left. + \sum_{D \neq H_2} C_{in_1 l_1 m_1}^{H_1} C_{an_2 l_2 m_2}^{H_1} C_{an_3 l_3 m_3}^{H_2} C_{in_4 l_4 m_4}^D \varphi_{n_1 l_1 m_1}^{H_1}(\mathbf{0}) \varphi_{n_2 l_2 m_2}^{H_1}(\mathbf{0}) \varphi_{n_3 l_3 m_3}^{H_2}(\mathbf{0}) \varphi_{n_4 l_4 m_4}^D(\mathbf{r}_{DH_2}) + \right.$$

$$\begin{aligned}
 & + \sum_{C \neq H_2} C_{in,1,1}^{H_1} C_{an,2,2}^{H_1} C_{an,3,3}^C C_{in,4,4}^{H_2} \varphi_{n,1,1}^{H_1}(\mathbf{0}) \varphi_{n,2,2}^{H_1}(\mathbf{0}) \varphi_{n,3,3}^C(\mathbf{r}_{CH_2}) \varphi_{n,4,4}^{H_2}(\mathbf{0}) + \\
 & + \sum_{\substack{C \neq H_2 \\ D \neq H_2}} C_{in,1,1}^{H_1} C_{an,2,2}^{H_1} C_{an,3,3}^C C_{in,4,4}^D \varphi_{n,1,1}^{H_1}(\mathbf{0}) \varphi_{n,2,2}^{H_1}(\mathbf{0}) \varphi_{n,3,3}^C(\mathbf{r}_{CH_2}) \varphi_{n,4,4}^D(\mathbf{r}_{DH_2}) + \\
 & + \sum_{B \neq H_1} C_{in,1,1}^{H_1} C_{an,2,2}^B C_{an,3,3}^{H_2} C_{in,4,4}^{H_2} \varphi_{n,1,1}^{H_1}(\mathbf{0}) \varphi_{n,2,2}^B(\mathbf{r}_{BH_1}) \varphi_{n,3,3}^{H_2}(\mathbf{0}) \varphi_{n,4,4}^{H_2}(\mathbf{0}) + \\
 & + \sum_{\substack{B \neq H_1 \\ D \neq H_2}} C_{in,1,1}^{H_1} C_{an,2,2}^B C_{an,3,3}^{H_2} C_{in,4,4}^D \varphi_{n,1,1}^{H_1}(\mathbf{0}) \varphi_{n,2,2}^B(\mathbf{r}_{BH_1}) \varphi_{n,3,3}^{H_2}(\mathbf{0}) \varphi_{n,4,4}^D(\mathbf{r}_{DH_2}) + \\
 & + \sum_{\substack{B \neq H_1 \\ C \neq H_2}} C_{in,1,1}^{H_1} C_{an,2,2}^B C_{an,3,3}^C C_{in,4,4}^{H_2} \varphi_{n,1,1}^{H_1}(\mathbf{0}) \varphi_{n,2,2}^B(\mathbf{r}_{BH_1}) \varphi_{n,3,3}^C(\mathbf{r}_{CH_2}) \varphi_{n,4,4}^{H_2}(\mathbf{0}) + \\
 & + \sum_{\substack{B \neq H_1 \\ C \neq H_2 \\ D \neq H_2}} C_{in,1,1}^{H_1} C_{an,2,2}^B C_{an,3,3}^C C_{in,4,4}^D \varphi_{n,1,1}^{H_1}(\mathbf{0}) \varphi_{n,2,2}^B(\mathbf{r}_{BH_1}) \varphi_{n,3,3}^C(\mathbf{r}_{CH_2}) \varphi_{n,4,4}^D(\mathbf{r}_{DH_2}) + \\
 & + \sum_{A \neq H_1} C_{in,1,1}^A C_{an,2,2}^{H_1} C_{an,3,3}^{H_2} C_{in,4,4}^{H_2} \varphi_{n,1,1}^A(\mathbf{r}_{AH_1}) \varphi_{n,2,2}^{H_1}(\mathbf{0}) \varphi_{n,3,3}^{H_2}(\mathbf{0}) \varphi_{n,4,4}^{H_2}(\mathbf{0}) + \\
 & + \sum_{\substack{A \neq H_1 \\ D \neq H_2}} C_{in,1,1}^A C_{an,2,2}^{H_1} C_{an,3,3}^{H_2} C_{in,4,4}^D \varphi_{n,1,1}^A(\mathbf{r}_{AH_1}) \varphi_{n,2,2}^{H_1}(\mathbf{0}) \varphi_{n,3,3}^{H_2}(\mathbf{0}) \varphi_{n,4,4}^D(\mathbf{r}_{DH_2}) + \\
 & + \sum_{\substack{A \neq H_1 \\ C \neq H_2}} C_{in,1,1}^A C_{an,2,2}^{H_1} C_{an,3,3}^C C_{in,4,4}^{H_2} \varphi_{n,1,1}^A(\mathbf{r}_{AH_1}) \varphi_{n,2,2}^{H_1}(\mathbf{0}) \varphi_{n,3,3}^C(\mathbf{r}_{CH_2}) \varphi_{n,4,4}^{H_2}(\mathbf{0}) + \\
 & + \sum_{\substack{A \neq H_1 \\ C \neq H_2 \\ D \neq H_2}} C_{in,1,1}^A C_{an,2,2}^{H_1} C_{an,3,3}^C C_{in,4,4}^D \varphi_{n,1,1}^A(\mathbf{r}_{AH_1}) \varphi_{n,2,2}^{H_1}(\mathbf{0}) \varphi_{n,3,3}^C(\mathbf{r}_{CH_2}) \varphi_{n,4,4}^D(\mathbf{r}_{DH_2}) + \\
 & + \sum_{\substack{A \neq H_1 \\ B \neq H_1}} C_{in,1,1}^A C_{an,2,2}^B C_{an,3,3}^{H_2} C_{in,4,4}^{H_2} \varphi_{n,1,1}^A(\mathbf{r}_{AH_1}) \varphi_{n,2,2}^B(\mathbf{r}_{BH_1}) \varphi_{n,3,3}^{H_2}(\mathbf{0}) \varphi_{n,4,4}^{H_2}(\mathbf{0}) + \\
 & + \sum_{\substack{A \neq H_1 \\ B \neq H_1 \\ D \neq H_2}} C_{in,1,1}^A C_{an,2,2}^B C_{an,3,3}^{H_2} C_{in,4,4}^D \varphi_{n,1,1}^A(\mathbf{r}_{AH_1}) \varphi_{n,2,2}^B(\mathbf{r}_{BH_1}) \varphi_{n,3,3}^{H_2}(\mathbf{0}) \varphi_{n,4,4}^D(\mathbf{r}_{DH_2}) + \\
 & + \sum_{\substack{A \neq H_1 \\ B \neq H_1 \\ C \neq H_2}} C_{in,1,1}^A C_{an,2,2}^B C_{an,3,3}^C C_{in,4,4}^{H_2} \varphi_{n,1,1}^A(\mathbf{r}_{AH_1}) \varphi_{n,2,2}^B(\mathbf{r}_{BH_1}) \varphi_{n,3,3}^C(\mathbf{r}_{CH_2}) \varphi_{n,4,4}^{H_2}(\mathbf{0}) + \\
 & + \left. \sum_{\substack{A \neq H_1 \\ B \neq H_1 \\ C \neq H_2 \\ D \neq H_2}} \sum_{C \neq H_2} C_{in,1,1}^A C_{an,2,2}^B C_{an,3,3}^C C_{in,4,4}^D \varphi_{n,1,1}^A(\mathbf{r}_{AH_1}) \varphi_{n,2,2}^B(\mathbf{r}_{BH_1}) \varphi_{n,3,3}^C(\mathbf{r}_{CH_2}) \varphi_{n,4,4}^D(\mathbf{r}_{DH_2}) \right\}
 \end{aligned}$$

(2)

Taking into account only the s-type functions on hydrogen atoms, one can eliminate the summations over the quantum numbers  $\{n_i, l_i, m_i\}$  in the terms containing  $\varphi_{n_i l_i m_i}^{H_{1,2}}(\mathbf{0})$  and replace

$\varphi_{n_i l_i m_i}^{H_{1,2}}(\mathbf{0})$  by  $\varphi_{100}^{H_{1,2}}(\mathbf{0}) = \frac{1}{a_0 \sqrt{\pi a_0}}$ . In that way, all sums in Eq. (2) can be combined into nine

groups:

$$\begin{aligned}
 J_{H_1 H_2}^{FC} [H_I^0] = & \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \frac{1}{\pi^2 a_0^6} C_{i100}^{H_1} C_{a100}^{H_1} C_{a100}^{H_2} C_{i100}^{H_2} + \right. \\
 & + \frac{1}{\pi a_0^4 \sqrt{\pi a_0}} \sum_{nlm} \sum_{A \neq H_1} C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{anlm}^A + i \leftrightarrow a \right) \varphi_{nlm}^A(\mathbf{r}_{AH_1}) + \\
 & + \frac{1}{\pi a_0^4 \sqrt{\pi a_0}} \sum_{nlm} \sum_{A \neq H_2} C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{anlm}^A + i \leftrightarrow a \right) \varphi_{nlm}^A(\mathbf{r}_{AH_2}) + \\
 & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \sum_{\substack{A \neq H_2 \\ B \neq H_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^A C_{in_2 l_2 m_2}^B \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_2}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_2}) + \\
 & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \sum_{\substack{A \neq H_1 \\ B \neq H_1}} C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1 l_1 m_1}^A C_{an_2 l_2 m_2}^B \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_1}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_1}) + \\
 & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \sum_{\substack{A \neq H_1 \\ B \neq H_2}} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^A + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^B + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_1}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_2}) \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \sum_{\substack{A \neq H_1 \\ B \neq H_2 \\ C \neq H_2}} C_{an_2 l_2 m_2}^B C_{in_3 l_3 m_3}^C \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^A + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_1}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_2}) \varphi_{n_3 l_3 m_3}^C(\mathbf{r}_{CH_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \sum_{\substack{A \neq H_1 \\ B \neq H_1 \\ C \neq H_2}} C_{in_1 l_1 m_1}^A C_{an_2 l_2 m_2}^B \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^C + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_1}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_1}) \varphi_{n_3 l_3 m_3}^C(\mathbf{r}_{CH_2}) + \\
 & + \left. \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} \sum_{\substack{A \neq H_1 \\ B \neq H_1 \\ D \neq H_2}} \sum_{C \neq H_2} C_{in_1 l_1 m_1}^A C_{an_2 l_2 m_2}^B C_{an_3 l_3 m_3}^C C_{in_4 l_4 m_4}^D \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_1}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_1}) \varphi_{n_3 l_3 m_3}^C(\mathbf{r}_{CH_2}) \varphi_{n_4 l_4 m_4}^D(\mathbf{r}_{DH_2}) \right\}
 \end{aligned}
 \tag{3}$$

Herewith, the Cartesian left-handed coordinate system is chosen, so that  $C_1 C_2$  bond lies on Z axis and  $C_1 H_1$  bond lies on Y axis. Provided that bond angles  $\angle HCC$  equal to  $\pi/2$ , the  $C_2 H_2$

bond lies in the plane parallel to XY plane and revolves around Z axis with the azimuth  $\phi$  which in that case equals to the dihedral angle  $\angle H_1C_1C_2H_2$ .

Further, the short notation  $\bar{\varphi}_{nlm}^C(\mathbf{r}_{CH})$  denoting the part of  $\varphi_{nlm}^C(\mathbf{r}_{CH})$  which is not depend on  $\phi$ , namely,  $\varphi_{nlm}^C(\mathbf{r}_{CH}) = \bar{\varphi}_{nlm}^C(\mathbf{r}_{CH}) \cdot \begin{Bmatrix} \sin \phi \\ \cos \phi \end{Bmatrix}$ , is used throughout.

