Supplementary data for Phys. Chem. Chem. Phys.

Supplementary Information

Equations of explicitly-correlated coupled-cluster methods

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Supplementary data for Phys. Chem. Chem. Phys.

Contents

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1. NOTE

This supplementary information compiles the equations and intermediates (computational sequences) of the CC-R12, Λ-CC-R12, and EOM-CC-R12 methods including through the connected quadruple excitation operators.

The equations and intermediates for the Λ-CC-R12 and left-hand-side EOM-CC-R12 methods turn out to be identical with the exceptions of $-f_{a_1}^{i_2} - v_{a_1 a_4}^{i_2 i_3} t_{i_3}^{a_4}$, $v_{a_1 a_2}^{i_3 i_4}$, and $\frac{1}{2} v_{\alpha_5 \alpha_6}^{i_3 i_4} F_{i_1 i_2}^{\alpha_5 \alpha_6}$ (or $V_{i_1 i_2}^{i_3 i_4}$) in the λ_1, λ_2, and geminal λ equations, respectively, while the λ_3 and λ_4 equations are always identical between Λ-CC-R12 and left-hand-side EOM-CC-R12 of the same rank. Therefore, we will omit the equations for the left-hand-side EOM-CC-R12 methods in the following.

Supplementary data for Phys. Chem. Chem. Phys.

2. EQUATIONS OBTAINED WITH THE MODIFIED ANSATZ 2

A. CCSD-R12

TABLE ESI.2.I: The energy equation of CCSD-R12 and higher-order CC-R12 obtained with the modified ansatz 2

$$e = +f^{i_1}_{a_2} t^{a_2}_{i_1} + \tfrac{1}{2} v^{i_1 i_2}_{a_3 a_4} t^{a_3}_{i_1} t^{a_4}_{i_2} + \tfrac{1}{4} v^{i_1 i_2}_{a_3 a_4} t^{a_3 a_4}_{i_1 i_2} + \tfrac{1}{8} v^{i_1 i_2}_{\alpha_3 \alpha_4} F^{\alpha_3 \alpha_4}_{i_5 i_6} t^{i_5 i_6}_{i_1 i_2}$$

TABLE ESI.2.II: The T_1 amplitude equation of CCSD-R12 obtained with the modified ansatz 2

$$\begin{aligned}
\delta^{a_2}_{i_1} &= +f^{a_2}_{i_1} - f^{i_3}_{i_1} t^{a_2}_{i_3} + f^{a_2}_{a_3} t^{a_3}_{i_1} - f^{i_3}_{a_4} t^{a_4}_{i_1} t^{a_2}_{i_3} + f^{i_3}_{a_4} t^{a_2 a_4}_{i_1 i_3} - \tfrac{1}{2} f^{i_3}_{a_4} F^{\alpha_4 a_2}_{i_5 i_6} t^{i_5 i_6}_{i_1 i_3} - v^{i_3 a_2}_{i_1 a_4} t^{a_4}_{i_3} + v^{i_3 i_4}_{i_1 a_5} t^{a_5}_{i_3} t^{a_2}_{i_4} + v^{i_3 a_2}_{a_4 a_5} t^{a_4}_{i_3} t^{a_5}_{i_1} - \tfrac{1}{2} v^{i_3 i_4}_{i_1 a_5} t^{a_2 a_5}_{i_3 i_4} - \tfrac{1}{2} v^{i_3 a_2}_{a_4 a_5} t^{a_4 a_5}_{i_1 i_3} \\
&\quad + \tfrac{1}{4} v^{i_3 i_4}_{i_1 \alpha_5} F^{\alpha_5 a_2}_{i_6 i_7} t^{i_6 i_7}_{i_3 i_4} - \tfrac{1}{4} v^{i_3 a_2}_{\alpha_4 \alpha_5} F^{\alpha_4 \alpha_5}_{i_6 i_7} t^{i_6 i_7}_{i_1 i_3} - v^{i_3 i_4}_{a_5 a_6} t^{a_5}_{i_3} t^{a_6}_{i_1} t^{a_2}_{i_4} + v^{i_3 i_4}_{a_5 a_6} t^{a_2 a_6}_{i_1 i_4} t^{a_5}_{i_3} - \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} t^{a_2 a_6}_{i_3 i_4} t^{a_5}_{i_1} - \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} t^{a_5 a_6}_{i_1 i_4} t^{a_2}_{i_3} - \tfrac{1}{2} v^{i_3 i_4}_{\alpha_5 a_6} F^{\alpha_5 a_2}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_3} t^{a_6}_{i_4} \\
&\quad - \tfrac{1}{4} v^{i_3 i_4}_{\alpha_5 a_6} F^{\alpha_5 a_2}_{i_7 i_8} t^{i_7 i_8}_{i_3 i_4} t^{a_6}_{i_1} + \tfrac{1}{4} v^{i_3 i_4}_{\alpha_5 \alpha_6} F^{\alpha_5 \alpha_6}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_3} t^{a_2}_{i_4}
\end{aligned}$$

TABLE ESI.2.III: The T_2 amplitude equation of CCSD-R12 obtained with the modified ansatz 2

$$\begin{aligned}
\delta^{a_3 a_4}_{i_1 i_2} &= +P_2 f^{i_5}_{i_1} t^{a_3 a_4}_{i_2 i_5} - P_2 f^{a_3}_{a_5} t^{a_4 a_5}_{i_1 i_2} + \tfrac{1}{2} P_2 f^{a_3}_{\alpha_5} F^{\alpha_5 a_4}_{i_6 i_7} t^{i_6 i_7}_{i_1 i_2} + \tfrac{1}{2} P_2 f^{i_5}_{\alpha_6} F^{\alpha_6 a_3}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_2} t^{a_4}_{i_5} + P_2 f^{i_5}_{a_6} t^{a_3}_{i_5} t^{a_4 a_6}_{i_1 i_2} + P_2 f^{i_5}_{a_6} t^{a_6}_{i_1} t^{a_3 a_4}_{i_2 i_5} + v^{a_3 a_4}_{i_1 i_2} + P_2 v^{i_5 a_3}_{i_1 i_2} t^{a_4}_{i_5} + P_2 v^{a_3 a_4}_{i_1 a_5} t^{a_5}_{i_2} \\
&\quad + \tfrac{1}{2} P_2 v^{i_5 i_6}_{i_1 i_2} t^{a_3}_{i_5} t^{a_4}_{i_6} + P_2 P_2 v^{i_5 a_3}_{i_1 a_6} t^{a_6}_{i_2} t^{a_4}_{i_5} + \tfrac{1}{2} P_2 v^{a_3 a_4}_{a_5 a_6} t^{a_5}_{i_1} t^{a_6}_{i_2} + \tfrac{1}{2} v^{i_5 i_6}_{i_1 i_2} t^{a_3 a_4}_{i_5 i_6} - P_2 P_2 v^{i_5 a_3}_{i_1 a_6} t^{a_4 a_6}_{i_2 i_5} + \tfrac{1}{2} v^{a_3 a_4}_{a_5 a_6} t^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{2} P_2 P_2 v^{i_5 a_3}_{i_7 a_6} F^{\alpha_6 a_4}_{i_8 i_9} t^{i_7 i_8}_{i_2 i_5} + \tfrac{1}{4} v^{a_3 a_4}_{\alpha_5 \alpha_6} F^{\alpha_5 \alpha_6}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_2} \\
&\quad + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{i_1 a_7} t^{a_7}_{i_2} t^{a_3}_{i_5} t^{a_4}_{i_6} + \tfrac{1}{2} P_2 P_2 v^{i_5 a_3}_{a_6 a_7} t^{a_6}_{i_1} t^{a_7}_{i_2} t^{a_4}_{i_5} - \tfrac{1}{2} P_2 v^{i_5 a_3}_{\alpha_6 a_7} F^{\alpha_6 a_4}_{i_8 i_9} t^{i_8 i_9}_{i_1 i_2} t^{a_7}_{i_5} + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{\alpha_6 a_7} F^{\alpha_7 a_3}_{i_8 i_9} t^{i_8 i_9}_{i_2 i_5} t^{a_4}_{i_6} + \tfrac{1}{2} P_2 P_2 v^{i_5 a_3}_{\alpha_6 a_7} F^{\alpha_6 a_4}_{i_8 i_9} t^{i_8 i_9}_{i_1 i_5} t^{a_7}_{i_2} \\
&\quad + \tfrac{1}{4} P_2 v^{i_5 a_3}_{a_6 \alpha_7} F^{\alpha_6 \alpha_7}_{i_8 i_9} t^{i_8 i_9}_{i_1 i_2} t^{a_4}_{i_5} - P_2 P_2 v^{i_5 i_6}_{i_1 a_7} t^{a_3}_{i_5} t^{a_4 a_7}_{i_2 i_6} + \tfrac{1}{2} P_2 v^{i_5 a_3}_{a_6 a_7} t^{a_4}_{i_5} t^{a_6 a_7}_{i_1 i_2} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{i_1 a_7} t^{a_7}_{i_2} t^{a_3 a_4}_{i_5 i_6} - P_2 P_2 v^{i_5 a_3}_{a_6 a_7} t^{a_6}_{i_1} t^{a_4 a_7}_{i_2 i_5} - P_2 v^{i_5 i_6}_{i_1 a_7} t^{a_7}_{i_5} t^{a_3 a_4}_{i_2 i_6} - P_2 v^{i_5 a_3}_{a_6 a_7} t^{a_6}_{i_5} t^{a_4 a_7}_{i_1 i_2} \\
&\quad + \tfrac{1}{4} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_7}_{i_2} t^{a_8}_{i_5} t^{a_3}_{i_6} t^{a_4}_{} - \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} t^{a_8}_{i_5} t^{a_4}_{i_6} + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_5} t^{a_8}_{i_2} t^{a_4}_{i_6} + \tfrac{1}{8} P_2 v^{i_5 i_6}_{a_7 a_8} F^{\alpha_7 a_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} t^{a_3}_{i_5} t^{a_4}_{i_6} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_3}_{i_5} t^{a_7 a_8}_{i_1 i_2} t^{a_4}_{i_6} \\
&\quad + \tfrac{1}{4} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_7}_{i_1} t^{a_3 a_4}_{i_5 i_6} t^{a_8}_{i_2} + P_2 P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_7}_{i_1} t^{a_3 a_8}_{i_2 i_6} t^{a_4}_{i_5} - P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_7}_{i_5} t^{a_3 a_4}_{i_1 i_6} t^{a_8}_{i_2} - P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_7}_{i_5} t^{a_3 a_8}_{i_1 i_2} t^{a_4}_{i_6} + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_3 a_7}_{i_1 i_5} t^{a_4 a_8}_{i_2 i_6} - \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_3 a_7}_{i_5 i_6} t^{a_4 a_8}_{i_1 i_2} \\
&\quad + \tfrac{1}{4} v^{i_5 i_6}_{a_7 a_8} t^{a_7 a_8}_{i_1 i_2} t^{a_3 a_4}_{i_5 i_6} - \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_7 a_8}_{i_1 i_5} t^{a_3 a_4}_{i_2 i_6} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{a_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} t^{a_4 a_8}_{i_5 i_6} - \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_5} t^{a_4 a_8}_{i_2 i_6} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{a_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} t^{a_4 a_8}_{i_1 i_2} \\
&\quad + \tfrac{1}{8} v^{i_5 i_6}_{a_7 a_8} F^{\alpha_7 a_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} t^{a_3 a_4}_{i_5 i_6} - \tfrac{1}{4} P_2 v^{i_5 i_6}_{a_7 a_8} F^{\alpha_7 a_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_5} t^{a_3 a_4}_{i_2 i_6} + \tfrac{1}{8} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_5} F^{\alpha_8 a_4}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_2 i_6} - \tfrac{1}{8} P_2 v^{i_5 i_6}_{a_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} F^{\alpha_8 a_4}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_2}
\end{aligned}$$

TABLE ESI.2.IV: The geminal t amplitude equation of CCSD-R12 obtained with the modified ansatz 2

$$\begin{aligned}
\delta^{i_3 i_4}_{i_1 i_2} &= -F^{i_3 i_4 *}_{\alpha_5 a_6} f^{\alpha_5}_{a_7} t^{a_6 a_7}_{i_1 i_2} + \tfrac{1}{4} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} f^{i_7}_{i_1} F^{\alpha_5 a_6}_{i_8 i_9} t^{i_8 i_9}_{i_2 i_7} + \tfrac{1}{2} F^{i_3 i_4 *}_{\alpha_5 a_6} f^{\alpha_6}_{a_7} F^{\alpha_5 \alpha_7}_{i_8 i_9} t^{i_8 i_9}_{i_1 i_2} - \tfrac{1}{4} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} f^{i_7}_{a_8} F^{\alpha_5 a_6}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_7} t^{a_8}_{i_2} - \tfrac{1}{2} F^{i_3 i_4 *}_{\alpha_5 a_6} f^{i_7}_{a_8} F^{\alpha_5 a_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} t^{a_6}_{i_7} + \tfrac{1}{2} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{\alpha_5 \alpha_6}_{i_1 i_2} \\
&\quad + F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{i_1 i_2} t^{a_6}_{i_7} + \tfrac{1}{2} P_2 F^{i_3 i_4 *}_{\alpha_5 \alpha_6} v^{\alpha_5 \alpha_6}_{i_1 a_7} t^{a_7}_{i_2} + P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{i_1 a_8} t^{a_8}_{i_2} t^{a_6}_{i_7} + \tfrac{1}{4} P_2 F^{i_3 i_4 *}_{\alpha_5 \alpha_6} v^{\alpha_5 \alpha_6}_{a_7 a_8} t^{a_7 a_8}_{i_1 i_2} - P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{i_1 a_8} t^{a_6 a_8}_{i_2 i_7} + \tfrac{1}{4} F^{i_3 i_4 *}_{\alpha_5 \alpha_6} v^{\alpha_5 \alpha_6}_{a_7 a_8} t^{a_7 a_8}_{i_1 i_2} \\
&\quad + \tfrac{1}{8} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{i_1 i_2} F^{\alpha_5 \alpha_6}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_7 i_8} + \tfrac{1}{2} P_2 F^{i_3 i_4 *}_{\alpha_5 \alpha_6} v^{i_7 \alpha_6}_{i_1 a_8} F^{\alpha_5 a_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_2 i_7} + \tfrac{1}{8} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{\alpha_5 \alpha_6}_{a_7 a_8} F^{\alpha_7 a_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} + \tfrac{1}{2} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} t^{a_8}_{i_1} t^{a_9}_{i_2} t^{a_6}_{i_7} - F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} t^{a_6 a_9}_{i_1 i_2} t^{a_8}_{i_7} \\
&\quad + P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} t^{a_6 a_9}_{i_1 i_7} t^{a_8}_{i_2} + \tfrac{1}{2} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} t^{a_8 a_9}_{i_1 i_2} t^{a_6}_{i_7} + \tfrac{1}{4} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{i_1 a_9} F^{\alpha_5 \alpha_6}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_2 i_7} t^{a_9}_{i_8} + \tfrac{1}{8} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{i_1 a_9} F^{\alpha_5 \alpha_6}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_7 i_8} t^{a_9}_{i_2} - \tfrac{1}{2} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 \alpha_6}_{a_8 a_9} F^{\alpha_5 a_8}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_1 i_2} t^{a_9}_{i_7} \\
&\quad - \tfrac{1}{2} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{i_1 a_9} F^{\alpha_5 a_9}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_2 i_7} t^{a_6}_{i_8} + \tfrac{1}{2} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 \alpha_6}_{a_8 a_9} F^{\alpha_5 a_8}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_1 i_7} t^{a_9}_{i_2} + \tfrac{1}{4} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} F^{\alpha_8 a_9}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_1 i_2} t^{a_6}_{i_7} + \tfrac{1}{4} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} t^{a_9 a_{10}}_{i_2} \\
&\quad + \tfrac{1}{16} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_2} t^{a_9}_{i_1} t^{a_{10}}_{i_2} + \tfrac{1}{2} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} t^{a_{10}}_{i_7} t^{a_6}_{i_8} - \tfrac{1}{2} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 a_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_7} t^{a_{10}}_{i_2} t^{a_6}_{i_8} - \tfrac{1}{8} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_7} t^{a_9 a_{10}}_{i_2 i_8} \\
&\quad + \tfrac{1}{16} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} t^{a_9 a_{10}}_{i_1 i_2} - \tfrac{1}{4} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 a_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_2} t^{a_6 a_{10}}_{i_7 i_8} + \tfrac{1}{2} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 a_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_7} t^{a_6 a_{10}}_{i_2 i_8} - \tfrac{1}{4} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 a_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} t^{a_6 a_{10}}_{i_1 i_2} \\
&\quad + \tfrac{1}{8} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 a_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_7} F^{\alpha_6 a_{10}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_2 i_8} - \tfrac{1}{8} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 a_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} F^{\alpha_6 a_{10}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_1 i_2} + \tfrac{1}{32} F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_9 a_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_2} F^{\alpha_5 \alpha_6}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_7 i_8} \\
&\quad - \tfrac{1}{16} P_2 F^{i_3 i_4 *}_{\alpha_5 a_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_9 a_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_7} F^{\alpha_5 \alpha_6}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_2 i_8}
\end{aligned}$$

Supplementary data for Phys. Chem. Chem. Phys.

B. CCSDT-R12

TABLE ESI.2.V: The T_1 amplitude equation of CCSDT-R12 and higher-order CC-R12 obtained with the modified ansatz 2

$$\delta_{i_1}^{a_2} = \text{CCSD-R12} + \tfrac{1}{4} v_{a_5 a_6}^{i_3 i_4} t_{i_1 i_3 i_4}^{a_2 a_5 a_6}$$

TABLE ESI.2.VI: The T_2 amplitude equation of CCSDT-R12 obtained with the modified ansatz 2

$$\begin{aligned}\delta_{i_1 i_2}^{a_3 a_4} = \text{CCSD-R12} &+ f_{a_6}^{i_5} t_{i_1 i_2 i_5}^{a_3 a_4 a_6} + \tfrac{1}{2} P_2 v_{i_1 a_7}^{i_5 i_6} t_{i_2 i_5 i_6}^{a_3 a_4 a_7} + \tfrac{1}{2} P_2 v_{a_6 a_7}^{i_5 a_3} t_{i_1 i_2 i_5}^{a_4 a_6 a_7} + v_{a_7 a_8}^{i_5 i_6} t_{i_1 i_2 i_6}^{a_3 a_4 a_8} t_{i_5}^{a_7} - \tfrac{1}{2} P_2 v_{a_7 a_8}^{i_5 i_6} t_{i_1 i_5 i_6}^{a_3 a_4 a_8} t_{i_2}^{a_7} - \tfrac{1}{2} P_2 v_{a_7 a_8}^{i_5 i_6} t_{i_1 i_2 i_6}^{a_3 a_7 a_8} t_{i_5}^{a_4}\end{aligned}$$

TABLE ESI.2.VII: The T_3 amplitude equation of CCSDT-R12 obtained with the modified ansatz 2

$$\begin{aligned}\delta_{i_1 i_2 i_3}^{a_4 a_5 a_6} = &-P_3 f_{i_1}^{i_7} t_{i_2 i_3 i_7}^{a_4 a_5 a_6} + P_3 f_{a_7}^{a_4} t_{i_1 i_2 i_3}^{a_5 a_6 a_7} - P_3 f_{a_8}^{i_7} t_{i_1 i_2 i_7}^{a_4 a_5 a_6} t_{i_3}^{a_8} - P_3 f_{a_8}^{i_7} t_{i_1 i_2 i_3}^{a_4 a_5 a_8} t_{i_7}^{a_6} + P_3 P_3 f_{a_8}^{i_7} t_{i_1 i_2}^{a_4 a_8} t_{i_3 i_7}^{a_5 a_6} - \tfrac{1}{2} P_3 P_3 f_{a_8}^{i_7} t_{i_1 i_7}^{a_4 a_5} F_{i_9 i_{10}}^{\alpha_8 a_6} t_{i_2 i_3}^{i_9 i_{10}} - P_3 P_3 v_{i_1 i_2}^{i_7 a_4} t_{i_3 i_7}^{a_5 a_6} \\
&-P_3 P_3 v_{i_1 a_7}^{a_4 a_5} t_{i_2 i_3}^{a_6 a_7} + \tfrac{1}{2} P_3 P_3 v_{i_1 a_7}^{a_4 a_5} F_{i_8 i_9}^{a_7 a_6} t_{i_2 i_3}^{i_8 i_9} - P_3 P_3 v_{i_1 i_2}^{i_7 i_8} t_{i_3 i_8}^{a_4 a_5} t_{i_7}^{a_6} + P_3 P_3 v_{i_1 a_8}^{i_7 a_4} t_{i_2 i_7}^{a_5 a_6} t_{i_3}^{a_8} + P_3 P_3 v_{i_1 a_8}^{i_7 a_4} t_{i_2 i_3}^{a_5 a_8} t_{i_7}^{a_6} - P_3 P_3 v_{a_7 a_8}^{a_4 a_5} t_{i_1 i_2}^{a_6 a_8} t_{i_3}^{a_7} + \tfrac{1}{2} P_3 v_{i_1 i_2}^{i_7 i_8} t_{i_3 i_7 i_8}^{a_4 a_5 a_6} \\
&-P_3 P_3 v_{i_1 a_8}^{i_7 a_4} t_{i_2 i_3 i_7}^{a_5 a_6 a_8} + \tfrac{1}{2} P_3 v_{a_7 a_8}^{a_4 a_5} t_{i_1 i_2 i_3}^{a_6 a_7 a_8} + \tfrac{1}{2} P_3 P_3 v_{i_1 a_8}^{i_7 a_4} t_{i_7}^{a_5} F_{i_9 i_{10}}^{\alpha_8 a_6} t_{i_2 i_3}^{i_9 i_{10}} - \tfrac{1}{2} P_3 P_3 v_{a_7 a_8}^{a_4 a_5} t_{i_1}^{a_8} F_{i_9 i_{10}}^{a_7 a_6} t_{i_2 i_3}^{i_9 i_{10}} + P_3 P_3 v_{i_1 a_9}^{i_7 i_8} t_{i_2 i_8}^{a_4 a_5} t_{i_3}^{a_9} t_{i_7}^{a_6} - \tfrac{1}{2} P_3 P_3 v_{a_8 a_9}^{i_7 a_4} t_{i_1 i_7}^{a_5 a_6} t_{i_2}^{a_8} t_{i_3}^{a_9} \\
&-\tfrac{1}{2} P_3 P_3 v_{i_1 a_9}^{i_7 i_8} t_{i_2 i_3}^{a_4 a_9} t_{i_7}^{a_5} t_{i_8}^{a_6} + P_3 P_3 v_{a_8 a_9}^{i_7 a_4} t_{i_1 i_2}^{a_5 a_9} t_{i_3}^{a_8} t_{i_7}^{a_6} + P_3 v_{i_1 a_9}^{i_7 i_8} t_{i_2 i_3 i_8}^{a_4 a_5 a_6} t_{i_7}^{a_9} - \tfrac{1}{2} P_3 v_{i_1 a_9}^{i_7 i_8} t_{i_2 i_7 i_8}^{a_4 a_5 a_6} t_{i_3}^{a_9} + P_3 v_{a_8 a_9}^{i_7 a_4} t_{i_1 i_2 i_3}^{a_5 a_6 a_9} t_{i_7}^{a_8} - P_3 P_3 v_{i_1 a_9}^{i_7 i_8} t_{i_2 i_3 i_8}^{a_4 a_5 a_9} t_{i_7}^{a_6} \\
&-P_3 P_3 v_{a_8 a_9}^{i_7 a_4} t_{i_1 i_2 i_7}^{a_5 a_6 a_9} t_{i_3}^{a_8} - \tfrac{1}{2} P_3 v_{a_8 a_9}^{i_7 a_4} t_{i_1 i_2 i_3}^{a_5 a_8 a_9} t_{i_7}^{a_6} - \tfrac{1}{2} P_3 P_3 v_{i_1 a_9}^{i_7 i_8} t_{i_2 i_7}^{a_4 a_9} t_{i_3 i_8}^{a_5 a_6} + P_3 P_3 v_{i_1 a_9}^{i_7 i_8} t_{i_2 i_7}^{a_4 a_9} t_{i_3 i_8}^{a_5 a_6} + P_3 P_3 v_{a_8 a_9}^{i_7 a_4} t_{i_1 i_7}^{a_5 a_8} t_{i_2 i_3}^{a_6 a_9} - \tfrac{1}{2} P_3 P_3 v_{a_8 a_9}^{i_7 a_4} t_{i_1 i_2}^{a_8 a_9} t_{i_3 i_7}^{a_5 a_6} \\
&-\tfrac{1}{4} P_3 P_3 v_{i_1 a_9}^{i_7 i_8} t_{i_7}^{a_4} F_{i_{10} i_{11}}^{\alpha_9 a_5} t_{i_2 i_3}^{i_{10} i_{11}} t_{i_8}^{a_6} + \tfrac{1}{2} P_3 P_3 v_{\alpha_8 a_9}^{i_7 a_4} t_{i_1}^{a_9} F_{i_{10} i_{11}}^{\alpha_8 a_5} t_{i_2 i_3}^{i_{10} i_{11}} t_{i_7}^{a_6} - \tfrac{1}{2} P_3 P_3 v_{i_1 a_9}^{i_7 i_8} t_{i_2 i_7}^{a_4 a_5} F_{i_{10} i_{11}}^{\alpha_9 a_6} t_{i_3 i_8}^{i_{10} i_{11}} - \tfrac{1}{4} P_3 P_3 v_{\alpha_8 a_9}^{i_7 a_4} t_{i_1 i_7}^{a_5 a_6} F_{i_{10} i_{11}}^{\alpha_8 a_9} t_{i_2 i_3}^{i_{10} i_{11}} \\
&+\tfrac{1}{4} P_3 P_3 v_{i_1 a_9}^{i_7 i_8} t_{i_7 i_8}^{a_4 a_5} F_{i_{10} i_{11}}^{\alpha_9 a_6} t_{i_2 i_3}^{i_{10} i_{11}} + \tfrac{1}{2} P_3 P_3 v_{\alpha_8 a_9}^{i_7 a_4} t_{i_1 i_2}^{a_5 a_9} F_{i_{10} i_{11}}^{\alpha_8 a_6} t_{i_3 i_7}^{i_{10} i_{11}} + \tfrac{1}{2} P_3 P_3 v_{\alpha_8 a_9}^{i_7 a_4} t_{i_1 i_7}^{a_5 a_9} F_{i_{10} i_{11}}^{\alpha_8 a_6} t_{i_2 i_3}^{i_{10} i_{11}} + \tfrac{1}{4} P_3 P_3 v_{\alpha_8 a_9}^{i_7 a_4} F_{i_{10} i_{11}}^{\alpha_8 a_5} t_{i_1 i_7}^{i_{10} i_{11}} F_{i_{12} i_{13}}^{\alpha_9 a_6} t_{i_2 i_3}^{i_{12} i_{13}} \\
&-\tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_8}^{a_4 a_5} t_{i_2}^{a_9} t_{i_3}^{a_{10}} t_{i_7}^{a_6} - \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2}^{a_4 a_{10}} t_{i_3}^{a_9} t_{i_7}^{a_5} t_{i_8}^{a_6} - P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2 i_8}^{a_4 a_5 a_6} t_{i_7}^{a_9} t_{i_3}^{a_{10}} + \tfrac{1}{4} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_7 i_8}^{a_4 a_5 a_6} t_{i_2}^{a_9} t_{i_3}^{a_{10}} - P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2 i_3}^{a_4 a_5 a_{10}} t_{i_7}^{a_9} t_{i_8}^{a_6} \\
&-P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2 i_8}^{a_4 a_5 a_{10}} t_{i_3}^{a_9} t_{i_7}^{a_6} + \tfrac{1}{4} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2 i_3}^{a_4 a_9 a_{10}} t_{i_7}^{a_5} t_{i_8}^{a_6} - \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2}^{a_4 a_{10}} t_{i_3}^{a_9} t_{i_7 i_8}^{a_5 a_6} + P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2}^{a_4 a_{10}} t_{i_7}^{a_9} t_{i_3 i_8}^{a_5 a_6} - P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_8}^{a_4 a_9} t_{i_7}^{a_5} t_{i_2 i_3}^{a_6 a_{10}} \\
&-P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_7}^{a_4 a_{10}} t_{i_2}^{a_9} t_{i_3 i_8}^{a_5 a_6} - \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2}^{a_9 a_{10}} t_{i_7}^{a_4} t_{i_3 i_8}^{a_5 a_6} + \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_7}^{a_4 a_5} t_{i_2 i_3 i_8}^{a_6 a_9 a_{10}} + \tfrac{1}{4} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_7 i_8}^{a_4 a_5} t_{i_1 i_2 i_3}^{a_6 a_9 a_{10}} + \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2}^{a_4 a_9} t_{i_3 i_7 i_8}^{a_5 a_6 a_{10}} \\
&+P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_7}^{a_4 a_9} t_{i_2 i_3 i_8}^{a_5 a_6 a_{10}} + \tfrac{1}{2} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_7 i_8}^{a_4 a_9} t_{i_1 i_2 i_3}^{a_5 a_6 a_{10}} + \tfrac{1}{4} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2}^{a_9 a_{10}} t_{i_3 i_7 i_8}^{a_4 a_5 a_6} + \tfrac{1}{2} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_7}^{a_9 a_{10}} t_{i_2 i_3 i_8}^{a_4 a_5 a_6} - \tfrac{1}{4} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1}^{a_{10}} F_{i_{11} i_{12}}^{\alpha_9 a_4} t_{i_2 i_3}^{i_{11} i_{12}} t_{i_7}^{a_5} t_{i_8}^{a_6} \\
&+\tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_8}^{a_4 a_5} F_{i_{11} i_{12}}^{\alpha_9 a_6} t_{i_2 i_3}^{i_{11} i_{12}} t_{i_7}^{a_{10}} + \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_7}^{a_4 a_{10}} F_{i_{11} i_{12}}^{\alpha_9 a_5} t_{i_2 i_8}^{i_{11} i_{12}} t_{i_3}^{a_6} - \tfrac{1}{4} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_8}^{a_4 a_5} F_{i_{11} i_{12}}^{\alpha_9 a_{10}} t_{i_2 i_3}^{i_{11} i_{12}} t_{i_7}^{a_6} - \tfrac{1}{4} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_7 i_8}^{a_4 a_5} F_{i_{11} i_{12}}^{\alpha_9 a_6} t_{i_1 i_2}^{i_{11} i_{12}} t_{i_3}^{a_{10}} \\
&-\tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2}^{a_4 a_{10}} F_{i_{11} i_{12}}^{\alpha_9 a_5} t_{i_3 i_7}^{i_{11} i_{12}} t_{i_8}^{a_6} + \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_8}^{a_4 a_{10}} F_{i_{11} i_{12}}^{\alpha_9 a_5} t_{i_2 i_3}^{i_{11} i_{12}} t_{i_7}^{a_6} + \tfrac{1}{4} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2 i_8}^{a_4 a_5 a_6} F_{i_{11} i_{12}}^{\alpha_9 a_{10}} t_{i_3 i_7}^{i_{11} i_{12}} + \tfrac{1}{8} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_7 i_8}^{a_4 a_5 a_6} F_{i_{11} i_{12}}^{\alpha_9 a_{10}} t_{i_2 i_3}^{i_{11} i_{12}} \\
&-\tfrac{1}{4} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2 i_3}^{a_4 a_5 a_{10}} F_{i_{11} i_{12}}^{\alpha_9 a_6} t_{i_7 i_8}^{i_{11} i_{12}} - \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2 i_8}^{a_4 a_5 a_{10}} F_{i_{11} i_{12}}^{\alpha_9 a_6} t_{i_3 i_7}^{i_{11} i_{12}} - \tfrac{1}{4} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_7 i_8}^{a_4 a_5 a_{10}} F_{i_{11} i_{12}}^{\alpha_9 a_6} t_{i_2 i_3}^{i_{11} i_{12}} - \tfrac{1}{4} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_8}^{a_4} F_{i_{11} i_{12}}^{\alpha_9 a_5} t_{i_1 i_7}^{i_{11} i_{12}} F_{i_{13} i_{14}}^{\alpha_{10} a_6} t_{i_2 i_3}^{i_{13} i_{14}}\end{aligned}$$

TABLE ESI.2.VIII: The geminal t amplitude equation of CCSDT-R12 and higher-order CC-R12 obtained with the modified ansatz 2

$$\delta_{i_1 i_2}^{i_3 i_4} = \text{CCSD-R12} + \tfrac{1}{2} F_{a_5 a_6}^{i_3 i_4 *} v_{a_8 a_9}^{i_7 \alpha_5} t_{i_1 i_2 i_7}^{a_6 a_8 a_9}$$

C. CCSDTQ-R12

TABLE ESI.2.IX: The T_2 amplitude equation of CCSDTQ-R12 obtained with the modified ansatz 2

$$\delta^{a_3a_4}_{i_1i_2} = \text{CCSDT-R12} + \tfrac{1}{4} v^{i_5i_6}_{a_7a_8} t^{a_3a_4a_7a_8}_{i_1i_2i_5i_6}$$

TABLE ESI.2.X: The T_3 amplitude equation of CCSDTQ-R12 obtained with the modified ansatz 2

$$\begin{aligned}\delta^{a_4a_5a_6}_{i_1i_2i_3} = \text{CCSDT-R12} &+ f^{i_7}_{a_8} t^{a_4a_5a_6a_8}_{i_1i_2i_3i_7} - \tfrac{1}{2} P_3 v^{i_7i_8}_{i_1a_9} t^{a_4a_5a_6a_9}_{i_2i_3i_7i_8} - \tfrac{1}{2} P_3 v^{i_7a_4}_{a_8a_9} t^{a_5a_6a_8a_9}_{i_1i_2i_3i_7} + v^{i_7i_8}_{a_9a_{10}} t^{a_4a_5a_6a_{10}}_{i_1i_2i_3i_8} t^{a_9}_{i_7} \\ &- \tfrac{1}{2} P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_4a_5a_6a_{10}}_{i_1i_2i_7i_8} t^{a_9}_{i_3} - \tfrac{1}{2} P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_4a_5a_9a_{10}}_{i_1i_2i_3i_8} t^{a_6}_{i_7}\end{aligned}$$

TABLE ESI.2.XI: The T_4 amplitude equation of CCSDTQ-R12 obtained with the modified ansatz 2

$$\begin{aligned}\delta^{a_5a_6a_7a_8}_{i_1i_2i_3i_4} = &+P_4 f^{i_9}_{i_1} t^{a_5a_6a_7a_8}_{i_2i_3i_4i_9} - P_4 f^{a_5}_{a_9} t^{a_6a_7a_8a_9}_{i_1i_2i_3i_4} - P_4 f^{i_9}_{a_{10}} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} t^{a_{10}}_{i_4} - P_4 f^{i_9}_{a_{10}} t^{a_5a_6a_7a_{10}}_{i_1i_2i_3i_4} t^{a_8}_{i_9} - P_4 P_4 f^{i_9}_{a_{10}} t^{a_5a_6}_{i_1i_9} t^{a_7a_8a_{10}}_{i_2i_3i_4} - P_4 P_4 f^{i_9}_{a_{10}} t^{a_5a_{10}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9} \\ &+\tfrac{1}{2} P_4 P_4 f^{i_9}_{\alpha_{10}} F^{\alpha_{10}a_5}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9} + P_4 P_4 v^{i_9a_5}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9} + P_4 P_4 v^{a_5a_6}_{i_1a_9} t^{a_7a_8a_9}_{i_2i_3i_4} - P_4 P_4 v^{i_9i_{10}}_{i_1i_2} t^{a_5a_6a_7}_{i_3i_4i_{10}} t^{a_8}_{i_9} + P_4 P_4 v^{i_9a_5}_{i_1a_{10}} t^{a_6a_7a_8}_{i_2i_3i_9} t^{a_{10}}_{i_4} + P_4 P_4 v^{i_9a_5}_{i_1a_{10}} t^{a_6a_7a_{10}}_{i_2i_3i_4} t^{a_8}_{i_9} \\ &-P_4 P_4 v^{a_5a_6}_{a_9a_{10}} t^{a_7a_8a_{10}}_{i_1i_2i_3} t^{a_9}_{i_4} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{i_1i_2} t^{a_5a_6}_{i_3i_9} t^{a_7a_8}_{i_4i_{10}} - P_4 P_4 v^{i_9a_5}_{i_1a_{10}} t^{a_6a_{10}}_{i_2i_3} t^{a_7a_8}_{i_4i_9} - \tfrac{1}{2} P_4 P_4 v^{a_5a_6}_{a_9a_{10}} t^{a_7a_9}_{i_1i_2} t^{a_8a_{10}}_{i_3i_4} + \tfrac{1}{2} P_4 P_4 v^{i_9a_5}_{i_1a_{10}} F^{\alpha_{10}a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3} t^{a_7a_8}_{i_4i_9} \\ &+\tfrac{1}{2} P_4 P_4 v^{a_5a_6}_{a_9a_{10}} F^{a_9a_7}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_1i_2} t^{a_8a_{10}}_{i_3i_4} + \tfrac{1}{2} P_4 v^{i_9i_{10}}_{i_1i_2} t^{a_5a_6a_7a_8}_{i_3i_4i_9i_{10}} - P_4 P_4 v^{i_9a_5}_{i_1a_{10}} t^{a_6a_7a_8a_{10}}_{i_2i_3i_4i_9} + \tfrac{1}{2} P_4 v^{a_5a_6}_{a_9a_{10}} t^{a_7a_8a_9a_{10}}_{i_1i_2i_3i_4} - \tfrac{1}{8} P_4 P_4 v^{a_5a_6}_{a_9a_{10}} F^{a_9a_7}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_1i_2} F^{\alpha_{10}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_3i_4} \\ &-P_4 P_4 v^{i_9i_{10}}_{i_1a_{11}} t^{a_5a_6a_7}_{i_2i_3i_{10}} t^{a_{11}}_{i_4} t^{a_8}_{i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_6a_7a_8}_{i_1i_2i_9} t^{a_{10}}_{i_3} t^{a_{11}}_{i_4} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{i_1a_{11}} t^{a_5a_6a_{11}}_{i_2i_3i_4} t^{a_7}_{i_9} t^{a_8}_{i_{10}} - P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_6a_7a_{11}}_{i_1i_2i_3} t^{a_{10}}_{i_4} t^{a_8}_{i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{i_1a_{11}} t^{a_5a_6a_{11}}_{i_2i_9i_{10}} t^{a_7a_8}_{i_3i_4} \\ &+P_4 P_4 v^{i_9i_{10}}_{i_1a_{11}} t^{a_5a_{11}}_{i_2i_3} t^{a_6}_{i_9} t^{a_7a_8}_{i_4i_{10}} + \tfrac{1}{2} P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_6a_{10}}_{i_1i_2} t^{a_7}_{i_9} t^{a_8a_{11}}_{i_3i_4} - P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_6a_{11}}_{i_1i_2} t^{a_{10}}_{i_3} t^{a_7a_8}_{i_4i_9} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{i_1\alpha_{11}} F^{\alpha_{11}a_5}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_2i_3} t^{a_6}_{i_9} t^{a_7a_8}_{i_4i_{10}} \\ &-\tfrac{1}{2} P_4 P_4 v^{i_9a_5}_{\alpha_{10}a_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_1i_2} t^{a_7}_{i_9} t^{a_8a_{11}}_{i_3i_4} - \tfrac{1}{2} P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_1i_2} t^{a_7}_{i_3} t^{a_7a_8}_{i_4i_9} - P_4 v^{i_9i_{10}}_{i_1a_{11}} t^{a_5a_6a_7a_8}_{i_2i_3i_4i_{10}} t^{a_{11}}_{i_9} + \tfrac{1}{2} P_4 v^{i_9a_5}_{i_1a_{11}} t^{a_6a_7a_8}_{i_2i_3i_9i_{10}} t^{a_{10}}_{i_4} - P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_6a_7a_8a_{11}}_{i_1i_2i_3i_4} t^{a_{10}}_{i_9} \\ &+P_4 P_4 v^{i_9i_{10}}_{i_1a_{11}} t^{a_5a_6a_7a_{11}}_{i_2i_3i_4i_{10}} t^{a_8}_{i_9} + P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_6a_7a_8a_{11}}_{i_1i_2i_3i_9} t^{a_{10}}_{i_4} + \tfrac{1}{2} P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_6a_7a_{10}a_{11}}_{i_1i_2i_3i_4} t^{a_8}_{i_9} + \tfrac{1}{8} P_4 P_4 v^{i_9a_5}_{\alpha_{10}\alpha_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_1i_2} t^{a_7}_{i_9} F^{\alpha_{11}a_8}_{i_{14}i_{15}} t^{i_{14}i_{15}}_{i_3i_4} \\ &+P_4 P_4 v^{i_9i_{10}}_{i_1a_{11}} t^{a_5a_6}_{i_2i_9} t^{a_7a_8a_{11}}_{i_3i_4i_{10}} - \tfrac{1}{2} P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_6a_7}_{i_1i_9} t^{a_8a_{10}a_{11}}_{i_2i_3i_4} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{i_1a_{11}} t^{a_5a_6}_{i_9i_{10}} t^{a_7a_8a_{11}}_{i_2i_3i_4} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{i_1a_{11}} t^{a_5a_{11}}_{i_2i_3} t^{a_6a_7a_8}_{i_4i_9i_{10}} + P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_6a_{10}}_{i_1i_2} t^{a_7a_8a_{11}}_{i_3i_4i_9} \\ &-P_4 P_4 v^{i_9i_{10}}_{i_1a_{11}} t^{a_5a_{11}}_{i_2i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} - P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_6a_{10}}_{i_1i_9} t^{a_7a_8a_{11}}_{i_2i_3i_4} + \tfrac{1}{2} P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} t^{a_{10}a_{11}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9} + \tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{i_1a_{11}} F^{\alpha_{11}a_5}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_2i_3} t^{a_6a_7a_8}_{i_4i_9i_{10}} \\ &-\tfrac{1}{2} P_4 P_4 v^{i_9a_5}_{\alpha_{10}a_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_1i_2} t^{a_7a_8a_{11}}_{i_3i_4i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{i_1\alpha_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_2i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} + \tfrac{1}{2} P_4 P_4 v^{i_9a_5}_{a_{10}a_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_1i_9} t^{a_7a_8a_{11}}_{i_2i_3i_4} + \tfrac{1}{4} P_4 P_4 v^{i_9a_5}_{\alpha_{10}\alpha_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9} \\ &-\tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_6a_7}_{i_1i_2i_{10}} t^{a_{11}}_{i_3} t^{a_{12}}_{i_4} t^{a_8}_{i_9} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_6a_{12}}_{i_1i_2i_3} t^{a_{11}}_{i_4} t^{a_7}_{i_9} t^{a_8}_{i_{10}} - \tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_6}_{i_1i_9} t^{a_{11}a_{12}}_{i_2i_3} t^{a_7a_8}_{i_4i_{10}} - \tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{11}}_{i_1i_2} t^{a_6}_{i_9} t^{a_7}_{i_{10}} t^{a_8a_{12}}_{i_3i_4} \\ &+P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{11}}_{i_1i_2} t^{a_{12}}_{i_3} t^{a_6}_{i_{10}} t^{a_7a_8}_{i_4i_9} + \tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_6}_{i_9} t^{a_7}_{i_{10}} t^{a_8a_{12}}_{i_3i_4} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_5a_6}_{i_3i_9} t^{a_7a_8}_{i_4i_{10}} - P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_6}_{i_1i_9} t^{a_7a_8a_{12}}_{i_2i_3i_4i_{10}} \\ &+P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{11}}_{i_1i_2} t^{a_6}_{i_9} t^{a_7a_8a_{12}}_{i_3i_4i_{10}} + P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{12}}_{i_2} t^{a_{11}}_{i_3i_4i_{10}} t^{a_6a_7a_8}_{i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{11}a_{12}}_{i_1i_2} t^{a_5}_{i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_6}_{i_9} t^{a_7a_8a_{12}}_{i_3i_4i_{10}} \\ &-\tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_{12}}_{i_3} t^{a_6a_7a_8}_{i_4i_9i_{10}} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_{12}}_{i_4} t^{a_6a_7a_8}_{i_3i_9i_{10}} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_9} t^{a_5}_{i_3} t^{a_6a_7a_8}_{i_4i_9i_{10}} \\ &+\tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_9} t^{a_{12}}_{i_2} t^{a_6a_7a_8}_{i_3i_4i_{10}} + \tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_{12}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_5}_{i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} - \tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{11}}_{i_1i_2} t^{a_6a_{12}}_{i_3i_4} t^{a_7a_8}_{i_9i_{10}} + P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{11}}_{i_1i_9} t^{a_6a_{12}}_{i_2i_3} t^{a_7a_8}_{i_4i_{10}} \\ &-\tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{11}a_{12}}_{i_1i_2} t^{a_5a_6}_{i_3i_9} t^{a_7a_8}_{i_4i_{10}} + \tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_6a_{12}}_{i_3i_4} t^{a_7a_8}_{i_9i_{10}} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_6a_7}_{i_9i_{10}} F^{\alpha_{12}a_8}_{i_{15}i_{16}} t^{i_{15}i_{16}}_{i_3i_4} \\ &-\tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_9} t^{a_6a_{12}}_{i_2i_3} t^{a_7a_8}_{i_4i_{10}} - \tfrac{1}{8} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_{12}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_5a_6}_{i_3i_9} t^{a_7a_8}_{i_4i_{10}} - \tfrac{1}{16} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_6a_7}_{i_9i_{10}} F^{\alpha_{12}a_8}_{i_{15}i_{16}} t^{i_{15}i_{16}}_{i_3i_4} \\ &+\tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_9} t^{a_6a_7}_{i_2i_{10}} F^{\alpha_{12}a_8}_{i_{15}i_{16}} t^{i_{15}i_{16}}_{i_3i_4} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_6a_{11}}_{i_1i_9i_{10}} t^{a_7a_8a_{12}}_{i_2i_3i_4} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_6a_{11}}_{i_1i_9i_{10}} t^{a_7a_8a_{12}}_{i_2i_3i_4} + \tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{11}a_{12}}_{i_1i_2i_3} t^{a_6a_7a_8}_{i_4i_9i_{10}} \\ &+\tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{11}a_{12}}_{i_1i_2i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_6}_{i_1i_9} t^{a_7a_8a_{11}a_{12}}_{i_2i_3i_4i_{10}} + \tfrac{1}{4} P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_6}_{i_9i_{10}} t^{a_7a_8a_{11}a_{12}}_{i_1i_2i_3i_4} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{11}}_{i_1i_2} t^{a_6a_7a_8a_{12}}_{i_3i_4i_9i_{10}} \\ &+P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{11}}_{i_1i_9} t^{a_6a_7a_8a_{12}}_{i_2i_3i_4i_{10}} - \tfrac{1}{2} P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_5a_{11}}_{i_9i_{10}} t^{a_6a_7a_8a_{12}}_{i_1i_2i_3i_4} + \tfrac{1}{4} P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{11}a_{12}}_{i_1i_2} t^{a_5a_6a_7a_8}_{i_3i_4i_9i_{10}} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{11}a_{12}}_{i_1i_9} t^{a_5a_6a_7a_8}_{i_2i_3i_4i_{10}} \\ &+\tfrac{1}{4} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9i_{10}} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_9} t^{a_6a_7a_8}_{i_2i_3i_4i_{10}} + \tfrac{1}{4} P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_{12}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_5a_6a_7a_8}_{i_3i_4i_9i_{10}} \\ &-\tfrac{1}{4} P_4 v^{i_9i_{10}}_{\alpha_{11}a_{12}} F^{\alpha_{11}a_{12}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_9} t^{a_5a_6a_7a_8}_{i_2i_3i_4i_{10}}\end{aligned}$$

D. Λ-CCSD-R12

TABLE ESI.2.XII: The Λ_1 amplitude equation of Λ-CCSD-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_2}_{a_1} = & -f^{i_2}_{a_1} - v^{i_2 i_3}_{a_1 a_4} t^{a_4}_{i_3} + \lambda^{i_3}_{a_1} f^{i_2}_{i_3} - \lambda^{i_2}_{a_3} f^{a_3}_{a_1} + \lambda^{i_3}_{a_1} f^{i_2}_{a_4} t^{a_4}_{i_3} + \lambda^{i_2}_{a_3} f^{i_4}_{a_1} t^{a_3}_{i_4} + \lambda^{i_3}_{a_4} v^{i_2 a_4}_{i_3 a_1} + \lambda^{i_3}_{a_1} v^{i_2 i_4}_{i_3 a_5} t^{a_5}_{i_4} + \lambda^{i_2}_{a_3} v^{i_4 a_3}_{a_1 a_5} t^{a_5}_{i_4} - \lambda^{i_3}_{a_4} v^{i_2 i_5}_{i_3 a_1} t^{a_4}_{i_5} - \lambda^{i_3}_{a_4} v^{i_2 a_4}_{a_1 a_5} t^{a_5}_{i_3} - \lambda^{i_3}_{a_1} v^{i_2 i_4}_{a_5 a_6} t^{a_5}_{i_4} t^{a_6}_{i_3} \\
& -\lambda^{i_2}_{a_3} v^{i_4 i_5}_{a_1 a_6} t^{a_6}_{i_4} t^{a_3}_{i_5} + \lambda^{i_3}_{a_4} v^{i_2 i_5}_{a_1 a_6} t^{a_6}_{i_3} t^{a_4}_{i_5} + \tfrac{1}{2}\lambda^{i_3}_{a_1} v^{i_2 i_4}_{a_5 a_6} t^{a_5 a_6}_{i_3 i_4} + \tfrac{1}{2}\lambda^{i_2}_{a_3} v^{i_4 i_5}_{a_1 a_6} t^{a_3 a_6}_{i_4 i_5} - \lambda^{i_3}_{a_4} v^{i_2 i_5}_{a_1 a_6} t^{a_4 a_6}_{i_3 i_5} + \tfrac{1}{4}\lambda^{i_3}_{a_1} v^{i_2 i_4}_{\alpha_5 \alpha_6} F^{\alpha_5 \alpha_6}_{i_7 i_8} t^{i_7 i_8}_{i_3 i_4} + \tfrac{1}{4}\lambda^{i_2}_{a_3} v^{i_4 i_5}_{\alpha_6 a_1} F^{\alpha_6 a_3}_{i_7 i_8} t^{i_7 i_8}_{i_4 i_5} \\
& -\tfrac{1}{2}\lambda^{i_3}_{a_4} v^{i_2 i_5}_{\alpha_6 a_1} F^{\alpha_6 a_4}_{i_7 i_8} t^{i_7 i_8}_{i_3 i_5} - \tfrac{1}{2}\lambda^{i_3 i_4}_{a_1 a_5} f^{i_2}_{a_6} t^{a_5 a_6}_{i_3 i_4} - \tfrac{1}{2}\lambda^{i_2 i_3}_{a_4 a_5} f^{i_6}_{a_1} t^{a_4 a_5}_{i_3 i_6} + \tfrac{1}{4}\lambda^{i_3 i_4}_{a_1 a_5} f^{i_2}_{\alpha_6} F^{\alpha_6 a_5}_{i_7 i_8} t^{i_7 i_8}_{i_3 i_4} + \tfrac{1}{8}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} f^{i_2}_{\alpha_8} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_4} - \tfrac{1}{8}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 \alpha_7} f^{i_8}_{a_1} F^{\alpha_6 \alpha_7}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_8} \\
& +\tfrac{1}{2}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 a_5}_{i_3 i_4} + \tfrac{1}{2}\lambda^{i_2 i_3}_{a_4 a_5} v^{a_4 a_5}_{i_3 a_1} - \tfrac{1}{4}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} v^{i_2 \alpha_7}_{i_3 i_4} + \tfrac{1}{4}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 \alpha_7} v^{\alpha_6 \alpha_7}_{i_3 a_1} - \tfrac{1}{2}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{i_3 i_4} t^{a_5}_{i_6} - \lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 a_5}_{i_4 a_6} t^{a_6}_{i_3} - \lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 a_5}_{i_3 a_1} t^{a_4}_{i_6} - \tfrac{1}{2}\lambda^{i_2 i_3}_{a_4 a_5} v^{a_4 a_5}_{a_1 a_6} t^{a_6}_{i_3} \\
& +\tfrac{1}{2}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} v^{i_2 \alpha_7}_{i_4 a_8} t^{a_8}_{i_3} + \tfrac{1}{2}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 a_7} v^{i_8 \alpha_6}_{i_3 a_1} t^{a_7}_{i_8} - \tfrac{1}{4}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 \alpha_7} v^{\alpha_6 \alpha_7}_{a_1 a_8} t^{a_8}_{i_3} + \lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{i_4 a_7} t^{a_7}_{i_3} t^{a_5}_{i_6} + \tfrac{1}{2}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 a_5}_{a_6 a_7} t^{a_6}_{i_3} t^{a_7}_{i_4} + \tfrac{1}{2}\lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 i_7}_{i_3 a_1} t^{a_4}_{i_6} t^{a_5}_{i_7} + \lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 a_5}_{a_1 a_7} t^{a_7}_{i_3} t^{a_4}_{i_6} \\
& -\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{i_4 a_7} t^{a_5 a_7}_{i_3 i_6} + \tfrac{1}{4}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 a_5}_{a_6 a_7} t^{a_6 a_7}_{i_3 i_4} + \tfrac{1}{4}\lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 i_7}_{i_3 a_1} t^{a_4 a_5}_{i_6 i_7} - \lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 a_5}_{a_1 a_7} t^{a_4 a_7}_{i_3 i_6} - \tfrac{1}{2}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_2 i_7}_{i_4 a_1} t^{a_5 a_6}_{i_3 i_7} - \tfrac{1}{2}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_2 a_6}_{a_1 a_7} t^{a_5 a_7}_{i_3 i_4} + \tfrac{1}{2}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{i_4 \alpha_7} F^{\alpha_7 a_5}_{i_8 i_9} t^{i_8 i_9}_{i_3 i_6} \\
& +\tfrac{1}{8}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 a_5}_{\alpha_6 \alpha_7} F^{\alpha_6 \alpha_7}_{i_8 i_9} t^{i_8 i_9}_{i_3 i_4} - \tfrac{1}{2}\lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 a_5}_{\alpha_7 a_1} F^{\alpha_7 a_4}_{i_8 i_9} t^{i_8 i_9}_{i_3 i_6} - \tfrac{1}{4}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_2 a_6}_{\alpha_7 a_1} F^{\alpha_7 a_5}_{i_8 i_9} t^{i_8 i_9}_{i_3 i_4} - \tfrac{1}{4}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} v^{i_2 \alpha_7}_{a_8 a_9} t^{a_8}_{i_3} t^{a_9}_{i_4} - \tfrac{1}{2}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 a_7} v^{i_8 \alpha_6}_{a_1 a_9} t^{a_9}_{i_3} t^{a_7}_{i_8} \\
& -\tfrac{1}{8}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} v^{i_2 \alpha_7}_{a_8 a_9} t^{a_8 a_9}_{i_3 i_4} + \tfrac{1}{2}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 a_7} v^{i_8 \alpha_6}_{a_1 a_9} t^{a_7 a_9}_{i_3 i_8} + \tfrac{1}{4}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_8} v^{i_2 \alpha_7}_{a_1 a_9} t^{a_8 a_9}_{i_3 i_4} + \tfrac{1}{4}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} v^{i_2 i_8}_{i_4 \alpha_9} F^{\alpha_7 \alpha_9}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_3 i_8} - \tfrac{1}{16}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} v^{i_2 \alpha_7}_{\alpha_8 \alpha_9} F^{\alpha_8 \alpha_9}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_3 i_4} \\
& +\tfrac{1}{16}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 \alpha_7} v^{i_8 i_9}_{i_3 a_1} F^{\alpha_6 \alpha_7}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_8 i_9} + \tfrac{1}{4}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 \alpha_7} v^{i_8 \alpha_7}_{\alpha_9 a_1} F^{\alpha_6 \alpha_9}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_3 i_8} - \tfrac{1}{8}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 \alpha_8} v^{i_2 i_9}_{i_4 a_1} F^{\alpha_7 \alpha_8}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_3 i_9} + \tfrac{1}{8}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 \alpha_8} v^{i_2 \alpha_8}_{\alpha_9 a_1} F^{\alpha_7 \alpha_9}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_3 i_4} \\
& -\tfrac{1}{2}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{a_7 a_8} t^{a_7}_{i_3} t^{a_8}_{i_4} t^{a_5}_{i_6} - \tfrac{1}{2}\lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 i_7}_{a_1 a_8} t^{a_8}_{i_3} t^{a_4}_{i_6} t^{a_5}_{i_7} - \tfrac{1}{4}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{a_7 a_8} t^{a_5}_{i_6} t^{a_7 a_8}_{i_3 i_4} + \lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{a_7 a_8} t^{a_7}_{i_3} t^{a_5 a_8}_{i_4 i_6} + \tfrac{1}{2}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{a_7 a_8} t^{a_7}_{i_6} t^{a_5 a_8}_{i_3 i_4} + \lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 i_7}_{a_1 a_8} t^{a_4}_{i_6} t^{a_5 a_8}_{i_3 i_7} \\
& -\tfrac{1}{4}\lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 i_7}_{a_1 a_8} t^{a_8}_{i_3} t^{a_4 a_5}_{i_6 i_7} + \tfrac{1}{2}\lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 i_7}_{a_1 a_8} t^{a_8}_{i_6} t^{a_4 a_5}_{i_3 i_7} - \tfrac{1}{2}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_2 i_7}_{a_1 a_8} t^{a_5}_{i_7} t^{a_6 a_8}_{i_3 i_4} - \tfrac{1}{2}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_2 i_7}_{a_1 a_8} t^{a_8}_{i_3} t^{a_5 a_6}_{i_4 i_7} - \tfrac{1}{8}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{\alpha_7 \alpha_8} t^{a_5}_{i_6} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_4} - \tfrac{1}{2}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{\alpha_7 a_8} t^{a_8}_{i_4} F^{\alpha_7 a_5}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_6} \\
& +\tfrac{1}{4}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{\alpha_7 a_8} t^{a_8}_{i_6} F^{\alpha_7 a_5}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_4} + \tfrac{1}{2}\lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 i_7}_{\alpha_8 a_1} t^{a_5}_{i_7} F^{\alpha_8 a_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_6} + \tfrac{1}{4}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_2 i_7}_{\alpha_8 a_1} t^{a_6}_{i_7} F^{\alpha_8 a_5}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_4} - \tfrac{1}{4}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} v^{i_2 i_8}_{\alpha_9 a_{10}} t^{a_{10}}_{i_4} F^{\alpha_7 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_8} \\
& +\tfrac{1}{8}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} v^{i_2 i_8}_{\alpha_9 a_{10}} t^{a_{10}}_{i_8} F^{\alpha_7 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_4} - \tfrac{1}{4}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 a_7} v^{i_8 i_9}_{\alpha_{10} a_1} t^{a_7}_{i_9} F^{\alpha_6 \alpha_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_8} - \tfrac{1}{16}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 \alpha_7} v^{i_8 i_9}_{a_1 a_{10}} t^{a_{10}}_{i_3} F^{\alpha_6 \alpha_7}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_8 i_9} - \tfrac{1}{8}\lambda^{i_2 i_3}_{i_4 i_5} F^{i_4 i_5}_{\alpha_6 \alpha_7} v^{i_8 i_9}_{a_1 a_{10}} t^{a_{10}}_{i_9} F^{\alpha_6 \alpha_7}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_8} \\
& -\tfrac{1}{8}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_8} v^{i_2 i_9}_{\alpha_{10} a_1} t^{a_8}_{i_9} F^{\alpha_7 \alpha_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_4} + \tfrac{1}{8}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 \alpha_8} v^{i_2 i_9}_{a_1 a_{10}} t^{a_{10}}_{i_4} F^{\alpha_7 \alpha_8}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_9}
\end{aligned}
$$

TABLE ESI.2.XIII: The Λ_2 amplitude equation of Λ-CCSD-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_3 i_4}_{a_1 a_2} = & +v^{i_3 i_4}_{a_1 a_2} + P_2 P_2 \lambda^{i_3}_{a_1} f^{i_4}_{a_2} - P_2 \lambda^{i_5}_{a_1} v^{i_3 i_4}_{i_5 a_2} - P_2 \lambda^{i_3}_{a_5} v^{i_4 a_5}_{a_1 a_2} + P_2 P_2 \lambda^{i_3}_{a_1} v^{i_4 i_5}_{a_2 a_6} t^{a_6}_{i_5} + P_2 \lambda^{i_5}_{a_1} v^{i_3 i_4}_{a_2 a_6} t^{a_6}_{i_5} + P_2 \lambda^{i_3}_{a_5} v^{i_4 i_6}_{a_1 a_2} t^{a_5}_{i_6} - P_2 \lambda^{i_3 i_5}_{a_1 a_2} f^{i_4}_{i_5} + P_2 \lambda^{i_3 i_4}_{a_1 a_5} f^{a_5}_{a_2} \\
& -\tfrac{1}{2} P_2 \lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} f^{\alpha_7}_{a_2} - P_2 \lambda^{i_3 i_5}_{a_1 a_2} f^{i_4}_{a_6} t^{a_6}_{i_5} - P_2 \lambda^{i_3 i_4}_{a_1 a_5} f^{i_6}_{a_2} t^{a_5}_{i_6} + \tfrac{1}{2}\lambda^{i_5 i_6}_{a_1 a_2} v^{i_3 i_4}_{i_5 i_6} - P_2 P_2 \lambda^{i_3 i_5}_{a_1 a_6} v^{i_4 a_6}_{i_5 a_2} + \tfrac{1}{2}\lambda^{i_3 i_4}_{a_5 a_6} v^{a_5 a_6}_{a_1 a_2} + \tfrac{1}{2} P_2 P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 a_1} v^{i_4 \alpha_8}_{i_5 a_2} \\
& +\tfrac{1}{4}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 \alpha_8} v^{\alpha_7 \alpha_8}_{a_1 a_2} - P_2 \lambda^{i_3 i_5}_{a_1 a_2} v^{i_4 i_6}_{i_5 a_7} t^{a_7}_{i_6} - \lambda^{i_5 i_6}_{a_1 a_2} v^{i_3 i_4}_{i_6 a_7} t^{a_7}_{i_5} - P_2 \lambda^{i_3 i_4}_{a_1 a_5} v^{i_6 a_5}_{a_2 a_7} t^{a_7}_{i_6} + P_2 P_2 \lambda^{i_3 i_5}_{a_1 a_6} v^{i_4 i_7}_{i_5 a_2} t^{a_6}_{i_7} + P_2 P_2 \lambda^{i_3 i_5}_{a_1 a_6} v^{i_4 a_6}_{a_2 a_7} t^{a_7}_{i_5} - \lambda^{i_3 i_4}_{a_5 a_6} v^{i_7 a_6}_{a_1 a_2} t^{a_5}_{i_7} \\
& +\tfrac{1}{2} P_2 \lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} v^{i_8 \alpha_7}_{a_2 a_9} t^{a_9}_{i_8} - \tfrac{1}{2} P_2 P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 a_1} v^{i_4 \alpha_8}_{a_2 a_9} t^{a_9}_{i_5} + \tfrac{1}{2}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_8} v^{i_9 \alpha_7}_{a_1 a_2} t^{a_8}_{i_9} + P_2 \lambda^{i_3 i_5}_{a_1 a_2} v^{i_4 i_6}_{a_7 a_8} t^{a_7}_{i_6} t^{a_8}_{i_5} + \tfrac{1}{2}\lambda^{i_5 i_6}_{a_1 a_2} v^{i_3 i_4}_{a_7 a_8} t^{a_7}_{i_5} t^{a_8}_{i_6} + P_2 \lambda^{i_3 i_4}_{a_1 a_5} v^{i_6 i_7}_{a_2 a_8} t^{a_8}_{i_6} t^{a_5}_{i_7} \\
& -P_2 P_2 \lambda^{i_3 i_5}_{a_1 a_6} v^{i_4 i_7}_{a_2 a_8} t^{a_8}_{i_5} t^{a_6}_{i_7} + \tfrac{1}{2}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_7 i_8}_{a_1 a_2} t^{a_5}_{i_7} t^{a_6}_{i_8} - \tfrac{1}{2} P_2 \lambda^{i_3 i_5}_{a_1 a_2} v^{i_4 i_6}_{a_7 a_8} t^{a_7 a_8}_{i_5 i_6} + \tfrac{1}{4}\lambda^{i_5 i_6}_{a_1 a_2} v^{i_3 i_4}_{a_7 a_8} t^{a_7 a_8}_{i_5 i_6} - \tfrac{1}{2} P_2 \lambda^{i_3 i_4}_{a_1 a_5} v^{i_6 i_7}_{a_2 a_8} t^{a_5 a_8}_{i_6 i_7} + P_2 P_2 \lambda^{i_3 i_5}_{a_1 a_6} v^{i_4 i_7}_{a_2 a_8} t^{a_6 a_8}_{i_5 i_7} \\
& -\tfrac{1}{2} P_2 \lambda^{i_5 i_6}_{a_1 a_7} v^{i_3 i_4}_{a_2 a_8} t^{a_7 a_8}_{i_5 i_6} + \tfrac{1}{4}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_7 i_8}_{a_1 a_2} t^{a_5 a_6}_{i_7 i_8} - \tfrac{1}{2} P_2 \lambda^{i_3 i_5}_{a_6 a_7} v^{i_4 i_8}_{a_1 a_2} t^{a_6 a_7}_{i_5 i_8} - \tfrac{1}{4} P_2 \lambda^{i_3 i_5}_{a_1 a_2} v^{i_4 i_6}_{\alpha_7 \alpha_8} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} + \tfrac{1}{8}\lambda^{i_5 i_6}_{a_1 a_2} v^{i_3 i_4}_{\alpha_7 \alpha_8} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} - \tfrac{1}{4} P_2 \lambda^{i_3 i_4}_{a_1 a_5} v^{i_6 i_7}_{\alpha_8 a_2} F^{\alpha_8 a_5}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_6 i_7} \\
& +\tfrac{1}{2} P_2 P_2 \lambda^{i_3 i_5}_{a_1 a_6} v^{i_4 i_7}_{\alpha_8 a_2} F^{\alpha_8 a_6}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_7} - \tfrac{1}{4} P_2 \lambda^{i_5 i_6}_{a_1 a_7} v^{i_3 i_4}_{\alpha_8 a_2} F^{\alpha_8 a_7}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} - \tfrac{1}{8} P_2 \lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_1} v^{i_8 i_9}_{\alpha_{10} a_2} F^{\alpha_7 \alpha_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_8 i_9} + \tfrac{1}{4} P_2 P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 a_1} v^{i_4 i_9}_{\alpha_{10} a_2} F^{\alpha_8 \alpha_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_9} \\
& -\tfrac{1}{8} P_2 \lambda^{i_5 i_6}_{i_7 i_8} F^{i_7 i_8}_{\alpha_9 a_1} v^{i_3 i_4}_{\alpha_{10} a_2} F^{\alpha_9 \alpha_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_6} + \tfrac{1}{16}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 \alpha_8} v^{i_9 i_{10}}_{a_1 a_2} F^{\alpha_7 \alpha_8}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_9 i_{10}} - \tfrac{1}{8} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} v^{i_4 i_{10}}_{a_1 a_2} F^{\alpha_8 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_{10}}
\end{aligned}
$$

TABLE ESI.2.XIV: The geminal λ amplitude equation of Λ-CCSD-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_3 i_4}_{i_1 i_2} = & +\tfrac{1}{2} v^{i_3 i_4}_{\alpha_5 \alpha_6} F^{\alpha_5 \alpha_6}_{i_1 i_2} - P_2 \lambda^{i_3}_{a_5} f^{i_4}_{\alpha_6} F^{\alpha_6 a_5}_{i_1 i_2} + \lambda^{i_5}_{a_6} v^{i_3 i_4}_{i_5 \alpha_7} F^{\alpha_7 a_6}_{i_1 i_2} - \tfrac{1}{2} P_2 \lambda^{i_3}_{a_5} v^{i_4 a_5}_{\alpha_6 \alpha_7} F^{\alpha_6 \alpha_7}_{i_1 i_2} - P_2 \lambda^{i_3}_{a_5} v^{i_4 i_6}_{\alpha_7 a_8} F^{\alpha_7 a_5}_{i_1 i_2} t^{a_8}_{i_6} - \lambda^{i_5}_{a_6} v^{i_3 i_4}_{\alpha_7 a_8} F^{\alpha_7 a_6}_{i_1 i_2} t^{a_8}_{i_5} + \tfrac{1}{2} P_2 \lambda^{i_3}_{a_5} v^{i_4 i_6}_{\alpha_7 \alpha_8} F^{\alpha_7 \alpha_8}_{i_1 i_2} t^{a_5}_{i_6} \\
& +\lambda^{i_3 i_4}_{a_5 a_6} f^{a_5}_{\alpha_7} F^{\alpha_7 a_6}_{i_1 i_2} - \tfrac{1}{4} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} f^{i_4}_{i_5} F^{\alpha_8 \alpha_9}_{i_1 i_2} - \tfrac{1}{2}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 \alpha_8} f^{\alpha_7}_{\alpha_9} F^{\alpha_8 \alpha_9}_{i_1 i_2} - \lambda^{i_3 i_4}_{a_5 a_6} f^{i_7}_{\alpha_8} F^{\alpha_8 a_6}_{i_1 i_2} t^{a_5}_{i_7} - \tfrac{1}{4} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} f^{i_4}_{a_{10}} F^{\alpha_8 \alpha_9}_{i_1 i_2} t^{a_{10}}_{i_5} - \tfrac{1}{2}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_8} f^{i_9}_{\alpha_{10}} F^{\alpha_7 \alpha_{10}}_{i_1 i_2} t^{a_8}_{i_9} \\
& -P_2 \lambda^{i_3 i_5}_{a_6 a_7} v^{i_4 a_6}_{i_5 \alpha_8} F^{\alpha_8 a_7}_{i_1 i_2} + \tfrac{1}{4}\lambda^{i_3 i_4}_{a_5 a_6} v^{a_5 a_6}_{\alpha_7 \alpha_8} F^{\alpha_7 \alpha_8}_{i_1 i_2} + \tfrac{1}{8}\lambda^{i_5 i_6}_{i_7 i_8} F^{i_7 i_8}_{\alpha_9 \alpha_{10}} v^{i_3 i_4}_{i_5 i_6} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} + \tfrac{1}{2} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} v^{i_4 \alpha_8}_{i_5 \alpha_{10}} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} + \tfrac{1}{8}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 \alpha_8} v^{\alpha_7 \alpha_8}_{\alpha_9 \alpha_{10}} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} - \lambda^{i_3 i_4}_{a_5 a_6} v^{i_7 a_5}_{\alpha_8 a_9} F^{\alpha_8 a_6}_{i_1 i_2} t^{a_9}_{i_7} \\
& +P_2 \lambda^{i_3 i_5}_{a_6 a_7} v^{i_4 i_8}_{i_5 \alpha_9} F^{\alpha_9 a_7}_{i_1 i_2} t^{a_6}_{i_8} + P_2 \lambda^{i_3 i_5}_{a_6 a_7} v^{i_4 a_6}_{\alpha_8 a_9} F^{\alpha_8 a_7}_{i_1 i_2} t^{a_9}_{i_5} - \tfrac{1}{2}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_7 a_6}_{\alpha_8 \alpha_9} F^{\alpha_8 \alpha_9}_{i_1 i_2} t^{a_5}_{i_7} - \tfrac{1}{4} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} v^{i_4 i_{10}}_{i_5 a_{11}} F^{\alpha_8 \alpha_9}_{i_1 i_2} t^{a_{11}}_{i_{10}} - \tfrac{1}{4}\lambda^{i_5 i_6}_{i_7 i_8} F^{i_7 i_8}_{\alpha_9 \alpha_{10}} v^{i_3 i_4}_{i_6 a_{11}} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} t^{a_{11}}_{i_5} \\
& +\tfrac{1}{2}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 \alpha_8} v^{i_9 \alpha_7}_{\alpha_{10} a_{11}} F^{\alpha_8 \alpha_{10}}_{i_1 i_2} t^{a_{11}}_{i_9} + \tfrac{1}{2} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 a_9} v^{i_4 i_{10}}_{i_5 \alpha_{11}} F^{\alpha_8 \alpha_{11}}_{i_1 i_2} t^{a_9}_{i_{10}} - \tfrac{1}{2} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} v^{i_4 \alpha_8}_{\alpha_{10} a_{11}} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} t^{a_{11}}_{i_5} + \tfrac{1}{4}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_8} v^{i_9 \alpha_7}_{\alpha_{10} \alpha_{11}} F^{\alpha_{10} \alpha_{11}}_{i_1 i_2} t^{a_8}_{i_9} \\
& +\lambda^{i_3 i_4}_{a_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} F^{\alpha_9 a_6}_{i_1 i_2} t^{a_{10}}_{i_7} t^{a_5}_{i_8} - P_2 \lambda^{i_3 i_5}_{a_6 a_7} v^{i_4 i_8}_{\alpha_9 a_{10}} F^{\alpha_9 a_7}_{i_1 i_2} t^{a_{10}}_{i_5} t^{a_6}_{i_8} + \tfrac{1}{4}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_7 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} t^{a_5}_{i_7} t^{a_6}_{i_8} - \tfrac{1}{2}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} F^{\alpha_9 a_6}_{i_1 i_2} t^{a_5 a_{10}}_{i_7 i_8} + P_2 \lambda^{i_3 i_5}_{a_6 a_7} v^{i_4 i_8}_{\alpha_9 a_{10}} F^{\alpha_9 a_7}_{i_1 i_2} t^{a_6 a_{10}}_{i_5 i_8} \\
& -\tfrac{1}{2}\lambda^{i_5 i_6}_{a_7 a_8} v^{i_3 i_4}_{\alpha_9 a_{10}} F^{\alpha_9 a_8}_{i_1 i_2} t^{a_7 a_{10}}_{i_5 i_6} + \tfrac{1}{8}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_7 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} t^{a_5 a_6}_{i_7 i_8} - \tfrac{1}{4} P_2 \lambda^{i_3 i_5}_{a_6 a_7} v^{i_4 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} t^{a_6 a_7}_{i_5 i_8} - \tfrac{1}{4}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_7 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_9 a_5}_{i_1 i_2} F^{\alpha_{10} a_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} \\
& +\tfrac{1}{2} P_2 \lambda^{i_3 i_5}_{a_6 a_7} v^{i_4 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_9 a_6}_{i_1 i_2} F^{\alpha_{10} a_7}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_8} - \tfrac{1}{4}\lambda^{i_5 i_6}_{a_7 a_8} v^{i_3 i_4}_{\alpha_9 \alpha_{10}} F^{\alpha_9 a_7}_{i_1 i_2} F^{\alpha_{10} a_8}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_6} + \tfrac{1}{4} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} v^{i_4 i_{10}}_{a_{11} a_{12}} F^{\alpha_8 \alpha_9}_{i_1 i_2} t^{a_{11}}_{i_{10}} t^{a_{12}}_{i_5} + \tfrac{1}{8}\lambda^{i_5 i_6}_{i_7 i_8} F^{i_7 i_8}_{\alpha_9 \alpha_{10}} v^{i_3 i_4}_{a_{11} a_{12}} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} t^{a_{11}}_{i_5} t^{a_{12}}_{i_6} \\
& +\tfrac{1}{2}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_8} v^{i_9 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_7 \alpha_{11}}_{i_1 i_2} t^{a_{12}}_{i_9} t^{a_8}_{i_{10}} - \tfrac{1}{2} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 a_9} v^{i_4 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_8 \alpha_{11}}_{i_1 i_2} t^{a_{12}}_{i_5} t^{a_9}_{i_{10}} - \tfrac{1}{8} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} v^{i_4 i_{10}}_{a_{11} a_{12}} F^{\alpha_8 \alpha_9}_{i_1 i_2} t^{a_{11} a_{12}}_{i_5 i_{10}} + \tfrac{1}{16}\lambda^{i_5 i_6}_{i_7 i_8} F^{i_7 i_8}_{\alpha_9 \alpha_{10}} v^{i_3 i_4}_{a_{11} a_{12}} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} t^{a_{11} a_{12}}_{i_5 i_6} \\
& -\tfrac{1}{4}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 a_8} v^{i_9 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_7 \alpha_{11}}_{i_1 i_2} t^{a_8 a_{12}}_{i_9 i_{10}} + \tfrac{1}{2} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 a_9} v^{i_4 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_8 \alpha_{11}}_{i_1 i_2} t^{a_9 a_{12}}_{i_5 i_{10}} - \tfrac{1}{4}\lambda^{i_5 i_6}_{i_7 i_8} F^{i_7 i_8}_{\alpha_9 a_{10}} v^{i_3 i_4}_{\alpha_{11} a_{12}} F^{\alpha_9 \alpha_{11}}_{i_1 i_2} t^{a_{10} a_{12}}_{i_5 i_6} - \tfrac{1}{16} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} v^{i_4 i_{10}}_{\alpha_{11} \alpha_{12}} F^{\alpha_8 \alpha_9}_{i_1 i_2} F^{\alpha_{11} \alpha_{12}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_5 i_{10}} \\
& +\tfrac{1}{32}\lambda^{i_5 i_6}_{i_7 i_8} F^{i_7 i_8}_{\alpha_9 \alpha_{10}} v^{i_3 i_4}_{\alpha_{11} \alpha_{12}} F^{\alpha_9 \alpha_{10}}_{i_1 i_2} F^{\alpha_{11} \alpha_{12}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_5 i_6} - \tfrac{1}{8}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 \alpha_8} v^{i_9 i_{10}}_{\alpha_{11} \alpha_{12}} F^{\alpha_7 \alpha_{11}}_{i_1 i_2} F^{\alpha_8 \alpha_{12}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_9 i_{10}} + \tfrac{1}{4} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} v^{i_4 i_{10}}_{\alpha_{11} \alpha_{12}} F^{\alpha_8 \alpha_{11}}_{i_1 i_2} F^{\alpha_9 \alpha_{12}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_5 i_{10}} \\
& -\tfrac{1}{8}\lambda^{i_5 i_6}_{i_7 i_8} F^{i_7 i_8}_{\alpha_9 \alpha_{10}} v^{i_3 i_4}_{\alpha_{11} \alpha_{12}} F^{\alpha_9 \alpha_{11}}_{i_1 i_2} F^{\alpha_{10} \alpha_{12}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_5 i_6} + \tfrac{1}{32}\lambda^{i_3 i_4}_{i_5 i_6} F^{i_5 i_6}_{\alpha_7 \alpha_8} v^{i_9 i_{10}}_{\alpha_{11} \alpha_{12}} F^{\alpha_{11} \alpha_{12}}_{i_1 i_2} F^{\alpha_7 \alpha_8}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_9 i_{10}} - \tfrac{1}{16} P_2 \lambda^{i_3 i_5}_{i_6 i_7} F^{i_6 i_7}_{\alpha_8 \alpha_9} v^{i_4 i_{10}}_{\alpha_{11} \alpha_{12}} F^{\alpha_{11} \alpha_{12}}_{i_1 i_2} F^{\alpha_8 \alpha_9}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_5 i_{10}}
\end{aligned}
$$

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E. Λ-CCSDT-R12

TABLE ESI.2.XV: The Λ_1 amplitude equation of Λ-CCSDT-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_2}_{a_1} &= \Lambda\text{-CCSD-F12} - \tfrac{1}{4}\lambda^{i_3 i_4}_{a_1 a_5} v^{i_2 i_6}_{a_7 a_8} t^{a_5 a_7 a_8}_{i_3 i_4 i_6} - \tfrac{1}{4}\lambda^{i_2 i_3}_{a_4 a_5} v^{i_6 i_7}_{a_1 a_8} t^{a_4 a_5 a_8}_{i_3 i_6 i_7} - \tfrac{1}{4}\lambda^{i_3 i_4}_{a_5 a_6} v^{i_2 i_7}_{a_1 a_8} t^{a_5 a_6 a_8}_{i_3 i_4 i_7} + \tfrac{1}{12}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} f^{i_2}_{a_8} t^{a_6 a_7 a_8}_{i_3 i_4 i_5} + \tfrac{1}{12}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} f^{i_8}_{a_1} t^{a_5 a_6 a_7}_{i_3 i_4 i_8} + \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{i_4 i_5} t^{a_6 a_7}_{i_3 i_8} \\
&+\tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 a_7}_{i_5 a_8} t^{a_6 a_8}_{i_3 i_4} + \tfrac{1}{2}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 a_7}_{i_4 a_1} t^{a_5 a_6}_{i_3 i_8} + \tfrac{1}{4}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{a_6 a_7}_{a_1 a_8} t^{a_5 a_8}_{i_3 i_4} - \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 a_7}_{i_5 a_8} F^{a_8 a_6}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_4} + \tfrac{1}{8}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{a_6 a_7}_{a_8 a_1} F^{a_8 a_5}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_4} + \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{i_5 a_9} t^{a_6 a_7}_{i_4 i_8} t^{a_9}_{i_3} \\
&+\tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{i_5 a_9} t^{a_7 a_9}_{i_3 i_4} t^{a_6}_{i_8} + \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 a_7}_{a_8 a_9} t^{a_6 a_9}_{i_4 i_5} t^{a_8}_{i_3} + \tfrac{1}{2}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{i_4 a_1} t^{a_6 a_7}_{i_3 i_9} t^{a_5}_{i_8} + \tfrac{1}{2}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 a_7}_{a_1 a_9} t^{a_5 a_6}_{i_4 i_8} t^{a_9}_{i_3} + \tfrac{1}{2}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 a_7}_{a_1 a_9} t^{a_6 a_9}_{i_3 i_4} t^{a_5}_{i_8} + \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{i_5 a_9} t^{a_6 a_7 a_9}_{i_3 i_4 i_8} \\
&-\tfrac{1}{12}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 a_7}_{a_8 a_9} t^{a_6 a_8 a_9}_{i_3 i_4 i_5} - \tfrac{1}{12}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{i_4 a_1} t^{a_5 a_6 a_7}_{i_3 i_4 i_8} + \tfrac{1}{4}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 a_7}_{a_1 a_9} t^{a_5 a_6 a_9}_{i_3 i_4 i_8} - \tfrac{1}{12}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_2 i_9}_{i_5 a_1} t^{a_6 a_7 a_8}_{i_3 i_4 i_9} - \tfrac{1}{12}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_2 a_8}_{a_1 a_9} t^{a_6 a_7 a_9}_{i_3 i_4 i_5} + \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{i_5 a_9} F^{a_9 a_6}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_3 i_4} t^{a_7}_{i_8} \\
&+\tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 a_7}_{a_8 a_9} F^{a_8 a_6}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_3 i_4} t^{a_9}_{i_5} - \tfrac{1}{4}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 a_7}_{a_9 a_1} F^{a_9 a_5}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_3 i_4} t^{a_6}_{i_8} + \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} t^{a_6 a_7}_{i_5 i_8} t^{a_9}_{i_3} + \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_9}_{a_9 a_{10}} t^{a_7 a_{10}}_{i_4 i_5} t^{a_9}_{i_3} t^{a_6}_{i_8} + \tfrac{1}{2}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{a_1 a_{10}} t^{a_6 a_7}_{i_4 i_9} t^{a_{10}}_{i_3} t^{a_5}_{i_8} \\
&+\tfrac{1}{4}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{a_1 a_{10}} t^{a_7 a_{10}}_{i_3 i_4} t^{a_5}_{i_8} t^{a_6}_{i_9} - \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} t^{a_6 a_9}_{i_3 i_8} t^{a_7 a_{10}}_{i_4 i_5} + \tfrac{1}{8}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} t^{a_9 a_{10}}_{i_3 i_4} t^{a_6 a_7}_{i_5 i_8} + \tfrac{1}{8}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{a_1 a_{10}} t^{a_6 a_7}_{i_8 i_9} t^{a_5 a_{10}}_{i_3 i_4} - \tfrac{1}{2}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{a_1 a_{10}} t^{a_5 a_{10}}_{i_4 i_9} t^{a_6 a_7}_{i_3 i_8} \\
&-\tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_2 i_9}_{a_1 a_{10}} t^{a_6 a_{10}}_{i_3 i_4} t^{a_7 a_8}_{i_5 i_9} - \tfrac{1}{12}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} t^{a_6 a_7 a_{10}}_{i_3 i_4 i_5} t^{a_9}_{i_8} + \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} t^{a_6 a_7 a_{10}}_{i_4 i_5 i_8} t^{a_9}_{i_3} - \tfrac{1}{12}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} t^{a_7 a_9 a_{10}}_{i_3 i_4 i_5} t^{a_6}_{i_8} - \tfrac{1}{12}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{a_1 a_{10}} t^{a_5 a_6 a_7}_{i_3 i_4 i_9} t^{a_{10}}_{i_8} \\
&-\tfrac{1}{12}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{a_1 a_{10}} t^{a_5 a_6 a_7}_{i_4 i_8 i_9} t^{a_{10}}_{i_3} + \tfrac{1}{4}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{a_1 a_{10}} t^{a_6 a_7 a_{10}}_{i_4 i_9} t^{a_5}_{i_8} + \tfrac{1}{12}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_2 i_9}_{a_1 a_{10}} t^{a_6 a_7 a_8}_{i_4 i_5 i_9} t^{a_{10}}_{i_3} + \tfrac{1}{12}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_2 i_9}_{a_1 a_{10}} t^{a_7 a_8 a_{10}}_{i_3 i_4 i_5} t^{a_6}_{i_9} - \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} F^{a_9 a_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_4} t^{a_{10}}_{i_5} t^{a_7}_{i_8} \\
&+\tfrac{1}{8}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{\alpha_{10} a_1} F^{\alpha_{10} a_5}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_4} t^{a_6 a_7}_{i_8 i_9} + \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} F^{a_9 a_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_4} t^{a_7 a_{10}}_{i_4 i_5} + \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} F^{a_9 a_6}_{i_{11} i_{12}} t^{a_7 a_{10}}_{i_3 i_8} + \tfrac{1}{16}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} F^{a_9 a_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_4} t^{a_6 a_7}_{i_5 i_8} \\
&+\tfrac{1}{16}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{\alpha_{10} a_1} F^{\alpha_{10} a_5}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_8 i_9} t^{a_6 a_7}_{i_3 i_4} - \tfrac{1}{4}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{\alpha_{10} a_1} F^{\alpha_{10} a_5}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_8} t^{a_6 a_7}_{i_4 i_9} - \tfrac{1}{8}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_2 i_9}_{\alpha_{10} a_1} F^{\alpha_{10} a_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_4} t^{a_7 a_8}_{i_5 i_9} - \tfrac{1}{8}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} F^{a_9 a_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_3 i_8} F^{\alpha_{10} a_7}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_4 i_5}
\end{aligned}
$$

TABLE ESI.2.XVI: The Λ_2 amplitude equation of Λ-CCSDT-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_3 i_4}_{a_1 a_2} &= \Lambda\text{-CCSD-F12} + \tfrac{1}{2}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} f^{i_4}_{a_8} t^{a_7 a_8}_{i_5 i_6} + \tfrac{1}{2}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} f^{i_8}_{a_2} t^{a_6 a_7}_{i_5 i_8} - \tfrac{1}{4}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} f^{i_4}_{a_8} F^{a_8 a_7}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} - \tfrac{1}{2}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 a_7}_{i_5 i_6} - \tfrac{1}{2}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{a_6 a_7}_{i_5 a_2} + \tfrac{1}{2}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{i_5 i_6} t^{a_7}_{i_8} \\
&+P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 a_7}_{i_6 a_8} t^{a_8}_{i_5} + P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 a_7}_{i_5 a_2} t^{a_6}_{i_8} + \tfrac{1}{2}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{a_6 a_7}_{a_2 a_8} t^{a_8}_{i_5} - P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{i_6 a_9} t^{a_9}_{i_5} t^{a_7}_{i_8} - \tfrac{1}{2}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 a_7}_{a_8 a_9} t^{a_8}_{i_5} t^{a_9}_{i_6} - \tfrac{1}{2}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 i_9}_{i_5 a_2} t^{a_6}_{i_8} t^{a_7}_{i_9} \\
&-P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 a_7}_{a_2 a_9} t^{a_9}_{i_5} t^{a_6}_{i_8} + P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{i_6 a_9} t^{a_7 a_9}_{i_5 i_8} - \tfrac{1}{4}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 a_7}_{a_8 a_9} t^{a_8 a_9}_{i_5 i_6} - \tfrac{1}{2}\lambda^{i_5 i_6 i_7}_{a_1 a_2 a_8} v^{i_3 i_4}_{i_7 a_9} t^{a_8 a_9}_{i_5 i_6} - \tfrac{1}{4}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 i_9}_{i_5 a_2} t^{a_6 a_7}_{i_8 i_9} + P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 a_7}_{a_2 a_9} t^{a_6 a_9}_{i_5 i_8} \\
&+\tfrac{1}{2}P_2P_2\lambda^{i_3 i_5 i_6}_{a_1 a_7 a_8} v^{i_4 i_9}_{i_6 a_2} t^{a_7 a_8}_{i_5 i_9} + \tfrac{1}{2}P_2P_2\lambda^{i_3 i_5 i_6}_{a_1 a_7 a_8} v^{i_4 a_8}_{a_2 a_9} t^{a_7 a_9}_{i_5 i_6} - \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 a_8}_{a_1 a_2} t^{a_6 a_7}_{i_5 i_9} - \tfrac{1}{2}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{i_6 a_9} F^{a_9 a_7}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_5 i_8} - \tfrac{1}{8}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 a_7}_{a_8 a_9} F^{a_8 a_9}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_5 i_6} \\
&+\tfrac{1}{4}\lambda^{i_5 i_6 i_7}_{a_1 a_2 a_8} v^{i_3 i_4}_{i_7 a_9} F^{a_9 a_8}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_5 i_6} + \tfrac{1}{2}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 a_7}_{a_9 a_2} F^{a_9 a_6}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_5 i_8} + \tfrac{1}{4}P_2P_2\lambda^{i_3 i_5 i_6}_{a_1 a_7 a_8} v^{i_4 a_8}_{a_9 a_2} F^{a_9 a_7}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_5 i_6} + \tfrac{1}{2}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{a_9 a_{10}} t^{a_9}_{i_5} t^{a_{10}}_{i_6} t^{a_7}_{i_8} \\
&+\tfrac{1}{2}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 i_9}_{a_2 a_{10}} t^{a_{10}}_{i_5} t^{a_6}_{i_8} t^{a_7}_{i_9} + \tfrac{1}{4}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{a_9 a_{10}} t^{a_7}_{i_8} t^{a_9 a_{10}}_{i_5 i_6} - P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{a_9 a_{10}} t^{a_9}_{i_5} t^{a_7 a_{10}}_{i_6 i_8} - \tfrac{1}{2}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{a_9 a_{10}} t^{a_9}_{i_5 i_6} t^{a_7 a_{10}}_{i_8} - \tfrac{1}{2}\lambda^{i_5 i_6 i_7}_{a_1 a_2 a_8} v^{i_3 i_4}_{a_9 a_{10}} t^{a_9}_{i_5 i_6} t^{a_8 a_{10}}_{i_7} \\
&-P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 i_9}_{a_2 a_{10}} t^{a_6}_{i_8} t^{a_7 a_{10}}_{i_5 i_9} + \tfrac{1}{4}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 i_9}_{a_2 a_{10}} t^{a_{10}}_{i_5} t^{a_6 a_7}_{i_8 i_9} - \tfrac{1}{2}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 i_9}_{a_2 a_{10}} t^{a_{10}}_{i_8} t^{a_6 a_7}_{i_5 i_9} + \tfrac{1}{2}P_2P_2\lambda^{i_3 i_5 i_6}_{a_1 a_7 a_8} v^{i_4 i_9}_{a_2 a_{10}} t^{a_7}_{i_5 i_6} t^{a_8 a_{10}}_{i_9} + \tfrac{1}{2}P_2P_2\lambda^{i_3 i_5 i_6}_{a_1 a_7 a_8} v^{i_4 i_9}_{a_2 a_{10}} t^{a_{10}}_{i_5} t^{a_7 a_8}_{i_6 i_9} \\
&-\tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{a_1 a_2} t^{a_6}_{i_9} t^{a_7 a_8}_{i_5 i_{10}} + \tfrac{1}{8}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{a_9 a_{10}} t^{a_7}_{i_8} F^{a_9 a_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_6} + \tfrac{1}{2}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{a_9 a_{10}} t^{a_{10}}_{i_6} F^{a_9 a_7}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_8} - \tfrac{1}{4}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{a_9 a_{10}} t^{a_{10}}_{i_8} F^{a_9 a_7}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_6} \\
&-\tfrac{1}{4}\lambda^{i_5 i_6 i_7}_{a_1 a_2 a_8} v^{i_3 i_4}_{a_9 a_{10}} t^{a_{10}}_{i_7} F^{a_9 a_8}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_6} - \tfrac{1}{2}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 i_9}_{a_{10} a_2} t^{a_7}_{i_9} F^{a_{10} a_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_8} - \tfrac{1}{4}P_2P_2\lambda^{i_3 i_5 i_6}_{a_1 a_7 a_8} v^{i_4 i_9}_{a_{10} a_2} t^{a_8}_{i_9} F^{a_{10} a_7}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_6} + \tfrac{1}{4}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} v^{i_4 i_8}_{a_9 a_{10}} t^{a_7 a_9 a_{10}}_{i_5 i_6 i_8} \\
&+\tfrac{1}{12}\lambda^{i_5 i_6 i_7}_{a_1 a_2 a_8} v^{i_3 i_4}_{a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_5 i_6 i_7} + \tfrac{1}{4}P_2\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_8 i_9}_{a_2 a_{10}} t^{a_6 a_7 a_{10}}_{i_5 i_8 i_9} + \tfrac{1}{4}P_2P_2\lambda^{i_3 i_5 i_6}_{a_1 a_7 a_8} v^{i_4 i_9}_{a_2 a_{10}} t^{a_7 a_8 a_{10}}_{i_5 i_6 i_9} + \tfrac{1}{12}P_2\lambda^{i_3 i_5 i_6}_{a_1 a_8 a_9} v^{i_4 i_9}_{a_2 a_{10}} t^{a_8 a_9 a_{10}}_{i_5 i_6 i_7} + \tfrac{1}{12}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{a_1 a_2} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} \\
&+\tfrac{1}{12}P_2\lambda^{i_3 i_5 i_6}_{a_7 a_8 a_9} v^{i_4 i_{10}}_{a_1 a_2} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}}
\end{aligned}
$$

TABLE ESI.2.XVII: The Λ_3 amplitude equation of Λ-CCSDT-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_4 i_5 i_6}_{a_1 a_2 a_3} &= -P_3P_3\lambda^{i_4}_{a_1} v^{i_5 i_6}_{a_2 a_3} - P_3P_3\lambda^{i_4 i_5}_{a_1 a_2} f^{i_6}_{a_3} + P_3P_3\lambda^{i_4 i_7}_{a_1 a_2} v^{i_5 i_6}_{i_7 a_3} + P_3P_3\lambda^{i_4 i_5}_{a_1 a_7} v^{i_6 a_7}_{a_2 a_3} - \tfrac{1}{2}P_3P_3\lambda^{i_4 i_5}_{i_7 i_8} F^{i_7 i_8}_{a_9 a_1} v^{i_6 a_9}_{a_2 a_3} - P_3P_3\lambda^{i_4 i_5}_{a_1 a_2} v^{i_6 i_7}_{a_3 a_8} t^{a_8}_{i_7} - P_3P_3\lambda^{i_4 i_7}_{a_1 a_2} v^{i_5 i_6}_{a_3 a_8} t^{a_8}_{i_7} \\
&-P_3P_3\lambda^{i_4 i_5}_{a_1 a_7} v^{i_6 i_8}_{a_2 a_3} t^{a_7}_{i_8} + P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_3} f^{i_6}_{i_7} - P_3\lambda^{i_4 i_5 i_6}_{a_1 a_2 a_7} f^{a_7}_{a_3} + P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_3} f^{i_6}_{a_8} t^{a_8}_{i_7} + P_3\lambda^{i_4 i_5 i_6}_{a_1 a_2 a_7} f^{i_8}_{a_3} t^{a_7}_{i_8} - \tfrac{1}{2}P_3\lambda^{i_4 i_7 i_8}_{a_1 a_2 a_3} v^{i_5 i_6}_{i_7 i_8} + P_3P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_8} v^{i_6 a_8}_{i_7 a_3} \\
&-\tfrac{1}{2}P_3\lambda^{i_4 i_5 i_6}_{a_1 a_7 a_8} v^{a_7 a_8}_{a_2 a_3} + P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_3} v^{i_6 i_8}_{i_7 a_9} t^{a_9}_{i_8} + P_3\lambda^{i_4 i_7 i_8}_{a_1 a_2 a_3} v^{i_5 i_6}_{i_8 a_9} t^{a_9}_{i_7} + P_3\lambda^{i_4 i_5 i_6}_{a_1 a_2 a_7} v^{i_8 a_7}_{a_3 a_9} t^{a_9}_{i_8} - P_3P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_8} v^{i_6 i_8}_{i_7 a_3} t^{a_8}_{i_9} - P_3P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_8} v^{i_6 a_8}_{a_3 a_9} t^{a_9}_{i_7} + P_3\lambda^{i_4 i_5 i_6}_{a_1 a_7 a_8} v^{i_9 a_8}_{a_2 a_3} t^{a_7}_{i_9} \\
&-P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_3} v^{i_6 i_8}_{a_9 a_{10}} t^{a_9}_{i_8} t^{a_{10}}_{i_7} - \tfrac{1}{2}P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_3} v^{i_8 i_9}_{a_9 a_{10}} t^{a_9}_{i_7} t^{a_{10}}_{i_8} - P_3\lambda^{i_4 i_5 i_6}_{a_1 a_2 a_7} v^{i_8 i_9}_{a_3 a_{10}} t^{a_{10}}_{i_8} t^{a_7}_{i_9} + P_3P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_8} v^{i_6 i_9}_{a_3 a_{10}} t^{a_{10}}_{i_7} t^{a_8}_{i_9} - \tfrac{1}{2}P_3\lambda^{i_4 i_5 i_6}_{a_1 a_7 a_8} v^{i_9 i_{10}}_{a_2 a_3} t^{a_7 a_8}_{i_9 i_{10}} \\
&+\tfrac{1}{2}P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_3} v^{i_6 i_8}_{a_9 a_{10}} t^{a_9 a_{10}}_{i_7 i_8} - \tfrac{1}{4}P_3\lambda^{i_4 i_7 i_8}_{a_1 a_2 a_3} v^{i_5 i_6}_{a_9 a_{10}} t^{a_9 a_{10}}_{i_7 i_8} + \tfrac{1}{2}P_3\lambda^{i_4 i_5 i_6}_{a_1 a_2 a_7} v^{i_8 i_9}_{a_3 a_{10}} t^{a_7 a_{10}}_{i_8 i_9} - P_3P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_8} v^{i_6 i_9}_{a_3 a_{10}} t^{a_8 a_{10}}_{i_7 i_9} + \tfrac{1}{2}P_3P_3\lambda^{i_4 i_7 i_8}_{a_1 a_2 a_9} v^{i_5 i_6}_{a_3 a_{10}} t^{a_9 a_{10}}_{i_7 i_8} \\
&-\tfrac{1}{4}P_3\lambda^{i_4 i_5 i_6}_{a_1 a_7 a_8} v^{i_9 i_{10}}_{a_2 a_3} t^{a_7 a_8}_{i_9 i_{10}} + \tfrac{1}{2}P_3P_3\lambda^{i_4 i_5 i_7}_{a_1 a_8 a_9} v^{i_6 i_{10}}_{a_2 a_3} t^{a_8 a_9}_{i_7 i_{10}} + \tfrac{1}{4}P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_3} v^{i_6 i_8}_{a_9 a_{10}} t^{a_9 a_{10}}_{i_7 i_8} F^{a_9 a_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} - \tfrac{1}{8}P_3\lambda^{i_4 i_7 i_8}_{a_1 a_2 a_9} v^{i_5 i_6}_{a_9 a_{10}} F^{a_9 a_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} \\
&+\tfrac{1}{4}P_3\lambda^{i_4 i_5 i_6}_{a_1 a_2 a_7} v^{i_8 i_9}_{\alpha_{10} a_3} F^{\alpha_{10} a_7}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_8 i_9} - \tfrac{1}{2}P_3P_3\lambda^{i_4 i_5 i_7}_{a_1 a_2 a_8} v^{i_6 i_9}_{\alpha_{10} a_3} F^{\alpha_{10} a_8}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_9} + \tfrac{1}{4}P_3P_3\lambda^{i_4 i_7 i_8}_{a_1 a_2 a_9} v^{i_5 i_6}_{\alpha_{10} a_3} F^{\alpha_{10} a_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8}
\end{aligned}
$$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.2.XVIII: The geminal λ amplitude equation of Λ-CCSDT-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_3 i_4}_{i_1 i_2} = \Lambda\text{-CCSD-R12} &- \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} f^{i_9}_{\alpha_{10}} F^{\alpha_{10} a_8}_{i_1 i_2} t^{a_6 a_7}_{i_5 i_9} + \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{a_6 a_7}_{i_5 a_9} F^{a_9 a_8}_{i_1 i_2} - \lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 a_7}_{i_5 \alpha_{10}} F^{\alpha_{10} a_8}_{i_1 i_2} t^{a_6}_{i_9} - \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{a_6 a_7}_{a_9 a_{10}} F^{a_9 a_8}_{i_1 i_2} t^{a_{10}}_{i_5} + \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{i_5 \alpha_{11}} F^{\alpha_{11} a_8}_{i_1 i_2} t^{a_6}_{i_9} t^{a_7}_{i_{10}} \\
&+ \lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 a_7}_{\alpha_{10} a_{11}} F^{\alpha_{10} a_8}_{i_1 i_2} t^{a_{11}}_{i_5} t^{a_6}_{i_9} + \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{i_5 \alpha_{11}} F^{\alpha_{11} a_8}_{i_1 i_2} t^{a_6 a_7}_{i_9 i_{10}} - \lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 a_7}_{\alpha_{10} a_{11}} F^{\alpha_{10} a_8}_{i_1 i_2} t^{a_6 a_{11}}_{i_5 i_9} - \tfrac{1}{2} P_2 \lambda^{i_3 i_5 i_6}_{a_7 a_8 a_9} v^{i_4 i_{10}}_{i_6 \alpha_{11}} F^{\alpha_{11} a_9}_{i_1 i_2} t^{a_7 a_8}_{i_5 i_{10}} \\
&- \tfrac{1}{2} P_2 \lambda^{i_3 i_5 i_6}_{a_7 a_8 a_9} v^{i_4 a_8}_{\alpha_{10} a_{11}} F^{\alpha_{10} a_9}_{i_1 i_2} t^{a_7 a_{11}}_{i_5 i_6} - \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 a_8}_{\alpha_{10} a_{11}} F^{\alpha_{10} a_{11}}_{i_1 i_2} t^{a_6 a_7}_{i_5 i_9} + \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 a_8}_{\alpha_{10} a_{11}} F^{\alpha_{10} a_6}_{i_1 i_2} F^{\alpha_{11} a_7}_{i_{12} i_{13}} t^{i_{12} i_{13}}_{i_5 i_9} + \tfrac{1}{4} P_2 \lambda^{i_3 i_5 i_6}_{a_7 a_8 a_9} v^{i_4 a_9}_{\alpha_{10} a_{11}} F^{\alpha_{10} a_7}_{i_1 i_2} F^{\alpha_{11} a_8}_{i_{12} i_{13}} t^{i_{12} i_{13}}_{i_5 i_6} \\
&- \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_8}_{i_1 i_2} t^{a_{12}}_{i_5} t^{a_6}_{i_9} t^{a_7}_{i_{10}} + \lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_8}_{i_1 i_2} t^{a_6}_{i_9} t^{a_7 a_{12}}_{i_5 i_{10}} - \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_8}_{i_1 i_2} t^{a_{12}}_{i_5} t^{a_6 a_7}_{i_9 i_{10}} + \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_8}_{i_1 i_2} t^{a_{12}}_{i_9} t^{a_6 a_7}_{i_5 i_{10}} \\
&- \tfrac{1}{2} P_2 \lambda^{i_3 i_5 i_6}_{a_7 a_8 a_9} v^{i_4 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_9}_{i_1 i_2} t^{a_7}_{i_{10}} t^{a_8 a_{12}}_{i_5 i_6} - \tfrac{1}{2} P_2 \lambda^{i_3 i_5 i_6}_{a_7 a_8 a_9} v^{i_4 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_9}_{i_1 i_2} t^{a_{12}}_{i_5} t^{a_7 a_8}_{i_6 i_{10}} - \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_{12}}_{i_1 i_2} t^{a_6}_{i_9} t^{a_7 a_8}_{i_5 i_{10}} - \tfrac{1}{2}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_7}_{i_1 i_2} t^{a_6}_{i_{10}} F^{\alpha_{12} a_8}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_5 i_9} \\
&- \tfrac{1}{4} P_2 \lambda^{i_3 i_5 i_6}_{a_7 a_8 a_9} v^{i_4 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_8}_{i_1 i_2} t^{a_7}_{i_{10}} F^{\alpha_{12} a_9}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_5 i_6} - \tfrac{1}{4}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_8}_{i_1 i_2} t^{a_{12}}_{i_5 i_9 i_{10}} - \tfrac{1}{4} P_2 \lambda^{i_3 i_5 i_6}_{a_7 a_8 a_9} v^{i_4 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_9}_{i_1 i_2} t^{a_7 a_8 a_{12}}_{i_5 i_6 i_{10}} - \tfrac{1}{12}\lambda^{i_3 i_5 i_6 i_7}_{a_8 a_9 a_{10}} v^{i_3 i_4}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_{10}}_{i_1 i_2} t^{a_8 a_9 a_{12}}_{i_5 i_6 i_7} \\
&+ \tfrac{1}{24}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_9 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_{12}}_{i_1 i_2} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} + \tfrac{1}{24} P_2 \lambda^{i_3 i_5 i_6}_{a_7 a_8 a_9} v^{i_4 i_{10}}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_{12}}_{i_1 i_2} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}}
\end{aligned}
$$

F. Λ-CCSDTQ-R12

TABLE ESI.2.XIX: The Λ_1 amplitude equation of Λ-CCSDTQ-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_2}_{a_1} = \Lambda\text{-CCSDT-R12} &+ \tfrac{1}{24}\lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} v^{i_2 i_8}_{a_9 a_{10}} t^{a_6 a_7 a_9 a_{10}}_{i_3 i_4 i_5 i_8} + \tfrac{1}{24}\lambda^{i_2 i_3 i_4}_{a_5 a_6 a_7} v^{i_8 i_9}_{a_1 a_{10}} t^{a_5 a_6 a_7 a_{10}}_{i_3 i_4 i_8 i_9} - \tfrac{1}{36}\lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} v^{i_2 i_9}_{a_1 a_{10}} t^{a_6 a_7 a_8 a_{10}}_{i_3 i_4 i_5 i_9} - \tfrac{1}{144}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} f^{i_2}_{a_{10}} t^{a_7 a_8 a_9 a_{10}}_{i_3 i_4 i_5 i_6} \\
&- \tfrac{1}{144}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} f^{i_{10}}_{a_1} t^{a_6 a_7 a_8 a_9}_{i_3 i_4 i_5 i_{10}} - \tfrac{1}{24}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{i_6 a_{10}} t^{a_7 a_8 a_9}_{i_3 i_4 i_{10}} - \tfrac{1}{12}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 a_9}_{i_6 a_{10}} t^{a_7 a_8 a_{10}}_{i_3 i_4 i_5} - \tfrac{1}{12}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} a_9}_{i_5 a_1} t^{a_6 a_7 a_8}_{i_3 i_4 i_{10}} - \tfrac{1}{24}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{a_8 a_9}_{a_1 a_{10}} t^{a_6 a_7 a_{10}}_{i_3 i_4 i_5} \\
&- \tfrac{1}{4}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{i_6 a_{11}} t^{a_7 a_{11}}_{i_3 i_4} t^{a_8 a_9}_{i_5 i_{10}} - \tfrac{1}{8}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 a_9}_{a_{10} a_{11}} t^{a_7 a_{10}}_{i_3 i_4} t^{a_8 a_{11}}_{i_5 i_6} - \tfrac{1}{8}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{i_3 i_{10}} t^{a_6 a_7}_{i_4 i_{11}} t^{a_8 a_9}_{i_5 i_{10}} - \tfrac{1}{4}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} a_9}_{a_1 a_{11}} t^{a_6 a_{11}}_{i_3 i_4} t^{a_7 a_8}_{i_5 i_{10}} \\
&+ \tfrac{1}{8}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{i_6 a_{11}} t^{a_8 a_9}_{i_3 i_{10}} F^{\alpha_{11} a_7}_{i_{12} i_{13}} t^{i_{12} i_{13}}_{i_4 i_5} + \tfrac{1}{8}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 a_9}_{\alpha_{10} a_{11}} t^{a_8 a_{11}}_{i_3 i_4} F^{\alpha_{10} a_7}_{i_{12} i_{13}} t^{i_{12} i_{13}}_{i_5 i_6} - \tfrac{1}{8}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} a_9}_{\alpha_{11} a_1} t^{a_7 a_8}_{i_3 i_{10}} F^{\alpha_{11} a_6}_{i_{12} i_{13}} t^{i_{12} i_{13}}_{i_4 i_5} + \tfrac{1}{12}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{i_6 a_{11}} t^{a_7 a_8 a_9}_{i_4 i_5 i_{10}} t^{a_{11}}_{i_3} \\
&+ \tfrac{1}{12}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{i_6 a_{11}} t^{a_8 a_9 a_{11}}_{i_3 i_4 i_5} t^{a_7}_{i_{10}} + \tfrac{1}{12}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 a_9}_{a_{10} a_{11}} t^{a_7 a_8 a_{11}}_{i_4 i_5 i_6} t^{a_{10}}_{i_3} + \tfrac{1}{12}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{i_5 a_1} t^{a_7 a_8 a_9}_{i_3 i_4 i_{11}} t^{a_6}_{i_{10}} + \tfrac{1}{12}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} a_9}_{a_1 a_{11}} t^{a_6 a_7 a_8}_{i_4 i_5 i_{10}} t^{a_{11}}_{i_3} \\
&+ \tfrac{1}{12}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} a_9}_{a_1 a_{11}} t^{a_7 a_8 a_{11}}_{i_3 i_4 i_5} t^{a_6}_{i_{10}} - \tfrac{1}{36}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{i_6 a_{11}} t^{a_7 a_8 a_9 a_{11}}_{i_3 i_4 i_5 i_{10}} + \tfrac{1}{96}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 a_9}_{a_{10} a_{11}} t^{a_7 a_8 a_{10} a_{11}}_{i_3 i_4 i_5 i_6} + \tfrac{1}{96}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{i_5 a_1} t^{a_6 a_7 a_8 a_9}_{i_3 i_4 i_{10} i_{11}} - \tfrac{1}{36}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} a_9}_{a_1 a_{11}} t^{a_6 a_7 a_8 a_{11}}_{i_3 i_4 i_5 i_{10}} \\
&- \tfrac{1}{144}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_2 i_{11}}_{i_6 a_1} t^{a_7 a_8 a_9 a_{10}}_{i_3 i_4 i_5 i_{11}} - \tfrac{1}{144}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_2 a_{10}}_{a_1 a_{11}} t^{a_7 a_8 a_9 a_{11}}_{i_3 i_4 i_5 i_6} - \tfrac{1}{32}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 a_9}_{\alpha_{10} a_{11}} F^{\alpha_{10} a_7}_{i_{12} i_{13}} t^{i_{12} i_{13}}_{i_3 i_4} F^{\alpha_{11} a_8}_{i_{14} i_{15}} t^{i_{14} i_{15}}_{i_5 i_6} \\
&+ \tfrac{1}{32}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{\alpha_{11} a_{12}} t^{a_9}_{i_{10}} F^{\alpha_{11} a_7}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_3 i_4} F^{\alpha_{12} a_8}_{i_{15} i_{16}} t^{i_{15} i_{16}}_{i_5 i_6} - \tfrac{1}{8}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{\alpha_{11} a_{12}} t^{a_8 a_9}_{i_3 i_{10}} t^{a_{12}}_{i_6} F^{\alpha_{11} a_7}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_4 i_5} + \tfrac{1}{8}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{\alpha_{11} a_{12}} t^{a_9 a_{12}}_{i_3 i_4} t^{a_8}_{i_{10}} F^{\alpha_{11} a_7}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_5 i_6} \\
&- \tfrac{1}{8}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{\alpha_{12} a_1} t^{a_8 a_9}_{i_3 i_{11}} t^{a_7}_{i_{10}} F^{\alpha_{12} a_6}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_4 i_5} + \tfrac{1}{4}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_7 a_{12}}_{i_4 i_5} t^{a_8 a_9}_{i_6 i_{10}} t^{a_{11}}_{i_3} + \tfrac{1}{8}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_8 a_{11}}_{i_3 i_4} t^{a_9 a_{12}}_{i_5 i_6} t^{a_7}_{i_{10}} + \tfrac{1}{8}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_1 a_{12}} t^{a_6 a_7}_{i_4 i_{10}} t^{a_8 a_9}_{i_5 i_{11}} t^{a_{12}}_{i_3} \\
&+ \tfrac{1}{4}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_1 a_{12}} t^{a_7 a_{12}}_{i_3 i_4} t^{a_8 a_9}_{i_5 i_{11}} t^{a_6}_{i_{10}} - \tfrac{1}{24}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}} t^{a_{11} a_{12}}_{i_3 i_4} - \tfrac{1}{12}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_8 a_9 a_{12}}_{i_4 i_5 i_6} t^{a_7 a_{11}}_{i_3 i_{10}} - \tfrac{1}{8}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_1 a_{12}} t^{a_8 a_9 a_{12}}_{i_4 i_5 i_{11}} t^{a_7 a_{11}}_{i_3 i_{10}} \\
&- \tfrac{1}{24}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_1 a_{12}} t^{a_8 a_9 a_{12}}_{i_3 i_4 i_5} t^{a_6}_{i_{10}} t^{a_7}_{i_{11}} - \tfrac{1}{48}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}} t^{a_{11} a_{12}}_{i_3 i_4} + \tfrac{1}{12}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_8 a_9 a_{12}}_{i_4 i_5 i_6} t^{a_7 a_{11}}_{i_3 i_{10}} - \tfrac{1}{8}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_8 a_9 a_{12}}_{i_5 i_6 i_{10}} t^{a_7 a_{11}}_{i_3 i_4} \\
&+ \tfrac{1}{24}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_9 a_{11} a_{12}}_{i_4 i_5 i_6} t^{a_7 a_8}_{i_3 i_{10}} + \tfrac{1}{12}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_1 a_{12}} t^{a_7 a_8 a_9}_{i_5 i_{10} i_{11}} t^{a_6 a_{12}}_{i_3 i_4} + \tfrac{1}{24}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_1 a_{12}} t^{a_8 a_9 a_{12}}_{i_3 i_4 i_5} t^{a_6 a_7}_{i_{10} i_{11}} \\
&- \tfrac{1}{8}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_1 a_{12}} t^{a_8 a_9 a_{12}}_{i_4 i_5 i_{11}} t^{a_6 a_7}_{i_3 i_{10}} + \tfrac{1}{24}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_2 i_{11}}_{a_1 a_{12}} t^{a_8 a_9 a_{10}}_{i_3 i_6 i_{11}} t^{a_7 a_{12}}_{i_3 i_4} + \tfrac{1}{24}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_2 i_{11}}_{a_1 a_{12}} t^{a_9 a_{10} a_{12}}_{i_4 i_5 i_6} t^{a_7 a_8}_{i_3 i_{11}} - \tfrac{1}{96}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}} F^{\alpha_{11} a_{12}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_3 i_4} \\
&- \tfrac{1}{24}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_8 a_9 a_{12}}_{i_4 i_5 i_6} F^{\alpha_{11} a_7}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_3 i_{10}} + \tfrac{1}{16}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_8 a_9 a_{12}}_{i_5 i_6 i_{10}} F^{\alpha_{11} a_7}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_3 i_4} + \tfrac{1}{24}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_{12} a_1} t^{a_7 a_8 a_9}_{i_4 i_5 i_{11}} F^{a_6 a_{12}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_3 i_{10}} \\
&+ \tfrac{1}{48}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{\alpha_{12} a_1} t^{a_7 a_8 a_9}_{i_5 i_{10} i_{11}} F^{\alpha_{12} a_6}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_3 i_4} + \tfrac{1}{48}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_2 i_{11}}_{\alpha_{12} a_1} t^{a_8 a_9 a_{10}}_{i_5 i_6 i_{11}} F^{\alpha_{12} a_7}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_3 i_4} + \tfrac{1}{144}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_7 a_8 a_9 a_{12}}_{i_3 i_4 i_5 i_6} t^{a_{11}}_{i_{10}} + \tfrac{1}{36}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_7 a_8 a_9 a_{11}}_{i_4 i_5 i_6 i_{10}} t^{a_{12}}_{i_3} \\
&- \tfrac{1}{96}\lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_8 a_9 a_{11} a_{12}}_{i_3 i_4 i_5 i_6} t^{a_7}_{i_{10}} + \tfrac{1}{144}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_1 a_{12}} t^{a_6 a_7 a_8 a_9}_{i_3 i_4 i_5 i_{11}} t^{a_{12}}_{i_{10}} - \tfrac{1}{96}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_1 a_{12}} t^{a_6 a_7 a_8 a_9}_{i_4 i_5 i_{10} i_{11}} t^{a_{12}}_{i_3} + \tfrac{1}{36}\lambda^{i_2 i_3 i_4 i_5}_{a_6 a_7 a_8 a_9} v^{i_{10} i_{11}}_{a_1 a_{12}} t^{a_7 a_8 a_9 a_{12}}_{i_3 i_4 i_5 i_{11}} t^{a_6}_{i_{10}} \\
&- \tfrac{1}{144}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_2 i_{11}}_{a_1 a_{12}} t^{a_7 a_8 a_9 a_{10}}_{i_4 i_5 i_6 i_{11}} t^{a_{12}}_{i_3} - \tfrac{1}{144}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_2 i_{11}}_{a_1 a_{12}} t^{a_8 a_9 a_{10} a_{12}}_{i_3 i_4 i_5 i_6} t^{a_7}_{i_{11}}
\end{aligned}
$$