A general form of  $\varphi_{nlm}^A(\mathbf{r}_{H_{1,2}} - \mathbf{r}_A)$  with a factorized  $\phi$ -dependence is as follows:

$$\varphi_{100}^{H_{1,2}}(|\mathbf{r}_{H_1} - \mathbf{r}_{H_2}|) = \frac{1}{a_0 \sqrt{\pi a_0}} \cdot e^{-\frac{1}{a_0}|\mathbf{r}_{H_1} - \mathbf{r}_{H_2}|} = \frac{1}{a_0 \sqrt{\pi a_0}} \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \quad (4)$$

$$\varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) = \bar{\varphi}_{200}^{C_1}(\mathbf{r}_{C_1H_1}) = \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) = \bar{\varphi}_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \quad (5)$$

$$\varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) = \bar{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \quad (6)$$

$$\varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) = \bar{\varphi}_{200}^{C_1}(\mathbf{r}_{C_1H_2}) = \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) = \bar{\varphi}_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \quad (7)$$

$$\varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) = \bar{\varphi}_{210}^{C_1}(\mathbf{r}_{C_1H_2}) = -\varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) = -\bar{\varphi}_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \quad (8)$$

$$\varphi_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) = \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \cdot \begin{Bmatrix} \sin \phi \\ \cos \phi \end{Bmatrix} \quad (9)$$

$$\varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) = \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \quad (10)$$

$$\varphi_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) = \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \cdot \begin{Bmatrix} \sin \phi \\ \cos \phi \end{Bmatrix} \quad (11)$$

$$\varphi_{210}^{C_1}(\mathbf{r}_{C_1H_1}) = \varphi_{21+1}^{C_1}(\mathbf{r}_{C_1H_1}) = \varphi_{21+1}^{C_2}(\mathbf{r}_{C_2H_1}) = \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_2}) = 0 \quad (12)$$

Further we consider each group in (3) using a set of Eqs. (4)-(12). If  $\varphi_{nlm}^C(\mathbf{r}_{CH}) = \bar{\varphi}_{nlm}^C(\mathbf{r}_{CH})$ , then notation  $\varphi_{nlm}^C(\mathbf{r}_{CH})$  is used for  $\bar{\varphi}_{nlm}^C(\mathbf{r}_{CH})$ .

### 1<sup>st</sup> sum

$$J_{H_1H_2}^{FC(1)}[H_I^0] = A = \left(\frac{16\pi\beta}{3}\right)^2 \frac{1}{\pi^2 a_0^6} \sum_{ia} \frac{C_{i100}^{H_1} C_{a100}^{H_1} C_{a100}^{H_2} C_{i100}^{H_2}}{\varepsilon_a - \varepsilon_i} = -\left(\frac{8\beta}{3a_0^3}\right)^2 \pi_{S_{H_1}, S_{H_2}} \quad (13)$$

Here  $\pi_{\mu\nu}$  is the **mutual polarizability** of atomic orbitals:

$$\pi_{\mu\nu} = -4 \sum_{ia} \frac{C_{i\mu} C_{iv} C_{a\mu} C_{av}}{\varepsilon_a - \varepsilon_i} \quad (14)$$

**2<sup>nd</sup> sum**

$$\begin{aligned} J_{NN'}^{FC(2)}[H_I^0] &= \frac{1}{\pi a_0^4 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \sum_{nlm} \sum_{A \neq H_1} C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{anlm}^A + i \leftrightarrow a \right) \varphi_{nlm}^A(\mathbf{r}_{AH_1}) = \\ &= \frac{256\pi\beta^2}{9a_0^4 \sqrt{\pi a_0}} \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \sum_{nlm} \left( C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{anlm}^{H_2} + i \leftrightarrow a \right) \varphi_{nlm}^{H_2}(\mathbf{r}_{H_2H_1}) + \right. \\ &+ C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{anlm}^{C_1} + i \leftrightarrow a \right) \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1H_1}) + C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{anlm}^{C_2} + i \leftrightarrow a \right) \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2H_1}) \Big) = \\ &= \frac{256\pi\beta^2}{9a_0^4 \sqrt{\pi a_0}} \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \left( C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \varphi_{100}^{H_2}(\mathbf{r}_{H_2H_1}) e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \right. \\ &+ C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{a200}^{C_1} + i \leftrightarrow a \right) \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) + C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{a21-1}^{C_1} + i \leftrightarrow a \right) \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) + \\ &+ C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{a200}^{C_2} + i \leftrightarrow a \right) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) + C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{a210}^{C_2} + i \leftrightarrow a \right) \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) + \\ &+ C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{a21-1}^{C_2} + i \leftrightarrow a \right) \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \Big) \quad (15) \end{aligned}$$

Eq. (15) takes a general form:

$$J_{H_1H_2}^{FC(2)}[H_I^0] = A + B e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \quad (16)$$

where coefficients  $A$  and  $B$  are as follows:

$$\begin{aligned} A &= \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \left( C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} + \right. \\ &+ C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \Big) \quad (17) \end{aligned}$$

$$B = \left( \frac{16\beta}{3a_0^3} \right)^2 \sum_{ia} \frac{C_{a100}^{H_2} C_{i100}^{H_2} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right)}{\varepsilon_a - \varepsilon_i} \quad (18)$$

### 3<sup>rd</sup> sum

$$\begin{aligned}
 J_{H_1 H_2}^{FC(3)}[H_I^0] &= \frac{1}{\pi a_0^4 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \sum_{nlm} \sum_{A \neq H_2} C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{anlm}^A + i \leftrightarrow a \right) \varphi_{nlm}^A(\mathbf{r}_{AH_2}) = \\
 &= \frac{256\pi\beta^2}{9a_0^4 \sqrt{\pi a_0}} \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \sum_{nlm} \left( C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{anlm}^{H_1} + i \leftrightarrow a \right) \varphi_{nlm}^{H_1}(\mathbf{r}_{H_1 H_2}) + \right. \\
 &+ C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{anlm}^{C_1} + i \leftrightarrow a \right) \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1 H_2}) + C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{anlm}^{C_2} + i \leftrightarrow a \right) \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2 H_2}) \left. \right) = \\
 &= \frac{256\pi\beta^2}{9a_0^4 \sqrt{\pi a_0}} \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a100}^{H_1} + i \leftrightarrow a \right) \overline{\varphi}_{100}^{H_1}(\mathbf{r}_{H_1 H_2}) \right)^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \\
 &+ C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a200}^{C_1} + i \leftrightarrow a \right) \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) + C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a210}^{C_1} + i \leftrightarrow a \right) \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 &+ C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a21+1}^{C_1} + i \leftrightarrow a \right) \overline{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1 H_2}) \sin\phi + \\
 &+ C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a21-1}^{C_1} + i \leftrightarrow a \right) \overline{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1 H_2}) \cos\phi + \\
 &+ C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a200}^{C_2} + i \leftrightarrow a \right) \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 &+ C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a21+1}^{C_2} + i \leftrightarrow a \right) \overline{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2 H_2}) \sin\phi + \\
 &+ C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a21-1}^{C_2} + i \leftrightarrow a \right) \overline{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2 H_2}) \cos\phi \left. \right) \quad (19)
 \end{aligned}$$

Eq. (19) takes a general form:

$$J_{H_1 H_2}^{FC(3)}[H_I^0] = A + B \sin\phi + C \cos\phi + D e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \quad (20)$$

The coefficients  $A$ ,  $B$ ,  $C$  and  $D$  are as follows:

$$\begin{aligned}
 A &= \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \left\{ C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( \begin{array}{l} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) \end{array} \right) + \right. \\
 &+ \left. \left( C_{i100}^{H_2} C_{a200}^{C_2} + i \leftrightarrow a \right) \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_2}) \right\} \quad (21)
 \end{aligned}$$

$$\begin{aligned}
 \left( \begin{array}{l} B \\ C \end{array} \right) &= \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \left( C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a21\pm 1}^{C_1} + i \leftrightarrow a \right) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1 H_2}) + \right. \\
 &+ \left. C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a21\pm 1}^{C_2} + i \leftrightarrow a \right) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2 H_2}) \right) \quad (22)
 \end{aligned}$$

$$D = \left( \frac{16\beta}{3a_0^3} \right)^2 \sum_{ia} \frac{C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{i100}^{H_2} C_{a100}^{H_1} + i \leftrightarrow a \right)}{\varepsilon_a - \varepsilon_i} \quad (23)$$

#### 4<sup>th</sup> sum

$$\begin{aligned} J_{H_1 H_2}^{FC(4)}[H_I^0] &= \frac{1}{\pi a_0^3} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \sum_{\substack{A \neq H_2 \\ B \neq H_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^A C_{in_2 l_2 m_2}^B \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_2}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_2}) = \\ &= \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^{H_1} C_{in_2 l_2 m_2}^{H_1} \varphi_{n_1 l_1 m_1}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_2 l_2 m_2}^{H_1}(\mathbf{r}_{H_1 H_2}) + \right. \\ &+ \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^{H_1} C_{in_2 l_2 m_2}^{C_1} \varphi_{n_1 l_1 m_1}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ &+ \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^{H_1} C_{in_2 l_2 m_2}^{C_2} \varphi_{n_1 l_1 m_1}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ &+ \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^{C_1} C_{in_2 l_2 m_2}^{H_1} \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_2 l_2 m_2}^{H_1}(\mathbf{r}_{H_1 H_2}) + \\ &+ \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^{C_1} C_{in_2 l_2 m_2}^{C_1} \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ &+ \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^{C_1} C_{in_2 l_2 m_2}^{C_2} \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ &+ \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^{C_2} C_{in_2 l_2 m_2}^{H_1} \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_2 l_2 m_2}^{H_1}(\mathbf{r}_{H_1 H_2}) + \\ &+ \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^{C_2} C_{in_2 l_2 m_2}^{C_1} \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ &+ \left. \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_1} C_{a100}^{H_1} C_{an_1 l_1 m_1}^{C_2} C_{in_2 l_2 m_2}^{C_2} \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \right) \quad (24) \end{aligned}$$

$$\begin{aligned} J_{H_1 H_2}^{FC(4)}[H_I^0] &= \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( \frac{1}{\pi a_0^3} C_{i100}^{H_1} C_{a100}^{H_1} C_{a100}^{H_1} C_{i100}^{H_1} e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \right. \\ &+ \frac{1}{a_0 \sqrt{\pi a_0}} e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \left\{ C_{i100}^{H_1} C_{a100}^{H_1} C_{a100}^{H_1} \left( C_{i200}^{C_1} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) + C_{i210}^{C_1} \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) + \right. \right. \end{aligned}$$

$$\begin{aligned}
 & + C_{i21+1}^{C_1} \overline{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \sin \phi + C_{i21-1}^{C_1} \overline{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) \cos \phi + i \leftrightarrow a \Big\} + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \left\{ C_{i100}^{H_1} C_{a100}^{H_1} C_{a100}^{H_1} \left( C_{i200}^{C_2} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \right. \right. \\
 & + C_{i21+1}^{C_2} \overline{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) \sin \phi + C_{i21-1}^{C_2} \overline{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) \cos \phi + i \leftrightarrow a \Big\} + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} \left[ \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \otimes \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \right] \cdot \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] \otimes \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21+1}^{C_1} + i \leftrightarrow a \right) \cdot \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \cdot \overline{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \sin \phi + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21-1}^{C_1} + i \leftrightarrow a \right) \cdot \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \cdot \overline{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) \cos \phi + \\
 & + \frac{1}{2} C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a21-1}^{C_1} C_{i21+1}^{C_1} + i \leftrightarrow a \right) \cdot \left( \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \right)^2 \sin 2\phi + \\
 & + \frac{1}{2} C_{i100}^{H_1} C_{a100}^{H_1} C_{a21+1}^{C_1} C_{i21+1}^{C_1} \cdot \left( \overline{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \right)^2 (1 - \cos 2\phi) + \\
 & + \frac{1}{2} C_{i100}^{H_1} C_{a100}^{H_1} C_{a21-1}^{C_1} C_{i21-1}^{C_1} \cdot \left( \overline{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) \right)^2 (1 + \cos 2\phi) + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21+1}^{C_2} + i \leftrightarrow a \right) \cdot \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \cdot \overline{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) \sin \phi + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a21+1}^{C_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \cdot \overline{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \sin \phi + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \cdot \overline{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) \cos \phi + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a21-1}^{C_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \cdot \overline{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) \cos \phi + \\
 & + \frac{1}{2} C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a21-1}^{C_1} C_{i21+1}^{C_2} + C_{a21+1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \sin 2\phi + \\
 & + \frac{1}{2} C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \cdot \overline{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) (1 - \cos 2\phi) +
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{2} C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \bar{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) (1 + \cos 2\phi) + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} C_{a200}^{C_2} C_{i200}^{C_2} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a200}^{C_2} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) \sin \phi + \\
 & + C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a200}^{C_2} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) \cos \phi + \\
 & + \frac{1}{2} C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a21+1}^{C_2} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \bar{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) \sin 2\phi + \\
 & + \frac{1}{2} C_{i100}^{H_1} C_{a100}^{H_1} C_{a21+1}^{C_2} C_{i21+1}^{C_2} \bar{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) (1 - \cos 2\phi) + \\
 & + \frac{1}{2} C_{i100}^{H_1} C_{a100}^{H_1} C_{a21-1}^{C_2} C_{i21-1}^{C_2} \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) (1 + \cos 2\phi) \Big) \quad (25)
 \end{aligned}$$