TABLE ESI.2.XX: The Λ_2 amplitude equation of Λ-CCSDTQ-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_3i_4}_{a_1a_2} = {} & \Lambda\text{-CCSDT-R12} - \tfrac{1}{12}P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} f^{i_4}_{a_{10}} t^{a_8a_9a_{10}}_{i_5i_6i_7} - \tfrac{1}{12}P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} f^{i_{10}}_{a_2} t^{a_7a_8a_9}_{i_5i_6i_{10}} - \tfrac14 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{i_6i_7} t^{a_8a_9}_{i_5i_{10}} - \tfrac12 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4a_9}_{i_7a_{10}} t^{a_8a_{10}}_{i_5i_6} \\
& -\tfrac12 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}a_9}_{i_6a_2} t^{a_7a_8}_{i_5i_{10}} - \tfrac14 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{a_8a_9}_{a_2a_{10}} t^{a_7a_{10}}_{i_5i_6} + \tfrac14 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4a_9}_{i_7\alpha_{10}} F^{\alpha_{10}a_8}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_5i_6} - \tfrac18 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{a_8a_9}_{\alpha_{10}a_2} F^{\alpha_{10}a_7}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_5i_6} \\
& -\tfrac12 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{i_7a_{11}} t^{a_8}_{i_{10}} t^{a_9a_{11}}_{i_5i_6} - \tfrac12 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{i_7a_{11}} t^{a_{11}}_{i_5} t^{a_8a_9}_{i_6i_{10}} - \tfrac12 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4a_9}_{a_{10}a_{11}} t^{a_{10}}_{i_5} t^{a_8a_{11}}_{i_6i_7} - \tfrac12 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{i_6a_2} t^{a_7}_{i_{10}} t^{a_8a_9}_{i_5i_{11}} \\
& -\tfrac12 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}a_9}_{a_2a_{11}} t^{a_7}_{i_{10}} t^{a_8a_{11}}_{i_5i_6} - \tfrac12 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}a_9}_{a_2a_{11}} t^{a_{11}}_{i_5} t^{a_7a_8}_{i_6i_{10}} - \tfrac14 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{i_7\alpha_{11}} t^{a_9}_{i_{10}} F^{\alpha_{11}a_8}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_5i_6} - \tfrac14 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4a_9}_{\alpha_{10}a_{11}} t^{a_{11}}_{i_7} F^{\alpha_{10}a_8}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_5i_6} \\
& +\tfrac14 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}a_9}_{\alpha_{11}a_2} t^{a_8}_{i_{10}} F^{\alpha_{11}a_7}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_5i_6} - \tfrac14 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{i_7a_{11}} t^{a_8a_9a_{11}}_{i_5i_6i_{10}} + \tfrac1{12} P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4a_9}_{a_{10}a_{11}} t^{a_8a_{10}a_{11}}_{i_5i_6i_7} - \tfrac1{12}\lambda^{i_5i_6i_7i_8}_{a_1a_2a_9a_{10}} v^{i_3i_4}_{i_8a_{11}} t^{a_9a_{10}a_{11}}_{i_5i_6i_7} \\
& +\tfrac1{12}P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{i_6a_2} t^{a_7a_8a_9}_{i_5i_{10}i_{11}} - \tfrac14 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}a_9}_{a_2a_{11}} t^{a_7a_8a_{11}}_{i_5i_6i_{10}} + \tfrac1{12}P_2P_2\lambda^{i_3i_5i_6i_7}_{a_1a_8a_9a_{10}} v^{i_4i_{11}}_{i_7a_2} t^{a_8a_9a_{10}}_{i_5i_6i_{11}} + \tfrac1{12}P_2P_2\lambda^{i_3i_5i_6i_7}_{a_1a_8a_9a_{10}} v^{i_4a_{10}}_{a_2a_{11}} t^{a_8a_9a_{11}}_{i_5i_6i_7} \\
& -\tfrac1{12}\lambda^{i_3i_4i_5i_6}_{a_7a_8a_9a_{10}} v^{i_{11}a_{10}}_{a_1a_2} t^{a_7a_8a_9}_{i_5i_6i_{11}} - \tfrac12 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{a_{11}a_{12}} t^{a_{11}}_{i_5} t^{a_8}_{i_{10}} t^{a_9a_{12}}_{i_6i_7} - \tfrac14 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{a_{11}a_{12}} t^{a_{11}}_{i_5} t^{a_{12}}_{i_6} t^{a_8a_9}_{i_7i_{10}} - \tfrac14 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{a_2a_{12}} t^{a_7}_{i_{10}} t^{a_8}_{i_{11}} t^{a_9a_{12}}_{i_5i_6} \\
& -\tfrac12 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{a_2a_{12}} t^{a_{12}}_{i_5} t^{a_7}_{i_{10}} t^{a_8a_9}_{i_6i_{11}} + \tfrac14 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{\alpha_{11}a_{12}} t^{a_{12}}_{i_7} t^{a_9}_{i_{10}} F^{\alpha_{11}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_5i_6} - \tfrac18 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{\alpha_{12}a_2} t^{a_8}_{i_{10}} t^{a_9}_{i_{11}} F^{\alpha_{12}a_7}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_5i_6} \\
& +\tfrac1{12}P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{a_{11}a_{12}} t^{a_8}_{i_{10}} t^{a_9a_{11}a_{12}}_{i_5i_6i_7} - \tfrac14 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{a_{11}a_{12}} t^{a_{11}}_{i_5} t^{a_8a_9a_{12}}_{i_6i_7i_{10}} + \tfrac1{12}P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{a_{11}a_{12}} t^{a_{11}}_{i_{10}} t^{a_8a_9a_{12}}_{i_5i_6i_7} + \tfrac1{12}\lambda^{i_5i_6i_7i_8}_{a_1a_2a_9a_{10}} v^{i_3i_4}_{a_{11}a_{12}} t^{a_{11}}_{i_5} t^{a_9a_{10}a_{12}}_{i_6i_7i_8} \\
& -\tfrac14 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{a_2a_{12}} t^{a_7}_{i_{10}} t^{a_8a_9a_{12}}_{i_5i_6i_{11}} + \tfrac1{12}P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{a_2a_{12}} t^{a_{12}}_{i_5} t^{a_7a_8a_9}_{i_6i_{10}i_{11}} + \tfrac1{12}P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{a_2a_{12}} t^{a_{12}}_{i_{10}} t^{a_7a_8a_9}_{i_5i_6i_{11}} - \tfrac1{12}P_2P_2\lambda^{i_3i_5i_6i_7}_{a_1a_8a_9a_{10}} v^{i_4i_{11}}_{a_2a_{12}} t^{a_8}_{i_{11}} t^{a_9a_{10}a_{12}}_{i_5i_6i_7} \\
& -\tfrac1{12}P_2P_2\lambda^{i_3i_5i_6i_7}_{a_1a_8a_9a_{10}} v^{i_4i_{11}}_{a_2a_{12}} t^{a_{12}}_{i_5} t^{a_8a_9a_{10}}_{i_6i_7i_{11}} + \tfrac1{12}\lambda^{i_3i_4i_5i_6}_{a_7a_8a_9a_{10}} v^{i_{11}i_{12}}_{a_1a_2} t^{a_7}_{i_{11}} t^{a_8a_9a_{10}}_{i_5i_6i_{12}} + \tfrac12 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{a_{11}a_{12}} t^{a_8a_{11}}_{i_5i_{10}} t^{a_9a_{12}}_{i_6i_7} - \tfrac18 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{a_{11}a_{12}} t^{a_{11}a_{12}}_{i_5i_6} t^{a_8a_9}_{i_7i_{10}} \\
& -\tfrac18\lambda^{i_5i_6i_7i_8}_{a_1a_2a_9a_{10}} v^{i_3i_4}_{a_{11}a_{12}} t^{a_9a_{11}}_{i_5i_6} t^{a_{10}a_{12}}_{i_7i_8} - \tfrac18 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{a_2a_{12}} t^{a_7a_{12}}_{i_5i_6} t^{a_8a_9}_{i_{10}i_{11}} + \tfrac12 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{a_2a_{12}} t^{a_7a_{12}}_{i_5i_{10}} t^{a_8a_9}_{i_6i_{11}} + \tfrac14 P_2P_2\lambda^{i_3i_5i_6i_7}_{a_1a_8a_9a_{10}} v^{i_4i_{11}}_{a_2a_{12}} t^{a_8a_{12}}_{i_5i_6} t^{a_9a_{10}}_{i_7i_{11}} \\
& -\tfrac18\lambda^{i_3i_4i_5i_6}_{a_7a_8a_9a_{10}} v^{i_{11}i_{12}}_{a_1a_2} t^{a_7a_8}_{i_5i_{11}} t^{a_9a_{10}}_{i_6i_{12}} - \tfrac1{16}P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{\alpha_{11}\alpha_{12}} t^{a_8a_9}_{i_5i_{10}} F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_6i_7} - \tfrac14 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{\alpha_{11}a_{12}} t^{a_9a_{12}}_{i_5i_6} F^{\alpha_{11}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_7i_{10}} \\
& -\tfrac14 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{\alpha_{11}a_{12}} t^{a_9a_{12}}_{i_5i_{10}} F^{\alpha_{11}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_6i_7} + \tfrac18\lambda^{i_5i_6i_7i_8}_{a_1a_2a_9a_{10}} v^{i_3i_4}_{\alpha_{11}a_{12}} t^{a_{10}a_{12}}_{i_5i_6} F^{\alpha_{11}a_9}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_7i_8} + \tfrac14 P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{\alpha_{12}a_2} t^{a_8a_9}_{i_5i_{10}} F^{\alpha_{12}a_7}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_6i_{11}} \\
& -\tfrac1{16}P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{\alpha_{12}a_2} t^{a_8a_9}_{i_{10}i_{11}} F^{\alpha_{12}a_7}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_5i_6} + \tfrac18 P_2P_2\lambda^{i_3i_5i_6i_7}_{a_1a_8a_9a_{10}} v^{i_4i_{11}}_{\alpha_{12}a_2} t^{a_9a_{10}}_{i_5i_{11}} F^{\alpha_{12}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_6i_7} - \tfrac1{24}P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{a_{11}a_{12}} t^{a_8a_9a_{11}a_{12}}_{i_5i_6i_7i_{10}} \\
& +\tfrac1{96}\lambda^{i_5i_6i_7i_8}_{a_1a_2a_9a_{10}} v^{i_3i_4}_{a_{11}a_{12}} t^{a_9a_{10}a_{11}a_{12}}_{i_5i_6i_7i_8} - \tfrac1{24}P_2\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9} v^{i_{10}i_{11}}_{a_2a_{12}} t^{a_7a_8a_9a_{12}}_{i_5i_6i_{10}i_{11}} + \tfrac1{36}P_2P_2\lambda^{i_3i_5i_6i_7}_{a_1a_8a_9a_{10}} v^{i_4i_{11}}_{a_2a_{12}} t^{a_8a_9a_{10}a_{12}}_{i_5i_6i_7i_{11}} - \tfrac1{144}P_2\lambda^{i_5i_6i_7i_8}_{a_1a_9a_{10}a_{11}} v^{i_3i_4}_{a_2a_{12}} t^{a_9a_{10}a_{11}a_{12}}_{i_5i_6i_7i_8} \\
& +\tfrac1{96}\lambda^{i_3i_4i_5i_6}_{a_7a_8a_9a_{10}} v^{i_{11}i_{12}}_{a_1a_2} t^{a_7a_8a_9a_{10}}_{i_5i_6i_{11}i_{12}} - \tfrac1{144}P_2\lambda^{i_3i_5i_6i_7}_{a_8a_9a_{10}a_{11}} v^{i_4i_{12}}_{a_1a_2} t^{a_8a_9a_{10}a_{11}}_{i_5i_6i_7i_{12}} + \tfrac18 P_2\lambda^{i_3i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_4i_{10}}_{\alpha_{11}\alpha_{12}} F^{\alpha_{11}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_5i_{10}} F^{\alpha_{12}a_9}_{i_{15}i_{16}} t^{i_{15}i_{16}}_{i_6i_7} \\
& -\tfrac1{32}\lambda^{i_5i_6i_7i_8}_{a_1a_2a_9a_{10}} v^{i_3i_4}_{\alpha_{11}\alpha_{12}} F^{\alpha_{11}a_9}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_5i_6} F^{\alpha_{12}a_{10}}_{i_{15}i_{16}} t^{i_{15}i_{16}}_{i_7i_8}
\end{aligned}
$$

TABLE ESI.2.XXI: The Λ_3 amplitude equation of Λ-CCSDTQ-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_4i_5i_6}_{a_1a_2a_3} = {} & \Lambda\text{-CCSDT-R12} - \tfrac12 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} f^{i_6}_{a_{10}} t^{a_9a_{10}}_{i_7i_8} - \tfrac12 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} f^{i_{10}}_{a_3} t^{a_8a_9}_{i_7i_{10}} + \tfrac14 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} f^{i_6}_{\alpha_{10}} F^{\alpha_{10}a_9}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_7i_8} + \tfrac12 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6a_9}_{i_7i_8} + \tfrac12 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{a_8a_9}_{i_7a_3} \\
& -\tfrac12 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{i_7i_8} t^{a_9}_{i_{10}} - P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6a_9}_{i_8a_{10}} t^{a_{10}}_{i_7} - P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}a_9}_{i_7a_3} t^{a_8}_{i_{10}} - \tfrac12 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{a_8a_9}_{a_3a_{10}} t^{a_{10}}_{i_7} + P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{i_8a_{11}} t^{a_{11}}_{i_7} t^{a_9}_{i_{10}} \\
& +\tfrac12 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6a_9}_{a_{10}a_{11}} t^{a_{10}}_{i_7} t^{a_{11}}_{i_8} + \tfrac12 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}i_{11}}_{i_7a_3} t^{a_8}_{i_{10}} t^{a_9}_{i_{11}} + P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}a_9}_{a_3a_{11}} t^{a_{11}}_{i_7} t^{a_8}_{i_{10}} - P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{i_8a_{11}} t^{a_9a_{11}}_{i_7i_{10}} + \tfrac14 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6a_9}_{a_{10}a_{11}} t^{a_{10}a_{11}}_{i_7i_8} \\
& +\tfrac12 P_3\lambda^{i_4i_7i_8i_9}_{a_1a_2a_3a_{10}} v^{i_5i_6}_{i_9a_{11}} t^{a_{10}a_{11}}_{i_7i_8} + \tfrac14 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}i_{11}}_{i_7a_3} t^{a_8a_9}_{i_{10}i_{11}} - P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}a_9}_{a_3a_{11}} t^{a_8a_{11}}_{i_7i_{10}} - \tfrac12 P_3P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_9a_{10}} v^{i_6i_{11}}_{i_8a_3} t^{a_9a_{10}}_{i_7i_{11}} - \tfrac12 P_3P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_9a_{10}} v^{i_6a_{10}}_{a_3a_{11}} t^{a_9a_{11}}_{i_7i_8} \\
& +\tfrac12 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_8a_9a_{10}} v^{i_{11}a_{10}}_{a_2a_3} t^{a_8a_9}_{i_7i_{11}} + \tfrac12 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{i_8\alpha_{11}} F^{\alpha_{11}a_9}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_7i_{10}} + \tfrac18 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6a_9}_{\alpha_{10}\alpha_{11}} F^{\alpha_{10}\alpha_{11}}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_7i_8} - \tfrac14 P_3\lambda^{i_4i_7i_8i_9}_{a_1a_2a_3a_{10}} v^{i_5i_6}_{i_9\alpha_{11}} F^{\alpha_{11}a_{10}}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_7i_8} \\
& -\tfrac12 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}a_9}_{\alpha_{11}a_3} F^{\alpha_{11}a_8}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_7i_{10}} - \tfrac14 P_3P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_9a_{10}} v^{i_6a_{10}}_{\alpha_{11}a_3} F^{\alpha_{11}a_9}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_7i_8} - \tfrac12 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{a_{11}a_{12}} t^{a_{11}}_{i_7} t^{a_{12}}_{i_8} t^{a_9}_{i_{10}} - \tfrac12 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}i_{11}}_{a_3a_{12}} t^{a_{12}}_{i_7} t^{a_8}_{i_{10}} t^{a_9}_{i_{11}} \\
& -\tfrac14 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{a_{11}a_{12}} t^{a_9}_{i_{10}} t^{a_{11}a_{12}}_{i_7i_8} + P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{a_{11}a_{12}} t^{a_{11}}_{i_7} t^{a_9a_{12}}_{i_8i_{10}} + \tfrac12 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{a_{11}a_{12}} t^{a_{11}}_{i_{10}} t^{a_9a_{12}}_{i_7i_8} + \tfrac12 P_3\lambda^{i_4i_7i_8i_9}_{a_1a_2a_3a_{10}} v^{i_5i_6}_{a_{11}a_{12}} t^{a_{11}}_{i_7} t^{a_{10}a_{12}}_{i_8i_9} \\
& +P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}i_{11}}_{a_3a_{12}} t^{a_8}_{i_{10}} t^{a_9a_{12}}_{i_7i_{11}} - \tfrac14 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}i_{11}}_{a_3a_{12}} t^{a_{12}}_{i_7} t^{a_8a_9}_{i_{10}i_{11}} + \tfrac12 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}i_{11}}_{a_3a_{12}} t^{a_{12}}_{i_{10}} t^{a_8a_9}_{i_7i_{11}} - \tfrac12 P_3P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_9a_{10}} v^{i_6i_{11}}_{a_3a_{12}} t^{a_9}_{i_{11}} t^{a_{10}a_{12}}_{i_7i_8} \\
& -\tfrac12 P_3P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_9a_{10}} v^{i_6i_{11}}_{a_3a_{12}} t^{a_{12}}_{i_7} t^{a_9a_{10}}_{i_8i_{11}} + \tfrac12 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_8a_9a_{10}} v^{i_{11}i_{12}}_{a_2a_3} t^{a_8}_{i_{11}} t^{a_9a_{10}}_{i_7i_{12}} - \tfrac18 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{\alpha_{11}\alpha_{12}} t^{a_9}_{i_{10}} F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_7i_8} - \tfrac12 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{\alpha_{11}a_{12}} t^{a_{12}}_{i_8} F^{\alpha_{11}a_9}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_7i_{10}} \\
& +\tfrac14 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{\alpha_{11}a_{12}} t^{a_{12}}_{i_{10}} F^{\alpha_{11}a_9}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_7i_8} + \tfrac14 P_3\lambda^{i_4i_7i_8i_9}_{a_1a_2a_3a_{10}} v^{i_5i_6}_{\alpha_{11}a_{12}} t^{a_{12}}_{i_9} F^{\alpha_{11}a_{10}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_7i_8} + \tfrac12 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}i_{11}}_{\alpha_{12}a_3} t^{a_9}_{i_{11}} F^{\alpha_{12}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_7i_{10}} \\
& +\tfrac14 P_3P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_9a_{10}} v^{i_6i_{11}}_{\alpha_{12}a_3} t^{a_{10}}_{i_{11}} F^{\alpha_{12}a_9}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_7i_8} - \tfrac14 P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_3a_9} v^{i_6i_{10}}_{a_{11}a_{12}} t^{a_9a_{11}a_{12}}_{i_7i_8i_{10}} - \tfrac1{12}P_3\lambda^{i_4i_7i_8i_9}_{a_1a_2a_3a_{10}} v^{i_5i_6}_{a_{11}a_{12}} t^{a_{10}a_{11}a_{12}}_{i_7i_8i_9} - \tfrac14 P_3\lambda^{i_4i_5i_6i_7}_{a_1a_2a_8a_9} v^{i_{10}i_{11}}_{a_3a_{12}} t^{a_8a_9a_{12}}_{i_7i_{10}i_{11}} \\
& -\tfrac14 P_3P_3\lambda^{i_4i_5i_7i_8}_{a_1a_2a_9a_{10}} v^{i_6i_{11}}_{a_3a_{12}} t^{a_9a_{10}a_{12}}_{i_7i_8i_{11}} - \tfrac1{12}P_3P_3\lambda^{i_4i_7i_8i_9}_{a_1a_2a_{10}a_{11}} v^{i_5i_6}_{a_3a_{12}} t^{a_{10}a_{11}a_{12}}_{i_7i_8i_9} - \tfrac1{12}P_3\lambda^{i_4i_5i_6i_7}_{a_1a_8a_9a_{10}} v^{i_{11}i_{12}}_{a_2a_3} t^{a_8a_9a_{10}}_{i_7i_{11}i_{12}} - \tfrac1{12}P_3P_3\lambda^{i_4i_5i_7i_8}_{a_1a_9a_{10}a_{11}} v^{i_6i_{12}}_{a_2a_3} t^{a_9a_{10}a_{11}}_{i_7i_8i_{12}}
\end{aligned}
$$

TABLE ESI.2.XXII: The Λ_4 amplitude equation of Λ-CCSDTQ-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_5i_6i_7i_8}_{a_1a_2a_3a_4} = {} & +P_4P_4\lambda^{i_5i_6}_{a_1a_2} v^{i_7i_8}_{a_3a_4} + P_4P_4\lambda^{i_5i_6i_7}_{a_1a_2a_3} f^{i_8}_{a_4} - P_4P_4\lambda^{i_5i_6i_9}_{a_1a_2a_3} v^{i_7i_8}_{i_9a_4} - P_4P_4\lambda^{i_5i_6i_7}_{a_1a_2a_9} v^{i_8a_9}_{a_3a_4} + P_4P_4\lambda^{i_5i_6i_7}_{a_1a_2a_3} v^{i_8i_9}_{a_4a_{10}} t^{a_{10}}_{i_9} + P_4P_4\lambda^{i_5i_6i_9}_{a_1a_2a_3} v^{i_7i_8}_{a_4a_{10}} t^{a_{10}}_{i_9} \\
& +P_4P_4\lambda^{i_5i_6i_7}_{a_1a_2a_9} v^{i_8i_{10}}_{a_3a_4} t^{a_9}_{i_{10}} - P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_4} f^{i_8}_{i_9} + P_4\lambda^{i_5i_6i_7i_8}_{a_1a_2a_3a_9} f^{a_9}_{a_4} - P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_4} f^{i_8}_{a_{10}} t^{a_{10}}_{i_9} - P_4\lambda^{i_5i_6i_7i_8}_{a_1a_2a_3a_9} f^{i_{10}}_{a_4} t^{a_9}_{i_{10}} + \tfrac12 P_4\lambda^{i_5i_6i_9i_{10}}_{a_1a_2a_3a_4} v^{i_7i_8}_{i_9i_{10}} \\
& -P_4P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_{10}} v^{i_8a_{10}}_{i_9a_4} + \tfrac12 P_4\lambda^{i_5i_6i_7i_8}_{a_1a_2a_9a_{10}} v^{a_9a_{10}}_{a_3a_4} - P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_4} v^{i_8i_{10}}_{i_9a_{11}} t^{a_{11}}_{i_{10}} - P_4\lambda^{i_5i_6i_9i_{10}}_{a_1a_2a_3a_4} v^{i_7i_8}_{i_{10}a_{11}} t^{a_{11}}_{i_9} - P_4\lambda^{i_5i_6i_7i_8}_{a_1a_2a_3a_9} v^{i_{10}a_9}_{a_4a_{11}} t^{a_{11}}_{i_{10}} + P_4P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_{10}} v^{i_8i_{11}}_{i_9a_4} t^{a_{10}}_{i_{11}} \\
& +P_4P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_{10}} v^{i_8a_{10}}_{a_4a_{11}} t^{a_{11}}_{i_9} - P_4\lambda^{i_5i_6i_7i_8}_{a_1a_2a_9a_{10}} v^{i_{11}a_{10}}_{a_3a_4} t^{a_9}_{i_{11}} + P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_4} v^{i_8i_{10}}_{a_{11}a_{12}} t^{a_{11}}_{i_{10}} t^{a_{12}}_{i_9} + \tfrac12 P_4\lambda^{i_5i_6i_9i_{10}}_{a_1a_2a_3a_4} v^{i_7i_8}_{a_{11}a_{12}} t^{a_{11}}_{i_9} t^{a_{12}}_{i_{10}} + P_4\lambda^{i_5i_6i_7i_8}_{a_1a_2a_3a_9} v^{i_{10}i_{11}}_{a_4a_{12}} t^{a_{12}}_{i_{10}} t^{a_9}_{i_{11}} \\
& -P_4P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_{10}} v^{i_8i_{11}}_{a_4a_{12}} t^{a_{12}}_{i_9} t^{a_{10}}_{i_{11}} + \tfrac12 P_4\lambda^{i_5i_6i_7i_8}_{a_1a_2a_9a_{10}} v^{i_{11}i_{12}}_{a_3a_4} t^{a_9}_{i_{11}} t^{a_{10}}_{i_{12}} - \tfrac12 P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_4} v^{i_8i_{10}}_{a_{11}a_{12}} t^{a_{11}a_{12}}_{i_9i_{10}} + \tfrac14 P_4\lambda^{i_5i_6i_9i_{10}}_{a_1a_2a_3a_4} v^{i_7i_8}_{a_{11}a_{12}} t^{a_{11}a_{12}}_{i_9i_{10}} - \tfrac12 P_4\lambda^{i_5i_6i_7i_8}_{a_1a_2a_3a_9} v^{i_{10}i_{11}}_{a_4a_{12}} t^{a_9a_{12}}_{i_{10}i_{11}} \\
& +P_4P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_{10}} v^{i_8i_{11}}_{a_4a_{12}} t^{a_{10}a_{12}}_{i_9i_{11}} - \tfrac12 P_4P_4\lambda^{i_5i_6i_9i_{10}}_{a_1a_2a_3a_{11}} v^{i_7i_8}_{a_4a_{12}} t^{a_{11}a_{12}}_{i_9i_{10}} + \tfrac14 P_4\lambda^{i_5i_6i_7i_8}_{a_1a_2a_9a_{10}} v^{i_{11}i_{12}}_{a_3a_4} t^{a_9a_{10}}_{i_{11}i_{12}} - \tfrac12 P_4P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_{10}a_{11}} v^{i_8i_{12}}_{a_3a_4} t^{a_{10}a_{11}}_{i_9i_{12}} \\
& -\tfrac14 P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_4} v^{i_8i_{10}}_{\alpha_{11}\alpha_{12}} F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_9i_{10}} + \tfrac18 P_4\lambda^{i_5i_6i_9i_{10}}_{a_1a_2a_3a_4} v^{i_7i_8}_{\alpha_{11}\alpha_{12}} F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_9i_{10}} - \tfrac14 P_4\lambda^{i_5i_6i_7i_8}_{a_1a_2a_3a_9} v^{i_{10}i_{11}}_{\alpha_{12}a_4} F^{\alpha_{12}a_9}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_{10}i_{11}} + \tfrac12 P_4P_4\lambda^{i_5i_6i_7i_9}_{a_1a_2a_3a_{10}} v^{i_8i_{11}}_{\alpha_{12}a_4} F^{\alpha_{12}a_{10}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_9i_{11}} \\
& -\tfrac14 P_4P_4\lambda^{i_5i_6i_9i_{10}}_{a_1a_2a_3a_{11}} v^{i_7i_8}_{\alpha_{12}a_4} F^{\alpha_{12}a_{11}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_9i_{10}}
\end{aligned}
$$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.2.XXIII: The geminal λ amplitude equation of Λ-CCSDTQ-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_3 i_4}_{i_1 i_2} = \Lambda\text{-CCSDT-R12} &- \tfrac{1}{12}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} f^{i_{11}}_{\alpha_{12}} F^{\alpha_{12} a_{10}}_{i_1 i_2} t^{a_7 a_8 a_9}_{i_5 i_6 i_{11}} - \tfrac{1}{2}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} a_9}_{i_6 \alpha_{12}} F^{\alpha_{12} a_{10}}_{i_1 i_2} t^{a_7 a_8}_{i_5 i_{11}} - \tfrac{1}{4}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{a_8 a_9}_{\alpha_{11} a_{12}} F^{\alpha_{11} a_{10}}_{i_1 i_2} t^{a_7 a_{12}}_{i_5 i_6} \\
&- \tfrac{1}{8}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{a_9 a_{10}}_{\alpha_{11} \alpha_{12}} F^{\alpha_{11} a_7}_{i_1 i_2} F^{\alpha_{12} a_8}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_5 i_6} - \tfrac{1}{2}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{i_6 \alpha_{13}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_7}_{i_{11}} t^{a_8 a_9}_{i_5 i_{12}} - \tfrac{1}{2}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} a_9}_{\alpha_{12} a_{13}} F^{\alpha_{12} a_{10}}_{i_1 i_2} t^{a_7 a_{13}}_{i_{11} i_5 i_6} - \tfrac{1}{2}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} a_9}_{\alpha_{12} a_{13}} F^{\alpha_{12} a_{10}}_{i_1 i_2} t^{a_{13} a_7 a_8}_{i_5 i_6 i_{11}} \\
&+ \tfrac{1}{4}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} a_8}_{\alpha_{12} \alpha_{13}} F^{\alpha_{12} a_9}_{i_1 i_2} t^{a_7}_{i_{11}} F^{\alpha_{13} a_{10}}_{i_{14} i_{15}} t^{i_{14} i_{15}}_{i_5 i_6} + \tfrac{1}{12}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{i_6 \alpha_{13}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_7 a_8 a_9}_{i_5 i_{11} i_{12}} - \tfrac{1}{4}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} a_9}_{\alpha_{12} a_{13}} F^{\alpha_{12} a_{10}}_{i_1 i_2} t^{a_7 a_8 a_{13}}_{i_5 i_6 i_{11}} \\
&+ \tfrac{1}{12} P_2 \lambda^{i_3 i_5 i_6 i_7}_{a_8 a_9 a_{10} a_{11}} v^{i_4 i_{12}}_{i_7 \alpha_{13}} F^{\alpha_{13} a_{11}}_{i_1 i_2} t^{a_8 a_9 a_{10}}_{i_5 i_6 i_{12}} + \tfrac{1}{12} P_2 \lambda^{i_3 i_5 i_6 i_7}_{a_8 a_9 a_{10} a_{11}} v^{i_4 a_{10}}_{\alpha_{12} a_{13}} F^{\alpha_{12} a_{11}}_{i_1 i_2} t^{a_8 a_9 a_{13}}_{i_5 i_6 i_7} - \tfrac{1}{24}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} a_{10}}_{\alpha_{12} \alpha_{13}} F^{\alpha_{12} \alpha_{13}}_{i_1 i_2} t^{a_7 a_8 a_9}_{i_5 i_6 i_{11}} \\
&- \tfrac{1}{4}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_7}_{i_{11}} t^{a_8}_{i_{12}} t^{a_9 a_{14}}_{i_5 i_6} - \tfrac{1}{2}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_{14}}_{i_5} t^{a_7}_{i_{11}} t^{a_8 a_9}_{i_6 i_{12}} + \tfrac{1}{8}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_7}_{i_1 i_2} t^{a_8}_{i_{11}} t^{a_{10}}_{i_{12}} F^{\alpha_{14} a_9}_{i_{15} i_{16}} t^{i_{15} i_{16}}_{i_5 i_6} \\
&- \tfrac{1}{4}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_7}_{i_{11}} t^{a_8 a_9 a_{14}}_{i_5 i_6 i_{12}} + \tfrac{1}{12}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_{14}}_{i_5} t^{a_7 a_8 a_9}_{i_6 i_{11} i_{12}} + \tfrac{1}{12}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_{14}}_{i_{11}} t^{a_7 a_8 a_9}_{i_5 i_6 i_{12}} \\
&- \tfrac{1}{12} P_2 \lambda^{i_3 i_5 i_6 i_7}_{a_8 a_9 a_{10} a_{11}} v^{i_4 i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{11}}_{i_1 i_2} t^{a_8}_{i_{12}} t^{a_9 a_{10} a_{14}}_{i_5 i_6 i_7} - \tfrac{1}{12} P_2 \lambda^{i_3 i_5 i_6 i_7}_{a_8 a_9 a_{10} a_{11}} v^{i_4 i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{11}}_{i_1 i_2} t^{a_{14}}_{i_5} t^{a_8 a_9 a_{10}}_{i_6 i_7 i_{12}} + \tfrac{1}{24}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} \alpha_{14}} F^{\alpha_{13} \alpha_{14}}_{i_1 i_2} t^{a_7}_{i_{11}} t^{a_8 a_9 a_{10}}_{i_5 i_6 i_{12}} \\
&- \tfrac{1}{8}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_7 a_{14}}_{i_5 i_6} t^{a_8 a_9}_{i_{11} i_{12}} + \tfrac{1}{2}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_7 a_{14}}_{i_5 i_{11}} t^{a_8 a_9}_{i_6 i_{12}} + \tfrac{1}{4} P_2 \lambda^{i_3 i_5 i_6 i_7}_{a_8 a_9 a_{10} a_{11}} v^{i_4 i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{11}}_{i_1 i_2} t^{a_8 a_{14}}_{i_5 i_6} t^{a_9 a_{10}}_{i_7 i_{12}} \\
&- \tfrac{1}{16}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{14}}_{i_1 i_2} t^{a_7 a_8}_{i_5 i_{11}} t^{a_9 a_{10}}_{i_6 i_{12}} + \tfrac{1}{4}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_9}_{i_1 i_2} t^{a_7 a_8}_{i_5 i_{11}} F^{\alpha_{14} a_{10}}_{i_{15} i_{16}} t^{i_{15} i_{16}}_{i_6 i_{12}} - \tfrac{1}{16}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} \alpha_{14}} F^{\alpha_{13} a_9}_{i_1 i_2} t^{a_7 a_8}_{i_{11} i_{12}} F^{\alpha_{14} a_{10}}_{i_{15} i_{16}} t^{i_{15} i_{16}}_{i_5 i_6} \\
&+ \tfrac{1}{8} P_2 \lambda^{i_3 i_5 i_6 i_7}_{a_8 a_9 a_{10} a_{11}} v^{i_4 i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_8 a_9}_{i_5 i_{12}} F^{\alpha_{14} a_{11}}_{i_{15} i_{16}} t^{i_{15} i_{16}}_{i_6 i_7} - \tfrac{1}{24}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{10}}_{i_1 i_2} t^{a_7 a_8 a_9 a_{14}}_{i_5 i_6 i_{11} i_{12}} + \tfrac{1}{36} P_2 \lambda^{i_3 i_5 i_6 i_7}_{a_8 a_9 a_{10} a_{11}} v^{i_4 i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{11}}_{i_1 i_2} t^{a_8 a_9 a_{10} a_{14}}_{i_5 i_6 i_7 i_{12}} \\
&- \tfrac{1}{144}\lambda^{i_5 i_6 i_7 i_8}_{a_9 a_{10} a_{11} a_{12}} v^{i_3 i_4}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{12}}_{i_1 i_2} t^{a_9 a_{10} a_{11} a_{14}}_{i_5 i_6 i_7 i_8} + \tfrac{1}{192}\lambda^{i_3 i_4 i_5 i_6}_{a_7 a_8 a_9 a_{10}} v^{i_{11} i_{12}}_{\alpha_{13} \alpha_{14}} F^{\alpha_{13} \alpha_{14}}_{i_1 i_2} t^{a_7 a_8 a_9 a_{10}}_{i_5 i_6 i_{11} i_{12}} - \tfrac{1}{288} P_2 \lambda^{i_3 i_5 i_6 i_7}_{a_8 a_9 a_{10} a_{11}} v^{i_4 i_{12}}_{\alpha_{13} a_{14}} F^{\alpha_{13} a_{14}}_{i_1 i_2} t^{a_8 a_9 a_{10} a_{11}}_{i_5 i_6 i_7 i_{12}}
\end{aligned}
$$

G. EOM-CCSD-R12

TABLE ESI.2.XXIV: The R_1 amplitude equation of EOM-CCSD-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{a_2}_{i_1} = & -f^{i_3}_{i_1} r^{a_2}_{i_3} + f^{a_2}_{a_3} r^{a_3}_{i_1} - f^{i_3}_{a_4} r^{a_2}_{i_3} t^{a_4}_{i_1} - f^{i_3}_{a_4} r^{a_4}_{i_1} t^{a_2}_{i_3} + f^{i_3}_{a_4} r^{a_2 a_4}_{i_1 i_3} - \tfrac{1}{2} f^{i_3}_{\alpha_4} F^{\alpha_4 a_2}_{i_5 i_6} r^{i_5 i_6}_{i_1 i_3} - v^{i_3 a_2}_{i_1 a_4} r^{a_4}_{i_3} - v^{i_3 i_4}_{i_1 a_5} r^{a_2}_{i_3} t^{a_5}_{i_4} - v^{i_3 a_2}_{a_4 a_5} r^{a_4}_{i_1} t^{a_5}_{i_3} + v^{i_3 i_4}_{i_1 a_5} r^{a_5}_{i_3} t^{a_2}_{i_4} + v^{i_3 a_2}_{a_4 a_5} r^{a_4}_{i_3} t^{a_5}_{i_1} \\
& + v^{i_3 i_4}_{a_5 a_6} r^{a_2}_{i_3} t^{a_5}_{i_4} t^{a_6}_{i_1} + v^{i_3 i_4}_{a_5 a_6} r^{a_5}_{i_1} t^{a_6}_{i_3} t^{a_2}_{i_4} - v^{i_3 i_4}_{a_5 a_6} r^{a_5}_{i_3} t^{a_6}_{i_1} t^{a_2}_{i_4} - \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} r^{a_2}_{i_3} t^{a_5 a_6}_{i_1 i_4} - \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} r^{a_5}_{i_1} t^{a_2 a_6}_{i_3 i_4} + v^{i_3 i_4}_{a_5 a_6} r^{a_5}_{i_3} t^{a_2 a_6}_{i_1 i_4} + \tfrac{1}{4} v^{i_3 i_4}_{\alpha_5 \alpha_6} r^{a_2}_{i_4} F^{\alpha_5 \alpha_6}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_3} - \tfrac{1}{4} v^{i_3 i_4}_{\alpha_5 a_6} r^{a_6}_{i_1} F^{\alpha_5 a_2}_{i_7 i_8} t^{i_7 i_8}_{i_3 i_4} \\
& - \tfrac{1}{2} v^{i_3 i_4}_{\alpha_5 a_6} r^{a_6}_{i_4} F^{\alpha_5 a_2}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_3} - \tfrac{1}{2} v^{i_3 i_4}_{i_1 a_5} r^{a_2 a_5}_{i_3 i_4} - \tfrac{1}{2} v^{i_3 a_2}_{a_4 a_5} r^{a_4 a_5}_{i_1 i_3} + \tfrac{1}{4} v^{i_3 i_4}_{i_1 \alpha_5} F^{\alpha_5 a_2}_{i_6 i_7} r^{i_6 i_7}_{i_3 i_4} - \tfrac{1}{4} v^{i_3 a_2}_{\alpha_4 \alpha_5} F^{\alpha_4 \alpha_5}_{i_6 i_7} r^{i_6 i_7}_{i_1 i_3} + v^{i_3 i_4}_{a_5 a_6} r^{a_2 a_5}_{i_1 i_3} t^{a_6}_{i_4} + \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} r^{a_2 a_5}_{i_3 i_4} t^{a_6}_{i_1} + \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} r^{a_5 a_6}_{i_1 i_3} t^{a_2}_{i_4} \\
& - \tfrac{1}{2} v^{i_3 i_4}_{\alpha_5 a_6} F^{\alpha_5 a_2}_{i_7 i_8} r^{i_7 i_8}_{i_1 i_3} t^{a_6}_{i_4} - \tfrac{1}{4} v^{i_3 i_4}_{\alpha_5 a_6} F^{\alpha_5 a_2}_{i_7 i_8} r^{i_7 i_8}_{i_3 i_4} t^{a_6}_{i_1} + \tfrac{1}{4} v^{i_3 i_4}_{\alpha_5 \alpha_6} F^{\alpha_5 \alpha_6}_{i_7 i_8} r^{i_7 i_8}_{i_1 i_3} t^{a_2}_{i_4}
\end{aligned}
$$

TABLE ESI.2.XXV: The R_2 amplitude equation of EOM-CCSD-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{a_3 a_4}_{i_1 i_2} = & +P_2 f^{i_5}_{a_6} r^{a_3}_{i_5} t^{a_4 a_6}_{i_1 i_2} + P_2 f^{i_5}_{a_6} r^{a_6}_{i_1} t^{a_3 a_4}_{i_2 i_5} - \tfrac{1}{2} P_2 f^{i_5}_{\alpha_6} r^{a_3}_{i_5} F^{\alpha_6 a_4}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_2} + P_2 f^{i_5}_{i_1} r^{a_3 a_4}_{i_2 i_5} - P_2 f^{a_3}_{a_5} r^{a_4 a_5}_{i_1 i_2} + \tfrac{1}{2} P_2 f^{a_3}_{\alpha_5} F^{\alpha_5 a_4}_{i_6 i_7} r^{i_6 i_7}_{i_1 i_2} - P_2 f^{i_5}_{a_6} r^{a_3 a_4}_{i_1 i_5} t^{a_6}_{i_2} - P_2 f^{i_5}_{a_6} r^{a_3 a_6}_{i_1 i_2} t^{a_4}_{i_5} \\
& + \tfrac{1}{2} P_2 f^{i_5}_{\alpha_6} F^{\alpha_6 a_3}_{i_7 i_8} r^{i_7 i_8}_{i_1 i_2} t^{a_4}_{i_5} + P_2 v^{i_5 a_3}_{i_1 i_2} r^{a_4}_{i_5} + P_2 v^{a_3 a_4}_{i_1 a_5} r^{a_5}_{i_2} + P_2 v^{i_5 i_6}_{i_1 i_2} r^{a_3}_{i_5} t^{a_4}_{i_6} + P_2 P_2 v^{i_5 a_3}_{i_1 a_6} r^{a_4}_{i_5} t^{a_6}_{i_2} + P_2 P_2 v^{i_5 a_3}_{i_1 a_6} r^{a_6}_{i_2} t^{a_4}_{i_5} + P_2 v^{a_3 a_4}_{a_5 a_6} r^{a_5}_{i_1} t^{a_6}_{i_2} + P_2 P_2 v^{i_5 i_6}_{i_1 a_7} r^{a_3}_{i_5} t^{a_7}_{i_2} t^{a_4}_{i_6} \\
& + \tfrac{1}{2} P_2 P_2 v^{i_5 a_3}_{a_6 a_7} r^{a_4}_{i_5} t^{a_6}_{i_1} t^{a_7}_{i_2} + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{i_1 a_7} r^{a_7}_{i_2} t^{a_3}_{i_5} t^{a_4}_{i_6} + P_2 P_2 v^{i_5 a_3}_{a_6 a_7} r^{a_6}_{i_1} t^{a_7}_{i_2} t^{a_4}_{i_5} - P_2 P_2 v^{i_5 i_6}_{i_1 a_7} r^{a_3}_{i_5} t^{a_4 a_7}_{i_2 i_6} + \tfrac{1}{2} P_2 v^{i_5 a_3}_{a_6 a_7} r^{a_4}_{i_5} t^{a_6 a_7}_{i_1 i_2} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{i_1 a_7} r^{a_7}_{i_2} t^{a_3 a_4}_{i_5 i_6} \\
& - P_2 P_2 v^{i_5 a_3}_{a_6 a_7} r^{a_6}_{i_1} t^{a_4 a_7}_{i_2 i_5} - P_2 v^{i_5 i_6}_{i_1 a_7} r^{a_7}_{i_5} t^{a_3 a_4}_{i_2 i_6} - P_2 v^{i_5 a_3}_{a_6 a_7} r^{a_6}_{i_5} t^{a_4 a_7}_{i_1 i_2} - \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{i_1 \alpha_7} r^{a_3}_{i_6} F^{\alpha_7 a_4}_{i_8 i_9} t^{i_8 i_9}_{i_2 i_5} + \tfrac{1}{4} P_2 v^{i_5 a_3}_{\alpha_6 \alpha_7} r^{a_4}_{i_5} F^{\alpha_6 \alpha_7}_{i_8 i_9} t^{i_8 i_9}_{i_1 i_2} - \tfrac{1}{2} P_2 P_2 v^{i_5 a_3}_{\alpha_6 a_7} r^{a_7}_{i_1} F^{\alpha_6 a_4}_{i_8 i_9} t^{i_8 i_9}_{i_2 i_5} \\
& - \tfrac{1}{2} P_2 v^{i_5 a_3}_{\alpha_6 a_7} r^{a_7}_{i_5} F^{\alpha_6 a_4}_{i_8 i_9} t^{i_8 i_9}_{i_1 i_2} + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3}_{i_5} t^{a_7}_{i_1} t^{a_8}_{i_2} t^{a_4}_{i_6} + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_7}_{i_1} t^{a_8}_{i_2} t^{a_3}_{i_5} t^{a_4}_{i_6} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3}_{i_5} t^{a_4}_{i_6} t^{a_7 a_8}_{i_1 i_2} - P_2 P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3}_{i_5} t^{a_7}_{i_1} t^{a_4 a_8}_{i_2 i_6} - P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3}_{i_5} t^{a_7}_{i_6} t^{a_4 a_8}_{i_1 i_2} \\
& - P_2 P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_7}_{i_1} t^{a_3}_{i_5} t^{a_4 a_8}_{i_2 i_6} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_7}_{i_1} t^{a_8}_{i_2} t^{a_3 a_4}_{i_5 i_6} - P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_7}_{i_1} t^{a_8}_{i_5} t^{a_3 a_4}_{i_2 i_6} + P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_7}_{i_5} t^{a_3}_{i_6} t^{a_4 a_8}_{i_1 i_2} + P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_7}_{i_5} t^{a_8}_{i_1} t^{a_3 a_4}_{i_2 i_6} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{\alpha_7 \alpha_8} r^{a_3}_{i_5} t^{a_4}_{i_6} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} \\
& + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{\alpha_7 a_8} r^{a_3}_{i_6} t^{a_8}_{i_1} F^{\alpha_7 a_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_2 i_5} - \tfrac{1}{2} P_2 v^{i_5 i_6}_{\alpha_7 a_8} r^{a_3}_{i_5} t^{a_8}_{i_6} F^{\alpha_7 a_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{\alpha_7 a_8} r^{a_8}_{i_1} t^{a_3}_{i_6} F^{\alpha_7 a_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_2 i_5} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{\alpha_7 a_8} r^{a_8}_{i_5} t^{a_3}_{i_6} F^{\alpha_7 a_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} + \tfrac{1}{2} v^{i_5 i_6}_{i_1 i_2} r^{a_3 a_4}_{i_5 i_6} \\
& - P_2 P_2 v^{i_5 a_3}_{i_1 a_6} r^{a_4 a_6}_{i_2 i_5} + \tfrac{1}{2} v^{a_3 a_4}_{a_5 a_6} r^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{2} P_2 P_2 v^{i_5 a_3}_{i_1 \alpha_6} F^{\alpha_6 a_4}_{i_7 i_8} r^{i_7 i_8}_{i_2 i_5} + \tfrac{1}{4} v^{a_3 a_4}_{\alpha_5 \alpha_6} F^{\alpha_5 \alpha_6}_{i_7 i_8} r^{i_7 i_8}_{i_1 i_2} + P_2 v^{i_5 i_6}_{i_1 a_7} r^{a_3 a_4}_{i_2 i_5} t^{a_7}_{i_6} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{i_1 a_7} r^{a_3 a_4}_{i_5 i_6} t^{a_7}_{i_2} + P_2 v^{i_5 a_3}_{a_6 a_7} r^{a_4 a_6}_{i_1 i_2} t^{a_7}_{i_5} \\
& - P_2 P_2 v^{i_5 i_6}_{i_1 a_7} r^{a_3 a_7}_{i_2 i_5} t^{a_4}_{i_6} - P_2 P_2 v^{i_5 a_3}_{a_6 a_7} r^{a_4 a_6}_{i_1 i_5} t^{a_7}_{i_2} + \tfrac{1}{2} P_2 v^{i_5 a_3}_{a_6 a_7} r^{a_6 a_7}_{i_1 i_2} t^{a_4}_{i_5} - \tfrac{1}{2} P_2 v^{i_5 a_3}_{\alpha_6 a_7} F^{\alpha_6 a_4}_{i_8 i_9} r^{i_8 i_9}_{i_1 i_2} t^{a_7}_{i_5} + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{i_1 \alpha_7} F^{\alpha_7 a_3}_{i_8 i_9} r^{i_8 i_9}_{i_2 i_5} t^{a_4}_{i_6} + \tfrac{1}{2} P_2 P_2 v^{i_5 a_3}_{\alpha_6 a_7} F^{\alpha_6 a_4}_{i_8 i_9} r^{i_8 i_9}_{i_1 i_5} t^{a_7}_{i_2} \\
& + \tfrac{1}{4} P_2 v^{i_5 a_3}_{\alpha_6 \alpha_7} F^{\alpha_6 \alpha_7}_{i_8 i_9} r^{i_8 i_9}_{i_1 i_2} t^{a_4}_{i_5} + P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3 a_4}_{i_1 i_5} t^{a_7}_{i_6} t^{a_8}_{i_2} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3 a_4}_{i_5 i_6} t^{a_7}_{i_1} t^{a_8}_{i_2} + P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3 a_7}_{i_1 i_2} t^{a_8}_{i_5} t^{a_4}_{i_6} - P_2 P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3 a_7}_{i_1 i_5} t^{a_8}_{i_2} t^{a_4}_{i_6} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_7 a_8}_{i_1 i_2} t^{a_3}_{i_5} t^{a_4}_{i_6} \\
& - \tfrac{1}{2} P_2 v^{i_5 i_6}_{\alpha_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_2} t^{a_8}_{i_5} t^{a_4}_{i_6} + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{\alpha_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_5} t^{a_8}_{i_2} t^{a_4}_{i_6} + \tfrac{1}{8} P_2 v^{i_5 i_6}_{\alpha_7 \alpha_8} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_2} t^{a_3}_{i_5} t^{a_4}_{i_6} - \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3 a_4}_{i_1 i_5} t^{a_7 a_8}_{i_2 i_6} + \tfrac{1}{4} v^{i_5 i_6}_{a_7 a_8} r^{a_3 a_4}_{i_5 i_6} t^{a_7 a_8}_{i_1 i_2} \\
& - \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3 a_7}_{i_1 i_2} t^{a_4 a_8}_{i_5 i_6} + P_2 P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3 a_7}_{i_1 i_5} t^{a_4 a_8}_{i_2 i_6} - \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_3 a_7}_{i_5 i_6} t^{a_4 a_8}_{i_1 i_2} + \tfrac{1}{4} v^{i_5 i_6}_{a_7 a_8} r^{a_7 a_8}_{i_1 i_2} t^{a_3 a_4}_{i_5 i_6} - \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_7 a_8}_{i_1 i_5} t^{a_3 a_4}_{i_2 i_6} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{\alpha_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_2} t^{a_4 a_8}_{i_5 i_6} \\
& - \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{\alpha_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_5} t^{a_4 a_8}_{i_2 i_6} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{\alpha_7 a_8} F^{\alpha_7 a_3}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_5 i_6} t^{a_4 a_8}_{i_1 i_2} + \tfrac{1}{8} v^{i_5 i_6}_{\alpha_7 \alpha_8} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_2} t^{a_3 a_4}_{i_5 i_6} - \tfrac{1}{4} P_2 v^{i_5 i_6}_{\alpha_7 \alpha_8} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_5} t^{a_3 a_4}_{i_2 i_6} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{\alpha_7 \alpha_8} r^{a_3 a_4}_{i_1 i_6} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_2 i_5} \\
& + \tfrac{1}{8} v^{i_5 i_6}_{\alpha_7 \alpha_8} r^{a_3 a_4}_{i_5 i_6} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} - \tfrac{1}{4} P_2 v^{i_5 i_6}_{\alpha_7 a_8} r^{a_3 a_8}_{i_1 i_2} F^{\alpha_7 a_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} - \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{\alpha_7 a_8} r^{a_3 a_8}_{i_1 i_6} F^{\alpha_7 a_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_2 i_5} - \tfrac{1}{4} P_2 v^{i_5 i_6}_{\alpha_7 a_8} r^{a_3 a_8}_{i_5 i_6} F^{\alpha_7 a_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} \\
& - \tfrac{1}{8} P_2 v^{i_5 i_6}_{\alpha_7 \alpha_8} F^{\alpha_7 a_3}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_2} F^{\alpha_8 a_4}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_5 i_6} - \tfrac{1}{4} P_2 P_2 v^{i_5 i_6}_{\alpha_7 \alpha_8} F^{\alpha_7 a_3}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_6} F^{\alpha_8 a_4}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_2 i_5} - \tfrac{1}{8} P_2 v^{i_5 i_6}_{\alpha_7 \alpha_8} F^{\alpha_7 a_3}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_5 i_6} F^{\alpha_8 a_4}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_2}
\end{aligned}
$$

TABLE ESI.2.XXVI: The geminal r amplitude equation of EOM-CCSD-R12 obtained with the modified ansatz 2

$$
\begin{aligned}
\delta^{i_3 i_4}_{i_1 i_2} = & -\tfrac{1}{2} F^{i_3 i_4}_{\alpha_5 a_6} f^{i_7}_{\alpha_8} r^{a_6}_{i_7} F^{\alpha_5 \alpha_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} + \tfrac{1}{4} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} f^{i_7}_{a_8} r^{a_8}_{i_1} F^{\alpha_5 \alpha_6}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_2 i_7} - F^{i_3 i_4}_{\alpha_5 a_6} f^{\alpha_5}_{a_7} r^{a_6 a_7}_{i_1 i_2} + \tfrac{1}{4} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} f^{i_7}_{i_1} F^{\alpha_5 \alpha_6}_{i_8 i_9} r^{i_8 i_9}_{i_2 i_7} + \tfrac{1}{2} F^{i_3 i_4}_{\alpha_5 \alpha_6} f^{\alpha_6}_{\alpha_7} F^{\alpha_5 \alpha_7}_{i_8 i_9} r^{i_8 i_9}_{i_1 i_2} \\
& - \tfrac{1}{4} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} f^{i_7}_{a_8} F^{\alpha_5 \alpha_6}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_7} t^{a_8}_{i_2} - \tfrac{1}{2} F^{i_3 i_4}_{\alpha_5 a_6} f^{i_7}_{\alpha_8} F^{\alpha_5 \alpha_8}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_2} t^{a_6}_{i_7} + F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{i_1 i_2} r^{a_6}_{i_7} + \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{\alpha_5 \alpha_6}_{i_1 a_7} r^{a_7}_{i_2} + P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{i_1 a_8} r^{a_6}_{i_7} t^{a_8}_{i_2} + P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{i_1 a_8} r^{a_8}_{i_2} t^{a_6}_{i_7} \\
& + \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{\alpha_5 \alpha_6}_{a_7 a_8} r^{a_7}_{i_1} t^{a_8}_{i_2} + \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} r^{a_6}_{i_7} t^{a_8}_{i_1} t^{a_9}_{i_2} + P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} r^{a_8}_{i_1} t^{a_9}_{i_2} t^{a_6}_{i_7} + \tfrac{1}{2} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} r^{a_6}_{i_7} t^{a_8 a_9}_{i_1 i_2} - P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} r^{a_8}_{i_1} t^{a_6 a_9}_{i_2 i_7} - F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} r^{a_8}_{i_7} t^{a_6 a_9}_{i_1 i_2} \\
& - \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{i_1 \alpha_9} r^{a_6}_{i_8} F^{\alpha_5 \alpha_9}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_2 i_7} + \tfrac{1}{4} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{\alpha_8 \alpha_9} r^{a_6}_{i_7} F^{\alpha_8 \alpha_9}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_1 i_2} + \tfrac{1}{8} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{i_1 a_9} r^{a_9}_{i_2} F^{\alpha_5 \alpha_6}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_7 i_8} - \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 \alpha_6}_{\alpha_8 a_9} r^{a_9}_{i_1} F^{\alpha_5 \alpha_8}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_2 i_7} \\
& + \tfrac{1}{4} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{i_1 a_9} r^{a_9}_{i_8} F^{\alpha_5 \alpha_6}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_2 i_7} - \tfrac{1}{2} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 \alpha_6}_{\alpha_8 a_9} r^{a_9}_{i_7} F^{\alpha_5 \alpha_8}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_1 i_2} + \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} r^{a_6}_{i_8} t^{a_{10}}_{i_1} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_2 i_7} - \tfrac{1}{2} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} r^{a_6}_{i_7} t^{a_{10}}_{i_8} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_2} \\
& + \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} r^{a_{10}}_{i_1} t^{a_6}_{i_8} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_2 i_7} + \tfrac{1}{8} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{a_9 a_{10}} r^{a_9}_{i_1} t^{a_{10}}_{i_2} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} + \tfrac{1}{4} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{a_9 a_{10}} r^{a_9}_{i_1} t^{a_{10}}_{i_8} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_2 i_7} + \tfrac{1}{2} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} r^{a_{10}}_{i_7} t^{a_6}_{i_8} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_2} \\
& - \tfrac{1}{4} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{a_9 a_{10}} r^{a_9}_{i_8} t^{a_{10}}_{i_1} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_2 i_7} - P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{i_1 a_8} r^{a_6 a_8}_{i_2 i_7} + \tfrac{1}{4} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{\alpha_5 \alpha_6}_{a_7 a_8} r^{a_7 a_8}_{i_1 i_2} + \tfrac{1}{8} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{i_1 i_2} F^{\alpha_5 \alpha_6}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_7 i_8} + \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 \alpha_6}_{i_1 \alpha_8} F^{\alpha_5 \alpha_8}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_2 i_7} \\
& + \tfrac{1}{8} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{\alpha_5 \alpha_6}_{\alpha_7 \alpha_8} F^{\alpha_7 \alpha_8}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_1 i_2} + F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} r^{a_6 a_8}_{i_1 i_2} t^{a_9}_{i_7} - P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} r^{a_6 a_8}_{i_1 i_7} t^{a_9}_{i_2} + \tfrac{1}{2} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{a_8 a_9} r^{a_8 a_9}_{i_1 i_2} t^{a_6}_{i_7} + \tfrac{1}{4} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{i_1 a_9} F^{\alpha_5 \alpha_6}_{i_{10} i_{11}} r^{i_{10} i_{11}}_{i_2 i_7} t^{a_9}_{i_8} \\
& + \tfrac{1}{8} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{i_1 a_9} F^{\alpha_5 \alpha_6}_{i_{10} i_{11}} r^{i_{10} i_{11}}_{i_7 i_8} t^{a_9}_{i_2} - \tfrac{1}{2} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 \alpha_6}_{\alpha_8 a_9} F^{\alpha_5 \alpha_8}_{i_{10} i_{11}} r^{i_{10} i_{11}}_{i_1 i_2} t^{a_9}_{i_7} - \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{i_1 \alpha_9} F^{\alpha_5 \alpha_9}_{i_{10} i_{11}} r^{i_{10} i_{11}}_{i_2 i_7} t^{a_6}_{i_8} + \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 \alpha_6}_{\alpha_8 a_9} F^{\alpha_5 \alpha_8}_{i_{10} i_{11}} r^{i_{10} i_{11}}_{i_1 i_7} t^{a_9}_{i_2} \\
& + \tfrac{1}{4} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 \alpha_5}_{\alpha_8 \alpha_9} F^{\alpha_8 \alpha_9}_{i_{10} i_{11}} r^{i_{10} i_{11}}_{i_1 i_2} t^{a_6}_{i_7} + \tfrac{1}{4} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_7} t^{a_9}_{i_8} t^{a_{10}}_{i_2} + \tfrac{1}{16} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_7 i_8} t^{a_9}_{i_1} t^{a_{10}}_{i_2} + \tfrac{1}{2} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_2} t^{a_{10}}_{i_7} t^{a_6}_{i_8} \\
& - \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_7} t^{a_{10}}_{i_2} t^{a_6}_{i_8} - \tfrac{1}{8} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_7} t^{a_9 a_{10}}_{i_2 i_8} + \tfrac{1}{16} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{a_9 a_{10}} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_7 i_8} t^{a_9 a_{10}}_{i_1 i_2} - \tfrac{1}{4} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_2} t^{a_6 a_{10}}_{i_7 i_8} \\
& + \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_7} t^{a_6 a_{10}}_{i_2 i_8} - \tfrac{1}{4} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_7 i_8} t^{a_6 a_{10}}_{i_1 i_2} - \tfrac{1}{4} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} r^{a_6 a_{10}}_{i_1 i_2} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} - \tfrac{1}{2} P_2 F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} r^{a_6 a_{10}}_{i_1 i_8} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_2 i_7} \\
& - \tfrac{1}{4} F^{i_3 i_4}_{\alpha_5 a_6} v^{i_7 i_8}_{\alpha_9 a_{10}} r^{a_6 a_{10}}_{i_7 i_8} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_1 i_2} + \tfrac{1}{16} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{a_9 a_{10}} r^{a_9 a_{10}}_{i_1 i_2} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} + \tfrac{1}{8} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{a_9 a_{10}} r^{a_9 a_{10}}_{i_1 i_8} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_2 i_7} \\
& + \tfrac{1}{16} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_8} F^{\alpha_9 \alpha_{10}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_2 i_7} + \tfrac{1}{32} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_5 \alpha_6}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_7 i_8} F^{\alpha_9 \alpha_{10}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_1 i_2} - \tfrac{1}{8} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_2} F^{\alpha_6 \alpha_{10}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_7 i_8} \\
& - \tfrac{1}{4} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_8} F^{\alpha_6 \alpha_{10}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_2 i_7} - \tfrac{1}{8} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_5 \alpha_9}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_7 i_8} F^{\alpha_6 \alpha_{10}}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_1 i_2} + \tfrac{1}{32} F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_9 \alpha_{10}}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_2} F^{\alpha_5 \alpha_6}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_7 i_8} \\
& + \tfrac{1}{16} P_2 F^{i_3 i_4}_{\alpha_5 \alpha_6} v^{i_7 i_8}_{\alpha_9 \alpha_{10}} F^{\alpha_9 \alpha_{10}}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_1 i_8} F^{\alpha_5 \alpha_6}_{i_{13} i_{14}} t^{i_{13} i_{14}}_{i_2 i_7}
\end{aligned}
$$

Supplementary data for Phys. Chem. Chem. Phys.

H. EOM-CCSDT-R12

TABLE ESI.2.XXVII: The R_1 amplitude equation of EOM-CCSDT-R12 obtained with the modified ansatz 2

$\delta_{i_1}^{a_2} = \text{EOM-CCSD-R12} + \frac{1}{4} v_{a_5 a_6}^{i_3 i_4} r_{i_1 i_3 i_4}^{a_2 a_5 a_6}$

TABLE ESI.2.XXVIII: The R_2 amplitude equation of EOM-CCSDT-R12 obtained with the modified ansatz 2

$\delta_{i_1 i_2}^{a_3 a_4} = \text{EOM-CCSD-R12} + f_{a_6}^{i_5} r_{i_1 i_2 i_5}^{a_3 a_4 a_6} + \frac{1}{2} P_2 v_{a_7 a_8}^{i_5 i_6} r_{i_5}^{a_3} t_{i_1 i_2 i_6}^{a_4 a_7 a_8} + \frac{1}{2} P_2 v_{a_7 a_8}^{i_5 i_6} r_{i_1}^{a_7} t_{i_2 i_5 i_6}^{a_3 a_4 a_8} + v_{a_7 a_8}^{i_5 i_6} r_{i_5}^{a_7} t_{i_1 i_2 i_6}^{a_3 a_4 a_8} + \frac{1}{2} P_2 v_{i_1 a_7}^{i_5 i_6} r_{i_2 i_5 i_6}^{a_3 a_4 a_7} + \frac{1}{2} P_2 v_{a_6 a_7}^{i_5 a_3} r_{i_1 i_2 i_5}^{a_4 a_6 a_7}$ $+ v_{a_7 a_8}^{i_5 i_6} r_{i_1 i_2 i_5}^{a_3 a_4 a_7} t_{i_6}^{a_8} + \frac{1}{2} P_2 v_{a_7 a_8}^{i_5 i_6} r_{i_1 i_5 i_6}^{a_3 a_4 a_7} t_{i_2}^{a_8} + \frac{1}{2} P_2 v_{a_7 a_8}^{i_5 i_6} r_{i_1 i_2 i_5}^{a_3 a_7 a_8} t_{i_6}^{a_4}$

TABLE ESI.2.XXIX: The geminal r amplitude equation of EOM-CCSDT-R12 obtained with the modified ansatz 2

$\delta_{i_1 i_2}^{i_3 i_4} = \text{EOM-CCSD-R12} + \frac{1}{2} F_{a_5 a_6}^{i_3 i_4 *} v_{a_8 a_9}^{i_7 a_5} r_{i_1 i_2 i_7}^{a_6 a_8 a_9}$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.2.XXX: The R_3 amplitude equation of EOM-CCSDT-R12 obtained with the modified ansatz 2

$$\delta^{a_4a_5a_6}_{i_1i_2i_3} = -P_3 f^{i_7}_{a_8} r^{a_4}_{i_7} t^{a_5a_6a_8}_{i_1i_2i_3} - P_3 f^{i_7}_{a_8} r^{a_8}_{i_1} t^{a_4a_5a_6}_{i_2i_3i_7} + P_3P_3 f^{i_7}_{a_8} r^{a_4a_5}_{i_1i_7} t^{a_6a_8}_{i_2i_3} + P_3P_3 f^{i_7}_{a_8} r^{a_4a_8}_{i_1i_2} t^{a_5a_6}_{i_3i_7} - \tfrac{1}{2}P_3P_3 f^{i_7}_{\alpha_8} F^{\alpha_8a_4}_{i_9i_{10}} r^{i_9i_{10}}_{i_1i_2} t^{a_5a_6}_{i_3i_7} - \tfrac{1}{2}P_3P_3 f^{i_7}_{\alpha_8} r^{a_4a_5}_{i_1i_7} F^{\alpha_8a_6}_{i_9i_{10}} t^{i_9i_{10}}_{i_2i_3}$$

$$-P_3 f^{i_7}_{i_1} r^{a_4a_5a_6}_{i_2i_3i_7} + P_3 f^{a_4}_{a_7} r^{a_5a_6a_7}_{i_1i_2i_3} - P_3 f^{i_7}_{a_8} r^{a_4a_5a_6}_{i_1i_2i_7} t^{a_8}_{i_3} - P_3 f^{i_7}_{a_8} r^{a_4a_5a_8}_{i_1i_2i_3} t^{a_6}_{i_7} - P_3P_3 v^{i_7i_8}_{i_1i_2} r^{a_4}_{i_7} t^{a_5a_6}_{i_3i_8} - P_3P_3 v^{i_7a_4}_{i_1a_8} r^{a_5}_{i_7} t^{a_6a_8}_{i_2i_3} - P_3P_3 v^{i_7a_4}_{i_1a_8} r^{a_8}_{i_2} t^{a_5a_6}_{i_3i_7}$$

$$-P_3P_3 v^{a_4a_5}_{a_7a_8} r^{a_7}_{i_1} t^{a_6a_8}_{i_2i_3} + \tfrac{1}{2}P_3P_3 v^{i_7a_4}_{i_1\alpha_8} r^{a_5}_{i_7} F^{\alpha_8a_6}_{i_9i_{10}} t^{i_9i_{10}}_{i_2i_3} - \tfrac{1}{2}P_3P_3 v^{a_4a_5}_{\alpha_7a_8} r^{a_8}_{i_1} F^{\alpha_7a_6}_{i_9i_{10}} t^{i_9i_{10}}_{i_2i_3} - P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_4}_{i_7} t^{a_5}_{i_8} t^{a_6a_9}_{i_2i_3} - P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_4}_{i_7} t^{a_9}_{i_2} t^{a_5a_6}_{i_3i_8}$$

$$-P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_5}_{i_7} t^{a_8}_{i_1} t^{a_6a_9}_{i_2i_3} - P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_9}_{i_2} t^{a_4}_{i_7} t^{a_5a_6}_{i_3i_8} - P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_8}_{i_1} t^{a_5}_{i_7} t^{a_6a_9}_{i_2i_3} - P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_8}_{i_1} t^{a_9}_{i_2} t^{a_5a_6}_{i_3i_7} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{i_1\alpha_9} r^{a_4}_{i_7} t^{a_5}_{i_8} F^{\alpha_9a_6}_{i_{10}i_{11}} t^{i_{10}i_{11}}_{i_2i_3}$$

$$-\tfrac{1}{2}P_3P_3 v^{i_7a_4}_{\alpha_8a_9} r^{a_5}_{i_7} t^{a_9}_{i_1} F^{\alpha_8a_6}_{i_{10}i_{11}} t^{i_{10}i_{11}}_{i_2i_3} - \tfrac{1}{2}P_3P_3 v^{i_7a_4}_{\alpha_8a_9} r^{a_9}_{i_1} t^{a_5}_{i_7} F^{\alpha_8a_6}_{i_{10}i_{11}} t^{i_{10}i_{11}}_{i_2i_3} - P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_4}_{i_7} t^{a_5a_6a_9}_{i_2i_3i_8} + \tfrac{1}{2}P_3 v^{i_7a_4}_{a_8a_9} r^{a_5}_{i_7} t^{a_6a_8a_9}_{i_1i_2i_3} + \tfrac{1}{2}P_3 v^{i_7i_8}_{i_1a_9} r^{a_9}_{i_2} t^{a_4a_5a_6}_{i_3i_7i_8}$$

$$-P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_8}_{i_1} t^{a_5a_6a_9}_{i_2i_3i_7} + P_3 v^{i_7i_8}_{i_1a_9} r^{a_9}_{i_7} t^{a_4a_5a_6}_{i_2i_3i_8} + P_3 v^{i_7a_4}_{a_8a_9} r^{a_8}_{i_7} t^{a_5a_6a_9}_{i_1i_2i_3} - P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4}_{i_7} t^{a_9}_{i_1} t^{a_5}_{i_8} t^{a_6a_{10}}_{i_2i_3} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4}_{i_7} t^{a_9}_{i_1} t^{a_{10}}_{i_2} t^{a_5a_6}_{i_3i_8}$$

$$-\tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_1} t^{a_4}_{i_7} t^{a_5}_{i_8} t^{a_6a_{10}}_{i_2i_3} - P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_1} t^{a_{10}}_{i_2} t^{a_4}_{i_7} t^{a_5a_6}_{i_3i_8} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4}_{i_7} t^{a_{10}}_{i_1} t^{a_5}_{i_8} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3} - \tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_{10}}_{i_1} t^{a_4}_{i_7} t^{a_5}_{i_8} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3}$$

$$+\tfrac{1}{2}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4}_{i_7} t^{a_5}_{i_8} t^{a_6a_9a_{10}}_{i_1i_2i_3} - P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4}_{i_7} t^{a_9}_{i_1} t^{a_5a_6a_{10}}_{i_2i_3i_8} + P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4}_{i_7} t^{a_9}_{i_8} t^{a_5a_6a_{10}}_{i_1i_2i_3} - P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_1} t^{a_4}_{i_7} t^{a_5a_6a_{10}}_{i_2i_3i_8} + \tfrac{1}{2}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_1} t^{a_{10}}_{i_2} t^{a_4a_5a_6}_{i_3i_7i_8}$$

$$+P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_1} t^{a_{10}}_{i_7} t^{a_4a_5a_6}_{i_2i_3i_8} - P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_7} t^{a_4}_{i_8} t^{a_5a_6a_{10}}_{i_1i_2i_3} - P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_7} t^{a_{10}}_{i_1} t^{a_4a_5a_6}_{i_2i_3i_8} + P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4}_{i_7} t^{a_5a_9}_{i_1i_8} t^{a_6a_{10}}_{i_2i_3} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4}_{i_7} t^{a_9a_{10}}_{i_1i_2} t^{a_5a_6}_{i_3i_8}$$

$$-\tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_1} t^{a_4a_{10}}_{i_2i_3} t^{a_5a_6}_{i_7i_8} + P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_1} t^{a_4a_{10}}_{i_2i_7} t^{a_5a_6}_{i_3i_8} + P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_7} t^{a_4a_{10}}_{i_1i_2} t^{a_5a_6}_{i_3i_8} - \tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9\alpha_{10}} r^{a_4}_{i_7} t^{a_5a_6}_{i_1i_8} F^{\alpha_9\alpha_{10}}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3}$$

$$-\tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4}_{i_8} t^{a_5a_{10}}_{i_1i_2} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_7} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4}_{i_7} t^{a_5a_{10}}_{i_1i_8} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_{10}}_{i_1} t^{a_4a_5}_{i_2i_7} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_8} - \tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_{10}}_{i_1} t^{a_4a_5}_{i_7i_8} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3}$$

$$+\tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_{10}}_{i_7} t^{a_4a_5}_{i_1i_8} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3} - \tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9\alpha_{10}} r^{a_4}_{i_8} F^{\alpha_9a_5}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_1i_7} F^{\alpha_{10}a_6}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_2i_3} - P_3P_3 v^{i_7a_4}_{i_1i_2} r^{a_5a_6}_{i_3i_7} - P_3P_3 v^{a_4a_5}_{i_1a_7} r^{a_6a_7}_{i_2i_3} + \tfrac{1}{2}P_3P_3 v^{a_4a_5}_{i_1\alpha_7} F^{\alpha_7a_6}_{i_8i_9} r^{i_8i_9}_{i_2i_3}$$

$$+P_3P_3 v^{i_7i_8}_{i_1i_2} r^{a_4a_5}_{i_3i_7} t^{a_6}_{i_8} + P_3P_3 v^{i_7a_4}_{i_1a_8} r^{a_5a_6}_{i_2i_7} t^{a_8}_{i_3} + P_3P_3 v^{i_7a_4}_{i_1a_8} r^{a_5a_8}_{i_2i_3} t^{a_6}_{i_7} + P_3P_3 v^{a_4a_5}_{a_7a_8} r^{a_6a_7}_{i_1i_2} t^{a_8}_{i_3} - \tfrac{1}{2}P_3P_3 v^{i_7a_4}_{i_1\alpha_8} F^{\alpha_8a_5}_{i_9i_{10}} r^{i_9i_{10}}_{i_2i_3} t^{a_6}_{i_7} - \tfrac{1}{2}P_3P_3 v^{a_4a_5}_{\alpha_7a_8} F^{\alpha_7a_6}_{i_9i_{10}} r^{i_9i_{10}}_{i_1i_2} t^{a_8}_{i_3}$$

$$-P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_4a_5}_{i_2i_7} t^{a_9}_{i_3} t^{a_6}_{i_8} - \tfrac{1}{2}P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_5a_6}_{i_1i_7} t^{a_8}_{i_2} t^{a_9}_{i_3} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_4a_9}_{i_2i_3} t^{a_5}_{i_7} t^{a_6}_{i_8} - P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_5a_8}_{i_1i_2} t^{a_9}_{i_3} t^{a_6}_{i_7} + \tfrac{1}{4}P_3P_3 v^{i_7i_8}_{i_1\alpha_9} F^{\alpha_9a_4}_{i_{10}i_{11}} r^{i_{10}i_{11}}_{i_2i_3} t^{a_5}_{i_7} t^{a_6}_{i_8}$$

$$+\tfrac{1}{2}P_3P_3 v^{i_7a_4}_{\alpha_8a_9} F^{\alpha_8a_5}_{i_{10}i_{11}} r^{i_{10}i_{11}}_{i_1i_2} t^{a_9}_{i_3} t^{a_6}_{i_7} + P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_4a_5}_{i_2i_7} t^{a_6a_9}_{i_3i_8} - \tfrac{1}{2}P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_5a_6}_{i_1i_7} t^{a_8a_9}_{i_2i_3} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_4a_5}_{i_7i_8} t^{a_6a_9}_{i_2i_3} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_4a_9}_{i_2i_3} t^{a_5a_6}_{i_7i_8}$$

$$+P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_5a_8}_{i_1i_2} t^{a_6a_9}_{i_3i_7} + P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_4a_9}_{i_2i_7} t^{a_5a_6}_{i_3i_8} + P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_5a_8}_{i_1i_7} t^{a_6a_9}_{i_2i_3} - \tfrac{1}{2}P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_8a_9}_{i_1i_2} t^{a_5a_6}_{i_3i_7} + \tfrac{1}{4}P_3P_3 v^{i_7i_8}_{i_1\alpha_9} F^{\alpha_9a_4}_{i_{10}i_{11}} r^{i_{10}i_{11}}_{i_2i_3} t^{a_5a_6}_{i_7i_8}$$

$$-\tfrac{1}{2}P_3P_3 v^{i_7a_4}_{\alpha_8a_9} F^{\alpha_8a_5}_{i_{10}i_{11}} r^{i_{10}i_{11}}_{i_1i_2} t^{a_6a_9}_{i_3i_7} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{i_1\alpha_9} F^{\alpha_9a_4}_{i_{10}i_{11}} r^{i_{10}i_{11}}_{i_2i_7} t^{a_5a_6}_{i_3i_8} - \tfrac{1}{2}P_3P_3 v^{i_7a_4}_{\alpha_8a_9} F^{\alpha_8a_5}_{i_{10}i_{11}} r^{i_{10}i_{11}}_{i_1i_7} t^{a_6a_9}_{i_2i_3} - \tfrac{1}{4}P_3P_3 v^{i_7a_4}_{\alpha_8\alpha_9} F^{\alpha_8\alpha_9}_{i_{10}i_{11}} r^{i_{10}i_{11}}_{i_1i_2} t^{a_5a_6}_{i_3i_7}$$

$$+\tfrac{1}{2}P_3P_3 v^{i_7i_8}_{i_1\alpha_9} r^{a_4a_5}_{i_2i_8} F^{\alpha_9a_6}_{i_{10}i_{11}} t^{i_{10}i_{11}}_{i_3i_7} - \tfrac{1}{4}P_3P_3 v^{i_7a_4}_{\alpha_8\alpha_9} r^{a_5a_6}_{i_1i_7} F^{\alpha_8\alpha_9}_{i_{10}i_{11}} t^{i_{10}i_{11}}_{i_2i_3} + \tfrac{1}{4}P_3P_3 v^{i_7i_8}_{i_1\alpha_9} r^{a_4a_5}_{i_7i_8} F^{\alpha_9a_6}_{i_{10}i_{11}} t^{i_{10}i_{11}}_{i_2i_3} + \tfrac{1}{2}P_3P_3 v^{i_7a_4}_{\alpha_8a_9} r^{a_5a_9}_{i_1i_2} F^{\alpha_8a_6}_{i_{10}i_{11}} t^{i_{10}i_{11}}_{i_3i_7}$$

$$+\tfrac{1}{2}P_3P_3 v^{i_7a_4}_{\alpha_8a_9} r^{a_5a_9}_{i_1i_7} F^{\alpha_8a_6}_{i_{10}i_{11}} t^{i_{10}i_{11}}_{i_2i_3} + \tfrac{1}{4}P_3P_3 v^{i_7a_4}_{\alpha_8\alpha_9} F^{\alpha_8a_5}_{i_{10}i_{11}} r^{i_{10}i_{11}}_{i_1i_2} F^{\alpha_9a_6}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_3i_7} + \tfrac{1}{4}P_3P_3 v^{i_7a_4}_{\alpha_8\alpha_9} F^{\alpha_8a_5}_{i_{10}i_{11}} r^{i_{10}i_{11}}_{i_1i_7} F^{\alpha_9a_6}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_2i_3} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5}_{i_1i_7} t^{a_9}_{i_2} t^{a_{10}}_{i_3} t^{a_6}_{i_8}$$

$$+\tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9}_{i_1i_2} t^{a_{10}}_{i_3} t^{a_5}_{i_7} t^{a_6}_{i_8} - \tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} t^{a_{10}}_{i_3} t^{a_5}_{i_7} t^{a_6}_{i_8} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5}_{i_1i_7} t^{a_6}_{i_8} t^{a_9a_{10}}_{i_2i_3} - P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5}_{i_1i_7} t^{a_9}_{i_2} t^{a_6a_{10}}_{i_3i_8}$$

$$-P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5}_{i_1i_7} t^{a_9}_{i_8} t^{a_6a_{10}}_{i_2i_3} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5}_{i_7i_8} t^{a_9}_{i_1} t^{a_6a_{10}}_{i_2i_3} - P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9}_{i_1i_2} t^{a_5}_{i_7} t^{a_6a_{10}}_{i_3i_8} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9}_{i_1i_2} t^{a_{10}}_{i_3} t^{a_5a_6}_{i_7i_8} - P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9}_{i_1i_2} t^{a_{10}}_{i_7} t^{a_5a_6}_{i_3i_8}$$

$$+P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9}_{i_1i_7} t^{a_5}_{i_8} t^{a_6a_{10}}_{i_2i_3} + P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9}_{i_1i_7} t^{a_{10}}_{i_2} t^{a_5a_6}_{i_3i_8} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9a_{10}}_{i_1i_2} t^{a_4}_{i_7} t^{a_5a_6}_{i_3i_8} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} t^{a_5}_{i_7} t^{a_6a_{10}}_{i_3i_8}$$

$$-\tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} t^{a_{10}}_{i_3} t^{a_5a_6}_{i_7i_8} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} t^{a_{10}}_{i_7} t^{a_5a_6}_{i_3i_8} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_7} t^{a_5}_{i_8} t^{a_6a_{10}}_{i_2i_3} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_7} t^{a_{10}}_{i_2} t^{a_5a_6}_{i_3i_8}$$

$$-\tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9\alpha_{10}} F^{\alpha_9\alpha_{10}}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} t^{a_4}_{i_7} t^{a_5a_6}_{i_3i_8} + \tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9\alpha_{10}} r^{a_4a_5}_{i_1i_7} t^{a_6}_{i_8} F^{\alpha_9\alpha_{10}}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4a_5}_{i_1i_8} t^{a_{10}}_{i_2} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_7} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4a_5}_{i_1i_7} t^{a_{10}}_{i_8} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3}$$

$$-\tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4a_5}_{i_7i_8} t^{a_{10}}_{i_1} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4a_{10}}_{i_1i_2} t^{a_5}_{i_8} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_7} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4a_{10}}_{i_1i_7} t^{a_5}_{i_8} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3}$$

$$+\tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9\alpha_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} t^{a_5}_{i_8} F^{\alpha_{10}a_6}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_3i_7} + \tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9\alpha_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_7} t^{a_5}_{i_8} F^{\alpha_{10}a_6}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_2i_3} + \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5}_{i_1i_7} t^{a_6a_9a_{10}}_{i_2i_3i_8} + \tfrac{1}{4}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5}_{i_7i_8} t^{a_6a_9a_{10}}_{i_1i_2i_3}$$

$$+\tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9}_{i_1i_2} t^{a_5a_6a_{10}}_{i_3i_7i_8} + P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9}_{i_1i_7} t^{a_5a_6a_{10}}_{i_2i_3i_8} + \tfrac{1}{2}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9}_{i_7i_8} t^{a_5a_6a_{10}}_{i_1i_2i_3} + \tfrac{1}{4}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9a_{10}}_{i_1i_2} t^{a_4a_5a_6}_{i_3i_7i_8} + \tfrac{1}{2}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9a_{10}}_{i_1i_7} t^{a_4a_5a_6}_{i_2i_3i_8}$$

$$-\tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} t^{a_5a_6a_{10}}_{i_3i_7i_8} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_7} t^{a_5a_6a_{10}}_{i_2i_3i_8} - \tfrac{1}{4}P_3 v^{i_7i_8}_{\alpha_9a_{10}} F^{\alpha_9a_4}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_7i_8} t^{a_5a_6a_{10}}_{i_1i_2i_3} + \tfrac{1}{8}P_3 v^{i_7i_8}_{\alpha_9\alpha_{10}} F^{\alpha_9\alpha_{10}}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} t^{a_4a_5a_6}_{i_3i_7i_8}$$

$$+\tfrac{1}{4}P_3 v^{i_7i_8}_{\alpha_9\alpha_{10}} F^{\alpha_9\alpha_{10}}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_7} t^{a_4a_5a_6}_{i_2i_3i_8} + \tfrac{1}{2}P_3 v^{i_7i_8}_{i_1i_2} r^{a_4a_5a_6}_{i_3i_7i_8} - P_3P_3 v^{i_7a_4}_{i_1a_8} r^{a_5a_6a_8}_{i_2i_3i_7} + \tfrac{1}{2}P_3 v^{a_4a_5}_{a_7a_8} r^{a_6a_7a_8}_{i_1i_2i_3} - P_3 v^{i_7i_8}_{i_1a_9} r^{a_4a_5a_6}_{i_2i_3i_7} t^{a_9}_{i_8} - \tfrac{1}{2}P_3 v^{i_7i_8}_{i_1a_9} r^{a_4a_5a_6}_{i_2i_7i_8} t^{a_9}_{i_3}$$

$$-P_3 v^{i_7a_4}_{a_8a_9} r^{a_5a_6a_8}_{i_1i_2i_3} t^{a_9}_{i_7} + P_3P_3 v^{i_7i_8}_{i_1a_9} r^{a_4a_5a_9}_{i_2i_3i_7} t^{a_6}_{i_8} + P_3P_3 v^{i_7a_4}_{a_8a_9} r^{a_5a_6a_8}_{i_1i_2i_7} t^{a_9}_{i_3} - \tfrac{1}{2}P_3 v^{i_7a_4}_{a_8a_9} r^{a_5a_8a_9}_{i_1i_2i_3} t^{a_6}_{i_7} + P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_6}_{i_1i_2i_7} t^{a_9}_{i_8} t^{a_{10}}_{i_3} + \tfrac{1}{4}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_6}_{i_1i_7i_8} t^{a_9}_{i_2} t^{a_{10}}_{i_3}$$

$$+P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_9}_{i_1i_2i_3} t^{a_{10}}_{i_7} t^{a_6}_{i_8} - P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_9}_{i_1i_2i_7} t^{a_{10}}_{i_3} t^{a_6}_{i_8} + \tfrac{1}{4}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9a_{10}}_{i_1i_2i_3} t^{a_5}_{i_7} t^{a_6}_{i_8} - \tfrac{1}{2}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_6}_{i_1i_2i_7} t^{a_9a_{10}}_{i_3i_8} + \tfrac{1}{4}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_6}_{i_1i_7i_8} t^{a_9a_{10}}_{i_2i_3}$$

$$-\tfrac{1}{2}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_9}_{i_1i_2i_3} t^{a_6a_{10}}_{i_7i_8} + P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_9}_{i_1i_2i_7} t^{a_6a_{10}}_{i_3i_8} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_9}_{i_1i_7i_8} t^{a_6a_{10}}_{i_2i_3} + \tfrac{1}{4}P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9a_{10}}_{i_1i_2i_3} t^{a_5a_6}_{i_7i_8} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_9a_{10}}_{i_1i_2i_7} t^{a_5a_6}_{i_3i_8}$$

$$+\tfrac{1}{4}P_3 v^{i_7i_8}_{\alpha_9\alpha_{10}} r^{a_4a_5a_6}_{i_1i_2i_8} F^{\alpha_9\alpha_{10}}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_7} + \tfrac{1}{8}P_3 v^{i_7i_8}_{\alpha_9\alpha_{10}} r^{a_4a_5a_6}_{i_1i_7i_8} F^{\alpha_9\alpha_{10}}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3} - \tfrac{1}{4}P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4a_5a_{10}}_{i_1i_2i_3} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_7i_8} - \tfrac{1}{2}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4a_5a_{10}}_{i_1i_2i_8} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_7}$$

$$-\tfrac{1}{4}P_3P_3 v^{i_7i_8}_{\alpha_9a_{10}} r^{a_4a_5a_{10}}_{i_1i_7i_8} F^{\alpha_9a_6}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_2i_3}$$

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I. EOM-CCSDTQ-R12

TABLE ESI.2.XXXI: The R_2 amplitude equation of EOM-CCSDTQ-R12 obtained with the modified ansatz 2

$$\delta^{a_3a_4}_{i_1i_2} = \text{EOM-CCSDT-R12} + \tfrac{1}{4} v^{i_5i_6}_{a_7a_8} r^{a_3a_4a_7a_8}_{i_1i_2i_5i_6}$$

TABLE ESI.2.XXXII: The R_3 amplitude equation of EOM-CCSDTQ-R12 obtained with the modified ansatz 2

$$\begin{aligned}\delta^{a_4a_5a_6}_{i_1i_2i_3} = \text{EOM-CCSDT-R12} &+ f^{i_7}_{a_8} r^{a_4a_5a_6a_8}_{i_1i_2i_3i_7} - \tfrac{1}{2} P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4}_{i_7} t^{a_5a_6a_9a_{10}}_{i_1i_2i_3i_8} - \tfrac{1}{2} P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_1} t^{a_4a_5a_6a_{10}}_{i_2i_3i_7i_8} + v^{i_7i_8}_{a_9a_{10}} r^{a_9}_{i_7} t^{a_4a_5a_6a_{10}}_{i_1i_2i_3i_8} - \tfrac{1}{2} P_3 v^{i_7i_8}_{i_1a_9} r^{a_4a_5a_6a_9}_{i_2i_3i_7i_8} \\ &- \tfrac{1}{2} P_3 v^{i_7a_4}_{a_8a_9} r^{a_5a_6a_8a_9}_{i_1i_2i_3i_7} + v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_6a_9}_{i_1i_2i_3i_7} t^{a_{10}}_{i_8} + \tfrac{1}{2} P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_9a_{10}}_{i_1i_2i_7i_8} t^{a_{10}}_{i_3} + \tfrac{1}{2} P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_4a_5a_9a_{10}}_{i_1i_2i_3i_7} t^{a_6}_{i_8}\end{aligned}$$

TABLE ESI.2.XXXIII: The R_4 amplitude equation of EOM-CCSDTQ-R12 obtained with the modified ansatz 2 [Part I]

$$\begin{aligned}\delta^{a_5a_6a_7a_8}_{i_1i_2i_3i_4} = &+P_4 f^{i_9}_{a_{10}} r^{a_5}_{i_9} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_4} + P_4 f^{i_9}_{a_{10}} r^{a_{10}}_{i_1} t^{a_5a_6a_7a_8}_{i_2i_3i_4i_9} - P_4P_4 f^{i_9}_{a_{10}} r^{a_5a_6}_{i_1i_9} t^{a_7a_8a_{10}}_{i_2i_3i_4} - P_4P_4 f^{i_9}_{a_{10}} r^{a_5a_{10}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9} + \tfrac{1}{2} P_4P_4 f^{i_9}_{a_{10}} F^{\alpha_{10}a_5}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9} \\ &+P_4P_4 f^{i_9}_{a_{10}} r^{a_5a_6a_7}_{i_1i_2i_9} t^{a_8a_{10}}_{i_3i_4} + P_4P_4 f^{i_9}_{a_{10}} r^{a_5a_6a_{10}}_{i_1i_9} t^{a_7a_8}_{i_2i_3i_4} - \tfrac{1}{2} P_4P_4 f^{i_9}_{a_{10}} r^{a_5a_6a_7}_{i_1i_2} F^{\alpha_{10}a_8}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_4} + P_4 f^{i_9}_{i_1} r^{a_5a_6a_7a_8}_{i_2i_3i_4i_9} - P_4 f^{a_5}_{a_9} r^{a_6a_7a_8a_9}_{i_1i_2i_3i_4} - P_4 f^{i_9}_{a_{10}} r^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} t^{a_{10}}_{i_4} \\ &-P_4 f^{i_9}_{a_{10}} r^{a_5a_6a_7a_{10}}_{i_1i_2i_3i_4} t^{a_8}_{i_9} + P_4P_4 v^{i_9i_{10}}_{i_1i_2} r^{a_5}_{i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} + P_4P_4 v^{i_9a_5}_{i_1a_{10}} r^{a_6}_{i_9} t^{a_7a_8a_{10}}_{i_2i_3i_4} + P_4P_4 v^{i_9a_5}_{i_1a_{10}} r^{a_{10}}_{i_2} t^{a_6a_7a_8}_{i_3i_4i_9} + P_4P_4 v^{a_5a_6}_{a_9a_{10}} r^{a_9}_{i_1} t^{a_7a_8a_{10}}_{i_2i_3i_4} + P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5}_{i_9} t^{a_6}_{i_{10}} t^{a_7a_8a_{11}}_{i_2i_3i_4} \\ &+P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5}_{i_9} t^{a_6a_7a_8}_{i_2i_3i_4i_{10}} + P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6}_{i_9} t^{a_7a_{10}}_{i_1i_2} t^{a_8a_{11}}_{i_3i_4} + P_4P_4 v^{i_9a_5}_{i_1a_{11}} r^{a_{10}}_{i_2} t^{a_6a_7a_8}_{i_3i_4i_{10}} + P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_{10}}_{i_1} t^{a_6a_7a_8}_{i_2i_3i_4i_9} \\ &-P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5}_{i_9} t^{a_6a_{11}}_{i_2i_3} t^{a_7a_8}_{i_4i_{10}} - \tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6}_{i_9} t^{a_{10}}_{i_1i_2} t^{a_8a_{11}}_{i_3i_4} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_{11}}_{i_2} t^{a_5a_6}_{i_3i_9} t^{a_7a_8}_{i_4i_{10}} - P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_{10}}_{i_1} t^{a_6a_{11}}_{i_2i_3} t^{a_7a_8}_{i_4i_9} \\ &+\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5}_{i_9} t^{a_6a_7}_{i_2i_{10}} F^{\alpha_{11}a_8}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_3i_4} - \tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6}_{i_9} t^{a_7a_{11}}_{i_1i_2} F^{\alpha_{10}a_8}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_3i_4} - \tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_{11}}_{i_1} t^{a_6a_7}_{i_2i_9} F^{\alpha_{10}a_8}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_3i_4} - P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5}_{i_9} t^{a_6a_7a_8a_{11}}_{i_2i_3i_4i_{10}} \\ &+\tfrac{1}{2} P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6}_{i_9} t^{a_7a_8a_{10}a_{11}}_{i_1i_2i_3i_4} + \tfrac{1}{2} P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_{11}}_{i_2} t^{a_5a_6a_7a_8}_{i_3i_4i_9i_{10}} - P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_{10}}_{i_1} t^{a_6a_7a_8a_{11}}_{i_2i_3i_4i_9} - P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_{11}}_{i_9} t^{a_5a_6a_7a_8}_{i_2i_3i_4i_{10}} - P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_{10}}_{i_9} t^{a_6a_7a_8a_{11}}_{i_1i_2i_3i_4} \\ &-\tfrac{1}{8} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6}_{i_9} F^{\alpha_{10}a_7}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_1i_2} F^{\alpha_{11}a_8}_{i_{14}i_{15}} t^{i_{14}i_{15}}_{i_3i_4} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_7}_{i_1} t^{a_6}_{i_{10}} t^{a_7a_8a_{12}}_{i_2i_3i_4} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_1} t^{a_{12}}_{i_2} t^{a_6a_7a_8}_{i_3i_4i_{10}} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_1} t^{a_{12}}_{i_9} t^{a_6}_{i_{10}} t^{a_7a_8a_{12}}_{i_2i_3i_4} \\ &+P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_1} t^{a_{12}}_{i_2} t^{a_5}_{i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} + \tfrac{1}{2} P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6}_{i_{10}} t^{a_7a_8a_{11}a_{12}}_{i_1i_2i_3i_4} - P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_7a_8a_{11}a_{12}}_{i_1i_2i_3i_4i_{10}} - P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_7a_8a_{11}a_{12}}_{i_1i_2i_3i_4i_{10}} \\ &-P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_1} t^{a_5}_{i_9} t^{a_6a_7a_8a_{12}}_{i_2i_3i_4i_{10}} + \tfrac{1}{2} P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_1} t^{a_{12}}_{i_2} t^{a_5a_6a_7a_8}_{i_3i_4i_9i_{10}} - P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_1} t^{a_{12}}_{i_9} t^{a_5}_{i_{10}} t^{a_6a_7a_8a_{12}}_{i_2i_3i_4} + P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_9} t^{a_{12}}_{i_1} t^{a_5a_6a_7a_8}_{i_2i_3i_4i_{10}} \\ &-\tfrac{1}{8} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6}_{i_{10}} F^{\alpha_{11}a_7}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} F^{\alpha_{12}a_8}_{i_{15}i_{16}} t^{i_{15}i_{16}}_{i_3i_4} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_7}_{i_1i_{10}} t^{a_{12}}_{i_2} F^{\alpha_{11}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_3i_4} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_{12}}_{i_1i_2} t^{a_7}_{i_{10}} F^{\alpha_{11}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_3i_4} \\ &-\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{12}}_{i_1} t^{a_5a_6}_{i_2i_{10}} t^{a_7}_{i_9} F^{\alpha_{11}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_3i_4} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_{12}}_{i_3i_{10}} t^{a_7a_8}_{i_4} t^{a_{11}}_{i_{10}} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_1} t^{a_6a_{11}}_{i_{10}} t^{a_7a_{12}}_{i_3i_4} t^{a_8}_{i_{10}} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_1} t^{a_5a_6}_{i_2i_9} t^{a_7a_8}_{i_3i_{10}} t^{a_{12}}_{i_4} \\ &+P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_1} t^{a_5a_{12}}_{i_2i_3} t^{a_6a_7}_{i_4i_{10}} t^{a_8}_{i_9} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_7}_{i_1i_{10}} t^{a_8a_{11}a_{12}}_{i_2i_3i_4} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_{11}}_{i_1i_2} t^{a_7a_8a_{12}}_{i_3i_4i_{10}} - P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_{11}}_{i_1i_{10}} t^{a_7a_8a_{12}}_{i_2i_3i_4} \\ &+\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_{11}a_{12}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_{10}} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_7}_{i_1i_2} t^{a_8a_{11}a_{12}}_{i_3i_4i_{10}} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_1} t^{a_6a_{11}}_{i_{10}} t^{a_7a_{12}}_{i_3i_4} t^{a_8}_{i_{10}} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_1} t^{a_5a_6}_{i_2i_9} t^{a_7a_8}_{i_3i_{10}} t^{a_{12}}_{i_4} \\ &+P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_1} t^{a_5a_{12}}_{i_2i_3} t^{a_6a_7}_{i_4i_{10}} t^{a_8}_{i_9} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_7}_{i_1i_{10}} t^{a_8a_{11}a_{12}}_{i_2i_3i_4} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_{11}}_{i_1i_2} t^{a_7a_8a_{12}}_{i_3i_4i_{10}} - P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_{11}}_{i_1i_{10}} t^{a_7a_8a_{12}}_{i_2i_3i_4} \\ &+\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_{11}a_{12}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_{10}} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} t^{a_6a_7}_{i_1i_{10}} t^{a_8a_{11}a_{12}}_{i_2i_3i_4} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_1} t^{a_6a_{11}}_{i_2i_9} t^{a_7a_8}_{i_3i_{10}} t^{a_{12}}_{i_4} \\ &-P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_1} t^{a_5a_{12}}_{i_2i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} - P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_9} t^{a_5a_6}_{i_1i_{10}} t^{a_7a_8a_{12}}_{i_2i_3i_4} - P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}}_{i_1} t^{a_5a_{12}}_{i_9} t^{a_6a_7a_8}_{i_2i_3i_4i_{10}} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} F^{\alpha_{11}a_6}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_7a_8a_{12}}_{i_3i_4i_{10}} \\ &-\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_{10}} F^{\alpha_{11}a_6}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_9} t^{a_7a_8a_{12}}_{i_2i_3i_4} + \tfrac{1}{4} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5}_{i_9} F^{\alpha_{11}a_{12}}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_{10}} - \tfrac{1}{4} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{12}}_{i_9} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_2i_3} t^{a_6a_7a_8}_{i_4i_9i_{10}} \\ &-\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{12}}_{i_1} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_2i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{12}}_{i_9} F^{\alpha_{11}a_5}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_{10}} - P_4P_4 v^{i_9i_{10}}_{i_1i_2} r^{a_5a_6}_{i_3i_9} t^{a_7a_8}_{i_4i_{10}} - P_4P_4 v^{i_9a_5}_{i_1a_{10}} r^{a_6}_{i_9} t^{a_8a_{10}}_{i_2i_3i_4} \\ &-P_4P_4 v^{i_9a_5}_{i_1a_{10}} r^{a_6a_{10}}_{i_2i_9} t^{a_7a_8}_{i_3i_4} - P_4P_4 v^{a_5a_6}_{a_9a_{10}} r^{a_7a_9}_{i_1i_2} t^{a_8a_{10}}_{i_3i_4} + \tfrac{1}{2} P_4P_4 v^{i_9a_5}_{i_1a_{10}} F^{\alpha_{10}a_6}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_2i_3} t^{a_7a_8}_{i_4i_9} + \tfrac{1}{2} P_4P_4 v^{a_5a_6}_{a_9a_{10}} F^{a_9a_7}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} t^{a_8a_{10}}_{i_3i_4} \\ &+\tfrac{1}{2} P_4P_4 v^{i_9a_5}_{i_1a_{10}} r^{a_6a_7}_{i_2i_9} F^{\alpha_{10}a_8}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_4} - \tfrac{1}{2} P_4P_4 v^{a_5a_6}_{a_9a_{10}} r^{a_7a_{10}}_{i_1i_2} F^{\alpha_9a_8}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_4} - \tfrac{1}{4} P_4P_4 v^{a_5a_6}_{a_9a_{10}} F^{a_9a_7}_{i_{11}i_{12}} r^{i_{11}i_{12}}_{i_1i_2} F^{\alpha_{10}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_3i_4} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5a_6}_{i_2i_9} t^{a_7}_{i_{10}} F^{\alpha_{11}a_8}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_3i_4} \\ &+\tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6a_7}_{i_1i_9} t^{a_{11}}_{i_2} F^{\alpha_{10}a_8}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_3i_4} + \tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_7}_{i_9} t^{a_6}_{i_1i_2} F^{\alpha_{10}a_8}_{i_{12}i_{13}} t^{i_{12}i_{13}}_{i_3i_4} + \tfrac{1}{4} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} r^{i_{12}i_{13}}_{i_1i_2} t^{a_7}_{i_9} F^{\alpha_{11}a_8}_{i_{14}i_{15}} t^{i_{14}i_{15}}_{i_3i_4} - P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5a_6}_{i_2i_9} t^{a_7a_8}_{i_3i_{10}} t^{a_{11}}_{i_4} \\ &-P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5a_6}_{i_2i_9} t^{a_7a_{11}}_{i_3i_4} t^{a_8}_{i_{10}} + P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6a_7}_{i_1i_9} t^{a_8a_{11}}_{i_2i_3} t^{a_{10}}_{i_4} + P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5a_{11}}_{i_2i_3} t^{a_6a_7}_{i_4i_{10}} t^{a_8}_{i_9} - P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6a_{10}}_{i_1i_2} t^{a_7a_{11}}_{i_3i_9} t^{a_8}_{i_4} - P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6a_{10}}_{i_1i_2} t^{a_7a_{11}}_{i_3i_4} t^{a_8}_{i_9} \\ &-\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} F^{\alpha_{11}a_5}_{i_{12}i_{13}} r^{i_{12}i_{13}}_{i_2i_3} t^{a_6a_7}_{i_4i_{10}} t^{a_8}_{i_9} + \tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} r^{i_{12}i_{13}}_{i_1i_2} t^{a_7a_8}_{i_3i_9} t^{a_{11}}_{i_4} + \tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{11}a_{12}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} r^{i_{12}i_{13}}_{i_1i_2} t^{a_7a_{11}}_{i_3i_4} t^{a_8}_{i_9} + P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5a_6}_{i_2i_9} t^{a_7a_8a_{11}}_{i_3i_4i_{10}} \\ &-\tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6a_7}_{i_1i_9} t^{a_8a_{10}a_{11}}_{i_2i_3i_4} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5a_6}_{i_2i_3i_4} t^{a_7a_8a_{11}}_{i_9i_{10}} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5a_{11}}_{i_2i_3} t^{a_6a_7a_8}_{i_4i_9i_{10}} + P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6a_{10}}_{i_1i_2} t^{a_7a_8a_{11}}_{i_3i_4i_9} - P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} r^{a_5a_{11}}_{i_2i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} \\ &-P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_6a_{10}}_{i_1i_9} t^{a_7a_8a_{11}}_{i_2i_3i_4} + \tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} r^{a_{10}a_{11}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9} + \tfrac{1}{4} P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} F^{\alpha_{11}a_5}_{i_{12}i_{13}} r^{i_{12}i_{13}}_{i_2i_3} t^{a_6a_7a_8}_{i_4i_9i_{10}} - \tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} r^{i_{12}i_{13}}_{i_1i_2} t^{a_7a_8a_{11}}_{i_3i_4i_9} \\ &+\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{i_1a_{11}} F^{\alpha_{11}a_5}_{i_{12}i_{13}} r^{i_{12}i_{13}}_{i_2i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} + \tfrac{1}{2} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} F^{\alpha_{10}a_6}_{i_{12}i_{13}} r^{i_{12}i_{13}}_{i_1i_9} t^{a_7a_8a_{11}}_{i_2i_3i_4} + \tfrac{1}{4} P_4P_4 v^{i_9a_5}_{a_{10}a_{11}} F^{\alpha_{10}\alpha_{11}}_{i_{12}i_{13}} r^{i_{12}i_{13}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9} \\ &-\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_6}_{i_1i_9} t^{a_{12}}_{i_2} t^{a_7}_{i_{10}} F^{\alpha_{11}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_3i_4} - \tfrac{1}{4} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_{12}}_{i_1i_2} t^{a_6}_{i_9} t^{a_7}_{i_{10}} F^{\alpha_{11}a_8}_{i_{13}i_{14}} t^{i_{13}i_{14}}_{i_3i_4} - \tfrac{1}{8} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} r^{i_{13}i_{14}}_{i_1i_2} t^{a_6}_{i_9} t^{a_7a_8a_{12}}_{i_{10}i_2i_3i_4} \\ &+\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_6}_{i_1i_9} t^{a_7}_{i_2} t^{a_8a_{11}a_{12}}_{i_{10}i_3i_4} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_6}_{i_1i_9} t^{a_7a_8a_{12}}_{i_2i_3i_{10}} t^{a_{11}}_{i_4} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_6}_{i_9i_{10}} t^{a_7a_8a_{11}}_{i_1i_2i_3i_4} \\ &-P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_{11}}_{i_1i_2} t^{a_6}_{i_9} t^{a_7a_8a_{12}}_{i_3i_4i_{10}} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_{11}}_{i_1i_2} t^{a_{12}}_{i_3} t^{a_6a_7a_8}_{i_4i_9i_{10}} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_{11}}_{i_1i_2} t^{a_{12}}_{i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} - P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_{11}}_{i_1i_9} t^{a_6a_7a_8}_{i_2i_3i_4} \\ &-P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_{11}}_{i_1i_9} t^{a_{12}}_{i_2} t^{a_6a_7a_8}_{i_3i_4i_{10}} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}a_{12}}_{i_1i_2} t^{a_5}_{i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} r^{i_{13}i_{14}}_{i_1i_2} t^{a_6}_{i_9} t^{a_7a_8a_{12}}_{i_3i_4i_{10}} - \tfrac{1}{4} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} r^{i_{13}i_{14}}_{i_1i_2} t^{a_{12}}_{i_3} t^{a_6a_7a_8}_{i_4i_9i_{10}} \\ &-\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} r^{i_{13}i_{14}}_{i_1i_2} t^{a_6a_7a_8}_{i_9} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} r^{i_{13}i_{14}}_{i_1i_9} t^{a_6}_{i_{10}} t^{a_7a_8a_{12}}_{i_2i_3i_4} + \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} r^{i_{13}i_{14}}_{i_2i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} \\ &+\tfrac{1}{4} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}} r^{i_{13}i_{14}}_{i_1i_2} t^{a_5}_{i_9} t^{a_6a_7a_8}_{i_3i_4i_{10}} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_6}_{i_1i_2} t^{a_7a_8}_{i_3i_9} t^{a_{11}a_{12}}_{i_4i_{10}} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_6}_{i_1i_9} t^{a_7a_8}_{i_2i_3i_4} t^{a_{11}a_{12}}_{i_{10}} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_{11}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_9} t^{a_{12}}_{i_{10}} \\ &-\tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_{11}}_{i_1i_2} t^{a_6a_{12}}_{i_3i_4} t^{a_7}_{i_9} t^{a_8}_{i_{10}} - \tfrac{1}{2} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} r^{i_{13}i_{14}}_{i_1i_2} t^{a_6a_7a_8}_{i_3i_4i_{10}} t^{a_{12}}_{i_9} + \tfrac{1}{4} P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} F^{\alpha_{11}a_5}_{i_{13}i_{14}} r^{i_{13}i_{14}}_{i_1i_2} t^{a_6a_{12}}_{i_3i_4} t^{a_7}_{i_9} t^{a_8}_{i_{10}} + P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_5a_6}_{i_1i_9} t^{a_7a_{11}}_{i_2i_{10}} t^{a_{12}}_{i_3i_4}\end{aligned}$$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.2.XXXIV: The R_4 amplitude equation of EOM-CCSDTQ-R12 obtained with the modified ansatz 2 [Part II]

$$
\begin{aligned}
&-\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6}_{i_1i_9}t^{a_{11}a_{12}}_{i_2i_3}t^{a_7a_8}_{i_4i_{10}} - \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6}_{i_9i_{10}}t^{a_7a_{11}}_{i_1i_2}t^{a_8a_{12}}_{i_3i_4} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_{11}}_{i_1i_2}t^{a_6a_{12}}_{i_3i_4}t^{a_7a_8}_{i_9i_{10}} + P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_{11}}_{i_1i_2}t^{a_6a_{12}}_{i_3i_9}t^{a_7a_8}_{i_4i_{10}}\\
&+P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_{11}}_{i_1i_9}t^{a_6a_{12}}_{i_2i_3}t^{a_7a_8}_{i_4i_{10}} - \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_{11}a_{12}}_{i_1i_2}t^{a_5a_6}_{i_3i_9}t^{a_7a_8}_{i_4i_{10}} + \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}F^{\alpha_{11}a_5}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_2}t^{a_6a_{12}}_{i_3i_4}t^{a_7a_8}_{i_9i_{10}} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}F^{\alpha_{11}a_5}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_2}t^{a_6a_{12}}_{i_3i_9}t^{a_7a_8}_{i_4i_{10}}\\
&-\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}F^{\alpha_{11}a_5}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_9}t^{a_6a_{12}}_{i_2i_3}t^{a_7a_8}_{i_4i_{10}} - \tfrac{1}{8}P_4P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_2}t^{a_5a_6}_{i_3i_9}t^{a_7a_8}_{i_4i_{10}} - \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}r^{a_5a_6}_{i_1i_9}t^{a_7a_8}_{i_2i_{10}}F^{\alpha_{11}a_{12}}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4}\\
&-\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6}_{i_1i_9}t^{a_7a_{12}}_{i_2i_3}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_4i_9} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6}_{i_1i_9}t^{a_7a_{12}}_{i_2i_{10}}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4} - \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6}_{i_9i_{10}}t^{a_7a_{12}}_{i_1i_2}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4}\\
&+\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_{12}}_{i_1i_2}t^{a_6a_7}_{i_3i_9}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_4i_{10}} - \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_{12}}_{i_1i_2}t^{a_6a_7}_{i_9i_{10}}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_{12}}_{i_1i_9}t^{a_6a_7}_{i_2i_{10}}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4}\\
&+\tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}F^{\alpha_{11}a_5}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_2}t^{a_6a_7}_{i_3i_9}F^{\alpha_{12}a_8}_{i_{15}i_{16}}t^{i_{15}i_{16}}_{i_4i_{10}} - \tfrac{1}{8}P_4P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}F^{\alpha_{11}a_5}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_2}t^{a_6a_7}_{i_9i_{10}}F^{\alpha_{12}a_8}_{i_{15}i_{16}}t^{i_{15}i_{16}}_{i_3i_4} + \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}F^{\alpha_{11}a_5}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_9}t^{a_6a_7}_{i_2i_{10}}F^{\alpha_{12}a_8}_{i_{15}i_{16}}t^{i_{15}i_{16}}_{i_3i_4}\\
&-\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6}_{i_1i_9}t^{a_7a_8a_{11}a_{12}}_{i_2i_3i_4i_{10}} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6}_{i_9i_{10}}t^{a_7a_8a_{11}a_{12}}_{i_1i_2i_3i_4} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_{11}}_{i_1i_2}t^{a_6a_7a_8a_{12}}_{i_3i_4i_9i_{10}} + P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_{11}}_{i_1i_9}t^{a_6a_7a_8a_{12}}_{i_2i_3i_4i_{10}}\\
&-\tfrac{1}{2}P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_{11}}_{i_9i_{10}}t^{a_6a_7a_8a_{12}}_{i_1i_2i_3i_4} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_{11}a_{12}}_{i_1i_2}t^{a_5a_6a_7a_8}_{i_3i_4i_9i_{10}} - \tfrac{1}{2}P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_{11}a_{12}}_{i_1i_9}t^{a_5a_6a_7a_8}_{i_2i_3i_4i_{10}} + \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}F^{\alpha_{11}a_5}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_2}t^{a_6a_7a_8a_{12}}_{i_3i_4i_9i_{10}}\\
&-\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}F^{\alpha_{11}a_5}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_9}t^{a_6a_7a_8a_{12}}_{i_2i_3i_4i_{10}} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}F^{\alpha_{11}a_5}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_9i_{10}}t^{a_6a_7a_8a_{12}}_{i_1i_2i_3i_4} + \tfrac{1}{8}P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_2}t^{a_5a_6a_7a_8}_{i_3i_4i_9i_{10}}\\
&-\tfrac{1}{4}P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}}r^{i_{13}i_{14}}_{i_1i_9}t^{a_5a_6a_7a_8}_{i_2i_3i_4i_{10}} - \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}r^{a_5a_6}_{i_1i_{10}}F^{\alpha_{11}a_7}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_2i_9}F^{\alpha_{12}a_8}_{i_{15}i_{16}}t^{i_{15}i_{16}}_{i_3i_4} - \tfrac{1}{16}P_4P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}r^{a_5a_6}_{i_9i_{10}}F^{\alpha_{11}a_7}_{i_{13}i_{14}}t^{i_1i_2}_{i_{15}i_{16}}F^{\alpha_{12}a_8}_{i_{15}i_{16}}t^{i_3i_4}_{i_1i_2}\\
&+P_4P_4v^{i_9a_5}_{i_1i_2}r^{a_6a_7a_8}_{i_3i_4i_9} + P_4P_4v^{a_5a_6}_{i_1a_9}r^{a_7a_8a_9}_{i_2i_3i_4} + P_4P_4v^{i_9i_{10}}_{i_1i_2}r^{a_5a_6a_7}_{i_3i_4i_9}t^{a_8}_{i_{10}} + P_4P_4v^{i_9a_5}_{i_1a_{10}}r^{a_6a_7a_8}_{i_2i_3i_9}t^{a_{10}}_{i_4} + P_4P_4v^{i_9a_5}_{i_1a_{10}}r^{a_6a_7a_{10}}_{i_2i_3i_4}t^{a_8}_{i_9} + P_4P_4v^{a_5a_6}_{a_9a_{10}}r^{a_7a_8a_9}_{i_1i_2i_3}t^{a_{10}}_{i_4}\\
&+P_4P_4v^{i_9i_{10}}_{i_1a_{11}}r^{a_5a_6a_7}_{i_2i_3i_9}t^{a_{11}}_{i_4}t^{a_8}_{i_{10}} + \tfrac{1}{2}P_4P_4v^{i_9a_5}_{a_{10}a_{11}}r^{a_6a_7a_8}_{i_1i_2i_9}t^{a_{10}}_{i_3}t^{a_{11}}_{i_4} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{i_1a_{11}}r^{a_5a_6a_{11}}_{i_2i_3i_4}t^{a_7}_{i_9}t^{a_8}_{i_{10}} + P_4P_4v^{i_9a_5}_{a_{10}a_{11}}r^{a_6a_7a_{10}}_{i_1i_2i_3}t^{a_{11}}_{i_4}t^{a_8}_{i_9} - P_4P_4v^{i_9i_{10}}_{i_1a_{11}}r^{a_5a_6a_7}_{i_2i_3i_9}t^{a_8a_{11}}_{i_4i_{10}}\\
&+\tfrac{1}{2}P_4P_4v^{i_9a_5}_{a_{10}a_{11}}r^{a_6a_7a_8}_{i_1i_2i_9}t^{a_{10}a_{11}}_{i_3i_4} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{i_1a_{11}}r^{a_5a_6a_7}_{i_2i_9i_{10}}t^{a_8a_{11}}_{i_3i_4} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{i_1a_{11}}r^{a_5a_6a_{11}}_{i_2i_3i_4}t^{a_7a_8}_{i_9i_{10}} - P_4P_4v^{i_9a_5}_{a_{10}a_{11}}r^{a_6a_7a_{10}}_{i_1i_2i_3}t^{a_8a_{11}}_{i_4i_9} - P_4P_4v^{i_9i_{10}}_{i_1a_{11}}r^{a_5a_6a_{11}}_{i_2i_3i_9}t^{a_7a_8}_{i_4i_{10}}\\
&-P_4P_4v^{i_9a_5}_{a_{10}a_{11}}r^{a_6a_7a_{10}}_{i_1i_2i_9}t^{a_8a_{11}}_{i_3i_4} + \tfrac{1}{2}P_4P_4v^{i_9a_5}_{a_{10}a_{11}}r^{a_6a_{10}a_{11}}_{i_1i_2i_3}t^{a_7a_8}_{i_4i_9} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{i_1a_{11}}r^{a_5a_6a_7}_{i_2i_3i_{10}}F^{\alpha_{11}a_8}_{i_{12}i_{13}}t^{i_{12}i_{13}}_{i_4i_9} + \tfrac{1}{4}P_4P_4v^{i_9a_5}_{\alpha_{10}a_{11}}r^{a_6a_7a_8}_{i_1i_2i_9}F^{\alpha_{10}a_{11}}_{i_{12}i_{13}}t^{i_{12}i_{13}}_{i_3i_4}\\
&-\tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{i_1a_{11}}r^{a_5a_6a_7}_{i_2i_9i_{10}}F^{\alpha_{11}a_8}_{i_{12}i_{13}}t^{i_{12}i_{13}}_{i_3i_4} - \tfrac{1}{2}P_4P_4v^{i_9a_5}_{\alpha_{10}a_{11}}r^{a_6a_7a_{11}}_{i_1i_2i_3}F^{\alpha_{10}a_8}_{i_{12}i_{13}}t^{i_{12}i_{13}}_{i_4i_9} - \tfrac{1}{2}P_4P_4v^{i_9a_5}_{\alpha_{10}a_{11}}r^{a_6a_7a_{11}}_{i_1i_2i_9}F^{\alpha_{10}a_8}_{i_{12}i_{13}}t^{i_{12}i_{13}}_{i_3i_4} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_2i_9}t^{a_{11}}_{i_3}t^{a_{12}}_{i_4}t^{a_8}_{i_{10}}\\
&+\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}}_{i_1i_2i_3}t^{a_{12}}_{i_4}t^{a_7}_{i_9}t^{a_8}_{i_{10}} + \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_2i_9}t^{a_8}_{i_{10}}F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_2i_{10}}t^{a_{12}}_{i_3}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_4i_9}\\
&-\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_2i_9}t^{a_{12}}_{i_{10}}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4} - \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_9i_{10}}t^{a_{12}}_{i_2}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_2i_3}t^{a_7}_{i_{10}}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_4i_9}\\
&+\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6a_{12}}_{i_1i_2i_9}t^{a_7}_{i_{10}}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4} - P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_2i_9}t^{a_8a_{12}}_{i_3i_4}t^{a_{11}}_{i_{10}} + P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_2i_9}t^{a_8a_{12}}_{i_3i_{10}}t^{a_{11}}_{i_4} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_2i_9}t^{a_{11}a_{12}}_{i_3i_4}t^{a_8}_{i_{10}}\\
&-\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_9i_{10}}t^{a_8a_{11}a_{12}}_{i_2i_3}t^{a_{11}}_{i_4} - P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}}_{i_1i_2i_3}t^{a_7a_8}_{i_4i_9}t^{a_{12}}_{i_{10}} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}}_{i_1i_2i_9}t^{a_7a_8}_{i_3i_{10}}t^{a_{12}}_{i_4} + P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}}_{i_1i_2i_9}t^{a_7a_8a_{12}}_{i_3i_4i_{10}}t^{a_{11}}_{i_9}\\
&-P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}}_{i_1i_2i_9}t^{a_7a_8}_{i_3i_{10}}t^{a_{12}}_{i_4} - P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_{11}a_{12}}_{i_1i_2i_9}t^{a_7a_8}_{i_3i_4}t^{a_6a_7}_{i_{10}} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_{11}a_{12}}_{i_1i_2i_3}t^{a_6a_7}_{i_4i_{10}}t^{a_8}_{i_9} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}}_{i_1i_2i_9}t^{a_7a_8a_{12}}_{i_3i_4i_9i_{10}}\\
&+\tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7}_{i_1i_2i_9}t^{a_8a_{11}a_{12}}_{i_3i_4i_{10}} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}}_{i_1i_2i_3}t^{a_7a_8a_{12}}_{i_4i_9i_{10}} + P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}}_{i_1i_2i_9}t^{a_7a_8a_{12}}_{i_3i_4i_{10}}t^{a_{11}}_{i_9} + P_4P_4v^{i_9a_5}_{i_1a_{10}}r^{a_6a_7a_8a_{10}}_{i_2i_3i_4i_9}t^{a_{11}}_{i_{10}} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{i_1i_2}r^{a_5a_6a_7a_8}_{i_3i_4i_9i_{10}}t^{a_{11}a_{12}}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_{15}i_{16}}t^{i_{15}i_{16}}_{i_{17}i_{18}}\\
&+\tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}}_{i_1i_2i_3}t^{a_7a_8}_{i_4i_9}t^{a_{12}}_{i_{10}} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7a_8}_{i_1i_2i_3i_9}t^{a_{11}a_{12}}_{i_4i_{10}} + \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}}t^{a_{11}a_{12}}_{i_3i_4} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7a_{11}}_{i_1i_2i_3i_4}t^{a_8a_{12}}_{i_9i_{10}} + P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7a_{11}}_{i_1i_2i_3i_9}t^{a_8a_{12}}_{i_4i_{10}}\\
&-\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_7a_{11}}_{i_1i_2i_9i_{10}}t^{a_8a_{12}}_{i_3i_4} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}a_{12}}_{i_1i_2i_3i_4}t^{a_7a_8}_{i_9i_{10}} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}r^{a_5a_6a_{11}a_{12}}_{i_1i_2i_3i_9}t^{a_7a_8}_{i_4i_{10}} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}r^{a_5a_6a_7a_8}_{i_1i_2i_3i_{10}}F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_4i_9}\\
&+\tfrac{1}{8}P_4v^{i_9i_{10}}_{\alpha_{11}\alpha_{12}}r^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}}F^{\alpha_{11}\alpha_{12}}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4} - \tfrac{1}{4}P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6a_7a_{12}}_{i_1i_2i_3i_4}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_9i_{10}} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6a_7a_{12}}_{i_1i_2i_3i_{10}}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_4i_9} - \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{\alpha_{11}a_{12}}r^{a_5a_6a_7a_{12}}_{i_1i_2i_9i_{10}}F^{\alpha_{11}a_8}_{i_{13}i_{14}}t^{i_{13}i_{14}}_{i_3i_4}
\end{aligned}
$$

Supplementary data for Phys. Chem. Chem. Phys.

3. EQUATIONS WITH SPECIAL INTERMEDIATES AND THE RI INSERTION USING THE CABS

A. CCSD-R12

TABLE ESI.3.I: The energy equation of CCSD-R12 and higher-order CC-R12 with special intermediates and the RI insertion using the CABS

$$e = +f^{i_2}_{a_1} t^{a_1}_{i_2} + \tfrac{1}{2} v^{i_2 i_4}_{a_1 a_3} t^{a_3}_{i_4} t^{a_1}_{i_2} + \tfrac{1}{4} v^{i_3 i_4}_{a_1 a_2} t^{a_1 a_2}_{i_3 i_4} + \tfrac{1}{4} V^{i_3 i_4}_{i_1 i_2} t^{i_1 i_2}_{i_3 i_4}$$

TABLE ESI.3.II: The T_1 amplitude equation of CCSD-R12 with special intermediates and the RI insertion using the CABS

$$\begin{aligned}\delta^{a_2}_{i_1} &= +f^{a_2}_{i_1} - f^{i_3}_{i_1} t^{a_2}_{i_3} + f^{a_2}_{a_3} t^{a_3}_{i_1} - f^{i_3}_{a_4} t^{a_4}_{i_1} t^{a_2}_{i_3} + f^{i_4}_{a_3} t^{a_2 a_3}_{i_1 i_4} - f^{i_4}_{a_3} \tilde{t}^{a'_3 a_2}_{i_1 i_4} - v^{i_4 a_2}_{i_1 a_3} t^{a_3}_{i_4} - v^{i_3 i_5}_{i_1 a_4} t^{a_4}_{i_5} t^{a_2}_{i_3} - v^{i_5 a_2}_{a_3 a_4} t^{a_4}_{i_5} t^{a_3}_{i_1} - \tfrac{1}{2} v^{i_4 i_5}_{i_1 a_3} t^{a_2 a_3}_{i_4 i_5} - \tfrac{1}{2} v^{i_5 a_2}_{a_3 a_4} t^{a_3 a_4}_{i_1 i_5} + \tfrac{1}{2} v^{i_4 i_5}_{i_1 a'_3} \tilde{t}^{a'_3 a_2}_{i_4 i_5} \\ &\quad - \tfrac{1}{2} V^{i_5 a_2}_{i_3 i_4} t^{i_3 i_4}_{i_1 i_5} - v^{i_3 i_6}_{a_4 a_5} t^{a_5}_{i_6} t^{a_4}_{i_1} t^{a_2}_{i_3} + v^{i_4 i_6}_{a_3 a_5} t^{a_5}_{i_6} t^{a_2 a_3}_{i_1 i_4} + \tfrac{1}{2} v^{i_4 i_5}_{a_3 a_6} t^{a_6}_{i_1} t^{a_2 a_3}_{i_4 i_5} - \tfrac{1}{2} v^{i_3 i_6}_{a_4 a_5} t^{a_4 a_5}_{i_1 i_6} t^{a_2}_{i_3} - v^{i_4 i_6}_{a'_3 a_5} t^{a_5}_{i_6} \tilde{t}^{a'_3 a_2}_{i_1 i_4} - \tfrac{1}{2} v^{i_4 i_5}_{a'_3 a_6} t^{a_6}_{i_1} \tilde{t}^{a'_3 a_2}_{i_4 i_5} - \tfrac{1}{2} V^{i_3 i_6}_{i_4 i_5} t^{i_4 i_5}_{i_1 i_6} t^{a_2}_{i_3}\end{aligned}$$

TABLE ESI.3.III: The T_2 amplitude equation of CCSD-R12 with special intermediates and the RI insertion using the CABS

$$\begin{aligned}\delta^{a_3 a_4}_{i_1 i_2} &= -P_2 f^{i_5}_{i_2} t^{a_3 a_4}_{i_1 i_5} + P_2 f^{a_4}_{a_5} t^{a_3 a_5}_{i_1 i_2} - P_2 f^{a_4}_{a'_5} \tilde{t}^{a'_5 a_3}_{i_1 i_2} - P_2 f^{i_5}_{a'_6} \tilde{t}^{a'_6 a_4}_{i_1 i_2} t^{a_3}_{i_5} + P_2 f^{i_5}_{a_6} t^{a_4 a_6}_{i_1 i_2} t^{a_3}_{i_5} - P_2 f^{i_5}_{a_6} t^{a_6}_{i_2} t^{a_3 a_4}_{i_1 i_5} + v^{a_3 a_4}_{i_1 i_2} - P_2 v^{i_5 a_4}_{i_1 i_2} t^{a_3}_{i_5} - P_2 v^{a_3 a_4}_{i_2 a_5} t^{a_5}_{i_1} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{i_1 i_2} t^{a_4}_{i_6} t^{a_3}_{i_5} \\ &\quad + P_2 P_2 v^{i_5 a_4}_{i_2 a_6} t^{a_6}_{i_1} t^{a_3}_{i_5} + \tfrac{1}{2} P_2 v^{a_3 a_4}_{a_5 a_6} t^{a_6}_{i_2} t^{a_5}_{i_1} + \tfrac{1}{2} v^{i_5 i_6}_{i_1 i_2} t^{a_3 a_4}_{i_5 i_6} - P_2 P_2 v^{i_6 a_4}_{i_2 a_5} t^{a_3 a_5}_{i_1 i_6} + \tfrac{1}{2} v^{a_3 a_4}_{a_5 a_6} t^{a_5 a_6}_{i_1 i_2} + P_2 P_2 v^{i_6 a_4}_{i_2 a'_5} \tilde{t}^{a'_5 a_3}_{i_1 i_6} + \tfrac{1}{2} V^{a_3 a_4}_{i_5 i_6} t^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{i_2 a_7} t^{a_7}_{i_1} t^{a_4}_{i_6} t^{a_3}_{i_5} \\ &\quad - \tfrac{1}{2} P_2 P_2 v^{i_5 a_4}_{a_6 a_7} t^{a_7}_{i_2} t^{a_6}_{i_1} t^{a_3}_{i_5} + P_2 v^{i_7 a_4}_{a'_5 a_6} t^{a_6}_{i_7} \tilde{t}^{a'_5 a_3}_{i_1 i_2} - P_2 P_2 v^{i_5 i_7}_{i_2 a'_6} \tilde{t}^{a'_6 a_4}_{i_1 i_7} t^{a_3}_{i_5} - P_2 P_2 v^{i_6 a_4}_{a'_5 a_7} t^{a_7}_{i_2} \tilde{t}^{a'_5 a_3}_{i_1 i_6} - \tfrac{1}{2} P_2 V^{i_5 a_4}_{i_6 i_7} t^{i_6 i_7}_{i_1 i_2} t^{a_3}_{i_5} + P_2 P_2 v^{i_5 i_7}_{i_2 a_6} t^{a_4 a_6}_{i_1 i_7} t^{a_3}_{i_5} - \tfrac{1}{2} P_2 v^{i_5 a_4}_{a_6 a_7} t^{a_6 a_7}_{i_1 i_2} t^{a_3}_{i_5} \\ &\quad - \tfrac{1}{2} P_2 v^{i_5 i_6}_{i_2 a_7} t^{a_7}_{i_1} t^{a_3 a_4}_{i_5 i_6} + P_2 P_2 v^{i_6 a_4}_{a_5 a_7} t^{a_7}_{i_2} t^{a_3 a_5}_{i_1 i_6} - P_2 v^{i_5 i_7}_{i_2 a_6} t^{a_6}_{i_7} t^{a_3 a_4}_{i_1 i_5} - P_2 v^{i_7 a_4}_{a_5 a_6} t^{a_6}_{i_7} t^{a_3 a_5}_{i_1 i_2} + \tfrac{1}{4} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_8}_{i_2} t^{a_7}_{i_1} t^{a_4}_{i_6} t^{a_3}_{i_5} - P_2 v^{i_5 i_8}_{a'_6 a_7} t^{a_7}_{i_8} \tilde{t}^{a'_6 a_4}_{i_1 i_2} t^{a_3}_{i_5} \\ &\quad + P_2 P_2 v^{i_5 i_7}_{a'_6 a_8} t^{a_8}_{i_2} \tilde{t}^{a'_6 a_4}_{i_1 i_7} t^{a_3}_{i_5} + \tfrac{1}{4} P_2 V^{i_5 i_6}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_2} t^{a_4}_{i_6} t^{a_3}_{i_5} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_7 a_8}_{i_1 i_2} t^{a_4}_{i_6} t^{a_3}_{i_5} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_8}_{i_2} t^{a_7}_{i_1} t^{a_3 a_4}_{i_5 i_6} - P_2 P_2 v^{i_5 i_7}_{a_6 a_8} t^{a_8}_{i_2} t^{a_4 a_6}_{i_1 i_7} t^{a_3}_{i_5} - P_2 v^{i_5 i_8}_{a_6 a_7} t^{a_7}_{i_8} t^{a_6}_{i_2} t^{a_3 a_4}_{i_1 i_5} \\ &\quad + P_2 v^{i_5 i_8}_{a_6 a_7} t^{a_7}_{i_8} t^{a_4 a_6}_{i_1 i_2} t^{a_3}_{i_5} + \tfrac{1}{2} P_2 P_2 v^{i_6 i_8}_{a_5 a_7} t^{a_4 a_7}_{i_2 i_8} t^{a_3 a_5}_{i_1 i_6} - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a_5 a_6} t^{a_6 a_7}_{i_7 i_8} t^{a_3 a_5}_{i_1 i_2} + \tfrac{1}{4} v^{i_5 i_6}_{a_7 a_8} t^{a_7 a_8}_{i_1 i_2} t^{a_3 a_4}_{i_5 i_6} - \tfrac{1}{2} P_2 v^{i_5 i_8}_{a_6 a_7} t^{a_6 a_7}_{i_2 i_8} t^{a_4 a_6}_{i_1 i_5} + \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_5 a_6} t^{a'_5 a_3}_{i_7 i_8} t^{a_4 a_6}_{i_1 i_2} \\ &\quad + P_2 P_2 v^{i_6 i_8}_{a'_7 a_5} \tilde{t}^{a'_7 a_4}_{i_2 i_8} t^{a_3 a_5}_{i_1 i_6} - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_6 a_5} \tilde{t}^{a'_6 a_4}_{i_7 i_8} t^{a_3 a_5}_{i_1 i_2} + \tfrac{1}{4} V^{i_5 i_6}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_2} t^{a_3 a_4}_{i_5 i_6} - \tfrac{1}{2} P_2 V^{i_5 i_8}_{i_6 i_7} t^{i_6 i_7}_{i_2 i_8} t^{a_3 a_4}_{i_1 i_5} + \tfrac{1}{2} P_2 P_2 v^{i_6 i_8}_{a'_5 a'_7} \tilde{t}^{a'_7 a_4}_{i_2 i_8} \tilde{t}^{a'_5 a_3}_{i_1 i_6} - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_5 a'_6} \tilde{t}^{a'_6 a_4}_{i_7 i_8} \tilde{t}^{a'_5 a_3}_{i_1 i_2}\end{aligned}$$

TABLE ESI.3.IV: The geminal t amplitude equation of CCSD-R12 with special intermediates and the RI insertion using the CABS

$$\begin{aligned}\delta^{i_3 i_4}_{i_1 i_2} &= +F^{i_3 i_4 *}_{a'_7 a_6} f^{a'_7}_{a_5} t^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{2} P_2 X^{i_3 i_4}_{i_6 i_7} t^{i_6 i_7}_{i_2 i_5} f^{i_5}_{i_1} + \tfrac{1}{2} B^{i_3 i_4}_{i_5 i_6} t^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{2} P_2 f^{i_7}_{a_8} t^{a_8}_{i_2} t^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} - f^{i_7}_{a_8} \tilde{t}^{a'_5 a'_8}_{i_1 i_2} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - f^{i_7}_{a_8} \tilde{t}^{a'_5 a'_8}_{i_1 i_2} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + (V^\dagger)^{i_3 i_4}_{i_1 i_2} + F^{i_3 i_4 *}_{a'_6 a_7} t^{a_7}_{i_5} v^{i_5 a'_6}_{i_1 i_2} \\ &\quad - P_2 (V^\dagger)^{i_3 i_4}_{i_2 a_5} t^{a_5}_{i_1} - P_2 F^{i_3 i_4 *}_{a'_7 a_8} t^{a_8}_{i_6} v^{i_6 a'_7}_{i_2 a_5} t^{a_5}_{i_1} + \tfrac{1}{2} P_2 (V^\dagger)^{i_3 i_4}_{a_5 a_6} t^{a_6}_{i_2} t^{a_5}_{i_1} + P_2 v^{i_8 a'_5}_{i_2 a_7} t^{a_6 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} (V^\dagger)^{i_3 i_4}_{a_5 a_6} t^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{4} v^{i_7 i_8}_{i_1 i_2} t^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} - P_2 v^{i_8 a'_6}_{i_2 a'_7} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} \\ &\quad - P_2 v^{i_8 a'_5}_{i_2 a'_7} \tilde{t}^{a'_7 a_6}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} - P_2 v^{i_8 a_6}_{i_2 a'_7} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} - P_2 v^{i_8 a'_6}_{i_2 a'_7} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} - P_2 v^{i_8 a_6}_{i_2 a'_7} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} P^{i_3 i_4}_{i_5 i_6} t^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} P_2 v^{i_7 a'_5}_{a_8 a_9} t^{a_9}_{i_2} t^{a_8}_{i_1} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + v^{i_9 a'_7}_{a_6 a_8} t^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_7 a_5} t^{a_5 a_6}_{i_1 i_2} \\ &\quad - P_2 v^{i_8 a'_5}_{a_7 a_9} t^{a_9}_{i_2} t^{a_6 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} F^{i_3 i_4 *}_{a'_8 a_9} t^{a_9}_{i_7} v^{i_7 a'_8}_{a_5 a_6} t^{a_5 a_6}_{i_1 i_2} - \tfrac{1}{2} P_2 v^{i_7 i_9}_{i_2 a_8} t^{a_8}_{i_9} t^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} - \tfrac{1}{4} P_2 v^{i_7 i_8}_{i_2 a_9} t^{a_9}_{i_1} t^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} - v^{i_9 a'_7}_{a'_6 a_8} t^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_8 a'_7} \tilde{t}^{a'_5 a'_6}_{i_1 i_2} - v^{i_9 a'_7}_{a'_5 a_8} t^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_7 a_6} t^{a_5 a_6}_{i_1 i_2} \\ &\quad - v^{i_9 a_6}_{a'_7 a_8} t^{a_8}_{i_9} \tilde{t}^{a'_5 a'_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} - v^{i_9 a'_7}_{a_6 a_8} t^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} - v^{i_9 a_6}_{a'_7 a_8} t^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} - P_2 v^{i_7 i_9}_{i_2 a'_8} \tilde{t}^{a'_5 a'_8}_{i_1 i_9} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - P_2 v^{i_7 i_9}_{i_2 a_8} \tilde{t}^{a'_5 a_8}_{i_1 i_9} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_8 a'_6}_{a'_7 a_9} t^{a_9}_{i_2} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} \\ &\quad + P_2 v^{i_8 a'_5}_{a'_7 a_9} t^{a_9}_{i_2} \tilde{t}^{a'_7 a_6}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_8 a_6}_{a'_7 a_9} t^{a_9}_{i_2} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} + P_2 v^{i_8 a'_6}_{a_7 a_9} t^{a_9}_{i_2} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} F^{i_3 i_4 *}_{a'_8 a_9} t^{a_9}_{i_7} V^{i_7 a'_8}_{i_5 i_6} t^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{2} P_2 v^{i_7 i_{10}}_{a_8 a_9} t^{a_9}_{i_{10}} t^{a_8}_{i_1} t^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} \\ &\quad + \tfrac{1}{8} P_2 v^{i_7 i_8}_{a_9 a_{10}} t^{a_{10}}_{i_2} t^{a_9}_{i_1} t^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} - v^{i_7 i_{10}}_{a'_8 a_9} t^{a_9}_{i_{10}} \tilde{t}^{a'_5 a'_8}_{i_1 i_2} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_7 i_9}_{a'_8 a_{10}} t^{a_{10}}_{i_2} \tilde{t}^{a'_5 a'_8}_{i_1 i_9} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_7 i_9}_{a_8 a_{10}} t^{a_{10}}_{i_2} \tilde{t}^{a'_5 a_8}_{i_1 i_9} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} \\ &\quad - \tfrac{1}{4} P_2 v^{i_7 i_{10}}_{a_8 a_9} t^{a_8 a_9}_{i_2 i_{10}} t^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{8} v^{i_7 i_8}_{a_9 a_{10}} t^{a_9 a_{10}}_{i_1 i_2} t^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} t^{a_6 a_8}_{i_9 i_{10}} \tilde{t}^{a'_5 a'_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a_6 a_8} t^{a_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} + P_2 v^{i_8 i_{10}}_{a'_7 a_9} t^{a_6 a_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} \\ &\quad + P_2 v^{i_8 i_{10}}_{a_7 a_9} t^{a_6 a_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_8 a_6} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_7 a_5} t^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{2} v^{i_9 i_{10}}_{a_6 a_8} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a_7} t^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{2} P_2 v^{i_8 i_{10}}_{a'_7 a'_9} \tilde{t}^{a'_6 a'_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} - P_2 v^{i_8 i_{10}}_{a'_7 a'_9} \tilde{t}^{a'_6 a_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} \\ &\quad - P_2 v^{i_8 i_{10}}_{a'_9 a_7} \tilde{t}^{a'_6 a'_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} + P_2 v^{i_8 i_{10}}_{a'_9 a_7} \tilde{t}^{a'_5 a_6}_{i_2 i_{10}} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} P_2 v^{i_8 i_{10}}_{a_7 a_9} \tilde{t}^{a'_6 a_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_6 a'_8} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a'_6}_{i_1 i_2} + \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a'_8} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} \tilde{t}^{a'_5 a'_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} \\ &\quad - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_5 a'_8} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_7 a_6} \tilde{t}^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_6 a_8} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2} v^{i_9 i_{10}}_{a_6 a_8} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_8 a_6} \tilde{t}^{a'_8 a_7}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} \\ &\quad - \tfrac{1}{2} v^{i_9 i_{10}}_{a_6 a_8} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{8} X^{i_3 i_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_7 i_8} V^{i_7 i_8}_{i_5 i_6} t^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{4} P_2 V^{i_7 i_{10}}_{i_8 i_9} t^{i_8 i_9}_{i_2 i_{10}} t^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6}\end{aligned}$$

B. CCSDT-R12

TABLE ESI.3.V: The T_1 amplitude equation of CCSDT-R12 and higher-order CC-R12 with special intermediates and the RI insertion using the CABS

$$\delta_{i_1}^{a_2} = \text{CCSD} + \tfrac{1}{4} v_{a_3 a_4}^{i_5 i_6} t_{i_1 i_5 i_6}^{a_2 a_3 a_4}$$

TABLE ESI.3.VI: The T_2 amplitude equation of CCSDT-R12 with special intermediates and the RI insertion using the CABS

$$\begin{aligned}\delta_{i_1 i_2}^{a_3 a_4} = {} & + f_{a_5}^{i_6} t_{i_1 i_2 i_6}^{a_3 a_4 a_5} - \tfrac{1}{2} P_2 v_{i_2 a_5}^{i_6 i_7} t_{i_1 i_6 i_7}^{a_3 a_4 a_5} - \tfrac{1}{2} P_2 v_{a_5 a_6}^{i_7 a_4} t_{i_1 i_2 i_7}^{a_3 a_5 a_6} + v_{a_5 a_7}^{i_6 i_8} t_{i_8}^{a_7} t_{i_1 i_2 i_6}^{a_3 a_4 a_5} + \tfrac{1}{2} P_2 v_{a_5 a_8}^{i_6 i_7} t_{i_2}^{a_8} t_{i_1 i_6 i_7}^{a_3 a_4 a_5} + \tfrac{1}{2} P_2 v_{a_6 a_7}^{i_5 i_8} t_{i_1 i_2 i_8}^{a_4 a_6 a_7} t_{i_5}^{a_3}\end{aligned}$$

TABLE ESI.3.VII: The T_3 amplitude equation of CCSDT-R12 with special intermediates and the RI insertion using the CABS

$$\begin{aligned}\delta_{i_1 i_2 i_3}^{a_4 a_5 a_6} = {} & -P_3 f_{i_3}^{i_7} t_{i_1 i_2 i_7}^{a_4 a_5 a_6} + P_3 f_{a_7}^{a_6} t_{i_1 i_2 i_3}^{a_4 a_5 a_7} - P_3 f_{a_8}^{i_7} t_{i_3}^{a_8} t_{i_1 i_2 i_7}^{a_4 a_5 a_6} - P_3 f_{a_8}^{i_7} t_{i_1 i_2 i_3}^{a_5 a_6 a_8} t_{i_7}^{a_4} + P_3 P_3 f_{a_8}^{i_7} t_{i_2 i_3}^{a_6 a_8} t_{i_1 i_7}^{a_4 a_5} - P_3 P_3 f_{a'_8}^{i_7} \tilde{t}_{i_2 i_3}^{a'_8 a_6} t_{i_1 i_7}^{a_4 a_5} - P_3 P_3 v_{i_2 i_3}^{i_7 a_6} t_{i_1 i_7}^{a_4 a_5} - P_3 P_3 v_{i_3 a_7}^{a_5 a_6} t_{i_1 i_2}^{a_4 a_7} \\ & + P_3 P_3 v_{i_3 a'_7}^{a_5 a_6} \tilde{t}_{i_1 i_2}^{a'_7 a_4} + P_3 P_3 v_{i_2 i_3}^{i_7 i_8} t_{i_8}^{a_6} t_{i_1 i_7}^{a_4 a_5} + P_3 P_3 v_{i_3 a_8}^{i_7 a_6} t_{i_2}^{a_8} t_{i_1 i_7}^{a_4 a_5} - P_3 P_3 v_{i_3 a_8}^{i_7 a_6} t_{i_1 i_2}^{a_5 a_8} t_{i_7}^{a_4} + P_3 P_3 v_{a_7 a_8}^{a_5 a_6} t_{i_3}^{a_8} t_{i_1 i_2}^{a_4 a_7} + \tfrac{1}{2} P_3 v_{i_2 i_3}^{i_7 i_8} t_{i_1 i_7 i_8}^{a_4 a_5 a_6} - P_3 P_3 v_{i_3 a_7}^{i_8 a_6} t_{i_1 i_2 i_8}^{a_4 a_5 a_7} \\ & + \tfrac{1}{2} P_3 v_{a_7 a_8}^{a_5 a_6} t_{i_1 i_2 i_3}^{a_4 a_7 a_8} + P_3 P_3 v_{i_3 a'_8}^{i_7 a_6} \tilde{t}_{i_1 i_2}^{a'_8 a_5} t_{i_7}^{a_4} - P_3 P_3 v_{a'_7 a_8}^{a_5 a_6} t_{i_3}^{a_8} \tilde{t}_{i_1 i_2}^{a'_7 a_4} - P_3 P_3 v_{i_3 a_9}^{i_7 i_8} t_{i_2}^{a_9} t_{i_8}^{a_6} t_{i_1 i_7}^{a_4 a_5} - \tfrac{1}{2} P_3 P_3 v_{a_8 a_9}^{i_7 a_6} t_{i_3}^{a_9} t_{i_2}^{a_8} t_{i_1 i_7}^{a_4 a_5} - \tfrac{1}{2} P_3 P_3 v_{i_3 a_9}^{i_7 i_8} t_{i_1 i_2}^{a_6 a_9} t_{i_8}^{a_5} t_{i_7}^{a_4} \\ & + P_3 P_3 v_{a_8 a_9}^{i_7 a_6} t_{i_3}^{a_9} t_{i_1 i_2}^{a_5 a_8} t_{i_7}^{a_4} - P_3 v_{i_3 a_8}^{i_7 i_9} t_{i_9}^{a_8} t_{i_1 i_2 i_7}^{a_4 a_5 a_6} - \tfrac{1}{2} P_3 v_{i_3 a_9}^{i_7 i_8} t_{i_2}^{a_9} t_{i_1 i_7 i_8}^{a_4 a_5 a_6} - P_3 v_{a_7 a_8}^{i_9 a_6} t_{i_9}^{a_8} t_{i_1 i_2 i_3}^{a_4 a_5 a_7} - P_3 P_3 v_{i_3 a_8}^{i_7 i_9} t_{i_1 i_2 i_9}^{a_5 a_6 a_8} t_{i_7}^{a_4} + P_3 P_3 v_{a_7 a_9}^{i_8 a_6} t_{i_3}^{a_9} t_{i_1 i_2 i_8}^{a_4 a_5 a_7} \\ & + \tfrac{1}{2} P_3 v_{a_8 a_9}^{i_7 a_6} t_{i_1 i_2 i_3}^{a_5 a_8 a_9} t_{i_7}^{a_4} - \tfrac{1}{2} P_3 P_3 v_{i_3 a_7}^{i_8 i_9} t_{i_8 i_9}^{a_5 a_6} t_{i_1 i_2}^{a_4 a_7} + P_3 P_3 v_{i_3 a_8}^{i_7 i_9} t_{i_2 i_9}^{a_6 a_8} t_{i_1 i_7}^{a_4 a_5} + P_3 P_3 v_{a_7 a_8}^{i_9 a_6} t_{i_3 i_9}^{a_5 a_8} t_{i_1 i_2}^{a_4 a_7} - \tfrac{1}{2} P_3 P_3 v_{i_3 a'_9}^{i_7 i_8} \tilde{t}_{i_1 i_2}^{a'_9 a_6} t_{i_8}^{a_5} t_{i_7}^{a_4} \\ & - P_3 P_3 v_{a'_8 a_9}^{i_7 a_6} t_{i_3}^{a_9} \tilde{t}_{i_1 i_2}^{a'_8 a_5} t_{i_7}^{a_4} - P_3 P_3 v_{i_3 a'_8}^{i_7 i_9} \tilde{t}_{i_2 i_9}^{a'_8 a_6} t_{i_1 i_7}^{a_4 a_5} - \tfrac{1}{2} P_3 P_3 V_{i_8 i_9}^{i_7 a_6} t_{i_2 i_3}^{i_8 i_9} t_{i_1 i_7}^{a_4 a_5} + \tfrac{1}{2} P_3 P_3 v_{i_3 a'_9}^{i_7 i_8} \tilde{t}_{i_1 i_2}^{a'_9 a_6} t_{i_7 i_8}^{a_4 a_5} + P_3 P_3 v_{a'_8 a_7}^{i_9 a_6} \tilde{t}_{i_3 i_9}^{a'_8 a_5} t_{i_1 i_2}^{a_4 a_7} - P_3 P_3 v_{a'_7 a_8}^{i_9 a_6} t_{i_3 i_9}^{a_5 a_8} \tilde{t}_{i_1 i_2}^{a'_7 a_4} \\ & + P_3 P_3 v_{a'_7 a'_8}^{i_9 a_6} \tilde{t}_{i_3 i_9}^{a'_8 a_5} \tilde{t}_{i_1 i_2}^{a'_7 a_4} + \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_3}^{a_{10}} t_{i_2}^{a_9} t_{i_8}^{a_6} t_{i_1 i_7}^{a_4 a_5} + \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_3}^{a_{10}} t_{i_1 i_2}^{a_6 a_9} t_{i_8}^{a_5} t_{i_7}^{a_4} - P_3 v_{a_8 a_9}^{i_7 i_{10}} t_{i_{10}}^{a_9} t_{i_3}^{a_8} t_{i_1 i_2 i_7}^{a_4 a_5 a_6} + \tfrac{1}{4} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_3}^{a_{10}} t_{i_2}^{a_9} t_{i_1 i_7 i_8}^{a_4 a_5 a_6} \\ & - P_3 v_{a_8 a_9}^{i_7 i_{10}} t_{i_{10}}^{a_9} t_{i_1 i_2 i_3}^{a_5 a_6 a_8} t_{i_7}^{a_4} + P_3 P_3 v_{a_8 a_{10}}^{i_7 i_9} t_{i_3}^{a_{10}} t_{i_1 i_2 i_9}^{a_5 a_6 a_8} t_{i_7}^{a_4} + \tfrac{1}{4} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2 i_3}^{a_6 a_9 a_{10}} t_{i_8}^{a_5} t_{i_7}^{a_4} + \tfrac{1}{2} P_3 P_3 v_{a_7 a_{10}}^{i_8 i_9} t_{i_3}^{a_{10}} t_{i_8 i_9}^{a_5 a_6} t_{i_1 i_2}^{a_4 a_7} + P_3 P_3 v_{a_8 a_9}^{i_7 i_{10}} t_{i_{10}}^{a_9} t_{i_2 i_3}^{a_6 a_8} t_{i_1 i_7}^{a_4 a_5} \\ & + P_3 P_3 v_{a_8 a_9}^{i_7 i_{10}} t_{i_3 i_{10}}^{a_6 a_9} t_{i_1 i_2}^{a_5 a_8} t_{i_7}^{a_4} - P_3 P_3 v_{a_8 a_{10}}^{i_7 i_9} t_{i_3}^{a_{10}} t_{i_2 i_9}^{a_6 a_8} t_{i_1 i_7}^{a_4 a_5} + \tfrac{1}{2} P_3 P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_2 i_3}^{a_9 a_{10}} t_{i_8}^{a_6} t_{i_1 i_7}^{a_4 a_5} + \tfrac{1}{2} P_3 P_3 v_{a_8 a_9}^{i_7 i_{10}} t_{i_2 i_3 i_{10}}^{a_6 a_8 a_9} t_{i_1 i_7}^{a_4 a_5} + \tfrac{1}{4} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_1 i_2 i_3}^{a_6 a_9 a_{10}} t_{i_7 i_8}^{a_4 a_5} \\ & + \tfrac{1}{2} P_3 P_3 v_{a_7 a_8}^{i_9 i_{10}} t_{i_3 i_9 i_{10}}^{a_5 a_6 a_8} t_{i_1 i_2}^{a_4 a_7} + P_3 P_3 v_{a_7 a_9}^{i_8 i_{10}} t_{i_3 i_{10}}^{a_6 a_9} t_{i_1 i_2 i_8}^{a_4 a_5 a_7} - \tfrac{1}{2} P_3 v_{a_7 a_8}^{i_9 i_{10}} t_{i_9 i_{10}}^{a_6 a_8} t_{i_1 i_2 i_3}^{a_4 a_5 a_7} + \tfrac{1}{4} P_3 v_{a_9 a_{10}}^{i_7 i_8} t_{i_2 i_3}^{a_9 a_{10}} t_{i_1 i_7 i_8}^{a_4 a_5 a_6} - \tfrac{1}{2} P_3 v_{a_8 a_9}^{i_7 i_{10}} t_{i_3 i_{10}}^{a_8 a_9} t_{i_1 i_2 i_7}^{a_4 a_5 a_6} \\ & - \tfrac{1}{2} P_3 P_3 v_{a'_9 a_{10}}^{i_7 i_8} t_{i_3}^{a_{10}} \tilde{t}_{i_1 i_2}^{a'_9 a_6} t_{i_8}^{a_5} t_{i_7}^{a_4} - P_3 P_3 v_{a'_8 a_9}^{i_7 i_{10}} t_{i_{10}}^{a_9} \tilde{t}_{i_2 i_3}^{a'_8 a_6} t_{i_1 i_7}^{a_4 a_5} + P_3 P_3 v_{a'_8 a_{10}}^{i_7 i_9} t_{i_3}^{a_{10}} \tilde{t}_{i_2 i_9}^{a'_8 a_6} t_{i_1 i_7}^{a_4 a_5} + \tfrac{1}{2} P_3 P_3 V_{i_9 i_{10}}^{i_7 i_8} t_{i_2 i_3}^{i_9 i_{10}} t_{i_8}^{a_6} t_{i_1 i_7}^{a_4 a_5} - \tfrac{1}{2} P_3 P_3 v_{a'_9 a_{10}}^{i_7 i_8} t_{i_3}^{a_{10}} \tilde{t}_{i_1 i_2}^{a'_9 a_6} t_{i_7 i_8}^{a_4 a_5} \\ & + P_3 P_3 v_{a'_9 a_8}^{i_7 i_{10}} \tilde{t}_{i_3 i_{10}}^{a'_9 a_6} t_{i_1 i_2}^{a_5 a_8} t_{i_7}^{a_4} - P_3 P_3 v_{a'_8 a_9}^{i_7 i_{10}} t_{i_3 i_{10}}^{a_6 a_9} \tilde{t}_{i_1 i_2}^{a'_8 a_5} t_{i_7}^{a_4} - \tfrac{1}{2} P_3 V_{i_8 i_9}^{i_7 i_{10}} t_{i_3 i_{10}}^{i_8 i_9} t_{i_1 i_2 i_7}^{a_4 a_5 a_6} + \tfrac{1}{4} P_3 V_{i_9 i_{10}}^{i_7 i_8} t_{i_2 i_3}^{i_9 i_{10}} t_{i_1 i_7 i_8}^{a_4 a_5 a_6} - \tfrac{1}{2} P_3 v_{a'_8 a_7}^{i_9 i_{10}} \tilde{t}_{i_9 i_{10}}^{a'_8 a_6} t_{i_1 i_2 i_3}^{a_4 a_5 a_7} \\ & + P_3 P_3 v_{a'_9 a_7}^{i_8 i_{10}} \tilde{t}_{i_3 i_{10}}^{a'_9 a_6} t_{i_1 i_2 i_8}^{a_4 a_5 a_7} - \tfrac{1}{2} P_3 P_3 v_{a'_7 a_8}^{i_9 i_{10}} t_{i_3 i_9 i_{10}}^{a_5 a_6 a_8} \tilde{t}_{i_1 i_2}^{a'_7 a_4} + P_3 P_3 v_{a'_8 a'_9}^{i_7 i_{10}} \tilde{t}_{i_3 i_{10}}^{a'_9 a_6} \tilde{t}_{i_1 i_2}^{a'_8 a_5} t_{i_7}^{a_4}\end{aligned}$$

TABLE ESI.3.VIII: The geminal t amplitude equation of CCSDT-R12 and higher-order CC-R12 with special intermediates and the RI insertion using the CABS

$$\delta_{i_1 i_2}^{i_3 i_4} = \text{CCSD-R12} + \tfrac{1}{2} v_{a_7 a_8}^{i_9 \alpha_5} t_{i_1 i_2 i_9}^{a_6 a_7 a_8} F_{\alpha_5 a_6}^{i_3 i_4 *}$$

C. CCSDTQ-R12

TABLE ESI.3.IX: The T_2 amplitude equation of CCSDTQ-R12 with special intermediates and the RI insertion using the CABS

$$\delta^{a_3a_4}_{i_1i_2} = \text{CCSDT-R12} + \tfrac{1}{4} v^{i_7i_8}_{a_5a_6} t^{a_3a_4a_5a_6}_{i_1i_2i_7i_8}$$

TABLE ESI.3.X: The T_3 amplitude equation of CCSDTQ-R12 with special intermediates and the RI insertion using the CABS

$$\delta^{a_4a_5a_6}_{i_1i_2i_3} = \text{CCSDT-R12} + f^{i_8}_{a_7} t^{a_4a_5a_6a_7}_{i_1i_2i_3i_8} - \tfrac12 P_3 v^{i_8i_9}_{i_3a_7} t^{a_4a_5a_6a_7}_{i_1i_2i_8i_9} - \tfrac12 P_3 v^{i_9a_6}_{a_7a_8} t^{a_4a_5a_7a_8}_{i_1i_2i_3i_9} + v^{i_8i_{10}}_{a_7a_9} t^{a_9}_{i_{10}} t^{a_4a_5a_6a_7}_{i_1i_2i_3i_8} + \tfrac12 P_3 v^{i_8i_9}_{a_7a_{10}} t^{a_{10}}_{i_3} t^{a_4a_5a_6a_7}_{i_1i_2i_8i_9} - \tfrac12 P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_5a_6a_8a_9}_{i_1i_2i_3i_{10}} t^{a_4}_{i_7}$$

TABLE ESI.3.XI: The T_4 amplitude equation of CCSDTQ-R12 with special intermediates and the RI insertion using the CABS

$$\delta^{a_5a_6a_7a_8}_{i_1i_2i_3i_4} = -P_4 f^{i_9}_{i_4} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} + P_4 f^{a_8}_{a_9} t^{a_5a_6a_7a_9}_{i_1i_2i_3i_4} - P_4 f^{i_9}_{a_{10}} t^{a_{10}}_{i_4} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} + P_4 f^{i_9}_{a_{10}} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_4} t^{a_5}_{i_9} - P_4P_4 f^{i_9}_{a_{10}} t^{a_7a_8a_{10}}_{i_2i_3i_4} t^{a_5a_6}_{i_1i_9} + P_4P_4 f^{i_9}_{a_{10}} t^{a_8a_{10}}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9}$$

$$-P_4P_4 f^{i_9}_{a'_{10}} \tilde{t}^{a'_{10}a_8}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4P_4 v^{i_9a_8}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4P_4 v^{a_7a_8}_{i_4a_9} t^{a_5a_6a_9}_{i_1i_2i_3} + P_4P_4 v^{i_9i_{10}}_{i_3i_4} t^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4P_4 v^{i_9a_8}_{i_4a_{10}} t^{a_{10}}_{i_3} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4P_4 v^{i_9a_8}_{i_4a_{10}} t^{a_6a_7a_{10}}_{i_1i_2i_3} t^{a_5}_{i_9}$$

$$+P_4P_4 v^{a_7a_8}_{a_9a_{10}} t^{a_{10}}_{i_4} t^{a_5a_6a_9}_{i_1i_2i_3} - \tfrac12 P_4P_4 v^{i_9i_{10}}_{i_3i_4} t^{a_7a_8}_{i_2i_{10}} t^{a_5a_6}_{i_1i_9} - P_4P_4 v^{i_9a_8}_{i_4a_{10}} t^{a_7a_{10}}_{i_2i_3} t^{a_5a_6}_{i_1i_9} - \tfrac12 P_4P_4 v^{a_7a_8}_{a_9a_{10}} t^{a_6a_{10}}_{i_3i_4} t^{a_5a_9}_{i_1i_2} + P_4P_4 v^{i_9a_8}_{i_4a'_{10}} \tilde{t}^{a'_{10}a_7}_{i_2i_3} t^{a_5a_6}_{i_1i_9}$$

$$-P_4P_4 v^{a_7a_8}_{a'_{10}a_9} \tilde{t}^{a'_{10}a_6}_{i_3i_4} t^{a_5a_9}_{i_1i_2} + \tfrac12 P_4 v^{i_9i_{10}}_{i_3i_4} t^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} - P_4P_4 v^{i_{10}a_8}_{i_4a_9} t^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}} + \tfrac12 P_4 v^{a_7a_8}_{a_9a_{10}} t^{a_5a_6a_9a_{10}}_{i_1i_2i_3i_4} - \tfrac12 P_4P_4 v^{a_7a_8}_{a'_9a'_{10}} \tilde{t}^{a'_{10}a_6}_{i_3i_4} \tilde{t}^{a'_9a_5}_{i_1i_2} - P_4P_4 v^{i_9i_{10}}_{i_4a_{11}} t^{a_{11}}_{i_3} t^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9}$$

$$-\tfrac12 P_4P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_{11}}_{i_4} t^{a_{10}}_{i_3} t^{a_5a_6a_7}_{i_1i_2i_9} - \tfrac12 P_4P_4 v^{i_9i_{10}}_{i_4a_{11}} t^{a_7a_8a_{11}}_{i_1i_2i_3} t^{a_6}_{i_{10}} t^{a_5}_{i_9} - P_4P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_{11}}_{i_4} t^{a_6a_7a_{10}}_{i_1i_2i_3} t^{a_5}_{i_9} + \tfrac12 P_4P_4 v^{i_9i_{10}}_{i_4a_{11}} t^{a_{11}}_{i_3} t^{a_7a_8}_{i_2i_{10}} t^{a_5a_6}_{i_1i_9} - P_4P_4 v^{i_9i_{10}}_{i_4a_{11}} t^{a_8a_{11}}_{i_2i_3} t^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9}$$

$$+\tfrac12 P_4P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_7a_{11}}_{i_3i_4} t^{a_6a_{10}}_{i_1i_2} t^{a_5}_{i_9} + P_4P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_{11}}_{i_4} t^{a_7a_{10}}_{i_2i_3} t^{a_5a_6}_{i_1i_9} + P_4P_4 v^{i_9i_{10}}_{i_4a'_{11}} \tilde{t}^{a'_{11}a_8}_{i_2i_3} t^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} + P_4P_4 v^{i_9a_8}_{a'_{11}a_{10}} \tilde{t}^{a'_{11}a_7}_{i_3i_4} t^{a_6a_{10}}_{i_1i_2} t^{a_5}_{i_9} - P_4P_4 v^{i_9a_8}_{a'_{10}a_{11}} t^{a_{11}}_{i_4} \tilde{t}^{a'_{10}a_7}_{i_2i_3} t^{a_5a_6}_{i_1i_9}$$

$$-P_4 v^{i_9i_{11}}_{i_4a_{10}} t^{a_{10}}_{i_{11}} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} - \tfrac12 P_4 v^{i_9i_{10}}_{i_4a_{11}} t^{a_{11}}_{i_3} t^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} - P_4 v^{i_{11}a_8}_{a_9a_{10}} t^{a_{10}}_{i_{11}} t^{a_5a_6a_7a_9}_{i_1i_2i_3i_4} + P_4P_4 v^{i_9i_{11}}_{i_4a_{10}} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_{11}} t^{a_5}_{i_9} + P_4P_4 v^{i_{10}a_8}_{a_9a_{11}} t^{a_{11}}_{i_4} t^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}}$$

$$-\tfrac12 P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_6a_7a_{10}a_{11}}_{i_1i_2i_3i_4} t^{a_5}_{i_9} + \tfrac12 P_4P_4 v^{i_9a_8}_{a'_{10}a'_{11}} \tilde{t}^{a'_{11}a_7}_{i_3i_4} \tilde{t}^{a'_{10}a_6}_{i_1i_2} t^{a_5}_{i_9} - P_4P_4 v^{i_9i_{11}}_{i_4a_{10}} t^{a_7a_8a_{10}}_{i_2i_3i_{11}} t^{a_5a_6}_{i_1i_9} + \tfrac12 P_4P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_7a_{10}a_{11}}_{i_2i_3i_4} t^{a_5a_6}_{i_1i_9} - \tfrac12 P_4P_4 v^{i_{10}i_{11}}_{i_4a_9} t^{a_7a_8}_{i_{10}i_{11}} t^{a_5a_6a_9}_{i_1i_2i_3}$$

$$+\tfrac12 P_4P_4 v^{i_{10}i_{11}}_{i_4a_9} t^{a_6a_7a_8}_{i_3i_{10}i_{11}} t^{a_5a_9}_{i_1i_2} - P_4P_4 v^{i_{11}a_8}_{a_9a_{10}} t^{a_6a_7a_{10}}_{i_3i_4i_{11}} t^{a_5a_9}_{i_1i_2} + P_4P_4 v^{i_9i_{11}}_{i_4a_{10}} t^{a_8a_{10}}_{i_3i_{11}} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4P_4 v^{i_{11}a_8}_{a_9a_{10}} t^{a_7a_{10}}_{i_4i_{11}} t^{a_5a_6a_9}_{i_1i_2i_3} - \tfrac12 P_4P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_{10}a_{11}}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9}$$

$$+\tfrac12 P_4P_4 v^{i_9i_{10}}_{i_4a'_{11}} \tilde{t}^{a'_{11}a_8}_{i_2i_3} t^{a_5a_6a_7}_{i_1i_9i_{10}} + P_4P_4 v^{i_{11}a_8}_{a'_9a_{10}} t^{a_6a_7a_{10}}_{i_3i_4i_{11}} \tilde{t}^{a'_9a_5}_{i_1i_2} - P_4P_4 v^{i_9i_{11}}_{i_4a'_{10}} \tilde{t}^{a'_{10}a_8}_{i_3i_{11}} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4P_4 v^{i_{11}a_8}_{a'_{10}a_9} \tilde{t}^{a'_{10}a_7}_{i_4i_{11}} t^{a_5a_6a_9}_{i_1i_2i_3} - \tfrac12 P_4P_4 V^{i_9a_8}_{i_{10}i_{11}} t^{i_{10}i_{11}}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9}$$

$$+\tfrac12 P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} t^{a_{11}}_{i_3} t^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} + \tfrac12 P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} t^{a_7a_8a_{11}}_{i_1i_2i_3} t^{a_6}_{i_{10}} t^{a_5}_{i_9} - \tfrac14 P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} t^{a_{11}}_{i_3} t^{a_7a_8}_{i_2i_{10}} t^{a_5a_6}_{i_1i_9} - \tfrac14 P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_8a_{12}}_{i_3i_4} t^{a_7a_{11}}_{i_1i_2} t^{a_6}_{i_{10}} t^{a_5}_{i_9}$$

$$+P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} t^{a_8a_{11}}_{i_2i_3} t^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} - \tfrac12 P_4P_4 v^{i_9i_{10}}_{a'_{12}a_{11}} \tilde{t}^{a'_{12}a_8}_{i_3i_4} t^{a_7a_{11}}_{i_1i_2} t^{a_6}_{i_{10}} t^{a_5}_{i_9} - P_4P_4 v^{i_9i_{10}}_{a'_{11}a_{12}} t^{a_{12}}_{i_4} \tilde{t}^{a'_{11}a_8}_{i_2i_3} t^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} - P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_{11}}_{i_{12}} t^{a_{10}}_{i_4} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9}$$

$$+\tfrac14 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} t^{a_{11}}_{i_3} t^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} + P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_{11}}_{i_{12}} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_4} t^{a_5}_{i_9} - P_4P_4 v^{i_9i_{11}}_{a_{10}a_{12}} t^{a_{12}}_{i_4} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_{11}} t^{a_5}_{i_9} + \tfrac14 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_7a_8a_{11}a_{12}}_{i_1i_2i_3i_4} t^{a_6}_{i_{10}} t^{a_5}_{i_9}$$

$$-\tfrac14 P_4P_4 v^{i_9i_{10}}_{a'_{11}a'_{12}} \tilde{t}^{a'_{12}a_8}_{i_3i_4} \tilde{t}^{a'_{11}a_7}_{i_1i_2} t^{a_6}_{i_{10}} t^{a_5}_{i_9} + \tfrac12 P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_8a_{11}a_{12}}_{i_2i_3i_4} t^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} + P_4P_4 v^{i_9i_{11}}_{a_{10}a_{12}} t^{a_{12}}_{i_4} t^{a_7a_8a_{10}}_{i_2i_3i_{11}} t^{a_5a_6}_{i_1i_9} - P_4P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_{11}}_{i_{12}} t^{a_7a_8a_{10}}_{i_2i_3i_4} t^{a_5a_6}_{i_1i_9}$$

$$+\tfrac12 P_4P_4 v^{i_{10}i_{11}}_{a_9a_{12}} t^{a_{12}}_{i_4} t^{a_7a_8}_{i_{10}i_{11}} t^{a_5a_6a_9}_{i_1i_2i_3} + P_4P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_7a_8a_{11}}_{i_3i_4i_{12}} t^{a_6a_{10}}_{i_1i_2} t^{a_5}_{i_9} - \tfrac12 P_4P_4 v^{i_{10}i_{11}}_{a_9a_{12}} t^{a_{12}}_{i_4} t^{a_6a_7a_8}_{i_3i_{10}i_{11}} t^{a_5a_9}_{i_1i_2} + P_4P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_{11}}_{i_{12}} t^{a_8a_{10}}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9}$$

$$-P_4P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_8a_{11}}_{i_4i_{12}} t^{a_6a_7a_{10}}_{i_1i_2i_3} t^{a_5}_{i_9} - P_4P_4 v^{i_9i_{11}}_{a_{10}a_{12}} t^{a_{12}}_{i_4} t^{a_8a_{10}}_{i_3i_{11}} t^{a_5a_6a_7}_{i_1i_2i_9} + \tfrac12 P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{11}a_{12}}_{i_3i_4} t^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4P_4 v^{i_9i_{12}}_{a'_{10}a_{11}} t^{a_7a_8a_{11}}_{i_3i_4i_{12}} \tilde{t}^{a'_{10}a_6}_{i_1i_2} t^{a_5}_{i_9}$$

$$-\tfrac12 P_4P_4 v^{i_9i_{10}}_{a'_{11}a_{12}} t^{a_{12}}_{i_4} \tilde{t}^{a'_{11}a_8}_{i_2i_3} t^{a_5a_6a_7}_{i_1i_9i_{10}} - P_4P_4 v^{i_9i_{12}}_{a'_{10}a_{11}} t^{a_{11}}_{i_{12}} \tilde{t}^{a'_{10}a_8}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4P_4 v^{i_9i_{12}}_{a'_{11}a_{10}} \tilde{t}^{a'_{11}a_8}_{i_4i_{12}} t^{a_6a_7a_{10}}_{i_1i_2i_3} t^{a_5}_{i_9} + P_4P_4 v^{i_9i_{11}}_{a'_{10}a_{12}} t^{a_{12}}_{i_4} \tilde{t}^{a'_{10}a_8}_{i_3i_{11}} t^{a_5a_6a_7}_{i_1i_2i_9}$$

$$+\tfrac12 P_4P_4 V^{i_9i_{10}}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_4} t^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} - \tfrac14 P_4P_4 v^{i_{11}i_{12}}_{a_9a_{10}} t^{a_7a_8}_{i_{11}i_{12}} t^{a_6a_{10}}_{i_3i_4} t^{a_5a_9}_{i_1i_2} + P_4P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_8a_{11}}_{i_4i_{12}} t^{a_7a_{10}}_{i_2i_3} t^{a_5a_6}_{i_1i_9} - \tfrac14 P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{11}a_{12}}_{i_3i_4} t^{a_7a_8}_{i_2i_{10}} t^{a_5a_6}_{i_1i_9}$$

$$-\tfrac12 P_4P_4 v^{i_{10}i_{11}}_{a'_{12}a_9} \tilde{t}^{a'_{12}a_8}_{i_3i_4} t^{a_6a_7}_{i_{10}i_{11}} t^{a_5a_9}_{i_1i_2} - P_4P_4 v^{i_9i_{12}}_{a'_{10}a_{11}} t^{a_8a_{11}}_{i_4i_{12}} \tilde{t}^{a'_{10}a_7}_{i_2i_3} t^{a_5a_6}_{i_1i_9} + P_4P_4 v^{i_9i_{12}}_{a'_{11}a_{10}} \tilde{t}^{a'_{11}a_8}_{i_4i_{12}} t^{a_7a_{10}}_{i_2i_3} t^{a_5a_6}_{i_1i_9} - \tfrac14 P_4P_4 V^{i_9i_{10}}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_4} t^{a_7a_8}_{i_2i_{10}} t^{a_5a_6}_{i_1i_9}$$

$$-\tfrac14 P_4P_4 v^{i_9i_{10}}_{a'_{11}a'_{12}} \tilde{t}^{a'_{12}a_8}_{i_3i_4} \tilde{t}^{a'_{11}a_7}_{i_1i_2} t^{a_5a_6}_{i_9i_{10}} + P_4P_4 v^{i_9i_{12}}_{a'_{10}a'_{11}} \tilde{t}^{a'_{11}a_8}_{i_4i_{12}} \tilde{t}^{a'_{10}a_7}_{i_2i_3} t^{a_5a_6}_{i_1i_9} + \tfrac12 P_4P_4 v^{i_{10}i_{12}}_{a_9a_{11}} t^{a_7a_8a_{11}}_{i_3i_4i_{12}} t^{a_5a_6a_9}_{i_1i_2i_{10}} + \tfrac12 P_4P_4 v^{i_{11}i_{12}}_{a_9a_{10}} t^{a_7a_8a_{10}}_{i_4i_{11}i_{12}} t^{a_5a_6a_9}_{i_1i_2i_3}$$

$$+\tfrac14 P_4P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_8a_{11}a_{12}}_{i_2i_3i_4} t^{a_5a_6a_7}_{i_1i_9i_{10}} + \tfrac12 P_4P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_8a_{10}a_{11}}_{i_3i_4i_{12}} t^{a_5a_6a_7}_{i_1i_2i_9} - \tfrac12 P_4P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_7a_8a_{10}a_{11}}_{i_2i_3i_4i_{12}} t^{a_5a_6}_{i_1i_9} + \tfrac14 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_7a_8a_{11}a_{12}}_{i_1i_2i_3i_4} t^{a_5a_6}_{i_9i_{10}}$$

$$-\tfrac12 P_4P_4 v^{i_{11}i_{12}}_{a_9a_{10}} t^{a_6a_7a_8a_{10}}_{i_3i_4i_{11}i_{12}} t^{a_5a_9}_{i_1i_2} + P_4P_4 v^{i_{10}i_{12}}_{a_9a_{11}} t^{a_8a_{11}}_{i_4i_{12}} t^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}} - \tfrac12 P_4 v^{i_{11}i_{12}}_{a_9a_{10}} t^{a_8a_{10}}_{i_{11}i_{12}} t^{a_5a_6a_7a_9}_{i_1i_2i_3i_4} + \tfrac14 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{11}a_{12}}_{i_3i_4} t^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} - \tfrac12 P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_{10}a_{11}}_{i_4i_{12}} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9}$$

$$+\tfrac12 P_4P_4 v^{i_{11}i_{12}}_{a'_9a_{10}} t^{a_6a_7a_8a_{10}}_{i_3i_4i_{11}i_{12}} \tilde{t}^{a'_9a_5}_{i_1i_2} + P_4P_4 v^{i_{10}i_{12}}_{a'_{11}a_9} \tilde{t}^{a'_{11}a_8}_{i_4i_{12}} t^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}} - \tfrac12 P_4 v^{i_{11}i_{12}}_{a'_{10}a_9} \tilde{t}^{a'_{10}a_8}_{i_{11}i_{12}} t^{a_5a_6a_7a_9}_{i_1i_2i_3i_4} + \tfrac14 P_4 V^{i_9i_{10}}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_4} t^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} - \tfrac12 P_4 V^{i_9i_{12}}_{i_{10}i_{11}} t^{i_{10}i_{11}}_{i_4i_{12}} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9}$$

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D. Λ-CCSD-R12

TABLE ESI.3.XII: The Λ_1 amplitude equation of Λ-CCSD-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{i_2}_{a_1} &= -f^{i_2}_{a_1} - v^{i_2 i_4}_{a_1 a_3} t^{a_3}_{i_4} + \lambda^{i_3}_{a_1} f^{i_2}_{i_3} - \lambda^{i_2}_{a_3} f^{a_3}_{a_1} + f^{i_2}_{a_4} t^{a_4}_{i_3} \lambda^{i_3}_{a_1} + \lambda^{i_2}_{a_4} t^{a_4}_{i_3} f^{i_3}_{a_1} + \lambda^{i_4}_{a_3} v^{i_2 a_3}_{i_4 a_1} + v^{i_2 i_5}_{i_3 a_4} t^{a_4}_{i_5} \lambda^{i_3}_{a_1} + v^{i_5 a_3}_{a_1 a_4} t^{a_4}_{i_5} \lambda^{i_2}_{a_3} - \lambda^{i_4}_{a_5} t^{a_5}_{i_3} v^{i_2 i_3}_{i_4 a_1} - \lambda^{i_5}_{a_3} t^{a_4}_{i_5} v^{i_2 a_3}_{a_1 a_4} + v^{i_2 i_6}_{a_4 a_5} t^{a_5}_{i_6} t^{a_4}_{i_3} \lambda^{i_3}_{a_1} \\
&+ v^{i_4 i_6}_{a_1 a_5} t^{a_5}_{i_6} t^{a_3}_{i_4} \lambda^{i_2}_{a_3} + \lambda^{i_5}_{a_6} t^{a_6}_{i_5} t^{a_4}_{i_3} v^{i_2 i_3}_{a_1 a_4} + \tfrac{1}{2} v^{i_2 i_6}_{a_4 a_5} t^{a_4 a_5}_{i_3 i_6} \lambda^{i_3}_{a_1} - \tfrac{1}{2} \lambda^{i_2}_{a_6} t^{a_5 a_6}_{i_3 i_4} v^{i_3 i_4}_{a_1 a_5} - \lambda^{i_6}_{a_5} t^{a_4 a_5}_{i_3 i_6} v^{i_2 i_3}_{a_1 a_4} + \tfrac{1}{2} V^{i_2 i_6}_{i_4 i_5} t^{i_4 i_5}_{i_3 i_6} \lambda^{i_3}_{a_1} + \tfrac{1}{2} \lambda^{i_2}_{a_6} \tilde{t}^{a'_5 a_6}_{i_3 i_4} v^{i_3 i_4}_{a'_5 a_1} + \lambda^{i_6}_{a_5} \tilde{t}^{a'_4 a_5}_{i_3 i_6} v^{i_2 i_3}_{a'_4 a_1} \\
&- \tfrac{1}{2} f^{i_2}_{a_6} t^{a_5 a_6}_{i_3 i_4} \lambda^{i_3 i_4}_{a_1 a_5} + \tfrac{1}{2} \lambda^{i_2 i_6}_{a_4 a_5} t^{a_4 a_5}_{i_3 i_6} f^{i_3}_{a_1} + \tfrac{1}{2} f^{i_2}_{a'_6} \tilde{t}^{a'_6 a_5}_{i_3 i_4} \lambda^{i_3 i_4}_{a_1 a_5} + \tfrac{1}{2} f^{i_2}_{a'_6} \tilde{t}^{a'_5 a'_6}_{i_3 i_4} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} + \tfrac{1}{2} f^{i_2}_{a_6} \tilde{t}^{a'_5 a_6}_{i_3 i_4} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} + \tfrac{1}{4} X^{i_5 i_6}_{i_7 i_8} t^{i_7 i_8}_{i_3 i_4} \lambda^{i_2 i_4}_{i_5 i_6} f^{i_3}_{a_1} + \tfrac{1}{2} \lambda^{i_4 i_5}_{a_1 a_3} v^{i_2 a_3}_{i_4 i_5} + \tfrac{1}{2} \lambda^{i_2 i_5}_{a_3 a_4} v^{a_3 a_4}_{i_5 a_1} \\
&- \tfrac{1}{2} \tilde{\lambda}^{i_4 i_5}_{a'_3 a_1} v^{i_2 a'_3}_{i_4 i_5} + \tfrac{1}{2} \lambda^{i_2 i_5}_{i_3 i_4} (V^\dagger)^{i_3 i_4}_{i_5 a_1} - \tfrac{1}{2} v^{i_2 i_6}_{i_3 i_4} t^{a_5}_{i_6} \lambda^{i_3 i_4}_{a_1 a_5} - v^{i_2 a_5}_{i_4 a_6} t^{a_6}_{i_3} \lambda^{i_3 i_4}_{a_1 a_5} + \lambda^{i_2 i_5}_{a_4 a_6} t^{a_6}_{i_3} v^{i_3 a_4}_{i_5 a_1} - \tfrac{1}{2} v^{a_4 a_5}_{a_1 a_6} t^{a_6}_{i_3} \lambda^{i_2 i_3}_{a_4 a_5} + v^{i_2 a'_5}_{i_4 a_6} t^{a_6}_{i_3} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} + \tilde{\lambda}^{i_2 i_5}_{a'_4 a_6} t^{a_6}_{i_3} v^{i_3 a'_4}_{i_5 a_1} \\
&- \tfrac{1}{2} (V^\dagger)^{i_4 i_5}_{a_1 a_6} t^{a_6}_{i_3} \lambda^{i_2 i_3}_{i_4 i_5} + v^{i_2 i_6}_{i_4 a_7} t^{a_7}_{i_3} t^{a_5}_{i_6} \lambda^{i_3 i_4}_{a_1 a_5} + \tfrac{1}{2} v^{i_2 a_5}_{a_6 a_7} t^{a_7}_{i_4} t^{a_6}_{i_3} \lambda^{i_3 i_4}_{a_1 a_5} - \lambda^{i_2 i_6}_{a_4 a_7} t^{a_7}_{i_3} t^{a_5}_{i_6} v^{i_3 a_4}_{a_1 a_5} - v^{i_2 i_7}_{i_4 a_6} t^{a_5 a_6}_{i_3 i_7} \lambda^{i_3 i_4}_{a_1 a_5} + \tfrac{1}{4} v^{i_2 a_5}_{a_6 a_7} t^{a_6 a_7}_{i_3 i_4} \lambda^{i_3 i_4}_{a_1 a_5} \\
&+ \tfrac{1}{4} \lambda^{i_2 i_5}_{a_6 a_7} t^{a_6 a_7}_{i_3 i_4} v^{i_3 i_4}_{i_5 a_1} + \lambda^{i_2 i_7}_{a_4 a_6} t^{a_5 a_6}_{a_1 a_5} v^{i_3 a_4}_{i_7 a_5} - \tfrac{1}{2} \lambda^{i_4 i_7}_{a_5 a_6} t^{a_5 a_6}_{i_3 i_7} v^{i_2 i_3}_{i_4 a_1} - \tfrac{1}{2} \lambda^{i_6 i_7}_{a_3 a_5} t^{a_4 a_5}_{i_6 i_7} v^{i_2 a_3}_{a_1 a_4} + v^{i_2 i_7}_{i_4 a'_6} \tilde{t}^{a'_6 a_5}_{i_3 i_7} \lambda^{i_3 i_4}_{a_1 a_5} + \tfrac{1}{4} V^{i_2 a_5}_{i_6 i_7} t^{i_6 i_7}_{i_3 i_4} \lambda^{i_3 i_4}_{a_1 a_5} - \lambda^{i_2 i_7}_{a_4 a_6} \tilde{t}^{a'_5 a_6}_{i_3 i_7} v^{i_3 a_4}_{a'_5 a_1} \\
&+ \tfrac{1}{2} \lambda^{i_6 i_7}_{a_3 a_5} \tilde{t}^{a'_4 a_5}_{i_6 i_7} v^{i_2 a_3}_{a'_4 a_1} - \tfrac{1}{2} v^{i_2 a'_5}_{a_6 a_7} t^{a_7}_{i_4} t^{a_6}_{i_3} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} - \tilde{\lambda}^{i_2 i_6}_{a'_4 a_7} t^{a_7}_{i_3} t^{a_5}_{i_6} v^{i_3 a'_4}_{a_1 a_5} - \tfrac{1}{4} v^{i_2 a'_5}_{a_6 a_7} t^{a_6 a_7}_{i_3 i_4} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} + \tilde{\lambda}^{i_2 i_7}_{a'_4 a_6} t^{a_5 a_6}_{i_3 i_7} v^{i_3 a'_4}_{a_1 a_5} - \tfrac{1}{2} \tilde{\lambda}^{i_6 i_7}_{a'_5 a_3} t^{a_4 a_5}_{i_6 i_7} v^{i_2 a'_3}_{a_1 a_4} + v^{i_2 i_7}_{i_4 a'_6} \tilde{t}^{a'_5 a'_6}_{i_3 i_7} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} \\
&+ v^{i_2 i_7}_{i_4 a_6} \tilde{t}^{a'_5 a_6}_{i_3 i_7} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} - \tfrac{1}{4} V^{i_2 a'_5}_{i_6 i_7} t^{i_6 i_7}_{i_3 i_4} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} + \tfrac{1}{8} X^{i_6 i_7}_{i_8 i_9} t^{i_8 i_9}_{i_3 i_5} \lambda^{i_4 i_5}_{i_6 i_7} v^{i_2 i_3}_{i_4 a_1} + \tfrac{1}{2} \tilde{\lambda}^{i_6 i_7}_{a'_3 a'_5} \tilde{t}^{a'_4 a'_5}_{i_6 i_7} v^{i_2 a'_3}_{a'_4 a_1} + \tfrac{1}{2} \tilde{\lambda}^{i_6 i_7}_{a'_3 a_5} \tilde{t}^{a'_4 a_5}_{i_6 i_7} v^{i_2 a_3}_{a'_4 a_1} - \tfrac{1}{2} \tilde{\lambda}^{i_6 i_7}_{a'_5 a_3} \tilde{t}^{a'_4 a'_5}_{i_6 i_7} v^{i_2 a_3}_{a'_4 a_1} + \tfrac{1}{2} \tilde{\lambda}^{i_6 i_7}_{a'_3 a'_5} \tilde{t}^{a'_5 a_4}_{i_6 i_7} v^{i_2 a'_3}_{a_1 a_4} - \tfrac{1}{2} \tilde{\lambda}^{i_6 i_7}_{a'_5 a_3} \tilde{t}^{a'_5 a_4}_{i_6 i_7} v^{i_2 a_3}_{a_1 a_4} \\
&- \tfrac{1}{2} v^{i_2 i_6}_{a_7 a_8} t^{a_8}_{i_4} t^{a_7}_{i_3} t^{a_5}_{i_6} \lambda^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{2} \lambda^{i_2 i_6}_{a_7 a_8} t^{a_8}_{i_4} t^{a_7}_{i_3} t^{a_5}_{i_6} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{4} v^{i_2 i_6}_{a_7 a_8} t^{a_7 a_8}_{i_3 i_4} t^{a_5}_{i_6} \lambda^{i_3 i_4}_{a_1 a_5} + v^{i_2 i_7}_{a_6 a_8} t^{a_8}_{i_4} t^{a_5 a_6}_{i_3 i_7} \lambda^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{2} v^{i_2 i_8}_{a_6 a_7} t^{a_7}_{i_8} t^{a_5 a_6}_{i_3 i_4} \lambda^{i_3 i_4}_{a_1 a_5} + \lambda^{i_2 i_6}_{a_6 a_8} t^{a_8}_{i_4} t^{a_5 a_6}_{i_3 i_7} v^{i_3 i_4}_{a_1 a_5} \\
&- \tfrac{1}{4} \lambda^{i_2 i_6}_{a_7 a_8} t^{a_7 a_8}_{i_3 i_4} t^{a_5}_{i_6} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{2} \lambda^{i_2 i_8}_{a_6 a_7} t^{a_6 a_7}_{i_4 i_8} t^{a_5}_{i_3} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{2} \lambda^{i_6 i_7}_{a_5 a_8} t^{a_8}_{i_3} t^{a_4 a_5}_{i_6 i_7} v^{i_2 i_3}_{a_1 a_4} + \tfrac{1}{2} \lambda^{i_5 i_8}_{a_6 a_7} t^{a_6 a_7}_{i_3 i_8} t^{a_4}_{i_5} v^{i_2 i_3}_{a_1 a_4} - \tfrac{1}{4} V^{i_2 i_6}_{i_7 i_8} t^{i_7 i_8}_{i_3 i_4} t^{a_5}_{i_6} \lambda^{i_3 i_4}_{a_1 a_5} - v^{i_2 i_7}_{a'_6 a_8} t^{a_8}_{i_4} \tilde{t}^{a'_6 a_5}_{i_3 i_7} \lambda^{i_3 i_4}_{a_1 a_5} \\
&+ \tfrac{1}{2} v^{i_2 i_8}_{a'_6 a_7} t^{a_7}_{i_8} \tilde{t}^{a'_6 a_5}_{i_3 i_4} \lambda^{i_3 i_4}_{a_1 a_5} - \lambda^{i_2 i_7}_{a_6 a_8} t^{a_8}_{i_4} \tilde{t}^{a'_5 a_6}_{i_3 i_7} v^{i_3 i_4}_{a'_5 a_1} + \tfrac{1}{2} \lambda^{i_6 i_7}_{a_5 a_8} t^{a_8}_{i_3} \tilde{t}^{a'_4 a_5}_{i_6 i_7} v^{i_2 i_3}_{a'_4 a_1} - v^{i_2 i_7}_{a'_6 a_8} t^{a_8}_{i_4} \tilde{t}^{a'_5 a'_6}_{i_3 i_7} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} - v^{i_2 i_8}_{a_6 a_8} t^{a_8}_{i_4} \tilde{t}^{a'_5 a_6}_{i_3 i_7} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} + \tfrac{1}{2} v^{i_2 i_8}_{a'_6 a_7} t^{a_7}_{i_8} \tilde{t}^{a'_5 a'_6}_{i_3 i_4} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} \\
&+ \tfrac{1}{2} v^{i_2 i_8}_{a_6 a_7} t^{a_7}_{i_8} \tilde{t}^{a'_5 a_6}_{i_3 i_4} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} - \tilde{\lambda}^{i_2 i_7}_{a'_6 a_8} t^{a_8}_{i_4} \tilde{t}^{a'_5 a'_6}_{i_3 i_7} v^{i_3 i_4}_{a'_5 a_1} - \tilde{\lambda}^{i_2 i_7}_{a'_6 a_8} t^{a_8}_{i_4} \tilde{t}^{a'_6 a_5}_{i_3 i_7} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{8} X^{i_7 i_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_4} \lambda^{i_2 i_6}_{i_7 i_8} t^{a_5}_{i_6} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{4} X^{i_7 i_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_4 i_6} \lambda^{i_2 i_6}_{i_7 i_8} t^{a_5}_{i_3} v^{i_3 i_4}_{a_1 a_5} + \tfrac{1}{2} \tilde{\lambda}^{i_6 i_7}_{a'_5 a_8} t^{a_8}_{i_3} \tilde{t}^{a'_4 a'_5}_{i_6 i_7} v^{i_2 i_3}_{a'_4 a_1} \\
&+ \tfrac{1}{2} \tilde{\lambda}^{i_6 i_7}_{a'_5 a_8} t^{a_8}_{i_3} \tilde{t}^{a'_5 a_4}_{i_6 i_7} v^{i_2 i_3}_{a_1 a_4} + \tfrac{1}{4} X^{i_7 i_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_3 i_6} \lambda^{i_3 i_6}_{i_7 i_8} t^{a_4}_{i_5} v^{i_2 i_3}_{a_1 a_4}
\end{aligned}
$$

TABLE ESI.3.XIII: The Λ_2 amplitude equation of Λ-CCSD-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{i_3 i_4}_{a_1 a_2} &= +v^{i_3 i_4}_{a_1 a_2} + P_2 P_2 \lambda^{i_4}_{a_2} f^{i_3}_{a_1} + P_2 \lambda^{i_5}_{a_2} v^{i_3 i_4}_{i_5 a_1} + P_2 \lambda^{i_4}_{a_5} v^{i_3 a_5}_{a_1 a_2} + P_2 P_2 v^{i_4 i_6}_{a_2 a_5} t^{a_5}_{i_6} \lambda^{i_3}_{a_1} + P_2 v^{i_3 i_4}_{a_2 a_6} t^{a_6}_{i_5} \lambda^{i_5}_{a_1} - P_2 \lambda^{i_4}_{a_6} t^{a_6}_{i_5} v^{i_3 i_5}_{a_1 a_2} + P_2 \lambda^{i_4 i_5}_{a_1 a_2} f^{i_3}_{i_5} - P_2 \lambda^{i_3 i_4}_{a_2 a_5} f^{a_5}_{a_1} \\
&+ P_2 \tilde{\lambda}^{i_3 i_4}_{a'_5 a_2} f^{a'_5}_{a_1} - P_2 f^{i_4}_{a_6} t^{a_6}_{i_5} \lambda^{i_3 i_5}_{a_1 a_2} + P_2 \lambda^{i_3 i_4}_{a_2 a_6} t^{a_6}_{i_5} f^{i_5}_{a_1} + \tfrac{1}{2} \lambda^{i_5 i_6}_{a_1 a_2} v^{i_3 i_4}_{i_5 i_6} - P_2 P_2 \lambda^{i_4 i_6}_{a_2 a_5} v^{i_3 a_5}_{i_6 a_1} + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_5 a_6} v^{a_5 a_6}_{a_1 a_2} + P_2 P_2 \tilde{\lambda}^{i_4 i_6}_{a'_5 a_2} v^{i_3 a'_5}_{i_6 a_1} + \tfrac{1}{2} \lambda^{i_3 i_4}_{i_5 i_6} (V^\dagger)^{i_5 i_6}_{a_1 a_2} \\
&- P_2 v^{i_4 i_7}_{i_5 a_6} t^{a_6}_{i_7} \lambda^{i_3 i_5}_{a_1 a_2} - v^{i_3 i_4}_{i_6 a_7} t^{a_7}_{i_5} \lambda^{i_5 i_6}_{a_1 a_2} - P_2 v^{i_7 a_5}_{a_2 a_6} t^{a_6}_{i_7} \lambda^{i_3 i_4}_{a_1 a_5} + P_2 P_2 \lambda^{i_4 i_6}_{a_2 a_7} t^{a_7}_{i_5} v^{i_3 i_5}_{i_6 a_1} + P_2 P_2 v^{i_4 a_6}_{a_2 a_7} t^{a_7}_{i_5} \lambda^{i_3 i_5}_{a_1 a_6} + \lambda^{i_3 i_4}_{a_6 a_7} t^{a_7}_{i_5} v^{i_5 a_6}_{a_1 a_2} + P_2 v^{i_7 a'_5}_{a_2 a_6} t^{a_6}_{i_7} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} \\
&- P_2 P_2 v^{i_4 a'_6}_{a_2 a_7} t^{a_7}_{i_5} \tilde{\lambda}^{i_3 i_5}_{a'_6 a_1} + \tilde{\lambda}^{i_3 i_4}_{a'_6 a_7} t^{a_7}_{i_5} v^{i_5 a'_6}_{a_1 a_2} - P_2 v^{i_4 i_8}_{a_6 a_7} t^{a_7}_{i_8} t^{a_6}_{i_5} \lambda^{i_3 i_5}_{a_1 a_2} + \tfrac{1}{2} v^{i_3 i_4}_{a_7 a_8} t^{a_8}_{i_6} t^{a_7}_{i_5} \lambda^{i_5 i_6}_{a_1 a_2} - P_2 v^{i_6 i_8}_{a_2 a_7} t^{a_7}_{i_8} t^{a_5}_{i_6} \lambda^{i_3 i_4}_{a_1 a_5} - P_2 P_2 v^{i_4 i_7}_{a_2 a_8} t^{a_8}_{i_5} t^{a_6}_{i_7} \lambda^{i_3 i_5}_{a_1 a_6} + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_7 a_8} t^{a_8}_{i_6} t^{a_7}_{i_5} v^{i_5 i_6}_{a_1 a_2} \\
&- \tfrac{1}{2} P_2 v^{i_4 i_8}_{a_6 a_7} t^{a_6 a_7}_{i_5 i_8} \lambda^{i_3 i_5}_{a_1 a_2} + \tfrac{1}{4} v^{i_3 i_4}_{a_7 a_8} t^{a_7 a_8}_{i_5 i_6} \lambda^{i_5 i_6}_{a_1 a_2} - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a_2 a_6} t^{a_5 a_6}_{i_7 i_8} \lambda^{i_3 i_4}_{a_1 a_5} + P_2 P_2 v^{i_4 i_8}_{a_2 a_7} t^{a_6 a_7}_{i_5 i_8} \lambda^{i_3 i_5}_{a_1 a_6} - \tfrac{1}{2} P_2 \lambda^{i_7 i_8}_{a_2 a_6} t^{a_5 a_6}_{i_7 i_8} v^{i_3 i_4}_{a_1 a_5} + \tfrac{1}{4} \lambda^{i_3 i_4}_{a_7 a_8} t^{a_7 a_8}_{i_5 i_6} v^{i_5 i_6}_{a_1 a_2} \\
&- \tfrac{1}{2} P_2 \lambda^{i_4 i_8}_{a_6 a_7} t^{a_6 a_7}_{i_5 i_8} v^{i_3 i_5}_{a_1 a_2} - \tfrac{1}{2} P_2 V^{i_4 i_8}_{i_6 i_7} t^{i_6 i_7}_{i_5 i_8} \lambda^{i_3 i_5}_{a_1 a_2} + \tfrac{1}{4} V^{i_3 i_4}_{i_7 i_8} t^{i_7 i_8}_{i_5 i_6} \lambda^{i_5 i_6}_{a_1 a_2} - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_6 a_2} \tilde{t}^{a'_6 a_5}_{i_7 i_8} \lambda^{i_3 i_4}_{a_1 a_5} + P_2 P_2 v^{i_4 i_8}_{a'_7 a_2} \tilde{t}^{a'_7 a_6}_{i_5 i_8} \lambda^{i_3 i_5}_{a_1 a_6} + \tfrac{1}{2} P_2 \lambda^{i_7 i_8}_{a_2 a_6} \tilde{t}^{a'_5 a_6}_{i_7 i_8} v^{i_3 i_4}_{a'_5 a_1} \\
&- \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_6 a_2} \tilde{t}^{a'_5 a'_6}_{i_7 i_8} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} + \tfrac{1}{2} P_2 v^{i_7 i_8}_{a_2 a_6} \tilde{t}^{a'_5 a_6}_{i_7 i_8} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} + P_2 P_2 v^{i_4 i_8}_{a'_7 a_2} \tilde{t}^{a'_6 a'_7}_{i_5 i_8} \tilde{\lambda}^{i_3 i_5}_{a'_6 a_1} + P_2 P_2 \tilde{\lambda}^{i_4 i_8}_{a'_7 a_2} \tilde{t}^{a'_7 a_6}_{i_5 i_8} v^{i_3 i_5}_{a_1 a_6} - \tfrac{1}{2} P_2 \tilde{\lambda}^{i_7 i_8}_{a'_6 a_2} \tilde{t}^{a'_5 a'_6}_{i_7 i_8} v^{i_3 i_4}_{a'_5 a_1} - \tfrac{1}{2} P_2 \tilde{\lambda}^{i_7 i_8}_{a'_6 a_2} \tilde{t}^{a'_6 a_5}_{i_7 i_8} v^{i_3 i_4}_{a_1 a_5} \\
&+ \tfrac{1}{8} X^{i_7 i_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} \lambda^{i_3 i_4}_{i_7 i_8} v^{i_5 i_6}_{a_1 a_2} - \tfrac{1}{4} P_2 X^{i_7 i_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} \lambda^{i_4 i_6}_{i_7 i_8} v^{i_3 i_5}_{a_1 a_2}
\end{aligned}
$$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.3.XIV: The geminal λ amplitude equation of Λ-CCSD-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{i_3 i_4}_{i_1 i_2} \;=\; & +V^{i_3 i_4}_{i_1 i_2} - P_2 f^{i_4}_{a'_6} F^{a'_6 a_5}_{i_1 i_2} \lambda^{i_3}_{a_5} + \lambda^{i_5}_{a_7} F^{a'_6 a_7}_{i_1 i_2} v^{i_3 i_4}_{i_5 a'_6} + P_2 \lambda^{i_4}_{a_5} V^{i_3 a_5}_{i_1 i_2} - P_2 v^{i_4 i_8}_{a'_6 a_7} t^{a_7}_{i_8} F^{a'_6 a_5}_{i_1 i_2} \lambda^{i_3}_{a_5} - v^{i_3 i_4}_{a'_5 a_8} t^{a_8}_{i_7} \lambda^{i_7}_{a_6} F^{a'_5 a_6}_{i_1 i_2} - P_2 \lambda^{i_4}_{a_6} t^{a_6}_{i_5} V^{i_3 i_5}_{i_1 i_2} - f^{a_6}_{a'_7} F^{a'_7 a_5}_{i_1 i_2} \lambda^{i_3 i_4}_{a_5 a_6} \\
& + \tfrac{1}{2} P_2 \lambda^{i_4 i_7}_{i_5 i_6} f^{i_3}_{i_7} X^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} \lambda^{i_3 i_4}_{i_5 i_6} B^{i_5 i_6}_{i_1 i_2} - f^{i_7}_{a'_8} F^{a'_8 a_6}_{i_1 i_2} t^{a_5}_{i_7} \lambda^{i_3 i_4}_{a_5 a_6} - \tfrac{1}{2} P_2 f^{i_4}_{a_8} t^{a_8}_{i_7} \lambda^{i_3 i_7}_{i_5 i_6} X^{i_5 i_6}_{i_1 i_2} - f^{i_7}_{a'_8} F^{a'_5 a'_8}_{i_1 i_2} t^{a_6}_{i_7} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} - f^{i_7}_{a_8} F^{a'_5 a_8}_{i_1 i_2} t^{a_6}_{i_7} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} - P_2 \lambda^{i_4 i_8}_{a_6 a_7} v^{i_3 a_7}_{i_8 a'_5} F^{a'_5 a_6}_{i_1 i_2} \\
& + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_5 a_6} V^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{4} \lambda^{i_7 i_8}_{i_5 i_6} v^{i_3 i_4}_{i_7 i_8} X^{i_5 i_6}_{i_1 i_2} - P_2 \tilde{\lambda}^{i_4 i_8}_{a'_6 a'_7} v^{i_3 a'_7}_{i_8 a'_5} F^{a'_5 a'_6}_{i_1 i_2} - P_2 \tilde{\lambda}^{i_4 i_8}_{a'_6 a_7} v^{i_3 a_7}_{i_8 a'_5} F^{a'_5 a'_6}_{i_1 i_2} + P_2 \tilde{\lambda}^{i_4 i_8}_{a'_7 a_6} v^{i_3 a'_7}_{i_8 a'_5} F^{a'_5 a_6}_{i_1 i_2} + P_2 \tilde{\lambda}^{i_4 i_8}_{a'_5 a'_7} v^{i_3 a'_7}_{i_8 a_6} F^{a'_5 a_6}_{i_1 i_2} + P_2 \tilde{\lambda}^{i_4 i_8}_{a'_5 a_7} v^{i_3 a_7}_{i_8 a_6} F^{a'_5 a_6}_{i_1 i_2} \\
& + \tfrac{1}{2} \lambda^{i_3 i_4}_{i_5 i_6} P^{i_5 i_6}_{i_1 i_2} + v^{i_9 a_6}_{a'_7 a_8} t^{a_8}_{i_9} F^{a'_7 a_5}_{i_1 i_2} \lambda^{i_3 i_4}_{a_5 a_6} + P_2 \lambda^{i_4 i_8}_{a_6 a_9} t^{a_9}_{i_7} v^{i_3 i_7}_{i_8 a'_5} F^{a'_5 a_6}_{i_1 i_2} - P_2 v^{i_4 a_8}_{a'_5 a_9} t^{a_9}_{i_7} \lambda^{i_3 i_7}_{a_6 a_8} F^{a'_5 a_6}_{i_1 i_2} + \lambda^{i_3 i_4}_{a_6 a_7} t^{a_7}_{i_5} V^{i_5 a_6}_{i_1 i_2} - \tfrac{1}{2} P_2 v^{i_4 i_9}_{i_7 a_8} t^{a_8}_{i_9} \lambda^{i_3 i_7}_{i_5 i_6} X^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_3 i_4}_{i_8 a_9} t^{a_9}_{i_7} \lambda^{i_7 i_8}_{i_5 i_6} X^{i_5 i_6}_{i_1 i_2} \\
& - v^{i_9 a'_6}_{a'_7 a_8} t^{a_8}_{i_9} F^{a'_5 a'_7}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_6} - v^{i_9 a_6}_{a'_7 a_8} t^{a_8}_{i_9} F^{a'_5 a'_7}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} - v^{i_9 a'_5}_{a'_7 a_8} t^{a_8}_{i_9} F^{a'_7 a_6}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} - v^{i_9 a'_7}_{a_6 a_8} t^{a_8}_{i_9} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_7} F^{a'_5 a_6}_{i_1 i_2} - v^{i_9 a_6}_{a_7 a_8} t^{a_8}_{i_9} F^{a'_5 a_7}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} + P_2 \tilde{\lambda}^{i_4 i_8}_{a'_6 a_9} t^{a_9}_{i_7} v^{i_3 i_7}_{i_8 a'_5} F^{a'_5 a'_6}_{i_1 i_2} \\
& - P_2 \tilde{\lambda}^{i_4 i_8}_{a'_5 a_9} t^{a_9}_{i_7} v^{i_3 i_7}_{i_8 a_6} F^{a'_5 a_6}_{i_1 i_2} + P_2 v^{i_4 a'_8}_{a'_6 a_9} t^{a_9}_{i_7} \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} F^{a'_5 a'_6}_{i_1 i_2} + P_2 v^{i_4 a_8}_{a'_6 a_9} t^{a_9}_{i_7} \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a'_6}_{i_1 i_2} + P_2 v^{i_4 a_8}_{a'_5 a_9} t^{a_9}_{i_7} \tilde{\lambda}^{i_3 i_7}_{a'_8 a_6} F^{a'_5 a_6}_{i_1 i_2} + P_2 v^{i_4 a'_8}_{a_6 a_9} t^{a_9}_{i_7} \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} F^{a'_5 a_6}_{i_1 i_2} \\
& + P_2 v^{i_4 a_8}_{a_6 a_9} t^{a_9}_{i_7} \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} + \tilde{\lambda}^{i_3 i_4}_{a'_6 a_7} t^{a_7}_{i_5} V^{i_5 a'_6}_{i_1 i_2} - v^{i_7 i_{10}}_{a'_8 a_9} t^{a_9}_{i_{10}} F^{a'_8 a_6}_{i_1 i_2} t^{a_5}_{i_7} \lambda^{i_3 i_4}_{a_5 a_6} - P_2 \lambda^{i_4 i_9}_{a_6 a_{10}} t^{a_{10}}_{i_7} t^{a_8}_{i_9} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_7 a_8} t^{a_8}_{i_6} t^{a_7}_{i_5} V^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} t^{a_6 a_8}_{i_9 i_{10}} F^{a'_7 a_5}_{i_1 i_2} \lambda^{i_3 i_4}_{a_5 a_6} \\
& + P_2 \lambda^{i_4 i_{10}}_{a_6 a_9} t^{a_8 a_9}_{i_7 i_{10}} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} \lambda^{i_9 i_{10}}_{a_6 a_8} t^{a_7 a_8}_{i_9 i_{10}} v^{i_3 i_4}_{a'_5 a_7} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{4} \lambda^{i_3 i_4}_{a_7 a_8} t^{a_7 a_8}_{i_5 i_6} V^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{2} P_2 \lambda^{i_4 i_8}_{a_6 a_7} t^{a_6 a_7}_{i_5 i_8} V^{i_3 i_5}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a'_8} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} F^{a'_7 a_5}_{i_1 i_2} \lambda^{i_3 i_4}_{a_5 a_6} + P_2 v^{i_4 i_{10}}_{a'_5 a'_9} \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} \lambda^{i_3 i_7}_{a_6 a_8} F^{a'_5 a_6}_{i_1 i_2} \\
& - \tfrac{1}{2} \lambda^{i_9 i_{10}}_{a_6 a_8} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} v^{i_3 i_4}_{a'_5 a'_7} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} P_2 v^{i_4 i_{10}}_{a_8 a_9} t^{a_9}_{i_{10}} t^{a_8}_{i_7} \lambda^{i_3 i_7}_{i_5 i_6} X^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{4} v^{i_3 i_4}_{a_9 a_{10}} t^{a_{10}}_{i_8} t^{a_9}_{i_7} \lambda^{i_7 i_8}_{i_5 i_6} X^{i_5 i_6}_{i_1 i_2} - v^{i_7 i_{10}}_{a'_8 a_9} t^{a_9}_{i_{10}} F^{a'_5 a'_8}_{i_1 i_2} t^{a_6}_{i_7} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} - v^{i_7 i_{10}}_{a_8 a_9} t^{a_9}_{i_{10}} F^{a'_5 a_8}_{i_1 i_2} t^{a_6}_{i_7} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} \\
& - P_2 v^{i_4 i_9}_{a'_6 a_{10}} t^{a_{10}}_{i_7} t^{a_8}_{i_9} \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a'_6}_{i_1 i_2} - P_2 v^{i_4 i_9}_{a_6 a_{10}} t^{a_{10}}_{i_7} t^{a_8}_{i_9} \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{4} P_2 v^{i_4 i_{10}}_{a_8 a_9} t^{a_8 a_9}_{i_7 i_{10}} \lambda^{i_3 i_7}_{i_5 i_6} X^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{8} v^{i_3 i_4}_{a_9 a_{10}} t^{a_9 a_{10}}_{i_7 i_8} \lambda^{i_7 i_8}_{i_5 i_6} X^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} t^{a_6 a_8}_{i_9 i_{10}} F^{a'_5 a'_7}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} \\
& - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} t^{a_6 a_8}_{i_9 i_{10}} F^{a'_5 a_7}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} + P_2 v^{i_4 i_{10}}_{a'_6 a_9} t^{a_8 a_9}_{i_7 i_{10}} \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a'_6}_{i_1 i_2} + P_2 v^{i_4 i_{10}}_{a_6 a_9} t^{a_8 a_9}_{i_7 i_{10}} \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a_8} t^{a_6 a_8}_{i_9 i_{10}} F^{a'_5 a'_7}_{i_1 i_2} v^{i_3 i_4}_{a'_5 a_6} + \tfrac{1}{2} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a_8} t^{a_6 a_8}_{i_9 i_{10}} F^{a'_7 a_5}_{i_1 i_2} v^{i_3 i_4}_{a_5 a_6} \\
& - \tfrac{1}{4} P_2 V^{i_4 i_{10}}_{i_8 i_9} t^{i_8 i_9}_{i_7 i_{10}} \lambda^{i_3 i_7}_{i_5 i_6} X^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{8} V^{i_3 i_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_7 i_8} \lambda^{i_7 i_8}_{i_5 i_6} X^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a'_8} \tilde{t}^{a'_6 a'_8}_{i_9 i_{10}} F^{a'_5 a'_7}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a'_8} \tilde{t}^{a'_5 a'_8}_{i_9 i_{10}} F^{a'_7 a_6}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} + \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a'_8} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} F^{a'_5 a'_7}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_6} \\
& + \tfrac{1}{2} v^{i_9 i_{10}}_{a'_8 a_6} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_7} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_8 a_7} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} F^{a'_5 a_7}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} \tilde{t}^{a'_6 a_8}_{i_9 i_{10}} F^{a'_5 a'_7}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} \tilde{t}^{a'_5 a_8}_{i_9 i_{10}} F^{a'_7 a_6}_{i_1 i_2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a_6 a_8} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_7} F^{a'_5 a_6}_{i_1 i_2} \\
& + P_2 v^{i_4 i_{10}}_{a'_6 a'_9} \tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} F^{a'_5 a'_6}_{i_1 i_2} - P_2 \tilde{\lambda}^{i_4 i_{10}}_{a'_9 a_6} \tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} v^{i_3 i_7}_{a'_5 a'_8} F^{a'_5 a_6}_{i_1 i_2} - P_2 v^{i_4 i_{10}}_{a'_6 a'_9} \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a'_6}_{i_1 i_2} - P_2 v^{i_4 i_{10}}_{a'_9 a_6} \tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} F^{a'_5 a_6}_{i_1 i_2} + P_2 v^{i_4 i_{10}}_{a'_9 a_6} \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} \\
& - P_2 \tilde{\lambda}^{i_4 i_{10}}_{a'_6 a'_9} \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a'_6}_{i_1 i_2} + P_2 \tilde{\lambda}^{i_4 i_{10}}_{a'_9 a_6} \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} + P_2 v^{i_4 i_{10}}_{a_6 a_9} \tilde{t}^{a'_8 a_9}_{i_7 i_{10}} \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} \tilde{\lambda}^{i_9 i_{10}}_{a'_6 a'_8} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_3 i_4}_{a'_5 a'_7} F^{a'_5 a'_6}_{i_1 i_2} + \tfrac{1}{2} \tilde{\lambda}^{i_9 i_{10}}_{a'_8 a_6} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_3 i_4}_{a'_5 a_7} F^{a'_5 a_6}_{i_1 i_2} \\
& - \tfrac{1}{2} \tilde{\lambda}^{i_9 i_{10}}_{a'_6 a'_8} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_3 i_4}_{a'_5 a'_7} F^{a'_5 a'_6}_{i_1 i_2} - \tfrac{1}{2} \tilde{\lambda}^{i_9 i_{10}}_{a'_5 a'_8} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_3 i_4}_{a'_7 a_6} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} \tilde{\lambda}^{i_9 i_{10}}_{a'_5 a_8} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_3 i_4}_{a'_7 a_6} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a'_8} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} F^{a'_5 a_7}_{i_1 i_2} v^{i_3 i_4}_{a'_5 a_6} - \tfrac{1}{2} \tilde{\lambda}^{i_9 i_{10}}_{a'_8 a_6} \tilde{t}^{a'_8 a_7}_{i_9 i_{10}} v^{i_3 i_4}_{a'_5 a_7} F^{a'_5 a_6}_{i_1 i_2} \\
& - \tfrac{1}{2} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a'_8} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} F^{a'_7 a_5}_{i_1 i_2} v^{i_3 i_4}_{a_5 a_6} + \tfrac{1}{8} X^{i_7 i_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} \lambda^{i_3 i_4}_{i_7 i_8} V^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{4} P_2 X^{i_7 i_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_5 i_6} \lambda^{i_4 i_6}_{i_7 i_8} V^{i_3 i_5}_{i_1 i_2}
\end{aligned}
$$

E. Λ-CCSDT-R12

TABLE ESI.3.XV: The Λ_1 amplitude equation of Λ-CCSDT-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{i_2}_{a_1} = {} & \Lambda\text{-CCSD-R12} - \tfrac14 v^{i_2i_8}_{a_6a_7} t^{a_5a_6a_7}_{i_3i_4i_8} \lambda^{i_3i_4}_{a_1a_5} - \tfrac14 \lambda^{i_2i_8}_{a_6a_7} t^{a_5a_6a_7}_{i_3i_4i_8} v^{i_3i_4}_{a_1a_5} - \tfrac14 \lambda^{i_7i_8}_{a_5a_6} t^{a_4a_5a_6}_{i_3i_7i_8} v^{i_2i_3}_{a_1a_4} + \tfrac1{12} f^{i_2}_{a_8} t^{a_6a_7a_8}_{i_3i_4i_5} \lambda^{i_3i_4i_5}_{a_1a_6a_7} + \tfrac1{12}\lambda^{i_2i_7i_8}_{a_4a_5a_6} t^{a_4a_5a_6}_{i_3i_7i_8} f^{i_3}_{a_1} - \tfrac14 \lambda^{i_4i_5i_8}_{a_1a_6a_7} t^{a_6a_7}_{i_3i_8} v^{i_2i_3}_{i_4i_5} \\
& + \tfrac12 v^{i_2a_7}_{i_5a_8} t^{a_6a_8}_{i_3i_4} \lambda^{i_3i_4i_5}_{a_1a_6a_7} + \tfrac12 \lambda^{i_2i_5i_8}_{a_4a_6a_7} t^{a_6a_7}_{i_3i_8} v^{i_3a_4}_{i_5a_1} - \tfrac14 \lambda^{i_2i_7i_8}_{a_3a_4a_6} t^{a_5a_6}_{i_7i_8} v^{a_3a_4}_{a_1a_5} - \tfrac12 v^{i_2a_7}_{i_5a'_8} \tilde t^{a'_8a_6}_{i_3i_4} \lambda^{i_3i_4i_5}_{a_1a_6a_7} + \tfrac14 \lambda^{i_2i_7i_8}_{a_3a_4a_6} \tilde t^{a'_5a_6}_{i_7i_8} v^{a_3a_4}_{a'_5a_1} - \tfrac12 \lambda^{i_4i_6i_9}_{a_1a_7a_8} t^{a_7a_8}_{i_3i_9} t^{a_5}_{i_6} v^{i_2i_3}_{i_4a_5} \\
& + \tfrac12 v^{i_2i_8}_{i_5a_9} t^{a_7a_9}_{i_3i_4} t^{a_6}_{i_8} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac12 v^{i_2a_7}_{a_8a_9} t^{a_9}_{i_5} t^{a_6a_8}_{i_3i_4} \lambda^{i_3i_4i_5}_{a_1a_6a_7} + \tfrac12 \lambda^{i_2i_5i_9}_{a_6a_7a_8} t^{a_7a_8}_{i_4i_9} t^{a_6}_{i_3} v^{i_3i_4}_{i_5a_1} - \tfrac12 \lambda^{i_2i_6i_9}_{a_4a_7a_8} t^{a_7a_8}_{i_3i_9} t^{a_5}_{i_6} v^{i_3a_4}_{a_1a_5} + \tfrac12 \lambda^{i_2i_7i_8}_{a_4a_6a_9} t^{a_9}_{i_3} t^{a_5a_6}_{i_7i_8} v^{i_3a_4}_{a_1a_5} + \tfrac14 v^{i_2i_9}_{i_5a_8} t^{a_6a_7a_8}_{i_3i_4i_9} \lambda^{i_3i_4i_5}_{a_1a_6a_7} \\
& - \tfrac1{12} v^{i_2a_7}_{a_8a_9} t^{a_6a_8a_9}_{i_3i_4i_5} \lambda^{i_3i_4i_5}_{a_1a_6a_7} + \tfrac1{12}\lambda^{i_2i_5i_9}_{a_6a_7a_8} t^{a_6a_7a_8}_{i_3i_4i_9} v^{i_3i_4}_{i_5a_1} + \tfrac14 \lambda^{i_2i_8i_9}_{a_4a_6a_7} t^{a_5a_6a_7}_{i_3i_8i_9} v^{i_3a_4}_{a_1a_5} - \tfrac1{12}\lambda^{i_4i_8i_9}_{a_5a_6a_7} t^{a_5a_6a_7}_{i_3i_8i_9} v^{i_2i_3}_{i_4a_1} - \tfrac1{12}\lambda^{i_7i_8i_9}_{a_3a_5a_6} t^{a_4a_5a_6}_{i_7i_8i_9} v^{i_2a_3}_{a_1a_4} - \tfrac12 v^{i_2i_8}_{i_5a'_9} \tilde t^{a'_9a_7}_{i_3i_4} t^{a_6}_{i_8} \lambda^{i_3i_4i_5}_{a_1a_6a_7} \\
& + \tfrac12 v^{i_2a_7}_{a'_8a_9} t^{a_9}_{i_5} \tilde t^{a'_8a_6}_{i_3i_4} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac12 \lambda^{i_2i_7i_8}_{a_4a_6a_9} t^{a_9}_{i_3} \tilde t^{a'_5a_6}_{i_7i_8} v^{i_3a_4}_{a'_5a_1} - \tfrac14 \lambda^{i_6i_7i_{10}}_{a_1a_8a_9} t^{a_8a_9}_{i_3i_{10}} t^{a_5}_{i_7} t^{a_4}_{i_6} v^{i_2i_3}_{a_4a_5} - \tfrac12 v^{i_2i_8}_{a_9a_{10}} t^{a_{10}}_{i_5} t^{a_7a_9}_{i_3i_4} t^{a_6}_{i_8} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac12 \lambda^{i_2i_6i_{10}}_{a_7a_8a_9} t^{a_8a_9}_{i_4i_{10}} t^{a_7}_{i_3} t^{a_5}_{i_6} v^{i_3i_4}_{a_1a_5} \\
& - \tfrac14 \lambda^{i_2i_7i_8}_{a_6a_9a_{10}} t^{a_{10}}_{i_4} t^{a_9}_{i_3} t^{a_5a_6}_{i_7i_8} v^{i_3i_4}_{a_1a_5} - \tfrac12 v^{i_2i_{10}}_{a_8a_9} t^{a_7a_9}_{i_5i_{10}} t^{a_6a_8}_{i_3i_4} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac18 \lambda^{i_6i_7i_{10}}_{a_1a_8a_9} t^{a_8a_9}_{i_3i_{10}} t^{a_4a_5}_{i_6i_7} v^{i_2i_3}_{a_4a_5} - \tfrac18 \lambda^{i_2i_9i_{10}}_{a_6a_7a_8} t^{a_5a_8}_{i_9i_{10}} t^{a_6a_7}_{i_3i_4} v^{i_3i_4}_{a_1a_5} + \tfrac12 \lambda^{i_2i_7i_{10}}_{a_6a_8a_9} t^{a_8a_9}_{i_4i_{10}} t^{a_5a_6}_{i_3i_7} v^{i_3i_4}_{a_1a_5} \\
& - \tfrac14 \lambda^{i_6i_7i_{10}}_{a_5a_8a_9} t^{a_8a_9}_{i_3i_{10}} t^{a_4a_5}_{i_6i_7} v^{i_2i_3}_{a_1a_4} + \tfrac1{12} v^{i_2i_{10}}_{a_8a_9} t^{a_9}_{i_{10}} t^{a_6a_7a_8}_{i_3i_4i_5} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac14 v^{i_2i_9}_{a_8a_{10}} t^{a_{10}}_{i_5} t^{a_6a_7a_8}_{i_3i_4i_9} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac1{12} v^{i_2i_8}_{a_9a_{10}} t^{a_7a_9a_{10}}_{i_3i_4i_5} t^{a_6}_{i_8} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac1{12}\lambda^{i_2i_9i_{10}}_{a_6a_7a_8} t^{a_6a_7a_8}_{i_4i_9i_{10}} t^{a_5}_{i_3} v^{i_3i_4}_{a_1a_5} \\
& - \tfrac1{12}\lambda^{i_2i_6i_{10}}_{a_7a_8a_9} t^{a_7a_8a_9}_{i_3i_4i_{10}} t^{a_5}_{i_6} v^{i_3i_4}_{a_1a_5} - \tfrac14 \lambda^{i_2i_8i_9}_{a_6a_7a_{10}} t^{a_{10}}_{i_4} t^{a_5a_6a_7}_{i_3i_8i_9} v^{i_3i_4}_{a_1a_5} + \tfrac1{12}\lambda^{i_5i_9i_{10}}_{a_6a_7a_8} t^{a_6a_7a_8}_{i_3i_9i_{10}} t^{a_4}_{i_5} v^{i_2i_3}_{a_1a_4} + \tfrac1{12}\lambda^{i_7i_8i_9}_{a_5a_6a_{10}} t^{a_{10}}_{i_3} t^{a_4a_5a_6}_{i_7i_8i_9} v^{i_2i_3}_{a_1a_4} + \tfrac12 v^{i_2i_8}_{a'_9a_{10}} t^{a_{10}}_{i_5} \tilde t^{a'_9a_7}_{i_3i_4} t^{a_6}_{i_8} \lambda^{i_3i_4i_5}_{a_1a_6a_7} \\
& + \tfrac14 \lambda^{i_2i_7i_8}_{a_6a_9a_{10}} t^{a_{10}}_{i_4} t^{a_9}_{i_3} \tilde t^{a'_5a_6}_{i_7i_8} v^{i_3i_4}_{a'_5a_1} + \tfrac12 v^{i_2i_{10}}_{a'_8a_9} t^{a_7a_9}_{i_5i_{10}} \tilde t^{a'_8a_6}_{i_3i_4} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac12 v^{i_2i_{10}}_{a'_9a_8} \tilde t^{a'_9a_7}_{i_5i_{10}} t^{a_6a_8}_{i_3i_4} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac18 \lambda^{i_6i_7i_{10}}_{a_1a_8a_9} t^{a_8a_9}_{i_3i_{10}} t^{i_4i_5}_{i_6i_7} V^{i_2i_3}_{i_4i_5} + \tfrac18 \lambda^{i_2i_7i_8}_{a_6a_9a_{10}} t^{a_9a_{10}}_{i_3i_4} \tilde t^{a'_5a_6}_{i_7i_8} v^{i_3i_4}_{a'_5a_1} \\
& - \tfrac12 \lambda^{i_2i_7i_{10}}_{a_6a_8a_9} t^{a_8a_9}_{i_4i_{10}} \tilde t^{a'_5a_6}_{i_3i_7} v^{i_3i_4}_{a'_5a_1} + \tfrac14 \lambda^{i_6i_7i_{10}}_{a_5a_8a_9} t^{a_8a_9}_{i_3i_{10}} \tilde t^{a'_4a_5}_{i_6i_7} v^{i_2i_3}_{a'_4a_1} - \tfrac12 v^{i_2i_{10}}_{a'_8a'_9} \tilde t^{a'_9a_7}_{i_5i_{10}} \tilde t^{a'_8a_6}_{i_3i_4} \lambda^{i_3i_4i_5}_{a_1a_6a_7}
\end{aligned}
$$