The  $\mathbf{a} \otimes \mathbf{b}$  arising in Eq. (25) denotes the Cartesian product of the two sets  $\mathbf{a}$  and  $\mathbf{b}$ , defined as:  $\mathbf{a} \otimes \mathbf{b} = (a_{11}, a_{12}, \dots, a_{1M}; a_{21}, a_{22}, \dots, a_{2M}; \dots; a_{N1}, a_{N2}, \dots, a_{NM})$  for the row vector and  $\mathbf{a} \otimes \mathbf{b} = \left( \mathbf{a}^T \otimes \mathbf{b}^T \right)^T$  for the column vector.

Thus Eq. (25) takes a general form:

$$\begin{aligned}
 J_{H_1H_2}^{FC(4)}[H_I^0] &= A + B \sin \phi + C \cos \phi + (A' + B' \sin \phi + C' \cos \phi) e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \\
 & + E e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \quad (26)
 \end{aligned}$$

where the first coefficient reads as follows:

$$\begin{aligned}
 A &= \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{C_{i100}^{H_1} C_{a100}^{H_1}}{\varepsilon_a - \varepsilon_i} \cdot \left( \left[ \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \otimes \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \right] \right. \\
 & \cdot \left[ \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \otimes \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \right] + \frac{1}{2} C_{a21+1}^{C_1} C_{i21+1}^{C_1} \cdot \left( \bar{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \right)^2 + \frac{1}{2} C_{a21-1}^{C_1} C_{i21-1}^{C_1} \cdot \\
 & \cdot \left( \bar{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) \right)^2 + \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \cdot \bar{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left( C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \bar{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{a200}^{C_2} C_{i200}^{C_2} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) +
 \end{aligned}$$

$$+ \frac{1}{2} C_{a21+1}^{C_2} C_{i21+1}^{C_2} \bar{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) + \frac{1}{2} C_{a21-1}^{C_2} C_{i21-1}^{C_2} \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) \quad (27)$$

Taking into account that  $\bar{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) = \bar{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) = \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2})$ ,

$$\begin{aligned} A = & \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{C_{i100}^{H_1} C_{a100}^{H_1}}{\varepsilon_a - \varepsilon_i} \cdot \left( \left[ \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \otimes \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \right] \cdot \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] \otimes \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] \right) + \\ & + \frac{1}{2} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_1} + C_{a21-1}^{C_1} C_{i21-1}^{C_1} \right) \cdot \left( \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \right)^2 + \\ & + \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\ & + \frac{1}{2} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\ & + C_{a200}^{C_2} C_{i200}^{C_2} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\ & + \frac{1}{2} \left( C_{a21+1}^{C_2} C_{i21+1}^{C_2} + C_{a21-1}^{C_2} C_{i21-1}^{C_2} \right) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \quad (28) \end{aligned}$$

$$\begin{aligned} B = & \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( C_{i100}^{H_1} C_{a100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21+1}^{C_1} + i \leftrightarrow a \right) \cdot \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] \cdot \right. \\ & \cdot \bar{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i100}^{H_1} C_{a100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21+1}^{C_2} + i \leftrightarrow a \right) \cdot \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] \cdot \bar{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\ & + C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a21+1}^{C_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \cdot \bar{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) + \\ & \left. + C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a200}^{C_2} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) \quad (29) \end{aligned}$$

$$\begin{aligned} C = & \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( C_{i100}^{H_1} C_{a100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21-1}^{C_1} + i \leftrightarrow a \right) \cdot \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] \cdot \right. \\ & \cdot \bar{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i100}^{H_1} C_{a100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] \cdot \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\ & \left. + C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a21-1}^{C_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \cdot \bar{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \end{aligned}$$

$$+ C_{i100}^{H_1} C_{a100}^{H_1} \left( C_{a200}^{C_2} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) \quad (30)$$

$$A' = \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( C_{i100}^{H_1} C_{a100}^{H_1} C_{a100}^{H_1} \left[ \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} + \right. \right. \\ \left. \left. + C_{i200}^{C_2} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \right] + i \leftrightarrow a \right) \quad (31)$$

$$\left( \begin{matrix} B' \\ C' \end{matrix} \right) = \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( C_{i100}^{H_1} C_{a100}^{H_1} C_{a100}^{H_1} \left( C_{i21\pm 1}^{C_1} \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i21\pm 1}^{C_2} \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \right. \right. \\ \left. \left. + i \leftrightarrow a \right) \right) \quad (32)$$

$$E = \left( \frac{16\beta}{3a_0^3} \right)^2 \sum_{ia} \frac{C_{i100}^{H_1} C_{a100}^{H_1} C_{a100}^{H_1} C_{i100}^{H_1}}{\varepsilon_a - \varepsilon_i} = - \left( \frac{8\beta}{3a_0^3} \right)^2 \pi_{S_{H_1}, S_{H_1}} \quad (33)$$

### 5<sup>th</sup> sum

$$J_{H_1H_2}^{FC(5)}[H_l^0] = \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \sum_{\substack{n_1l_1m_1 \\ n_2l_2m_2}} \sum_{\substack{A \neq H_1 \\ B \neq H_1}} C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1l_1m_1}^A C_{an_2l_2m_2}^B \varphi_{n_1l_1m_1}^A(\mathbf{r}_{AH_1}) \varphi_{n_2l_2m_2}^B(\mathbf{r}_{BH_1}) = \\ = \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \sum_{\substack{n_1l_1m_1 \\ n_2l_2m_2}} \left( C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{H_2} \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{H_2}(\mathbf{r}_{H_2H_1}) + \right. \\ + C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{C_1} \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) + \\ + C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{C_2} \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) + \\ + C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{H_2} \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{H_2}(\mathbf{r}_{H_2H_1}) + \\ + C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_1} \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) + \\ + C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) + \\ + C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{H_2} \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{H_2}(\mathbf{r}_{H_2H_1}) + \\ + C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_1} \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) + \\ \left. + C_{a100}^{H_2} C_{i100}^{H_2} C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \quad (34)$$

$$\begin{aligned}
 J_{H_1 H_2}^{FC(5)}[H_I^0] = & \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{C_{a100}^{H_2} C_{i100}^{H_2}}{\varepsilon_a - \varepsilon_i} \left( \frac{1}{\pi a_0^3} C_{i100}^{H_2} C_{a100}^{H_2} e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \right. \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{nlm} \left( C_{i100}^{H_2} C_{anlm}^{C_1} + i \leftrightarrow a \right) \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1 H_1}) e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{nlm} \left( C_{i100}^{H_2} C_{anlm}^{C_2} + i \leftrightarrow a \right) \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2 H_1}) e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) + \\
 & \left. + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{in_1 l_1 m_1}^{C_2} C_{an_2 l_2 m_2}^{C_2} \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \right) \quad (35)
 \end{aligned}$$

Summing up the terms in Eq. (35) over the quantum numbers, we obtain

$$\begin{aligned}
 J_{H_1 H_2}^{FC(5)}[H_I^0] = & \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{C_{a100}^{H_2} C_{i100}^{H_2}}{\varepsilon_a - \varepsilon_i} \left( \frac{1}{\pi a_0^3} C_{i100}^{H_2} C_{a100}^{H_2} e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \right. \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1 H_1}) \end{pmatrix} e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2 H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2 H_1}) \end{pmatrix} e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \\
 & + \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1 H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1 H_1}) \end{pmatrix} \right] + \\
 & + \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right] \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1 H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2 H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2 H_1}) \end{pmatrix} \right] +
 \end{aligned}$$

$$+ \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \quad (36)$$

As follows from Eq. (36), the fifth contribution takes a general form:

$$J_{H_1H_2}^{FC(5)}[H_I^0] = A + Be^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + Ce^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \quad (37)$$

where coefficients  $A$ ,  $B$  and  $C$  are as follows:

$$A = \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{C_{a100}^{H_2} C_{i100}^{H_2}}{\varepsilon_a - \varepsilon_i} \left[ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \right] + \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right] \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \right] + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \right] \quad (38)$$

$$B = \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{C_{a100}^{H_2} C_{i100}^{H_2}}{\varepsilon_a - \varepsilon_i} \left\{ \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) + \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \right\} \quad (39)$$

$$C = \left( \frac{16\beta}{3a_0^3} \right)^2 \sum_{ia} \frac{C_{a100}^{H_2} C_{i100}^{H_2} C_{i100}^{H_2} C_{a100}^{H_2}}{\varepsilon_a - \varepsilon_i} = - \left( \frac{8\beta}{3a_0^3} \right)^2 \pi_{S_{H_2}, S_{H_2}} \quad (40)$$

6th sum

$$J_{H_1 H_2}^{FC(6)}[H_I^0] = \frac{1}{\pi a_0^3} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \sum_{\substack{A \neq H_1 \\ B \neq H_2}} \frac{\left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^A + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^B + i \leftrightarrow a \right)}{\varepsilon_a - \varepsilon_i} \cdot \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_1}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_2}) \quad (41)$$

which gives

$$J_{H_1 H_2}^{FC(6)}[H_I^0] = \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_1}(\mathbf{r}_{H_1 H_2}) + \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) + \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{H_1}(\mathbf{r}_{H_1 H_2}) + \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_1 H_2}) + \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_1}(\mathbf{r}_{H_1 H_2}) + \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_1 H_2}) \right) \quad (42)$$

Taking off the abundant summations over the quantum numbers in some terms of Eq. (42), we have

$$J_{H_1 H_2}^{FC(6)}[H_I^0] = \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{100}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{100}^{H_1}(\mathbf{r}_{H_1 H_2}) + \sum_{nlm} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{inlm}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{100}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1 H_2}) \right)$$

$$\begin{aligned}
 & \cdot \varphi_{100}^{H_2}(\mathbf{r}_{H_2H_1})\varphi_{nlm}^{C_1}(\mathbf{r}_{C_1H_2}) + \sum_{nlm} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{inlm}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{100}^{H_2}(\mathbf{r}_{H_2H_1})\varphi_{nlm}^{C_2}(\mathbf{r}_{C_2H_2}) + \sum_{nlm} \left( C_{i100}^{H_1} C_{anlm}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1H_1})\varphi_{100}^{H_1}(\mathbf{r}_{H_1H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1H_1})\varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1H_1})\varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2H_2}) + \sum_{nlm} \left( C_{i100}^{H_1} C_{anlm}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2H_1})\varphi_{100}^{H_1}(\mathbf{r}_{H_1H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2H_1})\varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2H_1})\varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2H_2}) \Big) \tag{43}
 \end{aligned}$$

Substitution of  $\varphi_{100}^{H_{1,2}}(\mathbf{r}_{H_1H_2})$  into Eq. (43) gives

$$\begin{aligned}
 J_{H_1H_2}^{FC(6)}[H_I^0] &= \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( \frac{1}{\pi a_0^3} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \right. \\
 & \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{nlm} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{inlm}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1H_2}) \cdot \\
 & \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{nlm} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{inlm}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2H_2}) \cdot \\
 & \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{nlm} \left( C_{i100}^{H_1} C_{anlm}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1H_1}) \cdot \\
 & \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \cdot \\
 & \cdot \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \cdot \\
 & \cdot \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2H_2}) + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{nlm} \left( C_{i100}^{H_1} C_{anlm}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2H_1}) \cdot
 \end{aligned}$$

$$\begin{aligned}
 & \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi)+L_{CC}^2}} + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \quad (44)
 \end{aligned}$$

Taking the sum over the quantum numbers in Eq. (44) gives

$$\begin{aligned}
 J_{H_1 H_2}^{FC(6)}[H_I^0] &= \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left[ \frac{1}{\pi a_0^3} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \right. \\
 & \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi)+L_{CC}^2}} + \frac{1}{a_0 \sqrt{\pi a_0}} e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi)+L_{CC}^2}} \left\{ \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \right. \\
 & \left. \left( C_{a100}^{H_2} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) \end{pmatrix} + \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21+1}^{C_1} + i \leftrightarrow a \right) \cdot \right. \\
 & \left. \left. \cdot \varphi_{21+1}^{C_1}(\mathbf{r}_{C_1 H_2}) \sin\phi + \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21-1}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{21-1}^{C_1}(\mathbf{r}_{X_1 H_2}) \cos\phi \right\} + \right. \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi)+L_{CC}^2}} \left\{ \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \right. \\
 & \left. \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_2}) + \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{21+1}^{C_2}(\mathbf{r}_{C_2 H_2}) \sin\phi + \right. \\
 & \left. + \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2 H_2}) \cos\phi \right\} + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi)+L_{CC}^2}} \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1 H_1}) \end{pmatrix} + \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \otimes \left( C_{a100}^{H_2} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1 H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) \end{pmatrix} \right] + \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21+1}^{C_1} + i \leftrightarrow a \right) \cdot
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \cdot \sin\phi + \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21-1}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) \cdot \cos\phi + \\
 & + \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) \sin\phi + \\
 & + \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) \cos\phi + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} + \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left( C_{a100}^{H_2} \cdot \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] + \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21+1}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \overline{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \sin\phi + \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21-1}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \overline{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) \cos\phi + \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{X_2H_2}) + \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \varphi_{21+1}^{-C_1}(\mathbf{r}_{C_2H_2}) \sin \phi + \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \varphi_{21-1}^{-C_1}(\mathbf{r}_{C_2H_2}) \cos \phi \quad (45)
 \end{aligned}$$

Eq. (45) can be generalized into the following expression:

$$\begin{aligned}
 J_{H_1H_2}^{FC(6)}[H_I^0] = & A \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot (B + C \sin \phi + D \cos \phi) + \\
 & + B' + C' \sin \phi + D' \cos \phi \quad (46)
 \end{aligned}$$

Coefficient  $A$  in Eq. (46) takes the form:

$$\begin{aligned}
 A = & \left( \frac{16\beta}{3a_0^3} \right)^2 \sum_{ia} \frac{\left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right)}{\varepsilon_a - \varepsilon_i} = \\
 = & \left( \frac{16\beta}{3a_0^3} \right)^2 \sum_{ia} \frac{\left( C_{i100}^{H_1} C_{a100}^{H_2} + C_{a100}^{H_1} C_{i100}^{H_2} \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + C_{i100}^{H_2} C_{a100}^{H_1} \right)}{\varepsilon_a - \varepsilon_i} = \left( \frac{16\beta}{3a_0^3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \\
 & \cdot \left( C_{i100}^{H_1} C_{a100}^{H_2} C_{a100}^{H_2} C_{i100}^{H_1} + C_{i100}^{H_1} C_{a100}^{H_2} C_{i100}^{H_2} C_{a100}^{H_1} + C_{a100}^{H_1} C_{i100}^{H_2} C_{a100}^{H_2} C_{i100}^{H_1} + C_{a100}^{H_1} C_{i100}^{H_2} C_{i100}^{H_2} C_{a100}^{H_1} \right) \quad (47)
 \end{aligned}$$

Using the definition of the mutual polarizability given by Eq. (14), one can reduce Eq. (47) into a compact form:

$$A = \left( \frac{16\beta}{3a_0^3} \right)^2 \cdot \left( \sum_{ia} \frac{C_{i100}^{H_1} C_{a100}^{H_2} C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a}{\varepsilon_a - \varepsilon_i} - \frac{1}{2} \pi_{S_{H_1}, S_{H_2}} \right) \quad (48)$$

The coefficient  $B$  in Eq. (46) takes the form:

$$\begin{aligned}
 B = & \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right) \cdot \\
 & \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) + \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) + \\
 & + \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \quad (49)
 \end{aligned}$$

and coefficients  $C$  and  $D$  in Eq. (46) are

$$\begin{aligned}
 \left( \begin{array}{c} C \\ D \end{array} \right) = & \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{\left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right)}{\varepsilon_a - \varepsilon_i} \cdot \left( \left( C_{a100}^{H_2} C_{i21\pm 1}^{C_1} + i \leftrightarrow a \right) \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \\
 & \left. + \left( C_{a100}^{H_2} C_{i21\pm 1}^{C_2} + i \leftrightarrow a \right) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) \quad (50)
 \end{aligned}$$

Coefficients  $B'$ ,  $C'$  and  $D'$  in Eq. (46) take the form:

$$\begin{aligned}
 B' = & \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \otimes \left( C_{a100}^{H_2} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \right. \\
 & \cdot \left[ \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \right] + \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left( C_{a100}^{H_2} \cdot \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \left[ \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \right] +
 \end{aligned}$$

$$+ \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_2H_2}) \quad (51)$$

$$\begin{aligned} \left( \frac{C'}{D'} \right) &= \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21\pm 1}^{C_1} + i \leftrightarrow a \right) \cdot \right. \\ &\cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21\pm 1}^{C_2} + i \leftrightarrow a \right) \cdot \\ &\cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} \cdot C_{i21\pm 1}^{C_1} + i \leftrightarrow a \right) \cdot \\ &\cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i21\pm 1}^{C_2} + i \leftrightarrow a \right) \cdot \\ &\cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_2H_2}) \left. \right) \quad (52) \end{aligned}$$

The latter two coefficients can be simplified to a form:

$$\begin{aligned} \left( \frac{C'}{D'} \right) &= \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left( C_{a100}^{H_2} \left( C_{i21\pm 1}^{C_1} \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i21\pm 1}^{C_2} \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_2H_2}) \right) + i \leftrightarrow a \right) \cdot \\ &\cdot \left( C_{i100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} + \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right) + i \leftrightarrow a \right) \quad (53) \end{aligned}$$

**7th sum:**



$$\begin{aligned}
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{H_1} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{H_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) + C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{H_1} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) + C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{H_1} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) + C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{C_1} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{H_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{C_1} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{C_1} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{C_2} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{H_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{C_2} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{C_2} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left. \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) \right\} \quad (55)
 \end{aligned}$$

$$\begin{aligned}
 J_{H_1 H_2}^{FC(7)}[H_I^0] &= \frac{1}{a_0 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \frac{1}{\pi a_0^4 \sqrt{\pi a_0}} C_{a 100}^{H_1} C_{i 100}^{H_1} \left( C_{i 100}^{H_1} C_{a 100}^{H_2} + i \leftrightarrow a \right) \cdot \right. \\
 & \cdot e^{-\frac{3}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \frac{1}{a_0^3 \pi} \sum_{nlm} C_{a 100}^{H_1} C_{i 100}^{H_1} \left( C_{i 100}^{H_1} C_{a nlm}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \\
 & \cdot \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1 H_1}) + \frac{1}{a_0^3 \pi} \sum_{nlm} C_{a 100}^{H_1} C_{i 100}^{H_1} \left( C_{i 100}^{H_1} C_{a nlm}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2 H_1}) + \\
 & + \frac{1}{a_0^3 \pi} \sum_{nlm} \left( C_{a 100}^{H_1} C_{i nlm}^{C_1} + i \leftrightarrow a \right) \left( C_{i 100}^{H_1} C_{a 100}^{H_2} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{a 100}^{H_1} C_{i n_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{a 100}^{H_1} C_{i n_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) +
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{a_0^3 \pi} \sum_{nlm} \left( C_{a100}^{H_1} C_{inlm}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{a100}^{H_1} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2H_2}) + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{a100}^{H_1} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{an_1 l_1 m_1}^{C_1} C_{in_2 l_2 m_2}^{C_1} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{an_2 l_2 m_2}^{C_1} C_{in_3 l_3 m_3}^{C_1} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{an_2 l_2 m_2}^{C_1} C_{in_3 l_3 m_3}^{C_1} \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{an_1 l_1 m_1}^{C_1} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{an_2 l_2 m_2}^{C_1} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{an_2 l_2 m_2}^{C_1} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{an_1 l_1 m_1}^{C_2} C_{in_2 l_2 m_2}^{C_2} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{C_2} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{a n_2 l_2 m_2}^{C_2} C_{i n_3 l_3 m_3}^{C_2} \left( C_{i 100}^{H_1} C_{a n_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) \left. \right\} \quad (56)
 \end{aligned}$$

$$\begin{aligned}
 J_{H_1 H_2}^{FC(7)}[H_I^0] = & A \cdot e^{-\frac{3}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + (B + C \sin\phi + D \cos\phi) e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \\
 & + (B' + C' \sin\phi + D' \cos\phi + E' \sin 2\phi + F' \cos 2\phi) e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \\
 & + B'' + C'' \sin\phi + D'' \cos\phi + E'' \sin 2\phi + F'' \cos 2\phi \quad (57)
 \end{aligned}$$

$$A = \left( \frac{16\beta}{3a_0^3} \right)^2 \sum_{ia} \frac{C_{a100}^{H_1} C_{i100}^{H_1} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right)}{\varepsilon_a - \varepsilon_i} \quad (58)$$

$$\begin{aligned}
 B = & \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \left\{ C_{a100}^{H_1} C_{i100}^{H_1} \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1 H_1}) \end{pmatrix} + \right. \\
 & + C_{a100}^{H_1} C_{i100}^{H_1} \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2 H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2 H_1}) \end{pmatrix} + \\
 & + \left( C_{a100}^{H_1} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) \end{pmatrix} + \\
 & \left. + \left( C_{a100}^{H_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_2}) \right\} \quad (59)
 \end{aligned}$$

$$\begin{aligned}
 \left( \begin{matrix} C \\ D \end{matrix} \right) = & \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \left( C_{a100}^{H_1} C_{i21\pm 1}^{C_1} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1 H_2}) + \right. \\
 & \left. + \left( C_{a100}^{H_1} C_{i21\pm 1}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2 H_2}) \right\} \quad (60)
 \end{aligned}$$

$$\begin{aligned}
 B' = & \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \left\{ \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \otimes \left( C_{a100}^{H_1} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \right. \\
 & \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right] \otimes \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] + \\
 & + \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left( C_{a100}^{H_1} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \left[ \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right] \otimes \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] + \\
 & + \left( C_{a100}^{H_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left( C_{a100}^{H_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \otimes \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \right] \cdot \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] \otimes \left[ \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right] + \\
 & + \frac{1}{2} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_1} + C_{a21-1}^{C_1} C_{i21-1}^{C_1} \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i200}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{a200}^{C_2} C_{i200}^{C_2} \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left( C_{a21+1}^{C_2} C_{i21+1}^{C_2} + C_{a21-1}^{C_2} C_{i21-1}^{C_2} \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \left. \right\} \quad (61)
 \end{aligned}$$