TABLE ESI.3.XVI: The Λ_2 amplitude equation of Λ-CCSDT-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{i_3i_4}_{a_1a_2} = {} & \Lambda\text{-CCSD-R12} + \tfrac12 P_2 f^{i_4}_{a_8} t^{a_7a_8}_{i_5i_6} \lambda^{i_3i_5i_6}_{a_1a_2a_7} + \tfrac12 P_2 \lambda^{i_3i_4i_8}_{a_2a_6a_7} t^{a_6a_7}_{i_5i_8} f^{i_5}_{a_1} - \tfrac12 P_2 f^{i_4}_{a'_8} \tilde t^{a'_8a_7}_{i_5i_6} \lambda^{i_3i_5i_6}_{a_1a_2a_7} + \tfrac12 P_2 \lambda^{i_4i_6i_7}_{a_1a_2a_5} v^{i_3a_5}_{i_6i_7} + \tfrac12 P_2 \lambda^{i_3i_4i_7}_{a_2a_5a_6} v^{a_5a_6}_{i_7a_1} + \tfrac12 P_2 v^{i_4i_8}_{i_5i_6} t^{a_7}_{i_8} \lambda^{i_3i_5i_6}_{a_1a_2a_7} \\
& + P_2 v^{i_4a_7}_{i_6a_8} t^{a_8}_{i_5} \lambda^{i_3i_5i_6}_{a_1a_2a_7} + P_2 \lambda^{i_3i_4i_7}_{a_2a_6a_8} t^{a_8}_{i_5} v^{i_5a_6}_{i_7a_1} + \tfrac12 P_2 v^{a_6a_7}_{a_2a_8} t^{a_8}_{i_5} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - P_2 v^{i_4i_8}_{i_6a_9} t^{a_9}_{i_5} t^{a_7}_{i_8} \lambda^{i_3i_5i_6}_{a_1a_2a_7} - \tfrac12 P_2 v^{i_4a_7}_{a_8a_9} t^{a_9}_{i_6} t^{a_8}_{i_5} \lambda^{i_3i_5i_6}_{a_1a_2a_7} + \tfrac12 P_2 \lambda^{i_3i_4i_7}_{a_2a_8a_9} t^{a_9}_{i_6} t^{a_8}_{i_5} v^{i_5i_6}_{i_7a_1} \\
& - P_2 v^{i_8a_7}_{a_2a_9} t^{a_9}_{i_5} t^{a_6}_{i_8} \lambda^{i_3i_4i_5}_{a_1a_6a_7} + P_2 v^{i_4i_9}_{i_6a_8} t^{a_7a_8}_{i_5i_9} \lambda^{i_3i_5i_6}_{a_1a_2a_7} - \tfrac14 P_2 v^{i_4a_7}_{a_8a_9} t^{a_8a_9}_{i_5i_6} \lambda^{i_3i_5i_6}_{a_1a_2a_7} + \tfrac12 \lambda^{i_5i_8i_9}_{a_1a_2a_7} t^{a_6a_7}_{i_8i_9} v^{i_3i_4}_{i_5a_6} - \tfrac14 P_2 v^{i_8i_9}_{i_5a_2} t^{a_6a_7}_{i_8i_9} \lambda^{i_3i_4i_5}_{a_1a_6a_7} + P_2 v^{i_9a_7}_{a_2a_8} t^{a_6a_8}_{i_5i_9} \lambda^{i_3i_4i_5}_{a_1a_6a_7} \\
& + \tfrac12 P_2P_2 \lambda^{i_4i_6i_9}_{a_2a_7a_8} t^{a_7a_8}_{i_5i_9} v^{i_3i_5}_{i_6a_1} + \tfrac12 P_2P_2 \lambda^{i_4i_8i_9}_{a_2a_5a_7} t^{a_6a_7}_{i_8i_9} v^{i_3a_5}_{a_1a_6} + \tfrac12 \lambda^{i_3i_4i_9}_{a_6a_7a_8} t^{a_7a_8}_{i_5i_9} v^{i_5a_6}_{a_1a_2} - P_2 v^{i_4i_9}_{i_6a'_8} \tilde t^{a'_8a_7}_{i_5i_9} \lambda^{i_3i_5i_6}_{a_1a_2a_7} - \tfrac14 P_2 V^{i_4a_7}_{i_8i_9} t^{i_8i_9}_{i_5i_6} \lambda^{i_3i_5i_6}_{a_1a_2a_7} + \tfrac12 v^{i_3i_4}_{i_7a'_9} \tilde t^{a'_9a_8}_{i_5i_6} \lambda^{i_5i_6i_7}_{a_1a_2a_8} \\
& + P_2 v^{i_9a_7}_{a'_8a_2} \tilde t^{a'_8a_6}_{i_5i_9} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac12 P_2P_2 \lambda^{i_4i_8i_9}_{a_2a_5a_7} \tilde t^{a'_6a_7}_{i_8i_9} v^{i_3a_5}_{a'_6a_1} + \tfrac12 P_2 v^{i_4i_8}_{a_9a_{10}} t^{a_{10}}_{i_6} t^{a_9}_{i_5} t^{a_7}_{i_8} \lambda^{i_3i_5i_6}_{a_1a_2a_7} - \tfrac12 P_2 \lambda^{i_3i_4i_8}_{a_2a_9a_{10}} t^{a_{10}}_{i_6} t^{a_9}_{i_5} t^{a_7}_{i_8} v^{i_5i_6}_{a_1a_7} + \tfrac14 P_2 v^{i_4i_8}_{a_9a_{10}} t^{a_9a_{10}}_{i_5i_6} t^{a_7}_{i_8} \lambda^{i_3i_5i_6}_{a_1a_2a_7} \\
& - P_2 v^{i_4i_9}_{a_8a_{10}} t^{a_{10}}_{i_6} t^{a_7a_8}_{i_5i_9} \lambda^{i_3i_5i_6}_{a_1a_2a_7} + \tfrac12 P_2 v^{i_4i_{10}}_{a_8a_9} t^{a_9}_{i_{10}} t^{a_7a_8}_{i_5i_6} \lambda^{i_3i_5i_6}_{a_1a_2a_7} + \tfrac12 \lambda^{i_7i_9i_{10}}_{a_1a_2a_8} t^{a_6a_8}_{i_9i_{10}} t^{a_5}_{i_7} v^{i_3i_4}_{a_5a_6} - P_2 v^{i_8i_{10}}_{a_2a_9} t^{a_7a_9}_{i_5i_{10}} t^{a_6}_{i_8} \lambda^{i_3i_4i_5}_{a_1a_6a_7} + \tfrac14 P_2 v^{i_8i_9}_{a_2a_{10}} t^{a_{10}}_{i_5} t^{a_6a_7}_{i_8i_9} \lambda^{i_3i_4i_5}_{a_1a_6a_7} \\
& - \tfrac12 P_2 \lambda^{i_3i_4i_{10}}_{a_2a_8a_9} t^{a_8a_9}_{i_6i_{10}} t^{a_7}_{i_5} v^{i_5i_6}_{a_1a_7} + \tfrac12 P_2P_2 \lambda^{i_4i_8i_9}_{a_2a_7a_{10}} t^{a_{10}}_{i_5} t^{a_6a_7}_{i_8i_9} v^{i_3i_5}_{a_1a_6} - \tfrac12 P_2P_2 \lambda^{i_4i_7i_{10}}_{a_2a_8a_9} t^{a_8a_9}_{i_5i_{10}} t^{a_6}_{i_7} v^{i_3i_5}_{a_1a_6} + \tfrac12 \lambda^{i_3i_4i_{10}}_{a_7a_8a_9} t^{a_8a_9}_{i_6i_{10}} t^{a_7}_{i_5} v^{i_5i_6}_{a_1a_2} + \tfrac14 P_2 V^{i_4i_8}_{i_9i_{10}} t^{i_9i_{10}}_{i_5i_6} t^{a_7}_{i_8} \lambda^{i_3i_5i_6}_{a_1a_2a_7} \\
& + P_2 v^{i_4i_9}_{a'_8a_{10}} t^{a_{10}}_{i_6} \tilde t^{a'_8a_7}_{i_5i_9} \lambda^{i_3i_5i_6}_{a_1a_2a_7} - \tfrac12 P_2 v^{i_4i_{10}}_{a'_8a_9} t^{a_9}_{i_{10}} \tilde t^{a'_8a_7}_{i_5i_6} \lambda^{i_3i_5i_6}_{a_1a_2a_7} - \tfrac12 v^{i_3i_4}_{a'_9a_{10}} t^{a_{10}}_{i_7} \tilde t^{a'_9a_8}_{i_5i_6} \lambda^{i_5i_6i_7}_{a_1a_2a_8} - P_2 v^{i_8i_{10}}_{a'_9a_2} \tilde t^{a'_9a_7}_{i_5i_{10}} t^{a_6}_{i_8} \lambda^{i_3i_4i_5}_{a_1a_6a_7} - \tfrac12 P_2P_2 \lambda^{i_4i_8i_9}_{a_2a_7a_{10}} t^{a_{10}}_{i_5} \tilde t^{a'_6a_7}_{i_8i_9} v^{i_3i_5}_{a'_6a_1} \\
& + \tfrac14 P_2 v^{i_4i_{10}}_{a_8a_9} t^{a_7a_8a_9}_{i_5i_6i_{10}} \lambda^{i_3i_5i_6}_{a_1a_2a_7} + \tfrac1{12} v^{i_3i_4}_{a_9a_{10}} t^{a_8a_9a_{10}}_{i_5i_6i_7} \lambda^{i_5i_6i_7}_{a_1a_2a_8} + \tfrac14 P_2 v^{i_9i_{10}}_{a_2a_8} t^{a_6a_7a_8}_{i_5i_9i_{10}} \lambda^{i_3i_4i_5}_{a_1a_6a_7} + \tfrac14 P_2P_2 \lambda^{i_4i_9i_{10}}_{a_2a_7a_8} t^{a_6a_7a_8}_{i_5i_9i_{10}} v^{i_3i_5}_{a_1a_6} - \tfrac1{12} P_2 \lambda^{i_8i_9i_{10}}_{a_2a_6a_7} t^{a_5a_6a_7}_{i_8i_9i_{10}} v^{i_3i_4}_{a_1a_5} \\
& + \tfrac1{12}\lambda^{i_3i_4i_{10}}_{a_7a_8a_9} t^{a_7a_8a_9}_{i_5i_6i_{10}} v^{i_5i_6}_{a_1a_2} - \tfrac1{12} P_2 \lambda^{i_4i_9i_{10}}_{a_6a_7a_8} t^{a_6a_7a_8}_{i_5i_9i_{10}} v^{i_3i_5}_{a_1a_2}
\end{aligned}
$$

TABLE ESI.3.XVII: The Λ_3 amplitude equation of Λ-CCSDT-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{i_4i_5i_6}_{a_1a_2a_3} = {} & -P_3P_3 \lambda^{i_6}_{a_3} v^{i_4i_5}_{a_1a_2} - P_3P_3 \lambda^{i_5i_6}_{a_2a_3} f^{i_4}_{a_1} + P_3P_3 \lambda^{i_6i_7}_{a_2a_3} v^{i_4i_5}_{i_7a_1} + P_3P_3 \lambda^{i_5i_6}_{a_3a_7} v^{i_4a_7}_{a_1a_2} - P_3P_3 \tilde\lambda^{i_5i_6}_{a'_7a_3} v^{i_4a'_7}_{a_1a_2} - P_3P_3 v^{i_6i_8}_{a_3a_7} t^{a_7}_{i_8} \lambda^{i_4i_5}_{a_1a_2} - P_3P_3 v^{i_5i_6}_{a_3a_8} t^{a_8}_{i_7} \lambda^{i_4i_7}_{a_1a_2} \\
& - P_3P_3 \lambda^{i_5i_6}_{a_3a_8} t^{a_8}_{i_7} v^{i_4i_7}_{a_1a_2} + P_3 \lambda^{i_5i_6i_7}_{a_1a_2a_3} f^{i_4}_{i_7} - P_3 \lambda^{i_4i_5i_6}_{a_2a_3a_7} f^{a_7}_{a_1} + P_3 f^{i_6}_{a_8} t^{a_8}_{i_7} \lambda^{i_4i_5i_7}_{a_1a_2a_3} + P_3 \lambda^{i_4i_5i_6}_{a_2a_3a_8} t^{a_8}_{i_7} f^{i_7}_{a_1} - \tfrac12 P_3 \lambda^{i_6i_7i_8}_{a_1a_2a_3} v^{i_4i_5}_{i_7i_8} + P_3P_3 \lambda^{i_5i_6i_8}_{a_2a_3a_7} v^{i_4a_7}_{i_8a_1} \\
& - \tfrac12 P_3 \lambda^{i_4i_5i_6}_{a_3a_7a_8} v^{a_7a_8}_{a_1a_2} + P_3 v^{i_6i_9}_{i_7a_8} t^{a_8}_{i_9} \lambda^{i_4i_5i_7}_{a_1a_2a_3} + P_3 v^{i_5i_6}_{i_8a_9} t^{a_9}_{i_7} \lambda^{i_4i_7i_8}_{a_1a_2a_3} + P_3 v^{i_9a_7}_{a_3a_8} t^{a_8}_{i_9} \lambda^{i_4i_5i_6}_{a_1a_2a_7} - P_3P_3 \lambda^{i_5i_6i_8}_{a_2a_3a_9} t^{a_9}_{i_7} v^{i_4i_7}_{i_8a_1} - P_3P_3 v^{i_6a_8}_{a_3a_9} t^{a_9}_{i_7} \lambda^{i_4i_5i_7}_{a_1a_2a_8} \\
& - P_3 \lambda^{i_4i_5i_6}_{a_3a_8a_9} t^{a_9}_{i_7} v^{i_7a_8}_{a_1a_2} + P_3 v^{i_6i_{10}}_{a_8a_9} t^{a_9}_{i_{10}} t^{a_8}_{i_7} \lambda^{i_4i_5i_7}_{a_1a_2a_3} - \tfrac12 P_3 v^{i_5i_6}_{a_9a_{10}} t^{a_{10}}_{i_8} t^{a_9}_{i_7} \lambda^{i_4i_7i_8}_{a_1a_2a_3} + P_3 v^{i_8i_{10}}_{a_3a_9} t^{a_9}_{i_{10}} t^{a_7}_{i_8} \lambda^{i_4i_5i_6}_{a_1a_2a_7} + P_3P_3 v^{i_6i_9}_{a_3a_{10}} t^{a_{10}}_{i_7} t^{a_8}_{i_9} \lambda^{i_4i_5i_7}_{a_1a_2a_8} \\
& - \tfrac12 P_3 \lambda^{i_4i_5i_6}_{a_3a_9a_{10}} t^{a_{10}}_{i_8} t^{a_9}_{i_7} v^{i_7i_8}_{a_1a_2} + \tfrac12 P_3 v^{i_6i_{10}}_{a_8a_9} t^{a_8a_9}_{i_7i_{10}} \lambda^{i_4i_5i_7}_{a_1a_2a_3} - \tfrac14 P_3 v^{i_5i_6}_{a_9a_{10}} t^{a_9a_{10}}_{i_7i_8} \lambda^{i_4i_7i_8}_{a_1a_2a_3} + \tfrac12 P_3 v^{i_9i_{10}}_{a_3a_8} t^{a_7a_8}_{i_9i_{10}} \lambda^{i_4i_5i_6}_{a_1a_2a_7} - P_3P_3 v^{i_6i_{10}}_{a_3a_9} t^{a_8a_9}_{i_7i_{10}} \lambda^{i_4i_5i_7}_{a_1a_2a_8} \\
& - \tfrac12 P_3P_3 \lambda^{i_6i_9i_{10}}_{a_2a_3a_8} t^{a_7a_8}_{i_9i_{10}} v^{i_4i_5}_{a_1a_7} - \tfrac14 P_3 \lambda^{i_4i_5i_6}_{a_3a_9a_{10}} t^{a_9a_{10}}_{i_7i_8} v^{i_7i_8}_{a_1a_2} - \tfrac12 P_3P_3 \lambda^{i_5i_6i_{10}}_{a_3a_8a_9} t^{a_8a_9}_{i_7i_{10}} v^{i_4i_7}_{a_1a_2} + \tfrac12 P_3 V^{i_6i_{10}}_{i_8i_9} t^{i_8i_9}_{i_7i_{10}} \lambda^{i_4i_5i_7}_{a_1a_2a_3} - \tfrac14 P_3 V^{i_5i_6}_{i_9i_{10}} t^{i_9i_{10}}_{i_7i_8} \lambda^{i_4i_7i_8}_{a_1a_2a_3} \\
& + \tfrac12 P_3 v^{i_9i_{10}}_{a'_8a_3} \tilde t^{a'_8a_7}_{i_9i_{10}} \lambda^{i_4i_5i_6}_{a_1a_2a_7} - P_3P_3 v^{i_6i_{10}}_{a'_9a_3} \tilde t^{a'_9a_8}_{i_7i_{10}} \lambda^{i_4i_5i_7}_{a_1a_2a_8} + \tfrac12 P_3P_3 \lambda^{i_6i_9i_{10}}_{a_2a_3a_8} \tilde t^{a'_7a_8}_{i_9i_{10}} v^{i_4i_5}_{a'_7a_1}
\end{aligned}
$$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.3.XVIII: The geminal λ amplitude equation of Λ-CCSDT-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{i_3 i_4}_{i_1 i_2} = {} & \Lambda\text{-CCSD-R12} + \tfrac{1}{2}\lambda^{i_3 i_4 i_{10}}_{a_6 a_8 a_9} t^{a_8 a_9}_{i_7 i_{10}} f^{i_7}_{a'_5} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2}\lambda^{i_3 i_4 i_9}_{a_6 a_7 a_8} v^{a_7 a_8}_{i_9 a'_5} F^{a'_5 a_6}_{i_1 i_2} + \lambda^{i_3 i_4 i_9}_{a_6 a_8 a_{10}} t^{a_{10}}_{i_7} v^{i_7 a_8}_{i_9 a'_5} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} v^{a_8 a_9}_{a'_5 a_{10}} t^{a_{10}}_{i_7} \lambda^{i_3 i_4 i_7}_{a_6 a_8 a_9} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2}\lambda^{i_3 i_4 i_9}_{a_6 a_{10} a_{11}} t^{a_{11}}_{i_8} t^{a_{10}}_{i_7} v^{i_7 i_8}_{i_9 a'_5} F^{a'_5 a_6}_{i_1 i_2} \\
& - v^{i_9 a_8}_{a'_{10} a_{11}} t^{a_{11}}_{i_5} F^{a'_{10} a_7}_{i_1 i_2} t^{a_6}_{i_9} \lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} + \tfrac{1}{4}\lambda^{i_3 i_4 i_9}_{a_6 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_7 i_8} v^{i_7 i_8}_{i_9 a'_5} F^{a'_5 a_6}_{i_1 i_2} - v^{i_{11} a_9}_{a'_5 a_{10}} t^{a_8 a_{10}}_{i_7 i_{11}} \lambda^{i_3 i_4 i_7}_{a_6 a_8 a_9} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2} P_2 \lambda^{i_4 i_8 i_{11}}_{a_6 a_9 a_{10}} t^{a_9 a_{10}}_{i_7 i_{11}} v^{i_3 i_7}_{i_8 a'_5} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2} P_2 \lambda^{i_4 i_{10} i_{11}}_{a_6 a_7 a_9} t^{a_8 a_9}_{i_{10} i_{11}} v^{i_3 a_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} \\
& + \tfrac{1}{2}\lambda^{i_3 i_4 i_9}_{a_6 a_7 a_8} t^{a_7 a_8}_{i_5 i_9} V^{i_5 a_6}_{i_1 i_2} + v^{i_{11} a_9}_{a'_5 a'_{10}} \tilde{t}^{a'_{10} a_8}_{i_7 i_{11}} \lambda^{i_3 i_4 i_7}_{a_6 a_8 a_9} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2} P_2 \lambda^{i_4 i_{10} i_{11}}_{a_6 a_7 a_9} \tilde{t}^{a'_8 a_9}_{i_{10} i_{11}} v^{i_3 a_7}_{a'_5 a'_8} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2}\lambda^{i_3 i_4 i_{10}}_{a_6 a_{11} a_{12}} t^{a_{12}}_{i_8} t^{a_{11}}_{i_7} t^{a_9}_{i_{10}} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} + \lambda^{i_3 i_4 i_9}_{a_6 a_{10} a_{12}} t^{a_{12}}_{i_8} t^{a_9 a_{10}}_{i_7 i_{11}} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} \\
& - \tfrac{1}{4}\lambda^{i_3 i_4 i_{10}}_{a_6 a_{11} a_{12}} t^{a_{11} a_{12}}_{i_7 i_8} t^{a_9}_{i_{10}} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2}\lambda^{i_3 i_4 i_{12}}_{a_6 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_8 i_{12}} t^{a_9}_{i_7} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2} P_2 \lambda^{i_4 i_{10} i_{11}}_{a_6 a_9 a_{12}} t^{a_{12}}_{i_7} t^{a_8 a_9}_{i_{10} i_{11}} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} P_2 \lambda^{i_4 i_9 i_{12}}_{a_6 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_7 i_{12}} t^{a_8}_{i_9} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} \\
& + \tfrac{1}{2}\lambda^{i_3 i_4 i_{10}}_{a_7 a_8 a_9} t^{a_8 a_9}_{i_6 i_{10}} t^{a_7}_{i_5} V^{i_5 i_6}_{i_1 i_2} + v^{i_9 i_{12}}_{a'_{10} a'_{11}} \tilde{t}^{a'_{11} a_8}_{i_5 i_{12}} F^{a'_{10} a_7}_{i_1 i_2} t^{a_6}_{i_9} \lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} + \tfrac{1}{2} P_2 \lambda^{i_4 i_{10} i_{11}}_{a_6 a_9 a_{12}} t^{a_{12}}_{i_7} \tilde{t}^{a'_8 a_9}_{i_{10} i_{11}} v^{i_3 i_7}_{a'_5 a'_8} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{4} v^{i_{11} i_{12}}_{a'_5 a_{10}} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} \lambda^{i_3 i_4 i_7}_{a_6 a_8 a_9} F^{a'_5 a_6}_{i_1 i_2} \\
& + \tfrac{1}{4} P_2 \lambda^{i_4 i_{11} i_{12}}_{a_6 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{12}\lambda^{i_{10} i_{11} i_{12}}_{a_6 a_8 a_9} t^{a_7 a_8 a_9}_{i_{10} i_{11} i_{12}} v^{i_3 i_4}_{a'_5 a_7} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{12}\lambda^{i_3 i_4 i_{10}}_{a_7 a_8 a_9} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}} V^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{12} P_2 \lambda^{i_4 i_9 i_{10}}_{a_6 a_7 a_8} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} V^{i_3 i_5}_{i_1 i_2}
\end{aligned}
$$

F. Λ-CCSDTQ-R12

TABLE ESI.3.XIX: The Λ_1 amplitude equation of Λ-CCSDTQ-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{i_2}_{a_1} = {} & \Lambda\text{-CCSDT-R12} + \tfrac{1}{24} v^{i_2 i_{10}}_{a_8 a_9} t^{a_6 a_7 a_8 a_9}_{i_3 i_4 i_5 i_{10}} \lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} - \tfrac{1}{24}\lambda^{i_2 i_9 i_{10}}_{a_6 a_7 a_8} t^{a_5 a_6 a_7 a_8}_{i_3 i_4 i_9 i_{10}} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{36}\lambda^{i_8 i_9 i_{10}}_{a_5 a_6 a_7} t^{a_4 a_5 a_6 a_7}_{i_3 i_8 i_9 i_{10}} v^{i_2 i_3}_{a_1 a_4} - \tfrac{1}{144} f^{i_2}_{a_{10}} t^{a_7 a_8 a_9 a_{10}}_{i_3 i_4 i_5 i_6} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} \\
& + \tfrac{1}{144}\lambda^{i_2 i_8 i_9 i_{10}}_{a_4 a_5 a_6 a_7} t^{a_4 a_5 a_6 a_7}_{i_3 i_8 i_9 i_{10}} f^{i_3}_{a_1} - \tfrac{1}{24}\lambda^{i_4 i_5 i_9 i_{10}}_{a_1 a_6 a_7 a_8} t^{a_6 a_7 a_8}_{i_3 i_9 i_{10}} v^{i_2 i_3}_{i_4 i_5} - \tfrac{1}{12} v^{i_2 a_9}_{i_6 a_{10}} t^{a_7 a_8 a_{10}}_{i_3 i_4 i_5} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \tfrac{1}{12}\lambda^{i_2 i_5 i_9 i_{10}}_{a_4 a_6 a_7 a_8} t^{a_6 a_7 a_8}_{i_3 i_9 i_{10}} v^{i_3 a_4}_{i_5 a_1} - \tfrac{1}{24}\lambda^{i_2 i_8 i_9 i_{10}}_{a_3 a_4 a_6 a_7} t^{a_5 a_6 a_7}_{i_8 i_9 i_{10}} v^{a_3 a_4}_{a_1 a_5} \\
& + \tfrac{1}{4}\lambda^{i_4 i_7 i_8 i_{11}}_{a_1 a_6 a_9 a_{10}} t^{a_9 a_{10}}_{i_3 i_{11}} t^{a_5 a_6}_{i_7 i_8} v^{i_2 i_3}_{i_4 a_5} - \tfrac{1}{8} v^{i_2 a_9}_{a_{10} a_{11}} t^{a_8 a_{11}}_{i_5 i_6} t^{a_7 a_{10}}_{i_3 i_4} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} - \tfrac{1}{8}\lambda^{i_2 i_5 i_8 i_{11}}_{a_6 a_7 a_9 a_{10}} t^{a_9 a_{10}}_{i_4 i_{11}} t^{a_6 a_7}_{i_3 i_8} v^{i_3 i_4}_{i_5 a_1} + \tfrac{1}{4}\lambda^{i_2 i_7 i_8 i_{11}}_{a_4 a_6 a_9 a_{10}} t^{a_9 a_{10}}_{i_3 i_{11}} t^{a_5 a_6}_{i_7 i_8} v^{i_3 a_4}_{a_1 a_5} + \tfrac{1}{4}\lambda^{i_4 i_7 i_8 i_{11}}_{a_1 a_6 a_9 a_{10}} t^{a_9 a_{10}}_{i_3 i_{11}} \tilde{t}^{a'_5 a_6}_{i_7 i_8} v^{i_2 i_3}_{i_4 a'_5} \\
& - \tfrac{1}{4} v^{i_2 a_9}_{a'_{11} a_{10}} \tilde{t}^{a'_{11} a_8}_{i_5 i_6} t^{a_7 a_{10}}_{i_3 i_4} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} - \tfrac{1}{4}\lambda^{i_2 i_7 i_8 i_{11}}_{a_4 a_6 a_9 a_{10}} t^{a_9 a_{10}}_{i_3 i_{11}} \tilde{t}^{a'_5 a_6}_{i_7 i_8} v^{i_3 a_4}_{a'_5 a_1} - \tfrac{1}{12}\lambda^{i_4 i_6 i_{10} i_{11}}_{a_1 a_7 a_8 a_9} t^{a_7 a_8 a_9}_{i_3 i_{10} i_{11}} t^{a_5}_{i_6} v^{i_2 i_3}_{i_4 a_5} + \tfrac{1}{12} v^{i_2 i_{10}}_{i_6 a_{11}} t^{a_8 a_9 a_{11}}_{i_3 i_4 i_5} t^{a_7}_{i_{10}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} \\
& + \tfrac{1}{12} v^{i_2 a_9}_{a_{10} a_{11}} t^{a_{11}}_{i_6} t^{a_7 a_8 a_{10}}_{i_3 i_4 i_5} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \tfrac{1}{12}\lambda^{i_2 i_5 i_{10} i_{11}}_{a_6 a_7 a_8 a_9} t^{a_6 a_7 a_8 a_9}_{i_4 i_{10} i_{11}} t^{a_6}_{i_3} v^{i_3 i_4}_{i_5 a_1} - \tfrac{1}{12}\lambda^{i_2 i_6 i_{10} i_{11}}_{a_4 a_7 a_8 a_9} t^{a_7 a_8 a_9}_{i_3 i_{10} i_{11}} t^{a_5}_{i_6} v^{i_3 a_4}_{a_1 a_5} - \tfrac{1}{12}\lambda^{i_2 i_8 i_9 i_{10}}_{a_4 a_6 a_7 a_{11}} t^{a_{11}}_{i_3} t^{a_5 a_6 a_7}_{i_8 i_9 i_{10}} v^{i_3 a_4}_{a_1 a_5} \\
& - \tfrac{1}{36} v^{i_2 i_{11}}_{i_6 a_{10}} t^{a_7 a_8 a_9 a_{10}}_{i_3 i_4 i_5 i_{11}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \tfrac{1}{96} v^{i_2 a_9}_{a_{10} a_{11}} t^{a_7 a_8 a_{10} a_{11}}_{i_3 i_4 i_5 i_6} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \tfrac{1}{96}\lambda^{i_2 i_5 i_{10} i_{11}}_{a_6 a_7 a_8 a_9} t^{a_6 a_7 a_8 a_9}_{i_3 i_4 i_{10} i_{11}} v^{i_3 i_4}_{i_5 a_1} + \tfrac{1}{36}\lambda^{i_2 i_9 i_{10} i_{11}}_{a_4 a_6 a_7 a_8} t^{a_5 a_6 a_7 a_8}_{i_3 i_9 i_{10} i_{11}} v^{i_3 a_4}_{a_1 a_5} - \tfrac{1}{144}\lambda^{i_4 i_9 i_{10} i_{11}}_{a_5 a_6 a_7 a_8} t^{a_5 a_6 a_7 a_8}_{i_3 i_9 i_{10} i_{11}} v^{i_2 i_3}_{i_4 a_1} \\
& - \tfrac{1}{144}\lambda^{i_8 i_9 i_{10} i_{11}}_{a_3 a_5 a_6 a_7} t^{a_4 a_5 a_6 a_7}_{i_8 i_9 i_{10} i_{11}} v^{i_2 a_3}_{a_1 a_4} - \tfrac{1}{8} v^{i_2 a_9}_{a'_{10} a'_{11}} \tilde{t}^{a'_{11} a_8}_{i_5 i_6} \tilde{t}^{a'_{10} a_7}_{i_3 i_4} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \tfrac{1}{8} v^{i_2 i_{10}}_{a'_{11} a'_{12}} \tilde{t}^{a'_{12} a_9}_{i_5 i_6} \tilde{t}^{a'_{11} a_8}_{i_3 i_4} t^{a_7}_{i_{10}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} - \tfrac{1}{4}\lambda^{i_6 i_8 i_9 i_{12}}_{a_1 a_7 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_3 i_{12}} t^{a'_4 a_7}_{i_8 i_9} t^{a_5}_{i_6} v^{i_2 i_3}_{a'_4 a_5} \\
& + \tfrac{1}{4} v^{i_2 i_{10}}_{a'_{12} a_{11}} \tilde{t}^{a'_{12} a_9}_{i_5 i_6} t^{a_8 a_{11}}_{i_3 i_4} t^{a_7}_{i_{10}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \tfrac{1}{4}\lambda^{i_2 i_7 i_8 i_{12}}_{a_6 a_9 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_4 i_{12}} t^{a_9}_{i_3} \tilde{t}^{a'_5 a_6}_{i_7 i_8} v^{i_3 i_4}_{a'_5 a_1} + \tfrac{1}{4}\lambda^{i_6 i_8 i_9 i_{12}}_{a_1 a_7 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_3 i_{12}} t^{a_5 a_7}_{i_8 i_9} t^{a_4}_{i_6} v^{i_2 i_3}_{a_4 a_5} + \tfrac{1}{8} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_9 a_{12}}_{i_5 i_6} t^{a_8 a_{11}}_{i_3 i_4} t^{a_7}_{i_{10}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} \\
& + \tfrac{1}{8}\lambda^{i_2 i_6 i_9 i_{12}}_{a_7 a_8 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_4 i_{12}} t^{a_7 a_8}_{i_3 i_9} t^{a_5}_{i_6} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{4}\lambda^{i_2 i_7 i_8 i_{12}}_{a_6 a_9 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_4 i_{12}} t^{a_9}_{i_3} t^{a_5 a_6}_{i_7 i_8} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{24}\lambda^{i_6 i_7 i_{11} i_{12}}_{a_1 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_3 i_{11} i_{12}} t^{a_5}_{i_7} t^{a_4}_{i_6} v^{i_2 i_3}_{a_4 a_5} - \tfrac{1}{12} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_{12}}_{i_6} t^{a_8 a_9 a_{11}}_{i_3 i_4 i_5} t^{a_7}_{i_{10}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} \\
& - \tfrac{1}{12}\lambda^{i_2 i_6 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_4 i_{11} i_{12}} t^{a_7}_{i_3} t^{a_5}_{i_6} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{24}\lambda^{i_8 i_9 i_{10}}_{a_6 a_7 a_8} t^{a_{12}}_{i_4} t^{a_{11}}_{i_3} t^{a_5 a_6 a_7}_{i_8 i_9 i_{10}} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{48}\lambda^{i_6 i_7 i_{11} i_{12}}_{a_1 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_3 i_{11} i_{12}} t^{a_4 a_5}_{i_6 i_7} v^{i_2 i_3}_{a_4 a_5} + \tfrac{1}{12} v^{i_2 i_{12}}_{a_{10} a_{11}} t^{a_9 a_{11}}_{i_6 i_{12}} t^{a_7 a_8 a_{10}}_{i_3 i_4 i_5} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} \\
& - \tfrac{1}{8} v^{i_2 i_{12}}_{a_{10} a_{11}} t^{a_8 a_9 a_{11}}_{i_5 i_6 i_{12}} t^{a_7 a_{10}}_{i_3 i_4} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \tfrac{1}{24}\lambda^{i_7 i_8 i_9 i_{12}}_{a_1 a_6 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_3 i_{12}} t^{a_4 a_5 a_6}_{i_7 i_8 i_9} v^{i_2 i_3}_{a_4 a_5} + \tfrac{1}{12}\lambda^{i_2 i_7 i_{11} i_{12}}_{a_6 a_8 a_9 a_{10}} t^{a_5 a_6}_{i_{11} i_{12}} v^{i_3 i_4}_{a_1 a_5} + \tfrac{1}{24}\lambda^{i_2 i_9 i_{11} i_{12}}_{a_6 a_7 a_8 a_{10}} t^{a_5 a_{10}}_{i_{11} i_{12}} t^{a_6 a_7 a_8}_{i_3 i_4 i_9} v^{i_3 i_4}_{a_1 a_5} \\
& - \tfrac{1}{48}\lambda^{i_2 i_{10} i_{11} i_{12}}_{a_6 a_7 a_8 a_9} t^{a_8 a_9}_{i_{10} i_{11} i_{12}} t^{a_6 a_7}_{i_3 i_4} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{8}\lambda^{i_2 i_8 i_9 i_{12}}_{a_6 a_7 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_4 i_{12}} t^{a_5 a_6 a_7}_{i_3 i_8 i_9} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{24}\lambda^{i_6 i_7 i_{11} i_{12}}_{a_5 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_3 i_{11} i_{12}} t^{a_4 a_5}_{i_6 i_7} v^{i_2 i_3}_{a_1 a_4} + \tfrac{1}{24}\lambda^{i_7 i_8 i_9 i_{12}}_{a_5 a_6 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_3 i_{12}} t^{a_7 i_8 i_9}_{i_7 i_8 i_9} v^{i_2 i_3}_{a_1 a_4} \\
& - \tfrac{1}{48}\lambda^{i_6 i_7 i_{11} i_{12}}_{a_1 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_3 i_{11} i_{12}} t^{i_4 i_5}_{i_6 i_7} V^{i_2 i_3}_{i_4 i_5} + \tfrac{1}{12} v^{i_2 i_{12}}_{a'_{11} a_{10}} \tilde{t}^{a'_{11} a_9}_{i_6 i_{12}} t^{a_7 a_8 a_{10}}_{i_3 i_4 i_5} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \tfrac{1}{8} v^{i_2 i_{12}}_{a'_{10} a_{11}} t^{a_8 a_9 a_{11}}_{i_5 i_6 i_{12}} \tilde{t}^{a_{10} a_7}_{i_3 i_4} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} - \tfrac{1}{12}\lambda^{i_2 i_7 i_{11} i_{12}}_{a_6 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_4 i_{11} i_{12}} \tilde{t}^{a'_5 a_6}_{i_3 i_7} v^{i_3 i_4}_{a'_5 a_1} \\
& + \tfrac{1}{24}\lambda^{i_2 i_7 i_8 i_{12}}_{a_6 a_9 a_{10} a_{11}} t^{a_9 a_{10} a_{11}}_{i_3 i_4 i_{12}} \tilde{t}^{a'_5 a_6}_{i_7 i_8} v^{i_3 i_4}_{a'_5 a_1} + \tfrac{1}{24}\lambda^{i_6 i_7 i_{11} i_{12}}_{a_5 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_3 i_{11} i_{12}} \tilde{t}^{a'_4 a_5}_{i_6 i_7} v^{i_2 i_3}_{a'_4 a_1} - \tfrac{1}{144} v^{i_2 i_{12}}_{a_{10} a_{11}} t^{a_{11}}_{i_{12}} t^{a_7 a_8 a_9 a_{10}}_{i_3 i_4 i_5 i_6} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \tfrac{1}{36} v^{i_2 i_{11}}_{a_{10} a_{12}} t^{a_{12}}_{i_6} t^{a_7 a_8 a_9 a_{10}}_{i_3 i_4 i_5 i_{11}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} \\
& - \tfrac{1}{96} v^{i_2 i_{10}}_{a_{11} a_{12}} t^{a_8 a_9 a_{11} a_{12}}_{i_3 i_4 i_5 i_6} t^{a_7}_{i_{10}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} - \tfrac{1}{144}\lambda^{i_2 i_{10} i_{11} i_{12}}_{a_6 a_7 a_8 a_9} t^{a_6 a_7 a_8 a_9}_{i_4 i_{10} i_{11} i_{12}} t^{a_5}_{i_3} v^{i_3 i_4}_{a_1 a_5} - \tfrac{1}{96}\lambda^{i_2 i_6 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}} t^{a_7 a_8 a_9 a_{10}}_{i_3 i_4 i_{11} i_{12}} t^{a_5}_{i_6} v^{i_3 i_4}_{a_1 a_5} + \tfrac{1}{36}\lambda^{i_2 i_9 i_{10} i_{11}}_{a_6 a_7 a_8 a_{12}} t^{a_{12}}_{i_4} t^{a_5 a_6 a_7 a_8}_{i_3 i_9 i_{10} i_{11}} v^{i_3 i_4}_{a_1 a_5} \\
& + \tfrac{1}{144}\lambda^{i_5 i_{10} i_{11} i_{12}}_{a_6 a_7 a_8 a_9} t^{a_6 a_7 a_8 a_9}_{i_3 i_{10} i_{11} i_{12}} t^{a_4}_{i_5} v^{i_2 i_3}_{a_1 a_4} - \tfrac{1}{144}\lambda^{i_8 i_9 i_{10} i_{11}}_{a_5 a_6 a_7 a_{12}} t^{a_{12}}_{i_3} t^{a_4 a_5 a_6 a_7}_{i_8 i_9 i_{10} i_{11}} v^{i_2 i_3}_{a_1 a_4}
\end{aligned}
$$

TABLE ESI.3.XX: The Λ_2 amplitude equation of Λ-CCSDTQ-R12 with special intermediates and the RI insertion using the CABS

$$\delta^{i_3 i_4}_{a_1 a_2} = \Lambda\text{-CCSDT-R12} - \frac{1}{12} P_2 f^{i_4}_{a_{10}} t^{a_8 a_9 a_{10}}_{i_5 i_6 i_7} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} + \frac{1}{12} P_2 \lambda^{i_3 i_4 i_9 i_{10}}_{a_2 a_6 a_7 a_8} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} f^{i_5}_{a_1} - \frac{1}{4} P_2 v^{i_4 i_{10}}_{i_6 i_7} t^{a_8 a_9}_{i_5 i_{10}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{2} P_2 v^{i_4 a_9}_{i_7 a_{10}} t^{a_8 a_{10}}_{i_5 i_6} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9}$$
$$+\frac{1}{2} P_2 \lambda^{i_3 i_4 i_7 i_{10}}_{a_2 a_6 a_8 a_9} t^{a_8 a_9}_{i_5 i_{10}} v^{i_5 a_6}_{i_7 a_1} - \frac{1}{4} P_2 v^{a_8 a_9}_{a_2 a_{10}} t^{a_7 a_{10}}_{i_5 i_6} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \frac{1}{2} P_2 v^{i_4 a_9}_{i_7 a'_{10}} \tilde{t}^{a'_{10} a_8}_{i_5 i_6} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{4} P_2 v^{a_8 a_9}_{a'_{10} a_2} \tilde{t}^{a'_{10} a_7}_{i_5 i_6} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} - \frac{1}{2} P_2 v^{i_4 i_{10}}_{i_7 a_{11}} t^{a_9 a_{11}}_{i_5 i_6} t^{a_8}_{i_{10}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9}$$
$$+\frac{1}{2} P_2 v^{i_4 i_{10}}_{i_7 a_{11}} t^{a_{11}}_{i_6} t^{a_8 a_9}_{i_5 i_{10}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} + \frac{1}{2} P_2 v^{i_4 a_9}_{a_{10} a_{11}} t^{a_{11}}_{i_7} t^{a_8 a_{10}}_{i_5 i_6} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} + \frac{1}{2} P_2 \lambda^{i_3 i_4 i_7 i_{11}}_{a_2 a_8 a_9 a_{10}} t^{a_9 a_{10}}_{i_6 i_{11}} t^{a_8}_{i_5} v^{i_5 i_6}_{i_7 a_1} + \frac{1}{2} P_2 \lambda^{i_3 i_4 i_9 i_{10}}_{a_2 a_6 a_8 a_{11}} t^{a_{11}}_{i_5} t^{a_7 a_8}_{i_9 i_{10}} v^{i_5 a_6}_{a_1 a_7}$$
$$-\frac{1}{2} P_2 \lambda^{i_3 i_4 i_8 i_{11}}_{a_2 a_6 a_9 a_{10}} t^{a_9 a_{10}}_{i_5 i_{11}} t^{a_7}_{i_8} v^{i_5 a_6}_{a_1 a_7} + \frac{1}{2} P_2 v^{i_4 i_{10}}_{i_7 a'_{11}} \tilde{t}^{a'_{11} a_9}_{i_5 i_6} t^{a_8}_{i_{10}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{2} P_2 v^{i_4 a_9}_{a'_{10} a_{11}} t^{a_{11}}_{i_7} \tilde{t}^{a'_{10} a_8}_{i_5 i_6} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{2} P_2 \lambda^{i_3 i_4 i_9 i_{10}}_{a_2 a_6 a_8 a_{11}} t^{a_{11}}_{i_5} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} v^{i_5 a_6}_{a'_7 a_1}$$
$$-\frac{1}{4} P_2 v^{i_4 i_{11}}_{i_7 a_{10}} t^{a_8 a_9 a_{10}}_{i_5 i_6 i_{11}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} + \frac{1}{12} P_2 v^{i_4 a_9}_{a_{10} a_{11}} t^{a_8 a_{10} a_{11}}_{i_5 i_6 i_7} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} + \frac{1}{12} \lambda^{i_5 i_9 i_{10} i_{11}}_{a_1 a_2 a_7 a_8} t^{a_6 a_7 a_8}_{i_9 i_{10} i_{11}} v^{i_3 i_4}_{i_5 a_6} + \frac{1}{12} P_2 v^{i_{10} i_{11}}_{i_6 a_2} t^{a_7 a_8 a_9}_{i_5 i_{10} i_{11}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} - \frac{1}{4} P_2 v^{i_{11} a_9}_{a_2 a_{10}} t^{a_7 a_8 a_{10}}_{i_5 i_6 i_{11}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9}$$
$$+\frac{1}{12} P_2 P_2 \lambda^{i_4 i_6 i_{10} i_{11}}_{a_2 a_7 a_8 a_9} t^{a_7 a_8 a_9}_{i_5 i_{10} i_{11}} v^{i_3 i_5}_{i_6 a_1} + \frac{1}{12} P_2 P_2 \lambda^{i_4 i_9 i_{10} i_{11}}_{a_2 a_5 a_7 a_8} t^{a_6 a_7 a_8}_{i_9 i_{10} i_{11}} v^{i_3 a_5}_{a_1 a_6} + \frac{1}{12} \lambda^{i_3 i_4 i_{10} i_{11}}_{a_6 a_7 a_8 a_9} t^{a_7 a_8 a_9}_{i_5 i_{10} i_{11}} v^{i_5 a_6}_{a_1 a_2} + \frac{1}{2} P_2 v^{i_4 i_{10}}_{a_{11} a_{12}} t^{a_{12}}_{i_7} t^{a_9 a_{11}}_{i_5 i_6} t^{a_8}_{i_{10}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9}$$
$$-\frac{1}{4} P_2 v^{i_4 i_{10}}_{a_{11} a_{12}} t^{a_{12}}_{i_7} t^{a_{11}}_{i_6} t^{a_8 a_9}_{i_5 i_{10}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{4} P_2 \lambda^{i_3 i_4 i_9 i_{10}}_{a_2 a_8 a_{11} a_{12}} t^{a_{12}}_{i_6} t^{a_{11}}_{i_5} t^{a_7 a_8}_{i_9 i_{10}} v^{i_5 i_6}_{a_1 a_7} - \frac{1}{2} P_2 \lambda^{i_3 i_4 i_8 i_{12}}_{a_2 a_9 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_6 i_{12}} t^{a_9}_{i_5} t^{a_7}_{i_8} v^{i_5 i_6}_{a_1 a_7} - \frac{1}{2} P_2 v^{i_4 i_{10}}_{a'_{11} a_{12}} t^{a_{12}}_{i_7} \tilde{t}^{a'_{11} a_9}_{i_5 i_6} t^{a_8}_{i_{10}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9}$$
$$+\frac{1}{4} P_2 \lambda^{i_3 i_4 i_9 i_{10}}_{a_2 a_8 a_{11} a_{12}} t^{a_{12}}_{i_6} t^{a_{11}}_{i_5} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} v^{i_5 i_6}_{a'_7 a_1} + \frac{1}{12} P_2 v^{i_4 i_{10}}_{a_{11} a_{12}} t^{a_9 a_{11} a_{12}}_{i_5 i_6 i_7} t^{a_8}_{i_{10}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} + \frac{1}{4} P_2 v^{i_4 i_{11}}_{a_{10} a_{12}} t^{a_{12}}_{i_7} t^{a_8 a_9 a_{10}}_{i_5 i_6 i_{11}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{12} P_2 v^{i_4 i_{12}}_{a_{10} a_{11}} t^{a_{11}}_{i_{12}} t^{a_8 a_9 a_{10}}_{i_5 i_6 i_7} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9}$$
$$+\frac{1}{12} \lambda^{i_7 i_{10} i_{11} i_{12}}_{a_1 a_2 a_8 a_9} t^{a_6 a_8 a_9}_{i_{10} i_{11} i_{12}} t^{a_5}_{i_7} v^{i_3 i_4}_{a_5 a_6} - \frac{1}{4} P_2 v^{i_{10} i_{12}}_{a_2 a_{11}} t^{a_8 a_9 a_{11}}_{i_5 i_6 i_{12}} t^{a_7}_{i_{10}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} - \frac{1}{12} P_2 v^{i_{10} i_{11}}_{a_2 a_{12}} t^{a_{12}}_{i_6} t^{a_7 a_8 a_9}_{i_5 i_{10} i_{11}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} - \frac{1}{12} P_2 \lambda^{i_3 i_4 i_{11} i_{12}}_{a_2 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_6 i_{11} i_{12}} t^{a_7}_{i_5} v^{i_5 i_6}_{a_1 a_7}$$
$$-\frac{1}{12} P_2 P_2 \lambda^{i_4 i_9 i_{10} i_{11}}_{a_2 a_7 a_8 a_{12}} t^{a_{12}}_{i_5} t^{a_6 a_7 a_8}_{i_9 i_{10} i_{11}} v^{i_3 i_5}_{a_1 a_6} - \frac{1}{12} P_2 P_2 \lambda^{i_4 i_7 i_{11} i_{12}}_{a_2 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_5 i_{11} i_{12}} t^{a_6}_{i_7} v^{i_3 i_5}_{a_1 a_6} + \frac{1}{12} \lambda^{i_3 i_4 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_6 i_{11} i_{12}} t^{a_7}_{i_5} v^{i_5 i_6}_{a_1 a_2} + \frac{1}{2} P_2 v^{i_4 i_{12}}_{a_{10} a_{11}} t^{a_9 a_{11}}_{i_7 i_{12}} t^{a_8 a_{10}}_{i_5 i_6} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9}$$
$$-\frac{1}{8} P_2 v^{i_4 i_{10}}_{a_{11} a_{12}} t^{a_{11} a_{12}}_{i_6 i_7} t^{a_8 a_9}_{i_5 i_{10}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{8} \lambda^{i_8 i_9 i_{11} i_{12}}_{a_1 a_2 a_7 a_{10}} t^{a_6 a_{10}}_{i_{11} i_{12}} t^{a_5 a_7}_{i_8 i_9} v^{i_3 i_4}_{a_5 a_6} - \frac{1}{8} P_2 v^{i_{11} i_{12}}_{a_2 a_{10}} t^{a_8 a_9}_{i_{11} i_{12}} t^{a_7 a_{10}}_{i_5 i_6} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} + \frac{1}{2} P_2 \lambda^{i_3 i_4 i_9 i_{12}}_{a_2 a_8 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_6 i_{12}} t^{a_7 a_8}_{i_5 i_9} v^{i_5 i_6}_{a_1 a_7}$$
$$+\frac{1}{4} P_2 P_2 \lambda^{i_4 i_8 i_9 i_{12}}_{a_2 a_7 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_5 i_{12}} t^{a_6 a_7}_{i_8 i_9} v^{i_3 i_5}_{a_1 a_6} - \frac{1}{8} \lambda^{i_3 i_4 i_9 i_{12}}_{a_7 a_8 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_6 i_{12}} t^{a_7 a_8}_{i_5 i_9} v^{i_5 i_6}_{a_1 a_2} - \frac{1}{8} P_2 V^{i_4 i_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_6 i_7} t^{a_8 a_9}_{i_5 i_{10}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} + \frac{1}{2} P_2 v^{i_4 i_{12}}_{a'_{11} a_{10}} \tilde{t}^{a'_{11} a_9}_{i_7 i_{12}} t^{a_8 a_{10}}_{i_5 i_6} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9}$$
$$-\frac{1}{2} P_2 v^{i_4 i_{12}}_{a'_{10} a_{11}} t^{a_9 a_{11}}_{i_7 i_{12}} \tilde{t}^{a'_{10} a_8}_{i_5 i_6} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{4} \lambda^{i_8 i_9 i_{11} i_{12}}_{a_1 a_2 a_7 a_{10}} t^{a_6 a_{10}}_{i_{11} i_{12}} \tilde{t}^{a'_5 a_7}_{i_8 i_9} v^{i_3 i_4}_{a'_5 a_6} - \frac{1}{2} P_2 \lambda^{i_3 i_4 i_9 i_{12}}_{a_2 a_8 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_6 i_{12}} \tilde{t}^{a'_7 a_8}_{i_5 i_9} v^{i_5 i_6}_{a'_7 a_1} - \frac{1}{8} P_2 v^{i_{10} i_{11}}_{a'_{12} a_2} \tilde{t}^{a'_{12} a_9}_{i_5 i_6} t^{a_7 a_8}_{i_{10} i_{11}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9}$$
$$-\frac{1}{4} P_2 P_2 \lambda^{i_4 i_8 i_9 i_{12}}_{a_2 a_7 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_5 i_{12}} \tilde{t}^{a'_6 a_7}_{i_8 i_9} v^{i_3 i_5}_{a'_6 a_1} - \frac{1}{24} P_2 v^{i_4 i_{12}}_{a_{10} a_{11}} t^{a_8 a_9 a_{10} a_{11}}_{i_5 i_6 i_7 i_{12}} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} + \frac{1}{96} v^{i_3 i_4}_{a_{11} a_{12}} t^{a_9 a_{10} a_{11} a_{12}}_{i_5 i_6 i_7 i_8} \lambda^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_9 a_{10}} - \frac{1}{24} P_2 v^{i_{11} i_{12}}_{a_2 a_{10}} t^{a_7 a_8 a_9 a_{10}}_{i_5 i_6 i_{11} i_{12}} \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9}$$
$$+\frac{1}{36} P_2 P_2 \lambda^{i_4 i_{10} i_{11} i_{12}}_{a_2 a_7 a_8 a_9} t^{a_6 a_7 a_8 a_9}_{i_5 i_{10} i_{11} i_{12}} v^{i_3 i_5}_{a_1 a_6} - \frac{1}{144} P_2 \lambda^{i_9 i_{10} i_{11} i_{12}}_{a_2 a_6 a_7 a_8} t^{a_5 a_6 a_7 a_8}_{i_9 i_{10} i_{11} i_{12}} v^{i_3 i_4}_{a_1 a_5} + \frac{1}{96} \lambda^{i_3 i_4 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}} t^{a_7 a_8 a_9 a_{10}}_{i_5 i_6 i_{11} i_{12}} v^{i_5 i_6}_{a_1 a_2} - \frac{1}{144} P_2 \lambda^{i_4 i_{10} i_{11} i_{12}}_{a_6 a_7 a_8 a_9} t^{a_6 a_7 a_8 a_9}_{i_5 i_{10} i_{11} i_{12}} v^{i_3 i_5}_{a_1 a_2}$$
$$+\frac{1}{2} P_2 v^{i_4 i_{12}}_{a'_{10} a'_{11}} \tilde{t}^{a'_{11} a_9}_{i_7 i_{12}} \tilde{t}^{a'_{10} a_8}_{i_5 i_6} \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{8} v^{i_3 i_4}_{a'_{11} a'_{12}} \tilde{t}^{a'_{12} a_{10}}_{i_7 i_8} \tilde{t}^{a'_{11} a_9}_{i_5 i_6} \lambda^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_9 a_{10}}$$

TABLE ESI.3.XXI: The Λ_3 amplitude equation of Λ-CCSDTQ-R12 with special intermediates and the RI insertion using the CABS

$$\delta^{i_4 i_5 i_6}_{a_1 a_2 a_3} = \Lambda\text{-CCSDT-R12} - \frac{1}{2} P_3 f^{i_6}_{a_{10}} t^{a_9 a_{10}}_{i_7 i_8} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} + \frac{1}{2} P_3 \lambda^{i_4 i_5 i_6 i_{10}}_{a_2 a_3 a_8 a_9} t^{a_8 a_9}_{i_7 i_{10}} f^{i_7}_{a_1} + \frac{1}{2} P_3 f^{i_6}_{a'_{10}} \tilde{t}^{a'_{10} a_9}_{i_7 i_8} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} + \frac{1}{2} P_3 \lambda^{i_5 i_6 i_8 i_9}_{a_1 a_2 a_3 a_7} v^{i_4 a_7}_{i_8 i_9} + \frac{1}{2} P_3 \lambda^{i_4 i_5 i_6 i_9}_{a_2 a_3 a_7 a_8} v^{a_7 a_8}_{i_9 a_1}$$
$$-\frac{1}{2} P_3 v^{i_6 i_{10}}_{i_7 i_8} t^{a_9}_{i_{10}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} - P_3 v^{i_6 a_9}_{i_8 a_{10}} t^{a_{10}}_{i_7} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} + P_3 \lambda^{i_4 i_5 i_6 i_9}_{a_2 a_3 a_8 a_{10}} t^{a_{10}}_{i_7} v^{i_7 a_8}_{i_9 a_1} - \frac{1}{2} P_3 v^{a_8 a_9}_{a_3 a_{10}} t^{a_{10}}_{i_7} \lambda^{i_4 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} + P_3 v^{i_6 i_{10}}_{i_8 a_{11}} t^{a_{11}}_{i_7} t^{a_9}_{i_{10}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9}$$
$$+\frac{1}{2} P_3 v^{i_6 a_9}_{a_{10} a_{11}} t^{a_{11}}_{i_8} t^{a_{10}}_{i_7} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} + \frac{1}{2} P_3 \lambda^{i_4 i_5 i_6 i_9}_{a_2 a_3 a_{10} a_{11}} t^{a_{11}}_{i_8} t^{a_{10}}_{i_7} v^{i_7 i_8}_{i_9 a_1} + P_3 v^{i_{10} a_9}_{a_3 a_{11}} t^{a_{11}}_{i_7} t^{a_8}_{i_{10}} \lambda^{i_4 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - P_3 v^{i_6 i_{11}}_{i_8 a_{10}} t^{a_9 a_{10}}_{i_7 i_{11}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} + \frac{1}{4} P_3 v^{i_6 a_9}_{a_{10} a_{11}} t^{a_{10} a_{11}}_{i_7 i_8} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9}$$
$$-\frac{1}{2} P_3 \lambda^{i_6 i_7 i_{10} i_{11}}_{a_1 a_2 a_3 a_9} t^{a_8 a_9}_{i_{10} i_{11}} v^{i_4 i_5}_{i_7 a_8} + \frac{1}{4} P_3 v^{i_{10} i_{11}}_{i_7 a_3} t^{a_8 a_9}_{i_{10} i_{11}} \lambda^{i_4 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - P_3 v^{i_{11} a_9}_{a_3 a_{10}} t^{a_8 a_{10}}_{i_7 i_{11}} \lambda^{i_4 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{2} P_3 P_3 \lambda^{i_5 i_6 i_8 i_{11}}_{a_2 a_3 a_9 a_{10}} t^{a_9 a_{10}}_{i_7 i_{11}} v^{i_4 i_7}_{i_8 a_1} - \frac{1}{2} P_3 P_3 \lambda^{i_5 i_6 i_{10} i_{11}}_{a_2 a_3 a_7 a_9} t^{a_8 a_9}_{i_{10} i_{11}} v^{i_4 a_7}_{a_1 a_8}$$
$$-\frac{1}{2} P_3 \lambda^{i_4 i_5 i_6 i_{11}}_{a_3 a_8 a_9 a_{10}} t^{a_9 a_{10}}_{i_7 i_{11}} v^{i_7 a_8}_{a_1 a_2} + P_3 v^{i_6 i_{11}}_{i_8 a'_{10}} \tilde{t}^{a'_{10} a_9}_{i_7 i_{11}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} + \frac{1}{4} P_3 V^{i_6 a_9}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_7 i_8} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} - \frac{1}{2} P_3 v^{i_5 i_6}_{i_9 a'_{11}} \tilde{t}^{a'_{11} a_{10}}_{i_7 i_8} \lambda^{i_4 i_7 i_8 i_9}_{a_1 a_2 a_3 a_{10}} - P_3 v^{i_{11} a_9}_{a'_{10} a_3} \tilde{t}^{a'_{10} a_8}_{i_7 i_{11}} \lambda^{i_4 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9}$$
$$+\frac{1}{2} P_3 P_3 \lambda^{i_5 i_6 i_{10} i_{11}}_{a_2 a_3 a_7 a_9} \tilde{t}^{a'_8 a_9}_{i_{10} i_{11}} v^{i_4 a_7}_{a'_8 a_1} - \frac{1}{2} P_3 v^{i_6 i_{10}}_{a_{11} a_{12}} t^{a_{12}}_{i_8} t^{a_{11}}_{i_7} t^{a_9}_{i_{10}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} - \frac{1}{2} P_3 \lambda^{i_4 i_5 i_6 i_{10}}_{a_2 a_3 a_{11} a_{12}} t^{a_{12}}_{i_8} t^{a_{11}}_{i_7} t^{a_9}_{i_{10}} v^{i_7 i_8}_{a_1 a_9} - \frac{1}{4} P_3 v^{i_6 i_{10}}_{a_{11} a_{12}} t^{a_{11} a_{12}}_{i_7 i_8} t^{a_9}_{i_{10}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9}$$
$$+P_3 v^{i_6 i_{11}}_{a_{10} a_{12}} t^{a_{12}}_{i_8} t^{a_9 a_{10}}_{i_7 i_{11}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} - \frac{1}{2} P_3 v^{i_6 i_{12}}_{a_{10} a_{11}} t^{a_{11}}_{i_{12}} t^{a_9 a_{10}}_{i_7 i_8} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} - \frac{1}{2} P_3 \lambda^{i_6 i_9 i_{11} i_{12}}_{a_1 a_2 a_3 a_{10}} t^{a_8 a_{10}}_{i_{11} i_{12}} t^{a_7}_{i_9} v^{i_4 i_5}_{a_7 a_8} + P_3 v^{i_{10} i_{12}}_{a_3 a_{11}} t^{a_9 a_{11}}_{i_7 i_{12}} t^{a_8}_{i_{10}} \lambda^{i_4 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9}$$
$$-\frac{1}{4} P_3 v^{i_{10} i_{11}}_{a_3 a_{12}} t^{a_{12}}_{i_7} t^{a_8 a_9}_{i_{10} i_{11}} \lambda^{i_4 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{2} P_3 \lambda^{i_4 i_5 i_6 i_{12}}_{a_2 a_3 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_8 i_{12}} t^{a_9}_{i_7} v^{i_7 i_8}_{a_1 a_9} - \frac{1}{2} P_3 P_3 \lambda^{i_5 i_6 i_{10} i_{11}}_{a_2 a_3 a_9 a_{12}} t^{a_{12}}_{i_7} t^{a_8 a_9}_{i_{10} i_{11}} v^{i_4 i_7}_{a_1 a_8} + \frac{1}{2} P_3 P_3 \lambda^{i_5 i_6 i_9 i_{12}}_{a_2 a_3 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_7 i_{12}} t^{a_8}_{i_9} v^{i_4 i_7}_{a_1 a_8}$$
$$-\frac{1}{2} P_3 \lambda^{i_4 i_5 i_6 i_{12}}_{a_3 a_9 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_8 i_{12}} t^{a_9}_{i_7} v^{i_7 i_8}_{a_1 a_2} - \frac{1}{4} P_3 V^{i_6 i_{10}}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_7 i_8} t^{a_9}_{i_{10}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} - P_3 v^{i_6 i_{11}}_{a'_{10} a_{12}} t^{a_{12}}_{i_8} \tilde{t}^{a'_{10} a_9}_{i_7 i_{11}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} + \frac{1}{2} P_3 v^{i_6 i_{12}}_{a'_{10} a_{11}} t^{a_{11}}_{i_{12}} \tilde{t}^{a'_{10} a_9}_{i_7 i_8} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9}$$
$$+\frac{1}{2} P_3 v^{i_5 i_6}_{a'_{11} a_{12}} t^{a_{12}}_{i_9} \tilde{t}^{a'_{11} a_{10}}_{i_7 i_8} \lambda^{i_4 i_7 i_8 i_9}_{a_1 a_2 a_3 a_{10}} + P_3 v^{i_{10} i_{12}}_{a'_{11} a_3} \tilde{t}^{a'_{11} a_9}_{i_7 i_{12}} t^{a_8}_{i_{10}} \lambda^{i_4 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} + \frac{1}{2} P_3 P_3 \lambda^{i_5 i_6 i_{10} i_{11}}_{a_2 a_3 a_9 a_{12}} t^{a_{12}}_{i_7} \tilde{t}^{a'_8 a_9}_{i_{10} i_{11}} v^{i_4 i_7}_{a'_8 a_1} - \frac{1}{4} P_3 v^{i_6 i_{12}}_{a_{10} a_{11}} t^{a_9 a_{10} a_{11}}_{i_7 i_8 i_{12}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9}$$
$$-\frac{1}{12} P_3 v^{i_5 i_6}_{a_{11} a_{12}} t^{a_{10} a_{11} a_{12}}_{i_7 i_8 i_9} \lambda^{i_4 i_7 i_8 i_9}_{a_1 a_2 a_3 a_{10}} - \frac{1}{4} P_3 v^{i_{11} i_{12}}_{a_3 a_{10}} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} \lambda^{i_4 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} - \frac{1}{4} P_3 P_3 v^{i_6 i_{12}}_{a_3 a_{11}} t^{a_9 a_{10} a_{11}}_{i_7 i_8 i_{12}} \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_9 a_{10}} - \frac{1}{12} P_3 P_3 \lambda^{i_6 i_{10} i_{11} i_{12}}_{a_2 a_3 a_8 a_9} t^{a_7 a_8 a_9}_{i_{10} i_{11} i_{12}} v^{i_4 i_5}_{a_1 a_7}$$
$$-\frac{1}{12} P_3 \lambda^{i_4 i_5 i_6 i_{12}}_{a_3 a_9 a_{10} a_{11}} t^{a_9 a_{10} a_{11}}_{i_7 i_8 i_{12}} v^{i_7 i_8}_{a_1 a_2} - \frac{1}{12} P_3 P_3 \lambda^{i_5 i_6 i_{11} i_{12}}_{a_3 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} v^{i_4 i_7}_{a_1 a_2}$$

TABLE ESI.3.XXII: The Λ_4 amplitude equation of Λ-CCSDTQ-R12 with special intermediates and the RI insertion using the CABS

$$\delta^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_3 a_4} = +P_4 P_4 \lambda^{i_7 i_8}_{a_3 a_4} v^{i_5 i_6}_{a_1 a_2} + P_4 P_4 \lambda^{i_6 i_7 i_8}_{a_2 a_3 a_4} f^{i_5}_{a_1} + P_4 P_4 \lambda^{i_7 i_8 i_9}_{a_2 a_3 a_4} v^{i_5 i_6}_{i_9 a_1} + P_4 P_4 \lambda^{i_6 i_7 i_8}_{a_3 a_4 a_9} v^{i_5 a_9}_{a_1 a_2} + P_4 P_4 v^{i_8 i_{10}}_{a_4 a_9} t^{a_9}_{i_{10}} \lambda^{i_5 i_6 i_7}_{a_1 a_2 a_3} + P_4 P_4 v^{i_7 i_8}_{a_4 a_{10}} t^{a_{10}}_{i_9} \lambda^{i_5 i_6 i_9}_{a_1 a_2 a_3}$$
$$-P_4 P_4 \lambda^{i_6 i_7 i_8}_{a_3 a_4 a_{10}} t^{a_{10}}_{i_9} v^{i_5 i_9}_{a_1 a_2} + P_4 \lambda^{i_6 i_7 i_8 i_9}_{a_1 a_2 a_3 a_4} f^{i_5}_{i_9} - P_4 \lambda^{i_5 i_6 i_7 i_8}_{a_2 a_3 a_4 a_9} f^{a_9}_{a_1} - P_4 f^{i_8}_{a_{10}} t^{a_{10}}_{i_9} \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_4} + P_4 \lambda^{i_5 i_6 i_7 i_8}_{a_2 a_3 a_4 a_{10}} t^{a_{10}}_{i_9} f^{i_9}_{a_1} + \frac{1}{2} P_4 \lambda^{i_7 i_8 i_9 i_{10}}_{a_1 a_2 a_3 a_4} v^{i_5 i_6}_{i_9 i_{10}}$$
$$-P_4 P_4 \lambda^{i_6 i_7 i_8 i_{10}}_{a_2 a_3 a_4 a_9} v^{i_5 a_9}_{i_{10} a_1} + \frac{1}{2} P_4 \lambda^{i_5 i_6 i_7 i_8}_{a_3 a_4 a_9 a_{10}} v^{a_9 a_{10}}_{a_1 a_2} - P_4 v^{i_8 i_{11}}_{i_9 a_{10}} t^{a_{10}}_{i_{11}} \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_4} - P_4 v^{i_7 i_8}_{i_{10} a_{11}} t^{a_{11}}_{i_9} \lambda^{i_5 i_6 i_9 i_{10}}_{a_1 a_2 a_3 a_4} - P_4 v^{i_{11} a_9}_{a_4 a_{10}} t^{a_{10}}_{i_{11}} \lambda^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_3 a_9} + P_4 P_4 \lambda^{i_6 i_7 i_8 i_{10}}_{a_2 a_3 a_4 a_{11}} t^{a_{11}}_{i_9} v^{i_5 i_9}_{i_{10} a_1}$$
$$+P_4 P_4 v^{i_8 a_{10}}_{a_4 a_{11}} t^{a_{11}}_{i_9} \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_{10}} + P_4 \lambda^{i_5 i_6 i_7 i_8}_{a_3 a_4 a_{10} a_{11}} t^{a_{11}}_{i_9} v^{i_9 a_{10}}_{a_1 a_2} - P_4 v^{i_8 i_{12}}_{a_{10} a_{11}} t^{a_{11}}_{i_{12}} t^{a_{10}}_{i_9} \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_4} + \frac{1}{2} P_4 v^{i_7 i_8}_{a_{11} a_{12}} t^{a_{12}}_{i_{10}} t^{a_{11}}_{i_9} \lambda^{i_5 i_6 i_9 i_{10}}_{a_1 a_2 a_3 a_4} - P_4 v^{i_{10} i_{12}}_{a_4 a_{11}} t^{a_{11}}_{i_{12}} t^{a_9}_{i_{10}} \lambda^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_3 a_9}$$
$$-P_4 P_4 v^{i_8 i_{11}}_{a_4 a_{12}} t^{a_{12}}_{i_9} t^{a_{10}}_{i_{11}} \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_{10}} + \frac{1}{2} P_4 \lambda^{i_5 i_6 i_7 i_8}_{a_3 a_4 a_{11} a_{12}} t^{a_{12}}_{i_{10}} t^{a_{11}}_{i_9} v^{i_9 i_{10}}_{a_1 a_2} - \frac{1}{2} P_4 v^{i_8 i_{12}}_{a_{10} a_{11}} t^{a_{10} a_{11}}_{i_9 i_{12}} \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_4} + \frac{1}{4} P_4 v^{i_7 i_8}_{a_{11} a_{12}} t^{a_{11} a_{12}}_{i_9 i_{10}} \lambda^{i_5 i_6 i_9 i_{10}}_{a_1 a_2 a_3 a_4} - \frac{1}{2} P_4 v^{i_{11} i_{12}}_{a_4 a_{10}} t^{a_9 a_{10}}_{i_{11} i_{12}} \lambda^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_3 a_9}$$
$$+P_4 P_4 v^{i_8 i_{12}}_{a_4 a_{11}} t^{a_{10} a_{11}}_{i_9 i_{12}} \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_{10}} - \frac{1}{2} P_4 P_4 \lambda^{i_7 i_8 i_{11} i_{12}}_{a_2 a_3 a_4 a_{10}} t^{a_9 a_{10}}_{i_{11} i_{12}} v^{i_5 i_6}_{a_1 a_9} + \frac{1}{4} P_4 \lambda^{i_5 i_6 i_7 i_8}_{a_3 a_4 a_{11} a_{12}} t^{a_{11} a_{12}}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_1 a_2} - \frac{1}{2} P_4 P_4 \lambda^{i_6 i_7 i_8 i_{12}}_{a_3 a_4 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_9 i_{12}} v^{i_5 i_9}_{a_1 a_2}$$
$$-\frac{1}{2} P_4 V^{i_8 i_{12}}_{i_{10} i_{11}} t^{i_{10} i_{11}}_{i_9 i_{12}} \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_4} + \frac{1}{4} P_4 V^{i_7 i_8}_{i_{11} i_{12}} t^{i_{11} i_{12}}_{i_9 i_{10}} \lambda^{i_5 i_6 i_9 i_{10}}_{a_1 a_2 a_3 a_4} - \frac{1}{2} P_4 v^{i_{11} i_{12}}_{a'_{10} a_4} \tilde{t}^{a'_{10} a_9}_{i_{11} i_{12}} \lambda^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_3 a_9} + P_4 P_4 v^{i_8 i_{12}}_{a'_{11} a_4} \tilde{t}^{a'_{11} a_{10}}_{i_9 i_{12}} \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_{10}} + \frac{1}{2} P_4 P_4 \lambda^{i_7 i_8 i_{11} i_{12}}_{a_2 a_3 a_4 a_{10}} \tilde{t}^{a'_9 a_{10}}_{i_{11} i_{12}} v^{i_5 i_6}_{a'_9 a_1}$$

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TABLE ESI.3.XXIII: The geminal λ amplitude equation of Λ-CCSDTQ-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{i_3 i_4}_{i_1 i_2} &= \Lambda\text{-CCSDT-R12} + \tfrac{1}{12}\lambda^{i_3 i_4 i_{11} i_{12}}_{a_6 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} f^{i_7}_{a'_5} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2}\lambda^{i_3 i_4 i_9 i_{12}}_{a_6 a_8 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_7 i_{12}} v^{i_7 a_8}_{i_9 a'_5} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{4}\lambda^{i_3 i_4 i_{11} i_{12}}_{a_6 a_7 a_8 a_{10}} t^{a_9 a_{10}}_{i_{11} i_{12}} v^{a_7 a_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{4} v^{a_{10} a_{11}}_{a'_5 a'_{12}} \tilde{t}^{a'_{12} a_9}_{i_7 i_8} \lambda^{i_3 i_4 i_7 i_8}_{a_6 a_9 a_{10} a_{11}} F^{a'_5 a_6}_{i_1 i_2} \\
&+ \tfrac{1}{2}\lambda^{i_3 i_4 i_9 i_{13}}_{a_6 a_{10} a_{11} a_{12}} t^{a_{11} a_{12}}_{i_8 i_{13}} t^{a_{10}}_{i_7} v^{i_7 i_8}_{i_9 a'_5} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2}\lambda^{i_3 i_4 i_{11} i_{12}}_{a_6 a_8 a_{10} a_{13}} t^{a_{13}}_{i_7} t^{a_9 a_{10}}_{i_{11} i_{12}} v^{i_7 a_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2}\lambda^{i_3 i_4 i_{10} i_{13}}_{a_6 a_8 a_{11} a_{12}} t^{a_{11} a_{12}}_{i_7 i_{13}} t^{a_9}_{i_{10}} v^{i_7 a_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2}\lambda^{i_3 i_4 i_{11} i_{12}}_{a_6 a_8 a_{10} a_{13}} t^{a_{13}}_{i_7} \tilde{t}^{a'_9 a_{10}}_{i_{11} i_{12}} v^{i_7 a_8}_{a'_5 a'_9} F^{a'_5 a_6}_{i_1 i_2} \\
&+ \tfrac{1}{12}\lambda^{i_3 i_4 i_9 i_{13}}_{a_6 a_{10} a_{11} a_{12}} t^{a_{10} a_{11} a_{12}}_{i_7 i_8 i_{13}} v^{i_7 i_8}_{i_9 a'_5} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{4} v^{i_{13} a_{11}}_{a'_5 a_{12}} t^{a_9 a_{10} a_{12}}_{i_7 i_8 i_{13}} \lambda^{i_3 i_4 i_7 i_8}_{a_6 a_9 a_{10} a_{11}} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{12} P_2 \lambda^{i_4 i_8 i_{12} i_{13}}_{a_6 a_9 a_{10} a_{11}} t^{a_9 a_{10} a_{11}}_{i_7 i_{12} i_{13}} v^{i_3 i_7}_{i_8 a'_5} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{12} P_2 \lambda^{i_4 i_{11} i_{12} i_{13}}_{a_6 a_7 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_{11} i_{12} i_{13}} v^{i_3 a_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} \\
&+ \tfrac{1}{12}\lambda^{i_3 i_4 i_{10} i_{11}}_{a_6 a_7 a_8 a_9} t^{a_7 a_8 a_9}_{i_5 i_{10} i_{11}} V^{i_5 a_6}_{i_1 i_2} - \tfrac{1}{4}\lambda^{i_3 i_4 i_{11} i_{12}}_{a_6 a_{10} a_{13} a_{14}} t^{a_{14}}_{i_8} t^{a_{13}}_{i_7} t^{a_9 a_{10}}_{i_{11} i_{12}} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2}\lambda^{i_3 i_4 i_{10} i_{14}}_{a_6 a_{11} a_{12} a_{13}} t^{a_{12} a_{13}}_{i_8 i_{14}} t^{a_{11}}_{i_7} t^{a_9}_{i_{10}} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{4}\lambda^{i_3 i_4 i_{11} i_{12}}_{a_6 a_{10} a_{13} a_{14}} t^{a_{14}}_{i_8} t^{a_{13}}_{i_7} \tilde{t}^{a'_9 a_{10}}_{i_{11} i_{12}} v^{i_7 i_8}_{a'_5 a'_9} F^{a'_5 a_6}_{i_1 i_2} \\
&- \tfrac{1}{4}\lambda^{i_3 i_4 i_{12} i_{13}}_{a_6 a_{10} a_{11} a_{14}} t^{a_{14}}_{i_8} t^{a_9 a_{10} a_{11}}_{i_7 i_{12} i_{13}} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{12}\lambda^{i_3 i_4 i_{10} i_{14}}_{a_6 a_{11} a_{12} a_{13}} t^{a_{11} a_{12} a_{13}}_{i_7 i_8 i_{14}} t^{a_9}_{i_{10}} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{12}\lambda^{i_3 i_4 i_{13} i_{14}}_{a_6 a_{10} a_{11} a_{12}} t^{a_{10} a_{11} a_{12}}_{i_8 i_{13} i_{14}} t^{a_9}_{i_7} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} \\
&- \tfrac{1}{12} P_2 \lambda^{i_4 i_{11} i_{12} i_{13}}_{a_6 a_9 a_{10} a_{14}} t^{a_{14}}_{i_7} t^{a_8 a_9 a_{10}}_{i_{11} i_{12} i_{13}} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{12} P_2 \lambda^{i_4 i_9 i_{13} i_{14}}_{a_6 a_{10} a_{11} a_{12}} t^{a_{10} a_{11} a_{12}}_{i_7 i_{13} i_{14}} t^{a_8}_{i_9} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{12}\lambda^{i_3 i_4 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}} t^{a_8 a_9 a_{10}}_{i_6 i_{11} i_{12}} t^{a_7}_{i_5} V^{i_5 i_6}_{i_1 i_2} \\
&- \tfrac{1}{8}\lambda^{i_3 i_4 i_{13} i_{14}}_{a_6 a_{10} a_{11} a_{12}} t^{a_9 a_{12}}_{i_{13} i_{14}} t^{a_{10} a_{11}}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{2}\lambda^{i_3 i_4 i_{11} i_{14}}_{a_6 a_{10} a_{12} a_{13}} t^{a_{12} a_{13}}_{i_8 i_{14}} t^{a_9 a_{10}}_{i_7 i_{11}} v^{i_7 i_8}_{a'_5 a_9} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{4} P_2 \lambda^{i_4 i_{10} i_{11} i_{14}}_{a_6 a_9 a_{12} a_{13}} t^{a_{12} a_{13}}_{i_7 i_{14}} t^{a_8 a_9}_{i_{10} i_{11}} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} \\
&- \tfrac{1}{8}\lambda^{i_3 i_4 i_9 i_{12}}_{a_7 a_8 a_{10} a_{11}} t^{a_{10} a_{11}}_{i_6 i_{12}} t^{a_7 a_8}_{i_5 i_9} V^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2}\lambda^{i_3 i_4 i_{11} i_{14}}_{a_6 a_{10} a_{12} a_{13}} t^{a_{12} a_{13}}_{i_8 i_{14}} \tilde{t}^{a'_9 a_{10}}_{i_7 i_{11}} v^{i_7 i_8}_{a'_5 a'_9} F^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{8}\lambda^{i_3 i_4 i_{11} i_{12}}_{a_6 a_{10} a_{13} a_{14}} t^{a_{13} a_{14}}_{i_7 i_8} \tilde{t}^{a'_9 a_{10}}_{i_{11} i_{12}} v^{i_7 i_8}_{a'_5 a'_9} F^{a'_5 a_6}_{i_1 i_2} \\
&+ \tfrac{1}{4} P_2 \lambda^{i_4 i_{10} i_{11} i_{14}}_{a_6 a_9 a_{12} a_{13}} t^{a_{12} a_{13}}_{i_7 i_{14}} \tilde{t}^{a'_8 a_9}_{i_{10} i_{11}} v^{i_3 i_7}_{a'_5 a'_8} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{24} v^{i_{13} i_{14}}_{a'_5 a_{12}} t^{a_9 a_{10} a_{11} a_{12}}_{i_7 i_8 i_{13} i_{14}} \lambda^{i_3 i_4 i_7 i_8}_{a_6 a_9 a_{10} a_{11}} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{36} P_2 \lambda^{i_4 i_{12} i_{13} i_{14}}_{a_6 a_9 a_{10} a_{11}} t^{a_8 a_9 a_{10} a_{11}}_{i_7 i_{12} i_{13} i_{14}} v^{i_3 i_7}_{a'_5 a_8} F^{a'_5 a_6}_{i_1 i_2} \\
&- \tfrac{1}{144}\lambda^{i_{11} i_{12} i_{13} i_{14}}_{a_6 a_8 a_9 a_{10}} t^{a_7 a_8 a_9 a_{10}}_{i_{11} i_{12} i_{13} i_{14}} v^{i_3 i_4}_{a'_5 a_7} F^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{96}\lambda^{i_3 i_4 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}} t^{a_7 a_8 a_9 a_{10}}_{i_5 i_6 i_{11} i_{12}} V^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{144} P_2 \lambda^{i_4 i_{10} i_{11} i_{12}}_{a_6 a_7 a_8 a_9} t^{a_6 a_7 a_8 a_9}_{i_5 i_{10} i_{11} i_{12}} V^{i_3 i_5}_{i_1 i_2}
\end{aligned}
$$

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G. EOM-CCSD-R12

TABLE ESI.3.XXIV: The R_1 amplitude equation of EOM-CCSD-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{a_2}_{i_1} &= -f^{i_3}_{i_1} r^{a_2}_{i_3} + f^{a_2}_{a_3} r^{a_3}_{i_1} - f^{i_3}_{a_4} t^{a_4}_{i_1} r^{a_2}_{i_3} - f^{i_3}_{a_4} r^{a_4}_{i_1} t^{a_2}_{i_3} + f^{i_4}_{a_3} r^{a_2 a_3}_{i_1 i_4} - f^{i_4}_{a'_3} \tilde{r}^{a'_3 a_2}_{i_1 i_4} - v^{i_4 a_2}_{i_1 a_3} r^{a_3}_{i_4} - v^{i_3 i_5}_{i_1 a_4} t^{a_4}_{i_5} r^{a_2}_{i_3} - v^{i_5 a_2}_{a_3 a_4} t^{a_4}_{i_5} r^{a_3}_{i_1} - v^{i_3 i_5}_{i_1 a_4} r^{a_4}_{i_5} t^{a_2}_{i_3} - v^{i_5 a_2}_{a_3 a_4} r^{a_4}_{i_5} t^{a_3}_{i_1} \\
&\quad - v^{i_3 i_6}_{a_4 a_5} t^{a_5}_{i_6} t^{a_4}_{i_1} r^{a_2}_{i_3} - v^{i_3 i_6}_{a_4 a_5} t^{a_5}_{i_6} r^{a_4}_{i_1} t^{a_2}_{i_3} - v^{i_3 i_6}_{a_4 a_5} r^{a_5}_{i_6} t^{a_4}_{i_1} t^{a_2}_{i_3} - \tfrac{1}{2} v^{i_3 i_6}_{a_4 a_5} t^{a_4 a_5}_{i_1 i_6} r^{a_2}_{i_3} + \tfrac{1}{2} v^{i_4 i_5}_{a_3 a_6} r^{a_6}_{i_1} t^{a_2 a_3}_{i_4 i_5} + v^{i_4 i_6}_{a_3 a_5} r^{a_5}_{i_6} t^{a_2 a_3}_{i_1 i_4} - \tfrac{1}{2} V^{i_3 i_6}_{i_4 i_5} t^{i_4 i_5}_{i_1 i_6} r^{a_2}_{i_3} - \tfrac{1}{2} v^{i_4 i_5}_{a'_3 a_6} r^{a_6}_{i_1} \tilde{t}^{a'_3 a_2}_{i_4 i_5} \\
&\quad - v^{i_4 i_6}_{a'_3 a_5} r^{a_5}_{i_6} \tilde{t}^{a'_3 a_2}_{i_1 i_4} - \tfrac{1}{2} v^{i_4 i_5}_{i_1 a_3} r^{a_2 a_3}_{i_4 i_5} - \tfrac{1}{2} v^{i_5 a_2}_{a_3 a_4} r^{a_3 a_4}_{i_1 i_5} + \tfrac{1}{2} v^{i_4 i_5}_{i_1 a'_3} \tilde{r}^{a'_3 a_2}_{i_4 i_5} - \tfrac{1}{2} r^{i_4 i_5}_{i_1 i_3} V^{i_3 a_2}_{i_4 i_5} + v^{i_4 i_6}_{a_3 a_5} t^{a_5}_{i_6} r^{a_2 a_3}_{i_1 i_4} + \tfrac{1}{2} v^{i_4 i_5}_{a_3 a_6} t^{a_6}_{i_1} r^{a_2 a_3}_{i_4 i_5} - \tfrac{1}{2} v^{i_3 i_6}_{a_4 a_5} r^{a_4 a_5}_{i_1 i_6} t^{a_2}_{i_3} - v^{i_4 i_6}_{a'_3 a_5} t^{a_5}_{i_6} \tilde{r}^{a'_3 a_2}_{i_1 i_4} \\
&\quad - \tfrac{1}{2} v^{i_4 i_5}_{a'_3 a_6} t^{a_6}_{i_1} \tilde{r}^{a'_3 a_2}_{i_4 i_5} - \tfrac{1}{2} r^{i_5 i_6}_{i_1 i_4} V^{i_3 i_4}_{i_5 i_6} t^{a_2}_{i_3}
\end{aligned}
$$

TABLE ESI.3.XXV: The R_2 amplitude equation of EOM-CCSD-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{a_3 a_4}_{i_1 i_2} &= +P_2 f^{i_5}_{a_6} t^{a_4 a_6}_{i_1 i_2} r^{a_3}_{i_5} - P_2 f^{i_5}_{a_6} r^{a_6}_{i_2} t^{a_3 a_4}_{i_1 i_5} - P_2 f^{i_5}_{a'_6} \tilde{t}^{a'_6 a_4}_{i_1 i_2} r^{a_3}_{i_5} - P_2 f^{i_5}_{i_2} r^{a_3 a_4}_{i_1 i_5} + P_2 f^{a_4}_{a_5} r^{a_3 a_5}_{i_1 i_2} - P_2 f^{a_4}_{a'_5} \tilde{r}^{a'_5 a_3}_{i_1 i_2} - P_2 f^{i_5}_{a_6} t^{a_6}_{i_2} r^{a_3 a_4}_{i_1 i_5} + P_2 f^{i_5}_{a_6} r^{a_4 a_6}_{i_1 i_2} t^{a_3}_{i_5} - P_2 f^{i_5}_{a'_6} \tilde{r}^{a'_6 a_4}_{i_1 i_2} t^{a_3}_{i_5} \\
&\quad - P_2 v^{i_5 a_4}_{i_1 i_2} r^{a_3}_{i_5} - P_2 v^{a_3 a_4}_{i_2 a_5} r^{a_5}_{i_1} + P_2 v^{i_5 i_6}_{i_1 i_2} t^{a_4}_{i_6} r^{a_3}_{i_5} + P_2 P_2 v^{i_5 a_4}_{i_2 a_6} t^{a_6}_{i_1} r^{a_3}_{i_5} + P_2 P_2 v^{i_5 a_4}_{i_2 a_6} r^{a_6}_{i_1} t^{a_3}_{i_5} + P_2 v^{a_3 a_4}_{a_5 a_6} t^{a_6}_{i_2} r^{a_5}_{i_1} - P_2 P_2 v^{i_5 i_6}_{i_2 a_7} t^{a_7}_{i_1} t^{a_4}_{i_6} r^{a_3}_{i_5} - \tfrac{1}{2} P_2 P_2 v^{i_5 a_4}_{a_6 a_7} t^{a_7}_{i_2} t^{a_6}_{i_1} r^{a_3}_{i_5} \\
&\quad - \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{i_2 a_7} r^{a_7}_{i_1} t^{a_4}_{i_6} t^{a_3}_{i_5} - P_2 P_2 v^{i_5 a_4}_{a_6 a_7} t^{a_7}_{i_2} r^{a_6}_{i_1} t^{a_3}_{i_5} + P_2 P_2 v^{i_5 i_7}_{i_2 a_6} t^{a_4 a_6}_{i_1 i_7} r^{a_3}_{i_5} - \tfrac{1}{2} P_2 v^{i_5 a_4}_{a_6 a_7} t^{a_6 a_7}_{i_1 i_2} r^{a_3}_{i_5} - \tfrac{1}{2} P_2 v^{i_5 i_6}_{i_2 a_7} r^{a_7}_{i_1} t^{a_3 a_4}_{i_5 i_6} + P_2 P_2 v^{i_6 a_4}_{a_5 a_7} r^{a_7}_{i_2} t^{a_3 a_5}_{i_1 i_6} - P_2 v^{i_5 i_7}_{i_2 a_6} r^{a_6}_{i_7} t^{a_3 a_4}_{i_1 i_5} \\
&\quad - P_2 v^{i_7 a_4}_{a_5 a_6} r^{a_6}_{i_7} t^{a_3 a_5}_{i_1 i_2} - P_2 P_2 v^{i_5 i_7}_{i_2 a'_6} \tilde{t}^{a'_6 a_4}_{i_1 i_7} r^{a_3}_{i_5} - \tfrac{1}{2} P_2 V^{i_5 a_4}_{i_6 i_7} t^{i_6 i_7}_{i_1 i_2} r^{a_3}_{i_5} - P_2 P_2 v^{i_6 a_4}_{a'_5 a_7} r^{a_7}_{i_2} \tilde{t}^{a'_5 a_3}_{i_1 i_6} + P_2 v^{i_7 a_4}_{a'_5 a_6} r^{a_6}_{i_7} \tilde{t}^{a'_5 a_3}_{i_1 i_2} + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_8}_{i_2} t^{a_7}_{i_1} t^{a_4}_{i_6} r^{a_3}_{i_5} \\
&\quad + \tfrac{1}{2} P_2 P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_8}_{i_2} r^{a_7}_{i_1} t^{a_4}_{i_6} t^{a_3}_{i_5} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_7 a_8}_{i_1 i_2} t^{a_4}_{i_6} r^{a_3}_{i_5} - P_2 P_2 v^{i_5 i_7}_{a_6 a_8} t^{a_8}_{i_2} t^{a_4 a_6}_{i_1 i_7} r^{a_3}_{i_5} + P_2 v^{i_5 i_8}_{a_6 a_7} t^{a_7}_{i_8} t^{a_4 a_6}_{i_1 i_2} r^{a_3}_{i_5} - P_2 P_2 v^{i_5 i_7}_{a_6 a_8} r^{a_8}_{i_2} t^{a_4 a_6}_{i_1 i_7} t^{a_3}_{i_5} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_8}_{i_2} r^{a_7}_{i_1} t^{a_3 a_4}_{i_5 i_6} \\
&\quad - P_2 v^{i_5 i_8}_{a_6 a_7} t^{a_7}_{i_8} r^{a_6}_{i_2} t^{a_3 a_4}_{i_1 i_5} + P_2 v^{i_5 i_8}_{a_6 a_7} r^{a_7}_{i_8} t^{a_4 a_6}_{i_1 i_2} t^{a_3}_{i_5} - P_2 v^{i_5 i_8}_{a_6 a_7} r^{a_7}_{i_8} t^{a_6}_{i_2} t^{a_3 a_4}_{i_1 i_5} + \tfrac{1}{2} P_2 V^{i_5 i_6}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_2} t^{a_4}_{i_6} r^{a_3}_{i_5} + P_2 P_2 v^{i_5 i_7}_{a'_6 a_8} t^{a_8}_{i_2} \tilde{t}^{a'_6 a_4}_{i_1 i_7} r^{a_3}_{i_5} - P_2 v^{i_5 i_8}_{a'_6 a_7} t^{a_7}_{i_8} \tilde{t}^{a'_6 a_4}_{i_1 i_2} r^{a_3}_{i_5} \\
&\quad + P_2 P_2 v^{i_5 i_7}_{a'_6 a_8} r^{a_8}_{i_2} \tilde{t}^{a'_6 a_4}_{i_1 i_7} t^{a_3}_{i_5} - P_2 v^{i_5 i_8}_{a'_6 a_7} r^{a_7}_{i_8} \tilde{t}^{a'_6 a_4}_{i_1 i_2} t^{a_3}_{i_5} + \tfrac{1}{2} v^{i_5 i_6}_{i_1 i_2} r^{a_3 a_4}_{i_5 i_6} - P_2 P_2 v^{i_6 a_4}_{i_2 a_5} r^{a_3 a_5}_{i_1 i_6} + \tfrac{1}{2} v^{a_3 a_4}_{a_5 a_6} r^{a_5 a_6}_{i_1 i_2} + P_2 P_2 v^{i_6 a_4}_{i_2 a'_5} \tilde{r}^{a'_5 a_3}_{i_1 i_6} + \tfrac{1}{2} r^{i_5 i_6}_{i_1 i_2} V^{a_3 a_4}_{i_5 i_6} - P_2 v^{i_5 i_7}_{i_2 a_6} t^{a_6}_{i_7} r^{a_3 a_4}_{i_1 i_5} \\
&\quad - \tfrac{1}{2} P_2 v^{i_5 i_6}_{i_2 a_7} t^{a_7}_{i_1} r^{a_3 a_4}_{i_5 i_6} - P_2 v^{i_7 a_4}_{a_5 a_6} t^{a_6}_{i_7} r^{a_3 a_5}_{i_1 i_2} + P_2 P_2 v^{i_5 i_7}_{i_2 a_6} r^{a_4 a_6}_{i_1 i_7} t^{a_3}_{i_5} + P_2 P_2 v^{i_6 a_4}_{a_5 a_7} t^{a_7}_{i_2} r^{a_3 a_5}_{i_1 i_6} - \tfrac{1}{2} P_2 v^{i_5 a_4}_{a_6 a_7} r^{a_6 a_7}_{i_1 i_2} t^{a_3}_{i_5} + P_2 v^{i_7 a_4}_{a'_5 a_6} t^{a_6}_{i_7} \tilde{r}^{a'_5 a_3}_{i_1 i_2} - P_2 P_2 v^{i_5 i_7}_{i_2 a'_6} \tilde{r}^{a'_6 a_4}_{i_1 i_7} t^{a_3}_{i_5} \\
&\quad - P_2 P_2 v^{i_6 a_4}_{a'_5 a_7} t^{a_7}_{i_2} \tilde{r}^{a'_5 a_3}_{i_1 i_6} - \tfrac{1}{2} P_2 r^{i_6 i_7}_{i_1 i_2} V^{i_5 a_4}_{i_6 i_7} t^{a_3}_{i_5} - P_2 v^{i_5 i_8}_{a_6 a_7} t^{a_7}_{i_8} t^{a_6}_{i_2} r^{a_3 a_4}_{i_1 i_5} + \tfrac{1}{4} P_2 v^{i_5 i_6}_{a_7 a_8} t^{a_8}_{i_2} t^{a_7}_{i_1} r^{a_3 a_4}_{i_5 i_6} + P_2 v^{i_5 i_8}_{a_6 a_7} t^{a_7}_{i_8} r^{a_4 a_6}_{i_1 i_2} t^{a_3}_{i_5} - P_2 P_2 v^{i_5 i_7}_{a_6 a_8} t^{a_8}_{i_2} r^{a_4 a_6}_{i_1 i_7} t^{a_3}_{i_5} \\
&\quad + \tfrac{1}{4} P_2 v^{i_5 i_6}_{a_7 a_8} r^{a_7 a_8}_{i_1 i_2} t^{a_4}_{i_6} t^{a_3}_{i_5} - P_2 v^{i_5 i_8}_{a'_6 a_7} t^{a_7}_{i_8} \tilde{r}^{a'_6 a_4}_{i_1 i_2} t^{a_3}_{i_5} + P_2 P_2 v^{i_5 i_7}_{a'_6 a_8} t^{a_8}_{i_2} \tilde{r}^{a'_6 a_4}_{i_1 i_7} t^{a_3}_{i_5} + \tfrac{1}{4} P_2 r^{i_7 i_8}_{i_1 i_2} V^{i_5 i_6}_{i_7 i_8} t^{a_4}_{i_6} t^{a_3}_{i_5} - \tfrac{1}{2} P_2 v^{i_5 i_8}_{a_6 a_7} t^{a_6 a_7}_{i_2 i_8} r^{a_3 a_4}_{i_1 i_5} + \tfrac{1}{4} v^{i_5 i_6}_{a_7 a_8} t^{a_7 a_8}_{i_1 i_2} r^{a_3 a_4}_{i_5 i_6} \\
&\quad - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a_5 a_6} t^{a_4 a_6}_{i_7 i_8} r^{a_3 a_5}_{i_1 i_2} + P_2 P_2 v^{i_6 i_8}_{a_5 a_7} t^{a_4 a_7}_{i_2 i_8} r^{a_3 a_5}_{i_1 i_6} - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a_5 a_6} r^{a_4 a_6}_{i_7 i_8} t^{a_3 a_5}_{i_1 i_2} + \tfrac{1}{4} v^{i_5 i_6}_{a_7 a_8} r^{a_7 a_8}_{i_1 i_2} t^{a_3 a_4}_{i_5 i_6} - \tfrac{1}{2} P_2 v^{i_5 i_8}_{a_6 a_7} r^{a_6 a_7}_{i_2 i_8} t^{a_3 a_4}_{i_1 i_5} + \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_5 a_6} t^{a_4 a_6}_{i_7 i_8} \tilde{r}^{a'_5 a_3}_{i_1 i_2} \\
&\quad + P_2 P_2 v^{i_6 i_8}_{a'_7 a_5} \tilde{r}^{a'_7 a_4}_{i_2 i_8} t^{a_3 a_5}_{i_1 i_6} - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_6 a_5} \tilde{r}^{a'_6 a_4}_{i_7 i_8} t^{a_3 a_5}_{i_1 i_2} + \tfrac{1}{4} r^{i_7 i_8}_{i_1 i_2} V^{i_5 i_6}_{i_7 i_8} t^{a_3 a_4}_{i_5 i_6} - \tfrac{1}{2} P_2 r^{i_7 i_8}_{i_2 i_6} V^{i_5 i_6}_{i_7 i_8} t^{a_3 a_4}_{i_1 i_5} - \tfrac{1}{2} P_2 V^{i_5 i_8}_{i_6 i_7} t^{i_6 i_7}_{i_2 i_8} r^{a_3 a_4}_{i_1 i_5} + \tfrac{1}{4} V^{i_5 i_6}_{i_7 i_8} t^{i_7 i_8}_{i_1 i_2} r^{a_3 a_4}_{i_5 i_6} - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_6 a_5} \tilde{t}^{a'_6 a_4}_{i_7 i_8} r^{a_3 a_5}_{i_1 i_2} \\
&\quad + P_2 P_2 v^{i_6 i_8}_{a'_7 a_5} \tilde{t}^{a'_7 a_4}_{i_2 i_8} r^{a_3 a_5}_{i_1 i_6} + \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_5 a_6} r^{a_4 a_6}_{i_7 i_8} \tilde{t}^{a'_5 a_3}_{i_1 i_2} - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_5 a'_6} \tilde{t}^{a'_6 a_4}_{i_7 i_8} \tilde{r}^{a'_5 a_3}_{i_1 i_2} + P_2 P_2 v^{i_6 i_8}_{a'_5 a'_7} \tilde{r}^{a'_7 a_4}_{i_2 i_8} \tilde{t}^{a'_5 a_3}_{i_1 i_6} - \tfrac{1}{2} P_2 v^{i_7 i_8}_{a'_5 a'_6} \tilde{r}^{a'_6 a_4}_{i_7 i_8} \tilde{t}^{a'_5 a_3}_{i_1 i_2}
\end{aligned}
$$

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TABLE ESI.3.XXVI: The geminal r amplitude equation of EOM-CCSD-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{i_3 i_4}_{i_1 i_2} \;=\; & -f^{i_7}_{a'_8}\tilde{t}^{a'_5 a'_8}_{i_1 i_2} r^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - f^{i_7}_{a_8}\tilde{t}^{a'_5 a_8}_{i_1 i_2} r^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} P_2 f^{i_7}_{a_8} r^{a_8}_{i_2} t^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} + F^{i_3 i_4 *}_{a'_7 a_6} f^{a'_7}_{a_5} r^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{2} P_2 r^{i_6 i_7}_{i_2 i_5} X^{i_3 i_4}_{i_6 i_7} f^{i_5}_{i_1} + \tfrac{1}{2} r^{i_5 i_6}_{i_1 i_2} B^{i_3 i_4}_{i_5 i_6} - \tfrac{1}{2} P_2 f^{i_7}_{a_8} t^{a_8}_{i_2} r^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} \\
& - f^{i_7}_{a'_8}\tilde{r}^{a'_5 a'_8}_{i_1 i_2} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - f^{i_7}_{a_8}\tilde{r}^{a'_5 a_8}_{i_1 i_2} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + F^{i_3 i_4 *}_{a'_6 a_7} r^{a_7}_{i_5} v^{i_5 a'_6}_{i_1 i_2} + P_2 r^{a_5}_{i_2} (V^\dagger)^{i_3 i_4}_{i_1 a_5} - P_2 F^{i_3 i_4 *}_{a'_7 a_8} r^{a_8}_{i_6} v^{i_6 a'_7}_{i_2 a_5} t^{a_5}_{i_1} - P_2 F^{i_3 i_4 *}_{a'_7 a_8} t^{a_8}_{i_6} v^{i_6 a'_7}_{i_2 a_5} r^{a_5}_{i_1} + P_2 (V^\dagger)^{i_3 i_4}_{a_5 a_6} t^{a_6}_{i_2} r^{a_5}_{i_1} \\
& + \tfrac{1}{2} P_2 v^{i_7 a'_5}_{a_8 a_9} t^{a_9}_{i_2} t^{a_8}_{i_1} r^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_7 a'_5}_{a_8 a_9} t^{a_9}_{i_2} r^{a_8}_{i_1} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} F^{i_3 i_4 *}_{a'_8 a_9} r^{a_9}_{i_7} v^{i_7 a'_8}_{a_5 a_6} t^{a_5 a_6}_{i_1 i_2} - P_2 v^{i_8 a'_5}_{a_7 a_9} r^{a_9}_{i_2} t^{a_6 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + v^{i_9 a'_7}_{a_6 a_8} r^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_7 a_5} t^{a_5 a_6}_{i_1 i_2} - P_2 v^{i_7 i_9}_{i_2 a'_8} \tilde{t}^{a'_5 a'_8}_{i_1 i_9} r^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} \\
& - P_2 v^{i_7 i_9}_{i_2 a_8} \tilde{t}^{a'_5 a_8}_{i_1 i_9} r^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} F^{i_3 i_4 *}_{a'_8 a_9} r^{a_9}_{i_7} V^{i_7 a'_8}_{i_5 i_6} t^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{4} P_2 v^{i_7 i_8}_{i_2 a_9} r^{a_9}_{i_1} t^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} + P_2 v^{i_8 a'_6}_{a'_7 a_9} r^{a_9}_{i_2} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} + P_2 v^{i_8 a'_5}_{a'_7 a_9} r^{a_9}_{i_2} \tilde{t}^{a'_7 a_6}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_8 a_6}_{a'_7 a_9} r^{a_9}_{i_2} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} \\
& + P_2 v^{i_8 a'_6}_{a_7 a_9} r^{a_9}_{i_2} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} + P_2 v^{i_8 a_6}_{a_7 a_9} r^{a_9}_{i_2} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} P_2 v^{i_7 i_9}_{i_2 a_8} r^{a_8}_{i_9} t^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} - v^{i_9 a'_7}_{a'_6 a_8} r^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} - v^{i_9 a'_7}_{a'_5 a_8} r^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_7 a_6} \tilde{t}^{a'_5 a_6}_{i_1 i_2} - v^{i_9 a_6}_{a'_7 a_8} r^{a_8}_{i_9} \tilde{t}^{a'_5 a'_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} \\
& - v^{i_9 a'_7}_{a_6 a_8} r^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} - v^{i_9 a_7}_{a_6 a_8} r^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} + P_2 v^{i_7 i_9}_{a'_8 a_{10}} t^{a_{10}}_{i_2} \tilde{t}^{a'_5 a'_8}_{i_1 i_9} r^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_7 i_9}_{a_8 a_{10}} t^{a_{10}}_{i_2} \tilde{t}^{a'_5 a_8}_{i_1 i_9} r^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - v^{i_7 i_{10}}_{a'_8 a_9} t^{a_9}_{i_{10}} \tilde{t}^{a'_5 a'_8}_{i_1 i_2} r^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} \\
& - v^{i_7 i_{10}}_{a_8 a_9} t^{a_9}_{i_{10}} \tilde{t}^{a'_5 a_8}_{i_1 i_2} r^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_7 i_9}_{a'_8 a_{10}} r^{a_{10}}_{i_2} \tilde{t}^{a'_5 a'_8}_{i_1 i_9} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_7 i_9}_{a_8 a_{10}} r^{a_{10}}_{i_2} \tilde{t}^{a'_5 a_8}_{i_1 i_9} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{4} P_2 v^{i_7 i_8}_{a_9 a_{10}} t^{a_{10}}_{i_2} r^{a_9}_{i_1} t^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} - \tfrac{1}{2} P_2 v^{i_7 i_{10}}_{a_8 a_9} t^{a_9}_{i_{10}} r^{a_8}_{i_2} t^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} \\
& - v^{i_7 i_{10}}_{a'_8 a_9} r^{a_9}_{i_{10}} \tilde{t}^{a'_5 a'_8}_{i_1 i_2} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - v^{i_7 i_{10}}_{a_8 a_9} r^{a_9}_{i_{10}} \tilde{t}^{a'_5 a_8}_{i_1 i_2} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} P_2 v^{i_7 i_{10}}_{a_8 a_9} r^{a_9}_{i_{10}} t^{a_8}_{i_2} t^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} + P_2 v^{i_8 a'_5}_{i_2 a_7} r^{a_6 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} r^{a_5 a_6}_{i_1 i_2} (V^\dagger)^{i_3 i_4}_{a_5 a_6} + \tfrac{1}{4} v^{i_7 i_8}_{i_1 i_2} r^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} \\
& - P_2 v^{i_8 a'_6}_{i_2 a'_7} \tilde{r}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} - P_2 v^{i_8 a'_5}_{i_2 a'_7} \tilde{r}^{a'_7 a_6}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} - P_2 v^{i_8 a_6}_{i_2 a'_7} \tilde{r}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} - P_2 v^{i_8 a_6}_{i_2 a_7} \tilde{r}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} r^{i_5 i_6}_{i_1 i_2} P^{i_3 i_4}_{i_5 i_6} + v^{i_9 a'_7}_{a_6 a_8} t^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_7 a_5} r^{a_5 a_6}_{i_1 i_2} \\
& - P_2 v^{i_8 a'_5}_{a_7 a_9} t^{a_9}_{i_2} r^{a_6 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} F^{i_3 i_4 *}_{a'_8 a_9} t^{a_9}_{i_7} v^{i_7 a'_8}_{a_5 a_6} r^{a_5 a_6}_{i_1 i_2} - \tfrac{1}{2} P_2 v^{i_7 i_9}_{i_2 a_8} t^{a_8}_{i_9} r^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} - \tfrac{1}{4} P_2 v^{i_7 i_8}_{i_2 a_9} t^{a_9}_{i_1} r^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} - v^{i_9 a'_6}_{a'_7 a_8} t^{a_8}_{i_9} \tilde{r}^{a'_5 a'_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a'_6} - v^{i_9 a'_5}_{a'_7 a_8} t^{a_8}_{i_9} \tilde{r}^{a'_7 a_6}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} \\
& - v^{i_9 a_6}_{a'_7 a_8} t^{a_8}_{i_9} \tilde{r}^{a'_5 a'_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} - v^{i_9 a'_7}_{a_6 a_8} t^{a_8}_{i_9} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{r}^{a'_5 a_6}_{i_1 i_2} - v^{i_9 a_6}_{a_7 a_8} t^{a_8}_{i_9} \tilde{r}^{a'_5 a_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} - P_2 v^{i_7 i_9}_{i_2 a'_8} \tilde{r}^{a'_5 a'_8}_{i_1 i_9} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - P_2 v^{i_7 i_9}_{i_2 a_8} \tilde{r}^{a'_5 a_8}_{i_1 i_9} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_8 a'_6}_{a'_7 a_9} t^{a_9}_{i_2} \tilde{r}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} \\
& + P_2 v^{i_8 a'_5}_{a'_7 a_9} t^{a_9}_{i_2} \tilde{r}^{a'_7 a_6}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_8 a_6}_{a'_7 a_9} t^{a_9}_{i_2} \tilde{r}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_8 a'_6}_{a_7 a_9} t^{a_9}_{i_2} \tilde{r}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} + \tfrac{1}{2} F^{i_3 i_4 *}_{a'_8 a_9} t^{a_9}_{i_7} V^{i_7 a'_8}_{i_5 i_6} \tilde{r}^{i_5 i_6}_{i_1 i_2} \\
& - \tfrac{1}{2} P_2 v^{i_7 i_{10}}_{a_8 a_9} t^{a_9}_{i_{10}} t^{a_8}_{i_2} r^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{8} P_2 v^{i_7 i_8}_{a_9 a_{10}} t^{a_{10}}_{i_2} t^{a_9}_{i_1} r^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} - v^{i_7 i_{10}}_{a'_8 a_9} t^{a_9}_{i_{10}} \tilde{r}^{a'_5 a'_8}_{i_1 i_2} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - v^{i_7 i_{10}}_{a_8 a_9} t^{a_9}_{i_{10}} \tilde{r}^{a'_5 a_8}_{i_1 i_2} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_7 i_9}_{a'_8 a_{10}} t^{a_{10}}_{i_2} \tilde{r}^{a'_5 a'_8}_{i_1 i_9} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} \\
& + P_2 v^{i_7 i_9}_{a_8 a_{10}} t^{a_{10}}_{i_2} \tilde{r}^{a'_5 a_8}_{i_1 i_9} t^{a_6}_{i_7} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{4} P_2 v^{i_7 i_{10}}_{a_8 a_9} t^{a_8 a_9}_{i_2 i_{10}} r^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{8} v^{i_7 i_8}_{a_9 a_{10}} t^{a_9 a_{10}}_{i_1 i_2} r^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} t^{a_6 a_8}_{i_9 i_{10}} \tilde{r}^{a'_5 a'_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a_7 a_8} t^{a_6 a_8}_{i_9 i_{10}} \tilde{r}^{a'_5 a_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} \\
& + P_2 v^{i_8 i_{10}}_{a'_7 a_9} t^{a_6 a_9}_{i_2 i_{10}} \tilde{r}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_8 i_{10}}_{a'_7 a_9} t^{a_6 a_9}_{i_2 i_{10}} \tilde{r}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_8 a_6} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a_7} t^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{2} v^{i_9 i_{10}}_{a_6 a_8} \tilde{r}^{a'_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a_7} t^{a_5 a_6}_{i_1 i_2} \\
& + \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a_7} r^{a_5 a_6}_{i_1 i_2} + P_2 v^{i_8 i_{10}}_{a'_7 a_9} r^{a_6 a_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} r^{a_6 a_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a_6 a_8} \tilde{r}^{a'_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} \\
& + \tfrac{1}{8} V^{i_7 i_8}_{a_9 a_{10}} r^{a_9 a_{10}}_{i_1 i_2} t^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} - \tfrac{1}{4} P_2 v^{i_7 i_{10}}_{a_8 a_9} r^{a_8 a_9}_{i_2 i_{10}} t^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} - \tfrac{1}{4} P_2 V^{i_7 i_{10}}_{i_8 i_9} t^{i_8 i_9}_{i_2 i_{10}} r^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{8} V^{i_7 i_8}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_1 i_2} r^{i_5 i_6}_{i_7 i_8} X^{i_3 i_4}_{i_5 i_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a'_8} \tilde{r}^{a'_5 a'_7}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_6} \\
& - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a'_8} \tilde{t}^{a'_5 a'_8}_{i_9 i_{10}} \tilde{r}^{a'_7 a_6}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} + \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a'_8} \tilde{t}^{a'_6 a_6}_{i_9 i_{10}} \tilde{r}^{a'_5 a'_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a'_6} + \tfrac{1}{2} v^{i_9 i_{10}}_{a'_8 a_6} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{r}^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_8 a_7} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} \tilde{r}^{a'_5 a_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} \tilde{r}^{a'_5 a_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a'_6} \\
& - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a_8} \tilde{t}^{a'_5 a_8}_{i_9 i_{10}} \tilde{r}^{a'_7 a_6}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a_6 a_8} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{r}^{a'_5 a_6}_{i_1 i_2} + P_2 v^{i_8 i_{10}}_{a'_7 a'_9} \tilde{r}^{a'_6 a'_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} - P_2 v^{i_8 i_{10}}_{a'_7 a'_9} \tilde{r}^{a'_6 a_6}_{i_2 i_{10}} \tilde{t}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} - P_2 v^{i_8 i_{10}}_{a'_7 a'_9} \tilde{t}^{a'_6 a_6}_{i_2 i_{10}} \tilde{r}^{a'_5 a'_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} \\
& - P_2 v^{i_8 i_{10}}_{a'_9 a_7} \tilde{t}^{a'_6 a'_9}_{i_2 i_{10}} \tilde{r}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} + P_2 v^{i_8 i_{10}}_{a'_9 a_7} \tilde{t}^{a'_9 a_6}_{i_2 i_{10}} \tilde{r}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} - P_2 v^{i_8 i_{10}}_{a'_9 a_7} \tilde{r}^{a'_6 a'_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} + P_2 v^{i_8 i_{10}}_{a'_9 a_7} \tilde{r}^{a'_9 a_6}_{i_2 i_{10}} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a_6} + P_2 v^{i_8 i_{10}}_{a'_7 a_9} \tilde{r}^{a'_6 a_9}_{i_2 i_{10}} \tilde{t}^{a'_5 a_7}_{i_1 i_8} F^{i_3 i_4 *}_{a'_5 a'_6} \\
& - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_6 a'_8} \tilde{r}^{a'_7 a'_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a'_6}_{i_1 i_2} + \tfrac{1}{2} v^{i_9 i_{10}}_{a'_7 a'_8} \tilde{r}^{a'_8 a_6}_{i_9 i_{10}} \tilde{t}^{a'_5 a'_7}_{i_1 i_2} F^{i_3 i_4 *}_{a'_5 a_6} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_5 a'_8} \tilde{r}^{a'_7 a'_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_7 a_6} \tilde{t}^{a'_5 a'_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_6 a_8} \tilde{r}^{a'_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a'_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_5 a_8} \tilde{r}^{a'_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_7 a_6} \tilde{t}^{a'_5 a_6}_{i_1 i_2} \\
& + \tfrac{1}{2} v^{i_9 i_{10}}_{a'_8 a_6} \tilde{r}^{a'_7 a'_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a'_8 a_6} \tilde{r}^{a'_8 a_7}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} - \tfrac{1}{2} v^{i_9 i_{10}}_{a_6 a_8} \tilde{r}^{a'_7 a_8}_{i_9 i_{10}} F^{i_3 i_4 *}_{a'_5 a'_7} \tilde{t}^{a'_5 a_6}_{i_1 i_2} + \tfrac{1}{8} X^{i_3 i_4}_{i_9 i_{10}} t^{i_9 i_{10}}_{i_7 i_8} V^{i_7 i_8}_{i_5 i_6} r^{i_5 i_6}_{i_1 i_2} - \tfrac{1}{4} P_2 r^{i_9 i_{10}}_{i_2 i_8} V^{i_7 i_8}_{i_9 i_{10}} t^{i_5 i_6}_{i_1 i_7} X^{i_3 i_4}_{i_5 i_6}
\end{aligned}
$$

Supplementary data for Phys. Chem. Chem. Phys.

H. EOM-CCSDT-R12

TABLE ESI.3.XXVII: The R_1 amplitude equation of EOM-CCSDT-R12 and higher-order EOM-CC-R12 with special intermediates and the RI insertion using the CABS

$\delta_{i_1}^{a_2} = \text{EOM-CCSD-R12} + \frac{1}{4} v_{a_3 a_4}^{i_5 i_6} r_{i_1 i_5 i_6}^{a_2 a_3 a_4}$

TABLE ESI.3.XXVIII: The R_2 amplitude equation of EOM-CCSDT-R12 with special intermediates and the RI insertion using the CABS

$\delta_{i_1 i_2}^{a_3 a_4} = \text{EOM-CCSD-R12} + f_{a_5}^{i_6} r_{i_1 i_2 i_6}^{a_3 a_4 a_5} + \frac{1}{2} P_2 v_{a_6 a_7}^{i_5 i_8} t_{i_1 i_2 i_8}^{a_4 a_6 a_7} r_{i_5}^{a_3} + \frac{1}{2} P_2 v_{a_5 a_8}^{i_6 i_7} r_{i_2}^{a_8} t_{i_1 i_6 i_7}^{a_3 a_4 a_5} + v_{a_5 a_7}^{i_6 i_8} r_{i_8}^{a_7} t_{i_1 i_2 i_6}^{a_3 a_4 a_5} - \frac{1}{2} P_2 v_{i_2 a_5}^{i_6 i_7} r_{i_1 i_6 i_7}^{a_3 a_4 a_5} - \frac{1}{2} P_2 v_{a_5 a_6}^{i_7 a_4} r_{i_1 i_2 i_7}^{a_3 a_5 a_6}$ $+ v_{a_5 a_7}^{i_6 i_8} t_{i_8}^{a_7} r_{i_1 i_2 i_6}^{a_3 a_4 a_5} + \frac{1}{2} P_2 v_{a_5 a_8}^{i_6 i_7} t_{i_2}^{a_8} r_{i_1 i_6 i_7}^{a_3 a_4 a_5} + \frac{1}{2} P_2 v_{a_6 a_7}^{i_5 i_8} r_{i_1 i_2 i_8}^{a_4 a_6 a_7} t_{i_5}^{a_3}$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.3.XXIX: The R_3 amplitude equation of EOM-CCSDT-R12 with special intermediates and the RI insertion using the CABS

$$
\begin{aligned}
\delta^{a_4a_5a_6}_{i_1i_2i_3} = & -P_3 f^{i_7}_{a_8} t^{a_5a_6a_8}_{i_1i_2i_3} r^{a_4}_{i_7} - P_3 f^{i_7}_{a_8} r^{a_8}_{i_3} t^{a_4a_5a_6}_{i_1i_2i_7} + P_3P_3 f^{i_7}_{a_8} t^{a_6a_8}_{i_2i_3} r^{a_4a_5}_{i_1i_7} + P_3P_3 f^{i_7}_{a_8} r^{a_6a_8}_{i_2i_3} t^{a_4a_5}_{i_1i_7} - P_3P_3 f^{i_7}_{a'_8} \tilde{r}^{a'_8a_6}_{i_2i_3} t^{a_4a_5}_{i_1i_7} - P_3P_3 f^{i_7}_{a'_8} \tilde{t}^{a'_8a_6}_{i_2i_3} r^{a_4a_5}_{i_1i_7} - P_3 f^{i_7}_{i_3} r^{a_4a_5a_6}_{i_1i_2i_7} \\
& +P_3 f^{a_6}_{a_7} r^{a_4a_5a_7}_{i_1i_2i_3} - P_3 f^{i_7}_{a_8} t^{a_8}_{i_3} r^{a_4a_5a_6}_{i_1i_2i_7} - P_3 f^{i_7}_{a_8} r^{a_5a_6a_8}_{i_1i_2i_3} t^{a_4}_{i_7} + P_3P_3 v^{i_7i_8}_{i_2i_3} r^{a_6}_{i_8} t^{a_4a_5}_{i_1i_7} - P_3P_3 v^{i_7a_6}_{i_3a_8} t^{a_5a_8}_{i_1i_2} r^{a_4}_{i_7} + P_3P_3 v^{i_7a_6}_{i_3a_8} r^{a_8}_{i_2} t^{a_4a_5}_{i_1i_7} + P_3P_3 v^{a_5a_6}_{a_7a_8} r^{a_8}_{i_3} t^{a_4a_7}_{i_1i_2} \\
& +P_3P_3 v^{i_7a_6}_{i_3a'_8} \tilde{t}^{a'_8a_5}_{i_1i_2} r^{a_4}_{i_7} - P_3P_3 v^{a_5a_6}_{a'_7a_8} r^{a_8}_{i_3} \tilde{t}^{a'_7a_4}_{i_1i_2} - P_3P_3 v^{i_7i_8}_{i_3a_9} t^{a_6a_9}_{i_1i_2} t^{a_5}_{i_8} r^{a_4}_{i_7} - P_3P_3 v^{i_7i_8}_{i_3a_9} t^{a_9}_{i_2} r^{a_6}_{i_8} t^{a_4a_5}_{i_1i_7} + P_3P_3 v^{i_7a_6}_{a_8a_9} t^{a_9}_{i_3} t^{a_5a_8}_{i_1i_2} r^{a_4}_{i_7} - P_3P_3 v^{i_7i_8}_{i_3a_9} r^{a_9}_{i_2} t^{a_6}_{i_8} t^{a_4a_5}_{i_1i_7} \\
& +P_3P_3 v^{i_7a_6}_{a_8a_9} r^{a_9}_{i_3} t^{a_5a_8}_{i_1i_2} t^{a_4}_{i_7} - P_3P_3 v^{i_7a_6}_{a_8a_9} t^{a_9}_{i_3} r^{a_8}_{i_2} t^{a_4a_5}_{i_1i_7} + P_3P_3 v^{i_7i_8}_{i_3a'_9} \tilde{t}^{a'_9a_6}_{i_1i_2} t^{a_5}_{i_8} r^{a_4}_{i_7} - P_3P_3 v^{i_7a_6}_{a'_8a_9} t^{a_9}_{i_3} \tilde{t}^{a'_8a_5}_{i_1i_2} r^{a_4}_{i_7} - P_3P_3 v^{i_7a_6}_{a'_8a_9} r^{a_9}_{i_3} \tilde{t}^{a'_8a_5}_{i_1i_2} t^{a_4}_{i_7} - P_3P_3 v^{i_7i_9}_{i_3a_8} t^{a_5a_6a_8}_{i_1i_2i_9} r^{a_4}_{i_7} \\
& +\tfrac{1}{2} P_3 v^{i_7a_6}_{a_8a_9} t^{a_5a_8a_9}_{i_1i_2i_3} r^{a_4}_{i_7} - \tfrac{1}{2} P_3 v^{i_7i_8}_{i_3a_9} r^{a_9}_{i_2} t^{a_4a_5a_6}_{i_1i_7i_8} + P_3P_3 v^{i_8a_6}_{a_7a_9} r^{a_9}_{i_3} t^{a_4a_5a_7}_{i_1i_2i_8} - P_3 v^{i_7i_9}_{i_3a_8} r^{a_8}_{i_9} t^{a_4a_5a_6}_{i_1i_2i_7} - P_3 v^{i_9a_6}_{a_7a_8} r^{a_8}_{i_9} t^{a_4a_5a_7}_{i_1i_2i_3} + P_3P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_{10}}_{i_3} t^{a_6a_9}_{i_1i_2} t^{a_5}_{i_8} r^{a_4}_{i_7} \\
& +\tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_{10}}_{i_3} t^{a_9}_{i_2} r^{a_6}_{i_8} t^{a_4a_5}_{i_1i_7} + \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_{10}}_{i_3} t^{a_6a_9}_{i_1i_2} t^{a_5}_{i_8} t^{a_4}_{i_7} + P_3P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_{10}}_{i_3} r^{a_9}_{i_2} t^{a_6}_{i_8} t^{a_4a_5}_{i_1i_7} - P_3P_3 v^{i_7i_8}_{a'_9a_{10}} t^{a_{10}}_{i_3} \tilde{t}^{a'_9a_6}_{i_1i_2} t^{a_5}_{i_8} r^{a_4}_{i_7} \\
& -\tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a'_9a_{10}} r^{a_{10}}_{i_3} \tilde{t}^{a'_9a_6}_{i_1i_2} t^{a_5}_{i_8} t^{a_4}_{i_7} + \tfrac{1}{2} P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_6a_9a_{10}}_{i_1i_2i_3} t^{a_5}_{i_8} r^{a_4}_{i_7} + P_3P_3 v^{i_7i_9}_{a_8a_{10}} t^{a_{10}}_{i_3} t^{a_5a_6a_8}_{i_1i_2i_9} r^{a_4}_{i_7} - P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_9}_{i_{10}} t^{a_5a_6a_8}_{i_1i_2i_3} r^{a_4}_{i_7} + P_3P_3 v^{i_7i_9}_{a_8a_{10}} r^{a_{10}}_{i_3} t^{a_5a_6a_8}_{i_1i_2i_9} t^{a_4}_{i_7} \\
& +\tfrac{1}{2} P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_{10}}_{i_3} r^{a_9}_{i_2} t^{a_4a_5a_6}_{i_1i_7i_8} - P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_9}_{i_{10}} r^{a_8}_{i_3} t^{a_4a_5a_6}_{i_1i_2i_7} - P_3 v^{i_7i_{10}}_{a_8a_9} r^{a_9}_{i_{10}} t^{a_5a_6a_8}_{i_1i_2i_3} t^{a_4}_{i_7} - P_3 v^{i_7i_{10}}_{a_8a_9} r^{a_9}_{i_{10}} t^{a_8}_{i_3} t^{a_4a_5a_6}_{i_1i_2i_7} + P_3P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_6a_9}_{i_3i_{10}} t^{a_5a_8}_{i_1i_2} r^{a_4}_{i_7} \\
& +\tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_9a_{10}}_{i_2i_3} r^{a_6}_{i_8} t^{a_4a_5}_{i_1i_7} + \tfrac{1}{2} P_3P_3 v^{i_8i_9}_{a_7a_{10}} r^{a_{10}}_{i_3} t^{a_5a_6}_{i_8i_9} t^{a_4a_7}_{i_1i_2} - P_3P_3 v^{i_7i_9}_{a_8a_{10}} r^{a_{10}}_{i_3} t^{a_6a_8}_{i_2i_9} t^{a_4a_5}_{i_1i_7} + P_3P_3 v^{i_7i_{10}}_{a_8a_9} r^{a_9}_{i_{10}} t^{a_6a_8}_{i_2i_3} t^{a_4a_5}_{i_1i_7} + \tfrac{1}{2} P_3P_3 V^{i_7i_8}_{i_9i_{10}} t^{i_9i_{10}}_{i_2i_3} r^{a_6}_{i_8} t^{a_4a_5}_{i_1i_7} \\
& +P_3P_3 v^{i_7i_{10}}_{a'_9a_8} \tilde{t}^{a'_9a_6}_{i_3i_{10}} t^{a_5a_8}_{i_1i_2} r^{a_4}_{i_7} - P_3P_3 v^{i_7i_{10}}_{a'_8a_9} t^{a_6a_9}_{i_3i_{10}} \tilde{t}^{a'_8a_5}_{i_1i_2} r^{a_4}_{i_7} + P_3P_3 v^{i_7i_9}_{a'_8a_{10}} r^{a_{10}}_{i_3} \tilde{t}^{a'_8a_6}_{i_2i_9} t^{a_4a_5}_{i_1i_7} - \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a'_9a_{10}} r^{a_{10}}_{i_3} \tilde{t}^{a'_9a_6}_{i_1i_2} t^{a_4a_5}_{i_7i_8} - P_3P_3 v^{i_7i_{10}}_{a'_8a_9} r^{a_9}_{i_{10}} \tilde{t}^{a'_8a_6}_{i_2i_3} t^{a_4a_5}_{i_1i_7} \\
& +P_3P_3 v^{i_7i_{10}}_{a'_8a'_9} \tilde{t}^{a'_9a_6}_{i_3i_{10}} \tilde{t}^{a'_8a_5}_{i_1i_2} r^{a_4}_{i_7} - P_3P_3 v^{i_7a_6}_{i_2i_3} r^{a_4a_5}_{i_1i_7} - P_3P_3 v^{a_5a_6}_{i_3a_7} r^{a_4a_7}_{i_1i_2} + P_3P_3 v^{a_5a_6}_{i_3a'_7} \tilde{r}^{a'_7a_4}_{i_1i_2} + P_3P_3 v^{i_7i_8}_{i_2i_3} t^{a_6}_{i_8} r^{a_4a_5}_{i_1i_7} + P_3P_3 v^{i_7a_6}_{i_3a_8} t^{a_8}_{i_2} r^{a_4a_5}_{i_1i_7} - P_3P_3 v^{i_7a_6}_{i_3a_8} r^{a_5a_8}_{i_1i_2} t^{a_4}_{i_7} \\
& +P_3P_3 v^{a_5a_6}_{a_7a_8} t^{a_8}_{i_3} r^{a_4a_7}_{i_1i_2} + P_3P_3 v^{i_7a_6}_{i_3a'_8} \tilde{r}^{a'_8a_5}_{i_1i_2} t^{a_4}_{i_7} - P_3P_3 v^{a_5a_6}_{a'_7a_8} t^{a_8}_{i_3} \tilde{r}^{a'_7a_4}_{i_1i_2} - P_3P_3 v^{i_7i_8}_{i_3a_9} t^{a_9}_{i_2} t^{a_6}_{i_8} r^{a_4a_5}_{i_1i_7} - \tfrac{1}{2} P_3P_3 v^{i_7a_6}_{a_8a_9} t^{a_9}_{i_3} t^{a_8}_{i_2} r^{a_4a_5}_{i_1i_7} - \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{i_3a_9} r^{a_6a_9}_{i_1i_2} t^{a_5}_{i_8} t^{a_4}_{i_7} \\
& +P_3P_3 v^{i_7a_6}_{a_8a_9} t^{a_9}_{i_3} r^{a_5a_8}_{i_1i_2} t^{a_4}_{i_7} + \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{i_3a'_9} \tilde{r}^{a'_9a_6}_{i_1i_2} t^{a_5}_{i_8} t^{a_4}_{i_7} - P_3P_3 v^{i_7a_6}_{a'_8a_9} t^{a_9}_{i_3} \tilde{r}^{a'_8a_5}_{i_1i_2} t^{a_4}_{i_7} + P_3P_3 v^{i_7i_9}_{i_3a_8} t^{a_6a_8}_{i_2i_9} r^{a_4a_5}_{i_1i_7} - \tfrac{1}{2} P_3P_3 v^{i_7a_6}_{a_8a_9} t^{a_8a_9}_{i_2i_3} r^{a_4a_5}_{i_1i_7} - \tfrac{1}{2} P_3P_3 v^{i_8i_9}_{i_3a_7} r^{a_5a_6}_{i_8i_9} t^{a_4a_7}_{i_1i_2} \\
& -\tfrac{1}{2} P_3P_3 v^{i_8i_9}_{i_3a_7} t^{a_5a_6}_{i_8i_9} r^{a_4a_7}_{i_1i_2} + P_3P_3 v^{i_9a_6}_{a_7a_8} t^{a_5a_8}_{i_3i_9} r^{a_4a_7}_{i_1i_2} + P_3P_3 v^{i_7i_9}_{i_3a_8} r^{a_6a_8}_{i_2i_9} t^{a_4a_5}_{i_1i_7} + P_3P_3 v^{i_9a_6}_{a_7a_8} r^{a_5a_8}_{i_3i_9} t^{a_4a_7}_{i_1i_2} - \tfrac{1}{2} P_3P_3 v^{i_7a_6}_{a_8a_9} r^{a_8a_9}_{i_2i_3} t^{a_4a_5}_{i_1i_7} + \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{i_3a'_9} \tilde{r}^{a'_9a_6}_{i_1i_2} t^{a_4a_5}_{i_7i_8} \\
& -P_3P_3 v^{i_9a_6}_{a'_7a_8} t^{a_5a_8}_{i_3i_9} \tilde{r}^{a'_7a_4}_{i_1i_2} - P_3P_3 v^{i_7i_9}_{i_3a'_8} \tilde{r}^{a'_8a_6}_{i_2i_9} t^{a_4a_5}_{i_1i_7} + P_3P_3 v^{i_9a_6}_{a'_8a_7} \tilde{r}^{a'_8a_5}_{i_3i_9} t^{a_4a_7}_{i_1i_2} - \tfrac{1}{2} P_3P_3 r^{i_8i_9}_{i_2i_3} V^{i_7a_6}_{i_8i_9} t^{a_4a_5}_{i_1i_7} - P_3P_3 v^{i_7i_9}_{i_3a'_8} \tilde{t}^{a'_8a_6}_{i_2i_9} r^{a_4a_5}_{i_1i_7} - \tfrac{1}{2} P_3P_3 V^{i_7a_6}_{i_8i_9} t^{i_8i_9}_{i_2i_3} r^{a_4a_5}_{i_1i_7} \\
& +\tfrac{1}{2} P_3P_3 v^{i_7i_8}_{i_3a'_9} \tilde{t}^{a'_9a_6}_{i_1i_2} r^{a_4a_5}_{i_7i_8} + P_3P_3 v^{i_9a_6}_{a'_8a_7} \tilde{t}^{a'_8a_5}_{i_3i_9} r^{a_4a_7}_{i_1i_2} - P_3P_3 v^{i_9a_6}_{a'_7a_8} r^{a_5a_8}_{i_3i_9} \tilde{t}^{a'_7a_4}_{i_1i_2} + P_3P_3 v^{i_9a_6}_{a'_7a'_8} \tilde{t}^{a'_8a_5}_{i_3i_9} \tilde{r}^{a'_7a_4}_{i_1i_2} + P_3P_3 v^{i_9a_6}_{a'_7a'_8} \tilde{r}^{a'_8a_5}_{i_3i_9} \tilde{t}^{a'_7a_4}_{i_1i_2} \\
& +\tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_{10}}_{i_3} t^{a_9}_{i_2} t^{a_6}_{i_8} r^{a_4a_5}_{i_1i_7} + \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_{10}}_{i_3} r^{a_6a_9}_{i_1i_2} t^{a_5}_{i_8} t^{a_4}_{i_7} - \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a'_9a_{10}} t^{a_{10}}_{i_3} \tilde{r}^{a'_9a_6}_{i_1i_2} t^{a_5}_{i_8} t^{a_4}_{i_7} + \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_9a_{10}}_{i_2i_3} t^{a_6}_{i_8} r^{a_4a_5}_{i_1i_7} - P_3P_3 v^{i_7i_9}_{a_8a_{10}} t^{a_{10}}_{i_3} t^{a_6a_8}_{i_2i_9} r^{a_4a_5}_{i_1i_7} \\
& +P_3P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_9}_{i_{10}} t^{a_6a_8}_{i_2i_3} r^{a_4a_5}_{i_1i_7} + \tfrac{1}{2} P_3P_3 v^{i_8i_9}_{a_7a_{10}} t^{a_{10}}_{i_3} r^{a_5a_6}_{i_8i_9} t^{a_4a_7}_{i_1i_2} + P_3P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_6a_9}_{i_3i_{10}} r^{a_5a_8}_{i_1i_2} t^{a_4}_{i_7} + \tfrac{1}{2} P_3P_3 v^{i_8i_9}_{a_7a_{10}} t^{a_{10}}_{i_3} t^{a_5a_6}_{i_8i_9} r^{a_4a_7}_{i_1i_2} + P_3P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_9}_{i_{10}} r^{a_6a_8}_{i_2i_3} t^{a_4a_5}_{i_1i_7} \\
& +P_3P_3 v^{i_7i_{10}}_{a_8a_9} r^{a_6a_9}_{i_3i_{10}} t^{a_5a_8}_{i_1i_2} t^{a_4}_{i_7} - P_3P_3 v^{i_7i_9}_{a_8a_{10}} t^{a_{10}}_{i_3} r^{a_6a_8}_{i_2i_9} t^{a_4a_5}_{i_1i_7} + \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9a_{10}}_{i_2i_3} t^{a_6}_{i_8} t^{a_4a_5}_{i_1i_7} - P_3P_3 v^{i_7i_{10}}_{a'_8a_9} t^{a_6a_9}_{i_3i_{10}} \tilde{r}^{a'_8a_5}_{i_1i_2} t^{a_4}_{i_7} - \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a'_9a_{10}} t^{a_{10}}_{i_3} \tilde{r}^{a'_9a_6}_{i_1i_2} t^{a_4a_5}_{i_7i_8} \\
& -P_3P_3 v^{i_7i_{10}}_{a'_8a_9} t^{a_9}_{i_{10}} \tilde{r}^{a'_8a_6}_{i_2i_3} t^{a_4a_5}_{i_1i_7} + P_3P_3 v^{i_7i_{10}}_{a'_9a_8} \tilde{r}^{a'_9a_6}_{i_3i_{10}} t^{a_5a_8}_{i_1i_2} t^{a_4}_{i_7} + P_3P_3 v^{i_7i_9}_{a'_8a_{10}} t^{a_{10}}_{i_3} \tilde{r}^{a'_8a_6}_{i_2i_9} t^{a_4a_5}_{i_1i_7} + \tfrac{1}{2} P_3P_3 r^{i_9i_{10}}_{i_2i_3} V^{i_7i_8}_{i_9i_{10}} t^{a_6}_{i_8} t^{a_4a_5}_{i_1i_7} + \tfrac{1}{2} P_3P_3 V^{i_7i_8}_{i_9i_{10}} t^{i_9i_{10}}_{i_2i_3} t^{a_6}_{i_8} r^{a_4a_5}_{i_1i_7} \\
& +P_3P_3 v^{i_7i_9}_{a'_8a_{10}} t^{a_{10}}_{i_3} \tilde{t}^{a'_8a_6}_{i_2i_9} r^{a_4a_5}_{i_1i_7} - P_3P_3 v^{i_7i_{10}}_{a'_8a_9} t^{a_9}_{i_{10}} \tilde{t}^{a'_8a_6}_{i_2i_3} r^{a_4a_5}_{i_1i_7} - \tfrac{1}{2} P_3P_3 v^{i_7i_8}_{a'_9a_{10}} t^{a_{10}}_{i_3} \tilde{t}^{a'_9a_6}_{i_1i_2} r^{a_4a_5}_{i_7i_8} + P_3P_3 v^{i_7i_{10}}_{a'_9a_8} \tilde{t}^{a'_9a_6}_{i_3i_{10}} r^{a_5a_8}_{i_1i_2} t^{a_4}_{i_7} - P_3P_3 v^{i_7i_{10}}_{a'_8a_9} r^{a_6a_9}_{i_3i_{10}} \tilde{t}^{a'_8a_5}_{i_1i_2} t^{a_4}_{i_7} \\
& +P_3P_3 v^{i_7i_{10}}_{a'_8a'_9} \tilde{t}^{a'_9a_6}_{i_3i_{10}} \tilde{r}^{a'_8a_5}_{i_1i_2} t^{a_4}_{i_7} + P_3P_3 v^{i_7i_{10}}_{a'_8a'_9} \tilde{r}^{a'_9a_6}_{i_3i_{10}} \tilde{t}^{a'_8a_5}_{i_1i_2} t^{a_4}_{i_7} + \tfrac{1}{2} P_3P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_6a_8a_9}_{i_2i_3i_{10}} r^{a_4a_5}_{i_1i_7} + \tfrac{1}{4} P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_6a_9a_{10}}_{i_1i_2i_3} r^{a_4a_5}_{i_7i_8} + \tfrac{1}{2} P_3P_3 v^{i_9i_{10}}_{a_7a_8} t^{a_5a_6a_8}_{i_3i_9i_{10}} r^{a_4a_7}_{i_1i_2} \\
& +P_3P_3 v^{i_8i_{10}}_{a_7a_9} r^{a_6a_9}_{i_3i_{10}} t^{a_4a_5a_7}_{i_1i_2i_8} - \tfrac{1}{2} P_3 v^{i_9i_{10}}_{a_7a_8} r^{a_6a_8}_{i_9i_{10}} t^{a_4a_5a_7}_{i_1i_2i_3} + \tfrac{1}{4} P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_9a_{10}}_{i_2i_3} t^{a_4a_5a_6}_{i_1i_7i_8} - \tfrac{1}{2} P_3 v^{i_7i_{10}}_{a_8a_9} r^{a_8a_9}_{i_3i_{10}} t^{a_4a_5a_6}_{i_1i_2i_7} - \tfrac{1}{2} P_3P_3 v^{i_9i_{10}}_{a'_7a_8} t^{a_5a_6a_8}_{i_3i_9i_{10}} \tilde{r}^{a'_7a_4}_{i_1i_2} \\
& +P_3P_3 v^{i_8i_{10}}_{a'_9a_7} \tilde{r}^{a'_9a_6}_{i_3i_{10}} t^{a_4a_5a_7}_{i_1i_2i_8} - \tfrac{1}{2} P_3 v^{i_9i_{10}}_{a'_8a_7} \tilde{r}^{a'_8a_6}_{i_9i_{10}} t^{a_4a_5a_7}_{i_1i_2i_3} + \tfrac{1}{4} P_3 r^{i_9i_{10}}_{i_2i_3} V^{i_7i_8}_{i_9i_{10}} t^{a_4a_5a_6}_{i_1i_7i_8} - \tfrac{1}{2} P_3 r^{i_9i_{10}}_{i_3i_8} V^{i_7i_8}_{i_9i_{10}} t^{a_4a_5a_6}_{i_1i_2i_7} + \tfrac{1}{2} P_3 v^{i_7i_8}_{i_2i_3} r^{a_4a_5a_6}_{i_1i_7i_8} - P_3P_3 v^{i_8a_6}_{i_3a_7} r^{a_4a_5a_7}_{i_1i_2i_8} \\
& +\tfrac{1}{2} P_3 v^{a_5a_6}_{a_7a_8} r^{a_4a_7a_8}_{i_1i_2i_3} - P_3 v^{i_7i_9}_{i_3a_8} t^{a_8}_{i_9} r^{a_4a_5a_6}_{i_1i_2i_7} - \tfrac{1}{2} P_3 v^{i_7i_8}_{i_3a_9} t^{a_9}_{i_2} r^{a_4a_5a_6}_{i_1i_7i_8} - P_3 v^{i_9a_6}_{a_7a_8} t^{a_8}_{i_9} r^{a_4a_5a_7}_{i_1i_2i_3} - P_3P_3 v^{i_7i_9}_{i_3a_8} r^{a_5a_6a_8}_{i_1i_2i_9} t^{a_4}_{i_7} + P_3P_3 v^{i_8a_6}_{a_7a_9} t^{a_9}_{i_3} r^{a_4a_5a_7}_{i_1i_2i_8} \\
& +\tfrac{1}{2} P_3 v^{i_7a_6}_{a_8a_9} r^{a_5a_8a_9}_{i_1i_2i_3} t^{a_4}_{i_7} - P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_9}_{i_{10}} t^{a_8}_{i_3} r^{a_4a_5a_6}_{i_1i_2i_7} + \tfrac{1}{4} P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_{10}}_{i_3} t^{a_9}_{i_2} r^{a_4a_5a_6}_{i_1i_7i_8} - P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_9}_{i_{10}} r^{a_5a_6a_8}_{i_1i_2i_3} t^{a_4}_{i_7} + P_3P_3 v^{i_7i_9}_{a_8a_{10}} t^{a_{10}}_{i_3} r^{a_5a_6a_8}_{i_1i_2i_9} t^{a_4}_{i_7} \\
& +\tfrac{1}{4} P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_6a_9a_{10}}_{i_1i_2i_3} t^{a_5}_{i_8} t^{a_4}_{i_7} - \tfrac{1}{2} P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_8a_9}_{i_3i_{10}} r^{a_4a_5a_6}_{i_1i_2i_7} + \tfrac{1}{4} P_3 v^{i_7i_8}_{a_9a_{10}} t^{a_9a_{10}}_{i_2i_3} r^{a_4a_5a_6}_{i_1i_7i_8} - \tfrac{1}{2} P_3 v^{i_9i_{10}}_{a_7a_8} t^{a_6a_8}_{i_9i_{10}} r^{a_4a_5a_7}_{i_1i_2i_3} + P_3P_3 v^{i_8i_{10}}_{a_7a_9} t^{a_6a_9}_{i_3i_{10}} r^{a_4a_5a_7}_{i_1i_2i_8} \\
& +\tfrac{1}{2} P_3P_3 v^{i_9i_{10}}_{a_7a_8} r^{a_5a_6a_8}_{i_3i_9i_{10}} t^{a_4a_7}_{i_1i_2} + \tfrac{1}{4} P_3 v^{i_7i_8}_{a_9a_{10}} r^{a_6a_9a_{10}}_{i_1i_2i_3} t^{a_4a_5}_{i_7i_8} + \tfrac{1}{2} P_3P_3 v^{i_7i_{10}}_{a_8a_9} r^{a_6a_8a_9}_{i_2i_3i_{10}} t^{a_4a_5}_{i_1i_7} - \tfrac{1}{2} P_3 V^{i_7i_{10}}_{i_8i_9} t^{i_8i_9}_{i_3i_{10}} r^{a_4a_5a_6}_{i_1i_2i_7} + \tfrac{1}{4} P_3 V^{i_7i_8}_{i_9i_{10}} t^{i_9i_{10}}_{i_2i_3} r^{a_4a_5a_6}_{i_1i_7i_8} \\
& -\tfrac{1}{2} P_3 v^{i_9i_{10}}_{a'_8a_7} \tilde{t}^{a'_8a_6}_{i_9i_{10}} r^{a_4a_5a_7}_{i_1i_2i_3} + P_3P_3 v^{i_8i_{10}}_{a'_9a_7} \tilde{t}^{a'_9a_6}_{i_3i_{10}} r^{a_4a_5a_7}_{i_1i_2i_8} - \tfrac{1}{2} P_3P_3 v^{i_9i_{10}}_{a'_7a_8} r^{a_5a_6a_8}_{i_3i_9i_{10}} \tilde{t}^{a'_7a_4}_{i_1i_2}
\end{aligned}
$$

TABLE ESI.3.XXX: The geminal r amplitude equation of EOM-CCSDT-R12 and higher-order EOM-CC-R12 with special intermediates and the RI insertion using the CABS

$$
\delta^{i_3i_4}_{i_1i_2} = \text{EOM-CCSD-R12} + \tfrac{1}{2} v^{i_9a'_5}_{a_7a_8} r^{a_6a_7a_8}_{i_1i_2i_9} F^{i_3i_4*}_{a'_5a_6}
$$

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I. EOM-CCSDTQ-R12

TABLE ESI.3.XXXI: The R_2 amplitude equation of EOM-CCSDTQ-R12 with special intermediates and the RI insertion using the CABS

$$\delta^{a_3a_4}_{i_1i_2} = \text{EOM-CCSDT-R12} + \tfrac{1}{4} v^{i_7i_8}_{a_5a_6} r^{a_3a_4a_5a_6}_{i_1i_2i_7i_8}$$

TABLE ESI.3.XXXII: The R_3 amplitude equation of EOM-CCSDTQ-R12 with special intermediates and the RI insertion using the CABS

$$\begin{aligned}\delta^{a_4a_5a_6}_{i_1i_2i_3} = \text{EOM-CCSDT-R12} &+ f^{i_8}_{a_7} r^{a_4a_5a_6a_7}_{i_1i_2i_3i_8} - \tfrac{1}{2} P_3 v^{i_7i_{10}}_{a_8a_9} t^{a_5a_6a_8a_9}_{i_1i_2i_3i_{10}} r^{a_4}_{i_7} + \tfrac{1}{2} P_3 v^{i_8i_9}_{a_7a_{10}} r^{a_{10}}_{i_3} t^{a_4a_5a_6a_7}_{i_1i_2i_8i_9} + v^{i_8i_{10}}_{a_7a_9} r^{a_9}_{i_{10}} t^{a_4a_5a_6a_7}_{i_1i_2i_3i_8} - \tfrac{1}{2} P_3 v^{i_8i_9}_{i_3a_7} r^{a_4a_5a_6a_7}_{i_1i_2i_8i_9} - \tfrac{1}{2} P_3 v^{i_9a_6}_{a_7a_8} r^{a_4a_5a_7a_8}_{i_1i_2i_3i_9} \\ &+ v^{i_8i_{10}}_{a_7a_9} t^{a_9}_{i_{10}} r^{a_4a_5a_6a_7}_{i_1i_2i_3i_8} + \tfrac{1}{2} P_3 v^{i_8i_9}_{a_7a_{10}} t^{a_{10}}_{i_3} r^{a_4a_5a_6a_7}_{i_1i_2i_8i_9} - \tfrac{1}{2} P_3 v^{i_7i_{10}}_{a_8a_9} r^{a_5a_6a_8a_9}_{i_1i_2i_3i_{10}} t^{a_4}_{i_7}\end{aligned}$$

TABLE ESI.3.XXXIII: The R_4 amplitude equation of EOM-CCSDTQ-R12 with special intermediates and the RI insertion using the CABS [Part I]

$$\begin{aligned}\delta^{a_5a_6a_7a_8}_{i_1i_2i_3i_4} = &+P_4 f^{i_9}_{a_{10}} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_4} r^{a_5}_{i_9} - P_4 f^{i_9}_{a_{10}} r^{a_{10}}_{i_4} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} - P_4 P_4 f^{i_9}_{a_{10}} t^{a_7a_8a_{10}}_{i_2i_3i_4} r^{a_5a_6}_{i_1i_9} + P_4 P_4 f^{i_9}_{a_{10}} r^{a_8a_{10}}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4 P_4 f^{i_9}_{a'_{10}} \tilde{r}^{a'_{10}a_8}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4 P_4 f^{i_9}_{a_{10}} t^{a_8a_{10}}_{i_3i_4} r^{a_5a_6a_7}_{i_1i_2i_9} \\ &-P_4 P_4 f^{i_9}_{a_{10}} r^{a_7a_8a_{10}}_{i_2i_3i_4} t^{a_5a_6}_{i_1i_9} - P_4 P_4 f^{i_9}_{a'_{10}} \tilde{t}^{a'_{10}a_8}_{i_3i_4} r^{a_5a_6a_7}_{i_1i_2i_9} - P_4 f^{i_9}_{i_4} r^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} + P_4 f^{i_9}_{a_9} r^{a_5a_6a_7a_9}_{i_1i_2i_3i_4} - P_4 f^{i_9}_{a_{10}} t^{a_{10}}_{i_4} r^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} + P_4 f^{i_9}_{a_{10}} r^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_4} t^{a_5}_{i_9} \\ &+P_4 P_4 v^{i_9i_{10}}_{i_3i_4} r^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4 P_4 v^{i_9a_8}_{i_4a_{10}} t^{a_6a_7a_{10}}_{i_1i_2i_3} r^{a_5}_{i_9} + P_4 P_4 v^{i_9a_8}_{i_4a_{10}} r^{a_{10}}_{i_3} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4 P_4 v^{a_7a_8}_{a_9a_{10}} r^{a_{10}}_{i_4} t^{a_5a_6a_9}_{i_1i_2i_3} - P_4 P_4 v^{i_9i_{10}}_{i_4a_{11}} t^{a_7a_8a_{11}}_{i_3} t^{a_6}_{i_{10}} r^{a_5}_{i_9} \\ &-P_4 P_4 v^{i_9i_{10}}_{i_4a_{11}} t^{a_{11}}_{i_3} r^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4 P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_{11}}_{i_4} t^{a_6a_7a_{10}}_{i_1i_2i_3} r^{a_5}_{i_9} - P_4 P_4 v^{i_9i_{10}}_{i_4a_{11}} r^{a_{11}}_{i_3} t^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4 P_4 v^{i_9a_8}_{a_{10}a_{11}} r^{a_{11}}_{i_4} t^{a_6a_7a_{10}}_{i_1i_2i_3} t^{a_5}_{i_9} - P_4 P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_{11}}_{i_4} r^{a_{10}}_{i_3} t^{a_5a_6a_7}_{i_1i_2i_9} \\ &-P_4 P_4 v^{i_9i_{10}}_{i_4a_{11}} t^{a_8a_{11}}_{i_2i_3} r^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_7a_{11}}_{i_3i_4} t^{a_6a_{10}}_{i_1i_2} r^{a_5}_{i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{i_4a_{11}} r^{a_{11}}_{i_3} t^{a_7a_8}_{i_2i_{10}} t^{a_5a_6}_{i_1i_9} + P_4 P_4 v^{i_9a_8}_{a_{10}a_{11}} r^{a_{11}}_{i_4} t^{a_7a_{10}}_{i_2i_3} t^{a_5a_6}_{i_1i_9} + P_4 P_4 v^{i_9i_{10}}_{i_4a'_{11}} \tilde{t}^{a'_{11}a_8}_{i_2i_3} r^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} \\ &+P_4 P_4 v^{i_9a_8}_{a'_{11}a_{10}} \tilde{t}^{a'_{11}a_7}_{i_3i_4} t^{a_6a_{10}}_{i_1i_2} r^{a_5}_{i_9} - P_4 P_4 v^{i_9a_8}_{a'_{10}a_{11}} r^{a_{11}}_{i_4} \tilde{t}^{a'_{10}a_7}_{i_2i_3} t^{a_5a_6}_{i_1i_9} + P_4 P_4 v^{i_9i_{11}}_{i_4a_{10}} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_{11}} r^{a_5}_{i_9} - \tfrac{1}{2} P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_6a_7a_{10}a_{11}}_{i_1i_2i_3i_4} r^{a_5}_{i_9} - \tfrac{1}{2} P_4 v^{i_9i_{10}}_{i_4a_{11}} r^{a_{11}}_{i_3} t^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} \\ &+P_4 P_4 v^{i_{10}a_8}_{a_9a_{11}} r^{a_{11}}_{i_4} t^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}} - P_4 v^{i_9i_{11}}_{i_4a_{10}} r^{a_{10}}_{i_{11}} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} - P_4 v^{i_{11}a_8}_{a_9a_{10}} r^{a_{10}}_{i_{11}} t^{a_5a_6a_7a_9}_{i_1i_2i_3i_4} + \tfrac{1}{2} P_4 P_4 v^{i_9a_8}_{a'_{10}a'_{11}} \tilde{t}^{a'_{11}a_7}_{i_3i_4} \tilde{t}^{a'_{10}a_6}_{i_1i_2} r^{a_5}_{i_9} + P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} t^{a_7a_8a_{11}}_{i_1i_2i_3} t^{a_6}_{i_{10}} r^{a_5}_{i_9} \\ &+\tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} t^{a_{11}}_{i_3} r^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} t^{a_7a_8a_{11}}_{i_1i_2i_3} t^{a_6}_{i_{10}} t^{a_5}_{i_9} + P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} r^{a_{11}}_{i_3} t^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} + \tfrac{1}{2} P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_7a_8a_{11}a_{12}}_{i_1i_2i_3i_4} t^{a_6}_{i_{10}} r^{a_5}_{i_9} \\ &-P_4 P_4 v^{i_9i_{11}}_{a_{10}a_{12}} t^{a_{12}}_{i_4} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_{11}} r^{a_5}_{i_9} + P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_{11}}_{i_{12}} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_4} r^{a_5}_{i_9} - P_4 P_4 v^{i_9i_{11}}_{a_{10}a_{12}} r^{a_{12}}_{i_4} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_{11}} t^{a_5}_{i_9} + \tfrac{1}{2} P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} r^{a_{11}}_{i_3} t^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} \\ &-P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_{11}}_{i_{12}} r^{a_{10}}_{i_4} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} + P_4 v^{i_9i_{12}}_{a_{10}a_{11}} r^{a_{11}}_{i_{12}} t^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_4} t^{a_5}_{i_9} - P_4 v^{i_9i_{12}}_{a_{10}a_{11}} r^{a_{11}}_{i_{12}} t^{a_{10}}_{i_4} t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a'_{11}a'_{12}} \tilde{t}^{a'_{12}a_8}_{i_3i_4} \tilde{t}^{a'_{11}a_7}_{i_1i_2} t^{a_6}_{i_{10}} r^{a_5}_{i_9} \\ &-P_4 P_4 v^{i_9i_{10}}_{a'_{11}a_{12}} t^{a_{12}}_{i_4} \tilde{t}^{a'_{11}a_8}_{i_2i_3} r^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} - P_4 P_4 v^{i_9i_{10}}_{a'_{12}a_{11}} \tilde{t}^{a'_{12}a_8}_{i_3i_4} t^{a_7a_{11}}_{i_1i_2} t^{a_6}_{i_{10}} r^{a_5}_{i_9} - P_4 P_4 v^{i_9i_{10}}_{a'_{11}a_{12}} r^{a_{12}}_{i_4} \tilde{t}^{a'_{11}a_8}_{i_2i_3} t^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} + P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} t^{a_8a_{11}}_{i_2i_3} r^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} \\ &-\tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_8a_{12}}_{i_3i_4} t^{a_7a_{11}}_{i_1i_2} t^{a_6}_{i_{10}} r^{a_5}_{i_9} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_{12}}_{i_4} r^{a_{11}}_{i_3} t^{a_7a_8}_{i_2i_{10}} t^{a_5a_6}_{i_1i_9} + P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{12}}_{i_4} t^{a_8a_{11}}_{i_2i_3} t^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_8a_{11}a_{12}}_{i_2i_3i_4} r^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} \\ &+P_4 P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_7a_8a_{11}}_{i_3i_4i_{12}} t^{a_6a_{10}}_{i_1i_2} r^{a_5}_{i_9} - P_4 P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_8a_{11}}_{i_4i_{12}} t^{a_6a_7a_{10}}_{i_1i_2i_3} r^{a_5}_{i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_8}_{i_{10}} t^{a_{11}a_{12}}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4 P_4 v^{i_9i_{11}}_{a_{10}a_{12}} r^{a_{12}}_{i_4} t^{a_7a_8a_{10}}_{i_1i_2i_3i_{11}} t^{a_5a_6}_{i_1i_9} \\ &+\tfrac{1}{2} P_4 P_4 v^{i_{10}i_{11}}_{a_9a_{12}} t^{a_{12}}_{i_4} t^{a_7a_8}_{i_{10}i_{11}} t^{a_5a_6a_9}_{i_1i_2i_3} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{11}}_{a_9a_{12}} r^{a_{12}}_{i_4} t^{a_6a_7a_8}_{i_3i_{10}i_{11}} t^{a_5a_6}_{i_1i_2} - P_4 P_4 v^{i_9i_{11}}_{a_{10}a_{12}} r^{a_{12}}_{i_4} t^{a_8a_{10}}_{i_3i_{11}} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4 P_4 v^{i_9i_{11}}_{a_{10}a_{11}} r^{a_{11}}_{i_{12}} t^{a_7a_8a_{10}}_{i_2i_3i_4} t^{a_5a_6}_{i_1i_9} \\ &+P_4 P_4 v^{i_9i_{12}}_{a_{10}a_{11}} r^{a_{11}}_{i_{12}} t^{a_8a_{10}}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4 P_4 v^{i_9i_{12}}_{a'_{10}a_{11}} t^{a_7a_8a_{11}}_{i_3i_4i_{12}} \tilde{t}^{a'_{10}a_6}_{i_1i_2} r^{a_5}_{i_9} - P_4 P_4 v^{i_9i_{12}}_{a'_{11}a_{10}} \tilde{t}^{a'_{11}a_8}_{i_4i_{12}} t^{a_6a_7a_{10}}_{i_1i_2i_3} r^{a_5}_{i_9} + \tfrac{1}{2} P_4 P_4 V^{i_9i_{10}}_{i_{11}i_{12}} t^{i_{11}i_{12}}_{i_3i_4} r^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} \\ &-\tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a'_{11}a_{12}} r^{a_{12}}_{i_4} \tilde{t}^{a'_{11}a_8}_{i_2i_3} t^{a_5a_6a_7}_{i_1i_9i_{10}} + P_4 P_4 v^{i_9i_{11}}_{a'_{10}a_{12}} r^{a_{12}}_{i_4} \tilde{t}^{a'_{10}a_8}_{i_3i_{11}} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4 P_4 v^{i_9i_{12}}_{a'_{10}a_{11}} r^{a_{11}}_{i_{12}} \tilde{t}^{a'_{10}a_8}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4 P_4 v^{i_9a_8}_{i_3i_4} t^{a_7a_{10}}_{i_2i_{10}} t^{a_5a_6}_{i_1i_9} r^{a_5a_6}_{i_1i_9} \\ &-P_4 P_4 v^{i_9a_8}_{i_4a_{10}} r^{a_7a_{10}}_{i_2i_3} t^{a_5a_6}_{i_1i_9} - P_4 P_4 v^{a_7a_8}_{a_9a_{10}} t^{a_6a_{10}}_{i_3i_4} r^{a_5a_9}_{i_1i_2} + P_4 P_4 v^{i_9a_8}_{i_4a'_{10}} \tilde{r}^{a'_{10}a_7}_{i_2i_3} t^{a_5a_6}_{i_1i_9} - P_4 P_4 v^{a_7a_8}_{a'_{10}a_9} \tilde{r}^{a'_{10}a_6}_{i_3i_4} t^{a_5a_9}_{i_1i_2} + P_4 P_4 v^{i_9a_8}_{i_4a'_{10}} \tilde{t}^{a'_{10}a_7}_{i_2i_3} r^{a_5a_6}_{i_1i_9} \\ &-P_4 P_4 v^{a_7a_8}_{a'_{10}a_9} \tilde{t}^{a'_{10}a_6}_{i_3i_4} r^{a_5a_9}_{i_1i_2} - P_4 P_4 v^{a_7a_8}_{a'_9a'_{10}} \tilde{r}^{a'_{10}a_6}_{i_3i_4} \tilde{t}^{a'_9a_5}_{i_1i_2} + P_4 P_4 v^{i_9i_{10}}_{i_4a'_{11}} \tilde{t}^{a'_{11}a_8}_{i_2i_3} t^{a_7}_{i_{10}} r^{a_5a_6}_{i_1i_9} - P_4 P_4 v^{i_9a_8}_{a'_{10}a_{11}} t^{a_{11}}_{i_4} \tilde{t}^{a'_{10}a_7}_{i_2i_3} r^{a_5a_6}_{i_1i_9} + P_4 P_4 v^{i_9a_8}_{a'_{11}a_{10}} \tilde{t}^{a'_{11}a_7}_{i_3i_4} r^{a_6a_{10}}_{i_1i_2} t^{a_5}_{i_9} \\ &+P_4 P_4 v^{i_9a_8}_{a'_{10}a'_{11}} \tilde{r}^{a'_{11}a_7}_{i_3i_4} \tilde{t}^{a'_{10}a_6}_{i_1i_2} t^{a_5}_{i_9} + P_4 P_4 v^{i_9i_{10}}_{i_4a_{11}} t^{a_{11}}_{i_3} t^{a_7a_8}_{i_2i_{10}} r^{a_5a_6}_{i_1i_9} - P_4 P_4 v^{i_9i_{10}}_{i_4a_{11}} t^{a_8a_{11}}_{i_2i_3} t^{a_7}_{i_{10}} r^{a_5a_6}_{i_1i_9} + P_4 P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_{11}}_{i_4} t^{a_7a_{10}}_{i_2i_3} r^{a_5a_6}_{i_1i_9} - P_4 P_4 v^{i_9i_{10}}_{i_4a_{11}} r^{a_8a_{11}}_{i_2i_3} t^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} \\ &+P_4 P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_{11}}_{i_4} r^{a_7a_{10}}_{i_2i_3} t^{a_5a_6}_{i_1i_9} + P_4 P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_7a_{11}}_{i_3i_4} r^{a_6a_{10}}_{i_1i_2} t^{a_5}_{i_9} + P_4 P_4 v^{i_9i_{10}}_{i_4a'_{11}} \tilde{r}^{a'_{11}a_8}_{i_2i_3} t^{a_7}_{i_{10}} t^{a_5a_6}_{i_1i_9} - P_4 P_4 v^{i_9a_8}_{a'_{10}a_{11}} t^{a_{11}}_{i_4} \tilde{t}^{a'_{10}a_7}_{i_2i_3} r^{a_5a_6}_{i_1i_9} + P_4 P_4 v^{i_9a_8}_{a'_{11}a_{10}} \tilde{r}^{a'_{11}a_7}_{i_3i_4} t^{a_6a_{10}}_{i_1i_2} t^{a_5}_{i_9} \\ &-P_4 P_4 v^{i_9i_{11}}_{i_4a_{10}} t^{a_7a_8a_{10}}_{i_2i_3i_{11}} r^{a_5a_6}_{i_1i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9a_8}_{a_{10}a_{11}} t^{a_7a_{10}a_{11}}_{i_2i_3i_4} r^{a_5a_6}_{i_1i_9} - \tfrac{1}{2} P_4 P_4 v^{i_{10}i_{11}}_{i_4a_9} r^{a_7a_8}_{i_{10}i_{11}} t^{a_5a_6a_9}_{i_1i_2i_3} + \tfrac{1}{2} P_4 P_4 v^{i_{10}i_{11}}_{i_4a_9} t^{a_6a_7a_8}_{i_3i_{10}i_{11}} r^{a_5a_9}_{i_1i_2} - P_4 P_4 v^{i_{11}a_8}_{a_9a_{10}} t^{a_6a_7a_{10}}_{i_3i_4i_{11}} r^{a_5a_9}_{i_1i_2} \\ &+P_4 P_4 v^{i_9i_{11}}_{i_4a_{10}} r^{a_8a_{10}}_{i_3i_{11}} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4 P_4 v^{i_{11}a_8}_{a_9a_{10}} t^{a_7a_{10}}_{i_4i_{11}} t^{a_5a_6a_9}_{i_1i_2i_3} - \tfrac{1}{2} P_4 P_4 v^{i_9a_8}_{a_{10}a_{11}} r^{a_{10}a_{11}}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{i_4a'_{11}} \tilde{r}^{a'_{11}a_8}_{i_2i_3} t^{a_5a_6a_7}_{i_1i_9i_{10}} + P_4 P_4 v^{i_{11}a_8}_{a'_9a_{10}} t^{a_6a_7a_{10}}_{i_3i_4i_{11}} \tilde{r}^{a'_9a_5}_{i_1i_2} \\ &-P_4 P_4 v^{i_9i_{11}}_{i_4a'_{10}} \tilde{r}^{a'_{10}a_8}_{i_3i_{11}} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4 P_4 v^{i_{11}a_8}_{a'_{10}a_9} \tilde{r}^{a'_{10}a_7}_{i_4i_{11}} t^{a_5a_6a_9}_{i_1i_2i_3} - \tfrac{1}{2} P_4 P_4 r^{i_{10}i_{11}}_{i_3i_4} V^{i_9a_8}_{i_{10}i_{11}} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4 P_4 v^{i_9i_{10}}_{a'_{11}a_{12}} t^{a_{12}}_{i_4} \tilde{t}^{a'_{11}a_8}_{i_2i_3} t^{a_7}_{i_{10}} r^{a_5a_6}_{i_1i_9} \\ &-\tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a'_{12}a_{11}} \tilde{t}^{a'_{12}a_8}_{i_3i_4} r^{a_7a_{11}}_{i_1i_2} t^{a_6}_{i_{10}} t^{a_5}_{i_9} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a'_{11}a'_{12}} \tilde{r}^{a'_{12}a_8}_{i_3i_4} \tilde{t}^{a'_{11}a_7}_{i_1i_2} t^{a_6}_{i_{10}} t^{a_5}_{i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} t^{a_7}_{i_2i_3i_4} r^{a_5a_6}_{i_1i_9} + P_4 P_4 v^{i_9i_{11}}_{a_{10}a_{12}} t^{a_{12}}_{i_4} t^{a_7a_8a_{10}}_{i_2i_3i_{11}} r^{a_5a_6}_{i_1i_9} \\ &-P_4 P_4 v^{i_9i_{12}}_{a_{10}a_{11}} t^{a_{11}}_{i_{12}} r^{a_8a_{10}}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} + P_4 P_4 v^{i_9i_{12}}_{a_{10}a_{11}} r^{a_8a_{11}}_{i_4i_{12}} t^{a_6a_7a_{10}}_{i_1i_2i_3} t^{a_5}_{i_9} - P_4 P_4 v^{i_9i_{11}}_{a_{10}a_{12}} r^{a_{12}}_{i_4} t^{a_8a_{10}}_{i_3i_{11}} t^{a_5a_6a_7}_{i_1i_2i_9} + \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a_{11}a_{12}} r^{a_{11}a_{12}}_{i_3i_4} t^{a_8}_{i_{10}} t^{a_5a_6a_7}_{i_1i_2i_9} \\ &-P_4 P_4 v^{i_9i_{12}}_{a'_{10}a_{11}} t^{a_7a_8a_{11}}_{i_3i_4i_{12}} \tilde{r}^{a'_{10}a_6}_{i_1i_2} t^{a_5}_{i_9} - \tfrac{1}{2} P_4 P_4 v^{i_9i_{10}}_{a'_{11}a_{12}} t^{a_{12}}_{i_4} \tilde{r}^{a'_{11}a_8}_{i_2i_3} t^{a_5a_6a_7}_{i_1i_9i_{10}} - P_4 P_4 v^{i_9i_{12}}_{a'_{10}a_{11}} t^{a_{11}}_{i_{12}} \tilde{r}^{a'_{10}a_8}_{i_3i_4} t^{a_5a_6a_7}_{i_1i_2i_9} - P_4 P_4 v^{i_9i_{12}}_{a'_{11}a_{10}} \tilde{r}^{a'_{11}a_8}_{i_4i_{12}} t^{a_6a_7a_{10}}_{i_1i_2i_3} t^{a_5}_{i_9}\end{aligned}$$

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TABLE ESI.3.XXXIV: The R_4 amplitude equation of EOM-CCSDTQ-R12 with special intermediates and the RI insertion using the CABS [Part II]

$$
\begin{aligned}
&+P_4P_4v^{i_9i_{11}}_{a'_{10}a_{12}}\,t^{a_{12}}_{i_4}\tilde{r}^{a'_{10}a_8}_{i_3i_{11}}\,t^{a_5a_6a_7}_{i_1i_2i_9} + \tfrac{1}{2}P_4P_4r^{i_{11}i_{12}}_{i_3i_4}V^{i_9i_{10}}_{i_{11}i_{12}}\,t^{a_8}_{i_{10}}\,t^{a_5a_6a_7}_{i_1i_2i_9} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_{12}}_{i_4}\,t^{a_{11}}_{i_3}\,t^{a_7a_8}_{i_2i_{10}}\,r^{a_5a_6}_{i_1i_9} + P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_{12}}_{i_4}\,t^{a_8a_{11}}_{i_2i_3}\,t^{a_7}_{i_{10}}\,r^{a_5a_6}_{i_1i_9}\\
&+P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_{12}}_{i_4}\,r^{a_8a_{11}}_{i_2i_3}\,t^{a_7}_{i_{10}}\,t^{a_5a_6}_{i_1i_9} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_8a_{12}}_{i_3i_4}\,r^{a_7a_{11}}_{i_1i_2}\,t^{a_6}_{i_{10}}\,t^{a_5}_{i_9} - P_4P_4v^{i_9i_{10}}_{a'_{11}a_{12}}\,t^{a_{12}}_{i_4}\tilde{r}^{a'_{11}a_8}_{i_2i_3}\,t^{a_7}_{i_{10}}\,t^{a_5a_6}_{i_1i_9} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a'_{12}a_{11}}\,\tilde{r}^{a'_{12}a_8}_{i_3i_4}\,t^{a_7a_{11}}_{i_1i_2}\,t^{a_6}_{i_{10}}\,t^{a_5}_{i_9}\\
&+P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_8a_{11}}_{i_4i_{12}}\,t^{a_7a_{10}}_{i_2i_3}\,r^{a_5a_6}_{i_1i_9} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_{11}a_{12}}_{i_3i_4}\,t^{a_7a_8}_{i_2i_{10}}\,r^{a_5a_6}_{i_1i_9} - \tfrac{1}{4}P_4P_4v^{i_{11}i_{12}}_{a_9a_{10}}\,r^{a_7a_8}_{i_{11}i_{12}}\,t^{a_6a_{10}}_{i_3i_4}\,t^{a_5a_9}_{i_1i_2} - \tfrac{1}{2}P_4P_4v^{i_{11}i_{12}}_{a_9a_{10}}\,t^{a_7a_8}_{i_{11}i_{12}}\,t^{a_6a_{10}}_{i_3i_4}\,r^{a_5a_9}_{i_1i_2}\\
&+P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_8a_{11}}_{i_4i_{12}}\,r^{a_7a_{10}}_{i_2i_3}\,t^{a_5a_6}_{i_1i_9} + P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,r^{a_8a_{11}}_{i_4i_{12}}\,t^{a_7a_{10}}_{i_2i_3}\,t^{a_5a_6}_{i_1i_9} - \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,r^{a_{11}a_{12}}_{i_3i_4}\,t^{a_7a_8}_{i_2i_{10}}\,t^{a_5a_6}_{i_1i_9} - \tfrac{1}{2}P_4P_4v^{i_{10}i_{11}}_{a'_{12}a_9}\,\tilde{r}^{a'_{12}a_8}_{i_3i_4}\,t^{a_6a_7}_{i_{10}i_{11}}\,t^{a_5a_9}_{i_1i_2}\\
&-P_4P_4v^{i_9i_{12}}_{a'_{10}a_{11}}\,t^{a_8a_{11}}_{i_4i_{12}}\,\tilde{r}^{a'_{10}a_7}_{i_2i_3}\,t^{a_5a_6}_{i_1i_9} + P_4P_4v^{i_9i_{12}}_{a'_{11}a_{10}}\,\tilde{r}^{a'_{11}a_8}_{i_2i_3}\,t^{a_7a_{10}}_{i_1i_9}\,t^{a_5a_6}_{i_1i_9} - \tfrac{1}{4}P_4P_4r^{i_{11}i_{12}}_{i_3i_4}V^{i_9i_{10}}_{i_{11}i_{12}}\,t^{a_7a_8}_{i_2i_{10}}\,t^{a_5a_6}_{i_1i_9} - \tfrac{1}{2}P_4P_4V^{i_9i_{10}}_{i_{11}i_{12}}\,t^{i_{11}i_{12}}_{i_3i_4}\,t^{a_7a_8}_{i_2i_{10}}\,r^{a_5a_6}_{i_1i_9}\\
&+P_4P_4v^{i_9i_{12}}_{a'_{11}a_{10}}\,\tilde{t}^{a'_{11}a_8}_{i_4i_{12}}\,t^{a_7a_{10}}_{i_2i_3}\,r^{a_5a_6}_{i_1i_9} - P_4P_4v^{i_9i_{12}}_{a'_{10}a_{11}}\,t^{a_8a_{11}}_{i_4i_{12}}\,\tilde{t}^{a'_{10}a_7}_{i_2i_3}\,r^{a_5a_6}_{i_1i_9} - \tfrac{1}{2}P_4P_4v^{i_{10}i_{11}}_{a'_{12}a_9}\,\tilde{t}^{a'_{12}a_8}_{i_3i_4}\,r^{a_6a_7}_{i_{10}i_{11}}\,t^{a_5a_9}_{i_1i_2} + P_4P_4v^{i_9i_{12}}_{a'_{11}a_{10}}\,\tilde{r}^{a'_{11}a_8}_{i_4i_{12}}\,r^{a_7a_{10}}_{i_2i_3}\,t^{a_5a_6}_{i_1i_9}\\
&-\tfrac{1}{2}P_4P_4v^{i_{10}i_{11}}_{a'_{12}a_9}\,\tilde{r}^{a'_{12}a_8}_{i_3i_4}\,t^{a_6a_7}_{i_{10}i_{11}}\,r^{a_5a_9}_{i_1i_2} - P_4P_4v^{i_9i_{12}}_{a'_{10}a_{11}}\,r^{a_8a_{11}}_{i_4i_{12}}\,\tilde{t}^{a'_{10}a_7}_{i_2i_3}\,t^{a_5a_6}_{i_1i_9} + P_4P_4v^{i_9i_{12}}_{a'_{10}a'_{11}}\,\tilde{t}^{a'_{11}a_8}_{i_4i_{12}}\,\tilde{r}^{a'_{10}a_7}_{i_2i_3}\,t^{a_5a_6}_{i_1i_9} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a'_{11}a'_{12}}\,\tilde{r}^{a'_{12}a_8}_{i_3i_4}\,\tilde{t}^{a'_{11}a_7}_{i_1i_2}\,t^{a_5a_6}_{i_9i_{10}}\\
&+P_4P_4v^{i_9i_{12}}_{a'_{10}a'_{11}}\,\tilde{r}^{a'_{11}a_8}_{i_4i_{12}}\,\tilde{t}^{a'_{10}a_7}_{i_2i_3}\,t^{a_5a_6}_{i_1i_9} - \tfrac{1}{2}P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_7a_8a_{10}a_{11}}_{i_2i_3i_4i_{12}}\,r^{a_5a_6}_{i_1i_9} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_7a_8a_{11}a_{12}}_{i_1i_2i_3i_4}\,r^{a_5a_6}_{i_9i_{10}} - \tfrac{1}{2}P_4P_4v^{i_{11}i_{12}}_{a_9a_{10}}\,t^{a_6a_7a_8a_{10}}_{i_3i_4i_{11}i_{12}}\,r^{a_5a_9}_{i_1i_2}\\
&+P_4P_4v^{i_{10}i_{12}}_{a_9a_{11}}\,r^{a_8a_{11}}_{i_4i_{12}}\,t^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}} - \tfrac{1}{2}P_4v^{i_{11}i_{12}}_{a_9a_{10}}\,r^{a_8a_{10}}_{i_{11}i_{12}}\,t^{a_5a_6a_7a_9}_{i_1i_2i_3i_4} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,r^{a_{11}a_{12}}_{i_3i_4}\,t^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} - \tfrac{1}{2}P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,r^{a_{10}a_{11}}_{i_4i_{12}}\,t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} + \tfrac{1}{2}P_4P_4v^{i_{11}i_{12}}_{a'_9a_{10}}\,t^{a_6a_7a_8a_{10}}_{i_3i_4i_{11}i_{12}}\,\tilde{r}^{a'_9a_5}_{i_1i_2}\\
&+P_4P_4v^{i_{10}i_{12}}_{a'_{11}a_9}\,\tilde{r}^{a'_{11}a_8}_{i_4i_{12}}\,t^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}} - \tfrac{1}{2}P_4v^{i_{11}i_{12}}_{a'_{10}a_9}\,\tilde{r}^{a'_{10}a_8}_{i_{11}i_{12}}\,t^{a_5a_6a_7a_9}_{i_1i_2i_3i_4} + \tfrac{1}{4}P_4r^{i_{11}i_{12}}_{i_3i_4}V^{i_9i_{10}}_{i_{11}i_{12}}\,t^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} - \tfrac{1}{2}P_4r^{i_{11}i_{12}}_{i_4i_{10}}V^{i_9i_{10}}_{i_{11}i_{12}}\,t^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} + P_4P_4v^{i_9i_{12}}_{a'_{10}a'_{11}}\,\tilde{t}^{a'_{11}a_8}_{i_4i_{12}}\,\tilde{t}^{a'_{10}a_7}_{i_2i_3}\,r^{a_5a_6}_{i_1i_9}\\
&-\tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{a'_{11}a'_{12}}\,\tilde{t}^{a'_{12}a_8}_{i_3i_4}\,\tilde{t}^{a'_{11}a_7}_{i_1i_2}\,r^{a_5a_6}_{i_9i_{10}} - P_4P_4v^{i_9a_8}_{i_3i_4}\,r^{a_5a_6a_7}_{i_1i_2i_9} - P_4P_4v^{a_7a_8}_{i_4a_9}\,r^{a_5a_6a_9}_{i_1i_2i_3} + P_4P_4v^{i_9i_{10}}_{i_3i_4}\,t^{a_8}_{i_{10}}\,r^{a_5a_6a_7}_{i_1i_2i_9} + P_4P_4v^{i_9a_8}_{i_4a_{10}}\,t^{a_{10}}_{i_3}\,r^{a_5a_6a_7}_{i_1i_2i_9} + P_4P_4v^{i_9a_8}_{i_4a_{10}}\,r^{a_6a_7a_{10}}_{i_1i_2i_3}\,t^{a_5}_{i_9}\\
&+P_4P_4v^{a_7a_8}_{a_9a_{10}}\,t^{a_{10}}_{i_4}\,r^{a_5a_6a_9}_{i_1i_2i_3} - P_4P_4v^{i_9i_{10}}_{i_4a_{11}}\,t^{a_{11}}_{i_3}\,t^{a_8}_{i_{10}}\,r^{a_5a_6a_7}_{i_1i_2i_9} - \tfrac{1}{2}P_4P_4v^{i_9a_8}_{a_{10}a_{11}}\,t^{a_{11}}_{i_4}\,t^{a_{10}}_{i_3}\,r^{a_5a_6a_7}_{i_1i_2i_9} - \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{i_4a_{11}}\,r^{a_7a_8a_{11}}_{i_1i_2i_3}\,t^{a_6}_{i_{10}}\,t^{a_5}_{i_9} - P_4P_4v^{i_9a_8}_{a_{10}a_{11}}\,t^{a_{11}}_{i_4}\,r^{a_6a_7a_{10}}_{i_1i_2i_3}\,t^{a_5}_{i_9}\\
&+P_4P_4v^{i_9i_{11}}_{i_4a_{10}}\,t^{a_8a_{10}}_{i_3i_{11}}\,r^{a_5a_6a_7}_{i_1i_2i_9} - \tfrac{1}{2}P_4P_4v^{i_9a_8}_{a_{10}a_{11}}\,t^{a_{10}a_{11}}_{i_3i_4}\,r^{a_5a_6a_7}_{i_1i_2i_9} + \tfrac{1}{2}P_4P_4v^{i_{10}i_{11}}_{i_4a_9}\,r^{a_6a_7a_8}_{i_3i_{10}i_{11}}\,t^{a_5a_9}_{i_1i_2} - \tfrac{1}{2}P_4P_4v^{i_{10}i_{11}}_{i_4a_9}\,t^{a_7a_8}_{i_{10}i_{11}}\,r^{a_5a_6a_9}_{i_1i_2i_3} + P_4P_4v^{i_{11}a_8}_{a_9a_{10}}\,t^{a_7a_{10}}_{i_4i_{11}}\,r^{a_5a_6a_9}_{i_1i_2i_3}\\
&-P_4P_4v^{i_9i_{11}}_{i_4a_{10}}\,r^{a_7a_8a_{10}}_{i_2i_3i_{11}}\,t^{a_5a_6}_{i_1i_9} - P_4P_4v^{i_{11}a_8}_{a_9a_{10}}\,r^{a_6a_7a_{10}}_{i_3i_4i_{11}}\,t^{a_5a_9}_{i_1i_2} + \tfrac{1}{2}P_4P_4v^{i_9a_8}_{a_{10}a_{11}}\,r^{a_7a_{10}a_{11}}_{i_2i_3i_4}\,t^{a_5a_6}_{i_1i_9} - P_4P_4v^{i_9i_{11}}_{i_4a'_{10}}\,\tilde{t}^{a'_{10}a_8}_{i_3i_{11}}\,r^{a_5a_6a_7}_{i_1i_2i_9} - \tfrac{1}{2}P_4P_4V^{i_9a_8}_{i_{10}i_{11}}\,t^{i_{10}i_{11}}_{i_3i_4}\,r^{a_5a_6a_7}_{i_1i_2i_9}\\
&+\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{i_4a'_{11}}\,\tilde{t}^{a'_{11}a_8}_{i_2i_3}\,r^{a_5a_6a_7}_{i_1i_9i_{10}} + P_4P_4v^{i_{11}a_8}_{a'_{10}a_9}\,\tilde{t}^{a'_{10}a_7}_{i_4i_{11}}\,r^{a_5a_6a_9}_{i_1i_2i_3} + P_4P_4v^{i_{11}a_8}_{a'_9a_{10}}\,r^{a_6a_7a_{10}}_{i_3i_4i_{11}}\,\tilde{t}^{a'_9a_5}_{i_1i_2} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_{12}}_{i_4}\,t^{a_{11}}_{i_3}\,t^{a_8}_{i_{10}}\,r^{a_5a_6a_7}_{i_1i_2i_9}\\
&+\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_{12}}_{i_4}\,r^{a_7a_8a_{11}}_{i_1i_2i_3}\,t^{a_6}_{i_{10}}\,t^{a_5}_{i_9} + \tfrac{1}{2}P_4P_4V^{i_9i_{10}}_{i_{11}i_{12}}\,t^{i_{11}i_{12}}_{i_3i_4}\,t^{a_8}_{i_{10}}\,r^{a_5a_6a_7}_{i_1i_2i_9} + P_4P_4v^{i_9i_{11}}_{a'_{10}a_{12}}\,t^{a_{12}}_{i_4}\,\tilde{t}^{a'_{10}a_8}_{i_3i_{11}}\,r^{a_5a_6a_7}_{i_1i_2i_9} - P_4P_4v^{i_9i_{12}}_{a'_{10}a_{11}}\,t^{a_{11}}_{i_{12}}\,\tilde{t}^{a'_{10}a_8}_{i_3i_4}\,r^{a_5a_6a_7}_{i_1i_2i_9}\\
&-\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a'_{11}a_{12}}\,t^{a_{12}}_{i_4}\,\tilde{t}^{a'_{11}a_8}_{i_2i_3}\,r^{a_5a_6a_7}_{i_1i_9i_{10}} - P_4P_4v^{i_9i_{12}}_{a'_{11}a_{10}}\,\tilde{t}^{a'_{11}a_8}_{i_4i_{12}}\,r^{a_6a_7a_{10}}_{i_1i_2i_3}\,t^{a_5}_{i_9} - P_4P_4v^{i_9i_{12}}_{a'_{10}a_{11}}\,r^{a_7a_8a_{11}}_{i_3i_4i_{12}}\,\tilde{t}^{a'_{10}a_6}_{i_9}\,t^{a_5}_{i_9} + P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_{10}a_{11}}_{i_{12}}\,t^{a_{12}}_{i_3}\,r^{a_5a_6a_7}_{i_1i_2i_9}\\
&-P_4P_4v^{i_9i_{11}}_{a_{10}a_{12}}\,t^{a_{12}}_{i_4}\,t^{a_8a_{10}}_{i_3i_{11}}\,r^{a_5a_6a_7}_{i_1i_2i_9} + \tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{i_{11}i_{12}}_{i_3i_4}\,t^{a_8}_{i_{10}}\,r^{a_5a_6a_7}_{i_1i_2i_9} - \tfrac{1}{2}P_4P_4v^{i_{10}i_{11}}_{a_9a_{12}}\,t^{a_{12}}_{i_4}\,r^{a_6a_7a_8}_{i_3i_{10}i_{11}}\,t^{a_5a_9}_{i_1i_2} - P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_{10}a_{11}}_{i_{12}}\,t^{a_{11}a_{12}}_{i_3i_4}\,r^{a_5a_6a_9}_{i_1i_9}\\
&+\tfrac{1}{2}P_4P_4v^{i_{10}i_{11}}_{a_9a_{12}}\,t^{a_{12}}_{i_4}\,t^{a_7a_8}_{i_{10}i_{11}}\,r^{a_5a_6a_9}_{i_1i_2i_3} - P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_8a_{11}}_{i_4i_{12}}\,r^{a_6a_7a_{10}}_{i_1i_2i_3}\,t^{a_5}_{i_9} + P_4P_4v^{i_9i_{11}}_{a_{10}a_{12}}\,t^{a_{12}}_{i_4}\,r^{a_7a_8a_{10}}_{i_2i_3i_{11}}\,t^{a_5a_6}_{i_1i_9} + P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,r^{a_7a_8a_{11}}_{i_3i_4i_{12}}\,t^{a_6a_{10}}_{i_{11}i_{12}}\,t^{a_5}_{i_9}\\
&+\tfrac{1}{2}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,r^{a_8a_{11}a_{12}}_{i_2i_3i_4}\,t^{a_7}_{i_{10}}\,t^{a_5a_6}_{i_1i_9} + \tfrac{1}{2}P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_8a_{10}a_{11}}_{i_3i_4i_{12}}\,r^{a_5a_6a_9}_{i_1i_2i_9} + \tfrac{1}{4}P_4P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_8a_{11}a_{12}}_{i_3i_4}\,r^{a_5a_6a_7}_{i_1i_9i_{10}} + \tfrac{1}{2}P_4P_4v^{i_{11}i_{12}}_{a_9a_{10}}\,t^{a_7a_8a_{10}}_{i_4i_{11}i_{12}}\,r^{a_5a_6a_9}_{i_1i_2i_3}\\
&+P_4P_4v^{i_{10}i_{12}}_{a_9a_{11}}\,t^{a_7a_8a_{11}}_{i_3i_4i_{12}}\,r^{a_5a_6a_9}_{i_1i_2i_{10}} + \tfrac{1}{2}P_4P_4v^{i_{11}i_{12}}_{a_9a_{10}}\,r^{a_7a_8a_{10}}_{i_4i_{11}i_{12}}\,t^{a_5a_6}_{i_1i_2i_3} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,r^{a_{11}a_{12}}_{i_2i_3i_4}\,t^{a_5a_6a_7}_{i_1i_9i_{10}} + \tfrac{1}{2}P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,r^{a_{10}a_{11}}_{i_3i_4i_{12}}\,t^{a_5a_6a_7a_8}_{i_1i_2i_9} + \tfrac{1}{2}P_4v^{i_9i_{10}}_{i_3i_4}\,r^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}}\\
&-P_4P_4v^{i_{10}a_8}_{i_4a_9}\,r^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}} + \tfrac{1}{2}P_4v^{a_7a_8}_{a_9a_{10}}\,r^{a_5a_6a_9a_{10}}_{i_1i_2i_3i_4} - P_4v^{i_9i_{11}}_{i_4a_{10}}\,t^{a_{10}}_{i_{11}}\,r^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} - \tfrac{1}{2}P_4v^{i_9i_{10}}_{i_4a_{11}}\,t^{a_{11}}_{i_3}\,r^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} - P_4v^{i_{11}a_8}_{a_9a_{10}}\,t^{a_{10}}_{i_{11}}\,r^{a_5a_6a_7a_9}_{i_1i_2i_3i_4} + P_4P_4v^{i_9i_{11}}_{i_4a_{10}}\,r^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_{11}}\,t^{a_5}_{i_9}\\
&+P_4P_4v^{i_{10}a_8}_{a_9a_{11}}\,t^{a_{11}}_{i_4}\,r^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}} - \tfrac{1}{2}P_4v^{i_9a_8}_{a_{10}a_{11}}\,r^{a_6a_7a_{10}a_{11}}_{i_1i_2i_3i_4}\,t^{a_{12}}_{i_{10}}\,t^{a_5}_{i_9} - \tfrac{1}{2}P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_{10}a_{11}}_{i_4i_{12}}\,r^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_{12}}_{i_4}\,t^{a_{11}}_{i_3}\,r^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} + P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_{11}}_{i_{12}}\,r^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_4}\,t^{a_5}_{i_9}\\
&-P_4P_4v^{i_9i_{11}}_{a_{10}a_{12}}\,t^{a_{12}}_{i_4}\,r^{a_6a_7a_8a_{10}}_{i_1i_2i_3i_{11}}\,t^{a_5}_{i_9} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,r^{a_7a_8a_{11}a_{12}}_{i_1i_2i_3i_4}\,t^{a_6}_{i_{10}}\,t^{a_5}_{i_9} - \tfrac{1}{2}P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_{10}a_{11}}_{i_4i_{12}}\,r^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,t^{a_{11}a_{12}}_{i_3i_4}\,r^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} - \tfrac{1}{2}P_4v^{i_{11}i_{12}}_{a_9a_{10}}\,t^{a_8a_{11}}_{i_1i_{11}i_{12}}\,r^{a_5a_6a_7a_9}_{i_1i_2i_3i_4}\\
&+P_4P_4v^{i_9i_{12}}_{a_9a_{11}}\,t^{a_8a_{11}}_{i_4i_{12}}\,r^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}} - \tfrac{1}{2}P_4P_4v^{i_{11}i_{12}}_{a_9a_{10}}\,r^{a_6a_7a_8a_{10}}_{i_3i_4i_{11}i_{12}}\,t^{a_5a_9}_{i_1i_2} + \tfrac{1}{4}P_4v^{i_9i_{10}}_{a_{11}a_{12}}\,r^{a_7a_8a_{11}a_{12}}_{i_3i_4i_{11}i_{12}}\,t^{a_5a_6}_{i_9i_{10}} - \tfrac{1}{2}P_4P_4v^{i_9i_{12}}_{a_{10}a_{11}}\,t^{a_7a_8a_{10}a_{11}}_{i_2i_3i_4i_{12}}\,t^{a_5a_6}_{i_1i_9}\\
&-\tfrac{1}{2}P_4V^{i_9i_{12}}_{i_{10}i_{11}}\,t^{i_{10}i_{11}}_{i_4i_{12}}\,r^{a_5a_6a_7a_8}_{i_1i_2i_3i_9} + \tfrac{1}{4}P_4V^{i_9i_{10}}_{i_{11}i_{12}}\,t^{i_{11}i_{12}}_{i_3i_4}\,r^{a_5a_6a_7a_8}_{i_1i_2i_9i_{10}} - \tfrac{1}{2}P_4v^{i_{11}i_{12}}_{a'_{10}a_9}\,\tilde{t}^{a'_{10}a_8}_{i_{11}i_{12}}\,r^{a_5a_6a_7a_9}_{i_1i_2i_3i_4} + P_4P_4v^{i_{10}i_{12}}_{a'_{11}a_9}\,\tilde{t}^{a'_{11}a_8}_{i_4i_{12}}\,r^{a_5a_6a_7a_9}_{i_1i_2i_3i_{10}} + \tfrac{1}{2}P_4P_4v^{i_{11}i_{12}}_{a'_9a_{10}}\,r^{a_6a_7a_8a_{10}}_{i_3i_4i_{11}i_{12}}\,\tilde{t}^{a'_9a_5}_{i_1i_2}
\end{aligned}
$$

Supplementary data for Phys. Chem. Chem. Phys.

4. THE COMPUTATIONAL SEQUENCE AND INTERMEDIATES

A. CCSD-R12

TABLE ESI.4.I: The computational sequence and intermediates for the energy equation of CCSD-R12 and higher-order CC-R12

$$(\xi_0)^{i_2}_{a_1} = +f^{i_2}_{a_1} + \tfrac{1}{2} t^{a_3}_{i_4} v^{i_2 i_4}_{a_1 a_3} \qquad \mathrm{e} = +t^{a_1}_{i_2} (\xi_0)^{i_2}_{a_1} + \tfrac{1}{4} t^{a_1 a_2}_{i_3 i_4} v^{i_3 i_4}_{a_1 a_2} + \tfrac{1}{4} t^{i_1 i_2}_{i_3 i_4} V^{i_3 i_4}_{i_1 i_2}$$

TABLE ESI.4.II: The computational sequence and intermediates for the T_1 amplitude equation of CCSD-R12

$$(\Xi_0)^{i_4}_{a_3} = +t^{a_5}_{i_6} v^{i_4 i_6}_{a_3 a_5}$$
$$(\xi_7)^{i_4 i_5}_{i_1 a'_3} = +v^{i_4 i_5}_{i_1 a'_3} - t^{a_6}_{i_1} v^{i_4 i_5}_{a'_3 a_6}$$
$$(\xi_5)^{i_4 i_5}_{i_1 a_3} = -v^{i_4 i_5}_{i_1 a_3} + t^{a_6}_{i_1} v^{i_4 i_5}_{a_3 a_6}$$
$$(\xi_3)^{i_4}_{a'_3} = -f^{i_4}_{a'_3} - t^{a_5}_{i_6} v^{i_4 i_6}_{a'_3 a_5}$$
$$(\xi_2)^{i_4}_{a_3} = +f^{i_4}_{a_3} + (\Xi_0)^{i_4}_{a_3}$$
$$(\xi_1)^{a_2}_{a_3} = +f^{a_2}_{a_3} - t^{a_4}_{i_5} v^{i_5 a_2}_{a_3 a_4}$$
$$(\xi_{0,0})^{i_3}_{a_4} = -f^{i_3}_{a_4} - (\Xi_0)^{i_3}_{a_4}$$
$$(\xi_0)^{i_3}_{i_1} = -f^{i_3}_{i_1} + t^{a_4}_{i_1} (\xi_{0,0})^{i_3}_{a_4} - t^{a_4}_{i_5} v^{i_3 i_5}_{i_1 a_4} - \tfrac{1}{2} t^{a_4 a_5}_{i_1 i_6} v^{i_3 i_6}_{a_4 a_5} - \tfrac{1}{2} t^{i_4 i_5}_{i_1 i_6} V^{i_3 i_6}_{i_4 i_5}$$
$$\delta^{a_2}_{i_1} = +f^{a_2}_{i_1} + t^{a_2}_{i_3} (\xi_0)^{i_3}_{i_1} + t^{a_3}_{i_1} (\xi_1)^{a_2}_{a_3} + t^{a_2 a_3}_{i_1 i_4} (\xi_2)^{i_4}_{a_3} + \tilde{t}^{a'_3 a_2}_{i_1 i_4} (\xi_3)^{i_4}_{a'_3} - t^{a_3}_{i_4} v^{i_4 a_2}_{i_1 a_3}$$
$$+ \tfrac{1}{2} t^{a_2 a_3}_{i_4 i_5} (\xi_5)^{i_4 i_5}_{i_1 a_3} - \tfrac{1}{2} t^{a_3 a_4}_{i_1 i_5} v^{i_5 a_2}_{a_3 a_4} + \tfrac{1}{2} \tilde{t}^{a'_3 a_2}_{i_4 i_5} (\xi_7)^{i_4 i_5}_{i_1 a'_3} - \tfrac{1}{2} t^{i_3 i_4}_{i_1 i_5} V^{i_5 a_2}_{i_3 i_4}$$

TABLE ESI.4.III: The computational sequence and intermediates for the T_2 amplitude equation of CCSD-R12

$$(\Xi_0)^{i_5 i_6}_{i_1 i_2} = +P_2 t^{a_7}_{i_1} v^{i_5 i_6}_{i_2 a_7}$$
$$(\Xi_1)^{i_6 a_4}_{i_2 a_5} = +t^{a_7}_{i_2} v^{i_6 a_4}_{a_5 a_7}$$
$$(\Xi_2)^{i_5 i_7}_{i_2 a_6} = +t^{a_8}_{i_2} v^{i_5 i_7}_{a_6 a_8}$$
$$(\Xi_3)^{i_5 i_6}_{i_1 i_2} = +\tfrac{1}{2} t^{i_7 i_8}_{i_1 i_2} V^{i_5 i_6}_{i_7 i_8}$$
$$(\Xi_4)^{i_5 i_6}_{i_1 i_2} = +\tfrac{1}{2} t^{a_7 a_8}_{i_1 i_2} v^{i_5 i_6}_{a_7 a_8}$$
$$(\Xi_5)^{i_5}_{a_6} = +t^{a_7}_{i_8} v^{i_5 i_8}_{a_6 a_7}$$
$$(\Xi_6)^{i_5 i_6}_{i_1 i_2} = +P_2 t^{a_7}_{i_1} (\Xi_2)^{i_5 i_6}_{i_2 a_7}$$
$$(\xi_8)^{i_6 a_4}_{i_2 a'_5} = +v^{i_6 a_4}_{i_2 a'_5} - t^{a_7}_{i_2} v^{i_6 a_4}_{a'_5 a_7} + \tfrac{1}{2} \tilde{t}^{a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_5 a'_7}$$
$$(\xi_6)^{i_6 a_4}_{i_2 a_5} = -v^{i_6 a_4}_{i_2 a_5} + (\Xi_1)^{i_6 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_4 a_7}_{i_2 i_8} v^{i_6 i_8}_{a_5 a_7} + \tilde{t}^{a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_7 a_5}$$
$$(\xi_5)^{i_5 i_6}_{i_1 i_2} = +v^{i_5 i_6}_{i_1 i_2} - (\Xi_0)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} (\Xi_6)^{i_5 i_6}_{i_1 i_2} + (\Xi_4)^{i_5 i_6}_{i_1 i_2} + (\Xi_3)^{i_5 i_6}_{i_1 i_2}$$
$$(\xi_4)^{a_3 a_4}_{i_2 a_5} = -v^{a_3 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_6}_{i_2} v^{a_3 a_4}_{a_5 a_6}$$
$$(\xi_{3,6})^{i_5 i_7}_{i_2 a_6} = +v^{i_5 i_7}_{i_2 a_6} - (\Xi_2)^{i_5 i_7}_{i_2 a_6}$$
$$(\xi_{3,4})^{i_5 i_7}_{i_2 a'_6} = -v^{i_5 i_7}_{i_2 a'_6} + t^{a_8}_{i_2} v^{i_5 i_7}_{a'_6 a_8}$$
$$(\xi_{3,3})^{i_5 a_4}_{i_2 a_6} = +v^{i_5 a_4}_{i_2 a_6} - \tfrac{1}{2} (\Xi_1)^{i_5 a_4}_{i_2 a_6}$$
$$(\xi_{3,2})^{i_5 i_6}_{i_1 i_2} = +v^{i_5 i_6}_{i_1 i_2} - (\Xi_0)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} (\Xi_6)^{i_5 i_6}_{i_1 i_2} + (\Xi_3)^{i_5 i_6}_{i_1 i_2} + (\Xi_4)^{i_5 i_6}_{i_1 i_2}$$
$$(\xi_{3,1})^{i_5}_{a_6} = +f^{i_5}_{a_6} + (\Xi_5)^{i_5}_{a_6}$$
$$(\xi_{3,0})^{i_5}_{a'_6} = -f^{i_5}_{a'_6} - t^{a_7}_{i_8} v^{i_5 i_8}_{a'_6 a_7}$$
$$(\xi_3)^{i_5 a_4}_{i_1 i_2} = -v^{i_5 a_4}_{i_1 i_2} + \tilde{t}^{a'_6 a_4}_{i_1 i_2} (\xi_{3,0})^{i_5}_{a'_6} + t^{a_4 a_6}_{i_1 i_2} (\xi_{3,1})^{i_5}_{a_6} + \tfrac{1}{2} t^{a_4}_{i_6} (\xi_{3,2})^{i_5 i_6}_{i_1 i_2}$$
$$+ P_2 t^{a_6}_{i_1} (\xi_{3,3})^{i_5 a_4}_{i_2 a_6} + P_2 \tilde{t}^{a'_6 a_4}_{i_1 i_7} (\xi_{3,4})^{i_5 i_7}_{i_2 a'_6} - \tfrac{1}{2} t^{i_6 i_7}_{i_1 i_2} V^{i_5 a_4}_{i_6 i_7}$$
$$+ P_2 t^{a_4 a_6}_{i_1 i_7} (\xi_{3,6})^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_1 i_2} v^{i_5 a_4}_{a_6 a_7}$$
$$(\xi_2)^{a_4}_{a'_5} = -f^{a_4}_{a'_5} + t^{a_6}_{i_7} v^{i_7 a_4}_{a'_5 a_6} + \tfrac{1}{2} t^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a'_6}$$
$$(\xi_1)^{a_4}_{a_5} = +f^{a_4}_{a_5} - t^{a_6}_{i_7} v^{i_7 a_4}_{a_5 a_6} - \tfrac{1}{2} t^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_5 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_5}$$
$$(\xi_{0,0})^{i_5}_{a_6} = -f^{i_5}_{a_6} - (\Xi_5)^{i_5}_{a_6}$$
$$(\xi_0)^{i_5}_{i_2} = -f^{i_5}_{i_2} + t^{a_6}_{i_2} (\xi_{0,0})^{i_5}_{a_6} - t^{a_6}_{i_7} v^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_2 i_8} v^{i_5 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_2 i_8} V^{i_5 i_8}_{i_6 i_7}$$
$$\delta^{a_3 a_4}_{i_1 i_2} = +v^{a_3 a_4}_{i_1 i_2} + P_2 t^{a_3 a_4}_{i_1 i_5} (\xi_0)^{i_5}_{i_2} + P_2 t^{a_3 a_5}_{i_1 i_2} (\xi_1)^{a_4}_{a_5} + P_2 \tilde{t}^{a'_5 a_3}_{i_1 i_2} (\xi_2)^{a_4}_{a'_5}$$
$$+ P_2 t^{a_3}_{i_5} (\xi_3)^{i_5 a_4}_{i_1 i_2} + P_2 t^{a_5}_{i_1} (\xi_4)^{a_3 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_3 a_4}_{i_5 i_6} (\xi_5)^{i_5 i_6}_{i_1 i_2}$$
$$+ P_2 P_2 t^{a_3 a_5}_{i_1 i_6} (\xi_6)^{i_6 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_5 a_6}_{i_1 i_2} v^{a_3 a_4}_{a_5 a_6} + P_2 P_2 \tilde{t}^{a'_5 a_3}_{i_1 i_6} (\xi_8)^{i_6 a_4}_{i_2 a'_5}$$
$$+ \tfrac{1}{2} t^{i_5 i_6}_{i_1 i_2} V^{a_3 a_4}_{i_5 i_6}$$

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TABLE ESI.4.IV: The computational sequence and intermediates for the geminal t amplitude equation of CCSD-R12

$$(\Xi_0)^{i_3i_4}_{i_7a'_8} = +t^{a_9}_{i_7} F^{i_3i_4*}_{a'_8a_9}$$
$$(\Xi_1)^{i_8a'_6}_{i_2a_7} = +t^{a_9}_{i_2} v^{i_8a'_6}_{a_7a_9}$$
$$(\Xi_2)^{a'_7}_{a_6} = +t^{a_8}_{i_9} v^{i_9a'_7}_{a_6a_8}$$
$$(\Xi_3)^{a'_5}_{a'_7} = +t^{a_8}_{i_9} v^{i_9a'_5}_{a'_7a_8}$$
$$(\Xi_4)^{i_8a'_5}_{i_2a'_7} = +t^{a_9}_{i_2} v^{i_8a'_5}_{a'_7a_9}$$
$$(\Xi_5)^{i_7}_{a_8} = +t^{a_9}_{i_{10}} v^{i_7i_{10}}_{a_8a_9}$$
$$(\Xi_6)^{i_7i_9}_{i_2a_8} = +t^{a_{10}}_{i_2} v^{i_7i_9}_{a_8a_{10}}$$
$$(\Xi_7)^{i_8a'_6}_{i_2a_7} = +\tilde{t}^{a'_6a'_9}_{i_2i_{10}} v^{i_8i_{10}}_{a'_9a_7}$$
$$(\Xi_8)^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{t}^{a'_7a'_8}_{i_9i_{10}} v^{i_9i_{10}}_{a'_8a_6}$$
$$(\Xi_9)^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{t}^{a'_7a_8}_{i_9i_{10}} v^{i_9i_{10}}_{a_6a_8}$$
$$(\Xi_{10})^{a'_5}_{a'_7} = +\tfrac{1}{2}\tilde{t}^{a'_5a'_8}_{i_9i_{10}} v^{i_9i_{10}}_{a'_7a'_8}$$
$$(\Xi_{11})^{a'_5}_{a'_7} = +\tfrac{1}{2}\tilde{t}^{a'_5a_8}_{i_9i_{10}} v^{i_9i_{10}}_{a'_7a_8}$$
$$(\xi_{8,2})^{a'_6}_{a'_7} = -(\Xi_3)^{a'_6}_{a'_7} - (\Xi_{10})^{a'_6}_{a'_7} - (\Xi_{11})^{a'_6}_{a'_7}$$
$$(\xi_{8,1})^{i_8a'_6}_{i_2a'_7} = -v^{i_8a'_6}_{i_2a'_7} + (\Xi_1)^{i_8a'_6}_{i_2a'_7} - (\Xi_7)^{i_8a'_6}_{i_2a'_7} + \tfrac{1}{2}\tilde{t}^{a'_6a_9}_{i_2i_{10}} v^{i_8i_{10}}_{a_7a_9}$$
$$(\xi_{8,0})^{i_8a'_6}_{i_2a'_7} = -v^{i_8a'_6}_{i_2a'_7} + (\Xi_4)^{i_8a'_6}_{i_2a'_7} + \tfrac{1}{2}\tilde{t}^{a'_6a'_9}_{i_2i_{10}} v^{i_8i_{10}}_{a'_7a'_9}$$
$$(\xi_8)^{a'_5a'_6}_{i_1i_2} = +P_2P_2\tilde{t}^{a'_5a'_7}_{i_1i_8}(\xi_{8,0})^{i_8a'_6}_{i_2a'_7} + P_2P_2\tilde{t}^{a'_5a_7}_{i_1i_8}(\xi_{8,1})^{i_8a'_6}_{i_2a_7} + P_2\tilde{t}^{a'_5a'_7}_{i_1i_2}(\xi_{8,2})^{a'_6}_{a'_7}$$
$$(\xi_7)^{i_3i_4}_{i_5i_6} = +\tfrac{1}{2}t^{i_7i_8}_{i_5i_6} X^{i_3i_4}_{i_7i_8}$$
$$(\xi_6)^{i_3i_4}_{i_2a_5} = -(V^\dagger)^{i_3i_4}_{i_2a_5} - v^{i_6a'_7}_{i_2a_5}(\Xi_0)^{i_3i_4}_{i_6a'_7} + \tfrac{1}{2}t^{a_6}_{i_2}(V^\dagger)^{i_3i_4}_{a_5a_6}$$
$$(\xi_{4,1})^{a'_7}_{a_6} = -(\Xi_2)^{a'_7}_{a_6} + (\Xi_8)^{a'_7}_{a_6} - (\Xi_9)^{a'_7}_{a_6}$$
$$(\xi_4)^{i_3i_4}_{a'_5a_6} = -f^{i_7}_{a_6}(\Xi_0)^{i_3i_4}_{i_7a'_5} + F^{i_3i_4*}_{a'_5a'_7}(\xi_{4,1})^{a'_7}_{a_6}$$
$$(\xi_{3,7})^{a_6}_{a'_7} = -t^{a_8}_{i_9} v^{i_9a_6}_{a_7a_8} - \tfrac{1}{2}t^{a_6a_8}_{i_9i_{10}} v^{i_9i_{10}}_{a_7a_8} - \tfrac{1}{2}\tilde{t}^{a'_8a_6}_{i_9i_{10}} v^{i_9i_{10}}_{a'_8a_7}$$
$$(\xi_{3,6})^{a'_5}_{a'_7} = -(\Xi_3)^{a'_5}_{a'_7} - (\Xi_{10})^{a'_5}_{a'_7} - (\Xi_{11})^{a'_5}_{a'_7}$$
$$(\xi_{3,5})^{a_6}_{a'_7} = -t^{a_8}_{i_9} v^{i_9a_6}_{a'_7a_8} - \tfrac{1}{2}t^{a_6a_8}_{i_9i_{10}} v^{i_9i_{10}}_{a'_7a_8} + \tfrac{1}{2}\tilde{t}^{a'_8a_6}_{i_9i_{10}} v^{i_9i_{10}}_{a'_7a'_8}$$
$$(\xi_{3,4})^{i_8a_6}_{i_2a_7} = -v^{i_8a_6}_{i_2a_7} + t^{a_9}_{i_2} v^{i_8a_6}_{a_7a_9} + t^{a_6a_9}_{i_2i_{10}} v^{i_8i_{10}}_{a_7a_9} + \tilde{t}^{a'_9a_6}_{i_2i_{10}} v^{i_8i_{10}}_{a'_9a_7}$$
$$(\xi_{3,3})^{i_8a'_5}_{i_2a'_7} = -v^{i_8a'_5}_{i_2a'_7} + (\Xi_4)^{i_8a'_5}_{i_2a'_7}$$
$$(\xi_{3,2})^{i_8a_6}_{i_2a'_7} = -v^{i_8a_6}_{i_2a'_7} + t^{a_9}_{i_2} v^{i_8a_6}_{a'_7a_9} - \tilde{t}^{a'_9a_6}_{i_2i_{10}} v^{i_8i_{10}}_{a'_7a'_9}$$
$$(\xi_{3,1})^{i_8a'_5}_{i_2a_7} = +v^{i_8a'_5}_{i_2a_7} - (\Xi_1)^{i_8a'_5}_{i_2a_7} + (\Xi_7)^{i_8a'_5}_{i_2a_7}$$
$$(\xi_{3,0,3})^{i_7i_9}_{i_2a_8} = -v^{i_7i_9}_{i_2a_8} + (\Xi_6)^{i_7i_9}_{i_2a_8}$$
$$(\xi_{3,0,2})^{i_7i_9}_{i_2a'_8} = -v^{i_7i_9}_{i_2a'_8} + t^{a_{10}}_{i_2} v^{i_7i_9}_{a'_8a_{10}}$$
$$(\xi_{3,0,0})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - t^{a_9}_{i_{10}} v^{i_7i_{10}}_{a'_8a_9}$$
$$(\xi_{3,0})^{i_7a'_5}_{i_1i_2} = +\tilde{t}^{a'_5a'_8}_{i_1i_2}(\xi_{3,0,0})^{i_7}_{a'_8} + \tfrac{1}{2}P_2t^{a_8}_{i_1}(\Xi_1)^{i_7a'_5}_{i_2a_8} + P_2\tilde{t}^{a'_5a'_8}_{i_1i_9}(\xi_{3,0,2})^{i_7i_9}_{i_2a'_8} + P_2\tilde{t}^{a'_5a_8}_{i_1i_9}(\xi_{3,0,3})^{i_7i_9}_{i_2a_8} - \tilde{t}^{a'_5a_8}_{i_1i_2}(\Xi_5)^{i_7}_{a_8}$$
$$(\xi_3)^{a'_5a_6}_{i_1i_2} = +t^{a_6}_{i_7}(\xi_{3,0})^{i_7a'_5}_{i_1i_2} + P_2t^{a_6a_7}_{i_1i_8}(\xi_{3,1})^{i_8a'_5}_{i_2a_7} + P_2\tilde{t}^{a'_5a'_7}_{i_1i_8}(\xi_{3,2})^{i_8a_6}_{i_2a'_7} + P_2\tilde{t}^{a'_7a_6}_{i_1i_8}(\xi_{3,3})^{i_8a'_5}_{i_2a'_7} + P_2\tilde{t}^{a'_5a_7}_{i_1i_8}(\xi_{3,4})^{i_8a_6}_{i_2a_7} + \tilde{t}^{a'_5a'_7}_{i_1i_2}(\xi_{3,5})^{a_6}_{a'_7} + \tilde{t}^{a'_7a_6}_{i_1i_2}(\xi_{3,6})^{a'_5}_{a'_7} + \tilde{t}^{a'_5a_7}_{i_1i_2}(\xi_{3,7})^{a_6}_{a_7}$$
$$(\xi_{2,1})^{i_7i_8}_{i_5i_6} = +\tfrac{1}{2}t^{i_7i_8}_{i_9i_{10}} V^{i_9i_{10}}_{i_5i_6}$$
$$(\xi_2)^{i_3i_4}_{i_5i_6} = +B^{i_3i_4}_{i_5i_6} + P^{i_3i_4}_{i_5i_6} + V^{i_7a'_8}_{i_5i_6}(\Xi_0)^{i_3i_4}_{i_7a'_8} + \tfrac{1}{2}X^{i_3i_4}_{i_7i_8}(\xi_{2,1})^{i_7i_8}_{i_5i_6}$$
$$(\xi_{1,1,0})^{i_7i_8}_{i_2a_9} = -v^{i_7i_8}_{i_2a_9} + \tfrac{1}{2}(\Xi_6)^{i_7i_8}_{i_2a_9}$$
$$(\xi_{1,1})^{i_7i_8}_{i_1i_2} = +P_2t^{a_9}_{i_1}(\xi_{1,1,0})^{i_7i_8}_{i_2a_9} + \tfrac{1}{2}t^{a_9a_{10}}_{i_1i_2} v^{i_7i_8}_{a_9a_{10}}$$
$$(\xi_{1,0,0})^{i_7}_{a_8} = -f^{i_7}_{a_8} - (\Xi_5)^{i_7}_{a_8}$$
$$(\xi_{1,0})^{i_7}_{i_2} = -f^{i_7}_{i_2} + t^{a_8}_{i_2}(\xi_{1,0,0})^{i_7}_{a_8} - t^{a_8}_{i_9} v^{i_7i_9}_{i_2a_8} - \tfrac{1}{2}t^{a_8a_9}_{i_2i_{10}} v^{i_7i_{10}}_{a_8a_9} - \tfrac{1}{2}t^{i_8i_9}_{i_2i_{10}} V^{i_7i_{10}}_{i_8i_9}$$
$$(\xi_1)^{i_5i_6}_{i_1i_2} = +P_2t^{i_5i_6}_{i_1i_7}(\xi_{1,0})^{i_7}_{i_2} + \tfrac{1}{2}t^{i_5i_6}_{i_7i_8}(\xi_{1,1})^{i_7i_8}_{i_1i_2}$$
$$(\xi_{0,0})^{a'_7}_{a_6} = -f^{a'_7}_{a_6} + (\Xi_2)^{a'_7}_{a_6} - (\Xi_8)^{a'_7}_{a_6} + (\Xi_9)^{a'_7}_{a_6}$$
$$(\xi_0)^{i_3i_4}_{a_5a_6} = +(V^\dagger)^{i_3i_4}_{a_5a_6} + P_2F^{i_3i_4*}_{a'_7a_5}(\xi_{0,0})^{a'_7}_{a_6} + v^{i_7a'_8}_{a_5a_6}(\Xi_0)^{i_3i_4}_{i_7a'_8}$$
$$\delta^{i_3i_4}_{i_1i_2} = +(V^\dagger)^{i_3i_4}_{i_1i_2} + \tfrac{1}{2}t^{a_5a_6}_{i_1i_2}(\xi_0)^{i_3i_4}_{a_5a_6} + \tfrac{1}{2}X^{i_3i_4}_{i_5i_6}(\xi_1)^{i_5i_6}_{i_1i_2} + \tfrac{1}{2}t^{i_5i_6}_{i_1i_2}(\xi_2)^{i_3i_4}_{i_5i_6} + F^{i_3i_4*}_{a'_5a_6}(\xi_3)^{a'_5a_6}_{i_1i_2} + \tilde{t}^{a'_5a_6}_{i_1i_2}(\xi_4)^{i_3i_4}_{a'_5a_6} + v^{i_5a'_6}_{i_1i_2}(\Xi_0)^{i_3i_4}_{i_5a'_6} + P_2t^{a_5}_{i_1}(\xi_6)^{i_3i_4}_{i_2a_5} + \tfrac{1}{2}v^{i_5i_6}_{i_1i_2}(\xi_7)^{i_3i_4}_{i_5i_6} + \tfrac{1}{2}F^{i_3i_4*}_{a'_5a'_6}(\xi_8)^{a'_5a'_6}_{i_1i_2}$$

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B. CCSDT-R12

TABLE ESI.4.V: The computational sequence and intermediates for the T_1 amplitude equation of CCSDT-R12 and higher-order CC-R12

$$
\begin{aligned}
(\Xi_0)^{i_4}_{a_3} &= +t^{a_5}_{i_6} v^{i_4 i_6}_{a_3 a_5} \\
(\xi_7)^{i_4 i_5}_{i_1 a'_3} &= +v^{i_4 i_5}_{i_1 a'_3} - t^{a_6}_{i_1} v^{i_4 i_5}_{a'_3 a_6} \\
(\xi_5)^{i_4 i_5}_{i_1 a_3} &= -v^{i_4 i_5}_{i_1 a_3} + t^{a_6}_{i_1} v^{i_4 i_5}_{a_3 a_6} \\
(\xi_3)^{i_4}_{a'_3} &= -f^{i_4}_{a'_3} - t^{a_5}_{i_6} v^{i_4 i_6}_{a'_3 a_5} \\
(\xi_2)^{i_4}_{a_3} &= +f^{i_4}_{a_3} + (\Xi_0)^{i_4}_{a_3} \\
(\xi_1)^{a_2}_{a_3} &= +f^{a_2}_{a_3} - t^{a_4}_{i_5} v^{i_5 a_2}_{a_3 a_4}
\end{aligned}
$$

$$
\begin{aligned}
(\xi_{0,0})^{i_3}_{a_4} &= -f^{i_3}_{a_4} - (\Xi_0)^{i_3}_{a_4} \\
(\xi_0)^{i_3}_{i_1} &= -f^{i_3}_{i_1} + t^{a_4}_{i_1} (\xi_{0,0})^{i_3}_{a_4} - t^{a_4}_{i_5} v^{i_3 i_5}_{i_1 a_4} - \tfrac{1}{2} t^{a_4 a_5}_{i_1 i_6} v^{i_3 i_6}_{a_4 a_5} - \tfrac{1}{2} t^{i_4 i_5}_{i_1 i_6} V^{i_3 i_6}_{i_4 i_5} \\
\delta^{a_2}_{i_1} &= +f^{a_2}_{i_1} + t^{a_2}_{i_3} (\xi_0)^{i_3}_{i_1} + t^{a_3}_{i_1} (\xi_1)^{a_2}_{a_3} + t^{a_2 a_3}_{i_1 i_4} (\xi_2)^{i_4}_{a_3} + \tilde{t}^{a'_3 a_2}_{i_1 i_4} (\xi_3)^{i_4}_{a'_3} - t^{a_3}_{i_4} v^{i_4 a_2}_{i_1 a_3} \\
&\quad + \tfrac{1}{2} t^{a_2 a_3}_{i_4 i_5} (\xi_5)^{i_4 i_5}_{i_1 a_3} - \tfrac{1}{2} t^{a_3 a_4}_{i_1 i_5} v^{i_5 a_2}_{a_3 a_4} + \tfrac{1}{2} \tilde{t}^{a'_3 a_2}_{i_4 i_5} (\xi_7)^{i_4 i_5}_{i_1 a'_3} - \tfrac{1}{2} t^{i_3 i_4}_{i_1 i_5} V^{i_5 a_2}_{i_3 i_4} \\
&\quad + \tfrac{1}{4} t^{a_2 a_3 a_4}_{i_1 i_5 i_6} v^{i_5 i_6}_{a_3 a_4}
\end{aligned}
$$