$$\begin{aligned}
 \left( \frac{C'}{D'} \right) &= \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \left\{ \left( C_{a100}^{H_1} C_{i21\pm 1}^{C_1} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \right. \\
 &\cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left( C_{a100}^{H_1} C_{i21\pm 1}^{C_1} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \\
 &\cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left( C_{a100}^{H_1} C_{i21\pm 1}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \\
 &\cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \left( C_{a100}^{H_1} C_{i21\pm 1}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \\
 &\cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \cdot C_{i21\pm 1}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \\
 &\cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21\pm 1}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \\
 &\cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \left( C_{a21\pm 1}^{C_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \cdot \\
 &\cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \left( C_{a200}^{C_2} C_{i21\pm 1}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \left. \right\} \quad (62)
 \end{aligned}$$

which can be simplified as

$$\begin{aligned}
 \left( \frac{C'}{D'} \right) &= \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \left\{ \left[ C_{a100}^{H_1} \left( C_{i21\pm 1}^{C_1} \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i21\pm 1}^{C_2} \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) + i \leftrightarrow a \right] \cdot \right. \\
 &\cdot \left[ C_{i100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} + \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right) + i \leftrightarrow a \right] + \\
 &+ \left( C_{i100}^{H_1} C_{a100}^{H_2} + i \leftrightarrow a \right) \cdot \left[ \left( C_{i21\pm 1}^{C_1} \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i21\pm 1}^{C_2} \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) \right] \cdot
 \end{aligned}$$



$$\begin{aligned}
 & + \frac{1}{2} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_1} + C_{a21-1}^{C_1} C_{i21-1}^{C_1} \right) \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \\
 & \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \otimes \left( C_{i200}^{C_2} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) + i \leftrightarrow a \right) \right] \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \frac{1}{2} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \\
 & \cdot \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left( C_{i200}^{C_2} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] + \frac{1}{2} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \\
 & + \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{a200}^{C_2} C_{i200}^{C_2} \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left( C_{a21+1}^{C_2} C_{i21+1}^{C_2} + C_{a21-1}^{C_2} C_{i21-1}^{C_2} \right) \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \\
 & \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + C_{a200}^{C_2} C_{i200}^{C_2} \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix}
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \frac{1}{2} \left( C_{a21+1}^{C_2} C_{i21+1}^{C_2} + C_{a21-1}^{C_2} C_{i21-1}^{C_2} \right) \cdot \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + \right. \\
 & \left. + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \begin{pmatrix} \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \\ \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \end{pmatrix} \quad (66) \\
 \left( \frac{C''}{D''} \right) &= \frac{1}{a_0 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \otimes \right. \right. \\
 & \left. \left. \otimes \left( C_{i21\pm 1}^{C_1} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left( C_{i21\pm 1}^{C_1} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \otimes \right. \\
 & \left. \otimes \left( C_{i21\pm 1}^{C_2} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left( C_{a21\pm 1}^{C_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \left[ \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left( C_{i21+1}^{C_2} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \\
 & \cdot \left( C_{a21\pm 1}^{C_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left( C_{a200}^{C_2} C_{i21\pm 1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left( C_{i100}^{H_1} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) +
 \end{aligned}$$

$$\begin{aligned}
 & + \left( C_{a200}^{C_2} C_{i21\pm 1}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{i100}^{H_1} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \\
 & \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \} \quad (67)
 \end{aligned}$$

$$\begin{aligned}
 E''' = & \frac{1}{2} \cdot \frac{1}{a_0 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{i100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} + \right. \right. \\
 & \left. \left. + \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right) + i \leftrightarrow a \right\} \cdot \left\{ C_{a21+1}^{C_1} C_{i21-1}^{C_1} \overline{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21-1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \\
 & \left. + C_{a21+1}^{C_1} C_{i21-1}^{C_2} \overline{\varphi}_{21+1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) + C_{a21+1}^{C_2} C_{i21-1}^{C_2} \overline{\varphi}_{21+1}^{C_2}(\mathbf{r}_{C_2H_2}) \overline{\varphi}_{21-1}^{C_2}(\mathbf{r}_{C_2H_2}) + i \leftrightarrow a \right\} \quad (68)
 \end{aligned}$$

$$\begin{aligned}
 F''' = & \frac{1}{2} \cdot \frac{1}{a_0 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{i100}^{H_1} \left( \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} + \right. \right. \\
 & \left. \left. + \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right) + i \leftrightarrow a \right\} \cdot \left\{ \left( C_{a21-1}^{C_1} C_{i21-1}^{C_1} - C_{a21+1}^{C_1} C_{i21+1}^{C_1} \right) \cdot \right. \\
 & \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left( C_{a21-1}^{C_1} C_{i21-1}^{C_2} - C_{a21+1}^{C_1} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & \left. + \left( C_{a21-1}^{C_2} C_{i21-1}^{C_2} - C_{a21+1}^{C_2} C_{i21+1}^{C_2} \right) \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right\} \quad (69)
 \end{aligned}$$

**8th sum:**

$$J_{H_1 H_2}^{FC(8)}[H_I^0] = \frac{1}{a_0 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \sum_{\substack{A \neq H_1 \\ B \neq H_1 \\ C \neq H_2}} C_{in_1 l_1 m_1}^A C_{an_2 l_2 m_2}^B \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^C + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_1}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_1}) \varphi_{n_3 l_3 m_3}^C(\mathbf{r}_{CH_2}) \right\} \quad (70)$$

$$J_{H_1 H_2}^{FC(8)}[H_I^0] = \frac{1}{a_0 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left\{ C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{H_1} + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) + \right. \right. \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{H_1} + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ \left. + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) + \right\}$$

$$\begin{aligned}
 &+ C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 &+ C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 &+ C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 &+ C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 &+ C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 &+ C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 &+ C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 &+ C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 &+ C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 &+ C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 &+ C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) \} \quad (71)
 \end{aligned}$$

Eq. (71) can be simplified to give

$$\begin{aligned}
 J_{H_1H_2}^{FC(8)}[H_I^0] &= \frac{1}{a_0 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \\
 &\sum_{\substack{n_1l_1m_1 \\ n_2l_2m_2 \\ n_3l_3m_3}} \left\{ C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{H_1} + i \leftrightarrow a \right) \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) + \right. \\
 &+ C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_1} + i \leftrightarrow a \right) \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 &+ C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{H_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 &+ \left( C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{H_1} + i \leftrightarrow a \right) \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 &+ \left( C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_1} + i \leftrightarrow a \right) \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 &+ \left( C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{H_1} + i \leftrightarrow a \right) \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 &+ \left( C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) \}
 \end{aligned}$$

$$\begin{aligned}
 & + \left( C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{C_1} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{H_2} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{H_2}(\mathbf{r}_{H_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 & + C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{X_2} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{H_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 & + C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) \} \quad (72)
 \end{aligned}$$

Substitution  $\varphi_{100}^{H_1}(\mathbf{r}_{H_1H_2}) = \varphi_{100}^{H_2}(\mathbf{r}_{H_2H_1})$  into Eq. (72) gives:

$$\begin{aligned}
 J_{H_1H_2}^{FC(8)}[H_I^0] &= \frac{1}{a_0 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \frac{1}{a_0^4 \pi \sqrt{a_0 \pi}} C_{i100}^{H_2} C_{a100}^{H_2} \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \right. \\
 & \cdot e^{-\frac{3}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \frac{1}{\pi a_0^3} \sum_{nlm} C_{i100}^{H_2} C_{a100}^{H_2} \left( C_{a100}^{H_2} C_{inlm}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1H_2}) + \frac{1}{\pi a_0^3} \sum_{nlm} C_{i100}^{H_2} C_{a100}^{H_2} \left( C_{a100}^{H_2} C_{in_3l_3m_3}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & \left. + \frac{1}{\pi a_0^3} \sum_{nlm} \left( C_{i100}^{H_2} C_{anlm}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1H_1}) + \right.
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \\
 & \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) + \frac{1}{\pi a_0^3} \sum_{nlm} \left( C_{i100}^{H_2} C_{anlm}^{C_2} + i \leftrightarrow a \right) \\
 & \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2 H_1}) + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \\
 & \cdot \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \\
 & \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{in_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right)
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{i n_1 l_1 m_1}^{C_1} C_{a n_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left( C_{a i 100}^{H_2} C_{i n_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i n_1 l_1 m_1}^{C_2} C_{a n_2 l_2 m_2}^{C_2} \left( C_{a i 100}^{H_2} C_{i i 100}^{H_1} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{i n_1 l_1 m_1}^{C_2} C_{a n_2 l_2 m_2}^{C_2} \left( C_{a i 100}^{H_2} C_{i n_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{i n_1 l_1 m_1}^{C_2} C_{a n_2 l_2 m_2}^{C_2} \left( C_{a i 100}^{H_2} C_{i n_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) \left. \right\} \quad (73)
 \end{aligned}$$

$$\begin{aligned}
 J_{H_1 H_2}^{FC(8)}[H_I^0] = & A \cdot e^{-\frac{3}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + (B + C \sin \phi + D \cos \phi) e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \\
 & + (B' + C' \sin \phi + D' \cos \phi) e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + B'' + C'' \sin \phi + D'' \cos \phi \quad (74)
 \end{aligned}$$

The coefficients in Eq. (74) are as follows:

$$\begin{aligned}
 A = & \left( \frac{16\beta}{3a_0^3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot C_{i i 100}^{H_2} C_{a i 100}^{H_2} \left( C_{a i 100}^{H_2} C_{i i 100}^{H_1} + i \leftrightarrow a \right) \quad (75) \\
 B = & \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{i i 100}^{H_2} C_{a i 100}^{H_2} \left( C_{a i 100}^{H_2} \left( C_{i 200}^{C_1}, C_{i 210}^{C_1} \right) + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) \end{pmatrix} + \right. \\
 & + C_{i i 100}^{H_2} C_{a i 100}^{H_2} \left( C_{a i 100}^{H_2} C_{i 200}^{C_2} + i \leftrightarrow a \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & \left. + \left( C_{i i 100}^{H_2} \left( C_{a 200}^{C_1}, C_{a 21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a i 100}^{H_2} C_{i i 100}^{H_1} + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1 H_1}) \end{pmatrix} \right\}
 \end{aligned}$$

$$+ \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \left. \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right\} \quad (76)$$

$$\left( \frac{C}{D} \right) = \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{C_{i100}^{H_2} C_{a100}^{H_2}}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{a100}^{H_2} \left( C_{i21\pm 1}^{C_1} \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i21\pm 1}^{C_2} \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) + i \leftrightarrow a \right\} \quad (77)$$

$$B' = \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \left[ \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \otimes \left( C_{a100}^{H_2} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \right.$$

$$\cdot \left[ \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \right] + \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_2} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot$$

$$\cdot \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \left[ \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \right.$$

$$\left. \left( C_{a100}^{H_2} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \left[ \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \right] +$$

$$+ \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \left( C_{a100}^{H_2} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \left. \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right\} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) +$$

$$+ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \left[ \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \right] +$$

$$+ \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] + i \leftrightarrow a \cdot$$

$$\cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_1 \\ \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_2 \\ \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] + \left( C_{a100}^{H_2} C_{i100}^{H_1} + i \leftrightarrow a \right) \cdot$$

$$\cdot \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_2 \\ \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_2 \\ \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \quad (78)$$

$$\left( \frac{C'}{D'} \right) = \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{a100}^{H_2} \left( C_{i21\pm 1}^{C_1} \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i21\pm 1}^{C_2} \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) + i \leftrightarrow a \right\} \cdot$$

$$\cdot \left\{ C_{i100}^{H_2} \left( \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \cdot \left( \begin{array}{c} C_1 \\ \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) + \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \cdot \left( \begin{array}{c} C_2 \\ \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \right) + i \leftrightarrow a \right\}$$