TABLE ESI.4.VI: The computational sequence and intermediates for the T_2 amplitude equation of CCSDT-R12

$$
\begin{aligned}
(\Xi_0)^{i_5 i_6}_{i_1 i_2} &= +P_2 t^{a_7}_{i_1} v^{i_5 i_6}_{i_2 a_7} \\
(\Xi_1)^{i_6 a_4}_{i_2 a_5} &= +t^{a_7}_{i_2} v^{i_6 a_4}_{a_5 a_7} \\
(\Xi_2)^{i_6 i_7}_{i_2 a_5} &= +t^{a_8}_{i_2} v^{i_6 i_7}_{a_5 a_8} \\
(\Xi_3)^{i_6}_{a_5} &= +t^{a_7}_{i_8} v^{i_6 i_8}_{a_5 a_7} \\
(\Xi_4)^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} t^{a_7 a_8}_{i_1 i_2} v^{i_5 i_6}_{a_7 a_8} \\
(\Xi_5)^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} t^{i_7 i_8}_{i_1 i_2} V^{i_5 i_6}_{i_7 i_8} \\
(\Xi_6)^{i_5 i_6}_{i_1 i_2} &= +P_2 t^{a_7}_{i_1} (\Xi_2)^{i_5 i_6}_{i_2 a_7} \\
(\xi_9)^{i_6 a_4}_{i_2 a'_5} &= +v^{i_6 a_4}_{i_2 a'_5} - t^{a_7}_{i_2} v^{i_6 a_4}_{a'_5 a_7} + \tfrac{1}{2} \tilde{t}^{a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_5 a'_7} \\
(\xi_7)^{i_6 a_4}_{i_2 a_5} &= -v^{i_6 a_4}_{i_2 a_5} + (\Xi_1)^{i_6 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_4 a_7}_{i_2 i_8} v^{i_6 i_8}_{a_5 a_7} + \tilde{t}^{a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_7 a_5} \\
(\xi_6)^{i_5 i_6}_{i_1 i_2} &= +v^{i_5 i_6}_{i_1 i_2} - (\Xi_0)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} (\Xi_6)^{i_5 i_6}_{i_1 i_2} + (\Xi_4)^{i_5 i_6}_{i_1 i_2} + (\Xi_5)^{i_5 i_6}_{i_1 i_2} \\
(\xi_5)^{a_3 a_4}_{i_2 a_5} &= -v^{a_3 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_6}_{i_2} v^{a_3 a_4}_{a_5 a_6} \\
(\xi_4)^{i_6}_{a_5} &= +f^{i_6}_{a_5} + (\Xi_3)^{i_6}_{a_5} \\
(\xi_{3,6})^{i_5 i_7}_{i_2 a'_6} &= -v^{i_5 i_7}_{i_2 a'_6} + t^{a_8}_{i_2} v^{i_5 i_7}_{a'_6 a_8} \\
(\xi_{3,4})^{i_5 i_7}_{i_2 a_6} &= +v^{i_5 i_7}_{i_2 a_6} - (\Xi_2)^{i_5 i_7}_{i_2 a_6} \\
(\xi_{3,3})^{i_5 a_4}_{i_2 a_6} &= +v^{i_5 a_4}_{i_2 a_6} - \tfrac{1}{2} (\Xi_1)^{i_5 a_4}_{i_2 a_6} \\
(\xi_{3,2})^{i_5 i_6}_{i_1 i_2} &= +v^{i_5 i_6}_{i_1 i_2} - (\Xi_0)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} (\Xi_6)^{i_5 i_6}_{i_1 i_2} + (\Xi_4)^{i_5 i_6}_{i_1 i_2} + (\Xi_5)^{i_5 i_6}_{i_1 i_2}
\end{aligned}
$$

$$
\begin{aligned}
(\xi_{3,1})^{i_5}_{a'_6} &= -f^{i_5}_{a'_6} - t^{a_7}_{i_8} v^{i_5 i_8}_{a'_6 a_7} \\
(\xi_{3,0})^{i_5}_{a_6} &= +f^{i_5}_{a_6} + (\Xi_3)^{i_5}_{a_6} \\
(\xi_3)^{i_5 a_4}_{i_1 i_2} &= -v^{i_5 a_4}_{i_1 i_2} + t^{a_4 a_6}_{i_1 i_2} (\xi_{3,0})^{i_5}_{a_6} + \tilde{t}^{a'_6 a_4}_{i_1 i_2} (\xi_{3,1})^{i_5}_{a'_6} + \tfrac{1}{2} t^{a_4}_{i_6} (\xi_{3,2})^{i_5 i_6}_{i_1 i_2} \\
&\quad + P_2 t^{a_6}_{i_1} (\xi_{3,3})^{i_5 a_4}_{i_2 a_6} + P_2 t^{a_4 a_6}_{i_1 i_7} (\xi_{3,4})^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_1 i_2} v^{i_5 a_4}_{a_6 a_7} \\
&\quad + P_2 \tilde{t}^{a'_6 a_4}_{i_1 i_7} (\xi_{3,6})^{i_5 i_7}_{i_2 a'_6} - \tfrac{1}{2} t^{i_6 i_7}_{i_1 i_2} V^{i_5 a_4}_{i_6 i_7} + \tfrac{1}{2} t^{a_4 a_6 a_7}_{i_1 i_2 i_8} v^{i_5 i_8}_{a_6 a_7} \\
(\xi_2)^{a_4}_{a'_5} &= -f^{a_4}_{a'_5} + t^{a_6}_{i_7} v^{i_7 a_4}_{a'_5 a_6} + \tfrac{1}{2} t^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a'_6} \\
(\xi_{11})^{i_6 i_7}_{i_2 a_5} &= -v^{i_6 i_7}_{i_2 a_5} + (\Xi_2)^{i_6 i_7}_{i_2 a_5} \\
(\xi_1)^{a_4}_{a_5} &= +f^{a_4}_{a_5} - t^{a_6}_{i_7} v^{i_7 a_4}_{a_5 a_6} - \tfrac{1}{2} t^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_5 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_5} \\
(\xi_{0,0})^{i_5}_{a_6} &= -f^{i_5}_{a_6} - (\Xi_3)^{i_5}_{a_6} \\
(\xi_0)^{i_5}_{i_2} &= -f^{i_5}_{i_2} + t^{a_6}_{i_2} (\xi_{0,0})^{i_5}_{a_6} - t^{a_6}_{i_7} v^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_2 i_8} v^{i_5 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_2 i_8} V^{i_5 i_8}_{i_6 i_7} \\
\delta^{a_3 a_4}_{i_1 i_2} &= +v^{a_3 a_4}_{i_1 i_2} + P_2 t^{a_3 a_4}_{i_1 i_5} (\xi_0)^{i_5}_{i_2} + P_2 t^{a_3 a_5}_{i_1 i_2} (\xi_1)^{a_4}_{a_5} + P_2 \tilde{t}^{a'_5 a_3}_{i_1 i_2} (\xi_2)^{a_4}_{a'_5} \\
&\quad + P_2 t^{a_3}_{i_5} (\xi_3)^{i_5 a_4}_{i_1 i_2} + t^{a_3 a_4 a_5}_{i_1 i_2 i_6} (\xi_4)^{i_6}_{a_5} + P_2 t^{a_5}_{i_1} (\xi_5)^{a_3 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_3 a_4}_{i_5 i_6} (\xi_6)^{i_5 i_6}_{i_1 i_2} \\
&\quad + P_2 P_2 t^{a_3 a_5}_{i_1 i_6} (\xi_7)^{i_6 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_5 a_6}_{i_1 i_2} v^{a_3 a_4}_{a_5 a_6} + P_2 P_2 \tilde{t}^{a'_5 a_3}_{i_1 i_6} (\xi_9)^{i_6 a_4}_{i_2 a'_5} \\
&\quad + \tfrac{1}{2} t^{i_5 i_6}_{i_1 i_2} V^{a_3 a_4}_{i_5 i_6} + \tfrac{1}{2} P_2 t^{a_3 a_4 a_5}_{i_1 i_6 i_7} (\xi_{11})^{i_6 i_7}_{i_2 a_5} - \tfrac{1}{2} P_2 t^{a_3 a_5 a_6}_{i_1 i_2 i_7} v^{i_7 a_4}_{a_5 a_6}
\end{aligned}
$$

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TABLE ESI.4.VII: The computational sequence and intermediates for the T_3 amplitude equation of CCSDT-R12

$$
\begin{aligned}
(\Xi_0)^{i_7 i_8}_{i_2 i_3} &= +P_2 t^{a_9}_{i_2} v^{i_7 i_8}_{i_3 a_9} \\
(\Xi_1)^{i_8 a_6}_{i_3 a_7} &= +t^{a_9}_{i_3} v^{i_8 a_6}_{a_7 a_9} \\
(\Xi_2)^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= +P_3 \tilde{t}^{a'_9 a_6}_{i_1 i_2} v^{i_7 i_8}_{i_3 a'_9} \\
(\Xi_3)^{i_7 i_9}_{i_3 a_8} &= +t^{a_{10}}_{i_3} v^{i_7 i_9}_{a_8 a_{10}} \\
(\Xi_4)^{i_7}_{a_8} &= +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a_8 a_9} \\
(\Xi_5)^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= +\tfrac{1}{2} t^{a_6 a_9 a_{10}}_{i_1 i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}} \\
(\Xi_6)^{i_8 a_6}_{i_3 a_7} &= +t^{a_6 a_9}_{i_3 i_{10}} v^{i_8 i_{10}}_{a_7 a_9} \\
(\Xi_7)^{i_7 i_8}_{i_2 i_3} &= +\tfrac{1}{2} t^{a_9 a_{10}}_{i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}} \\
(\Xi_8)^{i_7 i_8}_{i_3 a'_9} &= +t^{a_{10}}_{i_3} v^{i_7 i_8}_{a'_9 a_{10}} \\
(\Xi_9)^{i_7 i_8}_{i_2 i_3} &= +\tfrac{1}{2} t^{i_9 i_{10}}_{i_2 i_3} V^{i_7 i_8}_{i_9 i_{10}} \\
(\Xi_{10})^{i_8 a_6}_{i_3 a_7} &= +\tilde{t}^{a'_9 a_6}_{i_3 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7} \\
(\Xi_{11})^{i_7 i_8}_{i_2 i_3} &= +P_2 t^{a_9}_{i_2} (\Xi_3)^{i_7 i_8}_{i_3 a_9} \\
(\Xi_{12})^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= +P_3 \tilde{t}^{a'_9 a_6}_{i_1 i_2} (\Xi_8)^{i_7 i_8}_{i_3 a'_9} \\
(\xi_9)^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= +(\Xi_2)^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_5)^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{12})^{i_7 i_8 a_6}_{i_1 i_2 i_3} \\
(\xi_7)^{i_8 a_6}_{i_3 a_7} &= -v^{i_8 a_6}_{i_3 a_7} + (\Xi_1)^{i_8 a_6}_{i_3 a_7} + (\Xi_6)^{i_8 a_6}_{i_3 a_7} + (\Xi_{10})^{i_8 a_6}_{i_3 a_7} \\
(\xi_6)^{i_7 i_8}_{i_2 i_3} &= +v^{i_7 i_8}_{i_2 i_3} - (\Xi_0)^{i_7 i_8}_{i_2 i_3} + \tfrac{1}{2}(\Xi_{11})^{i_7 i_8}_{i_2 i_3} + (\Xi_7)^{i_7 i_8}_{i_2 i_3} + (\Xi_9)^{i_7 i_8}_{i_2 i_3} \\
(\xi_5)^{a_5 a_6}_{i_3 a'_7} &= +v^{a_5 a_6}_{i_3 a'_7} - t^{a_8}_{i_3} v^{a_5 a_6}_{a'_7 a_8} - P_2 t^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a_8} + P_2 \tilde{t}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a'_8} \\
&\quad -\tfrac{1}{2} t^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8} \\
(\xi_{4,1})^{i_8 i_9}_{i_3 a_7} &= -v^{i_8 i_9}_{i_3 a_7} + (\Xi_3)^{i_8 i_9}_{i_3 a_7} \\
(\xi_4)^{a_5 a_6}_{i_3 a_7} &= -v^{a_5 a_6}_{i_3 a_7} + t^{a_8}_{i_3} v^{a_5 a_6}_{a_7 a_8} + \tfrac{1}{2} t^{a_5 a_6}_{i_8 i_9} (\xi_{4,1})^{i_8 i_9}_{i_3 a_7} + P_2 t^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a_7 a_8} \\
&\quad + P_2 \tilde{t}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_8 a_7} + \tfrac{1}{2} t^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8} \\
(\xi_{3,6})^{i_7 i_9}_{i_3 a'_8} &= -v^{i_7 i_9}_{i_3 a'_8} + (\Xi_8)^{i_7 i_9}_{i_3 a'_8} \\
(\xi_{3,4})^{i_7 i_9}_{i_3 a_8} &= +v^{i_7 i_9}_{i_3 a_8} - (\Xi_3)^{i_7 i_9}_{i_3 a_8} \\
(\xi_{3,3})^{i_7 a_6}_{i_3 a_8} &= +v^{i_7 a_6}_{i_3 a_8} - \tfrac{1}{2}(\Xi_1)^{i_7 a_6}_{i_3 a_8} \\
(\xi_{3,2})^{i_7 i_8}_{i_2 i_3} &= +v^{i_7 i_8}_{i_2 i_3} - (\Xi_0)^{i_7 i_8}_{i_2 i_3} + \tfrac{1}{2}(\Xi_{11})^{i_7 i_8}_{i_2 i_3} + (\Xi_7)^{i_7 i_8}_{i_2 i_3} + (\Xi_9)^{i_7 i_8}_{i_2 i_3} \\
(\xi_{3,1})^{i_7}_{a'_8} &= -f^{i_7}_{a'_8} - t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9} \\
(\xi_{3,0})^{i_7}_{a_8} &= +f^{i_7}_{a_8} + (\Xi_4)^{i_7}_{a_8} \\
(\xi_3)^{i_7 a_6}_{i_2 i_3} &= -v^{i_7 a_6}_{i_2 i_3} + t^{a_6 a_8}_{i_2 i_3} (\xi_{3,0})^{i_7}_{a_8} + \tilde{t}^{a'_8 a_6}_{i_2 i_3} (\xi_{3,1})^{i_7}_{a'_8} + t^{a_6}_{i_8} (\xi_{3,2})^{i_7 i_8}_{i_2 i_3} \\
&\quad + P_2 t^{a_8}_{i_2} (\xi_{3,3})^{i_7 a_6}_{i_3 a_8} + P_2 t^{a_6 a_8}_{i_2 i_9} (\xi_{3,4})^{i_7 i_9}_{i_3 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_2 i_3} v^{i_7 a_6}_{a_8 a_9} \\
&\quad + P_2 \tilde{t}^{a'_8 a_6}_{i_2 i_9} (\xi_{3,6})^{i_7 i_9}_{i_3 a'_8} - \tfrac{1}{2} t^{i_8 i_9}_{i_2 i_3} V^{i_7 a_6}_{i_8 i_9} + \tfrac{1}{2} t^{a_6 a_8 a_9}_{i_2 i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} \\
(\xi_{2,4})^{i_7 i_9}_{i_3 a_8} &= -v^{i_7 i_9}_{i_3 a_8} + (\Xi_3)^{i_7 i_9}_{i_3 a_8} \\
(\xi_{2,3,0})^{i_7 i_8}_{i_3 a_9} &= -v^{i_7 i_8}_{i_3 a_9} + (\Xi_3)^{i_7 i_8}_{i_3 a_9} \\
(\xi_{2,3})^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= +(\Xi_2)^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_5)^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{12})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 t^{a_6 a_9}_{i_1 i_2} (\xi_{2,3,0})^{i_7 i_8}_{i_3 a_9} \\
(\xi_{2,2})^{i_7 a_6}_{i_3 a'_8} &= +v^{i_7 a_6}_{i_3 a'_8} - t^{a_9}_{i_3} v^{i_7 a_6}_{a'_8 a_9} - t^{a_6 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a_9} + \tilde{t}^{a'_9 a_6}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a'_9} \\
(\xi_{2,1})^{i_7 a_6}_{i_3 a_8} &= -v^{i_7 a_6}_{i_3 a_8} + (\Xi_1)^{i_7 a_6}_{i_3 a_8} + (\Xi_6)^{i_7 a_6}_{i_3 a_8} + (\Xi_{10})^{i_7 a_6}_{i_3 a_8} \\
(\xi_{2,0})^{i_7}_{a_8} &= -f^{i_7}_{a_8} - (\Xi_4)^{i_7}_{a_8} \\
(\xi_2)^{i_7 a_5 a_6}_{i_1 i_2 i_3} &= +t^{a_5 a_6 a_8}_{i_1 i_2 i_3} (\xi_{2,0})^{i_7}_{a_8} + P_2 P_3 t^{a_5 a_8}_{i_1 i_2} (\xi_{2,1})^{i_7 a_6}_{i_3 a_8} + P_2 P_3 \tilde{t}^{a'_8 a_5}_{i_1 i_2} (\xi_{2,2})^{i_7 a_6}_{i_3 a'_8} \\
&\quad + \tfrac{1}{2} P_2 t^{a_5}_{i_8} (\xi_{2,3})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 t^{a_5 a_6 a_8}_{i_1 i_2 i_9} (\xi_{2,4})^{i_7 i_9}_{i_3 a_8} + \tfrac{1}{2} P_2 t^{a_5 a_8 a_9}_{i_1 i_2 i_3} v^{i_7 a_6}_{a_8 a_9} \\
(\xi_1)^{a_6}_{a_7} &= +f^{a_6}_{a_7} - t^{a_8}_{i_9} v^{i_9 a_6}_{a_7 a_8} - \tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_7} \\
(\xi_{0,0})^{i_7}_{a_8} &= -f^{i_7}_{a_8} - (\Xi_4)^{i_7}_{a_8} \\
(\xi_0)^{i_7}_{i_3} &= -f^{i_7}_{i_3} + t^{a_8}_{i_3} (\xi_{0,0})^{i_7}_{a_8} - t^{a_8}_{i_9} v^{i_7 i_9}_{i_3 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} t^{i_8 i_9}_{i_3 i_{10}} V^{i_7 i_{10}}_{i_8 i_9} \\
\delta^{a_4 a_5 a_6}_{i_1 i_2 i_3} &= +P_3 t^{a_4 a_5 a_6}_{i_1 i_2 i_7} (\xi_0)^{i_7}_{i_3} + P_3 t^{a_4 a_5 a_7}_{i_1 i_2 i_3} (\xi_1)^{a_6}_{a_7} + P_3 t^{a_4}_{i_7} (\xi_2)^{i_7 a_5 a_6}_{i_1 i_2 i_3} \\
&\quad + P_3 P_3 t^{a_4 a_5}_{i_1 i_7} (\xi_3)^{i_7 a_6}_{i_2 i_3} + P_3 P_3 t^{a_4 a_7}_{i_1 i_2} (\xi_4)^{a_5 a_6}_{i_3 a_7} + P_3 P_3 \tilde{t}^{a'_7 a_4}_{i_1 i_2} (\xi_5)^{a_5 a_6}_{i_3 a'_7} \\
&\quad + \tfrac{1}{2} P_3 t^{a_4 a_5 a_6}_{i_1 i_7 i_8} (\xi_6)^{i_7 i_8}_{i_2 i_3} + P_3 P_3 t^{a_4 a_5 a_7}_{i_1 i_2 i_8} (\xi_7)^{i_8 a_6}_{i_3 a_7} \\
&\quad + \tfrac{1}{2} P_3 t^{a_4 a_7 a_8}_{i_1 i_2 i_3} v^{a_5 a_6}_{a_7 a_8} + \tfrac{1}{2} P_3 t^{a_4 a_5}_{i_7 i_8} (\xi_9)^{i_7 i_8 a_6}_{i_1 i_2 i_3}
\end{aligned}
$$

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TABLE ESI.4.VIII: The computational sequence and intermediates for the geminal t amplitude equation of CCSDT-R12 and higher-order CC-R12

$$(\Xi_0)^{i_3 i_4}_{i_7 a'_8} = +t^{a_9}_{i_7} F^{i_3 i_4 *}_{a'_8 a_9}$$
$$(\Xi_1)^{i_8 a'_5}_{i_2 a'_7} = +t^{a_9}_{i_2} v^{i_8 a'_5}_{a_7 a_9}$$
$$(\Xi_2)^{a'_5}_{a'_7} = +t^{a_8}_{i_9} v^{i_9 a'_5}_{a'_7 a_8}$$
$$(\Xi_3)^{a'_7}_{a_6} = +t^{a_8}_{i_9} v^{i_9 a'_7}_{a_6 a_8}$$
$$(\Xi_4)^{i_8 a'_5}_{i_2 a'_7} = +t^{a_9}_{i_2} v^{i_8 a'_5}_{a'_7 a_9}$$
$$(\Xi_5)^{i_7}_{a_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\Xi_6)^{i_7 i_9}_{i_2 a_8} = +t^{a_{10}}_{i_2} v^{i_7 i_9}_{a_8 a_{10}}$$
$$(\Xi_7)^{i_8 a'_6}_{i_2 a_7} = +\tilde{t}^{a'_6 a'_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\Xi_8)^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\Xi_9)^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{t}^{a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8}$$
$$(\Xi_{10})^{a'_5}_{a'_7} = +\tfrac{1}{2}\tilde{t}^{a'_5 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{11})^{a'_5}_{a'_7} = +\tfrac{1}{2}\tilde{t}^{a'_5 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\xi_{8,2})^{a'_6}_{a'_7} = -(\Xi_2)^{a'_6}_{a'_7} - (\Xi_{10})^{a'_6}_{a'_7} - (\Xi_{11})^{a'_6}_{a'_7}$$
$$(\xi_{8,1})^{i_8 a'_6}_{i_2 a'_7} = -v^{i_8 a'_6}_{i_2 a'_7} + (\Xi_1)^{i_8 a'_6}_{i_2 a'_7} - (\Xi_7)^{i_8 a'_6}_{i_2 a'_7} + \tfrac{1}{2}\tilde{t}^{a'_6 a_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a_7 a_9}$$
$$(\xi_{8,0})^{i_8 a'_6}_{i_2 a'_7} = -v^{i_8 a'_6}_{i_2 a'_7} + (\Xi_4)^{i_8 a'_6}_{i_2 a'_7} + \tfrac{1}{2}\tilde{t}^{a'_6 a'_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_7 a'_9}$$
$$(\xi_8)^{a'_5 a'_6}_{i_1 i_2} = +P_2 P_2 \tilde{t}^{a'_5 a'_7}_{i_1 i_8} (\xi_{8,0})^{i_8 a'_6}_{i_2 a'_7} + P_2 P_2 \tilde{t}^{a'_5 a'_7}_{i_1 i_8} (\xi_{8,1})^{i_8 a'_6}_{i_2 a_7} + P_2 \tilde{t}^{a'_5 a'_7}_{i_1 i_2} (\xi_{8,2})^{a'_6}_{a'_7}$$
$$(\xi_7)^{i_3 i_4}_{i_5 i_6} = +\tfrac{1}{2} t^{i_7 i_8}_{i_5 i_6} X^{i_3 i_4}_{i_7 i_8}$$
$$(\xi_6)^{i_3 i_4}_{i_2 a_5} = -(V^\dagger)^{i_3 i_4}_{i_2 a_5} - v^{i_6 a'_7}_{i_2 a_5} (\Xi_0)^{i_3 i_4}_{i_6 a'_7} + \tfrac{1}{2} t^{a_6}_{i_2} (V^\dagger)^{i_3 i_4}_{a_5 a_6}$$
$$(\xi_{4,1})^{a'_7}_{a_6} = -(\Xi_3)^{a'_7}_{a_6} + (\Xi_8)^{a'_7}_{a_6} - (\Xi_9)^{a'_7}_{a_6}$$
$$(\xi_4)^{i_3 i_4}_{a'_5 a_6} = -f^{i_7}_{a_6} (\Xi_0)^{i_3 i_4}_{i_7 a'_5} + F^{i_3 i_4 *}_{a'_5 a'_7} (\xi_{4,1})^{a'_7}_{a_6}$$
$$(\xi_{3,7})^{a_6}_{a'_7} = -t^{a_8}_{i_9} v^{i_9 a_6}_{a_7 a_8} - \tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_7}$$
$$(\xi_{3,6})^{a'_5}_{a'_7} = -(\Xi_2)^{a'_5}_{a'_7} - (\Xi_{10})^{a'_5}_{a'_7} - (\Xi_{11})^{a'_5}_{a'_7}$$
$$(\xi_{3,5})^{a_6}_{a'_7} = -t^{a_8}_{i_9} v^{i_9 a_6}_{a'_7 a_8} - \tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8} + \tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\xi_{3,4})^{i_8 a_6}_{i_2 a_7} = -v^{i_8 a_6}_{i_2 a_7} + t^{a_9}_{i_2} v^{i_8 a_6}_{a_7 a_9} + t^{a_6 a_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a_7 a_9} + \tilde{t}^{a'_9 a_6}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\xi_{3,3})^{i_8 a'_5}_{i_2 a'_7} = -v^{i_8 a'_5}_{i_2 a'_7} + (\Xi_4)^{i_8 a'_5}_{i_2 a'_7}$$
$$(\xi_{3,2})^{i_8 a_6}_{i_2 a'_7} = -v^{i_8 a_6}_{i_2 a'_7} + t^{a_9}_{i_2} v^{i_8 a_6}_{a'_7 a_9} - \tilde{t}^{a'_9 a_6}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_7 a'_9}$$
$$(\xi_{3,1})^{i_8 a'_5}_{i_2 a_7} = +v^{i_8 a'_5}_{i_2 a_7} - (\Xi_1)^{i_8 a'_5}_{i_2 a_7} + (\Xi_7)^{i_8 a'_5}_{i_2 a_7}$$
$$(\xi_{3,0,3})^{i_7 i_9}_{i_2 a_8} = -v^{i_7 i_9}_{i_2 a_8} + (\Xi_6)^{i_7 i_9}_{i_2 a_8}$$
$$(\xi_{3,0,2})^{i_7 i_9}_{i_2 a'_8} = -v^{i_7 i_9}_{i_2 a'_8} + t^{a_{10}}_{i_2} v^{i_7 i_9}_{a'_8 a_{10}}$$
$$(\xi_{3,0,0})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\xi_{3,0})^{i_7 a'_5}_{i_1 i_2} = +\tilde{t}^{a'_5 a'_8}_{i_1 i_2} (\xi_{3,0,0})^{i_7}_{a'_8} + \tfrac{1}{2} P_2 t^{a_8}_{i_1} (\Xi_1)^{i_7 a'_5}_{i_2 a_8} + P_2 \tilde{t}^{a'_5 a'_8}_{i_1 i_9} (\xi_{3,0,2})^{i_7 i_9}_{i_2 a'_8} + P_2 \tilde{t}^{a'_5 a_8}_{i_1 i_9} (\xi_{3,0,3})^{i_7 i_9}_{i_2 a_8} - \tilde{t}^{a'_5 a_8}_{i_1 i_2} (\Xi_5)^{i_7}_{a_8}$$
$$(\xi_3)^{a'_5 a_6}_{i_1 i_2} = +t^{a_6}_{i_7} (\xi_{3,0})^{i_7 a'_5}_{i_1 i_2} + P_2 t^{a_6 a_7}_{i_1 i_8} (\xi_{3,1})^{i_8 a'_5}_{i_2 a_7} + P_2 \tilde{t}^{a'_5 a'_7}_{i_1 i_8} (\xi_{3,2})^{i_8 a_6}_{i_2 a'_7} + P_2 \tilde{t}^{a'_7 a_6}_{i_1 i_8} (\xi_{3,3})^{i_8 a'_5}_{i_2 a'_7} + P_2 \tilde{t}^{a'_5 a_7}_{i_1 i_8} (\xi_{3,4})^{i_8 a_6}_{i_2 a_7} + \tilde{t}^{a'_5 a'_7}_{i_1 i_2} (\xi_{3,5})^{a_6}_{a'_7} + \tilde{t}^{a'_7 a_6}_{i_1 i_2} (\xi_{3,6})^{a'_5}_{a'_7} + \tilde{t}^{a'_5 a_7}_{i_1 i_2} (\xi_{3,7})^{a_6}_{a_7} + \tfrac{1}{2} t^{a_6 a_7 a_8}_{i_1 i_2 i_9} v^{i_9 a'_5}_{a_7 a_8}$$
$$(\xi_{2,1})^{i_7 i_8}_{i_5 i_6} = +\tfrac{1}{2} t^{i_7 i_8}_{i_9 i_{10}} V^{i_9 i_{10}}_{i_5 i_6}$$
$$(\xi_2)^{i_3 i_4}_{i_5 i_6} = +B^{i_3 i_4}_{i_5 i_6} + P^{i_3 i_4}_{i_5 i_6} + V^{i_7 a'_8}_{i_5 i_6} (\Xi_0)^{i_3 i_4}_{i_7 a'_8} + \tfrac{1}{2} X^{i_3 i_4}_{i_7 i_8} (\xi_{2,1})^{i_7 i_8}_{i_5 i_6}$$
$$(\xi_{1,1,0})^{i_7 i_8}_{i_2 a_9} = -v^{i_7 i_8}_{i_2 a_9} + \tfrac{1}{2} (\Xi_6)^{i_7 i_8}_{i_2 a_9}$$
$$(\xi_{1,1})^{i_7 i_8}_{i_1 i_2} = +P_2 t^{a_9}_{i_1} (\xi_{1,1,0})^{i_7 i_8}_{i_2 a_9} + \tfrac{1}{2} t^{a_9 a_{10}}_{i_1 i_2} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\xi_{1,0,0})^{i_7}_{a_8} = -f^{i_7}_{a_8} - (\Xi_5)^{i_7}_{a_8}$$
$$(\xi_{1,0})^{i_7}_{i_2} = -f^{i_7}_{i_2} + t^{a_8}_{i_2} (\xi_{1,0,0})^{i_7}_{a_8} - t^{a_8}_{i_9} v^{i_7 i_9}_{i_2 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_2 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} t^{i_8 i_9}_{i_2 i_{10}} V^{i_7 i_{10}}_{i_8 i_9}$$
$$(\xi_1)^{i_5 i_6}_{i_1 i_2} = +P_2 t^{i_5 i_6}_{i_1 i_7} (\xi_{1,0})^{i_7}_{i_2} + \tfrac{1}{2} t^{i_5 i_6}_{i_7 i_8} (\xi_{1,1})^{i_7 i_8}_{i_1 i_2}$$
$$(\xi_{0,0})^{a'_7}_{a_6} = -f^{a'_7}_{a_6} + (\Xi_3)^{a'_7}_{a_6} - (\Xi_8)^{a'_7}_{a_6} + (\Xi_9)^{a'_7}_{a_6}$$
$$(\xi_0)^{i_3 i_4}_{a_5 a_6} = +(V^\dagger)^{i_3 i_4}_{a_5 a_6} + P_2 F^{i_3 i_4 *}_{a'_7 a_5} (\xi_{0,0})^{a'_7}_{a_6} + v^{i_7 a'_8}_{a_5 a_6} (\Xi_0)^{i_3 i_4}_{i_7 a'_8}$$
$$\delta^{i_3 i_4}_{i_1 i_2} = +(V^\dagger)^{i_3 i_4}_{i_1 i_2} + \tfrac{1}{2} t^{a_5 a_6}_{i_1 i_2} (\xi_0)^{i_3 i_4}_{a_5 a_6} + \tfrac{1}{2} X^{i_3 i_4}_{i_5 i_6} (\xi_1)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} t^{i_5 i_6}_{i_1 i_2} (\xi_2)^{i_3 i_4}_{i_5 i_6} + F^{i_3 i_4 *}_{a'_5 a_6} (\xi_3)^{a'_5 a_6}_{i_1 i_2} + \tilde{t}^{a'_5 a_6}_{i_1 i_2} (\xi_4)^{i_3 i_4}_{a'_5 a_6} + v^{i_5 a'_6}_{i_1 i_2} (\Xi_0)^{i_3 i_4}_{i_5 a'_6} + P_2 t^{a_5}_{i_1} (\xi_6)^{i_3 i_4}_{i_2 a_5} + \tfrac{1}{2} v^{i_5 i_6}_{i_1 i_2} (\xi_7)^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{2} F^{i_3 i_4 *}_{a'_5 a'_6} (\xi_8)^{a'_5 a'_6}_{i_1 i_2}$$

Supplementary data for Phys. Chem. Chem. Phys.

C. CCSDTQ-R12

TABLE ESI.4.IX: The computational sequence and intermediates for the T_2 amplitude equation of CCSDTQ-R12

$$(\Xi_0)^{i_5 i_6}_{i_1 i_2} = +P_2 t^{a_7}_{i_1} v^{i_5 i_6}_{i_2 a_7}$$
$$(\Xi_1)^{i_6 a_4}_{i_2 a_5} = +t^{a_7}_{i_2} v^{i_6 a_4}_{a_5 a_7}$$
$$(\Xi_2)^{i_6 i_7}_{i_2 a_5} = +t^{a_8}_{i_2} v^{i_6 i_7}_{a_5 a_8}$$
$$(\Xi_3)^{i_6}_{a_5} = +t^{a_7}_{i_8} v^{i_6 i_8}_{a_5 a_7}$$
$$(\Xi_4)^{i_5 i_6}_{i_1 i_2} = +\tfrac{1}{2} t^{a_7 a_8}_{i_1 i_2} v^{i_5 i_6}_{a_7 a_8}$$
$$(\Xi_5)^{i_5 i_6}_{i_1 i_2} = +\tfrac{1}{2} t^{i_7 i_8}_{i_1 i_2} V^{i_5 i_6}_{i_7 i_8}$$
$$(\Xi_6)^{i_5 i_6}_{i_1 i_2} = +P_2 t^{a_7}_{i_1} (\Xi_2)^{i_5 i_6}_{i_2 a_7}$$
$$(\xi_9)^{i_6 a_4}_{i_2 a'_5} = +v^{i_6 a_4}_{i_2 a'_5} - t^{a_7}_{i_2} v^{i_6 a_4}_{a'_5 a_7} + \tfrac{1}{2} \tilde{t}^{a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_5 a'_7}$$
$$(\xi_7)^{i_6 a_4}_{i_2 a_5} = -v^{i_6 a_4}_{i_2 a_5} + (\Xi_1)^{i_6 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_4 a_7}_{i_2 i_8} v^{i_6 i_8}_{a_5 a_7} + \tilde{t}^{a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_7 a_5}$$
$$(\xi_6)^{i_5 i_6}_{i_1 i_2} = +v^{i_5 i_6}_{i_1 i_2} - (\Xi_0)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} (\Xi_6)^{i_5 i_6}_{i_1 i_2} + (\Xi_4)^{i_5 i_6}_{i_1 i_2} + (\Xi_5)^{i_5 i_6}_{i_1 i_2}$$
$$(\xi_5)^{a_3 a_4}_{i_2 a_5} = -v^{a_3 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_6}_{i_2} v^{a_3 a_4}_{a_5 a_6}$$
$$(\xi_4)^{i_6}_{a_5} = +f^{i_6}_{a_5} + (\Xi_3)^{i_6}_{a_5}$$
$$(\xi_{3,6})^{i_5 i_7}_{i_2 a'_6} = -v^{i_5 i_7}_{i_2 a'_6} + t^{a_8}_{i_2} v^{i_5 i_7}_{a'_6 a_8}$$
$$(\xi_{3,4})^{i_5 i_7}_{i_2 a_6} = +v^{i_5 i_7}_{i_2 a_6} - (\Xi_2)^{i_5 i_7}_{i_2 a_6}$$
$$(\xi_{3,3})^{i_5 a_4}_{i_2 a_6} = +v^{i_5 a_4}_{i_2 a_6} - \tfrac{1}{2} (\Xi_1)^{i_5 a_4}_{i_2 a_6}$$
$$(\xi_{3,2})^{i_5 i_6}_{i_1 i_2} = +v^{i_5 i_6}_{i_1 i_2} - (\Xi_0)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} (\Xi_6)^{i_5 i_6}_{i_1 i_2} + (\Xi_4)^{i_5 i_6}_{i_1 i_2} + (\Xi_5)^{i_5 i_6}_{i_1 i_2}$$

$$(\xi_{3,1})^{i_5}_{a'_6} = -f^{i_5}_{a'_6} - t^{a_7}_{i_8} v^{i_5 i_8}_{a'_6 a_7}$$
$$(\xi_{3,0})^{i_5}_{a_6} = +f^{i_5}_{a_6} + (\Xi_3)^{i_5}_{a_6}$$
$$(\xi_3)^{i_5 a_4}_{i_1 i_2} = -v^{i_5 a_4}_{i_1 i_2} + t^{a_4 a_6}_{i_1 i_2} (\xi_{3,0})^{i_5}_{a_6} + \tilde{t}^{a'_6 a_4}_{i_1 i_2} (\xi_{3,1})^{i_5}_{a'_6} + \tfrac{1}{2} t^{a_4}_{i_6} (\xi_{3,2})^{i_5 i_6}_{i_1 i_2}$$
$$+P_2 t^{a_6}_{i_1} (\xi_{3,3})^{i_5 a_4}_{i_2 a_6} + P_2 t^{a_4 a_6}_{i_1 i_7} (\xi_{3,4})^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_1 i_2} v^{i_5 a_4}_{a_6 a_7}$$
$$+P_2 \tilde{t}^{a'_6 a_4}_{i_1 i_7} (\xi_{3,6})^{i_5 i_7}_{i_2 a'_6} - \tfrac{1}{2} t^{i_6 i_7}_{i_1 i_2} V^{i_5 a_4}_{i_6 i_7} + \tfrac{1}{2} t^{a_4 a_6 a_7}_{i_1 i_2 i_8} v^{i_5 i_8}_{a_6 a_7}$$
$$(\xi_2)^{a_4}_{a'_5} = -f^{a_4}_{a'_5} + t^{a_6}_{i_7} v^{i_7 a_4}_{a'_5 a_6} + \tfrac{1}{2} t^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a'_6}$$
$$(\xi_{11})^{i_6 i_7}_{i_2 a_5} = -v^{i_6 i_7}_{i_2 a_5} + (\Xi_2)^{i_6 i_7}_{i_2 a_5}$$
$$(\xi_1)^{a_4}_{a_5} = +f^{a_4}_{a_5} - t^{a_6}_{i_7} v^{i_7 a_4}_{a_5 a_6} - \tfrac{1}{2} t^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_5 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_5}$$
$$(\xi_{0,0})^{i_5}_{a_6} = -f^{i_5}_{a_6} - (\Xi_3)^{i_5}_{a_6}$$
$$(\xi_0)^{i_5}_{i_2} = -f^{i_5}_{i_2} + t^{a_6}_{i_2} (\xi_{0,0})^{i_5}_{a_6} - t^{a_6}_{i_7} v^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_2 i_8} v^{i_5 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_2 i_8} V^{i_5 i_8}_{i_6 i_7}$$
$$\delta^{a_3 a_4}_{i_1 i_2} = +v^{a_3 a_4}_{i_1 i_2} + P_2 t^{a_3 a_4}_{i_1 i_5} (\xi_0)^{i_5}_{i_2} + P_2 t^{a_3 a_5}_{i_1 i_2} (\xi_1)^{a_4}_{a_5} + P_2 \tilde{t}^{a'_5 a_3}_{i_1 i_2} (\xi_2)^{a_4}_{a'_5}$$
$$+P_2 t^{a_3}_{i_5} (\xi_3)^{i_5 a_4}_{i_1 i_2} + t^{a_3 a_4 a_5}_{i_1 i_2 i_6} (\xi_4)^{i_6}_{a_5} + P_2 t^{a_5}_{i_1} (\xi_5)^{a_3 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_3 a_4}_{i_5 i_6} (\xi_6)^{i_5 i_6}_{i_1 i_2}$$
$$+P_2 P_2 t^{a_3 a_5}_{i_1 i_6} (\xi_7)^{i_6 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_5 a_6}_{i_1 i_2} v^{a_3 a_4}_{a_5 a_6} + P_2 P_2 \tilde{t}^{a'_5 a_3}_{i_1 i_6} (\xi_9)^{i_6 a_4}_{i_2 a'_5}$$
$$+\tfrac{1}{2} t^{i_5 i_6}_{i_1 i_2} V^{a_3 a_4}_{i_5 i_6} + \tfrac{1}{2} P_2 t^{a_3 a_4 a_5}_{i_1 i_6 i_7} (\xi_{11})^{i_6 i_7}_{i_2 a_5} - \tfrac{1}{2} P_2 t^{a_3 a_5 a_6}_{i_1 i_2 i_7} v^{i_7 a_4}_{a_5 a_6}$$
$$+\tfrac{1}{4} t^{a_3 a_4 a_5 a_6}_{i_1 i_2 i_7 i_8} v^{i_7 i_8}_{a_5 a_6}$$

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TABLE ESI.4.X: The computational sequence and intermediates for the T_3 amplitude equation of CCSDTQ-R12

$$
\begin{aligned}
(\Xi_0)^{i_7 i_8}_{i_2 i_3} &= +P_2 t^{a_9}_{i_2} v^{i_7 i_8}_{i_3 a_9} \\
(\Xi_1)^{i_8 a_6}_{i_3 a_7} &= +t^{a_9}_{i_3} v^{i_8 a_6}_{a_7 a_9} \\
(\Xi_2)^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= +P_3 \tilde{t}^{a'_9 a_6}_{i_1 i_2} v^{i_7 i_8}_{i_3 a'_9} \\
(\Xi_3)^{i_8 i_9}_{i_3 a_7} &= +t^{a_{10}}_{i_3} v^{i_8 i_9}_{a_7 a_{10}} \\
(\Xi_4)^{i_7 i_8}_{i_3 a'_9} &= +t^{a_{10}}_{i_3} v^{i_7 i_8}_{a'_9 a_{10}} \\
(\Xi_5)^{i_8}_{a_7} &= +t^{a_9}_{i_{10}} v^{i_8 i_{10}}_{a_7 a_9} \\
(\Xi_6)^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= +\tfrac{1}{2} t^{a_6 a_9 a_{10}}_{i_1 i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}} \\
(\Xi_7)^{i_8 a_6}_{i_3 a_7} &= +t^{a_6 a_9}_{i_3 i_{10}} v^{i_8 i_{10}}_{a_7 a_9} \\
(\Xi_8)^{i_7 i_8}_{i_2 i_3} &= +\tfrac{1}{2} t^{a_9 a_{10}}_{i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}} \\
(\Xi_9)^{i_7 i_8}_{i_2 i_3} &= +\tfrac{1}{2} t^{i_9 i_{10}}_{i_2 i_3} V^{i_7 i_8}_{i_9 i_{10}} \\
(\Xi_{10})^{i_8 a_6}_{i_3 a_7} &= +\tilde{t}^{a'_9 a_6}_{i_3 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7} \\
(\Xi_{11})^{i_7 i_8}_{i_2 i_3} &= +P_2 t^{a_9}_{i_2} (\Xi_3)^{i_7 i_8}_{i_3 a_9} \\
(\Xi_{12})^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= +P_3 \tilde{t}^{a'_9 a_6}_{i_1 i_2} (\Xi_4)^{i_7 i_8}_{i_3 a'_9} \\
(\xi_8)^{i_8 a_6}_{i_3 a_7} &= -v^{i_8 a_6}_{i_3 a_7} + (\Xi_1)^{i_8 a_6}_{i_3 a_7} + (\Xi_7)^{i_8 a_6}_{i_3 a_7} + (\Xi_{10})^{i_8 a_6}_{i_3 a_7} \\
(\xi_7)^{i_7 i_8}_{i_2 i_3} &= +v^{i_7 i_8}_{i_2 i_3} - (\Xi_0)^{i_7 i_8}_{i_2 i_3} + \tfrac{1}{2}(\Xi_{11})^{i_7 i_8}_{i_2 i_3} + (\Xi_8)^{i_7 i_8}_{i_2 i_3} + (\Xi_9)^{i_7 i_8}_{i_2 i_3} \\
(\xi_6)^{a_5 a_6}_{i_3 a'_7} &= +v^{a_5 a_6}_{i_3 a'_7} - t^{a_8}_{i_3} v^{a_5 a_6}_{a'_7 a_8} - P_2 t^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a_8} + P_2 \tilde{t}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a'_8} \\
&\quad -\tfrac{1}{2} t^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8} \\
(\xi_{5,1})^{i_8 i_9}_{i_3 a_7} &= -v^{i_8 i_9}_{i_3 a_7} + (\Xi_3)^{i_8 i_9}_{i_3 a_7} \\
(\xi_5)^{a_5 a_6}_{i_3 a_7} &= -v^{a_5 a_6}_{i_3 a_7} + t^{a_8}_{i_3} v^{a_5 a_6}_{a_7 a_8} + \tfrac{1}{2} t^{a_5 a_6}_{i_8 i_9} (\xi_{5,1})^{i_8 i_9}_{i_3 a_7} + P_2 t^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a_7 a_8} \\
&\quad +P_2 \tilde{t}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_8 a_7} + \tfrac{1}{2} t^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8} \\
(\xi_4)^{i_8}_{a_7} &= +f^{i_8}_{a_7} + (\Xi_5)^{i_8}_{a_7} \\
(\xi_{3,6})^{i_7 i_9}_{i_3 a'_8} &= -v^{i_7 i_9}_{i_3 a'_8} + (\Xi_4)^{i_7 i_9}_{i_3 a'_8} \\
(\xi_{3,4})^{i_7 i_9}_{i_3 a_8} &= +v^{i_7 i_9}_{i_3 a_8} - (\Xi_3)^{i_7 i_9}_{i_3 a_8} \\
(\xi_{3,3})^{i_7 a_6}_{i_3 a_8} &= +v^{i_7 a_6}_{i_3 a_8} - \tfrac{1}{2}(\Xi_1)^{i_7 a_6}_{i_3 a_8} \\
(\xi_{3,2})^{i_7 i_8}_{i_2 i_3} &= +v^{i_7 i_8}_{i_2 i_3} - (\Xi_0)^{i_7 i_8}_{i_2 i_3} + \tfrac{1}{2}(\Xi_{11})^{i_7 i_8}_{i_2 i_3} + (\Xi_8)^{i_7 i_8}_{i_2 i_3} + (\Xi_9)^{i_7 i_8}_{i_2 i_3} \\
(\xi_{3,1})^{i_7}_{a'_8} &= -f^{i_7}_{a'_8} - t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9} \\
(\xi_{3,0})^{i_7}_{a_8} &= +f^{i_7}_{a_8} + (\Xi_5)^{i_7}_{a_8} \\
(\xi_3)^{i_7 a_6}_{i_2 i_3} &= -v^{i_7 a_6}_{i_2 i_3} + t^{a_6 a_8}_{i_2 i_3} (\xi_{3,0})^{i_7}_{a_8} + \tilde{t}^{a'_8 a_6}_{i_2 i_3} (\xi_{3,1})^{i_7}_{a'_8} + t^{a_6}_{i_8} (\xi_{3,2})^{i_7 i_8}_{i_2 i_3} \\
&\quad +P_2 t^{a_8}_{i_2} (\xi_{3,3})^{i_7 a_6}_{i_3 a_8} + P_2 t^{a_6 a_8}_{i_2 i_9} (\xi_{3,4})^{i_7 i_9}_{i_3 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_2 i_3} v^{i_7 a_6}_{a_8 a_9} \\
&\quad +P_2 \tilde{t}^{a'_8 a_6}_{i_2 i_9} (\xi_{3,6})^{i_7 i_9}_{i_3 a'_8} - \tfrac{1}{2} t^{i_8 i_9}_{i_2 i_3} V^{i_7 a_6}_{i_8 i_9} + \tfrac{1}{2} t^{a_6 a_8 a_9}_{i_2 i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} \\
(\xi_{2,4})^{i_7 i_9}_{i_3 a_8} &= -v^{i_7 i_9}_{i_3 a_8} + (\Xi_3)^{i_7 i_9}_{i_3 a_8} \\
(\xi_{2,3,0})^{i_7 i_8}_{i_3 a_9} &= -v^{i_7 i_8}_{i_3 a_9} + (\Xi_3)^{i_7 i_8}_{i_3 a_9} \\
(\xi_{2,3})^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= +(\Xi_2)^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{12})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_6)^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 t^{a_6 a_9}_{i_1 i_2} (\xi_{2,3,0})^{i_7 i_8}_{i_3 a_9} \\
(\xi_{2,2})^{i_7 a_6}_{i_3 a'_8} &= +v^{i_7 a_6}_{i_3 a'_8} - t^{a_9}_{i_3} v^{i_7 a_6}_{a'_8 a_9} - t^{a_6 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a_9} + \tilde{t}^{a'_9 a_6}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a'_9} \\
(\xi_{2,1})^{i_7 a_6}_{i_3 a_8} &= -v^{i_7 a_6}_{i_3 a_8} + (\Xi_1)^{i_7 a_6}_{i_3 a_8} + (\Xi_7)^{i_7 a_6}_{i_3 a_8} + (\Xi_{10})^{i_7 a_6}_{i_3 a_8} \\
(\xi_{2,0})^{i_7}_{a_8} &= -f^{i_7}_{a_8} - (\Xi_5)^{i_7}_{a_8} \\
(\xi_2)^{i_7 a_5 a_6}_{i_1 i_2 i_3} &= +t^{a_5 a_6 a_8}_{i_1 i_2 i_3} (\xi_{2,0})^{i_7}_{a_8} + P_2 P_3 t^{a_5 a_8}_{i_1 i_2} (\xi_{2,1})^{i_7 a_6}_{i_3 a_8} + P_2 P_3 \tilde{t}^{a'_8 a_5}_{i_1 i_2} (\xi_{2,2})^{i_7 a_6}_{i_3 a'_8} \\
&\quad +\tfrac{1}{2} P_2 t^{a_5}_{i_8} (\xi_{2,3})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 t^{a_5 a_6 a_8}_{i_1 i_2 i_9} (\xi_{2,4})^{i_7 i_9}_{i_3 a_8} + \tfrac{1}{2} P_2 t^{a_5 a_8 a_9}_{i_1 i_2 i_3} v^{i_7 a_6}_{a_8 a_9} \\
&\quad -\tfrac{1}{2} t^{a_5 a_6 a_8 a_9}_{i_1 i_2 i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} \\
(\xi_{12})^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= +(\Xi_2)^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{12})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_6)^{i_7 i_8 a_6}_{i_1 i_2 i_3} \\
(\xi_{10})^{i_8 i_9}_{i_3 a_7} &= -v^{i_8 i_9}_{i_3 a_7} + (\Xi_3)^{i_8 i_9}_{i_3 a_7} \\
(\xi_1)^{a_6}_{a_7} &= +f^{a_6}_{a_7} - t^{a_8}_{i_9} v^{i_9 a_6}_{a_7 a_8} - \tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_7} \\
(\xi_{0,0})^{i_7}_{a_8} &= -f^{i_7}_{a_8} - (\Xi_5)^{i_7}_{a_8} \\
(\xi_0)^{i_7}_{i_3} &= -f^{i_7}_{i_3} + t^{a_8}_{i_3} (\xi_{0,0})^{i_7}_{a_8} - t^{a_8}_{i_9} v^{i_7 i_9}_{i_3 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} t^{i_8 i_9}_{i_3 i_{10}} V^{i_7 i_{10}}_{i_8 i_9} \\
\delta^{a_4 a_5 a_6}_{i_1 i_2 i_3} &= +P_3 t^{a_4 a_5 a_6}_{i_1 i_2 i_3} (\xi_0)^{i_7}_{i_3} + P_3 t^{a_4 a_5 a_7}_{i_1 i_2 i_3} (\xi_1)^{a_6}_{a_7} + P_3 t^{a_4}_{i_7} (\xi_2)^{i_7 a_5 a_6}_{i_1 i_2 i_3} \\
&\quad +P_3 P_3 t^{a_4 a_5}_{i_1 i_7} (\xi_3)^{i_7 a_6}_{i_2 i_3} + t^{a_4 a_5 a_6 a_7}_{i_1 i_2 i_3 i_8} (\xi_4)^{i_8}_{a_7} + P_3 P_3 t^{a_4 a_7}_{i_1 i_2} (\xi_5)^{a_5 a_6}_{i_3 a_7} \\
&\quad +P_3 P_3 \tilde{t}^{a'_7 a_4}_{i_1 i_2} (\xi_6)^{a_5 a_6}_{i_3 a'_7} + \tfrac{1}{2} P_3 t^{a_4 a_5 a_6}_{i_1 i_7 i_8} (\xi_7)^{i_7 i_8}_{i_2 i_3} + P_3 P_3 t^{a_4 a_5 a_7}_{i_1 i_2 i_8} (\xi_8)^{i_8 a_6}_{i_3 a_7} \\
&\quad +\tfrac{1}{2} P_3 t^{a_4 a_7 a_8}_{i_1 i_2 i_3} v^{a_5 a_6}_{a_7 a_8} + \tfrac{1}{2} P_3 t^{a_4 a_5 a_6 a_7}_{i_1 i_2 i_8 i_9} (\xi_{10})^{i_8 i_9}_{i_3 a_7} - \tfrac{1}{2} P_3 t^{a_4 a_5 a_7 a_8}_{i_1 i_2 i_3 i_9} v^{i_9 a_6}_{a_7 a_8} \\
&\quad +\tfrac{1}{2} P_3 t^{a_4 a_5}_{i_7 i_8} (\xi_{12})^{i_7 i_8 a_6}_{i_1 i_2 i_3}
\end{aligned}
$$

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TABLE ESI.4.XI: The computational sequence and intermediates for the T_4 amplitude equation of CCSDTQ-R12

$$
\begin{aligned}
(\Xi_0)^{i_9 i_{10}}_{i_3 i_4} &= +P_2 t^{a_{11}}_{i_3} v^{i_9 i_{10}}_{i_4 a_{11}} \\
(\Xi_1)^{i_{10} a_8}_{i_4 a_9} &= +t^{a_{11}}_{i_4} v^{i_{10} a_8}_{a_9 a_{11}} \\
(\Xi_2)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} &= +P_3 \tilde{t}^{a'_{11} a_8}_{i_2 i_3} v^{i_9 i_{10}}_{i_4 a'_{11}} \\
(\Xi_3)^{i_9 i_{11}}_{i_4 a_{10}} &= +t^{a_{12}}_{i_4} v^{i_9 i_{11}}_{a_{10} a_{12}} \\
(\Xi_4)^{i_{10} i_{11} a_8}_{i_3 i_4 a_9} &= +\tilde{t}^{a'_{12} a_8}_{i_3 i_4} v^{i_{10} i_{11}}_{a'_{12} a_9} \\
(\Xi_5)^{i_9 i_{11}}_{i_4 a'_{10}} &= +t^{a_{12}}_{i_4} v^{i_9 i_{11}}_{a'_{10} a_{12}} \\
(\Xi_6)^{i_9}_{a_{10}} &= +t^{a_{11}}_{i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}} \\
(\Xi_7)^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} &= +\tfrac{1}{2} t^{a_7 a_8 a_{11} a_{12}}_{i_1 i_2 i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}} \\
(\Xi_8)^{i_9 i_{10} a_8}_{i_3 i_4 a'_{11}} &= +\tilde{t}^{a'_{12} a_8}_{i_3 i_4} v^{i_9 i_{10}}_{a'_{11} a'_{12}} \\
(\Xi_9)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} &= +\tfrac{1}{2} t^{a_8 a_{11} a_{12}}_{i_2 i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}} \\
(\Xi_{10})^{i_{10} a_7 a_8}_{i_3 i_4 a_9} &= +t^{a_7 a_8 a_{11}}_{i_3 i_4 i_{12}} v^{i_{10} i_{12}}_{a_9 a_{11}} \\
(\Xi_{11})^{i_{10} a_8}_{i_4 a_9} &= +t^{a_8 a_{11}}_{i_4 i_{12}} v^{i_{10} i_{12}}_{a_9 a_{11}} \\
(\Xi_{12})^{i_9 i_{10}}_{i_3 i_4} &= +\tfrac{1}{2} t^{a_{11} a_{12}}_{i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}} \\
(\Xi_{13})^{i_{10} a_8}_{i_4 a_9} &= +\tilde{t}^{a'_{11} a_8}_{i_4 i_{12}} v^{i_{10} i_{12}}_{a'_{11} a_9} \\
(\Xi_{14})^{i_9 i_{10}}_{i_3 i_4} &= +\tfrac{1}{2} t^{i_{11} i_{12}}_{i_3 i_4} V^{i_9 i_{10}}_{i_{11} i_{12}} \\
(\Xi_{15})^{i_9 i_{10}}_{i_3 i_4} &= +P_2 t^{a_{11}}_{i_3} (\Xi_3)^{i_9 i_{10}}_{i_4 a_{11}} \\
(\Xi_{16})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} &= +P_3 \tilde{t}^{a'_{11} a_8}_{i_2 i_3} (\Xi_5)^{i_9 i_{10}}_{i_4 a'_{11}} \\
(\Xi_{17})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} &= +P_2 P_4 \tilde{t}^{a'_{11} a_7}_{i_1 i_2} (\Xi_8)^{i_9 i_{10} a_8}_{i_3 i_4 a'_{11}} \\
(\xi_8)^{i_{10} a_8}_{i_4 a_9} &= -v^{i_{10} a_8}_{i_4 a_9} + (\Xi_1)^{i_{10} a_8}_{i_4 a_9} + (\Xi_{11})^{i_{10} a_8}_{i_4 a_9} + (\Xi_{13})^{i_{10} a_8}_{i_4 a_9} \\
(\xi_7)^{i_9 i_{10}}_{i_3 i_4} &= +v^{i_9 i_{10}}_{i_3 i_4} - (\Xi_0)^{i_9 i_{10}}_{i_3 i_4} + \tfrac{1}{2} (\Xi_{15})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{12})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{14})^{i_9 i_{10}}_{i_3 i_4} \\
(\xi_{6,2})^{i_{10} i_{11}}_{i_4 a_9} &= +v^{i_{10} i_{11}}_{i_4 a_9} - (\Xi_3)^{i_{10} i_{11}}_{i_4 a_9} \\
(\xi_{6,0})^{a_7 a_8}_{a_9 a_{10}} &= -v^{a_7 a_8}_{a_9 a_{10}} - \tfrac{1}{2} t^{a_7 a_8}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} \\
(\xi_6)^{a_6 a_7 a_8}_{i_3 i_4 a_9} &= +\tfrac{1}{2} P_3 t^{a_6 a_{10}}_{i_3 i_4} (\xi_{6,0})^{a_7 a_8}_{a_9 a_{10}} - P_3 \tilde{t}^{a'_{10} a_6}_{i_3 i_4} v^{a_7 a_8}_{a'_{10} a_9} \\
&\quad + \tfrac{1}{2} P_2 t^{a_6 a_7 a_8}_{i_3 i_{10} i_{11}} (\xi_{6,2})^{i_{10} i_{11}}_{i_4 a_9} - P_3 t^{a_6 a_7 a_{10}}_{i_3 i_4 i_{11}} v^{i_{11} a_8}_{a_9 a_{10}} \\
&\quad - \tfrac{1}{2} P_3 t^{a_6 a_7}_{i_{10} i_{11}} (\Xi_4)^{i_{10} i_{11} a_8}_{i_3 i_4 a_9} - \tfrac{1}{2} t^{a_6 a_7 a_8 a_{10}}_{i_3 i_4 i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} \\
(\xi_{5,1})^{i_{10} i_{11}}_{i_4 a_9} &= -v^{i_{10} i_{11}}_{i_4 a_9} + (\Xi_3)^{i_{10} i_{11}}_{i_4 a_9} \\
(\xi_5)^{a_7 a_8}_{i_4 a_9} &= -v^{a_7 a_8}_{i_4 a_9} + t^{a_{10}}_{i_4} v^{a_7 a_8}_{a_9 a_{10}} + \tfrac{1}{2} t^{a_7 a_8}_{i_{10} i_{11}} (\xi_{5,1})^{i_{10} i_{11}}_{i_4 a_9} + P_2 t^{a_7 a_{10}}_{i_4 i_{11}} v^{i_{11} a_8}_{a_9 a_{10}} \\
&\quad + P_2 \tilde{t}^{a'_{10} a_7}_{i_4 i_{11}} v^{i_{11} a_8}_{a'_{10} a_9} + \tfrac{1}{2} t^{a_7 a_8 a_{10}}_{i_4 i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} \\
(\xi_{5,1})^{i_{10} i_{11}}_{i_4 a_9} &= -v^{i_{10} i_{11}}_{i_4 a_9} + (\Xi_3)^{i_{10} i_{11}}_{i_4 a_9} \\
(\xi_5)^{a_7 a_8}_{i_4 a_9} &= -v^{a_7 a_8}_{i_4 a_9} + t^{a_{10}}_{i_4} v^{a_7 a_8}_{a_9 a_{10}} + \tfrac{1}{2} t^{a_7 a_8}_{i_{10} i_{11}} (\xi_{5,1})^{i_{10} i_{11}}_{i_4 a_9} + P_2 t^{a_7 a_{10}}_{i_4 i_{11}} v^{i_{11} a_8}_{a_9 a_{10}} \\
&\quad + P_2 \tilde{t}^{a'_{10} a_7}_{i_4 i_{11}} v^{i_{11} a_8}_{a'_{10} a_9} + \tfrac{1}{2} t^{a_7 a_8 a_{10}}_{i_4 i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} \\
(\xi_{4,6})^{i_9 i_{11}}_{i_4 a'_{10}} &= -v^{i_9 i_{11}}_{i_4 a'_{10}} + (\Xi_5)^{i_9 i_{11}}_{i_4 a'_{10}} \\
(\xi_{4,4})^{i_9 i_{11}}_{i_4 a_{10}} &= +v^{i_9 i_{11}}_{i_4 a_{10}} - (\Xi_3)^{i_9 i_{11}}_{i_4 a_{10}} \\
(\xi_{4,3})^{i_9 a_8}_{i_4 a_{10}} &= +v^{i_9 a_8}_{i_4 a_{10}} - \tfrac{1}{2} (\Xi_1)^{i_9 a_8}_{i_4 a_{10}} \\
(\xi_{4,2})^{i_9 i_{10}}_{i_3 i_4} &= +v^{i_9 i_{10}}_{i_3 i_4} - (\Xi_0)^{i_9 i_{10}}_{i_3 i_4} + \tfrac{1}{2} (\Xi_{15})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{12})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{14})^{i_9 i_{10}}_{i_3 i_4} \\
(\xi_{4,1})^{i_9}_{a'_{10}} &= -f^{i_9}_{a'_{10}} - t^{a_{11}}_{i_{12}} v^{i_9 i_{12}}_{a'_{10} a_{11}} \\
(\xi_{4,0})^{i_9}_{a_{10}} &= +f^{i_9}_{a_{10}} + (\Xi_6)^{i_9}_{a_{10}} \\
(\xi_4)^{i_9 a_8}_{i_3 i_4} &= -v^{i_9 a_8}_{i_3 i_4} + t^{a_8 a_{10}}_{i_3 i_4} (\xi_{4,0})^{i_9}_{a_{10}} + \tilde{t}^{a'_{10} a_8}_{i_3 i_4} (\xi_{4,1})^{i_9}_{a'_{10}} + t^{a_8}_{i_{10}} (\xi_{4,2})^{i_9 i_{10}}_{i_3 i_4} \\
&\quad + P_2 t^{a_{10}}_{i_3} (\xi_{4,3})^{i_9 a_8}_{i_4 a_{10}} + P_2 t^{a_8 a_{10}}_{i_3 i_{11}} (\xi_{4,4})^{i_9 i_{11}}_{i_4 a_{10}} - \tfrac{1}{2} t^{a_{10} a_{11}}_{i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} \\
&\quad + P_2 \tilde{t}^{a'_{10} a_8}_{i_3 i_{11}} (\xi_{4,6})^{i_9 i_{11}}_{i_4 a'_{10}} - \tfrac{1}{2} t^{i_{10} i_{11}}_{i_3 i_4} V^{i_9 a_8}_{i_{10} i_{11}} + \tfrac{1}{2} t^{a_8 a_{10} a_{11}}_{i_3 i_4 i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}} \\
(\xi_{3,5})^{i_9 i_{11}}_{i_4 a_{10}} &= -v^{i_9 i_{11}}_{i_4 a_{10}} + (\Xi_3)^{i_9 i_{11}}_{i_4 a_{10}} \\
(\xi_{3,4,0})^{i_9 i_{10}}_{i_4 a_{11}} &= -v^{i_9 i_{10}}_{i_4 a_{11}} + (\Xi_3)^{i_9 i_{10}}_{i_4 a_{11}} \\
(\xi_{3,4})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} &= +(\Xi_2)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} - (\Xi_{16})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + (\Xi_9)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + P_3 t^{a_8 a_{11}}_{i_2 i_3} (\xi_{3,4,0})^{i_9 i_{10}}_{i_4 a_{11}} \\
(\xi_{3,3})^{i_9 a_8}_{i_4 a'_{10}} &= +v^{i_9 a_8}_{i_4 a'_{10}} - t^{a_{11}}_{i_4} v^{i_9 a_8}_{a'_{10} a_{11}} - t^{a_8 a_{11}}_{i_4 i_{12}} v^{i_9 i_{12}}_{a'_{10} a_{11}} + \tilde{t}^{a'_{11} a_8}_{i_4 i_{12}} v^{i_9 i_{12}}_{a'_{10} a'_{11}} \\
(\xi_{3,2})^{i_9 a_8}_{i_4 a_{10}} &= -v^{i_9 a_8}_{i_4 a_{10}} + (\Xi_1)^{i_9 a_8}_{i_4 a_{10}} + (\Xi_{11})^{i_9 a_8}_{i_4 a_{10}} + (\Xi_{13})^{i_9 a_8}_{i_4 a_{10}} \\
(\xi_{3,1})^{i_9 i_{10}}_{i_3 i_4} &= -v^{i_9 i_{10}}_{i_3 i_4} + (\Xi_0)^{i_9 i_{10}}_{i_3 i_4} - \tfrac{1}{2} (\Xi_{15})^{i_9 i_{10}}_{i_3 i_4} - (\Xi_{12})^{i_9 i_{10}}_{i_3 i_4} - (\Xi_{14})^{i_9 i_{10}}_{i_3 i_4} \\
(\xi_{3,0})^{i_9}_{a_{10}} &= -f^{i_9}_{a_{10}} - (\Xi_6)^{i_9}_{a_{10}} \\
(\xi_3)^{i_9 a_7 a_8}_{i_2 i_3 i_4} &= +t^{a_7 a_8 a_{10}}_{i_2 i_3 i_4} (\xi_{3,0})^{i_9}_{a_{10}} + \tfrac{1}{2} P_3 t^{a_7 a_8}_{i_2 i_{10}} (\xi_{3,1})^{i_9 i_{10}}_{i_3 i_4} + P_2 P_3 t^{a_7 a_{10}}_{i_2 i_3} (\xi_{3,2})^{i_9 a_8}_{i_4 a_{10}} \\
&\quad + P_2 P_3 \tilde{t}^{a'_{10} a_7}_{i_2 i_3} (\xi_{3,3})^{i_9 a_8}_{i_4 a'_{10}} + P_2 t^{a_7}_{i_{10}} (\xi_{3,4})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
&\quad + P_3 t^{a_7 a_8 a_{10}}_{i_2 i_3 i_{11}} (\xi_{3,5})^{i_9 i_{11}}_{i_4 a_{10}} + \tfrac{1}{2} P_2 t^{a_7 a_{10} a_{11}}_{i_2 i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} - \tfrac{1}{2} t^{a_7 a_8 a_{10} a_{11}}_{i_2 i_3 i_4 i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}} \\
(\xi_{2,6})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} &= +\tfrac{1}{2} P_2 \tilde{t}^{a'_{11} a_7}_{i_3 i_4} v^{i_9 a_8}_{a'_{10} a'_{11}} - t^{a_7 a_8 a_{11}}_{i_3 i_4 i_{12}} v^{i_9 i_{12}}_{a'_{10} a_{11}} \\
(\xi_{2,4})^{i_9 i_{11}}_{i_4 a_{10}} &= +v^{i_9 i_{11}}_{i_4 a_{10}} - (\Xi_3)^{i_9 i_{11}}_{i_4 a_{10}} \\
(\xi_{2,3})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} &= +(\Xi_{10})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} + \tfrac{1}{2} P_2 t^{a_7 a_{11}}_{i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} + P_2 \tilde{t}^{a'_{11} a_7}_{i_3 i_4} v^{i_9 a_8}_{a'_{11} a_{10}} \\
(\xi_{2,2,1})^{i_9 i_{10} a_8}_{i_3 i_4 a_{11}} &= -(\Xi_4)^{i_9 i_{10} a_8}_{i_3 i_4 a_{11}} - \tfrac{1}{2} t^{a_8 a_{12}}_{i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}} \\
(\xi_{2,2,0})^{i_9 i_{10}}_{i_4 a_{11}} &= -v^{i_9 i_{10}}_{i_4 a_{11}} + (\Xi_3)^{i_9 i_{10}}_{i_4 a_{11}} \\
(\xi_{2,2})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} &= +(\Xi_7)^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} - \tfrac{1}{2} (\Xi_{17})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} \\
&\quad + P_4 t^{a_7 a_8 a_{11}}_{i_1 i_2 i_3} (\xi_{2,2,0})^{i_9 i_{10}}_{i_4 a_{11}} + P_2 P_4 t^{a_7 a_{11}}_{i_1 i_2} (\xi_{2,2,1})^{i_9 i_{10} a_8}_{i_3 i_4 a_{11}} \\
(\xi_{2,1})^{i_9 a_8}_{i_4 a_{10}} &= +v^{i_9 a_8}_{i_4 a_{10}} - (\Xi_1)^{i_9 a_8}_{i_4 a_{10}} - (\Xi_{11})^{i_9 a_8}_{i_4 a_{10}} - (\Xi_{13})^{i_9 a_8}_{i_4 a_{10}} \\
(\xi_{2,0})^{i_9}_{a_{10}} &= +f^{i_9}_{a_{10}} + (\Xi_6)^{i_9}_{a_{10}} \\
(\xi_2)^{i_9 a_6 a_7 a_8}_{i_1 i_2 i_3 i_4} &= +t^{a_6 a_7 a_8 a_{10}}_{i_1 i_2 i_3 i_4} (\xi_{2,0})^{i_9}_{a_{10}} + P_3 P_4 t^{a_6 a_7 a_{10}}_{i_1 i_2 i_3} (\xi_{2,1})^{i_9 a_8}_{i_4 a_{10}} \\
&\quad + \tfrac{1}{2} P_3 t^{a_6}_{i_{10}} (\xi_{2,2})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} + P_3 P_4 t^{a_6 a_{10}}_{i_1 i_2} (\xi_{2,3})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} \\
&\quad + P_4 t^{a_6 a_7 a_8 a_{10}}_{i_1 i_2 i_3 i_{11}} (\xi_{2,4})^{i_9 i_{11}}_{i_4 a_{10}} - \tfrac{1}{2} P_3 t^{a_6 a_7 a_{10} a_{11}}_{i_1 i_2 i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} \\
&\quad + P_3 P_4 \tilde{t}^{a'_{10} a_6}_{i_1 i_2} (\xi_{2,6})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} \\
(\xi_{12})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} &= -\tfrac{1}{2} (\Xi_{17})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} + (\Xi_7)^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} \\
(\xi_{11})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} &= +(\Xi_2)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} - (\Xi_{16})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + (\Xi_9)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
(\xi_{10})^{a_6 a_7 a_8}_{i_3 i_4 a'_9} &= -\tfrac{1}{2} P_3 \tilde{t}^{a'_{10} a_6}_{i_3 i_4} v^{a_7 a_8}_{a'_9 a'_{10}} + P_3 t^{a_6 a_7 a_{10}}_{i_3 i_4 i_{11}} v^{i_{11} a_8}_{a'_9 a_{10}} + \tfrac{1}{2} t^{a_6 a_7 a_8 a_{10}}_{i_3 i_4 i_{11} i_{12}} v^{i_{11} i_{12}}_{a'_9 a_{10}} \\
(\xi_1)^{a_8}_{a_9} &= +f^{a_8}_{a_9} - t^{a_{10}}_{i_{11}} v^{i_{11} a_8}_{a_9 a_{10}} - \tfrac{1}{2} t^{a_8 a_{10}}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} - \tfrac{1}{2} \tilde{t}^{a'_{10} a_8}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a'_{10} a_9} \\
(\xi_{0,0})^{i_9}_{a_{10}} &= -f^{i_9}_{a_{10}} - (\Xi_6)^{i_9}_{a_{10}} \\
(\xi_0)^{i_9}_{i_4} &= -f^{i_9}_{i_4} + t^{a_{10}}_{i_4} (\xi_{0,0})^{i_9}_{a_{10}} - t^{a_{10}}_{i_{11}} v^{i_9 i_{11}}_{i_4 a_{10}} - \tfrac{1}{2} t^{a_{10} a_{11}}_{i_4 i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}} - \tfrac{1}{2} t^{i_{10} i_{11}}_{i_4 i_{12}} V^{i_9 i_{12}}_{i_{10} i_{11}} \\
\delta^{a_5 a_6 a_7 a_8}_{i_1 i_2 i_3 i_4} &= +P_4 t^{a_5 a_6 a_7 a_8}_{i_1 i_2 i_3 i_9} (\xi_0)^{i_9}_{i_4} + P_4 t^{a_5 a_6 a_7 a_9}_{i_1 i_2 i_3 i_4} (\xi_1)^{a_8}_{a_9} \\
&\quad + P_4 t^{a_5}_{i_9} (\xi_2)^{i_9 a_6 a_7 a_8}_{i_1 i_2 i_3 i_4} + P_4 P_4 t^{a_5 a_6}_{i_1 i_9} (\xi_3)^{i_9 a_7 a_8}_{i_2 i_3 i_4} \\
&\quad + P_4 P_4 t^{a_5 a_6 a_7}_{i_1 i_2 i_9} (\xi_4)^{i_9 a_8}_{i_3 i_4} + P_4 P_4 t^{a_5 a_6 a_9}_{i_1 i_2 i_3} (\xi_5)^{a_7 a_8}_{i_4 a_9} \\
&\quad + P_4 P_4 t^{a_5 a_9}_{i_1 i_2} (\xi_6)^{a_6 a_7 a_8}_{i_3 i_4 a_9} + \tfrac{1}{2} P_4 t^{a_5 a_6 a_7 a_8}_{i_1 i_2 i_9 i_{10}} (\xi_7)^{i_9 i_{10}}_{i_3 i_4} \\
&\quad + P_4 P_4 t^{a_5 a_6 a_7 a_9}_{i_1 i_2 i_3 i_{10}} (\xi_8)^{i_{10} a_8}_{i_4 a_9} + \tfrac{1}{2} P_4 t^{a_5 a_6 a_9 a_{10}}_{i_1 i_2 i_3 i_4} v^{a_7 a_8}_{a_9 a_{10}} \\
&\quad + P_4 P_4 \tilde{t}^{a'_9 a_5}_{i_1 i_2} (\xi_{10})^{a_6 a_7 a_8}_{i_3 i_4 a'_9} + \tfrac{1}{2} P_4 P_4 t^{a_5 a_6 a_7}_{i_1 i_9 i_{10}} (\xi_{11})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
&\quad + \tfrac{1}{2} P_4 t^{a_5 a_6}_{i_9 i_{10}} (\xi_{12})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} + \tfrac{1}{2} P_4 P_4 t^{a_5 a_6 a_9}_{i_1 i_2 i_{10}} (\Xi_{10})^{i_{10} a_7 a_8}_{i_3 i_4 a_9}
\end{aligned}
$$

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D. Λ-CCSD-R12

TABLE ESI.4.XII: The computational sequence and intermediates for the Λ_1 amplitude equation of Λ-CCSD-R12

$$
\begin{aligned}
(\Xi_0)^{i_2}_{a_6} &= +t^{a_7}_{i_8} v^{i_2 i_8}_{a_6 a_7} \\
(\Xi_1)^{i_5}_{i_3} &= +t^{a_6}_{i_3} \lambda^{i_5}_{a_6} \\
(\Xi_2)^{i_5}_{i_3} &= +\tfrac{1}{2} t^{a_6 a_7}_{i_3 i_8} \lambda^{i_5 i_8}_{a_6 a_7} \\
(\Xi_3)^{i_5 i_8}_{i_6 i_7} &= +\tfrac{1}{2} \lambda^{i_5 i_8}_{i_9 i_{10}} X^{i_9 i_{10}}_{i_6 i_7} \\
(\Xi_4)^{i_6 i_7}_{i_3 a_5} &= +t^{a_8}_{i_3} \lambda^{i_6 i_7}_{a_5 a_8} \\
(\Xi_5)^{i_6 i_7}_{i_3 a'_5} &= +t^{a_8}_{i_3} \tilde{\lambda}^{i_6 i_7}_{a'_5 a_8} \\
(\Xi_6)^{i_2 i_6}_{i_3 i_4} &= +\tfrac{1}{2} t^{a_7 a_8}_{i_3 i_4} \lambda^{i_2 i_6}_{a_7 a_8} \\
(\Xi_7)^{i_2 i_7}_{i_4 a_6} &= +t^{a_8}_{i_4} v^{i_2 i_7}_{a_6 a_8} \\
(\Xi_8)^{i_2 i_7}_{i_4 a'_6} &= +t^{a_8}_{i_4} v^{i_2 i_7}_{a'_6 a_8} \\
(\Xi_9)^{i_2}_{a'_6} &= +t^{a_7}_{i_8} v^{i_2 i_8}_{a'_6 a_7} \\
(\Xi_{10})^{i_5}_{i_3} &= +\tfrac{1}{2} t^{i_6 i_7}_{i_3 i_8} (\Xi_3)^{i_5 i_8}_{i_6 i_7} \\
(\Xi_{11})^{i_2 i_6}_{i_3 i_4} &= +P_2 t^{a_7}_{i_3} (\Xi_4)^{i_2 i_6}_{i_4 a_7} \\
(\Xi_{12})^{i_2 i_6}_{i_3 i_4} &= +\tfrac{1}{2} t^{i_7 i_8}_{i_3 i_4} (\Xi_3)^{i_2 i_6}_{i_7 i_8} \\
(\xi_9)^{a'_4}_{i_3} &= +\lambda^{i_5}_{a_6} \tilde{t}^{a'_4 a_6}_{i_3 i_5} + \tfrac{1}{2} \tilde{t}^{a'_4 a'_5}_{i_6 i_7} (\Xi_4)^{i_6 i_7}_{i_3 a_5} + \tfrac{1}{2} \tilde{t}^{a'_4 a'_5}_{i_6 i_7} (\Xi_5)^{i_6 i_7}_{i_3 a'_5} \\
(\xi_8)^{i_2 a'_5}_{i_3 i_4} &= +\lambda^{i_2}_{a_6} \tilde{t}^{a'_5 a_6}_{i_3 i_4} - P_2 \tilde{t}^{a'_5 a_6}_{i_3 i_7} (\Xi_4)^{i_2 i_7}_{i_4 a_6} - P_2 \tilde{t}^{a'_5 a'_6}_{i_3 i_7} (\Xi_5)^{i_2 i_7}_{i_4 a'_6} \\
(\xi_{7,3})^{i_2}_{i_4} &= -(\Xi_2)^{i_2}_{i_4} - (\Xi_{10})^{i_2}_{i_4} \\
(\xi_{7,1})^{i_2 i_6}_{i_3 i_4} &= -\tfrac{1}{2} (\Xi_{11})^{i_2 i_6}_{i_3 i_4} - (\Xi_6)^{i_2 i_6}_{i_3 i_4} - (\Xi_{12})^{i_2 i_6}_{i_3 i_4} \\
(\xi_7)^{i_2 a_5}_{i_3 i_4} &= -t^{a_5 a_6}_{i_3 i_4} \lambda^{i_2}_{a_6} + t^{a_5}_{i_6} (\xi_{7,1})^{i_2 i_6}_{i_3 i_4} + P_2 t^{a_5 a_6}_{i_3 i_7} (\Xi_4)^{i_2 i_7}_{i_4 a_6} + P_2 t^{a_5}_{i_3} (\xi_{7,3})^{i_2}_{i_4} \\
&\quad - P_2 \tilde{t}^{a'_6 a_5}_{i_3 i_7} (\Xi_5)^{i_2 i_7}_{i_4 a'_6} \\
(\xi_{6,0})^{i_5}_{i_3} &= +(\Xi_1)^{i_5}_{i_3} + (\Xi_2)^{i_5}_{i_3} + (\Xi_{10})^{i_5}_{i_3} \\
(\xi_6)^{a_4}_{i_3} &= +t^{a_4}_{i_5} (\xi_{6,0})^{i_5}_{i_3} - t^{a_4 a_5}_{i_3 i_6} \lambda^{i_6}_{a_5} - \tfrac{1}{2} t^{a_4 a_5}_{i_6 i_7} (\Xi_4)^{i_6 i_7}_{i_3 a_5} + \tfrac{1}{2} \tilde{t}^{a'_5 a_4}_{i_6 i_7} (\Xi_5)^{i_6 i_7}_{i_3 a'_5} \\
(\xi_5)^{a_4}_{a_3} &= -t^{a_4}_{i_5} \lambda^{i_5}_{a_3} - \tfrac{1}{2} t^{a_4 a_5}_{i_6 i_7} \lambda^{i_6 i_7}_{a_3 a_5} - \tfrac{1}{2} \tilde{t}^{a'_5 a_4}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a'_5 a_3} \\
(\xi_4)^{i_4}_{i_3} &= -(\Xi_1)^{i_4}_{i_3} - (\Xi_2)^{i_4}_{i_3} - (\Xi_{10})^{i_4}_{i_3} \\
(\xi_{27})^{a'_4}_{a'_3} &= +\tfrac{1}{2} \tilde{t}^{a'_4 a'_5}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a'_3 a'_5} + \tfrac{1}{2} \tilde{t}^{a'_4 a_5}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a'_3 a_5} \\
(\xi_{26})^{i_2 a'_5}_{i_3 a'_4} &= -\tilde{t}^{a'_5 a'_6}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a'_4 a'_6} - \tilde{t}^{a'_5 a_6}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a'_4 a_6} \\
(\xi_{25})^{a_4}_{a'_3} &= -\tfrac{1}{2} t^{a_4 a_5}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a'_3 a_5} + \tfrac{1}{2} \tilde{t}^{a'_5 a_4}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a'_3 a'_5} \\
(\xi_{24})^{i_2 a_5}_{i_3 a'_4} &= -t^{a_5}_{i_6} (\Xi_5)^{i_2 i_6}_{i_3 a'_4} + t^{a_5 a_6}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a'_4 a_6} - \tilde{t}^{a'_6 a_5}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a'_4 a'_6} \\
(\xi_{23})^{a'_4}_{a'_3} &= +\tfrac{1}{2} \lambda^{i_5 i_6}_{a_3 a_7} \tilde{t}^{a'_4 a_7}_{i_5 i_6} - \tfrac{1}{2} \tilde{t}^{a'_4 a'_5}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a'_5 a_3} \\
(\xi_{22})^{i_2 a'_5}_{i_3 a_4} &= -\lambda^{i_2 i_6}_{a_4 a_7} \tilde{t}^{a'_5 a_7}_{i_3 i_6} + \tilde{t}^{a'_5 a'_6}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a'_6 a_4} \\
(\xi_{21})^{i_2 i_5}_{i_3 i_4} &= +(\Xi_6)^{i_2 i_5}_{i_3 i_4} + (\Xi_{12})^{i_2 i_5}_{i_3 i_4} \\
(\xi_{20})^{i_2 a_5}_{i_3 a_4} &= -t^{a_5}_{i_6} (\Xi_4)^{i_2 i_6}_{i_3 a_4} + t^{a_5 a_6}_{i_3 i_7} \lambda^{i_2 i_7}_{a_4 a_6} + \tilde{t}^{a'_6 a_5}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a'_6 a_4} \\
(\xi_2)^{i_2}_{i_3} &= +(\Xi_1)^{i_2}_{i_3} + (\Xi_2)^{i_2}_{i_3} + (\Xi_{10})^{i_2}_{i_3} \\
(\xi_{18})^{i_2 a_5}_{i_3 i_4} &= -t^{a_5}_{i_6} \lambda^{i_2 i_6}_{i_3 i_4} \\
(\xi_{16})^{i_2 a_5}_{a_3 a_4} &= -t^{a_5}_{i_6} \lambda^{i_2 i_6}_{a_3 a_4} \\
(\xi_{11,5})^{i_2 i_7}_{i_4 a_6} &= +v^{i_2 i_7}_{i_4 a_6} - (\Xi_7)^{i_2 i_7}_{i_4 a_6} \\
(\xi_{11,4})^{i_2 i_7}_{i_4 a'_6} &= +v^{i_2 i_7}_{i_4 a'_6} - (\Xi_8)^{i_2 i_7}_{i_4 a'_6} \\
(\xi_{11,2})^{i_2 a'_5}_{i_4 a_6} &= +v^{i_2 a'_5}_{i_4 a_6} - \tfrac{1}{2} t^{a_7}_{i_4} v^{i_2 a'_5}_{a_6 a_7} \\
(\xi_{11,1})^{i_2}_{a_6} &= +f^{i_2}_{a_6} + (\Xi_0)^{i_2}_{a_6} \\
(\xi_{11,0})^{i_2}_{a'_6} &= +f^{i_2}_{a'_6} + (\Xi_9)^{i_2}_{a'_6} \\
(\xi_{11})^{i_2 a'_5}_{i_3 i_4} &= -v^{i_2 a'_5}_{i_3 i_4} + \tilde{t}^{a'_5 a_6}_{i_3 i_4} (\xi_{11,0})^{i_2}_{a'_6} + \tilde{t}^{a'_5 a_6}_{i_3 i_4} (\xi_{11,1})^{i_2}_{a_6} + P_2 t^{a_6}_{i_3} (\xi_{11,2})^{i_2 a'_5}_{i_4 a_6} \\
&\quad - \tfrac{1}{2} t^{a_6 a_7}_{i_3 i_4} v^{i_2 a'_5}_{a_6 a_7} + P_2 \tilde{t}^{a'_5 a'_6}_{i_3 i_7} (\xi_{11,4})^{i_2 i_7}_{i_4 a'_6} + P_2 \tilde{t}^{a'_5 a_6}_{i_3 i_7} (\xi_{11,5})^{i_2 i_7}_{i_4 a_6} \\
&\quad - \tfrac{1}{2} t^{i_6 i_7}_{i_3 i_4} V^{i_2 a'_5}_{i_6 i_7} \\
(\xi_{10,6})^{i_2 i_7}_{i_4 a'_6} &= +v^{i_2 i_7}_{i_4 a'_6} - (\Xi_8)^{i_2 i_7}_{i_4 a'_6} \\
(\xi_{10,4})^{i_2 i_7}_{i_4 a_6} &= -v^{i_2 i_7}_{i_4 a_6} + (\Xi_7)^{i_2 i_7}_{i_4 a_6} \\
(\xi_{10,3,0})^{i_2 i_6}_{i_4 a_7} &= +v^{i_2 i_6}_{i_4 a_7} - \tfrac{1}{2} (\Xi_7)^{i_2 i_6}_{i_4 a_7} \\
(\xi_{10,3})^{i_2 i_6}_{i_3 i_4} &= +P_2 t^{a_7}_{i_3} (\xi_{10,3,0})^{i_2 i_6}_{i_4 a_7} - \tfrac{1}{2} t^{a_7 a_8}_{i_3 i_4} v^{i_2 i_6}_{a_7 a_8} - \tfrac{1}{2} t^{i_7 i_8}_{i_3 i_4} V^{i_2 i_6}_{i_7 i_8} \\
(\xi_{10,2})^{i_2 a_5}_{i_4 a_6} &= -v^{i_2 a_5}_{i_4 a_6} + \tfrac{1}{2} t^{a_7}_{i_4} v^{i_2 a_5}_{a_6 a_7} \\
(\xi_{10,1})^{i_2}_{a'_6} &= +f^{i_2}_{a'_6} + (\Xi_9)^{i_2}_{a'_6} \\
(\xi_{10,0})^{i_2}_{a_6} &= -f^{i_2}_{a_6} - (\Xi_0)^{i_2}_{a_6} \\
(\xi_{10})^{i_2 a_5}_{i_3 i_4} &= +v^{i_2 a_5}_{i_3 i_4} + t^{a_5 a_6}_{i_3 i_4} (\xi_{10,0})^{i_2}_{a_6} + \tilde{t}^{a'_6 a_5}_{i_3 i_4} (\xi_{10,1})^{i_2}_{a'_6} + P_2 t^{a_6}_{i_3} (\xi_{10,2})^{i_2 a_5}_{i_4 a_6} \\
&\quad + t^{a_5}_{i_6} (\xi_{10,3})^{i_2 i_6}_{i_3 i_4} + P_2 t^{a_5 a_6}_{i_3 i_7} (\xi_{10,4})^{i_2 i_7}_{i_4 a_6} + \tfrac{1}{2} t^{a_6 a_7}_{i_3 i_4} v^{i_2 a_5}_{a_6 a_7} \\
&\quad + P_2 \tilde{t}^{a'_6 a_5}_{i_3 i_7} (\xi_{10,6})^{i_2 i_7}_{i_4 a'_6} + \tfrac{1}{2} t^{i_6 i_7}_{i_3 i_4} V^{i_2 a_5}_{i_6 i_7} \\
(\xi_1)^{a_3}_{a_1} &= -f^{a_3}_{a_1} + t^{a_4}_{i_5} v^{i_5 a_3}_{a_1 a_4} + t^{a_3}_{i_4} (\Xi_0)^{i_4}_{a_1} \\
(\xi_{0,0})^{i_2}_{a_4} &= +f^{i_2}_{a_4} + (\Xi_0)^{i_2}_{a_4} \\
(\xi_0)^{i_2}_{i_3} &= +f^{i_2}_{i_3} + t^{a_4}_{i_3} (\xi_{0,0})^{i_2}_{a_4} + t^{a_4 a_5}_{i_5 i_3} v^{i_2 i_5}_{i_3 a_4} + \tfrac{1}{2} t^{a_4 a_5}_{i_3 i_6} v^{i_2 i_6}_{a_4 a_5} + \tfrac{1}{2} t^{i_4 i_5}_{i_3 i_6} V^{i_2 i_6}_{i_4 i_5} \\
\delta^{i_2}_{a_1} &= +f^{i_2}_{a_1} + (\Xi_0)^{i_2}_{a_1} + \lambda^{i_2}_{a_1} (\xi_0)^{i_2}_{i_3} + \lambda^{i_2}_{a_3} (\xi_1)^{a_3}_{a_1} + f^{i_3}_{a_1} (\xi_2)^{i_2}_{i_3} + \lambda^{i_3}_{a_4} v^{i_2 a_4}_{i_3 a_1} \\
&\quad + v^{i_2 i_3}_{i_4 a_1} (\xi_4)^{i_4}_{i_3} + v^{i_2 a_3}_{a_1 a_4} (\xi_5)^{a_4}_{a_3} + v^{i_2 i_3}_{a_1 a_4} (\xi_6)^{a_4}_{i_3} + \tfrac{1}{2} v^{i_3 i_4}_{a_1 a_5} (\xi_7)^{i_2 a_5}_{i_3 i_4} \\
&\quad + \tfrac{1}{2} v^{i_3 i_4}_{a'_5 a_1} (\xi_8)^{i_2 a'_5}_{i_3 i_4} + v^{i_2 i_3}_{a'_4 a_1} (\xi_9)^{a'_4}_{i_3} + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_1 a_5} (\xi_{10})^{i_2 a_5}_{i_3 i_4} \\
&\quad + \tfrac{1}{2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} (\xi_{11})^{i_2 a'_5}_{i_3 i_4} + \tfrac{1}{2} \lambda^{i_2 i_3}_{a_4 a_5} v^{a_4 a_5}_{i_3 a_1} + \tfrac{1}{2} \lambda^{i_2 i_3}_{i_4 i_5} (V^{\dagger})^{i_4 i_5}_{i_3 a_1} \\
&\quad - \tfrac{1}{2} v^{i_2 i_3}_{i_4 i_5} (\Xi_4)^{i_4 i_5}_{i_3 a_1} + v^{i_3 a_4}_{i_5 a_1} (\Xi_4)^{i_2 i_5}_{i_3 a_4} + \tfrac{1}{2} v^{a_3 a_4}_{a_1 a_5} (\xi_{16})^{i_2 a_5}_{a_3 a_4} \\
&\quad + v^{i_3 a'_4}_{i_5 a_1} (\Xi_5)^{i_2 i_5}_{i_3 a'_4} + \tfrac{1}{2} (V^{\dagger})^{i_3 i_4}_{a_1 a_5} (\xi_{18})^{i_2 a_5}_{i_3 i_4} + \tfrac{1}{2} v^{i_3 i_4}_{i_5 a_1} (\Xi_{11})^{i_2 i_5}_{i_3 i_4} \\
&\quad + v^{i_3 a_4}_{a_1 a_5} (\xi_{20})^{i_2 a_5}_{i_3 a_4} + \tfrac{1}{2} v^{i_3 i_4}_{i_5 a_1} (\xi_{21})^{i_2 i_5}_{i_3 i_4} + v^{i_3 a_4}_{a'_4 a_1} (\xi_{22})^{i_2 a'_5}_{i_3 a_4} + v^{i_2 a_3}_{a'_4 a_1} (\xi_{23})^{a'_4}_{a_3} \\
&\quad + v^{i_3 a'_4}_{a_1 a_5} (\xi_{24})^{i_2 a_5}_{i_3 a'_4} + v^{i_2 a'_3}_{a_1 a_4} (\xi_{25})^{a_4}_{a'_3} + v^{i_3 a'_4}_{a'_5 a_1} (\xi_{26})^{i_2 a'_5}_{i_3 a'_4} + v^{i_2 a'_3}_{a'_4 a_1} (\xi_{27})^{a'_4}_{a'_3}
\end{aligned}
$$

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TABLE ESI.4.XIII: The computational sequence and intermediates for the Λ_2 amplitude equation of Λ-CCSD-R12

$$
\begin{aligned}
(\Xi_0)^{i_6}_{a_2'} &= +t^{a_7}_{i_8} v^{i_6 i_8}_{a_2' a_7} \\
(\Xi_1)^{i_4 i_7}_{i_5 a_2'} &= +t^{a_8}_{i_5} v^{i_4 i_7}_{a_2' a_8} \\
(\Xi_2)^{i_3 i_4}_{i_6 a_7} &= +t^{a_8}_{i_6} \lambda^{i_3 i_4}_{a_7 a_8} \\
(\Xi_3)^{i_4 i_8}_{i_6 i_7} &= +\tfrac{1}{2} \lambda^{i_4 i_8}_{i_9 i_{10}} X^{i_9 i_{10}}_{i_6 i_7} \\
(\xi_9)^{i_4 a_6}_{i_5 a_2'} &= -v^{i_4 a_6}_{i_5 a_2'} + t^{a_7}_{i_5} v^{i_4 a_6}_{a_2' a_7} - t^{a_6}_{i_7} (\Xi_1)^{i_4 i_7}_{i_5 a_2'} + \tilde{t}^{a_7' a_6}_{i_5 i_8} v^{i_4 i_8}_{a_7' a_2'} \\
(\xi_{8,0})^{i_3 i_4}_{i_6 a_7} &= -v^{i_3 i_4}_{i_6 a_7} + \tfrac{1}{2} (\Xi_1)^{i_3 i_4}_{i_6 a_7} \\
(\xi_8)^{i_3 i_4}_{i_5 i_6} &= +v^{i_3 i_4}_{i_5 i_6} + P_2 t^{a_7}_{i_5} (\xi_{8,0})^{i_3 i_4}_{i_6 a_7} + \tfrac{1}{2} t^{a_7 a_8}_{i_5 i_6} v^{i_3 i_4}_{a_7 a_8} + \tfrac{1}{2} t^{i_7 i_8}_{i_5 i_6} V^{i_3 i_4}_{i_7 i_8} \\
(\xi_6)^{a_5'}_{a_2'} &= -f^{a_5'}_{a_2'} + t^{a_6}_{i_7} v^{i_7 a_5'}_{a_2' a_6} - \tfrac{1}{2} \tilde{t}^{a_5' a_6}_{i_7 i_8} v^{i_7 i_8}_{a_6' a_2'} + \tfrac{1}{2} \tilde{t}^{a_5' a_6}_{i_7 i_8} v^{i_7 i_8}_{a_2' a_6} \\
(\xi_5)^{a_5}_{a_2'} &= +f^{a_5}_{a_2'} - t^{a_6}_{i_7} v^{i_7 a_5}_{a_2' a_6} - t^{a_5}_{i_6} (\Xi_0)^{i_6}_{a_2'} - \tfrac{1}{2} t^{a_5 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_2' a_6} - \tfrac{1}{2} \tilde{t}^{a_6' a_5}_{i_7 i_8} v^{i_7 i_8}_{a_6' a_2'} \\
(\xi_{4,0})^{i_4}_{a_6'} &= -f^{i_4}_{a_6'} - (\Xi_0)^{i_4}_{a_6'} \\
(\xi_4)^{i_4}_{i_5} &= -f^{i_4}_{i_5} + t^{a_6}_{i_5} (\xi_{4,0})^{i_4}_{a_6'} - t^{a_6}_{i_7} v^{i_4 i_7}_{i_5 a_6'} - \tfrac{1}{2} t^{a_6 a_7}_{i_5 i_8} v^{i_4 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_5 i_8} V^{i_4 i_8}_{i_6 i_7} \\
(\xi_3)^{i_4}_{i_5} &= -t^{a_6}_{i_5} \lambda^{i_4}_{a_6'} - \tfrac{1}{2} t^{a_6 a_7}_{i_5 i_8} \lambda^{i_4 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_5 i_8} (\Xi_3)^{i_4 i_8}_{i_6 i_7} \\
(\xi_{20})^{i_4 a_6'}_{i_5 a_2'} &= +\tilde{t}^{a_6' a_7'}_{i_5 i_8} \tilde{\lambda}^{\,i_4 i_8}_{a_7' a_2'} \\
(\xi_{19})^{a_5'}_{a_2'} &= +\tfrac{1}{2} \lambda^{i_6 i_7}_{a_2' a_8} \tilde{t}^{a_5' a_8}_{i_6 i_7} - \tfrac{1}{2} \tilde{t}^{a_5' a_6'}_{i_7 i_8} \tilde{\lambda}^{\,i_7 i_8}_{a_6' a_2'} \\
(\xi_{18})^{a_5}_{a_2'} &= -\tfrac{1}{2} t^{a_5 a_6}_{i_7 i_8} \lambda^{i_7 i_8}_{a_2' a_6} - \tfrac{1}{2} \tilde{t}^{a_6' a_5}_{i_7 i_8} \tilde{\lambda}^{\,i_7 i_8}_{a_6' a_2'} \\
(\xi_{17})^{i_4 a_6}_{i_5 a_2'} &= +t^{a_6 a_7}_{i_5 i_8} \lambda^{i_4 i_8}_{a_2' a_7} + \tilde{t}^{a_7' a_6}_{i_5 i_8} \tilde{\lambda}^{\,i_4 i_8}_{a_7' a_2'} \\
(\xi_{16})^{i_3 i_4}_{i_5 i_6} &= +\tfrac{1}{2} P_2 t^{a_7}_{i_5} (\Xi_2)^{i_3 i_4}_{i_6 a_7} + \tfrac{1}{2} t^{a_7 a_8}_{i_5 i_6} \lambda^{i_3 i_4}_{a_7 a_8} + \tfrac{1}{2} t^{i_7 i_8}_{i_5 i_6} (\Xi_3)^{i_3 i_4}_{i_7 i_8} \\
(\xi_{15})^{i_3 i_4}_{i_5 a_6'} &= +t^{a_7}_{i_5} \tilde{\lambda}^{\,i_3 i_4}_{a_6' a_7} \\
(\xi_{11})^{i_4 a_6'}_{i_5 a_2'} &= +v^{i_4 a_6'}_{i_5 a_2'} - t^{a_7}_{i_5} v^{i_4 a_6'}_{a_2' a_7} \\
(\xi_1)^{i_3 i_4}_{i_5 a_2'} &= -v^{i_3 i_4}_{i_5 a_2'} + (\Xi_1)^{i_3 i_4}_{i_5 a_2'} \\
(\xi_0)^{i_4}_{a_2'} &= +f^{i_4}_{a_2'} + (\Xi_0)^{i_4}_{a_2'} \\
\delta^{i_3 i_4}_{a_1' a_2'} &= +v^{i_3 i_4}_{a_1' a_2'} + P_2 P_2 \lambda^{i_3}_{a_1'} (\xi_0)^{i_4}_{a_2'} + P_2 \lambda^{i_5}_{a_1'} (\xi_1)^{i_3 i_4}_{i_5 a_2'} - P_2 \lambda^{i_3}_{a_5'} v^{i_4 a_5}_{a_1' a_2'} \\
&\quad + P_2 v^{i_3 i_5}_{a_1' a_2'} (\xi_3)^{i_4}_{i_5} + P_2 \lambda^{i_3 i_5}_{a_1' a_2'} (\xi_4)^{i_4}_{i_5} + P_2 \lambda^{i_3 i_4}_{a_1' a_5'} (\xi_5)^{a_5}_{a_2'} \\
&\quad + P_2 \tilde{\lambda}^{\,i_3 i_4}_{a_5' a_1'} (\xi_6)^{a_5'}_{a_2'} + P_2 f^{i_5}_{a_1'} (\Xi_2)^{i_3 i_4}_{i_5 a_2'} + \tfrac{1}{2} \lambda^{i_5 i_6}_{a_1' a_2'} (\xi_8)^{i_3 i_4}_{i_5 i_6} \\
&\quad + P_2 P_2 \lambda^{i_3 i_5}_{a_1' a_6'} (\xi_9)^{i_4 a_6}_{i_5 a_2'} + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_5' a_6'} v^{a_5 a_6}_{a_1' a_2'} + P_2 P_2 \tilde{\lambda}^{\,i_3 i_5}_{a_6' a_1'} (\xi_{11})^{i_4 a_6'}_{i_5 a_2'} \\
&\quad + \tfrac{1}{2} \lambda^{i_3 i_4}_{i_5 i_6} (V^\dagger)^{i_5 i_6}_{a_1' a_2'} + P_2 P_2 v^{i_3 i_5}_{i_6 a_1'} (\Xi_2)^{i_4 i_6}_{i_5 a_2'} + v^{i_5 a_6}_{a_1' a_2'} (\Xi_2)^{i_3 i_4}_{i_5 a_6'} \\
&\quad + v^{i_5 a_6'}_{a_1' a_2'} (\xi_{15})^{i_3 i_4}_{i_5 a_6'} + \tfrac{1}{2} v^{i_5 i_6}_{a_1' a_2'} (\xi_{16})^{i_3 i_4}_{i_5 i_6} + P_2 P_2 v^{i_3 i_5}_{a_1' a_6'} (\xi_{17})^{i_4 a_6}_{i_5 a_2'} \\
&\quad + P_2 v^{i_3 i_4}_{a_1' a_5'} (\xi_{18})^{a_5}_{a_2'} + P_2 v^{i_3 i_4}_{a_5' a_1'} (\xi_{19})^{a_5'}_{a_2'} + P_2 P_2 v^{i_3 i_5}_{a_6' a_1'} (\xi_{20})^{i_4 a_6'}_{i_5 a_2'}
\end{aligned}
$$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.4.XIV: The computational sequence and intermediates for the geminal λ amplitude equation of Λ-CCSD-R12

$$(\Xi_0)^{i_7 a_6}_{i_1 i_2} = +F^{a'_8 a_6}_{i_1 i_2} f^{i_7}_{a'_8}$$
$$(\Xi_1)^{i_7 a'_5}_{i_1 i_2} = +\lambda^{i_7}_{a_8} F^{a'_5 a_8}_{i_1 i_2}$$
$$(\Xi_2)^{i_7}_{a'_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_3)^{i_4 i_8}_{i_6 i_7} = +\tfrac{1}{2}\lambda^{i_4 i_8}_{i_9 i_{10}} X^{i_9 i_{10}}_{i_6 i_7}$$
$$(\Xi_4)^{i_3 i_4}_{i_5 a'_6} = +t^{a_7}_{i_5} \tilde{\lambda}^{i_3 i_4}_{a'_6 a_7}$$
$$(\Xi_5)^{a_6}_{a'_7} = +t^{a_8}_{i_9} v^{i_9 a_6}_{a'_7 a_8}$$
$$(\Xi_6)^{i_3 i_4}_{i_6 a_7} = +t^{a_8}_{i_6} \lambda^{i_3 i_4}_{a_7 a_8}$$
$$(\Xi_7)^{i_4 a_8}_{i_7 a'_6} = +t^{a_9}_{i_7} v^{i_4 a_8}_{a'_6 a_9}$$
$$(\Xi_8)^{a'_7}_{a'_5} = +t^{a_8}_{i_9} v^{i_9 a'_7}_{a'_5 a_8}$$
$$(\Xi_9)^{i_4 a'_8}_{i_7 a'_5} = +t^{a_9}_{i_7} v^{i_4 a'_8}_{a'_5 a_9}$$
$$(\Xi_{10})^{a_6}_{a'_7} = +\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\Xi_{11})^{a_6}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{12})^{i_7}_{a'_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_{13})^{i_4 i_9}_{i_7 a_6} = +t^{a_{10}}_{i_7} v^{i_4 i_9}_{a_6 a_{10}}$$
$$(\Xi_{14})^{a_6}_{a'_7} = +\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\Xi_{15})^{a'_7}_{a'_5} = +\tfrac{1}{2} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_5 a'_8}$$
$$(\Xi_{16})^{a'_7}_{a'_5} = +\tfrac{1}{2} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_5 a_8}$$
$$(\Xi_{17})^{i_4 a_8}_{i_7 a'_5} = +\tilde{t}^{a'_9 a_8}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_5 a'_9}$$
$$(\Xi_{18})^{a'_5}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_5 a'_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{19})^{a'_5}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_5 a_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\Xi_{20})^{a_6}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{21})^{i_7 a_6}_{i_1 i_2} = +F^{a'_8 a_6}_{i_1 i_2} (\Xi_2)^{i_7}_{a'_8}$$

$$(\xi_{9,8})^{a_7}_{a_6} = -t^{a_8}_{i_9} v^{i_9 a_7}_{a_6 a_8} - \tfrac{1}{2} t^{a_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_7}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\xi_{9,7})^{a'_7}_{a_6} = -t^{a_8}_{i_9} v^{i_9 a'_7}_{a_6 a_8} + \tfrac{1}{2} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6} - \tfrac{1}{2} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8}$$
$$(\xi_{9,6})^{a'_7}_{a'_5} = -(\Xi_8)^{a'_7}_{a'_5} - (\Xi_{15})^{a'_7}_{a'_5} - (\Xi_{16})^{a'_7}_{a'_5}$$
$$(\xi_{9,4})^{i_4 a_8}_{i_7 a_6} = -v^{i_4 a_8}_{i_7 a_6} + t^{a_9}_{i_7} v^{i_4 a_8}_{a_6 a_9} - t^{a_8}_{i_9} (\Xi_{13})^{i_4 i_9}_{i_7 a_6} + t^{a_8 a_9}_{i_7 i_{10}} v^{i_4 i_{10}}_{a_6 a_9} + \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} v^{i_4 i_{10}}_{a'_9 a_6}$$
$$(\xi_{9,3})^{i_4 a'_8}_{i_7 a_6} = -v^{i_4 a'_8}_{i_7 a_6} + t^{a_9}_{i_7} v^{i_4 a'_8}_{a_6 a_9} - \tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} v^{i_4 i_{10}}_{a'_9 a_6}$$
$$(\xi_{9,2})^{i_4 a'_8}_{i_7 a'_5} = -v^{i_4 a'_8}_{i_7 a'_5} + (\Xi_9)^{i_4 a'_8}_{i_7 a'_5}$$
$$(\xi_{9,12})^{a'_7}_{a_6} = -\tfrac{1}{2} \lambda^{i_8 i_9}_{a_6 a_{10}} \tilde{t}^{a'_7 a_{10}}_{i_8 i_9} + \tfrac{1}{2} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\xi_{9,11})^{i_4 a'_8}_{i_7 a_6} = +\lambda^{i_4 i_9}_{a_6 a_{10}} \tilde{t}^{a'_8 a_{10}}_{i_7 i_9} - \tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_9 a_6}$$
$$(\xi_{9,10})^{i_4 a_8}_{i_7 a_6} = -t^{a_8}_{i_9} (\Xi_6)^{i_4 i_9}_{i_7 a_6} + t^{a_8 a_9}_{i_7 i_{10}} \lambda^{i_4 i_{10}}_{a_6 a_9} + \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_9 a_6}$$
$$(\xi_{9,1})^{i_4 a_8}_{i_7 a'_5} = +v^{i_4 a_8}_{i_7 a'_5} - (\Xi_7)^{i_4 a_8}_{i_7 a'_5}$$
$$\begin{aligned}(\xi_9)^{i_3 i_4}_{a'_5 a_6} &= -f^{i_7}_{a_6} (\Xi_4)^{i_3 i_4}_{i_7 a'_5} + P_2 \lambda^{i_3 i_7}_{a_6 a_8} (\xi_{9,1})^{i_4 a_8}_{i_7 a'_5} + P_2 \tilde{\lambda}^{i_3 i_7}_{a'_8 a_6} (\xi_{9,2})^{i_4 a'_8}_{i_7 a'_5} \\ &+ P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} (\xi_{9,3})^{i_4 a'_8}_{i_7 a_6} + P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} (\xi_{9,4})^{i_4 a_8}_{i_7 a_6} + P_2 v^{i_3 i_7}_{i_8 a'_5} (\Xi_6)^{i_4 i_8}_{i_7 a_6} \\ &+ \tilde{\lambda}^{i_3 i_4}_{a'_7 a_6} (\xi_{9,6})^{a'_7}_{a'_5} + \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_7} (\xi_{9,7})^{a'_7}_{a_6} + \tilde{\lambda}^{i_3 i_4}_{a'_5 a_7} (\xi_{9,8})^{a_7}_{a_6} \\ &- P_2 v^{i_3 i_7}_{i_8 a_6} (\Xi_4)^{i_4 i_8}_{i_7 a'_5} + P_2 v^{i_3 i_7}_{a'_5 a_8} (\xi_{9,10})^{i_4 a_8}_{i_7 a_6} + P_2 v^{i_3 i_7}_{a'_5 a'_8} (\xi_{9,11})^{i_4 a'_8}_{i_7 a_6} \\ &+ v^{i_3 i_4}_{a'_5 a'_7} (\xi_{9,12})^{a'_7}_{a_6} + P_2 v^{i_3 i_7}_{a_6 a_8} (\Xi_{17})^{i_4 a_8}_{i_7 a'_5}\end{aligned}$$
$$(\xi_{8,1})^{a_6}_{a'_7} = -(\Xi_5)^{a_6}_{a'_7} - (\Xi_{10})^{a_6}_{a'_7} + (\Xi_{11})^{a_6}_{a'_7}$$

$$(\xi_{8,0,0})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - (\Xi_2)^{i_7}_{a'_8}$$
$$(\xi_{8,0})^{i_7 a'_5}_{i_1 i_2} = +F^{a'_5 a'_8}_{i_1 i_2} (\xi_{8,0,0})^{i_7}_{a'_8} - F^{a'_5 a_8}_{i_1 i_2} (\Xi_{12})^{i_7}_{a_8}$$
$$(\xi_8)^{a'_5 a_6}_{i_1 i_2} = +t^{a_6}_{i_7} (\xi_{8,0})^{i_7 a'_5}_{i_1 i_2} + F^{a'_5 a'_7}_{i_1 i_2} (\xi_{8,1})^{a_6}_{a'_7}$$
$$(\xi_{7,1,0})^{i_3 i_4}_{i_8 a_9} = -v^{i_3 i_4}_{i_8 a_9} + \tfrac{1}{2} (\Xi_{13})^{i_3 i_4}_{i_8 a_9}$$
$$(\xi_{7,1})^{i_3 i_4}_{i_7 i_8} = +P_2 t^{a_9}_{i_7} (\xi_{7,1,0})^{i_3 i_4}_{i_8 a_9} + \tfrac{1}{2} t^{a_9 a_{10}}_{i_7 i_8} v^{i_3 i_4}_{a_9 a_{10}}$$
$$(\xi_{7,0,0})^{i_4}_{a'_8} = -f^{i_4}_{a'_8} - (\Xi_{12})^{i_4}_{a'_8}$$
$$(\xi_{7,0})^{i_4}_{i_7} = +t^{a_8}_{i_7} (\xi_{7,0,0})^{i_4}_{a'_8} - t^{a_8}_{i_9} v^{i_4 i_9}_{i_7 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_7 i_{10}} v^{i_4 i_{10}}_{a_8 a_9} - \tfrac{1}{2} t^{i_8 i_9}_{i_7 i_{10}} V^{i_4 i_{10}}_{i_8 i_9}$$
$$(\xi_7)^{i_3 i_4}_{i_5 i_6} = +P_2 \lambda^{i_3 i_7}_{i_5 i_6} (\xi_{7,0})^{i_4}_{i_7} + \tfrac{1}{2} \lambda^{i_7 i_8}_{i_5 i_6} (\xi_{7,1})^{i_3 i_4}_{i_7 i_8}$$
$$(\xi_6)^{i_5 i_6}_{i_1 i_2} = +B^{i_5 i_6}_{i_1 i_2} + P^{i_5 i_6}_{i_1 i_2}$$
$$(\xi_{4,1})^{i_7 a_6}_{i_1 i_2} = -(\Xi_0)^{i_7 a_6}_{i_1 i_2} - (\Xi_{21})^{i_7 a_6}_{i_1 i_2}$$
$$(\xi_{4,0})^{a_6}_{a'_7} = -f^{a_6}_{a'_7} + (\Xi_5)^{a_6}_{a'_7} + (\Xi_{10})^{a_6}_{a'_7} - (\Xi_{11})^{a_6}_{a'_7}$$
$$(\xi_4)^{a_5 a_6}_{i_1 i_2} = +V^{a_5 a_6}_{i_1 i_2} + P_2 F^{a'_7 a_5}_{i_1 i_2} (\xi_{4,0})^{a_6}_{a'_7} + P_2 t^{a_5}_{i_7} (\xi_{4,1})^{i_7 a_6}_{i_1 i_2}$$
$$(\xi_3)^{i_4}_{i_5} = -t^{a_6}_{i_5} \lambda^{i_4}_{a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_5 i_8} \lambda^{i_4 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_5 i_8} (\Xi_3)^{i_4 i_8}_{i_6 i_7}$$
$$(\xi_{2,3})^{a'_5}_{a'_7} = -(\Xi_{18})^{a'_5}_{a'_7} - (\Xi_{19})^{a'_5}_{a'_7}$$
$$(\xi_{2,2})^{a_6}_{a'_7} = -(\Xi_{14})^{a_6}_{a'_7} + (\Xi_{20})^{a_6}_{a'_7}$$
$$(\xi_{2,1})^{a_6}_{a_7} = -\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} \lambda^{i_9 i_{10}}_{a_7 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_8 a_7}$$
$$(\xi_2)^{a'_5 a_6}_{i_1 i_2} = -t^{a_6}_{i_7} (\Xi_1)^{i_7 a'_5}_{i_1 i_2} + F^{a'_5 a_7}_{i_1 i_2} (\xi_{2,1})^{a_6}_{a_7} + F^{a'_5 a'_7}_{i_1 i_2} (\xi_{2,2})^{a_6}_{a'_7} + F^{a'_7 a_6}_{i_1 i_2} (\xi_{2,3})^{a'_5}_{a'_7}$$
$$(\xi_{17,0})^{a'_6}_{a'_7} = -(\Xi_{18})^{a'_6}_{a'_7} - (\Xi_{19})^{a'_6}_{a'_7}$$
$$(\xi_{17})^{a'_5 a'_6}_{i_1 i_2} = +P_2 F^{a'_5 a'_7}_{i_1 i_2} (\xi_{17,0})^{a'_6}_{a'_7}$$
$$(\xi_{16})^{i_5 i_6}_{i_1 i_2} = +\tfrac{1}{2} t^{i_5 i_6}_{i_7 i_8} (\Xi_3)^{i_7 i_8}_{i_1 i_2}$$
$$(\xi_{15,0})^{a_6}_{a'_7} = +(\Xi_{14})^{a_6}_{a'_7} - (\Xi_{20})^{a_6}_{a'_7}$$
$$(\xi_{15})^{a_5 a_6}_{i_1 i_2} = +P_2 F^{a'_7 a_5}_{i_1 i_2} (\xi_{15,0})^{a_6}_{a'_7}$$
$$(\xi_{14})^{i_3 i_4}_{i_5 i_6} = +\tfrac{1}{2} P_2 t^{a_7}_{i_5} (\Xi_6)^{i_3 i_4}_{i_6 a_7} + \tfrac{1}{2} t^{a_7 a_8}_{i_5 i_6} \lambda^{i_3 i_4}_{a_7 a_8} + \tfrac{1}{2} t^{i_7 i_8}_{i_5 i_6} (\Xi_3)^{i_3 i_4}_{i_7 i_8}$$
$$(\xi_{11,5})^{i_4 a'_8}_{i_7 a'_6} = +\tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_6 a'_9}$$
$$(\xi_{11,4})^{i_4 a_8}_{i_7 a'_6} = -(\Xi_{17})^{i_4 a_8}_{i_7 a'_6} + t^{a_8 a_9}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_6 a_9}$$
$$(\xi_{11,2})^{a'_7}_{a'_6} = -(\Xi_8)^{a'_7}_{a'_6} - (\Xi_{15})^{a'_7}_{a'_6} - (\Xi_{16})^{a'_7}_{a'_6}$$
$$(\xi_{11,1,0})^{i_4 i_9}_{i_7 a'_6} = -t^{a_{10}}_{i_7} v^{i_4 i_9}_{a'_6 a_{10}}$$
$$(\xi_{11,1})^{i_4 a_8}_{i_7 a'_6} = -v^{i_4 a_8}_{i_7 a'_6} + (\Xi_7)^{i_4 a_8}_{i_7 a'_6} + t^{a_8}_{i_9} (\xi_{11,1,0})^{i_4 i_9}_{i_7 a'_6} - \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} v^{i_4 i_{10}}_{a'_6 a'_9}$$
$$(\xi_{11,0})^{i_4 a'_8}_{i_7 a'_6} = -v^{i_4 a'_8}_{i_7 a'_6} + (\Xi_9)^{i_4 a'_8}_{i_7 a'_6}$$
$$\begin{aligned}(\xi_{11})^{i_3 i_4}_{a'_5 a'_6} &= +P_2 P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} (\xi_{11,0})^{i_4 a'_8}_{i_7 a'_6} + P_2 P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} (\xi_{11,1})^{i_4 a_8}_{i_7 a'_6} \\ &+ P_2 \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_7} (\xi_{11,2})^{a'_7}_{a'_6} + P_2 P_2 v^{i_3 i_7}_{i_8 a'_5} (\Xi_4)^{i_4 i_8}_{i_7 a'_6} \\ &+ P_2 P_2 v^{i_3 i_7}_{a'_5 a_8} (\xi_{11,4})^{i_4 a_8}_{i_7 a'_6} + P_2 P_2 v^{i_3 i_7}_{a'_5 a'_8} (\xi_{11,5})^{i_4 a'_8}_{i_7 a'_6}\end{aligned}$$
$$(\xi_0)^{i_4 a_5}_{i_1 i_2} = -(\Xi_0)^{i_4 a_5}_{i_1 i_2} - V^{i_4 a_5}_{i_1 i_2} - (\Xi_{21})^{i_4 a_5}_{i_1 i_2}$$
$$\begin{aligned}\delta^{i_3 i_4}_{i_1 i_2} &= +V^{i_3 i_4}_{i_1 i_2} + P_2 \lambda^{i_3}_{a_5} (\xi_0)^{i_4 a_5}_{i_1 i_2} + v^{i_3 i_4}_{i_5 a'_6} (\Xi_1)^{i_5 a'_6}_{i_1 i_2} + v^{i_3 i_4}_{a'_5 a_6} (\xi_2)^{a'_5 a_6}_{i_1 i_2} \\ &+ P_2 V^{i_3 i_5}_{i_1 i_2} (\xi_3)^{i_4}_{i_5} + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_5 a_6} (\xi_4)^{a_5 a_6}_{i_1 i_2} + P_2 f^{i_3}_{i_5} (\Xi_3)^{i_4 i_5}_{i_1 i_2} + \tfrac{1}{2} \lambda^{i_3 i_4}_{i_5 i_6} (\xi_6)^{i_5 i_6}_{i_1 i_2} \\ &+ \tfrac{1}{2} X^{i_5 i_6}_{i_1 i_2} (\xi_7)^{i_3 i_4}_{i_5 i_6} + \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} (\xi_8)^{a'_5 a_6}_{i_1 i_2} + F^{a'_5 a_6}_{i_1 i_2} (\xi_9)^{i_3 i_4}_{a'_5 a_6} + \tfrac{1}{2} v^{i_3 i_4}_{i_5 i_6} (\Xi_3)^{i_5 i_6}_{i_1 i_2} \\ &+ \tfrac{1}{2} F^{a'_5 a'_6}_{i_1 i_2} (\xi_{11})^{i_3 i_4}_{a'_5 a'_6} + V^{i_5 a_6}_{i_1 i_2} (\Xi_6)^{i_3 i_4}_{i_5 a_6} + V^{i_5 a'_6}_{i_1 i_2} (\Xi_4)^{i_3 i_4}_{i_5 a'_6} \\ &+ \tfrac{1}{2} V^{i_5 i_6}_{i_1 i_2} (\xi_{14})^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} (\xi_{15})^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{2} V^{i_3 i_4}_{i_5 i_6} (\xi_{16})^{i_5 i_6}_{i_1 i_2} \\ &+ \tfrac{1}{2} v^{i_3 i_4}_{a'_5 a'_6} (\xi_{17})^{a'_5 a'_6}_{i_1 i_2}\end{aligned}$$