(79)

$$B'' = \frac{1}{a_0 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \right.$$

$$+ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \otimes \left( C_{a100}^{H_2} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot$$

$$\cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_1 \\ \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_1 \\ \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_1 \\ \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \end{array} \right] +$$

$$+ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left( C_{a100}^{H_2} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot$$

$$\cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_1 \\ \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_1 \\ \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \end{array} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) +$$

$$+ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right] \otimes \left( C_{a100}^{H_2} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \cdot$$

$$\cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_1 \\ \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_2 \\ \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_1 \\ \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \end{array} \right] +$$

$$\begin{aligned}
 & + \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right] \cdot \left( C_{a100}^{H_2}, C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{X_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{X_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \otimes \left( C_{a100}^{H_2} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \end{array} \right] + \\
 & + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left( C_{a100}^{H_2}, C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \} \quad (80)
 \end{aligned}$$

$$\begin{aligned}
 \left( \begin{array}{c} C''' \\ D'' \end{array} \right) & = \frac{1}{a_0 \sqrt{\pi a_0}} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{a100}^{H_2} \left( C_{i21\pm 1}^{C_1} \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i21\pm 1}^{C_2} \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) + \right. \\
 & + i \leftrightarrow a \left. \right\} \cdot \left\{ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \right] \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \end{array} \right] + \right. \\
 & + \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \right] \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] + \\
 & + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \left. \right\} \quad (81)
 \end{aligned}$$

**9th sum:**

$$J_{H_1 H_2}^{FC(9)}[H_I^0] = \left(\frac{16\pi\beta}{3}\right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} \sum_{\substack{A \neq H_1 \\ B \neq H_1 \\ C \neq H_2 \\ D \neq H_2}} C_{in_1 l_1 m_1}^A C_{an_2 l_2 m_2}^B C_{an_3 l_3 m_3}^C C_{in_4 l_4 m_4}^D \varphi_{n_1 l_1 m_1}^A(\mathbf{r}_{AH_1}) \varphi_{n_2 l_2 m_2}^B(\mathbf{r}_{BH_1}) \varphi_{n_3 l_3 m_3}^C(\mathbf{r}_{CH_2}) \varphi_{n_4 l_4 m_4}^D(\mathbf{r}_{DH_2}) \right\} \quad (82)$$

$$J_{H_1 H_2}^{FC(9)}[H_I^0] = \left(\frac{16\pi\beta}{3}\right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \sum_{\substack{n_3 l_3 m_3 \\ n_4 l_4 m_4}} \left\{ C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{H_2} C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{H_1} \cdot \right. \\ \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{H_1}(\mathbf{r}_{H_1 H_2}) + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{H_2} \cdot \\ \cdot \left( C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{C_1} + i \leftrightarrow a \right) \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{H_2} \left( C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\ \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{H_2} C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_1} \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{H_2} \left( C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\ \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ + C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{H_2} C_{an_3 l_3 m_3}^{C_2} C_{in_4 l_4 m_4}^{C_2} \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{H_1} \cdot \\ \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{H_1}(\mathbf{r}_{H_1 H_2}) + \\ + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{C_1} + i \leftrightarrow a \right) \cdot \\ \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\ \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_1} \cdot \\ \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) +$$

$$\begin{aligned}
 & + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot C_{an_3 l_3 m_3}^{C_2} C_{in_4 l_4 m_4}^{C_2} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{H_1} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{H_1}(\mathbf{r}_{H_1 H_2}) + \\
 & + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_1} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \left( C_{in_1 l_1 m_1}^{H_2} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot C_{an_3 l_3 m_3}^{C_2} C_{in_4 l_4 m_4}^{C_2} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{H_2}(\mathbf{r}_{H_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{H_1} \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{H_1}(\mathbf{r}_{H_1 H_2}) + \\
 & + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{an_3 l_3 m_3}^{H_1} C_{in_4 l_4 m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{H_1}(\mathbf{r}_{H_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_1} \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) +
 \end{aligned}$$

$$\begin{aligned}
 & + C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_1} \left( C_{an_3l_3m_3}^{C_1} C_{in_4l_4m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_4l_4m_4}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_1} C_{an_3l_3m_3}^{C_2} C_{in_4l_4m_4}^{C_2} \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{n_4l_4m_4}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \cdot C_{an_3l_3m_3}^{H_1} C_{in_4l_4m_4}^{H_1} \cdot \\
 & \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) \varphi_{n_4l_4m_4}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{an_3l_3m_3}^{H_1} C_{in_4l_4m_4}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) \varphi_{n_4l_4m_4}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{an_3l_3m_3}^{H_1} C_{in_4l_4m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) \varphi_{n_4l_4m_4}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \cdot C_{an_3l_3m_3}^{C_1} C_{in_4l_4m_4}^{C_1} \cdot \\
 & \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_4l_4m_4}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{an_3l_3m_3}^{C_1} C_{in_4l_4m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_4l_4m_4}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left( C_{in_1l_1m_1}^{C_1} C_{an_2l_2m_2}^{C_2} + i \leftrightarrow a \right) \cdot C_{an_3l_3m_3}^{C_2} C_{in_4l_4m_4}^{C_2} \cdot \\
 & \cdot \varphi_{n_1l_1m_1}^{C_1}(\mathbf{r}_{C_1H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{n_4l_4m_4}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} C_{an_3l_3m_3}^{H_1} C_{in_4l_4m_4}^{H_1} \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) \varphi_{n_4l_4m_4}^{H_1}(\mathbf{r}_{H_1H_2}) + \\
 & + C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} \left( C_{an_3l_3m_3}^{H_1} C_{in_4l_4m_4}^{C_1} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) \varphi_{n_4l_4m_4}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} \left( C_{an_3l_3m_3}^{H_1} C_{in_4l_4m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{H_1}(\mathbf{r}_{H_1H_2}) \varphi_{n_4l_4m_4}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} C_{an_3l_3m_3}^{C_1} C_{in_4l_4m_4}^{C_1} \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_4l_4m_4}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + C_{in_1l_1m_1}^{C_2} C_{an_2l_2m_2}^{C_2} \left( C_{an_3l_3m_3}^{C_1} C_{in_4l_4m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1l_1m_1}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_2l_2m_2}^{C_2}(\mathbf{r}_{C_2H_1}) \varphi_{n_3l_3m_3}^{C_1}(\mathbf{r}_{C_1H_2}) \varphi_{n_4l_4m_4}^{C_2}(\mathbf{r}_{C_2H_2}) +
 \end{aligned}$$

$$+ C_{i1_1 m_1}^{C_2} C_{a n_2 l_2 m_2}^{C_2} C_{a n_3 l_3 m_3}^{C_2} C_{i n_4 l_4 m_4}^{C_2} \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) \left. \right\} \quad (83)$$

Substitution  $\varphi_{100}^{H_1}(\mathbf{r}_{H_1 H_2}) = \varphi_{100}^{H_2}(\mathbf{r}_{H_2 H_1})$  into Eq. (83) gives

$$\begin{aligned} J_{H_1 H_2}^{FC(9)}[H_I^0] = & \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \frac{1}{\pi^2 a_0^6} \cdot C_{i100}^{H_2} C_{a100}^{H_2} C_{a100}^{H_1} C_{i100}^{H_1} \cdot e^{-\frac{4}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} + \right. \\ & + \frac{1}{\pi a_0^4 \sqrt{\pi a_0}} \sum_{nlm} C_{i100}^{H_2} C_{a100}^{H_2} \left( C_{a100}^{H_1} C_{inlm}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{3}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ & + \frac{1}{\pi a_0^4 \sqrt{\pi a_0}} \sum_{nlm} C_{i100}^{H_2} C_{a100}^{H_2} \left( C_{a100}^{H_1} C_{inlm}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{3}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_2} C_{a100}^{H_2} C_{a n_1 l_1 m_1}^{C_1} C_{i n_2 l_2 m_2}^{C_1} \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\ & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_2} C_{a100}^{H_2} \left( C_{a n_1 l_1 m_1}^{C_1} C_{i n_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \\ & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{i100}^{H_2} C_{a100}^{H_2} C_{a n_1 l_1 m_1}^{C_2} C_{i n_2 l_2 m_2}^{C_2} \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\ & + \frac{1}{\pi a_0^4 \sqrt{\pi a_0}} \sum_{nlm} \left( C_{i100}^{H_2} C_{anlm}^{C_1} + i \leftrightarrow a \right) C_{a100}^{H_1} C_{i100}^{H_1} \cdot e^{-\frac{3}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{nlm}^{C_1}(\mathbf{r}_{C_1 H_1}) + \\ & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 m_1 l_1 \\ n_2 m_2 l_2}} \left( C_{i100}^{H_2} C_{a n_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_1} C_{i n_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \\ & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 m_1 l_1 \\ n_2 m_2 l_2}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_1} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot C_{an_2 l_2 m_2}^{C_1} C_{in_3 l_3 m_3}^{C_1} \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot \left( C_{an_2 l_2 m_2}^{C_1} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_1} + i \leftrightarrow a \right) \cdot C_{an_2 l_2 m_2}^{C_2} C_{in_3 l_3 m_3}^{C_2} \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \frac{1}{\pi a_0^4 \sqrt{\pi a_0}} \sum_{nlm} \left( C_{i100}^{H_2} C_{anlm}^{C_2} + i \leftrightarrow a \right) \cdot C_{a100}^{H_1} C_{i100}^{H_1} \cdot e^{-\frac{3}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{nlm}^{C_2}(\mathbf{r}_{C_2 H_1}) + \\
 & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 m_1 l_1 \\ n_2 m_2 l_2}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_1} C_{in_2 l_2 m_2}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 m_1 l_1 \\ n_2 m_2 l_2}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_1} C_{in_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) +
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot C_{an_2 l_2 m_2}^{H_1} C_{an_3 l_3 m_3}^{H_1} \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{an_2 l_2 m_2}^{C_1} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{i100}^{H_2} C_{an_1 l_1 m_1}^{C_2} + i \leftrightarrow a \right) \cdot C_{an_2 l_2 m_2}^{C_2} C_{in_3 l_3 m_3}^{C_2} \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} C_{a100}^{H_1} C_{i100}^{H_1} \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_1} C_{in_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{a100}^{H_1} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_1} \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) +
 \end{aligned}$$

$$\begin{aligned}
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} \left( C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_1} C_{an_3 l_3 m_3}^{C_2} C_{in_4 l_4 m_4}^{C_2} \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} \left( C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot C_{a100}^{H_1} C_{i100}^{H_1} \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_1} C_{in_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} \left( C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_1} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} \left( C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_1} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} \left( C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot \left( C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) +
 \end{aligned}$$

$$\begin{aligned}
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} \left( C_{in_1 l_1 m_1}^{C_1} C_{an_2 l_2 m_2}^{C_2} + i \leftrightarrow a \right) \cdot C_{an_3 l_3 m_3}^{C_2} C_{in_4 l_4 m_4}^{C_2} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_1}(\mathbf{r}_{C_1 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \frac{1}{\pi a_0^3} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2}} C_{in_1 l_1 m_1}^{C_2} C_{an_2 l_2 m_2}^{C_2} C_{a100}^{H_1} C_{i100}^{H_1} \cdot e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{in_1 l_1 m_1}^{C_2} C_{an_2 l_2 m_2}^{C_2} \left( C_{a100}^{H_1} C_{in_3 l_3 m_3}^{C_1} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \frac{1}{a_0 \sqrt{\pi a_0}} \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3}} C_{in_1 l_1 m_1}^{C_2} C_{an_2 l_2 m_2}^{C_2} \left( C_{a100}^{H_1} C_{in_3 l_3 m_3}^{C_2} + i \leftrightarrow a \right) \cdot e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} C_{in_1 l_1 m_1}^{C_2} C_{an_2 l_2 m_2}^{C_2} C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_1} \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_1}(\mathbf{r}_{C_1 H_2}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} C_{in_1 l_1 m_1}^{C_2} C_{an_2 l_2 m_2}^{C_2} \left( C_{an_3 l_3 m_3}^{C_1} C_{in_4 l_4 m_4}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_1}(\mathbf{r}_{C_1 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \sum_{\substack{n_1 l_1 m_1 \\ n_2 l_2 m_2 \\ n_3 l_3 m_3 \\ n_4 l_4 m_4}} C_{in_1 l_1 m_1}^{C_2} C_{an_2 l_2 m_2}^{C_2} C_{an_3 l_3 m_3}^{C_2} C_{in_4 l_4 m_4}^{C_2} \cdot \varphi_{n_1 l_1 m_1}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_2 l_2 m_2}^{C_2}(\mathbf{r}_{C_2 H_1}) \varphi_{n_3 l_3 m_3}^{C_2}(\mathbf{r}_{C_2 H_2}) \varphi_{n_4 l_4 m_4}^{C_2}(\mathbf{r}_{C_2 H_2}) \}
 \end{aligned}$$