E. Λ-CCSDT-R12

TABLE ESI.4.XV: The computational sequence and intermediates for the Λ_3 amplitude equation of Λ-CCSDT-R12

$$
\begin{aligned}
(\Xi_0)^{i_8}_{a_3} &= +t^{a_9}_{i_{10}} v^{i_8 i_{10}}_{a_3 a_9} \\
(\Xi_1)^{i_6 i_9}_{i_7 a_3} &= +t^{a_{10}}_{i_7} v^{i_6 i_9}_{a_3 a_{10}} \\
(\Xi_2)^{i_4 i_5 i_6}_{i_8 a_3 a_9} &= +t^{a_{10}}_{i_8} \lambda^{i_4 i_5 i_6}_{a_3 a_9 a_{10}} \\
(\xi_{9,0})^{i_5 i_6}_{i_8 a_9} &= +v^{i_5 i_6}_{i_8 a_9} - \tfrac{1}{2} (\Xi_1)^{i_5 i_6}_{i_8 a_9} \\
(\xi_9)^{i_5 i_6}_{i_7 i_8} &= -v^{i_5 i_6}_{i_7 i_8} + P_2 t^{a_9}_{i_7} (\xi_{9,0})^{i_5 i_6}_{i_8 a_9} - \tfrac{1}{2} t^{a_9 a_{10}}_{i_7 i_8} v^{i_5 i_6}_{a_9 a_{10}} - \tfrac{1}{2} t^{i_9 i_{10}}_{i_7 i_8} V^{i_5 i_6}_{i_9 i_{10}} \\
(\xi_7)^{a_7}_{a_3} &= -f^{a_7}_{a_3} + t^{a_8}_{i_9} v^{i_9 a_7}_{a_3 a_8} + t^{a_7}_{i_8} (\Xi_0)^{i_8}_{a_3} + \tfrac{1}{2} t^{a_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_3 a_8} + \tfrac{1}{2} \tilde{t}^{a'_8 a_7}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_3} \\
(\xi_{6,0})^{i_6}_{a_8} &= +f^{i_6}_{a_8} + (\Xi_0)^{i_6}_{a_8} \\
(\xi_6)^{i_6}_{i_7} &= +f^{i_6}_{i_7} + t^{a_8}_{i_7} (\xi_{6,0})^{i_6}_{a_8} + t^{a_8}_{i_9} v^{i_6 i_9}_{i_7 a_8} + \tfrac{1}{2} t^{a_8 a_9}_{i_7 i_{10}} v^{i_6 i_{10}}_{a_8 a_9} + \tfrac{1}{2} t^{i_8 i_9}_{i_7 i_{10}} V^{i_6 i_{10}}_{i_8 i_9} \\
(\xi_5)^{i_5 i_6}_{i_7 a_3} &= -t^{a_8}_{i_7} \lambda^{i_5 i_6}_{a_3 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_7 i_{10}} \lambda^{i_5 i_6 i_{10}}_{a_3 a_8 a_9} \\
(\xi_2)^{i_5 i_6}_{i_7 a_3} &= +v^{i_5 i_6}_{i_7 a_3} - (\Xi_1)^{i_5 i_6}_{i_7 a_3} \\
(\xi_{16})^{i_6 a'_7}_{a_2 a_3} &= +\tfrac{1}{2} \lambda^{i_6 i_8 i_9}_{a_2 a_3 a_{10}} \tilde{t}^{a'_7 a_{10}}_{i_8 i_9} \\
(\xi_{15})^{i_6 a_7}_{a_2 a_3} &= -\tfrac{1}{2} t^{a_7 a_8}_{i_9 i_{10}} \lambda^{i_6 i_9 i_{10}}_{a_2 a_3 a_8} \\
(\xi_{14})^{i_4 i_5 i_6}_{i_7 i_8 a_3} &= -\tfrac{1}{2} P_2 t^{a_9}_{i_7} (\Xi_2)^{i_4 i_5 i_6}_{i_8 a_3 a_9} - \tfrac{1}{2} t^{a_9 a_{10}}_{i_7 i_8} \lambda^{i_4 i_5 i_6}_{a_3 a_9 a_{10}} \\
(\xi_{10})^{i_6 a_8}_{i_7 a_3} &= +v^{i_6 a_8}_{i_7 a_3} - t^{a_9}_{i_7} v^{i_6 a_8}_{a_3 a_9} + t^{a_8}_{i_9} (\Xi_1)^{i_6 i_9}_{i_7 a_3} - t^{a_8 a_9}_{i_7 i_{10}} v^{i_6 i_{10}}_{a_3 a_9} - \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} v^{i_6 i_{10}}_{a'_9 a_3} \\
(\xi_1)^{i_6}_{a_3} &= -f^{i_6}_{a_3} - (\Xi_0)^{i_6}_{a_3} \\
\delta^{i_4 i_5 i_6}_{a_1 a_2 a_3} &= -P_3 P_3 \lambda^{i_4}_{a_1} v^{i_5 i_6}_{a_2 a_3} + P_3 P_3 \lambda^{i_4 i_5}_{a_1 a_2} (\xi_1)^{i_6}_{a_3} + P_3 P_3 \lambda^{i_4 i_7}_{a_1 a_2} (\xi_2)^{i_5 i_6}_{i_7 a_3} \\
&\quad + P_3 P_3 \lambda^{i_4 i_5}_{a_1 a_7} v^{i_6 a_7}_{a_2 a_3} - P_3 P_3 \tilde{\lambda}^{i_4 i_5}_{a'_7 a_1} v^{i_6 a'_7}_{a_2 a_3} + P_3 P_3 v^{i_4 i_7}_{a_1 a_2} (\xi_5)^{i_5 i_6}_{i_7 a_3} \\
&\quad + P_3 \lambda^{i_4 i_5 i_7}_{a_1 a_2 a_3} (\xi_6)^{i_6}_{i_7} + P_3 \lambda^{i_4 i_5 i_6}_{a_1 a_2 a_7} (\xi_7)^{a_7}_{a_3} + P_3 f^{i_7}_{a_1} (\Xi_2)^{i_4 i_5 i_6}_{i_7 a_2 a_3} \\
&\quad + \tfrac{1}{2} P_3 \lambda^{i_4 i_7 i_8}_{a_1 a_2 a_3} (\xi_9)^{i_5 i_6}_{i_7 i_8} + P_3 P_3 \lambda^{i_4 i_5 i_7}_{a_1 a_2 a_8} (\xi_{10})^{i_6 a_8}_{i_7 a_3} - \tfrac{1}{2} P_3 \lambda^{i_4 i_5 i_6}_{a_1 a_7 a_8} v^{a_7 a_8}_{a_2 a_3} \\
&\quad - P_3 P_3 v^{i_4 i_7}_{i_8 a_1} (\Xi_2)^{i_5 i_6 i_8}_{i_7 a_2 a_3} - P_3 v^{i_7 a_8}_{a_1 a_2} (\Xi_2)^{i_4 i_5 i_6}_{i_7 a_3 a_8} \\
&\quad + \tfrac{1}{2} P_3 v^{i_7 i_8}_{a_1 a_2} (\xi_{14})^{i_4 i_5 i_6}_{i_7 i_8 a_3} + P_3 P_3 v^{i_4 i_5}_{a_1 a_7} (\xi_{15})^{i_6 a_7}_{a_2 a_3} \\
&\quad + P_3 P_3 v^{i_4 i_5}_{a'_7 a_1} (\xi_{16})^{i_6 a'_7}_{a_2 a_3}
\end{aligned}
$$

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TABLE ESI.4.XVI: The computational sequence and intermediates for the Λ_1 amplitude equation of Λ-CCSDT-R12 [Part I]

$$
\begin{aligned}
(\Xi_0)^{i_2}_{a_8^{\prime}} &= +t^{a_9}_{i_{10}} v^{i_2 i_{10}}_{a_8 a_9} \\
(\Xi_1)^{i_5}_{i_3} &= +t^{a_6}_{i_3} \lambda^{i_5}_{a_6} \\
(\Xi_2)^{i_5}_{i_3} &= +\tfrac{1}{2} t^{a_6 a_7}_{i_3 i_8^{\prime}} \lambda^{i_5 i_8}_{a_6 a_7} \\
(\Xi_3)^{i_5 i_8}_{i_6 i_7} &= +\tfrac{1}{2} \lambda^{i_5 i_8}_{i_9 i_{10}} X^{i_9 i_{10}}_{i_6 i_7} \\
(\Xi_4)^{i_6 i_7}_{i_3 a_5} &= +t^{a_8}_{i_3} \lambda^{i_6 i_7}_{a_5 a_8} \\
(\Xi_5)^{i_6 i_7}_{i_3 a_5^{\prime}} &= +t^{a_8}_{i_3} \tilde{\lambda}^{i_6 i_7}_{a_5^{\prime} a_8} \\
(\Xi_6)^{i_2 a_7}_{i_5 a_8} &= +t^{a_9}_{i_5} v^{i_2 a_7}_{a_8 a_9} \\
(\Xi_7)^{i_2 i_6}_{i_3 i_4} &= +\tfrac{1}{2} t^{a_7 a_8}_{i_3 i_4} \lambda^{i_2 i_6}_{a_7 a_8} \\
(\Xi_8)^{i_2 i_9}_{i_5 a_8} &= +t^{a_{10}}_{i_5} v^{i_2 i_9}_{a_8 a_{10}} \\
(\Xi_9)^{i_2}_{a_6^{\prime}} &= +t^{a_7}_{i_8} v^{i_2 i_8}_{a_6^{\prime} a_7} \\
(\Xi_{10})^{i_2 i_8}_{i_5 a_9^{\prime}} &= +t^{a_{10}}_{i_5} v^{i_2 i_8}_{a_9^{\prime} a_{10}} \\
(\Xi_{11})^{i_5}_{i_3} &= +\tfrac{1}{12} t^{a_6 a_7 a_8}_{i_3 i_9 i_{10}} \lambda^{i_5 i_9 i_{10}}_{a_6 a_7 a_8} \\
(\Xi_{12})^{i_6 i_7}_{i_3 a_5} &= +\tfrac{1}{2} t^{a_8 a_9}_{i_3 i_{10}} \lambda^{i_6 i_7 i_{10}}_{a_5 a_8 a_9} \\
(\Xi_{13})^{i_2 a_5}_{a_6 a_7} &= +\tfrac{1}{2} t^{a_5 a_8}_{i_9 i_{10}} \lambda^{i_2 i_9 i_{10}}_{a_6 a_7 a_8} \\
(\Xi_{14})^{i_2 i_7 i_8}_{i_4 a_6 a_9} &= +t^{a_{10}}_{i_4} \lambda^{i_2 i_7 i_8}_{a_6 a_9 a_{10}} \\
(\Xi_{15})^{i_2 i_6}_{i_3 i_4} &= +\tfrac{1}{6} t^{a_7 a_8 a_9}_{i_3 i_4 i_{10}} \lambda^{i_2 i_6 i_{10}}_{a_7 a_8 a_9} \\
(\Xi_{16})^{i_5}_{i_3} &= +\tfrac{1}{2} t^{i_6 i_7}_{i_3 i_8} (\Xi_3)^{i_5 i_8}_{i_6 i_7} \\
(\Xi_{17})^{i_2 i_6}_{i_3 i_4} &= +P_2 t^{a_7}_{i_3} (\Xi_4)^{i_2 i_6}_{i_4 a_7} \\
(\Xi_{18})^{i_2 i_6}_{i_3 i_4} &= +\tfrac{1}{2} t^{i_7 i_8}_{i_3 i_4} (\Xi_3)^{i_2 i_6}_{i_7 i_8} \\
(\Xi_{19})^{i_6 a_5}_{i_3 a_1} &= +t^{a_5}_{i_7} (\Xi_{12})^{i_6 i_7}_{i_3 a_1} \\
(\Xi_{20})^{i_2 i_6}_{i_3 i_4} &= +P_2 t^{a_7}_{i_3} (\Xi_{12})^{i_2 i_6}_{i_4 a_7} \\
(\Xi_{21})^{i_2 i_7 i_8}_{i_3 i_4 a_6} &= +P_2 t^{a_9}_{i_3} (\Xi_{14})^{i_2 i_7 i_8}_{i_4 a_6 a_9} \\
(\xi_{9,1})^{i_6 i_7}_{i_3 a_5} &= +(\Xi_4)^{i_6 i_7}_{i_3 a_5} + (\Xi_{12})^{i_6 i_7}_{i_3 a_5} \\
(\xi_9)^{a_4^{\prime}}_{i_3} &= +\lambda^{i_5}_{a_6} \tilde{t}^{a_4^{\prime} a_6}_{i_3 i_5} + \tfrac{1}{2} \tilde{t}^{a_4^{\prime} a_5}_{i_6 i_7} (\xi_{9,1})^{i_6 i_7}_{i_3 a_5} + \tfrac{1}{2} \tilde{t}^{a_4^{\prime} a_5^{\prime}}_{i_6 i_7} (\Xi_5)^{i_6 i_7}_{i_3 a_5^{\prime}} \\
(\xi_{8,3})^{i_2 i_7 i_8}_{i_3 i_4 a_6} &= +\tfrac{1}{2} (\Xi_{21})^{i_2 i_7 i_8}_{i_3 i_4 a_6} + \tfrac{1}{2} t^{a_9 a_{10}}_{i_3 i_4} \lambda^{i_2 i_7 i_8}_{a_6 a_9 a_{10}} \\
(\xi_{8,1})^{i_2 i_7}_{i_4 a_6} &= -(\Xi_4)^{i_2 i_7}_{i_4 a_6} - (\Xi_{12})^{i_2 i_7}_{i_4 a_6} \\
(\xi_8)^{i_2 a_5^{\prime}}_{i_3 i_4} &= +\lambda^{i_2}_{a_6} \tilde{t}^{a_5^{\prime} a_6}_{i_3 i_4} + P_2 \tilde{t}^{a_5^{\prime} a_6}_{i_3 i_7} (\xi_{8,1})^{i_2 i_7}_{i_4 a_6} \\
&\quad - P_2 \tilde{t}^{a_5^{\prime} a_6^{\prime}}_{i_3 i_7} (\Xi_5)^{i_2 i_7}_{i_4 a_6^{\prime}} + \tfrac{1}{2} \tilde{t}^{a_5^{\prime} a_6}_{i_7 i_8} (\xi_{8,3})^{i_2 i_7 i_8}_{i_3 i_4 a_6} \\
(\xi_{7,3})^{i_2 i_7}_{i_4 a_6} &= +(\Xi_4)^{i_2 i_7}_{i_4 a_6} + (\Xi_{12})^{i_2 i_7}_{i_4 a_6} \\
(\xi_{7,2})^{i_2}_{i_4} &= -(\Xi_2)^{i_2}_{i_4} - (\Xi_{16})^{i_2}_{i_4} - (\Xi_{11})^{i_2}_{i_4} \\
(\xi_{7,1})^{i_2 i_6}_{i_3 i_4} &= -\tfrac{1}{2} (\Xi_{17})^{i_2 i_6}_{i_3 i_4} - (\Xi_7)^{i_2 i_6}_{i_3 i_4} - (\Xi_{18})^{i_2 i_6}_{i_3 i_4} - (\Xi_{20})^{i_2 i_6}_{i_3 i_4} - (\Xi_{15})^{i_2 i_6}_{i_3 i_4} \\
(\xi_7)^{i_2 a_5}_{i_3 i_4} &= -t^{a_5 a_6}_{i_3 i_4} \lambda^{i_2}_{a_6} + t^{a_5}_{i_6} (\xi_{7,1})^{i_2 i_6}_{i_3 i_4} + P_2 t^{a_5}_{i_3} (\xi_{7,2})^{i_2}_{i_4} + P_2 t^{a_5 a_6}_{i_3 i_7} (\xi_{7,3})^{i_2 i_7}_{i_4 a_6} \\
&\quad - \tfrac{1}{2} t^{a_5 a_6 a_7}_{i_3 i_4 i_8} \lambda^{i_2 i_8}_{a_6 a_7} - P_2 \tilde{t}^{a_6^{\prime} a_5}_{i_3 i_7} (\Xi_5)^{i_2 i_7}_{i_4 a_6^{\prime}} - \tfrac{1}{4} t^{a_5 a_6}_{i_7 i_8} (\Xi_{21})^{i_2 i_7 i_8}_{i_3 i_4 a_6} \\
&\quad - \tfrac{1}{2} t^{a_6 a_7}_{i_3 i_4} (\Xi_{13})^{i_2 a_5}_{a_6 a_7} - \tfrac{1}{4} P_2 t^{a_5 a_6 a_7}_{i_3 i_8 i_9} (\Xi_{14})^{i_2 i_8 i_9}_{i_4 a_6 a_7} \\
(\xi_{6,2})^{i_6 i_7}_{i_3 a_5} &= -(\Xi_4)^{i_6 i_7}_{i_3 a_5} - (\Xi_{12})^{i_6 i_7}_{i_3 a_5} \\
(\xi_{6,0})^{i_5}_{i_3} &= +(\Xi_1)^{i_5}_{i_3} + (\Xi_2)^{i_5}_{i_3} + (\Xi_{16})^{i_5}_{i_3} + (\Xi_{11})^{i_5}_{i_3} \\
(\xi_6)^{a_4}_{i_3} &= +t^{a_4}_{i_5} (\xi_{6,0})^{i_5}_{i_3} - t^{a_4 a_5}_{i_3 i_6} \lambda^{i_6}_{a_5} + \tfrac{1}{2} t^{a_4 a_5}_{i_6 i_7} (\xi_{6,2})^{i_6 i_7}_{i_3 a_5} - \tfrac{1}{4} t^{a_4 a_5 a_6}_{i_3 i_7 i_8} \lambda^{i_7 i_8}_{a_5 a_6} \\
&\quad + \tfrac{1}{2} \tilde{t}^{a_5^{\prime} a_4}_{i_6 i_7} (\Xi_5)^{i_6 i_7}_{i_3 a_5^{\prime}} + \tfrac{1}{12} t^{a_4 a_5 a_6}_{i_7 i_8 i_9} (\Xi_{14})^{i_7 i_8 i_9}_{i_3 a_5 a_6} \\
(\xi_5)^{a_4}_{a_3} &= -t^{a_4}_{i_5} \lambda^{i_5}_{a_3} - \tfrac{1}{2} t^{a_4 a_5}_{i_6 i_7} \lambda^{i_6 i_7}_{a_3 a_5} - \tfrac{1}{2} \tilde{t}^{a_5^{\prime} a_4}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a_5^{\prime} a_3} - \tfrac{1}{12} t^{a_4 a_5 a_6}_{i_7 i_8 i_9} \lambda^{i_7 i_8 i_9}_{a_3 a_5 a_6} \\
(\xi_4)^{i_4}_{i_3} &= -(\Xi_1)^{i_4}_{i_3} - (\Xi_2)^{i_4}_{i_3} - (\Xi_{16})^{i_4}_{i_3} - (\Xi_{11})^{i_4}_{i_3} \\
(\xi_{32})^{i_4 i_5}_{i_3 a_1} &= -\tfrac{1}{2} t^{i_4 i_5}_{i_6 i_7} (\Xi_{12})^{i_6 i_7}_{i_3 a_1} \\
(\xi_{31})^{a_4 a_5}_{i_3 a_1} &= -\tfrac{1}{2} P_2 t^{a_4}_{i_6} (\Xi_{19})^{i_6 a_5}_{i_3 a_1} - \tfrac{1}{2} t^{a_4 a_5}_{i_6 i_7} (\Xi_{12})^{i_6 i_7}_{i_3 a_1} \\
(\xi_{29})^{i_2 a_5^{\prime}}_{a_3 a_4} &= +\tfrac{1}{2} \lambda^{i_2 i_6 i_7}_{a_3 a_4 a_8} \tilde{t}^{a_5^{\prime} a_8}_{i_6 i_7} \\
(\xi_{28,4})^{i_2 i_9}_{i_5 a_8} &= +v^{i_2 i_9}_{i_5 a_8} - (\Xi_8)^{i_2 i_9}_{i_5 a_8} \\
(\xi_{28,3,1})^{i_2 i_8}_{i_5 a_9^{\prime}} &= -v^{i_2 i_8}_{i_5 a_9^{\prime}} + (\Xi_{10})^{i_2 i_8}_{i_5 a_9^{\prime}} \\
(\xi_{28,3,0})^{i_2 i_8}_{i_5 a_9} &= +v^{i_2 i_8}_{i_5 a_9} - (\Xi_8)^{i_2 i_8}_{i_5 a_9} \\
(\xi_{28,3})^{i_2 i_8 a_7}_{i_3 i_4 i_5} &= +P_3 t^{a_7 a_9}_{i_3 i_4} (\xi_{28,3,0})^{i_2 i_8}_{i_5 a_9} + P_3 \tilde{t}^{a_9^{\prime} a_7}_{i_3 i_4} (\xi_{28,3,1})^{i_2 i_8}_{i_5 a_9^{\prime}} - \tfrac{1}{2} t^{a_7 a_9 a_{10}}_{i_3 i_4 i_5} v^{i_2 i_8}_{a_9 a_{10}} \\
(\xi_{28,2})^{i_2 a_7}_{i_5 a_8^{\prime}} &= -v^{i_2 a_7}_{i_5 a_8^{\prime}} + t^{a_9}_{i_5} v^{i_2 a_7}_{a_8^{\prime} a_9} + t^{a_7 a_9}_{i_5 i_{10}} v^{i_2 i_{10}}_{a_8^{\prime} a_9} - \tilde{t}^{a_9^{\prime} a_7}_{i_5 i_{10}} v^{i_2 i_{10}}_{a_8^{\prime} a_9^{\prime}} \\
(\xi_{28,1})^{i_2 a_7}_{i_5 a_8} &= +v^{i_2 a_7}_{i_5 a_8} - (\Xi_6)^{i_2 a_7}_{i_5 a_8} - t^{a_7 a_9}_{i_5 i_{10}} v^{i_2 i_{10}}_{a_8 a_9} - \tilde{t}^{a_9^{\prime} a_7}_{i_5 i_{10}} v^{i_2 i_{10}}_{a_9^{\prime} a_8} \\
(\xi_{28,0})^{i_2}_{a_8} &= +f^{i_2}_{a_8} + (\Xi_0)^{i_2}_{a_8} \\
(\xi_{28})^{i_2 a_6 a_7}_{i_3 i_4 i_5} &= +t^{a_6 a_7 a_8}_{i_3 i_4 i_5} (\xi_{28,0})^{i_2}_{a_8} + P_2 P_3 t^{a_6 a_8}_{i_3 i_4} (\xi_{28,1})^{i_2 a_7}_{i_5 a_8} + P_2 P_3 \tilde{t}^{a_8^{\prime} a_6}_{i_3 i_4} (\xi_{28,2})^{i_2 a_7}_{i_5 a_8^{\prime}} \\
&\quad + P_2 t^{a_6}_{i_8} (\xi_{28,3})^{i_2 i_8 a_7}_{i_3 i_4 i_5} + P_3 t^{a_6 a_7 a_8}_{i_3 i_4 i_9} (\xi_{28,4})^{i_2 i_9}_{i_5 a_8} - \tfrac{1}{2} P_2 t^{a_6 a_8 a_9}_{i_3 i_4 i_5} v^{i_2 a_7}_{a_8 a_9} \\
(\xi_{27})^{a_4^{\prime}}_{a_3^{\prime}} &= +\tfrac{1}{2} \tilde{t}^{a_4^{\prime} a_5^{\prime}}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a_3^{\prime} a_5^{\prime}} + \tfrac{1}{2} \tilde{t}^{a_4^{\prime} a_5}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a_3^{\prime} a_5} \\
(\xi_{26})^{i_2 a_5^{\prime}}_{i_3 a_4^{\prime}} &= -\tilde{t}^{a_5^{\prime} a_6^{\prime}}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a_4^{\prime} a_6^{\prime}} - \tilde{t}^{a_5^{\prime} a_6}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a_4^{\prime} a_6} \\
(\xi_{25})^{a_4}_{a_3^{\prime}} &= -\tfrac{1}{2} t^{a_4 a_5}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a_3^{\prime} a_5} + \tfrac{1}{2} \tilde{t}^{a_5^{\prime} a_4}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a_3^{\prime} a_5^{\prime}} \\
(\xi_{24})^{i_2 a_5}_{i_3 a_4^{\prime}} &= -t^{a_5}_{i_6} (\Xi_5)^{i_2 i_6}_{i_3 a_4^{\prime}} + t^{a_5 a_6}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a_4^{\prime} a_6} - \tilde{t}^{a_6^{\prime} a_5}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a_4^{\prime} a_6^{\prime}} \\
(\xi_{23})^{a_4^{\prime}}_{a_3^{\prime}} &= +\tfrac{1}{2} \lambda^{i_5 i_6}_{a_3 a_7} \tilde{t}^{a_4^{\prime} a_7}_{i_5 i_6} - \tfrac{1}{2} \tilde{t}^{a_4^{\prime} a_5^{\prime}}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a_5^{\prime} a_3} \\
(\xi_{22})^{i_2 a_5^{\prime}}_{i_3 a_4} &= -\lambda^{i_2 i_6}_{a_4 a_7} \tilde{t}^{a_5^{\prime} a_7}_{i_3 i_6} + \tilde{t}^{a_5^{\prime} a_6^{\prime}}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a_6^{\prime} a_4} - \tfrac{1}{2} \tilde{t}^{a_5^{\prime} a_6}_{i_7 i_8} (\Xi_{14})^{i_2 i_7 i_8}_{i_3 a_4 a_6} \\
(\xi_{21})^{i_2 i_5}_{i_3 i_4} &= +(\Xi_7)^{i_2 i_5}_{i_3 i_4} + (\Xi_{18})^{i_2 i_5}_{i_3 i_4} + (\Xi_{15})^{i_2 i_5}_{i_3 i_4} \\
(\xi_{20})^{i_2 a_5}_{i_3 a_4} &= -(\Xi_{19})^{i_2 a_5}_{i_3 a_4} - t^{a_5}_{i_6} (\Xi_4)^{i_2 i_6}_{i_3 a_4} + t^{a_5 a_6}_{i_3 i_7} \lambda^{i_2 i_7}_{a_4 a_6} + \tilde{t}^{a_6^{\prime} a_5}_{i_3 i_7} \tilde{\lambda}^{i_2 i_7}_{a_6^{\prime} a_4} \\
&\quad + \tfrac{1}{2} t^{a_5 a_6}_{i_7 i_8} (\Xi_{14})^{i_2 i_7 i_8}_{i_3 a_4 a_6} + \tfrac{1}{4} t^{a_5 a_6 a_7}_{i_3 i_8 i_9} \lambda^{i_2 i_8 i_9}_{a_4 a_6 a_7} \\
(\xi_2)^{i_2}_{i_3} &= +(\Xi_1)^{i_2}_{i_3} + (\Xi_2)^{i_2}_{i_3} + (\Xi_{16})^{i_2}_{i_3} + (\Xi_{11})^{i_2}_{i_3} \\
(\xi_{19})^{i_2 i_5}_{i_3 i_4} &= +\tfrac{1}{2} (\Xi_{17})^{i_2 i_5}_{i_3 i_4} + (\Xi_{20})^{i_2 i_5}_{i_3 i_4} \\
(\xi_{18})^{i_2 a_5}_{i_3 i_4} &= -t^{a_5}_{i_6} \lambda^{i_2 i_6}_{i_3 i_4} \\
(\xi_{16})^{i_2 a_5}_{a_3 a_4} &= -(\Xi_{13})^{i_2 a_5}_{a_3 a_4} - t^{a_5}_{i_6} \lambda^{i_2 i_6}_{a_3 a_4} \\
(\xi_{15})^{i_2 i_5}_{i_3 a_4} &= +(\Xi_4)^{i_2 i_5}_{i_3 a_4} + (\Xi_{12})^{i_2 i_5}_{i_3 a_4} \\
(\xi_{14})^{i_4 i_5}_{i_3 a_1} &= -(\Xi_4)^{i_4 i_5}_{i_3 a_1} - (\Xi_{12})^{i_4 i_5}_{i_3 a_1} \\
(\xi_{11,5})^{i_2 i_7}_{i_4 a_6} &= +v^{i_2 i_7}_{i_4 a_6} - (\Xi_8)^{i_2 i_7}_{i_4 a_6} \\
(\xi_{11,4})^{i_2 i_7}_{i_4 a_6^{\prime}} &= +v^{i_2 i_7}_{i_4 a_6^{\prime}} - (\Xi_{10})^{i_2 i_7}_{i_4 a_6^{\prime}} \\
(\xi_{11,2})^{i_2 a_5^{\prime}}_{i_4 a_6} &= +v^{i_2 a_5^{\prime}}_{i_4 a_6} - \tfrac{1}{2} t^{a_7}_{i_4} v^{i_2 a_5^{\prime}}_{a_6 a_7} \\
(\xi_{11,1})^{i_2}_{a_6} &= +f^{i_2}_{a_6} + (\Xi_0)^{i_2}_{a_6} \\
(\xi_{11,0})^{i_2}_{a_6^{\prime}} &= +f^{i_2}_{a_6^{\prime}} + (\Xi_9)^{i_2}_{a_6^{\prime}} \\
(\xi_{11})^{i_2 a_5^{\prime}}_{i_3 i_4} &= -v^{i_2 a_5^{\prime}}_{i_3 i_4} + \tilde{t}^{a_5^{\prime} a_6}_{i_3 i_4} (\xi_{11,0})^{i_2}_{a_6^{\prime}} + \tilde{t}^{a_5^{\prime} a_6}_{i_3 i_4} (\xi_{11,1})^{i_2}_{a_6} + P_2 t^{a_6}_{i_3} (\xi_{11,2})^{i_2 a_5^{\prime}}_{i_4 a_6} \\
&\quad - \tfrac{1}{2} t^{a_6 a_7}_{i_3 i_4} v^{i_2 a_5^{\prime}}_{a_6 a_7} + P_2 \tilde{t}^{a_5^{\prime} a_5^{\prime}}_{i_3 i_7} (\xi_{11,4})^{i_2 i_7}_{i_4 a_6^{\prime}} + P_2 \tilde{t}^{a_5^{\prime} a_6}_{i_3 i_7} (\xi_{11,5})^{i_2 i_7}_{i_4 a_6} \\
&\quad - \tfrac{1}{2} t^{i_6 i_7}_{i_3 i_4} V^{i_2 a_5^{\prime}}_{i_6 i_7} \\
(\xi_{10,6})^{i_2 i_7}_{i_4 a_6^{\prime}} &= +v^{i_2 i_7}_{i_4 a_6^{\prime}} - (\Xi_{10})^{i_2 i_7}_{i_4 a_6^{\prime}} \\
(\xi_{10,4})^{i_2 i_7}_{i_4 a_6} &= -v^{i_2 i_7}_{i_4 a_6} + (\Xi_8)^{i_2 i_7}_{i_4 a_6} \\
(\xi_{10,3,0})^{i_2 i_6}_{i_4 a_7} &= +v^{i_2 i_6}_{i_4 a_7} - \tfrac{1}{2} (\Xi_8)^{i_2 i_6}_{i_4 a_7} \\
(\xi_{10,3})^{i_2 i_6}_{i_3 i_4} &= +P_2 t^{a_7}_{i_3} (\xi_{10,3,0})^{i_2 i_6}_{i_4 a_7} - \tfrac{1}{2} t^{a_7 a_8}_{i_3 i_4} v^{i_2 i_6}_{a_7 a_8} - \tfrac{1}{2} t^{i_7 i_8}_{i_3 i_4} V^{i_2 i_6}_{i_7 i_8} \\
(\xi_{10,2})^{i_2 a_5}_{i_4 a_6} &= -v^{i_2 a_5}_{i_4 a_6} + \tfrac{1}{2} (\Xi_6)^{i_2 a_5}_{i_4 a_6} \\
(\xi_{10,1})^{i_2}_{a_6^{\prime}} &= +f^{i_2}_{a_6^{\prime}} + (\Xi_9)^{i_2}_{a_6^{\prime}} \\
(\xi_{10,0})^{i_2}_{a_6} &= -f^{i_2}_{a_6} - (\Xi_0)^{i_2}_{a_6} \\
(\xi_{10})^{i_2 a_5}_{i_3 i_4} &= +v^{i_2 a_5}_{i_3 i_4} + t^{a_5 a_6}_{i_3 i_4} (\xi_{10,0})^{i_2}_{a_6} + \tilde{t}^{a_6^{\prime} a_5}_{i_3 i_4} (\xi_{10,1})^{i_2}_{a_6^{\prime}} + P_2 t^{a_6}_{i_3} (\xi_{10,2})^{i_2 a_5}_{i_4 a_6} \\
&\quad + t^{a_5}_{i_6} (\xi_{10,3})^{i_2 i_6}_{i_3 i_4} + P_2 t^{a_5 a_6}_{i_3 i_7} (\xi_{10,4})^{i_2 i_7}_{i_4 a_6} + \tfrac{1}{2} t^{a_6 a_7}_{i_3 i_4} v^{i_2 a_5}_{a_6 a_7} \\
&\quad + P_2 \tilde{t}^{a_6^{\prime} a_5}_{i_3 i_7} (\xi_{10,6})^{i_2 i_7}_{i_4 a_6^{\prime}} + \tfrac{1}{2} t^{i_6 i_7}_{i_3 i_4} V^{i_2 a_5}_{i_6 i_7} - \tfrac{1}{2} t^{a_5 a_6 a_7}_{i_3 i_4 i_8} v^{i_2 i_8}_{a_6 a_7}
\end{aligned}
$$

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TABLE ESI.4.XVII: The computational sequence and intermediates for the Λ_1 amplitude equation of Λ-CCSDT-R12 [Part II]

$$
\begin{aligned}
(\xi_1)^{a_3}_{a_1} &= -f^{a_3}_{a_1} + t^{a_4}_{i_5} v^{i_5 a_3}_{a_1 a_4} + t^{a_3}_{i_4} (\Xi_0)^{i_4}_{a_1} \\
(\xi_{0,0})^{i_2}_{a_4} &= +f^{i_2}_{a_4} + (\Xi_0)^{i_2}_{a_4} \\
(\xi_0)^{i_2}_{i_3} &= +f^{i_2}_{i_3} + t^{a_4}_{i_3} (\xi_{0,0})^{i_2}_{a_4} + t^{a_4}_{i_5} v^{i_2 i_5}_{i_3 a_4} + \tfrac{1}{2} t^{a_4 a_5}_{i_3 i_6} v^{i_2 i_6}_{a_4 a_5} + \tfrac{1}{2} t^{i_4 i_5}_{i_3 i_6} V^{i_2 i_6}_{i_4 i_5} \\
\delta^{i_2}_{a_1} &= +f^{i_2}_{a_1} + (\Xi_0)^{i_2}_{a_1} + \lambda^{i_3}_{a_1} (\xi_0)^{i_2}_{i_3} + \lambda^{i_2}_{a_3} (\xi_1)^{a_3}_{a_1} + f^{i_3}_{a_1} (\xi_2)^{i_2}_{i_3} + \lambda^{i_3}_{a_4} v^{i_2 a_4}_{i_3 a_1} \\
&\quad + v^{i_2 i_3}_{i_4 a_1} (\xi_4)^{i_4}_{i_3} + v^{i_2 a_3}_{a_1 a_4} (\xi_5)^{a_4}_{a_3} + v^{i_2 i_3}_{a_1 a_4} (\xi_6)^{a_4}_{i_3} + \tfrac{1}{2} v^{i_3 i_4}_{a_1 a_5} (\xi_7)^{i_2 a_5}_{i_3 i_4} \\
&\quad + \tfrac{1}{2} v^{i_3 i_4}_{a'_5 a_1} (\xi_8)^{i_2 a'_5}_{i_3 i_4} + v^{i_2 i_3}_{a'_4 a_1} (\xi_9)^{a'_4}_{i_3} + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_1 a_5} (\xi_{10})^{i_2 a_5}_{i_3 i_4} + \tfrac{1}{2} \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} (\xi_{11})^{i_2 a'_5}_{i_3 i_4} \\
&\quad + \tfrac{1}{2} \lambda^{i_2 i_3}_{a_4 a_5} v^{a_4 a_5}_{i_3 a_1} + \tfrac{1}{2} \lambda^{i_2 i_3}_{i_4 i_5} (V^\dagger)^{i_4 i_5}_{i_3 a_1} + \tfrac{1}{2} v^{i_2 i_3}_{i_4 i_5} (\xi_{14})^{i_4 i_5}_{i_3 a_1} + v^{i_3 a_4}_{i_5 a_1} (\xi_{15})^{i_2 i_5}_{i_3 a_4} \\
&\quad + \tfrac{1}{2} v^{a_3 a_4}_{a_1 a_5} (\xi_{16})^{i_2 a_5}_{a_3 a_4} + v^{i_3 a'_4}_{i_5 a_1} (\Xi_5)^{i_2 i_5}_{i_3 a'_4} + \tfrac{1}{2} (V^\dagger)^{i_3 i_4}_{a_1 a_5} (\xi_{18})^{i_2 a_5}_{i_3 i_4} \\
&\quad + v^{i_3 i_4}_{i_5 a_1} (\xi_{19})^{i_2 i_5}_{i_3 i_4} + v^{i_3 a_4}_{a_1 a_5} (\xi_{20})^{i_2 a_5}_{i_3 a_4} + \tfrac{1}{2} v^{i_3 i_4}_{i_5 a_1} (\xi_{21})^{i_2 i_5}_{i_3 i_4} \\
&\quad + v^{i_3 a_4}_{a'_5 a_1} (\xi_{22})^{i_2 a'_5}_{i_3 a_4} + v^{i_2 a_3}_{a'_4 a_1} (\xi_{23})^{a'_4}_{a_3} + v^{i_3 a'_4}_{a_1 a_5} (\xi_{24})^{i_2 a_5}_{i_3 a'_4} \\
&\quad + v^{i_2 a'_5}_{a_1 a_4} (\xi_{25})^{a_4}_{a'_5} + v^{i_3 a'_4}_{a'_5 a_1} (\xi_{26})^{i_2 a'_5}_{i_3 a'_4} + v^{i_2 a'_5}_{a'_4 a_1} (\xi_{27})^{a'_4}_{a'_5} \\
&\quad + \tfrac{1}{12} \lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} (\xi_{28})^{i_2 a_6 a_7}_{i_3 i_4 i_5} + \tfrac{1}{2} v^{a_3 a_4}_{a'_5 a_1} (\xi_{29})^{i_2 a'_5}_{a_3 a_4} - v^{i_2 i_3}_{i_4 a_5} (\Xi_{19})^{i_4 a_5}_{i_3 a_1} \\
&\quad + \tfrac{1}{2} v^{i_2 i_3}_{a_4 a_5} (\xi_{31})^{a_4 a_5}_{i_3 a_1} + \tfrac{1}{2} V^{i_2 i_3}_{i_4 i_5} (\xi_{32})^{i_4 i_5}_{i_3 a_1}
\end{aligned}
$$

TABLE ESI.4.XVIII: The computational sequence and intermediates for the Λ_2 amplitude equation of Λ-CCSDT-R12

$$
\begin{aligned}
(\Xi_0)^{i_4}_{a_8} &= +t^{a_9}_{i_{10}} v^{i_4 i_{10}}_{a_8 a_9} \\
(\Xi_1)^{i_8 i_9}_{i_5 a_2} &= +t^{a_{10}}_{i_5} v^{i_8 i_9}_{a_2 a_{10}} \\
(\Xi_2)^{i_3 i_4}_{i_6 a_7} &= +t^{a_8}_{i_6} \lambda^{i_3 i_4}_{a_7 a_8} \\
(\Xi_3)^{i_4 i_8}_{i_5 i_6} &= +P_2 t^{a_9}_{i_5} v^{i_4 i_8}_{i_6 a_9} \\
(\Xi_4)^{i_8 a_7}_{i_5 a_2} &= +t^{a_9}_{i_5} v^{i_8 a_7}_{a_2 a_9} \\
(\Xi_5)^{i_4 i_8}_{i_5 i_6} &= +\tfrac{1}{2} t^{a_9 a_{10}}_{i_5 i_6} v^{i_4 i_8}_{a_9 a_{10}} \\
(\Xi_6)^{i_4 i_8}_{i_5 i_6} &= +\tfrac{1}{2} t^{i_9 i_{10}}_{i_5 i_6} V^{i_4 i_8}_{i_9 i_{10}} \\
(\Xi_7)^{i_8 a_7}_{i_5 a_2} &= +\tilde{t}^{a'_9 a_7}_{i_5 i_{10}} v^{i_8 i_{10}}_{a'_9 a_2} \\
(\Xi_8)^{i_4 i_8}_{i_6 i_7} &= +\tfrac{1}{2} \lambda^{i_4 i_8}_{i_9 i_{10}} X^{i_9 i_{10}}_{i_6 i_7} \\
(\Xi_9)^{i_3 i_4}_{i_6 a_7} &= +\tfrac{1}{2} t^{a_8 a_9}_{i_6 i_{10}} \lambda^{i_3 i_4 i_{10}}_{a_7 a_8 a_9} \\
(\Xi_{10})^{i_4 i_8 i_9}_{i_5 a_2 a_7} &= +t^{a_{10}}_{i_5} \lambda^{i_4 i_8 i_9}_{a_2 a_7 a_{10}} \\
(\Xi_{11})^{i_7 a_6}_{a_1 a_2} &= +\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} \lambda^{i_7 i_9 i_{10}}_{a_1 a_2 a_8} \\
(\Xi_{12})^{i_3 i_4}_{i_7 a'_9} &= +t^{a_{10}}_{i_7} v^{i_3 i_4}_{a'_9 a_{10}} \\
(\Xi_{13})^{i_4 i_8}_{i_5 i_6} &= +P_2 t^{a_9}_{i_5} (\Xi_1)^{i_4 i_8}_{i_6 a_9} \\
(\Xi_{14})^{i_3 i_4 i_8}_{i_5 i_6 a_2} &= +P_2 t^{a_9}_{i_5} (\Xi_{10})^{i_3 i_4 i_8}_{i_6 a_2 a_9} \\
(\xi_9)^{i_4 a_6}_{i_5 a_2} &= -v^{i_4 a_6}_{i_5 a_2} + (\Xi_4)^{i_4 a_6}_{i_5 a_2} + (\Xi_7)^{i_4 a_6}_{i_5 a_2} - t^{a_6}_{i_7} (\Xi_1)^{i_4 i_7}_{i_5 a_2} \\
(\xi_8)^{i_3 i_4}_{i_5 i_6} &= +v^{i_3 i_4}_{i_5 i_6} + (\Xi_5)^{i_3 i_4}_{i_5 i_6} + (\Xi_6)^{i_3 i_4}_{i_5 i_6} \\
(\xi_7)^{i_3 i_4}_{i_5 a_2} &= +(\Xi_2)^{i_3 i_4}_{i_5 a_2} + (\Xi_9)^{i_3 i_4}_{i_5 a_2} \\
(\xi_6)^{a'_5}_{a_2} &= -f^{a'_5}_{a_2} + t^{a_6}_{i_7} v^{i_7 a'_5}_{a_2 a_6} - \tfrac{1}{2} \tilde{t}^{a'_5 a'_6}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_2} + \tfrac{1}{2} \tilde{t}^{a'_5 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_2 a_6} \\
(\xi_5)^{a_5}_{a_2} &= +f^{a_5}_{a_2} - t^{a_6}_{i_7} v^{i_7 a_5}_{a_2 a_6} - t^{a_5}_{i_6} (\Xi_0)^{i_6}_{a_2} - \tfrac{1}{2} t^{a_5 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_2 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_5}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_2} \\
(\xi_{4,0})^{i_4}_{a_6} &= -f^{i_4}_{a_6} - (\Xi_0)^{i_4}_{a_6} \\
(\xi_4)^{i_4}_{i_5} &= -f^{i_4}_{i_5} + t^{a_6}_{i_5} (\xi_{4,0})^{i_4}_{a_6} - t^{a_6}_{i_7} v^{i_4 i_7}_{i_5 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_5 i_8} v^{i_4 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_5 i_8} V^{i_4 i_8}_{i_6 i_7} \\
(\xi_{31})^{a_5 a_6}_{a_1 a_2} &= +P_2 t^{a_5}_{i_7} (\Xi_{11})^{i_7 a_6}_{a_1 a_2} \\
(\xi_{30})^{i_3 i_4 a_7}_{i_5 i_6 a_2} &= -\tfrac{1}{2} t^{a_7}_{i_8} (\Xi_{14})^{i_3 i_4 i_8}_{i_5 i_6 a_2} - P_2 t^{a_7}_{i_5} (\Xi_9)^{i_3 i_4}_{i_6 a_2} \\
(\xi_3)^{i_4}_{i_5} &= -t^{a_6}_{i_5} \lambda^{i_4}_{a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_5 i_8} \lambda^{i_4 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_5 i_8} (\Xi_8)^{i_4 i_8}_{i_6 i_7} - \tfrac{1}{12} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} \lambda^{i_4 i_9 i_{10}}_{a_6 a_7 a_8} \\
(\xi_{29})^{i_4 a'_6}_{a_2 a_5} &= -\tfrac{1}{2} \lambda^{i_4 i_7 i_8}_{a_2 a_5 a_9} \tilde{t}^{a'_6 a_9}_{i_7 i_8} \\
(\xi_{28,0})^{i_3 i_4}_{i_7 a'_9} &= +v^{i_3 i_4}_{i_7 a'_9} - (\Xi_{12})^{i_3 i_4}_{i_7 a'_9} \\
(\xi_{28})^{i_3 i_4 a_8}_{i_5 i_6 i_7} &= +P_3 \tilde{t}^{a'_9 a_8}_{i_5 i_6} (\xi_{28,0})^{i_3 i_4}_{i_7 a'_9} + \tfrac{1}{2} t^{a_8 a_9 a_{10}}_{i_5 i_6 i_7} v^{i_3 i_4}_{a_9 a_{10}} \\
(\xi_{23,2})^{i_8 i_9}_{i_5 a_2} &= -v^{i_8 i_9}_{i_5 a_2} + (\Xi_1)^{i_8 i_9}_{i_5 a_2} \\
(\xi_{23,1})^{i_8 a_7}_{i_5 a_2} &= -(\Xi_4)^{i_8 a_7}_{i_5 a_2} - (\Xi_7)^{i_8 a_7}_{i_5 a_2} - t^{a_7 a_9}_{i_5 i_{10}} v^{i_8 i_{10}}_{a_2 a_9} \\
(\xi_{23})^{a_6 a_7}_{i_5 a_2} &= -v^{a_6 a_7}_{i_5 a_2} + t^{a_8}_{i_5} v^{a_6 a_7}_{a_2 a_8} + P_2 t^{a_6}_{i_8} (\xi_{23,1})^{i_8 a_7}_{i_5 a_2} + \tfrac{1}{2} t^{a_6 a_7}_{i_8 i_9} (\xi_{23,2})^{i_8 i_9}_{i_5 a_2} \\
&\quad + P_2 t^{a_6 a_8}_{i_5 i_9} v^{i_9 a_7}_{a_2 a_8} + P_2 \tilde{t}^{a'_8 a_6}_{i_5 i_9} v^{i_9 a_7}_{a'_8 a_2} + \tfrac{1}{2} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} v^{i_9 i_{10}}_{a_2 a_8} \\
(\xi_{22,6})^{i_4 i_9}_{i_6 a'_8} &= -v^{i_4 i_9}_{i_6 a'_8} + (\Xi_{12})^{i_4 i_9}_{i_6 a'_8} \\
(\xi_{22,4})^{i_4 i_9}_{i_6 a_8} &= +v^{i_4 i_9}_{i_6 a_8} - (\Xi_1)^{i_4 i_9}_{i_6 a_8} \\
(\xi_{22,3})^{i_4 a_7}_{i_6 a_8} &= +v^{i_4 a_7}_{i_6 a_8} - \tfrac{1}{2} (\Xi_4)^{i_4 a_7}_{i_6 a_8} \\
(\xi_{22,2})^{i_4 i_8}_{i_5 i_6} &= +v^{i_4 i_8}_{i_5 i_6} - (\Xi_3)^{i_4 i_8}_{i_5 i_6} + \tfrac{1}{2} (\Xi_{13})^{i_4 i_8}_{i_5 i_6} + (\Xi_5)^{i_4 i_8}_{i_5 i_6} + (\Xi_6)^{i_4 i_8}_{i_5 i_6} \\
(\xi_{22,1})^{i_4}_{a'_8} &= -f^{i_4}_{a'_8} - t^{a_9}_{i_{10}} v^{i_4 i_{10}}_{a'_8 a_9} \\
(\xi_{22,0})^{i_4}_{a_8} &= +f^{i_4}_{a_8} + (\Xi_0)^{i_4}_{a_8} \\
(\xi_{22})^{i_4 a_7}_{i_5 i_6} &= -v^{i_4 a_7}_{i_5 i_6} + t^{a_7 a_8}_{i_5 i_6} (\xi_{22,0})^{i_4}_{a_8} + \tilde{t}^{a'_8 a_7}_{i_5 i_6} (\xi_{22,1})^{i_4}_{a'_8} + t^{a_7}_{i_8} (\xi_{22,2})^{i_4 i_8}_{i_5 i_6} \\
&\quad + P_2 t^{a_8}_{i_5} (\xi_{22,3})^{i_4 a_7}_{i_6 a_8} + P_2 t^{a_7 a_8}_{i_5 i_9} (\xi_{22,4})^{i_4 i_9}_{i_6 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_5 i_6} v^{i_4 a_7}_{a_8 a_9} \\
&\quad + P_2 \tilde{t}^{a'_8 a_7}_{i_5 i_9} (\xi_{22,6})^{i_4 i_9}_{i_6 a'_8} - \tfrac{1}{2} t^{i_8 i_9}_{i_5 i_6} V^{i_4 a_7}_{i_8 i_9} + \tfrac{1}{2} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}} v^{i_4 i_{10}}_{a_8 a_9} \\
(\xi_{21})^{i_4 a'_6}_{i_5 a_2} &= +\tilde{t}^{a'_6 a'_7}_{i_5 i_8} \tilde{\lambda}^{i_4 i_8}_{a'_7 a_2} - \tfrac{1}{2} \tilde{t}^{a'_6 a_7}_{i_8 i_9} (\Xi_{10})^{i_4 i_8 i_9}_{i_5 a_2 a_7} \\
(\xi_{20})^{a'_5}_{a_2} &= +\tfrac{1}{2} \lambda^{i_6 i_7}_{a_2 a_8} \tilde{t}^{a'_5 a_8}_{i_6 i_7} - \tfrac{1}{2} \tilde{t}^{a'_5 a'_6}_{i_7 i_8} \tilde{\lambda}^{i_7 i_8}_{a'_6 a_2} \\
(\xi_{19})^{a_5}_{a_2} &= -\tfrac{1}{2} t^{a_5 a_6}_{i_7 i_8} \lambda^{i_7 i_8}_{a_2 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_5}_{i_7 i_8} \tilde{\lambda}^{i_7 i_8}_{a'_6 a_2} - \tfrac{1}{12} t^{a_5 a_6 a_7}_{i_8 i_9 i_{10}} \lambda^{i_8 i_9 i_{10}}_{a_2 a_6 a_7} \\
(\xi_{18})^{i_4 a_6}_{i_5 a_2} &= +t^{a_6 a_7}_{i_5 i_8} \lambda^{i_4 i_8}_{a_2 a_7} + \tilde{t}^{a'_7 a_6}_{i_5 i_8} \tilde{\lambda}^{i_4 i_8}_{a'_7 a_2} + \tfrac{1}{2} t^{a_6 a_7}_{i_8 i_9} (\Xi_{10})^{i_4 i_8 i_9}_{i_5 a_2 a_7} - t^{a_6}_{i_7} (\Xi_9)^{i_4 i_7}_{i_5 a_2} \\
&\quad + \tfrac{1}{4} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} \lambda^{i_4 i_9 i_{10}}_{a_2 a_7 a_8} \\
(\xi_{17,0})^{i_3 i_4}_{i_6 a_7} &= +\tfrac{1}{2} (\Xi_2)^{i_3 i_4}_{i_6 a_7} + (\Xi_9)^{i_3 i_4}_{i_6 a_7} \\
(\xi_{17})^{i_3 i_4}_{i_5 i_6} &= +P_2 t^{a_7}_{i_5} (\xi_{17,0})^{i_3 i_4}_{i_6 a_7} + \tfrac{1}{2} t^{a_7 a_8}_{i_5 i_6} \lambda^{i_3 i_4}_{a_7 a_8} + \tfrac{1}{2} t^{i_7 i_8}_{i_5 i_6} (\Xi_8)^{i_3 i_4}_{i_7 i_8} + \tfrac{1}{6} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}} \lambda^{i_3 i_4 i_{10}}_{a_7 a_8 a_9} \\
(\xi_{16})^{i_3 i_4}_{i_5 a'_6} &= +t^{a_7}_{i_5} \tilde{\lambda}^{i_3 i_4}_{a'_6 a_7} \\
(\xi_{15})^{i_3 i_4}_{i_5 a_6} &= +(\Xi_2)^{i_3 i_4}_{i_5 a_6} + (\Xi_9)^{i_3 i_4}_{i_5 a_6} \\
(\xi_{14})^{i_4 i_6}_{i_5 a_2} &= +(\Xi_2)^{i_4 i_6}_{i_5 a_2} + (\Xi_9)^{i_4 i_6}_{i_5 a_2} \\
(\xi_{13})^{i_3 i_4}_{i_5 i_6} &= -(\Xi_3)^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{2} (\Xi_{13})^{i_3 i_4}_{i_5 i_6} \\
(\xi_{11})^{i_4 a'_6}_{i_5 a_2} &= +v^{i_4 a'_6}_{i_5 a_2} - t^{a_7}_{i_5} v^{i_4 a'_6}_{a_2 a_7} \\
(\xi_1)^{i_3 i_4}_{i_5 a_2} &= -v^{i_3 i_4}_{i_5 a_2} + (\Xi_1)^{i_3 i_4}_{i_5 a_2} \\
(\xi_0)^{i_4}_{a_2} &= +f^{i_4}_{a_2} + (\Xi_0)^{i_4}_{a_2} \\
\delta^{i_3 i_4}_{a_1 a_2} &= +v^{i_3 i_4}_{a_1 a_2} + P_2 P_2 \lambda^{i_3}_{a_1} (\xi_0)^{i_4}_{a_2} + P_2 \lambda^{i_5}_{a_1} (\xi_1)^{i_3 i_4}_{i_5 a_2} - P_2 \lambda^{i_3}_{a_5} v^{i_4 a_5}_{a_1 a_2} \\
&\quad + P_2 v^{i_3 i_5}_{a_1 a_2} (\xi_3)^{i_4}_{i_5} + P_2 \lambda^{i_3 i_5}_{a_1 a_2} (\xi_4)^{i_4}_{i_5} + P_2 \lambda^{i_3 i_4}_{a_1 a_5} (\xi_5)^{a_5}_{a_2} + P_2 \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} (\xi_6)^{a'_5}_{a_2} \\
&\quad + P_2 t^{i_5}_{a_1} (\xi_7)^{i_3 i_4}_{i_5 a_2} + \tfrac{1}{2} \lambda^{i_5 i_6}_{a_1 a_2} (\xi_8)^{i_3 i_4}_{i_5 i_6} + P_2 P_2 \lambda^{i_3 i_5}_{a_1 a_6} (\xi_9)^{i_4 a_6}_{i_5 a_2} \\
&\quad + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_5 a_6} v^{a_5 a_6}_{a_1 a_2} + P_2 P_2 \tilde{\lambda}^{i_3 i_5}_{a'_6 a_1} (\xi_{11})^{i_4 a'_6}_{i_5 a_2} + \tfrac{1}{2} \lambda^{i_3 i_4}_{i_5 i_6} (V^\dagger)^{i_5 i_6}_{a_1 a_2} \\
&\quad + \lambda^{i_5 i_6}_{a_1 a_2} (\xi_{13})^{i_3 i_4}_{i_5 i_6} + P_2 P_2 v^{i_3 i_5}_{i_6 a_1} (\xi_{14})^{i_4 i_6}_{i_5 a_2} + v^{i_5 a_6}_{a_1 a_2} (\xi_{15})^{i_3 i_4}_{i_5 a_6} \\
&\quad + v^{i_5 a'_6}_{a_1 a_2} (\xi_{16})^{i_3 i_4}_{i_5 a'_6} + \tfrac{1}{2} v^{i_5 i_6}_{a_1 a_2} (\xi_{17})^{i_3 i_4}_{i_5 i_6} + P_2 P_2 v^{i_3 i_5}_{a_1 a_6} (\xi_{18})^{i_4 a_6}_{i_5 a_2} \\
&\quad + P_2 v^{i_3 i_4}_{a_1 a_5} (\xi_{19})^{a_5}_{a_2} + P_2 v^{i_3 i_4}_{a'_5 a_1} (\xi_{20})^{a'_5}_{a_2} + P_2 P_2 v^{i_3 i_5}_{a'_6 a_1} (\xi_{21})^{i_4 a'_6}_{i_5 a_2} \\
&\quad + \tfrac{1}{2} P_2 \lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} (\xi_{22})^{i_4 a_7}_{i_5 i_6} + \tfrac{1}{2} P_2 \lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} (\xi_{23})^{a_6 a_7}_{i_5 a_2} + P_2 v^{i_5 a_6}_{i_7 a_1} (\Xi_{10})^{i_3 i_4 i_7}_{i_5 a_2 a_6} \\
&\quad + \tfrac{1}{2} P_2 v^{i_5 i_6}_{i_7 a_1} (\Xi_{14})^{i_3 i_4 i_7}_{i_5 i_6 a_2} + v^{i_3 i_4}_{i_5 a_6} (\Xi_{11})^{i_5 a_6}_{a_1 a_2} + P_2 P_2 v^{i_3 i_5}_{a_1 a_6} (\Xi_{11})^{i_4 a_6}_{a_2 a_5} \\
&\quad + \tfrac{1}{6} \lambda^{i_5 i_6 i_7}_{a_1 a_2 a_8} (\xi_{28})^{i_3 i_4 a_8}_{i_5 i_6 i_7} + P_2 P_2 v^{i_3 a_5}_{a'_6 a_1} (\xi_{29})^{i_4 a'_6}_{a_2 a_5} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_1 a_7} (\xi_{30})^{i_3 i_4 a_7}_{i_5 i_6 a_2} \\
&\quad + \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} (\xi_{31})^{a_5 a_6}_{a_1 a_2}
\end{aligned}
$$

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TABLE ESI.4.XIX: The computational sequence and intermediates for the geminal λ amplitude equation of Λ-CCSDT-R12 [Part I]

$$(\Xi_0)^{i_7 a_6}_{i_1 i_2} = +F^{a'_8 a_6}_{i_1 i_2} f^{i_7}_{a'_8}$$
$$(\Xi_1)^{i_7 a'_5}_{i_1 i_2} = +\lambda^{i_7}_{a_8} F^{a'_5 a_8}_{i_1 i_2}$$
$$(\Xi_2)^{i_7}_{a'_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_3)^{i_4 i_8}_{i_6 i_7} = +\tfrac{1}{2}\lambda^{i_4 i_8}_{i_9 i_{10}} X^{i_9 i_{10}}_{i_6 i_7}$$
$$(\Xi_4)^{i_3 i_4}_{i_5 a'_6} = +t^{a_7}_{i_5} \tilde{\lambda}^{i_3 i_4}_{a'_6 a_7}$$
$$(\Xi_5)^{a_6}_{a'_7} = +t^{a_8}_{i_9} v^{i_9 a_6}_{a'_7 a_8}$$
$$(\Xi_6)^{i_3 i_4}_{i_6 a_7} = +t^{a_8}_{i_6} \lambda^{i_3 i_4}_{a_7 a_8}$$
$$(\Xi_7)^{i_9 a_8}_{i_5 a'_{10}} = +t^{a_{11}}_{i_5} v^{i_9 a_8}_{a'_{10} a_{11}}$$
$$(\Xi_8)^{a'_7}_{a'_5} = +t^{a_8}_{i_9} v^{i_9 a'_7}_{a'_5 a_8}$$
$$(\Xi_9)^{i_4 a'_8}_{i_7 a'_5} = +t^{a_9}_{i_7} v^{i_4 a'_8}_{a'_5 a_9}$$
$$(\Xi_{10})^{a_6}_{a'_7} = +\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\Xi_{11})^{a_6}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{12})^{i_7}_{a'_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_{13})^{i_4 i_9}_{i_7 a_6} = +f^{a_{10}}_{i_7} v^{i_4 i_9}_{a_6 a_{10}}$$
$$(\Xi_{14})^{a_6}_{a'_7} = +\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\Xi_{15})^{a'_7}_{a'_5} = +\tfrac{1}{2} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_5 a'_8}$$
$$(\Xi_{16})^{a'_7}_{a'_5} = +\tfrac{1}{2} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_5 a_8}$$
$$(\Xi_{17})^{i_9 a_8}_{i_5 a'_{10}} = +\tilde{t}^{a'_{11} a_8}_{i_5 i_{12}} v^{i_9 i_{12}}_{a'_{10} a'_{11}}$$
$$(\Xi_{18})^{i_4 a_8}_{i_7 a'_5} = +\tilde{t}^{a'_9 a_8}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_5 a'_9}$$
$$(\Xi_{19})^{a'_5}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_5 a'_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{20})^{a'_5}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_5 a_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\Xi_{21})^{a_6}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{22})^{i_3 i_4}_{i_6 a_7} = +\tfrac{1}{2} t^{a_8 a_9}_{i_6 i_{10}} \lambda^{i_3 i_4 i_{10}}_{a_7 a_8 a_9}$$
$$(\Xi_{23})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9} = +f^{a_{12}}_{i_7} \lambda^{i_4 i_{10} i_{11}}_{a_6 a_9 a_{12}}$$
$$(\Xi_{24})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} = +\tfrac{1}{2} t^{a_{11} a_{12}}_{i_7 i_8} \lambda^{i_3 i_4 i_{10}}_{a_6 a_{11} a_{12}}$$
$$(\Xi_{25})^{i_7 a_6}_{i_1 i_2} = +F^{a'_8 a_6}_{i_1 i_2} (\Xi_2)^{i_7}_{a'_8}$$
$$(\Xi_{26})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} = +P_2 t^{a_{11}}_{i_7} (\Xi_{23})^{i_3 i_4 i_{10}}_{i_8 a_6 a_{11}}$$
$$(\xi_{9,8})^{a_7}_{a_6} = -t^{a_8}_{i_9} v^{i_9 a_7}_{a_6 a_8} - \tfrac{1}{2} t^{a_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_7}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\xi_{9,7})^{a'_7}_{a_6} = -t^{a_8}_{i_9} v^{i_9 a'_7}_{a_6 a_8} + \tfrac{1}{2} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6} - \tfrac{1}{2} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8}$$
$$(\xi_{9,6})^{a'_7}_{a'_5} = -(\Xi_8)^{a'_7}_{a'_5} - (\Xi_{15})^{a'_7}_{a'_5} - (\Xi_{16})^{a'_7}_{a'_5}$$
$$(\xi_{9,5})^{i_4 i_8}_{i_7 a_6} = +(\Xi_6)^{i_4 i_8}_{i_7 a_6} + (\Xi_{22})^{i_4 i_8}_{i_7 a_6}$$
$$(\xi_{9,4})^{i_4 a_8}_{i_7 a_6} = -v^{i_4 a_8}_{i_7 a_6} + t^{a_9}_{i_7} v^{i_4 a_8}_{a_6 a_9} - t^{a_8}_{i_9} (\Xi_{13})^{i_4 i_9}_{i_7 a_6} + t^{a_8 a_9}_{i_7 i_{10}} v^{i_4 i_{10}}_{a_6 a_9} + \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} v^{i_4 i_{10}}_{a'_9 a_6}$$
$$(\xi_{9,3})^{i_4 a'_8}_{i_7 a_6} = -v^{i_4 a'_8}_{i_7 a_6} + t^{a_9}_{i_7} v^{i_4 a'_8}_{a_6 a_9} - \tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} v^{i_4 i_{10}}_{a'_9 a_6}$$
$$(\xi_{9,21,0})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} = -\tfrac{1}{2} (\Xi_{26})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} - (\Xi_{24})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6}$$
$$(\xi_{9,21})^{i_3 i_4 a_9}_{i_7 i_8 a_6} = +t^{a_9}_{i_{10}} (\xi_{9,21,0})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} + P_2 t^{a_9 a_{10}}_{i_7 i_{11}} (\Xi_{23})^{i_3 i_4 i_{11}}_{i_8 a_6 a_{10}} - P_2 t^{a_9}_{i_7} (\Xi_{22})^{i_3 i_4}_{i_8 a_6}$$
$$(\xi_{9,20})^{i_4 a'_8}_{a_6 a_7} = +\tfrac{1}{2} \lambda^{i_4 i_9 i_{10}}_{a_6 a_7 a_{11}} \tilde{t}^{a'_8 a_{11}}_{i_9 i_{10}}$$
$$(\xi_{9,2})^{i_4 a'_8}_{i_7 a'_5} = -v^{i_4 a'_8}_{i_7 a'_5} + (\Xi_9)^{i_4 a'_8}_{i_7 a'_5}$$
$$(\xi_{9,19})^{i_4 a_8}_{a_6 a_7} = +\tfrac{1}{2} t^{a_8 a_9}_{i_{10} i_{11}} \lambda^{i_4 i_{10} i_{11}}_{a_6 a_7 a_9}$$
$$(\xi_{9,15})^{a_8 a_9}_{i_7 a'_5} = +v^{a_8 a_9}_{i_7 a'_5} - t^{a_{10}}_{i_7} v^{a_8 a_9}_{a'_5 a_{10}} - P_2 t^{a_8 a_{10}}_{i_7 i_{11}} v^{i_{11} a_9}_{a'_5 a_{10}} + P_2 \tilde{t}^{a'_{10} a_8}_{i_7 i_{11}} v^{i_{11} a_9}_{a'_5 a'_{10}} - \tfrac{1}{2} \tilde{t}^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} v^{i_{11} i_{12}}_{a'_5 a_{10}}$$
$$(\xi_{9,12})^{a'_7}_{a_6} = -\tfrac{1}{2} \lambda^{i_8 i_9}_{a_6 a_{10}} \tilde{t}^{a'_7 a_{10}}_{i_8 i_9} + \tfrac{1}{2} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\xi_{9,11})^{i_4 a'_8}_{i_7 a_6} = +\lambda^{i_4 i_9}_{a_6 a_{10}} \tilde{t}^{a'_8 a_{10}}_{i_7 i_9} - \tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_9 a_6} + \tfrac{1}{2} \tilde{t}^{a'_8 a_9}_{i_{10} i_{11}} (\Xi_{23})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9}$$
$$(\xi_{9,10,0})^{i_4 i_9}_{i_7 a_6} = -(\Xi_6)^{i_4 i_9}_{i_7 a_6} - (\Xi_{22})^{i_4 i_9}_{i_7 a_6}$$
$$(\xi_{9,10})^{i_4 a_8}_{i_7 a_6} = +t^{a_8}_{i_9} (\xi_{9,10,0})^{i_4 i_9}_{i_7 a_6} + t^{a_8 a_9}_{i_7 i_{10}} \lambda^{i_4 i_{10}}_{a_6 a_9} + \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_9 a_6} + \tfrac{1}{2} t^{a_8 a_9}_{i_{10} i_{11}} (\Xi_{23})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9} + \tfrac{1}{4} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} \lambda^{i_4 i_{11} i_{12}}_{a_6 a_9 a_{10}}$$
$$(\xi_{9,1})^{i_4 a_8}_{i_7 a'_5} = +v^{i_4 a_8}_{i_7 a'_5} - (\Xi_7)^{i_4 a_8}_{i_7 a'_5}$$
$$(\xi_9)^{i_3 i_4}_{a'_5 a_6} = -f^{i_7}_{a_6} (\Xi_4)^{i_3 i_4}_{i_7 a'_5} + P_2 \lambda^{i_3 i_7}_{a_6 a_8} (\xi_{9,1})^{i_4 a_8}_{i_7 a'_5} + P_2 \tilde{\lambda}^{i_3 i_7}_{a'_8 a_6} (\xi_{9,2})^{i_4 a'_8}_{i_7 a'_5} + P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} (\xi_{9,3})^{i_4 a'_8}_{i_7 a_6} + P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} (\xi_{9,4})^{i_4 a_8}_{i_7 a_6} + P_2 v^{i_3 i_7}_{i_8 a'_5} (\xi_{9,5})^{i_4 i_8}_{i_7 a_6} + \tilde{\lambda}^{i_3 i_4}_{a'_7 a_6} (\xi_{9,6})^{a'_7}_{a'_5} + \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_7} (\xi_{9,7})^{a'_7}_{a_6} + \tilde{\lambda}^{i_3 i_4}_{a'_5 a_7} (\xi_{9,8})^{a_7}_{a_6} - P_2 v^{i_3 i_7}_{i_8 a_6} (\Xi_4)^{i_4 i_8}_{i_7 a'_5} + P_2 v^{i_3 i_7}_{a'_5 a_8} (\xi_{9,10})^{i_4 a_8}_{i_7 a_6} + P_2 v^{i_3 i_7}_{a'_5 a'_8} (\xi_{9,11})^{i_4 a'_8}_{i_7 a_6} + v^{i_3 i_4}_{a'_5 a_7} (\xi_{9,12})^{a'_7}_{a_6} + P_2 v^{i_3 i_7}_{a_6 a_8} (\Xi_{18})^{i_4 a_8}_{i_7 a'_5} + f^{i_7}_{a'_5} (\Xi_{22})^{i_3 i_4}_{i_7 a_6} + \tfrac{1}{2} \lambda^{i_3 i_4 i_7}_{a_6 a_8 a_9} (\xi_{9,15})^{a_8 a_9}_{i_7 a'_5} + v^{i_7 a_8}_{i_9 a'_5} (\Xi_{23})^{i_3 i_4 i_9}_{i_7 a_6 a_8} + \tfrac{1}{2} v^{i_7 i_8}_{i_9 a'_5} (\Xi_{26})^{i_3 i_4 i_9}_{i_7 i_8 a_6} + \tfrac{1}{2} v^{i_7 i_8}_{i_9 a'_5} (\Xi_{24})^{i_3 i_4 i_9}_{i_7 i_8 a_6} + P_2 v^{i_3 a_7}_{a'_5 a_8} (\xi_{9,19})^{i_4 a_8}_{a_6 a_7} + P_2 v^{i_3 a_7}_{a'_5 a'_8} (\xi_{9,20})^{i_4 a'_8}_{a_6 a_7} + \tfrac{1}{2} v^{i_7 i_8}_{a'_5 a_9} (\xi_{9,21})^{i_3 i_4 a_9}_{i_7 i_8 a_6}$$
$$(\xi_{8,1})^{a_6}_{a'_7} = -(\Xi_5)^{a_6}_{a'_7} - (\Xi_{10})^{a_6}_{a'_7} + (\Xi_{11})^{a_6}_{a'_7}$$
$$(\xi_{8,0,0})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - (\Xi_2)^{i_7}_{a'_8}$$
$$(\xi_{8,0})^{i_7 a'_5}_{i_1 i_2} = +F^{a'_5 a'_8}_{i_1 i_2} (\xi_{8,0,0})^{i_7}_{a'_8} - F^{a'_5 a_8}_{i_1 i_2} (\Xi_{12})^{i_7}_{a_8}$$
$$(\xi_8)^{a'_5 a_6}_{i_1 i_2} = +t^{a_6}_{i_7} (\xi_{8,0})^{i_7 a'_5}_{i_1 i_2} + F^{a'_5 a'_7}_{i_1 i_2} (\xi_{8,1})^{a_6}_{a'_7}$$
$$(\xi_{7,1,0})^{i_3 i_4}_{i_8 a_9} = -v^{i_3 i_4}_{i_8 a_9} + \tfrac{1}{2} (\Xi_{13})^{i_3 i_4}_{i_8 a_9}$$
$$(\xi_{7,1})^{i_3 i_4}_{i_7 i_8} = +P_2 t^{a_9}_{i_7} (\xi_{7,1,0})^{i_3 i_4}_{i_8 a_9} + \tfrac{1}{2} t^{a_9 a_{10}}_{i_7 i_8} v^{i_3 i_4}_{a_9 a_{10}}$$
$$(\xi_{7,0,0})^{i_4}_{a_8} = -f^{i_4}_{a_8} - (\Xi_{12})^{i_4}_{a_8}$$
$$(\xi_{7,0})^{i_4}_{i_7} = +t^{a_8}_{i_7} (\xi_{7,0,0})^{i_4}_{a_8} - t^{a_8}_{i_9} v^{i_4 i_9}_{i_7 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_7 i_{10}} v^{i_4 i_{10}}_{a_8 a_9} - \tfrac{1}{2} t^{i_8 i_9}_{i_7 i_{10}} V^{i_4 i_{10}}_{i_8 i_9}$$
$$(\xi_7)^{i_3 i_4}_{i_5 i_6} = +P_2 \lambda^{i_3 i_7}_{i_5 i_6} (\xi_{7,0})^{i_4}_{i_7} + \tfrac{1}{2} \lambda^{i_7 i_8}_{i_5 i_6} (\xi_{7,1})^{i_3 i_4}_{i_7 i_8}$$
$$(\xi_6)^{i_5 i_6}_{i_1 i_2} = +B^{i_5 i_6}_{i_1 i_2} + P^{i_5 i_6}_{i_1 i_2}$$
$$(\xi_{4,1})^{i_7 a_6}_{i_1 i_2} = -(\Xi_0)^{i_7 a_6}_{i_1 i_2} - (\Xi_{25})^{i_7 a_6}_{i_1 i_2}$$
$$(\xi_{4,0})^{a_6}_{a'_7} = -f^{a_6}_{a'_7} + (\Xi_5)^{a_6}_{a'_7} + (\Xi_{10})^{a_6}_{a'_7} - (\Xi_{11})^{a_6}_{a'_7}$$
$$(\xi_4)^{a_5 a_6}_{i_1 i_2} = +V^{a_5 a_6}_{i_1 i_2} + P_2 F^{a'_7 a_5}_{i_1 i_2} (\xi_{4,0})^{a_6}_{a'_7} + P_2 t^{a_5}_{i_7} (\xi_{4,1})^{i_7 a_6}_{i_1 i_2}$$
$$(\xi_3)^{i_4}_{i_5} = -t^{a_6}_{i_5} \lambda^{i_4}_{a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_5 i_8} \lambda^{i_4 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_5 i_8} (\Xi_3)^{i_4 i_8}_{i_6 i_7} - \tfrac{1}{12} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} \lambda^{i_4 i_9 i_{10}}_{a_6 a_7 a_8}$$
$$(\xi_{2,3})^{a'_5}_{a'_7} = -(\Xi_{19})^{a'_5}_{a'_7} - (\Xi_{20})^{a'_5}_{a'_7}$$
$$(\xi_{2,2})^{a_6}_{a'_7} = -(\Xi_{14})^{a_6}_{a'_7} + (\Xi_{21})^{a_6}_{a'_7}$$
$$(\xi_{2,1})^{a_6}_{a_7} = -\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} \lambda^{i_9 i_{10}}_{a_7 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_8 a_7} - \tfrac{1}{12} t^{a_6 a_8 a_9}_{i_{10} i_{11} i_{12}} \lambda^{i_{10} i_{11} i_{12}}_{a_7 a_8 a_9}$$
$$(\xi_2)^{a'_5 a_6}_{i_1 i_2} = -t^{a_6}_{i_7} (\Xi_1)^{i_7 a'_5}_{i_1 i_2} + F^{a'_5 a_7}_{i_1 i_2} (\xi_{2,1})^{a_6}_{a_7} + F^{a'_5 a'_7}_{i_1 i_2} (\xi_{2,2})^{a_6}_{a'_7} + F^{a'_7 a_6}_{i_1 i_2} (\xi_{2,3})^{a'_5}_{a'_7}$$
$$(\xi_{18,0,0})^{i_9 a_8}_{i_5 a'_{10}} = -(\Xi_7)^{i_9 a_8}_{i_5 a'_{10}} + (\Xi_{17})^{i_9 a_8}_{i_5 a'_{10}}$$
$$(\xi_{18,0})^{i_9 a_7 a_8}_{i_1 i_2 i_5} = +P_2 F^{a'_{10} a_7}_{i_1 i_2} (\xi_{18,0,0})^{i_9 a_8}_{i_5 a'_{10}}$$
$$(\xi_{18})^{a_6 a_7 a_8}_{i_1 i_2 i_5} = +P_3 t^{a_6}_{i_9} (\xi_{18,0})^{i_9 a_7 a_8}_{i_1 i_2 i_5}$$
$$(\xi_{17,0})^{a'_6}_{a'_7} = -(\Xi_{19})^{a'_6}_{a'_7} - (\Xi_{20})^{a'_6}_{a'_7}$$
$$(\xi_{17})^{a'_5 a'_6}_{i_1 i_2} = +P_2 F^{a'_5 a'_7}_{i_1 i_2} (\xi_{17,0})^{a'_6}_{a'_7}$$
$$(\xi_{16})^{i_5 i_6}_{i_1 i_2} = +\tfrac{1}{2} t^{i_5 i_6}_{i_7 i_8} (\Xi_3)^{i_7 i_8}_{i_1 i_2}$$
$$(\xi_{15,0})^{a_6}_{a'_7} = +(\Xi_{14})^{a_6}_{a'_7} - (\Xi_{21})^{a_6}_{a'_7}$$
$$(\xi_{15})^{a_5 a_6}_{i_1 i_2} = +P_2 F^{a'_7 a_5}_{i_1 i_2} (\xi_{15,0})^{a_6}_{a'_7}$$
$$(\xi_{14,0})^{i_3 i_4}_{i_6 a_7} = +\tfrac{1}{2} (\Xi_6)^{i_3 i_4}_{i_6 a_7} + (\Xi_{22})^{i_3 i_4}_{i_6 a_7}$$
$$(\xi_{14})^{i_3 i_4}_{i_5 i_6} = +P_2 t^{a_7}_{i_5} (\xi_{14,0})^{i_3 i_4}_{i_6 a_7} + \tfrac{1}{2} t^{a_7 a_8}_{i_5 i_6} \lambda^{i_3 i_4}_{a_7 a_8} + \tfrac{1}{2} t^{i_7 i_8}_{i_5 i_6} (\Xi_3)^{i_3 i_4}_{i_7 i_8} + \tfrac{1}{6} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}} \lambda^{i_3 i_4 i_{10}}_{a_7 a_8 a_9}$$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.4.XX: The computational sequence and intermediates for the geminal λ amplitude equation of Λ-CCSDT-R12 [Part II]

$$
\begin{aligned}
(\xi_{12})^{i_3 i_4}_{i_5 a_6} &= +(\Xi_6)^{i_3 i_4}_{i_5 a_6} + (\Xi_{22})^{i_3 i_4}_{i_5 a_6} \\
(\xi_{11,5})^{i_4 a'_8}_{i_7 a'_6} &= +\tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_6 a'_9} \\
(\xi_{11,4})^{i_4 a_8}_{i_7 a'_6} &= -(\Xi_{18})^{i_4 a_8}_{i_7 a'_6} + t^{a_8 a_9}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_6 a_9} \\
(\xi_{11,2})^{a'_7}_{a'_6} &= -(\Xi_8)^{a'_7}_{a'_6} - (\Xi_{15})^{a'_7}_{a'_6} - (\Xi_{16})^{a'_7}_{a'_6} \\
(\xi_{11,1,0})^{i_4 i_9}_{i_7 a'_6} &= -t^{a_{10}}_{i_7} v^{i_4 i_9}_{a'_6 a_{10}} \\
(\xi_{11,1})^{i_4 a_8}_{i_7 a'_6} &= -v^{i_4 a_8}_{i_7 a'_6} + (\Xi_7)^{i_4 a_8}_{i_7 a'_6} - (\Xi_{17})^{i_4 a_8}_{i_7 a'_6} + t^{a_8}_{i_9} (\xi_{11,1,0})^{i_4 i_9}_{i_7 a'_6} \\
(\xi_{11,0})^{i_4 a'_8}_{i_7 a'_6} &= -v^{i_4 a'_8}_{i_7 a'_6} + (\Xi_9)^{i_4 a'_8}_{i_7 a'_6} \\
(\xi_{11})^{i_3 i_4}_{a'_5 a'_6} &= +P_2 P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} (\xi_{11,0})^{i_4 a'_8}_{i_7 a'_6} + P_2 P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} (\xi_{11,1})^{i_4 a_8}_{i_7 a'_6} \\
&\quad + P_2 \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_7} (\xi_{11,2})^{a'_7}_{a'_6} + P_2 P_2 v^{i_3 i_7}_{i_8 a'_5} (\Xi_4)^{i_4 i_8}_{i_7 a'_6} \\
&\quad + P_2 P_2 v^{i_3 i_7}_{a'_5 a_8} (\xi_{11,4})^{i_4 a_8}_{i_7 a'_6} + P_2 P_2 v^{i_3 i_7}_{a'_5 a'_8} (\xi_{11,5})^{i_4 a'_8}_{i_7 a'_6}
\end{aligned}
$$

$$
\begin{aligned}
\delta^{i_3 i_4}_{i_1 i_2} &= +V^{i_3 i_4}_{i_1 i_2} + P_2 \lambda^{i_3}_{a_5} (\xi_0)^{i_4 a_5}_{i_1 i_2} + v^{i_3 i_4}_{i_5 a'_6} (\Xi_1)^{i_5 a'_6}_{i_1 i_2} + v^{i_3 i_4}_{a'_5 a_6} (\xi_2)^{a'_5 a_6}_{i_1 i_2} \\
&\quad + P_2 V^{i_3 i_5}_{i_1 i_2} (\xi_3)^{i_4}_{i_5} + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_5 a_6} (\xi_4)^{a_5 a_6}_{i_1 i_2} + P_2 f^{i_3}_{i_5} (\Xi_3)^{i_4 i_5}_{i_1 i_2} \\
&\quad + \tfrac{1}{2} \lambda^{i_3 i_4}_{i_5 i_6} (\xi_6)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} X^{i_5 i_6}_{i_1 i_2} (\xi_7)^{i_3 i_4}_{i_5 i_6} + \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} (\xi_8)^{a'_5 a_6}_{i_1 i_2} \\
&\quad + F^{a'_5 a_6}_{i_1 i_2} (\xi_9)^{i_3 i_4}_{a'_5 a_6} + \tfrac{1}{2} v^{i_3 i_4}_{i_5 i_6} (\Xi_3)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} F^{a'_5 a'_6}_{i_1 i_2} (\xi_{11})^{i_3 i_4}_{a'_5 a'_6} + V^{i_5 a_6}_{i_1 i_2} (\xi_{12})^{i_3 i_4}_{i_5 a_6} \\
&\quad + V^{i_5 a'_6}_{i_1 i_2} (\Xi_4)^{i_3 i_4}_{i_5 a'_6} + \tfrac{1}{2} V^{i_5 i_6}_{i_1 i_2} (\xi_{14})^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} (\xi_{15})^{a_5 a_6}_{i_1 i_2} \\
&\quad + \tfrac{1}{2} V^{i_3 i_4}_{i_5 i_6} (\xi_{16})^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} v^{i_3 i_4}_{a'_5 a'_6} (\xi_{17})^{a'_5 a'_6}_{i_1 i_2} + \tfrac{1}{6} \lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} (\xi_{18})^{a_6 a_7 a_8}_{i_1 i_2 i_5}
\end{aligned}
$$

F. Λ-CCSDTQ-R12

TABLE ESI.4.XXI: The computational sequence and intermediates for the Λ_4 amplitude equation of Λ-CCSDTQ-R12

$$
\begin{aligned}
(\Xi_0)^{i_{10}}_{a_4} &= +t^{a_{11}}_{i_{12}} v^{i_{10} i_{12}}_{a_4 a_{11}} \\
(\Xi_1)^{i_8 i_{11}}_{i_9 a_4} &= +t^{a_{12}}_{i_9} v^{i_8 i_{11}}_{a_4 a_{12}} \\
(\Xi_2)^{i_5 i_6 i_7 i_8}_{i_{10} a_3 a_4 a_{11}} &= +t^{a_{12}}_{i_{10}} \lambda^{i_5 i_6 i_7 i_8}_{a_3 a_4 a_{11} a_{12}} \\
(\xi_9)^{i_8 a_{10}}_{i_9 a_4} &= -v^{i_8 a_{10}}_{i_9 a_4} + t^{a_{11}}_{i_9} v^{i_8 a_{10}}_{a_4 a_{11}} - t^{a_{10}}_{i_{11}} (\Xi_1)^{i_8 i_{11}}_{i_9 a_4} + t^{a_{10} a_{11}}_{i_9 i_{12}} v^{i_8 i_{12}}_{a_4 a_{11}} \\
&\quad + \tilde{t}^{a'_{11} a_{10}}_{i_9 i_{12}} v^{i_8 i_{12}}_{a'_{11} a_4} \\
(\xi_{8,0})^{i_7 i_8}_{i_{10} a_{11}} &= -v^{i_7 i_8}_{i_{10} a_{11}} + \tfrac{1}{2} (\Xi_1)^{i_7 i_8}_{i_{10} a_{11}} \\
(\xi_8)^{i_7 i_8}_{i_9 i_{10}} &= +v^{i_7 i_8}_{i_9 i_{10}} + P_2 t^{a_{11}}_{i_9} (\xi_{8,0})^{i_7 i_8}_{i_{10} a_{11}} + \tfrac{1}{2} t^{a_{11} a_{12}}_{i_9 i_{10}} v^{i_7 i_8}_{a_{11} a_{12}} + \tfrac{1}{2} t^{i_{11} i_{12}}_{i_9 i_{10}} V^{i_7 i_8}_{i_{11} i_{12}} \\
(\xi_6)^{a_9}_{a_4} &= +f^{a_9}_{a_4} - t^{a_{10}}_{i_{11}} v^{i_{11} a_9}_{a_4 a_{10}} - t^{a_9}_{i_{10}} (\Xi_0)^{i_{10}}_{a_4} - \tfrac{1}{2} t^{a_9 a_{10}}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a_4 a_{10}} - \tfrac{1}{2} \tilde{t}^{a'_{10} a_9}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a'_{10} a_4} \\
(\xi_{5,0})^{i_8}_{a_{10}} &= -f^{i_8}_{a_{10}} - (\Xi_0)^{i_8}_{a_{10}} \\
(\xi_5)^{i_8}_{i_9} &= -f^{i_8}_{i_9} + t^{a_{10}}_{i_9} (\xi_{5,0})^{i_8}_{a_{10}} - t^{a_{10}}_{i_{11}} v^{i_8 i_{11}}_{i_9 a_{10}} - \tfrac{1}{2} t^{a_{10} a_{11}}_{i_9 i_{12}} v^{i_8 i_{12}}_{a_{10} a_{11}} - \tfrac{1}{2} t^{i_{10} i_{11}}_{i_9 i_{12}} V^{i_8 i_{12}}_{i_{10} i_{11}} \\
(\xi_4)^{i_6 i_7 i_8}_{i_9 a_3 a_4} &= -t^{a_{10}}_{i_9} \lambda^{i_6 i_7 i_8}_{a_3 a_4 a_{10}} - \tfrac{1}{2} t^{a_{10} a_{11}}_{i_9 i_{12}} \lambda^{i_6 i_7 i_8 i_{12}}_{a_3 a_4 a_{10} a_{11}}
\end{aligned}
$$

$$
\begin{aligned}
(\xi_2)^{i_7 i_8}_{i_9 a_4} &= -v^{i_7 i_8}_{i_9 a_4} + (\Xi_1)^{i_7 i_8}_{i_9 a_4} \\
(\xi_{15})^{i_7 i_8 a'_9}_{a_2 a_3 a_4} &= +\tfrac{1}{2} \lambda^{i_7 i_8 i_{10} i_{11}}_{a_2 a_3 a_4 a_{12}} \tilde{t}^{a'_9 a_{12}}_{i_{10} i_{11}} \\
(\xi_{14})^{i_7 i_8 a_9}_{a_2 a_3 a_4} &= -\tfrac{1}{2} t^{a_9 a_{10}}_{i_{11} i_{12}} \lambda^{i_7 i_8 i_{11} i_{12}}_{a_2 a_3 a_4 a_{10}} \\
(\xi_{13})^{i_5 i_6 i_7 i_8}_{i_9 i_{10} a_3 a_4} &= +\tfrac{1}{2} P_2 t^{a_{11}}_{i_9} (\Xi_2)^{i_5 i_6 i_7 i_8}_{i_{10} a_3 a_4 a_{11}} + \tfrac{1}{2} t^{a_{11} a_{12}}_{i_9 i_{10}} \lambda^{i_5 i_6 i_7 i_8}_{a_3 a_4 a_{11} a_{12}} \\
(\xi_1)^{i_8}_{a_4} &= +f^{i_8}_{a_4} + (\Xi_0)^{i_8}_{a_4} \\
\delta^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_3 a_4} &= +P_4 P_4 \lambda^{i_5 i_6}_{a_1 a_2} v^{i_7 i_8}_{a_3 a_4} + P_4 P_4 \lambda^{i_5 i_6 i_7}_{a_1 a_2 a_3} (\xi_1)^{i_8}_{a_4} + P_4 P_4 \lambda^{i_5 i_6 i_9}_{a_1 a_2 a_3} (\xi_2)^{i_7 i_8}_{i_9 a_4} \\
&\quad - P_4 P_4 \lambda^{i_5 i_6 i_7}_{a_1 a_2 a_9} v^{i_8 a_9}_{a_3 a_4} + P_4 P_4 v^{i_5 i_9}_{a_1 a_2} (\xi_4)^{i_6 i_7 i_8}_{i_9 a_3 a_4} + P_4 \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_4} (\xi_5)^{i_8}_{i_9} \\
&\quad + P_4 \lambda^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_3 a_9} (\xi_6)^{a_9}_{a_4} + P_4 f^{i_9}_{a_1} (\Xi_2)^{i_5 i_6 i_7 i_8}_{i_9 a_2 a_3 a_4} + \tfrac{1}{2} P_4 \lambda^{i_5 i_6 i_9 i_{10}}_{a_1 a_2 a_3 a_4} (\xi_8)^{i_7 i_8}_{i_9 i_{10}} \\
&\quad + P_4 P_4 \lambda^{i_5 i_6 i_7 i_9}_{a_1 a_2 a_3 a_{10}} (\xi_9)^{i_8 a_{10}}_{i_9 a_4} + \tfrac{1}{2} P_4 \lambda^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_9 a_{10}} v^{a_9 a_{10}}_{a_3 a_4} \\
&\quad + P_4 P_4 v^{i_5 i_9}_{i_{10} a_1} (\Xi_2)^{i_6 i_7 i_8 i_{10}}_{i_9 a_2 a_3 a_4} + P_4 v^{i_9 a_{10}}_{a_1 a_2} (\Xi_2)^{i_5 i_6 i_7 i_8}_{i_9 a_3 a_4 a_{10}} \\
&\quad + \tfrac{1}{2} P_4 v^{i_9 i_{10}}_{a_1 a_2} (\xi_{13})^{i_5 i_6 i_7 i_8}_{i_9 i_{10} a_3 a_4} + P_4 P_4 v^{i_5 i_6}_{a_1 a_9} (\xi_{14})^{i_7 i_8 a_9}_{a_2 a_3 a_4} \\
&\quad + P_4 P_4 v^{i_5 i_6}_{a'_9 a_1} (\xi_{15})^{i_7 i_8 a'_9}_{a_2 a_3 a_4}
\end{aligned}
$$

TABLE ESI.4.XXII: The computational sequence and intermediates for the Λ_1 amplitude equation of Λ-CCSDTQ-R12 [Part I]

$$(\Xi_0)^{i_2}_{a_{10}} = +t^{a_{11}}_{i_{12}} v^{i_2 i_{12}}_{a_{10} a_{11}}$$
$$(\Xi_1)^{i_5}_{i_3} = +t^{a_6}_{i_3} \lambda^{i_5}_{a_6}$$
$$(\Xi_2)^{i_5}_{i_3} = +\tfrac{1}{2} t^{a_6 a_7}_{i_3 i_8} \lambda^{i_5 i_8}_{a_6 a_7}$$
$$(\Xi_3)^{i_5 i_8}_{i_6 i_7} = +\tfrac{1}{2} \lambda^{i_5 i_8}_{i_9 i_{10}} X^{i_9 i_{10}}_{i_6 i_7}$$
$$(\Xi_4)^{i_6 i_7}_{i_3 a_5} = +t^{a_8}_{i_3} \lambda^{i_6 i_7}_{a_5 a_8}$$
$$(\Xi_5)^{i_6 i_7}_{i_3 a'_5} = +t^{a_8}_{i_3} \tilde{\lambda}^{i_6 i_7}_{a'_5 a_8}$$
$$(\Xi_6)^{i_2 a_9}_{i_6 a_{10}} = +t^{a_{11}}_{i_6} v^{i_2 a_9}_{a_{10} a_{11}}$$
$$(\Xi_7)^{i_2 i_6}_{i_3 i_4} = +\tfrac{1}{2} t^{a_7 a_8}_{i_3 i_4} \lambda^{i_2 i_6}_{a_7 a_8}$$
$$(\Xi_8)^{i_2 i_{11}}_{i_6 a_{10}} = +t^{a_{12}}_{i_6} v^{i_2 i_{11}}_{a_{10} a_{12}}$$
$$(\Xi_9)^{i_2 i_8}_{i_5 a'_9} = +t^{a_{10}}_{i_5} v^{i_2 i_8}_{a'_9 a_{10}}$$
$$(\Xi_{10})^{i_2}_{a'_6} = +t^{a_7}_{i_8} v^{i_2 i_8}_{a'_6 a_7}$$
$$(\Xi_{11})^{i_5}_{i_3} = +\tfrac{1}{12} t^{a_6 a_7 a_8}_{i_3 i_9 i_{10}} \lambda^{i_5 i_9 i_{10}}_{a_6 a_7 a_8}$$
$$(\Xi_{12})^{i_6 i_7}_{i_3 a_5} = +\tfrac{1}{2} t^{a_8 a_9}_{i_3 i_{10}} \lambda^{i_6 i_7 i_{10}}_{a_5 a_8 a_9}$$
$$(\Xi_{13})^{i_2 a_5}_{a_6 a_7} = +\tfrac{1}{2} t^{a_5 a_8}_{i_9 i_{10}} \lambda^{i_2 i_9 i_{10}}_{a_6 a_7 a_8}$$
$$(\Xi_{14})^{i_7 i_8 i_9}_{i_3 a_5 a_6} = +t^{a_{10}}_{i_3} \lambda^{i_7 i_8 i_9}_{a_5 a_6 a_{10}}$$
$$(\Xi_{15})^{i_2 i_6}_{i_3 i_4} = +\tfrac{1}{6} t^{a_7 a_8 a_9}_{i_3 i_4 i_{10}} \lambda^{i_2 i_6 i_{10}}_{a_7 a_8 a_9}$$
$$(\Xi_{16})^{i_2 a_9}_{i_6 a_{10}} = +t^{a_9 a_{11}}_{i_6 i_{12}} v^{i_2 i_{12}}_{a_{10} a_{11}}$$
$$(\Xi_{17})^{i_2 a_9}_{i_6 a_{10}} = +\tilde{t}^{a'_{11} a_9}_{i_6 i_{12}} v^{i_2 i_{12}}_{a'_{11} a_{10}}$$
$$(\Xi_{18})^{i_5}_{i_3} = +\tfrac{1}{144} t^{a_6 a_7 a_8 a_9}_{i_3 i_{10} i_{11} i_{12}} \lambda^{i_5 i_{10} i_{11} i_{12}}_{a_6 a_7 a_8 a_9}$$
$$(\Xi_{19})^{i_6 i_7}_{i_3 a_5} = +\tfrac{1}{12} t^{a_8 a_9 a_{10}}_{i_3 i_{11} i_{12}} \lambda^{i_6 i_7 i_{11} i_{12}}_{a_5 a_8 a_9 a_{10}}$$
$$(\Xi_{20})^{i_2 a_5}_{a_6 a_7} = +\tfrac{1}{12} t^{a_5 a_8 a_9}_{i_{10} i_{11} i_{12}} \lambda^{i_2 i_{10} i_{11} i_{12}}_{a_6 a_7 a_8 a_9}$$
$$(\Xi_{21})^{i_7 i_8 i_9}_{i_3 a_5 a_6} = +\tfrac{1}{2} t^{a_{10} a_{11}}_{i_3 i_{12}} \lambda^{i_7 i_8 i_9 i_{12}}_{a_5 a_6 a_{10} a_{11}}$$
$$(\Xi_{22})^{i_8 i_9 i_{10} i_{11}}_{i_3 a_5 a_6 a_7} = +t^{a_{12}}_{i_3} \lambda^{i_8 i_9 i_{10} i_{11}}_{a_5 a_6 a_7 a_{12}}$$
$$(\Xi_{23})^{i_2 i_6}_{i_3 i_4} = +\tfrac{1}{48} t^{a_7 a_8 a_9 a_{10}}_{i_3 i_4 i_{11} i_{12}} \lambda^{i_2 i_6 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}}$$
$$(\Xi_{24})^{i_5}_{i_3} = +\tfrac{1}{2} t^{i_6 i_7}_{i_3 i_8} (\Xi_3)^{i_5 i_8}_{i_6 i_7}$$
$$(\Xi_{25})^{i_2 i_6}_{i_3 i_4} = +P_2 t^{a_7}_{i_3} (\Xi_4)^{i_2 i_6}_{i_4 a_7}$$
$$(\Xi_{26})^{i_2 i_6}_{i_3 i_4} = +\tfrac{1}{2} t^{i_7 i_8}_{i_3 i_4} (\Xi_3)^{i_2 i_6}_{i_7 i_8}$$
$$(\Xi_{27})^{i_6 a_5}_{i_3 a_1} = +t^{a_5}_{i_7} (\Xi_{12})^{i_6 i_7}_{i_3 a_1}$$
$$(\Xi_{28})^{i_2 i_6}_{i_3 i_4} = +P_2 t^{a_7}_{i_3} (\Xi_{12})^{i_2 i_6}_{i_4 a_7}$$
$$(\Xi_{29})^{i_2 i_7 i_8}_{i_3 i_4 a_6} = +P_2 t^{a_9}_{i_3} (\Xi_{14})^{i_2 i_7 i_8}_{i_4 a_6 a_9}$$
$$(\Xi_{30})^{i_6 a_5}_{i_3 a_1} = +\tfrac{1}{2} t^{a_5 a_7}_{i_8 i_9} (\Xi_{21})^{i_6 i_8 i_9}_{i_3 a_1 a_7}$$
$$(\Xi_{31})^{i_2 i_6}_{i_3 i_4} = +\tfrac{1}{2} P_2 t^{a_7 a_8}_{i_3 i_9} (\Xi_{21})^{i_2 i_6 i_9}_{i_4 a_7 a_8}$$
$$(\Xi_{32})^{i_6 a'_4}_{i_3 a_1} = +\tfrac{1}{2} \tilde{t}^{a'_4 a_7}_{i_8 i_9} (\Xi_{21})^{i_6 i_8 i_9}_{i_3 a_1 a_7}$$
$$(\Xi_{33})^{i_6 a_5}_{i_3 a_1} = +t^{a_5}_{i_7} (\Xi_{19})^{i_6 i_7}_{i_3 a_1}$$
$$(\Xi_{34})^{i_2 i_6}_{i_3 i_4} = +P_2 t^{a_7}_{i_3} (\Xi_{19})^{i_2 i_6}_{i_4 a_7}$$
$$(\Xi_{35})^{i_2 i_7 i_8}_{i_3 i_4 a_6} = +P_2 t^{a_9}_{i_3} (\Xi_{21})^{i_2 i_7 i_8}_{i_4 a_6 a_9}$$
$$(\xi_{9,1})^{i_6 i_7}_{i_3 a_5} = +(\Xi_4)^{i_6 i_7}_{i_3 a_5} + (\Xi_{12})^{i_6 i_7}_{i_3 a_5} + (\Xi_{19})^{i_6 i_7}_{i_3 a_5}$$
$$(\xi_9)^{a'_4}_{i_3} = +\lambda^{i_5}_{a_6} \tilde{t}^{a'_4 a_6}_{i_3 i_5} + \tfrac{1}{2} \tilde{t}^{a'_4 a_5}_{i_6 i_7} (\xi_{9,1})^{i_6 i_7}_{i_3 a_5} + \tfrac{1}{2} \tilde{t}^{a'_4 a'_5}_{i_6 i_7} (\Xi_5)^{i_6 i_7}_{i_3 a'_5}$$
$$\begin{aligned}(\xi_{8,3})^{i_2 i_7 i_8}_{i_3 i_4 a_6} &= +\tfrac{1}{2} (\Xi_{29})^{i_2 i_7 i_8}_{i_3 i_4 a_6} + (\Xi_{35})^{i_2 i_7 i_8}_{i_3 i_4 a_6} \\ &\quad + \tfrac{1}{2} t^{a_9 a_{10}}_{i_3 i_4} \lambda^{i_2 i_7 i_8}_{a_6 a_9 a_{10}} + \tfrac{1}{6} t^{a_9 a_{10} a_{11}}_{i_3 i_4 i_{12}} \lambda^{i_2 i_7 i_8 i_{12}}_{a_6 a_9 a_{10} a_{11}}\end{aligned}$$
$$(\xi_{8,1})^{i_2 i_7}_{i_4 a_6} = -(\Xi_4)^{i_2 i_7}_{i_4 a_6} - (\Xi_{12})^{i_2 i_7}_{i_4 a_6} - (\Xi_{19})^{i_2 i_7}_{i_4 a_6}$$
$$\begin{aligned}(\xi_8)^{i_2 a'_5}_{i_3 i_4} &= +\lambda^{i_2}_{a_6} \tilde{t}^{a'_5 a_6}_{i_3 i_4} + P_2 \tilde{t}^{a'_5 a_6}_{i_3 i_7} (\xi_{8,1})^{i_2 i_7}_{i_4 a_6} \\ &\quad - P_2 \tilde{t}^{a'_5 a'_6}_{i_3 i_7} (\Xi_5)^{i_2 i_7}_{i_4 a'_6} + \tfrac{1}{2} \tilde{t}^{a'_5 a_6}_{i_7 i_8} (\xi_{8,3})^{i_2 i_7 i_8}_{i_3 i_4 a_6}\end{aligned}$$
$$(\xi_{7,8})^{i_2 i_8 i_9}_{i_4 a_6 a_7} = -(\Xi_{14})^{i_2 i_8 i_9}_{i_4 a_6 a_7} - (\Xi_{21})^{i_2 i_8 i_9}_{i_4 a_6 a_7}$$
$$(\xi_{7,7})^{i_2 a_5}_{a_6 a_7} = -(\Xi_{13})^{i_2 a_5}_{a_6 a_7} - (\Xi_{20})^{i_2 a_5}_{a_6 a_7}$$
$$(\xi_{7,6})^{i_2 i_7 i_8}_{i_3 i_4 a_6} = -\tfrac{1}{2} (\Xi_{29})^{i_2 i_7 i_8}_{i_3 i_4 a_6} - (\Xi_{35})^{i_2 i_7 i_8}_{i_3 i_4 a_6}$$
$$(\xi_{7,3})^{i_2 i_7}_{i_4 a_6} = +(\Xi_4)^{i_2 i_7}_{i_4 a_6} + (\Xi_{12})^{i_2 i_7}_{i_4 a_6} + (\Xi_{19})^{i_2 i_7}_{i_4 a_6}$$
$$(\xi_{7,2})^{i_2}_{i_4} = -(\Xi_2)^{i_2}_{i_4} - (\Xi_{24})^{i_2}_{i_4} - (\Xi_{11})^{i_2}_{i_4} - (\Xi_{18})^{i_2}_{i_4}$$
$$(\xi_{7,11})^{i_2 i_9 a_5}_{a_6 a_7 a_8} = +\tfrac{1}{2} t^{a_5 a_{10}}_{i_{11} i_{12}} \lambda^{i_2 i_9 i_{11} i_{12}}_{a_6 a_7 a_8 a_{10}}$$
$$(\xi_{7,10})^{i_2 i_8 i_9 i_{10}}_{i_3 i_4 a_6 a_7} = -\tfrac{1}{2} P_2 t^{a_{11}}_{i_3} (\Xi_{22})^{i_2 i_8 i_9 i_{10}}_{i_4 a_6 a_7 a_{11}}$$
$$\begin{aligned}(\xi_{7,1})^{i_2 i_6}_{i_3 i_4} &= -\tfrac{1}{2} (\Xi_{25})^{i_2 i_6}_{i_3 i_4} - (\Xi_7)^{i_2 i_6}_{i_3 i_4} - (\Xi_{26})^{i_2 i_6}_{i_3 i_4} - (\Xi_{28})^{i_2 i_6}_{i_3 i_4} - (\Xi_{15})^{i_2 i_6}_{i_3 i_4} + \\ &\quad \tfrac{1}{2} (\Xi_{31})^{i_2 i_6}_{i_3 i_4} - (\Xi_{34})^{i_2 i_6}_{i_3 i_4} - (\Xi_{23})^{i_2 i_6}_{i_3 i_4}\end{aligned}$$
$$\begin{aligned}(\xi_7)^{i_2 a_5}_{i_3 i_4} &= -t^{a_5 a_6}_{i_3 i_4} \lambda^{i_2}_{a_6} + t^{a_5}_{i_6} (\xi_{7,1})^{i_2 i_6}_{i_3 i_4} + P_2 t^{a_5}_{i_3} (\xi_{7,2})^{i_2}_{i_4} + P_2 t^{a_5 a_6}_{i_3 i_7} (\xi_{7,3})^{i_2 i_7}_{i_4 a_6} \\ &\quad - \tfrac{1}{2} t^{a_5 a_6 a_7}_{i_3 i_4 i_8} \lambda^{i_2 i_8}_{a_6 a_7} - P_2 \tilde{t}^{a'_6 a_5}_{i_3 i_7} (\Xi_5)^{i_2 i_7}_{i_4 a'_6} + \tfrac{1}{2} t^{a_5 a_6}_{i_7 i_8} (\xi_{7,6})^{i_2 i_7 i_8}_{i_3 i_4 a_6} \\ &\quad + \tfrac{1}{2} t^{a_6 a_7}_{i_3 i_4} (\xi_{7,7})^{i_2 a_5}_{a_6 a_7} + \tfrac{1}{4} P_2 t^{a_5 a_6 a_7}_{i_3 i_8 i_9} (\xi_{7,8})^{i_2 i_8 i_9}_{i_4 a_6 a_7} - \tfrac{1}{12} t^{a_5 a_6 a_7 a_8}_{i_3 i_4 i_9 i_{10}} \lambda^{i_2 i_9 i_{10}}_{a_6 a_7 a_8} \\ &\quad + \tfrac{1}{12} t^{a_5 a_6 a_7}_{i_8 i_9 i_{10}} (\xi_{7,10})^{i_2 i_8 i_9 i_{10}}_{i_3 i_4 a_6 a_7} + \tfrac{1}{6} t^{a_6 a_7 a_8}_{i_3 i_4 i_9} (\xi_{7,11})^{i_2 i_9 a_5}_{a_6 a_7 a_8} \\ &\quad + \tfrac{1}{36} P_2 t^{a_5 a_6 a_7 a_8}_{i_3 i_9 i_{10} i_{11}} (\Xi_{22})^{i_2 i_9 i_{10} i_{11}}_{i_4 a_6 a_7 a_8}\end{aligned}$$
$$(\xi_{6,5})^{i_7 i_8 i_9}_{i_3 a_5 a_6} = +(\Xi_{14})^{i_7 i_8 i_9}_{i_3 a_5 a_6} + (\Xi_{21})^{i_7 i_8 i_9}_{i_3 a_5 a_6}$$
$$(\xi_{6,2})^{i_6 i_7}_{i_3 a_5} = -(\Xi_4)^{i_6 i_7}_{i_3 a_5} - (\Xi_{12})^{i_6 i_7}_{i_3 a_5} - (\Xi_{19})^{i_6 i_7}_{i_3 a_5}$$
$$(\xi_{6,0})^{i_5}_{i_3} = +(\Xi_1)^{i_5}_{i_3} + (\Xi_2)^{i_5}_{i_3} + (\Xi_{24})^{i_5}_{i_3} + (\Xi_{11})^{i_5}_{i_3} + (\Xi_{18})^{i_5}_{i_3}$$
$$\begin{aligned}(\xi_6)^{a_4}_{i_3} &= +t^{a_4}_{i_5} (\xi_{6,0})^{i_5}_{i_3} - t^{a_4 a_5}_{i_3 i_6} \lambda^{i_6}_{a_5} + \tfrac{1}{2} t^{a_4 a_5}_{i_6 i_7} (\xi_{6,2})^{i_6 i_7}_{i_3 a_5} - \tfrac{1}{4} t^{a_4 a_5 a_6}_{i_3 i_7 i_8} \lambda^{i_7 i_8}_{a_5 a_6} \\ &\quad + \tfrac{1}{2} \tilde{t}^{a'_5 a_4}_{i_6 i_7} (\Xi_5)^{i_6 i_7}_{i_3 a'_5} + \tfrac{1}{12} t^{a_4 a_5 a_6}_{i_7 i_8 i_9} (\xi_{6,5})^{i_7 i_8 i_9}_{i_3 a_5 a_6} \\ &\quad - \tfrac{1}{36} t^{a_4 a_5 a_6 a_7}_{i_3 i_8 i_9 i_{10}} \lambda^{i_8 i_9 i_{10}}_{a_5 a_6 a_7} - \tfrac{1}{144} t^{a_4 a_5 a_6 a_7}_{i_8 i_9 i_{10} i_{11}} (\Xi_{22})^{i_8 i_9 i_{10} i_{11}}_{i_3 a_5 a_6 a_7}\end{aligned}$$
$$\begin{aligned}(\xi_5)^{a_4}_{a_3} &= -t^{a_4}_{i_5} \lambda^{i_5}_{a_3} - \tfrac{1}{2} t^{a_4 a_5}_{i_6 i_7} \lambda^{i_6 i_7}_{a_3 a_5} - \tfrac{1}{2} \tilde{t}^{a'_5 a_4}_{i_6 i_7} \tilde{\lambda}^{i_6 i_7}_{a'_5 a_3} - \tfrac{1}{12} t^{a_4 a_5 a_6}_{i_7 i_8 i_9} \lambda^{i_7 i_8 i_9}_{a_3 a_5 a_6} \\ &\quad - \tfrac{1}{144} t^{a_4 a_5 a_6 a_7}_{i_8 i_9 i_{10} i_{11}} \lambda^{i_8 i_9 i_{10} i_{11}}_{a_3 a_5 a_6 a_7}\end{aligned}$$
$$(\xi_4)^{i_4}_{i_3} = -(\Xi_1)^{i_4}_{i_3} - (\Xi_2)^{i_4}_{i_3} - (\Xi_{24})^{i_4}_{i_3} - (\Xi_{11})^{i_4}_{i_3} - (\Xi_{18})^{i_4}_{i_3}$$
$$(\xi_{35})^{a'_4 a_5}_{i_3 a_1} = -t^{a_5}_{i_6} (\Xi_{32})^{i_6 a'_4}_{i_3 a_1}$$
$$(\xi_{33,6})^{i_2 a_8 a_9}_{i_5 i_6 a'_{10}} = -\tfrac{1}{2} P_2 \tilde{t}^{a'_{11} a_8}_{i_5 i_6} v^{i_2 a_9}_{a'_{10} a'_{11}} + t^{a_8 a_9 a_{11}}_{i_5 i_6 i_{12}} v^{i_2 i_{12}}_{a'_{10} a_{11}}$$
$$(\xi_{33,4})^{i_2 i_{11}}_{i_6 a_{10}} = -v^{i_2 i_{11}}_{i_6 a_{10}} + (\Xi_8)^{i_2 i_{11}}_{i_6 a_{10}}$$
$$(\xi_{33,3,2})^{i_2 i_{10} a_9}_{i_5 i_6 a_{11}} = +\tilde{t}^{a'_{12} a_9}_{i_5 i_6} v^{i_2 i_{10}}_{a'_{12} a_{11}} + \tfrac{1}{2} t^{a_9 a_{12}}_{i_5 i_6} v^{i_2 i_{10}}_{a_{11} a_{12}}$$
$$(\xi_{33,3,1})^{i_2 i_{10} a_9}_{i_5 i_6 a'_{11}} = +\tfrac{1}{2} \tilde{t}^{a'_{12} a_9}_{i_5 i_6} v^{i_2 i_{10}}_{a'_{11} a'_{12}}$$
$$(\xi_{33,3,0})^{i_2 i_{10}}_{i_6 a_{11}} = +v^{i_2 i_{10}}_{i_6 a_{11}} - (\Xi_8)^{i_2 i_{10}}_{i_6 a_{11}}$$
$$\begin{aligned}(\xi_{33,3})^{i_2 i_{10} a_8 a_9}_{i_3 i_4 i_5 i_6} &= +P_4 t^{a_8 a_9 a_{11}}_{i_3 i_4 i_5} (\xi_{33,3,0})^{i_2 i_{10}}_{i_6 a_{11}} + P_2 P_4 \tilde{t}^{a'_{11} a_8}_{i_3 i_4} (\xi_{33,3,1})^{i_2 i_{10} a_9}_{i_5 i_6 a'_{11}} \\ &\quad + P_2 P_4 t^{a_8 a_{11}}_{i_3 i_4} (\xi_{33,3,2})^{i_2 i_{10} a_9}_{i_5 i_6 a_{11}} - \tfrac{1}{2} t^{a_8 a_9 a_{11} a_{12}}_{i_3 i_4 i_5 i_6} v^{i_2 i_{10}}_{a_{11} a_{12}}\end{aligned}$$
$$(\xi_{33,2})^{i_2 a_8 a_9}_{i_5 i_6 a_{10}} = -\tfrac{1}{2} P_2 t^{a_8 a_{11}}_{i_5 i_6} v^{i_2 a_9}_{a_{10} a_{11}} - P_2 \tilde{t}^{a'_{11} a_8}_{i_5 i_6} v^{i_2 a_9}_{a'_{11} a_{10}} - t^{a_8 a_9 a_{11}}_{i_5 i_6 i_{12}} v^{i_2 i_{12}}_{a_{10} a_{11}}$$
$$(\xi_{33,1})^{i_2 a_9}_{i_6 a_{10}} = -v^{i_2 a_9}_{i_6 a_{10}} + (\Xi_6)^{i_2 a_9}_{i_6 a_{10}} + (\Xi_{16})^{i_2 a_9}_{i_6 a_{10}} + (\Xi_{17})^{i_2 a_9}_{i_6 a_{10}}$$
$$(\xi_{33,0})^{i_2}_{a_{10}} = -f^{i_2}_{a_{10}} - (\Xi_0)^{i_2}_{a_{10}}$$
$$\begin{aligned}(\xi_{33})^{i_2 a_7 a_8 a_9}_{i_3 i_4 i_5 i_6} &= +t^{a_7 a_8 a_9 a_{10}}_{i_3 i_4 i_5 i_6} (\xi_{33,0})^{i_2}_{a_{10}} + P_3 P_4 t^{a_7 a_8 a_{10}}_{i_3 i_4 i_5} (\xi_{33,1})^{i_2 a_9}_{i_6 a_{10}} \\ &\quad + P_3 P_4 t^{a_7 a_{10}}_{i_3 i_4} (\xi_{33,2})^{i_2 a_8 a_9}_{i_5 i_6 a_{10}} + P_3 t^{a_7}_{i_{10}} (\xi_{33,3})^{i_2 i_{10} a_8 a_9}_{i_3 i_4 i_5 i_6} \\ &\quad + P_4 t^{a_7 a_8 a_9 a_{10}}_{i_3 i_4 i_5 i_{11}} (\xi_{33,4})^{i_2 i_{11}}_{i_6 a_{10}} + \tfrac{1}{2} P_3 t^{a_7 a_8 a_{10} a_{11}}_{i_3 i_4 i_5 i_6} v^{i_2 a_9}_{a_{10} a_{11}} \\ &\quad + P_3 P_4 \tilde{t}^{a'_{10} a_7}_{i_3 i_4} (\xi_{33,6})^{i_2 a_8 a_9}_{i_5 i_6 a'_{10}}\end{aligned}$$
$$(\xi_{32,0})^{i_6 i_7}_{i_3 a_1} = -(\Xi_{12})^{i_6 i_7}_{i_3 a_1} - (\Xi_{19})^{i_6 i_7}_{i_3 a_1}$$
$$(\xi_{32})^{i_4 i_5}_{i_3 a_1} = +\tfrac{1}{2} t^{i_4 i_5}_{i_6 i_7} (\xi_{32,0})^{i_6 i_7}_{i_3 a_1}$$
$$(\xi_{31,1})^{i_6 i_7}_{i_3 a_1} = -(\Xi_{12})^{i_6 i_7}_{i_3 a_1} - (\Xi_{19})^{i_6 i_7}_{i_3 a_1}$$
$$(\xi_{31,0})^{i_6 a_5}_{i_3 a_1} = -\tfrac{1}{2} (\Xi_{27})^{i_6 a_5}_{i_3 a_1} + (\Xi_{30})^{i_6 a_5}_{i_3 a_1} - \tfrac{1}{2} (\Xi_{33})^{i_6 a_5}_{i_3 a_1}$$
$$(\xi_{31})^{a_4 a_5}_{i_3 a_1} = +P_2 t^{a_4}_{i_6} (\xi_{31,0})^{i_6 a_5}_{i_3 a_1} + \tfrac{1}{2} t^{a_4 a_5}_{i_6 i_7} (\xi_{31,1})^{i_6 i_7}_{i_3 a_1} + \tfrac{1}{6} t^{a_4 a_5 a_6}_{i_7 i_8 i_9} (\Xi_{21})^{i_7 i_8 i_9}_{i_3 a_1 a_6}$$
$$(\xi_{30})^{i_4 a_5}_{i_3 a_1} = -(\Xi_{27})^{i_4 a_5}_{i_3 a_1} + (\Xi_{30})^{i_4 a_5}_{i_3 a_1} - (\Xi_{33})^{i_4 a_5}_{i_3 a_1}$$
$$(\xi_{29})^{i_2 a'_5}_{a_3 a_4} = +\tfrac{1}{2} \lambda^{i_2 i_6 i_7}_{a_3 a_4 a_8} \tilde{t}^{a'_5 a_8}_{i_6 i_7}$$
$$(\xi_{28,4})^{i_2 i_9}_{i_5 a_8} = +v^{i_2 i_9}_{i_5 a_8} - (\Xi_8)^{i_2 i_9}_{i_5 a_8}$$