(84)

Eq. (84) can be represented in a generalized form:

$$\begin{aligned}
 J_{H_1 H_2}^{FC(9)}[H_I^0] = & A \cdot e^{-\frac{4}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + (B + C \sin\phi + D \cos\phi) e^{-\frac{3}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \\
 & + (B' + C' \sin\phi + D' \cos\phi + E' \sin 2\phi + F' \cos 2\phi) e^{-\frac{2}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \\
 & + (B'' + C'' \sin\phi + D'' \cos\phi + E'' \sin 2\phi + F'' \cos 2\phi) e^{-\frac{1}{a_0} \sqrt{2L_{CH}^2 (1-\cos\phi) + L_{CC}^2}} + \\
 & + B''' + C''' \sin\phi + D''' \cos\phi + E''' \sin 2\phi + F''' \cos 2\phi
 \end{aligned} \tag{85}$$

The coefficients in Eq. (85) are as follows:

$$A = \left( \frac{16\beta}{3a_0^3} \right)^2 \sum_{ia} \frac{C_{i100}^{H_2} C_{a100}^{H_2} C_{a100}^{H_1} C_{i100}^{H_1}}{\varepsilon_a - \varepsilon_i} = - \left( \frac{8\beta}{3a_0^3} \right)^2 \pi_{S_{H_2}, S_{H_1}} \tag{86}$$

$$\begin{aligned}
 B = & \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{i100}^{H_2} C_{a100}^{H_2} \left( C_{a100}^{H_1} \left( \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) \end{pmatrix} \right) + \right. \right. \\
 & + \left. \left. C_{i200}^{C_2} \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_2}) \right) + i \leftrightarrow a \right\} + C_{a100}^{H_1} C_{i100}^{H_1} \left( C_{i100}^{H_2} \left( \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1 H_1}) \end{pmatrix} \right) + \right. \\
 & \left. \left. \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2 H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2 H_1}) \end{pmatrix} \right) + i \leftrightarrow a \right\}
 \end{aligned} \tag{87}$$

$$\left( \begin{matrix} C \\ D \end{matrix} \right) = \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3a_0^2} \right)^2 \sum_{ia} \frac{C_{i100}^{H_2} C_{a100}^{H_2}}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{a100}^{H_1} \left( C_{i21\pm 1}^{C_1} \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1 H_2}) + C_{i21\pm 1}^{C_2} \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2 H_2}) \right) + i \leftrightarrow a \right\} \tag{88}$$

$$\begin{aligned}
 B' = & \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{i100}^{H_2} C_{a100}^{H_2} \cdot \left[ \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \otimes \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \right] \cdot \right. \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) \end{pmatrix} \right] + \frac{1}{2} C_{i100}^{H_2} C_{a100}^{H_2} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_1} + C_{a21-1}^{C_1} C_{i21-1}^{C_1} \right) \cdot \\
 & \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1 H_2}) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1 H_2}) + C_{i100}^{H_2} C_{a100}^{H_2} \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1 H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1 H_2}) \end{pmatrix} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2 H_2}) + \\
 & + \frac{1}{2} C_{i100}^{H_2} C_{a100}^{H_2} \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1 H_2}) \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2 H_2}) +
 \end{aligned}$$

$$\begin{aligned}
 & + C_{i100}^{H_2} C_{a100}^{H_2} C_{a200}^{C_2} C_{i200}^{C_2} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} C_{i100}^{H_2} C_{a100}^{H_2} \left( C_{a21+1}^{C_2} C_{i21+1}^{C_2} + C_{a21-1}^{C_2} C_{i21-1}^{C_2} \right) \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \otimes \left( C_{a100}^{H_1} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \right] \otimes \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \\ \left( \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \end{array} \right] + \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \left[ \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \right. \\
 & \left. \otimes \left( C_{a100}^{H_1} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \left[ \begin{array}{c} \left( \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \\ \left( \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \\ \left( \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \end{array} \right] \otimes \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \\ \left( \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \end{array} \right] + \\
 & + \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a100}^{H_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \left[ \begin{array}{c} \left( \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \\ \left( \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \\ \left( \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \end{array} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{a100}^{H_1} C_{i100}^{H_1} \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \right] \otimes \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \right] + \\
 & + C_{a100}^{H_1} C_{i100}^{H_1} \left[ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] + i \leftrightarrow a \right] \cdot
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \left[ \begin{pmatrix} C_1^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right] + C_{a100}^{H_1} C_{i100}^{H_1} \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \\
 & \cdot \left. \left[ \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right] \right\} \quad (89)
 \end{aligned}$$

$$\begin{aligned}
 \left( \frac{C'}{D'} \right) &= \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \left( C_{i21\pm 1}^{C_1} \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i21\pm 1}^{C_2} \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) \cdot \right. \\
 & \cdot \left[ C_{i100}^{H_2} C_{a100}^{H_2} \cdot \left[ \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} + C_{a200}^{C_2} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \right] + \right. \\
 & + C_{a100}^{H_1} \cdot \left[ C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \right] + \\
 & \left. \left. + C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} + i \leftrightarrow a \right] \right\} + i \leftrightarrow a \quad (90)
 \end{aligned}$$

$$\begin{aligned}
 E' &= \frac{1}{2} \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{C_{i100}^{H_2} C_{a100}^{H_2}}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{a21+1}^{C_1} C_{i21-1}^{C_1} \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \\
 & + \left( C_{a21+1}^{C_1} C_{i21-1}^{C_2} + C_{a21-1}^{C_1} C_{i21+1}^{C_2} \right) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + C_{a21+1}^{C_2} C_{i21-1}^{C_2} \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & \left. + i \leftrightarrow a \right\} \quad (91)
 \end{aligned}$$

$$\begin{aligned}
 F' &= \frac{1}{2} \frac{\pi}{a_0^3} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{C_{i100}^{H_2} C_{a100}^{H_2}}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \left( C_{a21-1}^{C_1} C_{i21-1}^{C_1} - C_{a21+1}^{C_1} C_{i21+1}^{C_1} \right) \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \\
 & \left. + \left( C_{a21-1}^{C_1} C_{i21-1}^{C_2} - C_{a21+1}^{C_1} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \right.
 \end{aligned}$$

$$+ \left( C_{a21-1}^{C_2} C_{i21-1}^{C_2} - C_{a21+1}^{C_2} C_{i21+1}^{C_2} \right) \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \left. \right\} \quad (92)$$

$$\begin{aligned}
 B'' = & \frac{\pi}{a_0} \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \right. \\
 & + \left[ \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \otimes \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \otimes \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \right] \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \right] \otimes \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \\ \left( \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \end{array} \right] \otimes \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \\ \left( \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \end{array} \right] \Bigg] + \\
 & + \frac{1}{2} \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a21+1}^{C_1} C_{i21+1}^{C_1} + C_{a21-1}^{C_1} C_{i21-1}^{C_1} \right) \cdot \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \cdot \\
 & \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \right] \otimes \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \\ \left( \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \end{array} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \frac{1}{2} \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \\
 & \cdot \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot C_{a200}^{C_2} C_{i200}^{C_2} \cdot \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \cdot \left( C_{a21+1}^{C_2} C_{i21+1}^{C_2} + C_{a21-1}^{C_2} C_{i21-1}^{C_2} \right) \cdot \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \cdot \\
 & \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \left[ \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \otimes \right. \\
 & \left. \otimes \left( C_{i200}^{X_1}, C_{i210}^{X_1} \right) \right] \cdot \left[ \begin{array}{c} \left( \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \\ \left( \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \\ \left( \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \end{array} \right] \otimes \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \\ \left( \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \end{array} \right] \otimes \left[ \begin{array}{c} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \\ \left( \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \right) \end{array} \right] \Bigg] + \\
 & + \frac{1}{2} \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a21+1}^{C_1} C_{i21+1}^{C_1} + C_{a21-1}^{C_1} C_{i21-1}^{C_1} \right) \cdot
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \\
 & \cdot \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \begin{bmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{bmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + C_{a200}^{C_2} C_{i200}^{C_2} \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \\
 & \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \frac{1}{2} \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \\
 & \cdot \left( C_{a21+1}^{C_2} C_{i21+1}^{C_2} + C_{a21-1}^{C_2} C_{i21-1}^{C_2} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \otimes \left( C_{a100}^{H_1} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] + \\
 & + \left( C_{a100}^{H_1} C_{i200}^{C_2} + i \leftrightarrow a \right) \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left( C_{a100}^{H_1} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_1 \\ \varphi_{200}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_2 \\ \varphi_{200}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_1 \\ \varphi_{200}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}(\mathbf{r}_{C_1H_2}) \end{array} \right) \end{array} \right] + \\
 & + \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right] \cdot \left( C_{a100}^{H_1}, C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_1 \\ \varphi_{200}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_2 \\ \varphi_{200}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \otimes \left( C_{a100}^{H_1} \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_2 \\ \varphi_{200}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_2 \\ \varphi_{200}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_1 \\ \varphi_{200}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}(\mathbf{r}_{C_1H_2}) \end{array} \right) \end{array} \right] + \\
 & + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left( C_{a100}^{H_1}, C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_2 \\ \varphi_{200}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_2 \\ \varphi_{200}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \} \quad (93)
 \end{aligned}$$

$$\begin{aligned}
 \left( \begin{array}{c} C'' \\ D'' \end{array} \right) &= \frac{\pi}{a_0} \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \left( C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) + i \leftrightarrow a \right) \otimes \right. \\
 & \otimes \left\{ \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \left( C_{i21\pm 1}^{C_1} \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i21\pm 1}^{C_2} \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) + i \leftrightarrow a \right\} \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_1 \\ \varphi_{200}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_1 \\ \varphi_{200}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}(\mathbf{r}_{C_1H_2}) \end{array} \right) \end{array} \right] + \\
 & \left( C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left\{ \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \left( C_{i21\pm 1}^{C_1} \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \right. \\
 & \left. \left. + C_{i21\pm 1}^{C_2} \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) + i \leftrightarrow a \right\} \cdot \left[ \begin{array}{c} \left( \begin{array}{c} C_2 \\ \varphi_{200}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} C_1 \\ \varphi_{200}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}(\mathbf{r}_{C_1H_2}) \end{array} \right) \end{array} \right] +
 \end{aligned}$$

$$\begin{aligned}
 & + \left( C_{i100}^{H_2} \left\{ \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} + \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right\} + i \leftrightarrow a \right) \cdot \\
 & \left\{ C_{i200}^{C_2} \left( C_{a21+1}^{C_1} \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{a21\pm 1}^{C_2} \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) + i \leftrightarrow a \right\} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left\{ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \right] + \right. \\
 & \left[ \left( \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \right] \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right] + \\
 & + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right] \left. \right\} \cdot \\
 & \cdot \left\{ C_{a100}^{H_1} \left( C_{i21\pm 1}^{C_1} \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{i21\pm 1}^{C_2} \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) + i \leftrightarrow a \right\} \quad (94)
 \end{aligned}$$

$$\begin{aligned}
 E'' = & \frac{1}{2} \frac{\pi}{a_0} \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ C_{a21+1}^{C_1} C_{i21-1}^{C_1} \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \\
 & + \left( C_{a21+1}^{C_1} C_{i21-1}^{C_2} + C_{a21-1}^{C_1} C_{i21+1}^{C_2} \right) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + C_{a21+1}^{C_2} C_{i21-1}^{C_2} \cdot \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + i \leftrightarrow a \left. \right\} \cdot \\
 & \cdot \left\{ C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} + C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} + i \leftrightarrow a \right\} \quad (95)
 \end{aligned}$$

$$\begin{aligned}
 F''' = & \frac{1}{2} \frac{\pi}{a_0} \sqrt{\frac{\pi}{a_0}} \left( \frac{16\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \left( C_{a21-1}^{C_1} C_{i21-1}^{C_1} - C_{a21+1}^{C_1} C_{i21+1}^{C_1} \right) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \\
 & + \left( C_{a21-1}^{C_1} C_{i21-1}^{C_2} - C_{a21+1}^{C_1} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & \left. + \left( C_{a21-1}^{C_2} C_{i21-1}^{C_2} - C_{a21+1}^{C_2} C_{i21+1}^{C_2} \right) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right\} \\
 & \cdot \left\{ C_{i100}^{H_2} \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} + C_{i100}^{H_2} \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \cdot \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} + i \leftrightarrow a \right\} \quad (96)
 \end{aligned}$$

$$\begin{aligned}
 B''' = & \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \right. \\
 & \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \otimes \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \right] \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] + \\
 & + \frac{1}{2} \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left( C_{a21+1}^{C_1} C_{i21+1}^{C_1} + C_{a21-1}^{C_1} C_{i21-1}^{C_1} \right) \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \right] \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \otimes \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i200}^{C_2} + i \leftrightarrow a \right) \right] \\
 & \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \right] \cdot \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot C_{a200}^{C_2} C_{i200}^{C_2} \cdot
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left( C_{a21+1}^{C_2}, C_{i21+1}^{C_2} + C_{a21-1}^{C_2}, C_{i21-1}^{C_2} \right) \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \right] \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \otimes \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \right] \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] + \\
 & + \frac{1}{2} \left( C_{a21+1}^{C_1}, C_{i21+1}^{C_1} + C_{a21-1}^{C_1}, C_{i21-1}^{C_1} \right) \cdot \left[ \left( \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right] \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \left( \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \cdot C_{i200}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left( \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a21+1}^{C_1}, C_{i21+1}^{C_2} + C_{a21-1}^{C_1}, C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right] \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) +
 \end{aligned}$$

$$\begin{aligned}
 & + \left( \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot C_{a200}^{C_2} C_{i200}^{C_2} \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left( \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \cdot \left( C_{a21+1}^{C_2} C_{i21+1}^{C_2} + C_{a21-1}^{C_2} C_{i21-1}^{C_2} \right) \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \otimes \left( C_{i200}^{C_1}, C_{i210}^{C_1} \right) \right] \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \end{array} \right] + \\
 & + \frac{1}{2} \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left( C_{a21+1}^{C_1} C_{i21+1}^{C_1} + C_{a21-1}^{C_1} C_{i21-1}^{C_1} \right) \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \\
 & + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \otimes \left( \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i200}^{C_2} + i \leftrightarrow a \right) \right] \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \end{array} \right] \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\
 & + \frac{1}{2} \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left( C_{a21+1}^{C_1} C_{i21+1}^{C_2} + C_{a21-1}^{C_1} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \end{array} \right] \cdot \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) +
 \end{aligned}$$

$$\begin{aligned}
 & + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot C_{a200}^{C_2} C_{i200}^{C_2} \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \\ \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) + \\ \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \cdot \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \overline{\varphi}_{2\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \end{array} \right\} \quad (97)
 \end{aligned}$$

$$\begin{aligned}
 \left( \frac{C'''}{D'''} \right) & = \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \right. \\
 & \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \otimes \left[ C_{i21\pm 1}^{C_1} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \\
 & \left. + C_{i21\pm 1}^{C_2} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + i \leftrightarrow a \right] \cdot \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \\ \left. + \left[ \left( \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) + i \leftrightarrow a \right) \otimes \left[ C_{i21\pm 1}^{C_1} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \right. \right. \\
 & \left. \left. + C_{i21\pm 1}^{C_2} \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + i \leftrightarrow a \right] \cdot \right. \\
 & \cdot \left[ \begin{array}{c} \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{array} \right) \otimes \left( \begin{array}{c} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{array} \right) \\ \left. + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \otimes \left[ \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21\pm 1}^{C_1} \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \right. \\
 & \left. \left. + \left( C_{a200}^{C_1}, C_{a210}^{C_1} \right) C_{i21\pm 1}^{C_2} \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + i \leftrightarrow a \right] \cdot \right.
 \end{array} \right\}
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_2}) \\ \varphi_{210}^{C_1}(\mathbf{r}_{C_1H_2}) \end{pmatrix} \right] + \\
 & + \left\{ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \right] + \right. \\
 & + \left. \left[ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] + i \leftrightarrow a \right] \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right] + \right. \\
 & + \left. \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right] \right\} \cdot \\
 & \cdot \left\{ C_{i200}^{C_2} \left( C_{a21\pm 1}^{C_1} \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + C_{a21\pm 1}^{C_2} \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right) + i \leftrightarrow a \right\} \cdot \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_2}) \quad (98)
 \end{aligned}$$

$$\begin{aligned}
 E''' &= \frac{1}{2} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \right. \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \right] + \left[ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] + i \leftrightarrow a \right] \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \\ \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right] + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \\
 & \cdot \left[ \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \otimes \begin{pmatrix} \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \\ \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \end{pmatrix} \right] \left. \right\} \cdot \left\{ \left( C_{i21+1}^{C_1} C_{a21-1}^{C_1} + i \leftrightarrow a \right) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \\
 & + \left. \left( C_{a21+1}^{C_1} C_{i21-1}^{C_2} + C_{a21-1}^{C_1} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \bar{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \bar{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \right.
 \end{aligned}$$

$$+ \left( C_{a21+1}^{C_2} C_{i21-1}^{C_2} + i \leftrightarrow a \right) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \left. \right\} \quad (99)$$

$$F''' = \frac{1}{2} \left( \frac{16\pi\beta}{3} \right)^2 \sum_{ia} \frac{1}{\varepsilon_a - \varepsilon_i} \cdot \left\{ \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_1}, C_{a21-1}^{C_1} \right) \right] \cdot \left[ \begin{array}{l} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \otimes \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \otimes \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \end{array} \right] + \left[ \left( C_{i200}^{C_1}, C_{i21-1}^{C_1} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] + i \leftrightarrow a \right\} \cdot \left[ \begin{array}{l} \left( \varphi_{200}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \otimes \left( \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \otimes \left( \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \\ \left( \varphi_{21-1}^{C_1}(\mathbf{r}_{C_1H_1}) \right) \otimes \left( \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \end{array} \right] + \left[ \left( C_{i200}^{C_2}, C_{i210}^{C_2}, C_{i21-1}^{C_2} \right) \otimes \left( C_{a200}^{C_2}, C_{a210}^{C_2}, C_{a21-1}^{C_2} \right) \right] \cdot \left[ \begin{array}{l} \left( \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \otimes \left( \varphi_{200}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \\ \left( \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \otimes \left( \varphi_{210}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \\ \left( \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \otimes \left( \varphi_{21-1}^{C_2}(\mathbf{r}_{C_2H_1}) \right) \end{array} \right] \left. \right\} \cdot \left\{ \left( C_{i21-1}^{C_1} C_{a21-1}^{C_1} - C_{i21+1}^{C_1} C_{a21+1}^{C_1} \right) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) + \right. \\ \left. + \left( C_{a21-1}^{C_1} C_{i21-1}^{C_2} - C_{a21+1}^{C_1} C_{i21+1}^{C_2} + i \leftrightarrow a \right) \overline{\varphi}_{21\pm 1}^{C_1}(\mathbf{r}_{C_1H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) + \right. \\ \left. + \left( C_{a21-1}^{C_2} C_{i21-1}^{C_2} - C_{a21+1}^{C_2} C_{i21+1}^{C_2} \right) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \overline{\varphi}_{21\pm 1}^{C_2}(\mathbf{r}_{C_2H_2}) \right\} \quad (100)$$

In that way, the final vicinal spin-spin coupling constant (FC term) can be expressed in a general form:

$$J_{H_1H_2}^{FC} [H_I^0] = \sum_{n=0}^4 (A_n + B_n \sin \phi + C_n \cos \phi + D_n \sin 2\phi + E_n \cos 2\phi) e^{-\frac{n}{a_0} \sqrt{2L_{CH}^2(1-\cos\phi) + L_{CC}^2}} \quad (101)$$

where the coefficients  $A_n$ ,  $B_n$ ,  $C_n$ ,  $D_n$  and  $E_n$  are obtained by collecting the corresponding coefficients in the following nine terms: (13), (16), (20), (26), (37), (46), (57), (74) and (85) to give

$$A_0 = A(13) + A(16) + A(20) + A(26) + A(37) + B'(46) + B''(57) + B'''(74) + B''''(85) \quad (102)$$

$$\begin{pmatrix} B_0 \\ C_0 \end{pmatrix} = \begin{pmatrix} B \\ C \end{pmatrix} (20) + \begin{pmatrix} B \\ C \end{pmatrix} (26) + \begin{pmatrix} C' \\ D' \end{pmatrix} (46) + \begin{pmatrix} C'' \\ D'' \end{pmatrix} (57) + \begin{pmatrix} C''' \\ D''' \end{pmatrix} (74) + \begin{pmatrix} C'''' \\ D'''' \end{pmatrix} (85) \quad (103)$$

$$\begin{pmatrix} D_0 \\ E_0 \end{pmatrix} = \begin{pmatrix} E'' \\ F'' \end{pmatrix} (57) + \begin{pmatrix} E'''' \\ F'''' \end{pmatrix} (85) \quad (104)$$

$$A_1 = B(16) + D(20) + A'(26) + B(37) + B(46) + B'(57) + B'(74) + B''(85) \quad (105)$$

$$\begin{pmatrix} B_1 \\ C_1 \end{pmatrix} = \begin{pmatrix} B' \\ C' \end{pmatrix}(26) + \begin{pmatrix} C \\ D \end{pmatrix}(46) + \begin{pmatrix} C' \\ D' \end{pmatrix}(57) + \begin{pmatrix} C' \\ D' \end{pmatrix}(74) + \begin{pmatrix} C'' \\ D'' \end{pmatrix}(85) \quad (106)$$

$$\begin{pmatrix} D_1 \\ E_1 \end{pmatrix} = \begin{pmatrix} E' \\ F' \end{pmatrix}(57) + \begin{pmatrix} E'' \\ F'' \end{pmatrix}(85) \quad (107)$$

$$A_2 = E(26) + C(37) + A(46) + B(57) + B(74) + B'(85) \quad (108)$$

$$\begin{pmatrix} B_2 \\ C_2 \end{pmatrix} = \begin{pmatrix} C \\ D \end{pmatrix}(57) + \begin{pmatrix} C \\ D \end{pmatrix}(74) + \begin{pmatrix} C' \\ D' \end{pmatrix}(85) \quad (109)$$

$$\begin{pmatrix} D_2 \\ E_2 \end{pmatrix} = \begin{pmatrix} E' \\ F' \end{pmatrix}(85) \quad (110)$$

$$A_3 = A(57) + A(74) + B(85) \quad (111)$$

$$\begin{pmatrix} B_3 \\ C_3 \end{pmatrix} = \begin{pmatrix} C \\ D \end{pmatrix}(85) \quad (112)$$

$$\begin{pmatrix} D_3 \\ E_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (113)$$

$$A_4 = A(85) \quad (114)$$

$$\begin{pmatrix} B_4 \\ C_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (115)$$

$$\begin{pmatrix} D_4 \\ E_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (116)$$