TABLE ESI.4.XXIII: The computational sequence and intermediates for the Λ_1 amplitude equation of Λ-CCSDTQ-R12 [Part II]

$$(\xi_{28,3,1})^{i_2i_8}_{i_5a_9} = +v^{i_2i_8}_{i_5a_9} - (\Xi_8)^{i_2i_8}_{i_5a_9}$$

$$(\xi_{28,3,0})^{i_2i_8}_{i_5a'_9} = -v^{i_2i_8}_{i_5a'_9} + (\Xi_9)^{i_2i_8}_{i_5a'_9}$$

$$(\xi_{28,3})^{i_2i_8a_7}_{i_3i_4i_5} = +P_3\tilde{t}^{a'_9a_7}_{i_3i_4}(\xi_{28,3,0})^{i_2i_8}_{i_5a'_9} + P_3t^{a_7a_9}_{i_3i_4}(\xi_{28,3,1})^{i_2i_8}_{i_5a_9} - \tfrac{1}{2}t^{a_7a_9a_{10}}_{i_3i_4i_5}v^{i_2i_8}_{a_9a_{10}}$$

$$(\xi_{28,2})^{i_2a_7}_{i_5a'_8} = -v^{i_2a_7}_{i_5a'_8} + t^{a_9}_{i_5}v^{i_2a_7}_{a'_8a_9} + t^{a_7a_9}_{i_5i_{10}}v^{i_2i_{10}}_{a'_8a_9} - \tilde{t}^{a'_9a_7}_{i_5i_{10}}v^{i_2i_{10}}_{a'_8a'_9}$$

$$(\xi_{28,1})^{i_2a_7}_{i_5a_8} = +v^{i_2a_7}_{i_5a_8} - (\Xi_6)^{i_2a_7}_{i_5a_8} - (\Xi_{16})^{i_2a_7}_{i_5a_8} - (\Xi_{17})^{i_2a_7}_{i_5a_8}$$

$$(\xi_{28,0})^{i_2}_{a_8} = +f^{i_2}_{a_8} + (\Xi_0)^{i_2}_{a_8}$$

$$\begin{aligned}(\xi_{28})^{i_2a_6a_7}_{i_3i_4i_5} = &+t^{a_6a_7a_8}_{i_3i_4i_5}(\xi_{28,0})^{i_2}_{a_8} + P_2P_3t^{a_6a_8}_{i_3i_4}(\xi_{28,1})^{i_2a_7}_{i_5a_8}\\ &+P_2P_3\tilde{t}^{a'_8a_6}_{i_3i_4}(\xi_{28,2})^{i_2a_7}_{i_5a'_8} + P_2t^{a_6}_{i_8}(\xi_{28,3})^{i_2i_8a_7}_{i_3i_4i_5}\\ &+P_3t^{a_6a_7a_8}_{i_3i_4i_9}(\xi_{28,4})^{i_2i_9}_{i_5a_8} - \tfrac{1}{2}P_2t^{a_6a_8a_9}_{i_3i_4i_5}v^{i_2a_7}_{a_8a_9}\\ &+\tfrac{1}{2}t^{a_6a_7a_8a_9}_{i_3i_4i_5i_{10}}v^{i_2i_{10}}_{a_8a_9}\end{aligned}$$

$$(\xi_{27})^{a'_4}_{a'_3} = +\tfrac{1}{2}\tilde{t}^{a'_4a'_5}_{i_6i_7}\tilde{\lambda}^{i_6i_7}_{a'_3a'_5} + \tfrac{1}{2}\tilde{t}^{a'_4a_5}_{i_6i_7}\tilde{\lambda}^{i_6i_7}_{a'_3a_5}$$

$$(\xi_{26})^{i_2a'_5}_{i_3a'_4} = -\tilde{t}^{a'_5a'_6}_{i_3i_7}\tilde{\lambda}^{i_2i_7}_{a'_4a'_6} - \tilde{t}^{a'_5a_6}_{i_3i_7}\tilde{\lambda}^{i_2i_7}_{a'_4a_6}$$

$$(\xi_{25})^{a_4}_{a'_3} = -\tfrac{1}{2}t^{a_4a_5}_{i_6i_7}\tilde{\lambda}^{i_6i_7}_{a'_3a_5} + \tfrac{1}{2}\tilde{t}^{a'_5a_4}_{i_6i_7}\tilde{\lambda}^{i_6i_7}_{a'_3a'_5}$$

$$(\xi_{24})^{i_2a_5}_{i_3a'_4} = -t^{a_5}_{i_6}(\Xi_5)^{i_2i_6}_{i_3a'_4} + t^{a_5a_6}_{i_3i_7}\tilde{\lambda}^{i_2i_7}_{a'_4a_6} - \tilde{t}^{a'_6a_5}_{i_3i_7}\tilde{\lambda}^{i_2i_7}_{a'_4a'_6}$$

$$(\xi_{23})^{a'_4}_{a_3} = +\tfrac{1}{2}\lambda^{i_5i_6}_{a_3a_7}\tilde{t}^{a'_4a_7}_{i_5i_6} - \tfrac{1}{2}\tilde{t}^{a'_4a'_5}_{i_6i_7}\tilde{\lambda}^{i_6i_7}_{a'_5a_3}$$

$$(\xi_{22})^{i_2a'_5}_{i_3a_4} = -(\Xi_{32})^{i_2a'_5}_{i_3a_4} - \lambda^{i_2i_6}_{a_4a_7}\tilde{t}^{a'_5a_7}_{i_3i_6} + \tilde{t}^{a'_5a'_6}_{i_3i_7}\tilde{\lambda}^{i_2i_7}_{a'_6a_4} - \tfrac{1}{2}\tilde{t}^{a'_5a_6}_{i_7i_8}(\Xi_{14})^{i_2i_7i_8}_{i_3a_4a_6}$$

$$(\xi_{21})^{i_2i_5}_{i_3i_4} = +(\Xi_7)^{i_2i_5}_{i_3i_4} + (\Xi_{26})^{i_2i_5}_{i_3i_4} + (\Xi_{15})^{i_2i_5}_{i_3i_4} + (\Xi_{23})^{i_2i_5}_{i_3i_4}$$

$$\begin{aligned}(\xi_{20})^{i_2a_5}_{i_3a_4} = &-(\Xi_{27})^{i_2a_5}_{i_3a_4} + (\Xi_{30})^{i_2a_5}_{i_3a_4} - (\Xi_{33})^{i_2a_5}_{i_3a_4} - t^{a_5}_{i_6}(\Xi_4)^{i_2i_6}_{i_3a_4}\\ &+t^{a_5a_6}_{i_3i_7}\lambda^{i_2i_7}_{a_4a_6} + \tilde{t}^{a'_6a_5}_{i_3i_7}\tilde{\lambda}^{i_2i_7}_{a'_6a_4} + \tfrac{1}{2}t^{a_5a_6}_{i_7i_8}(\Xi_{14})^{i_2i_7i_8}_{i_3a_4a_6} + \tfrac{1}{4}t^{a_5a_6a_7}_{i_3i_8i_9}\lambda^{i_2i_8i_9}_{a_4a_6a_7}\\ &-\tfrac{1}{12}t^{a_5a_6a_7}_{i_8i_9i_{10}}(\Xi_{22})^{i_2i_8i_9i_{10}}_{i_3a_4a_6a_7} + \tfrac{1}{36}t^{a_5a_6a_7a_8}_{i_3i_9i_{10}i_{11}}\lambda^{i_2i_9i_{10}i_{11}}_{a_4a_6a_7a_8}\end{aligned}$$

$$(\xi_2)^{i_2}_{i_3} = +(\Xi_1)^{i_2}_{i_3} + (\Xi_2)^{i_2}_{i_3} + (\Xi_{24})^{i_2}_{i_3} + (\Xi_{11})^{i_2}_{i_3} + (\Xi_{18})^{i_2}_{i_3}$$

$$(\xi_{19})^{i_2i_5}_{i_3i_4} = +\tfrac{1}{2}(\Xi_{25})^{i_2i_5}_{i_3i_4} + (\Xi_{28})^{i_2i_5}_{i_3i_4} - \tfrac{1}{2}(\Xi_{31})^{i_2i_5}_{i_3i_4} + (\Xi_{34})^{i_2i_5}_{i_3i_4}$$

$$(\xi_{18})^{i_2a_5}_{i_3i_4} = -t^{a_5}_{i_6}\lambda^{i_2i_6}_{i_3i_4}$$

$$(\xi_{16})^{i_2a_5}_{a_3a_4} = -(\Xi_{13})^{i_2a_5}_{a_3a_4} - (\Xi_{20})^{i_2a_5}_{a_3a_4} - t^{a_5}_{i_6}\lambda^{i_2i_6}_{a_3a_4}$$

$$(\xi_{15})^{i_2i_5}_{i_3a_4} = +(\Xi_4)^{i_2i_5}_{i_3a_4} + (\Xi_{12})^{i_2i_5}_{i_3a_4} + (\Xi_{19})^{i_2i_5}_{i_3a_4}$$

$$(\xi_{14})^{i_4i_5}_{i_3a_1} = -(\Xi_4)^{i_4i_5}_{i_3a_1} - (\Xi_{12})^{i_4i_5}_{i_3a_1} - (\Xi_{19})^{i_4i_5}_{i_3a_1}$$

$$(\xi_{11,5})^{i_2i_7}_{i_4a_6} = +v^{i_2i_7}_{i_4a_6} - (\Xi_8)^{i_2i_7}_{i_4a_6}$$

$$(\xi_{11,4})^{i_2i_7}_{i_4a'_6} = +v^{i_2i_7}_{i_4a'_6} - (\Xi_9)^{i_2i_7}_{i_4a'_6}$$

$$(\xi_{11,2})^{i_2a'_5}_{i_4a_6} = +v^{i_2a'_5}_{i_4a_6} - \tfrac{1}{2}t^{a_7}_{i_4}v^{i_2a'_5}_{a_6a_7}$$

$$(\xi_{11,1})^{i_2}_{a_6} = +f^{i_2}_{a_6} + (\Xi_0)^{i_2}_{a_6}$$

$$(\xi_{11,0})^{i_2}_{a'_6} = +f^{i_2}_{a'_6} + (\Xi_{10})^{i_2}_{a'_6}$$

$$\begin{aligned}(\xi_{11})^{i_2a'_5}_{i_3i_4} = &-v^{i_2a'_5}_{i_3i_4} + \tilde{t}^{a'_5a'_6}_{i_3i_4}(\xi_{11,0})^{i_2}_{a'_6} + \tilde{t}^{a'_5a_6}_{i_3i_4}(\xi_{11,1})^{i_2}_{a_6} + P_2t^{a_6}_{i_3}(\xi_{11,2})^{i_2a'_5}_{i_4a_6}\\ &-\tfrac{1}{2}t^{a_6a_7}_{i_3i_4}v^{i_2a'_5}_{a_6a_7} + P_2\tilde{t}^{a'_5a'_6}_{i_3i_7}(\xi_{11,4})^{i_2i_7}_{i_4a'_6}\\ &+P_2\tilde{t}^{a'_5a_6}_{i_3i_7}(\xi_{11,5})^{i_2i_7}_{i_4a_6} - \tfrac{1}{2}t^{i_6i_7}_{i_3i_4}V^{i_2a'_5}_{i_6i_7}\end{aligned}$$

$$(\xi_{10,6})^{i_2i_7}_{i_4a'_6} = +v^{i_2i_7}_{i_4a'_6} - (\Xi_9)^{i_2i_7}_{i_4a'_6}$$

$$(\xi_{10,4})^{i_2i_7}_{i_4a_6} = -v^{i_2i_7}_{i_4a_6} + (\Xi_8)^{i_2i_7}_{i_4a_6}$$

$$(\xi_{10,3,0})^{i_2i_6}_{i_4a_7} = +v^{i_2i_6}_{i_4a_7} - \tfrac{1}{2}(\Xi_8)^{i_2i_6}_{i_4a_7}$$

$$(\xi_{10,3})^{i_2i_6}_{i_3i_4} = +P_2t^{a_7}_{i_3}(\xi_{10,3,0})^{i_2i_6}_{i_4a_7} - \tfrac{1}{2}t^{i_7i_8}_{i_3i_4}V^{i_2i_6}_{i_7i_8} - \tfrac{1}{2}t^{a_7a_8}_{i_3i_4}v^{i_2i_6}_{a_7a_8}$$

$$(\xi_{10,2})^{i_2a_5}_{i_4a_6} = -v^{i_2a_5}_{i_4a_6} + \tfrac{1}{2}(\Xi_6)^{i_2a_5}_{i_4a_6}$$

$$(\xi_{10,1})^{i_2}_{a'_6} = +f^{i_2}_{a'_6} + (\Xi_{10})^{i_2}_{a'_6}$$

$$(\xi_{10,0})^{i_2}_{a_6} = -f^{i_2}_{a_6} - (\Xi_0)^{i_2}_{a_6}$$

$$\begin{aligned}(\xi_{10})^{i_2a_5}_{i_3i_4} = &+v^{i_2a_5}_{i_3i_4} + t^{a_5a_6}_{i_3i_4}(\xi_{10,0})^{i_2}_{a_6} + \tilde{t}^{a'_6a_5}_{i_3i_4}(\xi_{10,1})^{i_2}_{a'_6} + P_2t^{a_6}_{i_3}(\xi_{10,2})^{i_2a_5}_{i_4a_6}\\ &+t^{a_5}_{i_6}(\xi_{10,3})^{i_2i_6}_{i_3i_4} + P_2t^{a_5a_6}_{i_3i_7}(\xi_{10,4})^{i_2i_7}_{i_4a_6} + \tfrac{1}{2}t^{a_6a_7}_{i_3i_4}v^{i_2a_5}_{a_6a_7}\\ &+P_2\tilde{t}^{a'_6a_5}_{i_3i_7}(\xi_{10,6})^{i_2i_7}_{i_4a'_6} + \tfrac{1}{2}t^{i_6i_7}_{i_3i_4}V^{i_2a_5}_{i_6i_7} - \tfrac{1}{2}t^{a_5a_6a_7}_{i_3i_4i_8}v^{i_2i_8}_{a_6a_7}\end{aligned}$$

$$(\xi_1)^{a_3}_{a_1} = -f^{a_3}_{a_1} + t^{a_4}_{i_5}v^{i_5a_3}_{a_1a_4} + t^{a_3}_{i_4}(\Xi_0)^{i_4}_{a_1}$$

$$(\xi_{0,0})^{i_2}_{a_4} = +f^{i_2}_{a_4} + (\Xi_0)^{i_2}_{a_4}$$

$$(\xi_0)^{i_2}_{i_3} = +f^{i_2}_{i_3} + t^{a_4}_{i_3}(\xi_{0,0})^{i_2}_{a_4} + t^{a_4}_{i_5}v^{i_2i_5}_{i_3a_4} + \tfrac{1}{2}t^{a_4a_5}_{i_3i_6}v^{i_2i_6}_{a_4a_5} + \tfrac{1}{2}t^{i_4i_5}_{i_3i_6}V^{i_2i_6}_{i_4i_5}$$

$$\begin{aligned}\delta^{i_2}_{a_1} = &+f^{i_2}_{a_1} + (\Xi_0)^{i_2}_{a_1} + \lambda^{i_3}_{a_1}(\xi_0)^{i_2}_{i_3} + \lambda^{i_2}_{a_3}(\xi_1)^{a_3}_{a_1} + f^{i_3}_{a_1}(\xi_2)^{i_2}_{i_3} + \lambda^{i_3}_{a_4}v^{i_2a_4}_{i_3a_1}\\ &+v^{i_2i_3}_{i_4a_1}(\xi_4)^{i_4}_{i_3} + v^{i_2a_3}_{a_1a_4}(\xi_5)^{a_4}_{a_3} + v^{i_2i_3}_{a_1a_4}(\xi_6)^{a_4}_{i_3} + \tfrac{1}{2}v^{i_3i_4}_{a_1a_5}(\xi_7)^{i_2a_5}_{i_3i_4}\\ &+\tfrac{1}{2}v^{i_3i_4}_{a'_5a_1}(\xi_8)^{i_2a'_5}_{i_3i_4} + v^{i_2i_3}_{a'_4a_1}(\xi_9)^{a'_4}_{i_3} + \tfrac{1}{2}\lambda^{i_3i_4}_{a_1a_5}(\xi_{10})^{i_2a_5}_{i_3i_4} + \tfrac{1}{2}\tilde{\lambda}^{i_3i_4}_{a'_5a_1}(\xi_{11})^{i_2a'_5}_{i_3i_4}\\ &+\tfrac{1}{2}\lambda^{i_2i_3}_{a_4a_5}v^{a_4a_5}_{i_3a_1} + \tfrac{1}{2}\lambda^{i_2i_3}_{i_4i_5}(V^{\dagger})^{i_4i_5}_{i_3a_1} + \tfrac{1}{2}v^{i_2i_3}_{i_4i_5}(\xi_{14})^{i_4i_5}_{i_3a_1} + v^{i_3a_4}_{i_5a_1}(\xi_{15})^{i_2i_5}_{i_3a_4}\\ &+\tfrac{1}{2}v^{a_3a_4}_{a_1a_5}(\xi_{16})^{i_2a_5}_{a_3a_4} + v^{i_3a'_4}_{i_5a_1}(\Xi_5)^{i_2i_5}_{i_3a'_4} + \tfrac{1}{2}(V^{\dagger})^{i_3i_4}_{a_1a_5}(\xi_{18})^{i_2a_5}_{i_3i_4}\\ &+v^{i_3i_4}_{i_5a_1}(\xi_{19})^{i_2i_5}_{i_3i_4} + v^{i_3a_4}_{a_1a_5}(\xi_{20})^{i_2a_5}_{i_3a_4} + \tfrac{1}{2}v^{i_3i_4}_{i_5a_1}(\xi_{21})^{i_2i_5}_{i_3i_4}\\ &+v^{i_3a_4}_{a'_5a_1}(\xi_{22})^{i_2a'_5}_{i_3a_4} + v^{i_2a_3}_{a'_4a_1}(\xi_{23})^{a'_4}_{a_3} + v^{i_3a'_4}_{a_1a_5}(\xi_{24})^{i_2a_5}_{i_3a'_4} + v^{i_2a'_3}_{a_1a_4}(\xi_{25})^{a_4}_{a'_3}\\ &+v^{i_3a'_4}_{a'_5a_1}(\xi_{26})^{i_2a'_5}_{i_3a'_4} + v^{i_2a'_3}_{a'_4a_1}(\xi_{27})^{a'_4}_{a'_3} + \tfrac{1}{12}\lambda^{i_3i_4i_5}_{a_1a_6a_7}(\xi_{28})^{i_2a_6a_7}_{i_3i_4i_5}\\ &+\tfrac{1}{2}v^{a_3a_4}_{a'_5a_1}(\xi_{29})^{i_2a'_5}_{a_3a_4} + v^{i_2i_3}_{i_4a_5}(\xi_{30})^{i_4a_5}_{i_3a_1} + \tfrac{1}{2}v^{i_2i_3}_{a_4a_5}(\xi_{31})^{a_4a_5}_{i_3a_1}\\ &+\tfrac{1}{2}V^{i_2i_3}_{i_4i_5}(\xi_{32})^{i_4i_5}_{i_3a_1} + \tfrac{1}{144}\lambda^{i_3i_4i_5i_6}_{a_1a_7a_8a_9}(\xi_{33})^{i_2a_7a_8a_9}_{i_3i_4i_5i_6} + v^{i_2i_3}_{i_4a'_5}(\Xi_{32})^{i_4a'_5}_{i_3a_1}\\ &+v^{i_2i_3}_{a'_4a_5}(\xi_{35})^{a'_4a_5}_{i_3a_1}\end{aligned}$$

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TABLE ESI.4.XXIV: The computational sequence and intermediates for the Λ_2 amplitude equation of Λ-CCSDTQ-R12 [Part I]

$$(\Xi_0)^{i_4}_{a_{10}} = +t^{a_{11}}_{i_{12}} v^{i_4 i_{12}}_{a_{10}a_{11}}$$
$$(\Xi_1)^{i_{10}i_{11}}_{i_6 a_2} = +t^{a_{12}}_{i_6} v^{i_{10}i_{11}}_{a_2 a_{12}}$$
$$(\Xi_2)^{i_3 i_4}_{i_6 a_7} = +t^{a_8}_{i_6} \lambda^{i_3 i_4}_{a_7 a_8}$$
$$(\Xi_3)^{i_4 i_{10}}_{i_6 i_7} = +P_2 t^{a_{11}}_{i_6} v^{i_4 i_{10}}_{i_7 a_{11}}$$
$$(\Xi_4)^{i_4 a_9}_{i_7 a_{10}} = +t^{a_{11}}_{i_7} v^{i_4 a_9}_{a_{10} a_{11}}$$
$$(\Xi_5)^{i_4 i_{10}}_{i_6 i_7} = +\tfrac{1}{2} t^{a_{11}a_{12}}_{i_6 i_7} v^{i_4 i_{10}}_{a_{11}a_{12}}$$
$$(\Xi_6)^{i_4 i_{10}}_{i_6 i_7} = +\tfrac{1}{2} t^{i_{11}i_{12}}_{i_6 i_7} V^{i_4 i_{10}}_{i_{11}i_{12}}$$
$$(\Xi_7)^{i_4 a_9}_{i_7 a_{10}} = +\tilde{t}^{a'_{11}a_9}_{i_7 i_{12}} v^{i_4 i_{12}}_{a'_{11}a_{10}}$$
$$(\Xi_8)^{i_4 i_8}_{i_6 i_7} = +\tfrac{1}{2} \lambda^{i_4 i_8}_{i_9 i_{10}} X^{i_9 i_{10}}_{i_6 i_7}$$
$$(\Xi_9)^{i_3 i_4}_{i_6 a_7} = +\tfrac{1}{2} t^{a_8 a_9}_{i_6 i_{10}} \lambda^{i_3 i_4 i_{10}}_{a_7 a_8 a_9}$$
$$(\Xi_{10})^{i_4 i_8 i_9}_{i_5 a_2 a_7} = +t^{a_{10}}_{i_5} \lambda^{i_4 i_8 i_9}_{a_2 a_7 a_{10}}$$
$$(\Xi_{11})^{i_7 a_6}_{a_1 a_2} = +\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} \lambda^{i_7 i_9 i_{10}}_{a_1 a_2 a_8}$$
$$(\Xi_{12})^{i_4 i_{10} a_9}_{i_5 i_6 i_7} = +P_3 \tilde{t}^{a'_{11}a_9}_{i_5 i_6} v^{i_4 i_{10}}_{i_7 a'_{11}}$$
$$(\Xi_{13})^{i_4 a_9}_{i_7 a_{10}} = +t^{a_9 a_{11}}_{i_7 i_{12}} v^{i_4 i_{12}}_{a_{10} a_{11}}$$
$$(\Xi_{14})^{i_4 i_{10}}_{i_7 a'_{11}} = +t^{a_{12}}_{i_7} v^{i_4 i_{10}}_{a'_{11} a_{12}}$$
$$(\Xi_{15})^{i_4 i_{10} a_9}_{i_5 i_6 i_7} = +\tfrac{1}{2} t^{a_9 a_{11} a_{12}}_{i_5 i_6 i_7} v^{i_4 i_{10}}_{a_{11} a_{12}}$$
$$(\Xi_{16})^{i_3 i_4}_{i_6 a_7} = +\tfrac{1}{12} t^{a_8 a_9 a_{10}}_{i_6 i_{11} i_{12}} \lambda^{i_3 i_4 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}}$$
$$(\Xi_{17})^{i_4 i_8 i_9}_{i_5 a_2 a_7} = +\tfrac{1}{2} t^{a_{10} a_{11}}_{i_5 i_{12}} \lambda^{i_4 i_8 i_9 i_{12}}_{a_2 a_7 a_{10} a_{11}}$$
$$(\Xi_{18})^{i_8 i_9 a_6}_{a_1 a_2 a_7} = +\tfrac{1}{2} t^{a_6 a_{10}}_{i_{11} i_{12}} \lambda^{i_8 i_9 i_{11} i_{12}}_{a_1 a_2 a_7 a_{10}}$$
$$(\Xi_{19})^{i_4 i_9 i_{10} i_{11}}_{i_5 a_2 a_7 a_8} = +t^{a_{12}}_{i_5} \lambda^{i_4 i_9 i_{10} i_{11}}_{a_2 a_7 a_8 a_{12}}$$
$$(\Xi_{20})^{i_7 a_6}_{a_1 a_2} = +\tfrac{1}{12} t^{a_6 a_8 a_9}_{i_{10} i_{11} i_{12}} \lambda^{i_7 i_{10} i_{11} i_{12}}_{a_1 a_2 a_8 a_9}$$
$$(\Xi_{21})^{i_4 i_{10}}_{i_6 i_7} = +P_2 t^{a_{11}}_{i_6} (\Xi_1)^{i_4 i_{10}}_{i_7 a_{11}}$$
$$(\Xi_{22})^{i_3 i_4 i_8}_{i_5 i_6 a_2} = +P_2 t^{a_9}_{i_5} (\Xi_{10})^{i_3 i_4 i_8}_{i_6 a_2 a_9}$$
$$(\Xi_{23})^{i_4 i_{10} a_9}_{i_5 i_6 i_7} = +P_3 \tilde{t}^{a'_{11}a_9}_{i_5 i_6} (\Xi_{14})^{i_4 i_{10}}_{i_7 a'_{11}}$$
$$(\Xi_{24})^{i_3 i_4 i_8}_{i_5 i_6 a_2} = +P_2 t^{a_9}_{i_5} (\Xi_{17})^{i_3 i_4 i_8}_{i_6 a_2 a_9}$$
$$(\Xi_{25})^{i_3 i_4 i_9 i_{10}}_{i_5 i_6 a_2 a_8} = +P_2 t^{a_{11}}_{i_5} (\Xi_{19})^{i_3 i_4 i_9 i_{10}}_{i_6 a_2 a_8 a_{11}}$$
$$(\xi_9)^{i_4 a_6}_{i_5 a_2} = -v^{i_4 a_6}_{i_5 a_2} + (\Xi_4)^{i_4 a_6}_{i_5 a_2} + (\Xi_7)^{i_4 a_6}_{i_5 a_2} - t^{a_6}_{i_7} (\Xi_1)^{i_4 i_7}_{i_5 a_2}$$
$$(\xi_8)^{i_3 i_4}_{i_5 i_6} = +v^{i_3 i_4}_{i_5 i_6} + (\Xi_5)^{i_3 i_4}_{i_5 i_6} + (\Xi_6)^{i_3 i_4}_{i_5 i_6}$$
$$(\xi_7)^{i_3 i_4}_{i_5 a_2} = +(\Xi_2)^{i_3 i_4}_{i_5 a_2} + (\Xi_9)^{i_3 i_4}_{i_5 a_2} + (\Xi_{16})^{i_3 i_4}_{i_5 a_2}$$
$$(\xi_6)^{a'_5}_{a_2} = -f^{a'_5}_{a_2} + t^{a_6}_{i_7} v^{i_7 a'_5}_{a_2 a_6} - \tfrac{1}{2} \tilde{t}^{a'_5 a_6}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_2} + \tfrac{1}{2} \tilde{t}^{a'_5 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_2 a_6}$$
$$(\xi_5)^{a_5}_{a_2} = +f^{a_5}_{a_2} - t^{a_6}_{i_7} v^{i_7 a_5}_{a_2 a_6} - t^{a_5}_{i_6} (\Xi_0)^{i_6}_{a_2} - \tfrac{1}{2} t^{a_5 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_2 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_5}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_2}$$
$$(\xi_{41,1})^{i_3 i_4 a_{10}}_{i_7 i_8 a'_{11}} = -\tfrac{1}{2} \tilde{t}^{a'_{12}a_{10}}_{i_7 i_8} v^{i_3 i_4}_{a'_{11}a'_{12}}$$
$$(\xi_{41})^{i_3 i_4 a_9 a_{10}}_{i_5 i_6 i_7 i_8} = +\tfrac{1}{2} t^{a_9 a_{10} a_{11} a_{12}}_{i_5 i_6 i_7 i_8} v^{i_3 i_4}_{a_{11} a_{12}} + P_2 P_4 \tilde{t}^{a'_{11}a_9}_{i_5 i_6} (\xi_{41,1})^{i_3 i_4 a_{10}}_{i_7 i_8 a'_{11}}$$
$$(\xi_{40})^{a'_5 a_6}_{a_1 a_2} = -\tfrac{1}{2} \tilde{t}^{a'_5 a_7}_{i_8 i_9} (\Xi_{18})^{i_8 i_9 a_6}_{a_1 a_2 a_7}$$
$$(\xi_{4,0})^{i_4}_{a_6} = -f^{i_4}_{a_6} - (\Xi_0)^{i_4}_{a_6}$$
$$(\xi_4)^{i_4}_{i_5} = -f^{i_4}_{i_5} + t^{a_6}_{i_5} (\xi_{4,0})^{i_4}_{a_6} - t^{a_6}_{i_7} v^{i_4 i_7}_{i_5 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_5 i_8} v^{i_4 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_5 i_8} V^{i_4 i_8}_{i_6 i_7}$$
$$(\xi_{39})^{i_3 i_4 a'_7}_{i_5 i_6 a_2} = +\tfrac{1}{4} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} (\Xi_{25})^{i_3 i_4 i_9 i_{10}}_{i_5 i_6 a_2 a_8} - P_2 \tilde{t}^{a'_7 a_8}_{i_5 i_9} (\Xi_{17})^{i_3 i_4 i_9}_{i_6 a_2 a_8}$$
$$(\xi_{38})^{i_3 i_4 a'_7}_{i_5 a_2 a_6} = -\tfrac{1}{2} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} (\Xi_{19})^{i_3 i_4 i_9 i_{10}}_{i_5 a_2 a_6 a_8}$$
$$(\xi_{37})^{i_3 i_4 a_7}_{i_5 a_2 a_6} = +\tfrac{1}{2} t^{a_7 a_8}_{i_9 i_{10}} (\Xi_{19})^{i_3 i_4 i_9 i_{10}}_{i_5 a_2 a_6 a_8} - t^{a_7}_{i_8} (\Xi_{17})^{i_3 i_4 i_8}_{i_5 a_2 a_6}$$
$$(\xi_{36,5})^{i_{10} i_{11} a_9}_{i_5 i_6 a_2} = -\tilde{t}^{a'_{12}a_9}_{i_5 i_6} v^{i_{10} i_{11}}_{a'_{12} a_2}$$
$$(\xi_{36,4})^{a_8 a_9}_{a_2 a_{10}} = -\tfrac{1}{2} t^{a_8 a_9}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a_2 a_{10}}$$
$$(\xi_{36,3})^{i_{10} a_8 a_9}_{i_5 i_6 a_2} = -t^{a_8 a_9 a_{11}}_{i_5 i_6 i_{12}} v^{i_{10} i_{12}}_{a_2 a_{11}}$$
$$(\xi_{36,1})^{i_{10} i_{11}}_{i_6 a_2} = +v^{i_{10} i_{11}}_{i_6 a_2} - (\Xi_1)^{i_{10} i_{11}}_{i_6 a_2}$$
$$(\xi_{36})^{a_7 a_8 a_9}_{i_5 i_6 a_2} = -P_3 \tilde{t}^{a'_{10}a_7}_{i_5 i_6} v^{a_8 a_9}_{a'_{10} a_2} + \tfrac{1}{2} P_2 t^{a_7 a_8 a_9}_{i_5 i_{10} i_{11}} (\xi_{36,1})^{i_{10} i_{11}}_{i_6 a_2} - P_3 t^{a_7 a_8 a_{10}}_{i_5 i_6 i_{11}} v^{i_{11} a_9}_{a_2 a_{10}}$$
$$+P_3 t^{a_7}_{i_{10}} (\xi_{36,3})^{i_{10} a_8 a_9}_{i_5 i_6 a_2} + P_3 t^{a_7 a_{10}}_{i_5 i_6} (\xi_{36,4})^{a_8 a_9}_{a_2 a_{10}}$$
$$+\tfrac{1}{2} P_3 t^{a_7 a_8}_{i_{10} i_{11}} (\xi_{36,5})^{i_{10} i_{11} a_9}_{i_5 i_6 a_2} - \tfrac{1}{2} t^{a_7 a_8 a_9 a_{10}}_{i_5 i_6 i_{11} i_{12}} v^{i_{11} i_{12}}_{a_2 a_{10}}$$
$$(\xi_{33,5})^{i_4 i_{11}}_{i_7 a_{10}} = -v^{i_4 i_{11}}_{i_7 a_{10}} + (\Xi_1)^{i_4 i_{11}}_{i_7 a_{10}}$$
$$(\xi_{33,4})^{i_4 i_{10}}_{i_6 i_7} = +(\Xi_3)^{i_4 i_{10}}_{i_6 i_7} - \tfrac{1}{2} (\Xi_{21})^{i_4 i_{10}}_{i_6 i_7} - (\Xi_5)^{i_4 i_{10}}_{i_6 i_7} - (\Xi_6)^{i_4 i_{10}}_{i_6 i_7}$$
$$(\xi_{33,3,0})^{i_4 i_{10}}_{i_7 a_{11}} = -v^{i_4 i_{10}}_{i_7 a_{11}} + (\Xi_1)^{i_4 i_{10}}_{i_7 a_{11}}$$
$$(\xi_{33,3})^{i_4 i_{10} a_9}_{i_5 i_6 i_7} = +(\Xi_{12})^{i_4 i_{10} a_9}_{i_5 i_6 i_7} - (\Xi_{23})^{i_4 i_{10} a_9}_{i_5 i_6 i_7} + (\Xi_{15})^{i_4 i_{10} a_9}_{i_5 i_6 i_7} + P_3 t^{a_9 a_{11}}_{i_5 i_6} (\xi_{33,3,0})^{i_4 i_{10}}_{i_7 a_{11}}$$
$$(\xi_{33,2})^{i_4 a_9}_{i_7 a'_{10}} = +v^{i_4 a_9}_{i_7 a'_{10}} - t^{a_{11}}_{i_7} v^{i_4 a_9}_{a'_{10} a_{11}} - t^{a_9 a_{11}}_{i_7 i_{12}} v^{i_4 i_{12}}_{a'_{10} a_{11}} + \tilde{t}^{a'_{11}a_9}_{i_7 i_{12}} v^{i_4 i_{12}}_{a'_{10} a'_{11}}$$
$$(\xi_{33,1})^{i_4 a_9}_{i_7 a_{10}} = -v^{i_4 a_9}_{i_7 a_{10}} + (\Xi_4)^{i_4 a_9}_{i_7 a_{10}} + (\Xi_{13})^{i_4 a_9}_{i_7 a_{10}} + (\Xi_7)^{i_4 a_9}_{i_7 a_{10}}$$
$$(\xi_{33,0})^{i_4}_{a_{10}} = -f^{i_4}_{a_{10}} - (\Xi_0)^{i_4}_{a_{10}}$$
$$(\xi_{33})^{i_4 a_8 a_9}_{i_5 i_6 i_7} = +t^{a_8 a_9 a_{10}}_{i_5 i_6 i_7} (\xi_{33,0})^{i_4}_{a_{10}} + P_2 P_3 t^{a_8 a_{10}}_{i_5 i_6} (\xi_{33,1})^{i_4 a_9}_{i_7 a_{10}}$$
$$+P_2 P_3 \tilde{t}^{a'_{10}a_8}_{i_5 i_6} (\xi_{33,2})^{i_4 a_9}_{i_7 a'_{10}} + P_2 t^{a_8}_{i_{10}} (\xi_{33,3})^{i_4 i_{10} a_9}_{i_5 i_6 i_7}$$
$$+P_3 t^{a_8 a_9}_{i_5 i_{10}} (\xi_{33,4})^{i_4 i_{10}}_{i_6 i_7} + P_3 t^{a_8 a_9 a_{10}}_{i_5 i_6 i_{11}} (\xi_{33,5})^{i_4 i_{11}}_{i_7 a_{10}}$$
$$+\tfrac{1}{2} P_2 t^{a_8 a_9 a_{10} a_{11}}_{i_5 i_6 i_7 i_{12}} v^{i_4 i_{12}}_{a_{10} a_{11}} - \tfrac{1}{2} t^{a_8 a_9 a_{10} a_{11}}_{i_5 i_6 i_7 i_{12}} v^{i_4 i_{12}}_{a_{10} a_{11}}$$
$$(\xi_{31,0})^{i_7 a_6}_{a_1 a_2} = +(\Xi_{11})^{i_7 a_6}_{a_1 a_2} + (\Xi_{20})^{i_7 a_6}_{a_1 a_2}$$
$$(\xi_{31})^{a_5 a_6}_{a_1 a_2} = +P_2 t^{a_5}_{i_7} (\xi_{31,0})^{i_7 a_6}_{a_1 a_2} - \tfrac{1}{4} P_2 t^{a_5 a_7}_{i_8 i_9} (\Xi_{18})^{i_8 i_9 a_6}_{a_1 a_2 a_7}$$
$$(\xi_{30,1})^{i_3 i_4}_{i_6 a_2} = -(\Xi_9)^{i_3 i_4}_{i_6 a_2} - (\Xi_{16})^{i_3 i_4}_{i_6 a_2}$$
$$(\xi_{30,0})^{i_3 i_4 i_8}_{i_5 i_6 a_2} = -\tfrac{1}{2} (\Xi_{22})^{i_3 i_4 i_8}_{i_5 i_6 a_2} - (\Xi_{24})^{i_3 i_4 i_8}_{i_5 i_6 a_2}$$
$$(\xi_{30})^{i_3 i_4 a_7}_{i_5 i_6 a_2} = +t^{a_7}_{i_8} (\xi_{30,0})^{i_3 i_4 i_8}_{i_5 i_6 a_2} + P_2 t^{a_7}_{i_5} (\xi_{30,1})^{i_3 i_4}_{i_6 a_2} - \tfrac{1}{4} t^{a_7 a_8}_{i_9 i_{10}} (\Xi_{25})^{i_3 i_4 i_9 i_{10}}_{i_5 i_6 a_2 a_8}$$
$$+P_2 t^{a_7 a_8}_{i_5 i_9} (\Xi_{17})^{i_3 i_4 i_9}_{i_6 a_2 a_8}$$
$$(\xi_3)^{i_4}_{i_5} = -t^{a_6}_{i_5} \lambda^{i_4}_{a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_5 i_8} \lambda^{i_4 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_5 i_8} (\Xi_8)^{i_4 i_8}_{i_6 i_7} - \tfrac{1}{12} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} \lambda^{i_4 i_9 i_{10}}_{a_6 a_7 a_8}$$
$$-\tfrac{1}{144} t^{a_6 a_7 a_8 a_9}_{i_5 i_{10} i_{11} i_{12}} \lambda^{i_4 i_{10} i_{11} i_{12}}_{a_6 a_7 a_8 a_9}$$
$$(\xi_{29})^{i_4 a'_6}_{a_2 a_5} = -\tfrac{1}{2} \lambda^{i_4 i_7 i_8}_{a_2 a_5 a_9} \tilde{t}^{a'_6 a_9}_{i_7 i_8}$$
$$(\xi_{28})^{i_3 i_4 a_8}_{i_5 i_6 i_7} = +(\Xi_{12})^{i_3 i_4 a_8}_{i_5 i_6 i_7} - (\Xi_{23})^{i_3 i_4 a_8}_{i_5 i_6 i_7}$$
$$(\xi_{27})^{i_4 a_6}_{a_2 a_5} = +(\Xi_{11})^{i_4 a_6}_{a_2 a_5} + (\Xi_{20})^{i_4 a_6}_{a_2 a_5}$$
$$(\xi_{26})^{i_5 a_6}_{a_1 a_2} = +(\Xi_{11})^{i_5 a_6}_{a_1 a_2} + (\Xi_{20})^{i_5 a_6}_{a_1 a_2}$$
$$(\xi_{25})^{i_3 i_4 i_7}_{i_5 i_6 a_2} = +\tfrac{1}{2} (\Xi_{22})^{i_3 i_4 i_7}_{i_5 i_6 a_2} + (\Xi_{24})^{i_3 i_4 i_7}_{i_5 i_6 a_2}$$
$$(\xi_{24})^{i_3 i_4 i_7}_{i_5 a_2 a_6} = +(\Xi_{10})^{i_3 i_4 i_7}_{i_5 a_2 a_6} + (\Xi_{17})^{i_3 i_4 i_7}_{i_5 a_2 a_6}$$
$$(\xi_{23,2})^{i_8 i_9}_{i_5 a_2} = -v^{i_8 i_9}_{i_5 a_2} + (\Xi_1)^{i_8 i_9}_{i_5 a_2}$$
$$(\xi_{23,1})^{i_8 a_7}_{i_5 a_2} = -(\Xi_4)^{i_8 a_7}_{i_5 a_2} - (\Xi_{13})^{i_8 a_7}_{i_5 a_2} - (\Xi_7)^{i_8 a_7}_{i_5 a_2}$$
$$(\xi_{23})^{a_6 a_7}_{i_5 a_2} = -v^{a_6 a_7}_{i_5 a_2} + t^{a_8}_{i_5} v^{a_6 a_7}_{a_2 a_8} + P_2 t^{a_6}_{i_8} (\xi_{23,1})^{i_8 a_7}_{i_5 a_2} + \tfrac{1}{2} t^{a_6 a_7}_{i_8 i_9} (\xi_{23,2})^{i_8 i_9}_{i_5 a_2}$$
$$+P_2 t^{a_6 a_8}_{i_5 i_9} v^{i_9 a_7}_{a_2 a_8} + P_2 \tilde{t}^{a'_8 a_6}_{i_5 i_9} v^{i_9 a_7}_{a'_8 a_2} + \tfrac{1}{2} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} v^{i_9 i_{10}}_{a_2 a_8}$$
$$(\xi_{22,6})^{i_4 i_9}_{i_6 a'_8} = -v^{i_4 i_9}_{i_6 a'_8} + (\Xi_{14})^{i_4 i_9}_{i_6 a'_8}$$
$$(\xi_{22,4})^{i_4 i_9}_{i_6 a_8} = +v^{i_4 i_9}_{i_6 a_8} - (\Xi_1)^{i_4 i_9}_{i_6 a_8}$$
$$(\xi_{22,3})^{i_4 a_7}_{i_6 a_8} = +v^{i_4 a_7}_{i_6 a_8} - \tfrac{1}{2} (\Xi_4)^{i_4 a_7}_{i_6 a_8}$$
$$(\xi_{22,2})^{i_4 i_8}_{i_5 i_6} = +v^{i_4 i_8}_{i_5 i_6} - (\Xi_3)^{i_4 i_8}_{i_5 i_6} + \tfrac{1}{2} (\Xi_{21})^{i_4 i_8}_{i_5 i_6} + (\Xi_5)^{i_4 i_8}_{i_5 i_6} + (\Xi_6)^{i_4 i_8}_{i_5 i_6}$$
$$(\xi_{22,1})^{i_4}_{a'_8} = -f^{i_4}_{a'_8} - t^{a_9}_{i_{10}} v^{i_4 i_{10}}_{a'_8 a_9}$$
$$(\xi_{22,0})^{i_4}_{a_8} = +f^{i_4}_{a_8} + (\Xi_0)^{i_4}_{a_8}$$
$$(\xi_{22})^{i_4 a_7}_{i_5 i_6} = -v^{i_4 a_7}_{i_5 i_6} + t^{a_7 a_8}_{i_5 i_6} (\xi_{22,0})^{i_4}_{a_8} + \tilde{t}^{a'_8 a_7}_{i_5 i_6} (\xi_{22,1})^{i_4}_{a'_8} + t^{a_7}_{i_8} (\xi_{22,2})^{i_4 i_8}_{i_5 i_6}$$
$$+P_2 t^{a_8}_{i_5} (\xi_{22,3})^{i_4 a_7}_{i_6 a_8} + P_2 t^{a_7 a_8}_{i_5 i_9} (\xi_{22,4})^{i_4 i_9}_{i_6 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_5 i_6} v^{i_4 a_7}_{a_8 a_9}$$
$$+P_2 \tilde{t}^{a'_8 a_7}_{i_5 i_9} (\xi_{22,6})^{i_4 i_9}_{i_6 a'_8} - \tfrac{1}{2} t^{i_8 i_9}_{i_5 i_6} V^{i_4 a_7}_{i_8 i_9} + \tfrac{1}{2} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}} v^{i_4 i_{10}}_{a_8 a_9}$$
$$(\xi_{21,1})^{i_4 i_8 i_9}_{i_5 a_2 a_7} = -(\Xi_{10})^{i_4 i_8 i_9}_{i_5 a_2 a_7} - (\Xi_{17})^{i_4 i_8 i_9}_{i_5 a_2 a_7}$$
$$(\xi_{21})^{i_4 a'_6}_{i_5 a_2} = +\tilde{t}^{a'_6 a_7}_{i_5 i_8} \tilde{\lambda}^{i_4 i_8}_{a'_7 a_2} + \tfrac{1}{2} \tilde{t}^{a'_6 a_7}_{i_8 i_9} (\xi_{21,1})^{i_4 i_8 i_9}_{i_5 a_2 a_7}$$
$$(\xi_{20})^{a'_5}_{a_2} = +\tfrac{1}{2} \lambda^{i_6 i_7}_{a_2 a_8} \tilde{t}^{a'_5 a_8}_{i_6 i_7} - \tfrac{1}{2} \tilde{t}^{a'_5 a'_6}_{i_7 i_8} \tilde{\lambda}^{i_7 i_8}_{a'_6 a_2}$$

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TABLE ESI.4.XXV: The computational sequence and intermediates for the Λ_2 amplitude equation of Λ-CCSDTQ-R12 [Part II]

$$
\begin{aligned}
(\xi_{19})^{a_5}_{a_2} &= -\tfrac{1}{2} t^{a_5 a_6}_{i_7 i_8} \lambda^{i_7 i_8}_{a_2 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_5}_{i_7 i_8} \tilde{\lambda}^{i_7 i_8}_{a'_6 a_2} - \tfrac{1}{12} t^{a_5 a_6 a_7}_{i_8 i_9 i_{10}} \lambda^{i_8 i_9 i_{10}}_{a_2 a_6 a_7} \\
&\quad - \tfrac{1}{144} t^{a_5 a_6 a_7 a_8}_{i_9 i_{10} i_{11} i_{12}} \lambda^{i_9 i_{10} i_{11} i_{12}}_{a_2 a_6 a_7 a_8} \\
(\xi_{18,3})^{i_4 i_7}_{i_5 a_2} &= -(\Xi_9)^{i_4 i_7}_{i_5 a_2} - (\Xi_{16})^{i_4 i_7}_{i_5 a_2} \\
(\xi_{18,2})^{i_4 i_8 i_9}_{i_5 a_2 a_7} &= +(\Xi_{10})^{i_4 i_8 i_9}_{i_5 a_2 a_7} + (\Xi_{17})^{i_4 i_8 i_9}_{i_5 a_2 a_7} \\
(\xi_{18})^{i_4 a_6}_{i_5 a_2} &= +t^{a_6 a_7}_{i_5 i_8} \lambda^{i_4 i_8}_{a_2 a_7} + \tilde{t}^{a'_7 a_6}_{i_5 i_8} \tilde{\lambda}^{i_4 i_8}_{a'_7 a_2} + \tfrac{1}{2} t^{a_6 a_7}_{i_8 i_9} (\xi_{18,2})^{i_4 i_8 i_9}_{i_5 a_2 a_7} + t^{a_6}_{i_7} (\xi_{18,3})^{i_4 i_7}_{i_5 a_2} \\
&\quad + \tfrac{1}{4} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} \lambda^{i_4 i_9 i_{10}}_{a_2 a_7 a_8} - \tfrac{1}{12} t^{a_6 a_7 a_8}_{i_9 i_{10} i_{11}} (\Xi_{19})^{i_4 i_9 i_{10} i_{11}}_{i_5 a_2 a_7 a_8} + \tfrac{1}{36} t^{a_6 a_7 a_8 a_9}_{i_5 i_{10} i_{11} i_{12}} \lambda^{i_4 i_{10} i_{11} i_{12}}_{a_2 a_7 a_8 a_9} \\
(\xi_{17,0})^{i_3 i_4}_{i_6 a_7} &= +\tfrac{1}{2} (\Xi_2)^{i_3 i_4}_{i_6 a_7} + (\Xi_9)^{i_3 i_4}_{i_6 a_7} + (\Xi_{16})^{i_3 i_4}_{i_6 a_7} \\
(\xi_{17})^{i_3 i_4}_{i_5 i_6} &= +P_2 t^{a_7}_{i_5} (\xi_{17,0})^{i_3 i_4}_{i_6 a_7} + \tfrac{1}{2} t^{a_7 a_8}_{i_5 i_6} \lambda^{i_3 i_4}_{a_7 a_8} + \tfrac{1}{2} t^{i_7 i_8}_{i_5 i_6} (\Xi_8)^{i_3 i_4}_{i_7 i_8} + \tfrac{1}{6} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}} \lambda^{i_3 i_4 i_{10}}_{a_7 a_8 a_9} \\
&\quad - \tfrac{1}{4} P_2 t^{a_7 a_8}_{i_5 i_9} (\Xi_{17})^{i_3 i_4 i_9}_{i_6 a_7 a_8} + \tfrac{1}{48} t^{a_7 a_8 a_9 a_{10}}_{i_5 i_6 i_{11} i_{12}} \lambda^{i_3 i_4 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}} \\
(\xi_{16})^{i_3 i_4}_{i_5 a'_6} &= +t^{a_7}_{i_5} \tilde{\lambda}^{i_3 i_4}_{a'_6 a_7} \\
(\xi_{15})^{i_3 i_4}_{i_5 a_6} &= +(\Xi_2)^{i_3 i_4}_{i_5 a_6} + (\Xi_9)^{i_3 i_4}_{i_5 a_6} + (\Xi_{16})^{i_3 i_4}_{i_5 a_6} \\
(\xi_{14})^{i_4 i_6}_{i_5 a_2} &= +(\Xi_2)^{i_4 i_6}_{i_5 a_2} + (\Xi_9)^{i_4 i_6}_{i_5 a_2} + (\Xi_{16})^{i_4 i_6}_{i_5 a_2} \\
(\xi_{13})^{i_3 i_4}_{i_5 i_6} &= -(\Xi_3)^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{2} (\Xi_{21})^{i_3 i_4}_{i_5 i_6} \\
(\xi_{11})^{i_4 a'_6}_{i_5 a_2} &= +v^{i_4 a'_6}_{i_5 a_2} - t^{a_7}_{i_5} v^{i_4 a'_6}_{a_2 a_7} \\
(\xi_1)^{i_3 i_4}_{i_5 a_2} &= -v^{i_3 i_4}_{i_5 a_2} + (\Xi_1)^{i_3 i_4}_{i_5 a_2} \\
(\xi_0)^{i_4}_{a_2} &= +f^{i_4}_{a_2} + (\Xi_0)^{i_4}_{a_2}
\end{aligned}
$$

$$
\begin{aligned}
\delta^{i_3 i_4}_{a_1 a_2} &= +v^{i_3 i_4}_{a_1 a_2} + P_2 P_2 \lambda^{i_3}_{a_1} (\xi_0)^{i_4}_{a_2} + P_2 \lambda^{i_5}_{a_1} (\xi_1)^{i_3 i_4}_{i_5 a_2} - P_2 \lambda^{i_3}_{a_5} v^{i_4 a_5}_{a_1 a_2} \\
&\quad + P_2 v^{i_3 i_5}_{a_1 a_2} (\xi_3)^{i_4}_{i_5} + P_2 \lambda^{i_3 i_5}_{a_1 a_2} (\xi_4)^{i_4}_{i_5} + P_2 \lambda^{i_3 i_4}_{a_1 a_5} (\xi_5)^{a_5}_{a_2} \\
&\quad + P_2 \tilde{\lambda}^{i_3 i_4}_{a'_5 a_1} (\xi_6)^{a'_5}_{a_2} + P_2 f^{i_5}_{a_1} (\xi_7)^{i_3 i_4}_{i_5 a_2} + \tfrac{1}{2} \lambda^{i_5 i_6}_{a_1 a_2} (\xi_8)^{i_3 i_4}_{i_5 i_6} \\
&\quad + P_2 P_2 \lambda^{i_3 i_5}_{a_1 a_6} (\xi_9)^{i_4 a_6}_{i_5 a_2} + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_5 a_6} v^{a_5 a_6}_{a_1 a_2} + P_2 P_2 \tilde{\lambda}^{i_3 i_5}_{a'_6 a_1} (\xi_{11})^{i_4 a'_6}_{i_5 a_2} \\
&\quad + \tfrac{1}{2} \lambda^{i_3 i_4}_{i_5 i_6} (V^\dagger)^{i_5 i_6}_{a_1 a_2} + \lambda^{i_5 i_6}_{a_1 a_2} (\xi_{13})^{i_3 i_4}_{i_5 i_6} + P_2 P_2 v^{i_3 i_5}_{i_6 a_1} (\xi_{14})^{i_4 i_6}_{i_5 a_2} \\
&\quad + v^{i_5 a_6}_{a_1 a_2} (\xi_{15})^{i_3 i_4}_{i_5 a_6} + v^{i_5 a'_6}_{a_1 a_2} (\xi_{16})^{i_3 i_4}_{i_5 a'_6} + \tfrac{1}{2} v^{i_5 i_6}_{a_1 a_2} (\xi_{17})^{i_3 i_4}_{i_5 i_6} \\
&\quad + P_2 P_2 v^{i_3 i_5}_{a_1 a_6} (\xi_{18})^{i_4 a_6}_{i_5 a_2} + P_2 v^{i_3 i_4}_{a_1 a_5} (\xi_{19})^{a_5}_{a_2} + P_2 v^{i_3 i_4}_{a'_5 a_1} (\xi_{20})^{a'_5}_{a_2} \\
&\quad + P_2 P_2 v^{i_3 i_5}_{a'_6 a_1} (\xi_{21})^{i_4 a'_6}_{i_5 a_2} + \tfrac{1}{2} P_2 \lambda^{i_3 i_5 i_6}_{a_1 a_2 a_7} (\xi_{22})^{i_4 a_7}_{i_5 i_6} \\
&\quad + \tfrac{1}{2} P_2 \lambda^{i_3 i_4 i_5}_{a_1 a_6 a_7} (\xi_{23})^{a_6 a_7}_{i_5 a_2} + P_2 v^{i_5 a_6}_{i_7 a_1} (\xi_{24})^{i_3 i_4 i_7}_{i_5 a_2 a_6} + P_2 v^{i_5 i_6}_{i_7 a_1} (\xi_{25})^{i_3 i_4 i_7}_{i_5 i_6 a_2} \\
&\quad + v^{i_3 i_4}_{i_5 a_6} (\xi_{26})^{i_5 a_6}_{a_1 a_2} + P_2 P_2 v^{i_3 a_5}_{a_1 a_6} (\xi_{27})^{i_4 a_6}_{a_2 a_5} + \lambda^{i_5 i_6 i_7}_{a_1 a_2 a_8} (\xi_{28})^{i_3 i_4 a_8}_{i_5 i_6 i_7} \\
&\quad + P_2 P_2 v^{i_3 a_5}_{a'_6 a_1} (\xi_{29})^{i_4 a'_6}_{a_2 a_5} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{a_1 a_7} (\xi_{30})^{i_3 i_4 a_7}_{i_5 i_6 a_2} + \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} (\xi_{31})^{a_5 a_6}_{a_1 a_2} \\
&\quad + \tfrac{1}{6} \lambda^{i_5 i_6 i_7}_{a_1 a_2 a_8} (\Xi_{15})^{i_3 i_4 a_8}_{i_5 i_6 i_7} + \tfrac{1}{12} P_2 \lambda^{i_3 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} (\xi_{33})^{i_4 a_8 a_9}_{i_5 i_6 i_7} \\
&\quad - \tfrac{1}{2} P_2 v^{i_3 i_5}_{i_6 i_7} (\Xi_{17})^{i_4 i_6 i_7}_{i_5 a_1 a_2} - \tfrac{1}{2} P_2 v^{a_5 a_6}_{a_1 a_7} (\Xi_{18})^{i_3 i_4 a_7}_{a_2 a_5 a_6} \\
&\quad + \tfrac{1}{12} P_2 \lambda^{i_3 i_4 i_5 i_6}_{a_1 a_7 a_8 a_9} (\xi_{36})^{a_7 a_8 a_9}_{i_5 i_6 a_2} + P_2 v^{i_5 a_6}_{a_1 a_7} (\xi_{37})^{i_3 i_4 a_7}_{i_5 a_2 a_6} \\
&\quad + P_2 v^{i_5 a_6}_{a'_7 a_1} (\xi_{38})^{i_3 i_4 a'_7}_{i_5 a_2 a_6} + \tfrac{1}{2} P_2 v^{i_5 i_6}_{a'_7 a_1} (\xi_{39})^{i_3 i_4 a'_7}_{i_5 i_6 a_2} \\
&\quad + v^{i_3 i_4}_{a'_5 a_6} (\xi_{40})^{a'_5 a_6}_{a_1 a_2} + \tfrac{1}{48} \lambda^{i_5 i_6 i_7 i_8}_{a_1 a_2 a_9 a_{10}} (\xi_{41})^{i_3 i_4 a_9 a_{10}}_{i_5 i_6 i_7 i_8}
\end{aligned}
$$

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TABLE ESI.4.XXVI: The computational sequence and intermediates for the Λ_3 amplitude equation of Λ-CCSDTQ-R12

$$
\begin{aligned}
(\Xi_0)^{i_6}_{a_{10}} &= +t^{a_{11}}_{i_{12}} v^{i_6 i_{12}}_{a_{10} a_{11}} \\
(\Xi_1)^{i_{10} i_{11}}_{i_7 a_3} &= +t^{a_{12}}_{i_7} v^{i_{10} i_{11}}_{a_3 a_{12}} \\
(\Xi_2)^{i_4 i_5 i_6}_{i_8 a_3 a_9} &= +t^{a_{10}}_{i_8} \lambda^{i_4 i_5 i_6}_{a_3 a_9 a_{10}} \\
(\Xi_3)^{i_6 i_{10}}_{i_7 i_8} &= +P_2 t^{a_{11}}_{i_7} v^{i_6 i_{10}}_{i_8 a_{11}} \\
(\Xi_4)^{i_{10} a_9}_{i_7 a_3} &= +t^{a_{11}}_{i_7} v^{i_{10} a_9}_{a_3 a_{11}} \\
(\Xi_5)^{i_6 i_{10}}_{i_7 i_8} &= +\tfrac{1}{2} t^{a_{11} a_{12}}_{i_7 i_8} v^{i_6 i_{10}}_{a_{11} a_{12}} \\
(\Xi_6)^{i_{10} a_9}_{i_7 a_3} &= +t^{a_9 a_{11}}_{i_7 i_{12}} v^{i_{10} i_{12}}_{a_3 a_{11}} \\
(\Xi_7)^{i_6 i_{10}}_{i_7 i_8} &= +\tfrac{1}{2} t^{i_{11} i_{12}}_{i_7 i_8} V^{i_6 i_{10}}_{i_{11} i_{12}} \\
(\Xi_8)^{i_{10} a_9}_{i_7 a_3} &= +\tilde{t}^{a'_{11} a_9}_{i_7 i_{12}} v^{i_{10} i_{12}}_{a'_{11} a_3} \\
(\Xi_9)^{i_4 i_5 i_6}_{i_8 a_3 a_9} &= +\tfrac{1}{2} t^{a_{10} a_{11}}_{i_8 i_{12}} \lambda^{i_4 i_5 i_6 i_{12}}_{a_3 a_9 a_{10} a_{11}} \\
(\Xi_{10})^{i_5 i_6 i_{10} i_{11}}_{i_7 a_2 a_3 a_9} &= +t^{a_{12}}_{i_7} \lambda^{i_5 i_6 i_{10} i_{11}}_{a_2 a_3 a_9 a_{12}} \\
(\Xi_{11})^{i_6 i_9 a_8}_{a_1 a_2 a_3} &= +\tfrac{1}{2} t^{a_8 a_{10}}_{i_{11} i_{12}} \lambda^{i_6 i_9 i_{11} i_{12}}_{a_1 a_2 a_3 a_{10}} \\
(\Xi_{12})^{i_5 i_6}_{i_9 a'_{11}} &= +t^{a_{12}}_{i_9} v^{i_5 i_6}_{a'_{11} a_{12}} \\
(\Xi_{13})^{i_6 i_{10}}_{i_7 i_8} &= +P_2 t^{a_{11}}_{i_7} (\Xi_1)^{i_6 i_{10}}_{i_8 a_{11}} \\
(\Xi_{14})^{i_4 i_5 i_6 i_{10}}_{i_7 i_8 a_2 a_3} &= +P_2 t^{a_{11}}_{i_7} (\Xi_{10})^{i_4 i_5 i_6 i_{10}}_{i_8 a_2 a_3 a_{11}} \\
(\xi_9)^{i_5 i_6}_{i_7 i_8} &= -v^{i_5 i_6}_{i_7 i_8} - (\Xi_5)^{i_5 i_6}_{i_7 i_8} - (\Xi_7)^{i_5 i_6}_{i_7 i_8} \\
(\xi_8)^{i_4 i_5 i_6}_{i_7 a_2 a_3} &= +(\Xi_2)^{i_4 i_5 i_6}_{i_7 a_2 a_3} + (\Xi_9)^{i_4 i_5 i_6}_{i_7 a_2 a_3} \\
(\xi_7)^{a_7}_{a_3} &= -f^{a_7}_{a_3} + t^{a_8}_{i_9} v^{i_9 a_7}_{a_3 a_8} + t^{a_7}_{i_8} (\Xi_0)^{i_8}_{a_3} + \tfrac{1}{2} t^{a_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_3 a_8} + \tfrac{1}{2} \tilde{t}^{a'_8 a_7}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_3} \\
(\xi_{6,0})^{i_6}_{a_8} &= +f^{i_6}_{a_8} + (\Xi_0)^{i_6}_{a_8} \\
(\xi_6)^{i_6}_{i_7} &= +f^{i_6}_{i_7} + t^{a_8}_{i_7} (\xi_{6,0})^{i_6}_{a_8} + t^{a_8}_{i_9} v^{i_6 i_9}_{i_7 a_8} + \tfrac{1}{2} t^{a_8 a_9}_{i_7 i_{10}} v^{i_6 i_{10}}_{a_8 a_9} + \tfrac{1}{2} t^{i_8 i_9}_{i_7 i_{10}} V^{i_6 i_{10}}_{i_8 i_9} \\
(\xi_5)^{i_5 i_6}_{i_7 a_3} &= -t^{a_8}_{i_7} \lambda^{i_5 i_6}_{a_3 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_7 i_{10}} \lambda^{i_5 i_6 i_{10}}_{a_3 a_8 a_9} - \tfrac{1}{12} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} \lambda^{i_5 i_6 i_{11} i_{12}}_{a_3 a_8 a_9 a_{10}} \\
(\xi_{29})^{i_5 i_6 a'_8}_{i_7 a_2 a_3} &= +\tfrac{1}{2} \tilde{t}^{a'_8 a_9}_{i_{10} i_{11}} (\Xi_{10})^{i_5 i_6 i_{10} i_{11}}_{i_7 a_2 a_3 a_9} \\
(\xi_{28})^{i_5 i_6 a_8}_{i_7 a_2 a_3} &= -\tfrac{1}{2} t^{a_8 a_9}_{i_{10} i_{11}} (\Xi_{10})^{i_5 i_6 i_{10} i_{11}}_{i_7 a_2 a_3 a_9} + t^{a_8}_{i_9} (\Xi_9)^{i_5 i_6 i_9}_{i_7 a_2 a_3} - \tfrac{1}{4} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} \lambda^{i_5 i_6 i_{11} i_{12}}_{a_2 a_3 a_9 a_{10}} \\
(\xi_{27})^{i_6 a_7 a_8}_{a_1 a_2 a_3} &= -P_2 t^{a_7}_{i_9} (\Xi_{11})^{i_6 i_9 a_8}_{a_1 a_2 a_3} \\
(\xi_{26})^{i_4 i_5 i_6 a_9}_{i_7 i_8 a_2 a_3} &= -\tfrac{1}{2} t^{a_9}_{i_{10}} (\Xi_{14})^{i_4 i_5 i_6 i_{10}}_{i_7 i_8 a_2 a_3} - P_2 t^{a_9}_{i_7} (\Xi_9)^{i_4 i_5 i_6}_{i_8 a_2 a_3} \\
(\xi_{25})^{i_5 i_6 a'_8}_{a_2 a_3 a_7} &= +\tfrac{1}{2} \lambda^{i_5 i_6 i_9 i_{10}}_{a_2 a_3 a_7 a_{11}} \tilde{t}^{a'_8 a_{11}}_{i_9 i_{10}} \\
(\xi_{24,0})^{i_5 i_6}_{i_9 a'_{11}} &= -v^{i_5 i_6}_{i_9 a'_{11}} + (\Xi_{12})^{i_5 i_6}_{i_9 a'_{11}} \\
(\xi_{24})^{i_5 i_6 a_{10}}_{i_7 i_8 i_9} &= +P_3 \tilde{t}^{a'_{11} a_{10}}_{i_7 i_8} (\xi_{24,0})^{i_5 i_6}_{i_9 a'_{11}} - \tfrac{1}{2} t^{a_{10} a_{11} a_{12}}_{i_7 i_8 i_9} v^{i_5 i_6}_{a_{11} a_{12}} \\
(\xi_2)^{i_5 i_6}_{i_7 a_3} &= +v^{i_5 i_6}_{i_7 a_3} - (\Xi_1)^{i_5 i_6}_{i_7 a_3} \\
(\xi_{19,2})^{i_{10} i_{11}}_{i_7 a_3} &= +v^{i_{10} i_{11}}_{i_7 a_3} - (\Xi_1)^{i_{10} i_{11}}_{i_7 a_3} \\
(\xi_{19,1})^{i_{10} a_9}_{i_7 a_3} &= +(\Xi_4)^{i_{10} a_9}_{i_7 a_3} + (\Xi_6)^{i_{10} a_9}_{i_7 a_3} + (\Xi_8)^{i_{10} a_9}_{i_7 a_3} \\
(\xi_{19})^{a_8 a_9}_{i_7 a_3} &= +v^{a_8 a_9}_{i_7 a_3} - t^{a_{10}}_{i_7} v^{a_8 a_9}_{a_3 a_{10}} + P_2 t^{a_8}_{i_{10}} (\xi_{19,1})^{i_{10} a_9}_{i_7 a_3} + \tfrac{1}{2} t^{a_8 a_9}_{i_{10} i_{11}} (\xi_{19,2})^{i_{10} i_{11}}_{i_7 a_3} \\
&\quad - P_2 t^{a_8 a_{10}}_{i_7 i_{11}} v^{i_{11} a_9}_{a_3 a_{10}} - P_2 \tilde{t}^{a'_{10} a_8}_{i_7 i_{11}} v^{i_{11} a_9}_{a'_{10} a_3} - \tfrac{1}{2} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} v^{i_{11} i_{12}}_{a_3 a_{10}} \\
(\xi_{18,6})^{i_6 i_{11}}_{i_8 a'_{10}} &= +v^{i_6 i_{11}}_{i_8 a'_{10}} - (\Xi_{12})^{i_6 i_{11}}_{i_8 a'_{10}} \\
(\xi_{18,4})^{i_6 i_{11}}_{i_8 a_{10}} &= -v^{i_6 i_{11}}_{i_8 a_{10}} + (\Xi_1)^{i_6 i_{11}}_{i_8 a_{10}} \\
(\xi_{18,3})^{i_6 a_9}_{i_8 a_{10}} &= -v^{i_6 a_9}_{i_8 a_{10}} + \tfrac{1}{2} (\Xi_4)^{i_6 a_9}_{i_8 a_{10}} \\
(\xi_{18,2})^{i_6 i_{10}}_{i_7 i_8} &= -v^{i_6 i_{10}}_{i_7 i_8} + (\Xi_3)^{i_6 i_{10}}_{i_7 i_8} - \tfrac{1}{2} (\Xi_{13})^{i_6 i_{10}}_{i_7 i_8} - (\Xi_5)^{i_6 i_{10}}_{i_7 i_8} - (\Xi_7)^{i_6 i_{10}}_{i_7 i_8} \\
(\xi_{18,1})^{i_6}_{a'_{10}} &= +f^{i_6}_{a'_{10}} + t^{a_{11}}_{i_{12}} v^{i_6 i_{12}}_{a'_{10} a_{11}} \\
(\xi_{18,0})^{i_6}_{a_{10}} &= -f^{i_6}_{a_{10}} - (\Xi_0)^{i_6}_{a_{10}} \\
(\xi_{18})^{i_6 a_9}_{i_7 i_8} &= +v^{i_6 a_9}_{i_7 i_8} + t^{a_9 a_{10}}_{i_7 i_8} (\xi_{18,0})^{i_6}_{a_{10}} + \tilde{t}^{a'_{10} a_9}_{i_7 i_8} (\xi_{18,1})^{i_6}_{a'_{10}} + t^{a_9}_{i_{10}} (\xi_{18,2})^{i_6 i_{10}}_{i_7 i_8} \\
&\quad + P_2 t^{a_{10}}_{i_7} (\xi_{18,3})^{i_6 a_9}_{i_8 a_{10}} + P_2 t^{a_9 a_{10}}_{i_7 i_{11}} (\xi_{18,4})^{i_6 i_{11}}_{i_8 a_{10}} + \tfrac{1}{2} t^{a_{10} a_{11}}_{i_7 i_8} v^{i_6 a_9}_{a_{10} a_{11}} \\
&\quad + P_2 \tilde{t}^{a'_{10} a_9}_{i_7 i_{11}} (\xi_{18,6})^{i_6 i_{11}}_{i_8 a'_{10}} + \tfrac{1}{2} t^{i_{10} i_{11}}_{i_7 i_8} V^{i_6 a_9}_{i_{10} i_{11}} - \tfrac{1}{2} t^{a_9 a_{10} a_{11}}_{i_7 i_8 i_{12}} v^{i_6 i_{12}}_{a_{10} a_{11}} \\
(\xi_{17})^{i_6 a'_7}_{a_2 a_3} &= +\tfrac{1}{2} \lambda^{i_6 i_8 i_9}_{a_2 a_3 a_{10}} \tilde{t}^{a'_7 a_{10}}_{i_8 i_9} \\
(\xi_{16})^{i_6 a_7}_{a_2 a_3} &= -\tfrac{1}{2} t^{a_7 a_8}_{i_9 i_{10}} \lambda^{i_6 i_9 i_{10}}_{a_2 a_3 a_8} - \tfrac{1}{12} t^{a_7 a_8 a_9}_{i_{10} i_{11} i_{12}} \lambda^{i_6 i_{10} i_{11} i_{12}}_{a_2 a_3 a_8 a_9} \\
(\xi_{15,0})^{i_4 i_5 i_6}_{i_8 a_3 a_9} &= -\tfrac{1}{2} (\Xi_2)^{i_4 i_5 i_6}_{i_8 a_3 a_9} - (\Xi_9)^{i_4 i_5 i_6}_{i_8 a_3 a_9} \\
(\xi_{15})^{i_4 i_5 i_6}_{i_7 i_8 a_3} &= +P_2 t^{a_9}_{i_7} (\xi_{15,0})^{i_4 i_5 i_6}_{i_8 a_3 a_9} - \tfrac{1}{2} t^{a_9 a_{10}}_{i_7 i_8} \lambda^{i_4 i_5 i_6}_{a_3 a_9 a_{10}} - \tfrac{1}{6} t^{a_9 a_{10} a_{11}}_{i_7 i_8 i_{12}} \lambda^{i_4 i_5 i_6 i_{12}}_{a_3 a_9 a_{10} a_{11}} \\
(\xi_{14})^{i_4 i_5 i_6}_{i_7 a_3 a_8} &= -(\Xi_2)^{i_4 i_5 i_6}_{i_7 a_3 a_8} - (\Xi_9)^{i_4 i_5 i_6}_{i_7 a_3 a_8} \\
(\xi_{13})^{i_5 i_6 i_8}_{i_7 a_2 a_3} &= -(\Xi_2)^{i_5 i_6 i_8}_{i_7 a_2 a_3} - (\Xi_9)^{i_5 i_6 i_8}_{i_7 a_2 a_3} \\
(\xi_{12})^{i_5 i_6}_{i_7 i_8} &= +(\Xi_3)^{i_5 i_6}_{i_7 i_8} - \tfrac{1}{2} (\Xi_{13})^{i_5 i_6}_{i_7 i_8} \\
(\xi_{10})^{i_6 a_8}_{i_7 a_3} &= +v^{i_6 a_8}_{i_7 a_3} - (\Xi_4)^{i_6 a_8}_{i_7 a_3} - (\Xi_6)^{i_6 a_8}_{i_7 a_3} - (\Xi_8)^{i_6 a_8}_{i_7 a_3} + t^{a_8}_{i_9} (\Xi_1)^{i_6 i_9}_{i_7 a_3} \\
(\xi_1)^{i_6}_{a_3} &= -f^{i_6}_{a_3} - (\Xi_0)^{i_6}_{a_3} \\
\delta^{i_4 i_5 i_6}_{a_1 a_2 a_3} &= -P_3 P_3 \lambda^{i_4}_{a_1} v^{i_5 i_6}_{a_2 a_3} + P_3 P_3 \lambda^{i_4 i_5}_{a_1 a_2} (\xi_1)^{i_6}_{a_3} + P_3 P_3 \lambda^{i_4 i_7}_{a_1 a_2} (\xi_2)^{i_5 i_6}_{i_7 a_3} \\
&\quad + P_3 P_3 \lambda^{i_4 i_5}_{a_1 a_7} v^{i_6 a_7}_{a_2 a_3} - P_3 P_3 \tilde{\lambda}^{i_4 i_5}_{a'_7 a_1} v^{i_6 a'_7}_{a_2 a_3} + P_3 P_3 v^{i_4 i_7}_{a_1 a_2} (\xi_5)^{i_5 i_6}_{i_7 a_3} \\
&\quad + P_3 \lambda^{i_4 i_5 i_7}_{a_1 a_2 a_3} (\xi_6)^{i_6}_{i_7} + P_3 \lambda^{i_4 i_5 i_6}_{a_1 a_2 a_7} (\xi_7)^{a_7}_{a_3} + P_3 f^{i_7}_{a_1} (\xi_8)^{i_4 i_5 i_6}_{i_7 a_2 a_3} \\
&\quad + \tfrac{1}{2} P_3 \lambda^{i_4 i_7 i_8}_{a_1 a_2 a_3} (\xi_9)^{i_5 i_6}_{i_7 i_8} + P_3 P_3 \lambda^{i_4 i_5 i_7}_{a_1 a_2 a_8} (\xi_{10})^{i_6 a_8}_{i_7 a_3} - \tfrac{1}{2} P_3 \lambda^{i_4 i_5 i_6}_{a_1 a_7 a_8} v^{a_7 a_8}_{a_2 a_3} \\
&\quad + P_3 \lambda^{i_4 i_7 i_8}_{a_1 a_2 a_3} (\xi_{12})^{i_5 i_6}_{i_7 i_8} + P_3 P_3 v^{i_4 i_7}_{i_8 a_1} (\xi_{13})^{i_5 i_6 i_8}_{i_7 a_2 a_3} \\
&\quad + P_3 v^{i_7 a_8}_{a_1 a_2} (\xi_{14})^{i_4 i_5 i_6}_{i_7 a_3 a_8} + \tfrac{1}{2} P_3 v^{i_7 i_8}_{a_1 a_2} (\xi_{15})^{i_4 i_5 i_6}_{i_7 i_8 a_3} \\
&\quad + P_3 P_3 v^{i_4 i_5}_{a_1 a_7} (\xi_{16})^{i_6 a_7}_{a_2 a_3} + P_3 P_3 v^{i_4 i_5}_{a'_7 a_1} (\xi_{17})^{i_6 a'_7}_{a_2 a_3} \\
&\quad + \tfrac{1}{2} P_3 \lambda^{i_4 i_5 i_7 i_8}_{a_1 a_2 a_3 a_9} (\xi_{18})^{i_6 a_9}_{i_7 i_8} + \tfrac{1}{2} P_3 \lambda^{i_4 i_5 i_6 i_7}_{a_1 a_2 a_8 a_9} (\xi_{19})^{a_8 a_9}_{i_7 a_3} \\
&\quad + P_3 v^{i_7 a_8}_{i_9 a_1} (\Xi_{10})^{i_4 i_5 i_6 i_9}_{i_7 a_2 a_3 a_8} + \tfrac{1}{2} P_3 v^{i_7 i_8}_{i_9 a_1} (\Xi_{14})^{i_4 i_5 i_6 i_9}_{i_7 i_8 a_2 a_3} \\
&\quad - P_3 v^{i_4 i_5}_{i_7 a_8} (\Xi_{11})^{i_6 i_7 a_8}_{a_1 a_2 a_3} - P_3 P_3 v^{i_4 a_7}_{a_1 a_8} (\Xi_{11})^{i_5 i_6 a_8}_{a_2 a_3 a_7} \\
&\quad + \tfrac{1}{6} P_3 \lambda^{i_4 i_7 i_8 i_9}_{a_1 a_2 a_3 a_{10}} (\xi_{24})^{i_5 i_6 a_{10}}_{i_7 i_8 i_9} + P_3 P_3 v^{i_4 a_7}_{a'_8 a_1} (\xi_{25})^{i_5 i_6 a'_8}_{a_2 a_3 a_7} \\
&\quad + \tfrac{1}{2} P_3 v^{i_7 i_8}_{a_1 a_9} (\xi_{26})^{i_4 i_5 i_6 a_9}_{i_7 i_8 a_2 a_3} + \tfrac{1}{2} P_3 v^{i_4 i_5}_{a_7 a_8} (\xi_{27})^{i_6 a_7 a_8}_{a_1 a_2 a_3} \\
&\quad + P_3 P_3 v^{i_4 i_7}_{a_1 a_8} (\xi_{28})^{i_5 i_6 a_8}_{i_7 a_2 a_3} + P_3 P_3 v^{i_4 i_7}_{a'_8 a_1} (\xi_{29})^{i_5 i_6 a'_8}_{i_7 a_2 a_3}
\end{aligned}
$$

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TABLE ESI.4.XXVII: The computational sequence and intermediates for the geminal λ amplitude equation of Λ-CCSDTQ-R12 [Part I]

$$(\Xi_0)^{i_7 a_6}_{i_1 i_2} = +F^{a'_8 a_6}_{i_1 i_2} f^{i_7}_{a'_8}$$
$$(\Xi_1)^{i_7 a'_5}_{i_1 i_2} = +\lambda^{i_7}_{a_8} F^{a'_5 a_8}_{i_1 i_2}$$
$$(\Xi_2)^{i_7}_{a'_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_3)^{i_4 i_8}_{i_6 i_7} = +\tfrac{1}{2}\lambda^{i_4 i_8}_{i_9 i_{10}} X^{i_9 i_{10}}_{i_6 i_7}$$
$$(\Xi_4)^{i_3 i_4}_{i_5 a'_6} = +t^{a_7}_{i_5} \tilde{\lambda}^{i_3 i_4}_{a'_6 a_7}$$
$$(\Xi_5)^{a_6}_{a'_7} = +t^{a_8}_{i_9} v^{i_9 a_6}_{a'_7 a_8}$$
$$(\Xi_6)^{i_3 i_4}_{i_6 a_7} = +t^{a_8}_{i_6} \lambda^{i_3 i_4}_{a_7 a_8}$$
$$(\Xi_7)^{i_9 a_8}_{i_5 a'_{10}} = +t^{a_{11}}_{i_5} v^{i_9 a_8}_{a'_{10} a_{11}}$$
$$(\Xi_8)^{a'_7}_{a'_5} = +t^{a_8}_{i_9} v^{i_9 a'_7}_{a'_5 a_8}$$
$$(\Xi_9)^{i_4 a'_8}_{i_7 a'_5} = +t^{a_9}_{i_7} v^{i_4 a'_8}_{a'_5 a_9}$$
$$(\Xi_{10})^{a_6}_{a'_7} = +\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\Xi_{11})^{a_6}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{12})^{i_7}_{a'_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_{13})^{i_4 i_9}_{i_7 a_6} = +t^{a_{10}}_{i_7} v^{i_4 i_9}_{a_6 a_{10}}$$
$$(\Xi_{14})^{a_6}_{a'_7} = +\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\Xi_{15})^{a'_7}_{a'_5} = +\tfrac{1}{2} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_5 a'_8}$$
$$(\Xi_{16})^{a'_7}_{a'_5} = +\tfrac{1}{2} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_5 a_8}$$
$$(\Xi_{17})^{i_9 a_8}_{i_5 a'_{10}} = +\tilde{t}^{a'_{11} a_8}_{i_5 i_{12}} v^{i_9 i_{12}}_{a'_{10} a'_{11}}$$
$$(\Xi_{18})^{i_4 a_8}_{i_7 a'_5} = +\tilde{t}^{a'_9 a_8}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_5 a'_9}$$
$$(\Xi_{19})^{a'_5}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_5 a'_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{20})^{a'_5}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_5 a_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\Xi_{21})^{a_6}_{a'_7} = +\tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{22})^{i_3 i_4}_{i_6 a_7} = +\tfrac{1}{2} t^{a_8 a_9}_{i_6 i_{10}} \lambda^{i_3 i_4 i_{10}}_{a_7 a_8 a_9}$$
$$(\Xi_{23})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9} = +f^{a_{12}}_{i_7} \lambda^{i_4 i_{10} i_{11}}_{a_6 a_9 a_{12}}$$
$$(\Xi_{24})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} = +\tfrac{1}{2} t^{a_{11} a_{12}}_{i_7 i_8} \lambda^{i_3 i_4 i_{10}}_{a_6 a_{11} a_{12}}$$
$$(\Xi_{25})^{i_3 i_4}_{i_6 a_7} = +\tfrac{1}{12} t^{a_8 a_9 a_{10}}_{i_6 i_{11} i_{12}} \lambda^{i_3 i_4 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}}$$
$$(\Xi_{26})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9} = +\tfrac{1}{2} t^{a_{12} a_{13}}_{i_7 i_{14}} \lambda^{i_4 i_{10} i_{11} i_{14}}_{a_6 a_9 a_{12} a_{13}}$$
$$(\Xi_{27})^{i_3 i_4 a_9}_{a_6 a_{10} a_{11}} = +\tfrac{1}{2} t^{a_9 a_{12}}_{i_{13} i_{14}} \lambda^{i_3 i_4 i_{13} i_{14}}_{a_6 a_{10} a_{11} a_{12}}$$
$$(\Xi_{28})^{i_4 i_{11} i_{12} i_{13}}_{i_7 a_6 a_9 a_{10}} = +t^{a_{14}}_{i_7} \lambda^{i_4 i_{11} i_{12} i_{13}}_{a_6 a_9 a_{10} a_{14}}$$
$$(\Xi_{29})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} = +\tfrac{1}{6} t^{a_{11} a_{12} a_{13}}_{i_7 i_8 i_{14}} \lambda^{i_3 i_4 i_{10} i_{14}}_{a_6 a_{11} a_{12} a_{13}}$$
$$(\Xi_{30})^{i_7 a_6}_{i_1 i_2} = +F^{a'_8 a_6}_{i_1 i_2} (\Xi_2)^{i_7}_{a'_8}$$
$$(\Xi_{31})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} = +P_2 t^{a_{11}}_{i_7} (\Xi_{23})^{i_3 i_4 i_{10}}_{i_8 a_6 a_{11}}$$
$$(\Xi_{32})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} = +P_2 t^{a_{11}}_{i_7} (\Xi_{26})^{i_3 i_4 i_{10}}_{i_8 a_6 a_{11}}$$
$$(\Xi_{33})^{i_3 i_4 i_{11} i_{12}}_{i_7 i_8 a_6 a_{10}} = +P_2 t^{a_{13}}_{i_7} (\Xi_{28})^{i_3 i_4 i_{11} i_{12}}_{i_8 a_6 a_{10} a_{13}}$$
$$(\xi_{9,8})^{a_7}_{a_6} = -t^{a_8}_{i_9} v^{i_9 a_7}_{a_6 a_8} - \tfrac{1}{2} t^{a_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_7}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\xi_{9,7})^{a'_7}_{a_6} = -t^{a_8}_{i_9} v^{i_9 a'_7}_{a_6 a_8} + \tfrac{1}{2} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6} - \tfrac{1}{2} \tilde{t}^{a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8}$$
$$(\xi_{9,6})^{a'_7}_{a'_5} = -(\Xi_8)^{a'_7}_{a'_5} - (\Xi_{15})^{a'_7}_{a'_5} - (\Xi_{16})^{a'_7}_{a'_5}$$
$$(\xi_{9,5})^{i_4 i_8}_{i_7 a_6} = +(\Xi_6)^{i_4 i_8}_{i_7 a_6} + (\Xi_{22})^{i_4 i_8}_{i_7 a_6} + (\Xi_{25})^{i_4 i_8}_{i_7 a_6}$$
$$(\xi_{9,4})^{i_4 a_8}_{i_7 a_6} = -v^{i_4 a_8}_{i_7 a_6} + t^{a_9}_{i_7} v^{i_4 a_8}_{a_6 a_9} - t^{a_8}_{i_9} (\Xi_{13})^{i_4 i_9}_{i_7 a_6} + t^{a_8 a_9}_{i_7 i_{10}} v^{i_4 i_{10}}_{a_6 a_9} + \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} v^{i_4 i_{10}}_{a'_9 a_6}$$
$$(\xi_{9,3})^{i_4 a'_8}_{i_7 a_6} = -v^{i_4 a'_8}_{i_7 a_6} + t^{a_9}_{i_7} v^{i_4 a'_8}_{a_6 a_9} - \tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} v^{i_4 i_{10}}_{a'_9 a_6}$$
$$(\xi_{9,27,0})^{i_3 i_4 i_{11} i_{12}}_{i_7 i_8 a_6 a_{10}} = -\tfrac{1}{2} (\Xi_{33})^{i_3 i_4 i_{11} i_{12}}_{i_7 i_8 a_6 a_{10}} - \tfrac{1}{2} t^{a_{13} a_{14}}_{i_7 i_8} \lambda^{i_3 i_4 i_{11} i_{12}}_{a_6 a_{10} a_{13} a_{14}}$$
$$(\xi_{9,27})^{i_3 i_4 a'_9}_{i_7 i_8 a_6} = +\tfrac{1}{2} \tilde{t}^{a'_9 a_{10}}_{i_{11} i_{12}} (\xi_{9,27,0})^{i_3 i_4 i_{11} i_{12}}_{i_7 i_8 a_6 a_{10}} + P_2 \tilde{t}^{a'_9 a_{10}}_{i_7 i_{11}} (\Xi_{26})^{i_3 i_4 i_{11}}_{i_8 a_6 a_{10}}$$

$$(\xi_{9,26})^{a_9 a_{10} a_{11}}_{i_7 i_8 a'_5} = +P_3 t^{a_9 a_{10} a_{12}}_{i_7 i_8 i_{13}} v^{i_{13} a_{11}}_{a'_5 a_{12}} + \tfrac{1}{2} t^{a_9 a_{10} a_{11} a_{12}}_{i_7 i_8 i_{13} i_{14}} v^{i_{13} i_{14}}_{a'_5 a_{12}}$$
$$(\xi_{9,25})^{i_3 i_4 a'_9}_{i_7 a_6 a_8} = +\tfrac{1}{2} \tilde{t}^{a'_9 a_{10}}_{i_{11} i_{12}} (\Xi_{28})^{i_3 i_4 i_{11} i_{12}}_{i_7 a_6 a_8 a_{10}}$$
$$(\xi_{9,24})^{i_3 i_4 a_9}_{i_7 a_6 a_8} = +\tfrac{1}{2} t^{a_9 a_{10}}_{i_{11} i_{12}} (\Xi_{28})^{i_3 i_4 i_{11} i_{12}}_{i_7 a_6 a_8 a_{10}} - t^{a_9}_{i_{10}} (\Xi_{26})^{i_3 i_4 i_{10}}_{i_7 a_6 a_8}$$
$$(\xi_{9,23})^{i_3 i_4 a'_9}_{a_6 a_7 a_8} = -\tfrac{1}{2} \lambda^{i_3 i_4 i_{10} i_{11}}_{a_6 a_7 a_8 a_{12}} \tilde{t}^{a'_9 a_{12}}_{i_{10} i_{11}}$$
$$(\xi_{9,21,2})^{i_3 i_4}_{i_8 a_6} = -(\Xi_{22})^{i_3 i_4}_{i_8 a_6} - (\Xi_{25})^{i_3 i_4}_{i_8 a_6}$$
$$(\xi_{9,21,1})^{i_3 i_4 i_{11}}_{i_8 a_6 a_{10}} = +(\Xi_{23})^{i_3 i_4 i_{11}}_{i_8 a_6 a_{10}} + (\Xi_{26})^{i_3 i_4 i_{11}}_{i_8 a_6 a_{10}}$$
$$(\xi_{9,21,0})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} = -\tfrac{1}{2} (\Xi_{31})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} - (\Xi_{24})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} - (\Xi_{32})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} - (\Xi_{29})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6}$$
$$\begin{aligned}(\xi_{9,21})^{i_3 i_4 a_9}_{i_7 i_8 a_6} &= +t^{a_9}_{i_{10}} (\xi_{9,21,0})^{i_3 i_4 i_{10}}_{i_7 i_8 a_6} + P_2 t^{a_9 a_{10}}_{i_7 i_{11}} (\xi_{9,21,1})^{i_3 i_4 i_{11}}_{i_8 a_6 a_{10}} \\ &\quad + P_2 t^{a_9}_{i_7} (\xi_{9,21,2})^{i_3 i_4}_{i_8 a_6} - \tfrac{1}{4} t^{a_9 a_{10}}_{i_{11} i_{12}} (\Xi_{33})^{i_3 i_4 i_{11} i_{12}}_{i_7 i_8 a_6 a_{10}} \\ &\quad - \tfrac{1}{4} P_2 t^{a_9 a_{10} a_{11}}_{i_7 i_{12} i_{13}} (\Xi_{28})^{i_3 i_4 i_{12} i_{13}}_{i_8 a_6 a_{10} a_{11}} - \tfrac{1}{2} t^{a_{10} a_{11}}_{i_7 i_8} (\Xi_{27})^{i_3 i_4 a_9}_{a_6 a_{10} a_{11}}\end{aligned}$$
$$(\xi_{9,20})^{i_4 a'_8}_{a_6 a_7} = +\tfrac{1}{2} \lambda^{i_4 i_9 i_{10}}_{a_6 a_7 a_{11}} \tilde{t}^{a'_8 a_{11}}_{i_9 i_{10}}$$
$$(\xi_{9,2})^{i_4 a'_8}_{i_7 a'_5} = -v^{i_4 a'_8}_{i_7 a'_5} + (\Xi_9)^{i_4 a'_8}_{i_7 a'_5}$$
$$(\xi_{9,19})^{i_4 a_8}_{a_6 a_7} = +\tfrac{1}{2} t^{a_8 a_9}_{i_{10} i_{11}} \lambda^{i_4 i_{10} i_{11}}_{a_6 a_7 a_9} + \tfrac{1}{12} t^{a_8 a_9 a_{10}}_{i_{11} i_{12} i_{13}} \lambda^{i_4 i_{11} i_{12} i_{13}}_{a_6 a_7 a_9 a_{10}}$$
$$(\xi_{9,18})^{i_3 i_4 i_9}_{i_7 i_8 a_6} = +(\Xi_{24})^{i_3 i_4 i_9}_{i_7 i_8 a_6} + (\Xi_{29})^{i_3 i_4 i_9}_{i_7 i_8 a_6}$$
$$(\xi_{9,17})^{i_3 i_4 i_9}_{i_7 i_8 a_6} = +\tfrac{1}{2} (\Xi_{31})^{i_3 i_4 i_9}_{i_7 i_8 a_6} + (\Xi_{32})^{i_3 i_4 i_9}_{i_7 i_8 a_6}$$
$$(\xi_{9,16})^{i_3 i_4 i_9}_{i_7 a_6 a_8} = +(\Xi_{23})^{i_3 i_4 i_9}_{i_7 a_6 a_8} + (\Xi_{26})^{i_3 i_4 i_9}_{i_7 a_6 a_8}$$
$$\begin{aligned}(\xi_{9,15})^{a_8 a_9}_{i_7 a'_5} &= +v^{a_8 a_9}_{i_7 a'_5} - t^{a_{10}}_{i_7} v^{a_8 a_9}_{a'_5 a_{10}} - P_2 t^{a_8 a_{10}}_{i_7 i_{11}} v^{i_{11} a_9}_{a'_5 a_{10}} + P_2 \tilde{t}^{a'_{10} a_8}_{i_7 i_{11}} v^{i_{11} a_9}_{a'_5 a'_{10}} \\ &\quad - \tfrac{1}{2} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} v^{i_{11} i_{12}}_{a'_5 a_{10}}\end{aligned}$$
$$(\xi_{9,14})^{i_3 i_4}_{i_7 a_6} = +(\Xi_{22})^{i_3 i_4}_{i_7 a_6} + (\Xi_{25})^{i_3 i_4}_{i_7 a_6}$$
$$(\xi_{9,12})^{a'_7}_{a_6} = -\tfrac{1}{2} \lambda^{i_8 i_9}_{a_6 a_{10}} \tilde{t}^{a'_7 a_{10}}_{i_8 i_9} + \tfrac{1}{2} \tilde{t}^{a'_7 a'_8}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\xi_{9,11,2})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9} = +(\Xi_{23})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9} + (\Xi_{26})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9}$$
$$(\xi_{9,11})^{i_4 a'_8}_{i_7 a_6} = +\lambda^{i_4 i_9}_{a_6 a_{10}} \tilde{t}^{a'_8 a_{10}}_{i_7 i_9} - \tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_9 a_6} + \tfrac{1}{2} \tilde{t}^{a'_8 a_9}_{i_{10} i_{11}} (\xi_{9,11,2})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9}$$
$$(\xi_{9,10,3})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9} = +(\Xi_{23})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9} + (\Xi_{26})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9}$$
$$(\xi_{9,10,0})^{i_4 i_9}_{i_7 a_6} = -(\Xi_6)^{i_4 i_9}_{i_7 a_6} - (\Xi_{22})^{i_4 i_9}_{i_7 a_6} - (\Xi_{25})^{i_4 i_9}_{i_7 a_6}$$
$$\begin{aligned}(\xi_{9,10})^{i_4 a_8}_{i_7 a_6} &= +t^{a_8}_{i_9} (\xi_{9,10,0})^{i_4 i_9}_{i_7 a_6} + t^{a_8 a_9}_{i_7 i_{10}} \lambda^{i_4 i_{10}}_{a_6 a_9} + \tilde{t}^{a'_9 a_8}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_9 a_6} + \tfrac{1}{2} t^{a_8 a_9}_{i_{10} i_{11}} (\xi_{9,10,3})^{i_4 i_{10} i_{11}}_{i_7 a_6 a_9} \\ &\quad + \tfrac{1}{4} t^{a_8 a_9 a_{10}}_{i_7 i_{11} i_{12}} \lambda^{i_4 i_{11} i_{12}}_{a_6 a_9 a_{10}} - \tfrac{1}{12} t^{a_8 a_9 a_{10}}_{i_{11} i_{12} i_{13}} (\Xi_{28})^{i_4 i_{11} i_{12} i_{13}}_{i_7 a_6 a_9 a_{10}} \\ &\quad + \tfrac{1}{36} t^{a_8 a_9 a_{10} a_{11}}_{i_7 i_{12} i_{13} i_{14}} \lambda^{i_4 i_{12} i_{13} i_{14}}_{a_6 a_9 a_{10} a_{11}}\end{aligned}$$
$$(\xi_{9,1})^{i_4 a_8}_{i_7 a'_5} = +v^{i_4 a_8}_{i_7 a'_5} - (\Xi_7)^{i_4 a_8}_{i_7 a'_5}$$
$$\begin{aligned}(\xi_9)^{i_3 i_4}_{a'_5 a_6} &= -f^{i_7}_{a_6} (\Xi_4)^{i_3 i_4}_{i_7 a'_5} + P_2 \lambda^{i_3 i_7}_{a_6 a_8} (\xi_{9,1})^{i_4 a_8}_{i_7 a'_5} + P_2 \tilde{\lambda}^{i_3 i_7}_{a'_8 a_6} (\xi_{9,2})^{i_4 a'_8}_{i_7 a'_5} \\ &\quad + P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} (\xi_{9,3})^{i_4 a'_8}_{i_7 a_6} + P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} (\xi_{9,4})^{i_4 a_8}_{i_7 a_6} + P_2 v^{i_3 i_7}_{i_8 a'_5} (\xi_{9,5})^{i_4 i_8}_{i_7 a_6} \\ &\quad + \tilde{\lambda}^{i_3 i_4}_{a'_7 a_6} (\xi_{9,6})^{a'_7}_{a'_5} + \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_7} (\xi_{9,7})^{a'_7}_{a_6} + \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_7} (\xi_{9,8})^{a_7}_{a_6} - P_2 v^{i_3 i_7}_{i_8 a_6} (\Xi_4)^{i_4 i_8}_{i_7 a'_5} \\ &\quad + P_2 v^{i_3 i_7}_{a'_5 a_8} (\xi_{9,10})^{i_4 a_8}_{i_7 a_6} + P_2 v^{i_3 i_7}_{a'_5 a'_8} (\xi_{9,11})^{i_4 a'_8}_{i_7 a_6} + v^{i_3 i_4}_{a'_5 a_7} (\xi_{9,12})^{a'_7}_{a_6} \\ &\quad + P_2 v^{i_3 i_7}_{a_6 a_8} (\Xi_{18})^{i_4 a_8}_{i_7 a'_5} + f^{i_7}_{a'_5} (\xi_{9,14})^{i_3 i_4}_{i_7 a_6} + \tfrac{1}{2} \lambda^{i_3 i_4 i_7}_{a_6 a_8 a_9} (\xi_{9,15})^{a_8 a_9}_{i_7 a'_5} \\ &\quad + v^{i_7 a_8}_{i_9 a'_5} (\xi_{9,16})^{i_3 i_4 i_9}_{i_7 a_6 a_8} + v^{i_7 i_8}_{i_9 a'_5} (\xi_{9,17})^{i_3 i_4 i_9}_{i_7 i_8 a_6} + \tfrac{1}{2} v^{i_7 i_8}_{i_9 a'_5} (\xi_{9,18})^{i_3 i_4 i_9}_{i_7 i_8 a_6} \\ &\quad + P_2 v^{i_3 a_7}_{a'_5 a_8} (\xi_{9,19})^{i_4 a_8}_{a_6 a_7} + P_2 v^{i_3 a_7}_{a'_5 a'_8} (\xi_{9,20})^{i_4 a'_8}_{a_6 a_7} + \tfrac{1}{2} v^{i_7 i_8}_{a'_5 a_9} (\xi_{9,21})^{i_3 i_4 a_9}_{i_7 i_8 a_6} \\ &\quad - \tfrac{1}{2} v^{a_7 a_8}_{a'_5 a_9} (\Xi_{27})^{i_3 i_4 a_9}_{a_6 a_7 a_8} + \tfrac{1}{2} v^{a_7 a_8}_{a'_5 a_9} (\xi_{9,23})^{i_3 i_4 a'_9}_{a_6 a_7 a_8} + v^{i_7 a_8}_{a'_5 a_9} (\xi_{9,24})^{i_3 i_4 a_9}_{i_7 a_6 a_8} \\ &\quad + v^{i_7 a_8}_{a'_5 a'_9} (\xi_{9,25})^{i_3 i_4 a'_9}_{i_7 a_6 a_8} + \tfrac{1}{12} \lambda^{i_3 i_4 i_7 i_8}_{a_6 a_9 a_{10} a_{11}} (\xi_{9,26})^{a_9 a_{10} a_{11}}_{i_7 i_8 a'_5} \\ &\quad + \tfrac{1}{2} v^{i_7 i_8}_{a'_5 a'_9} (\xi_{9,27})^{i_3 i_4 a'_9}_{i_7 i_8 a_6}\end{aligned}$$
$$(\xi_{8,1})^{a_6}_{a'_7} = -(\Xi_5)^{a_6}_{a'_7} - (\Xi_{10})^{a_6}_{a'_7} + (\Xi_{11})^{a_6}_{a'_7}$$
$$(\xi_{8,0,0})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - (\Xi_2)^{i_7}_{a'_8}$$
$$(\xi_{8,0})^{i_7 a'_5}_{i_1 i_2} = +F^{a'_5 a'_8}_{i_1 i_2} (\xi_{8,0,0})^{i_7}_{a'_8} - F^{a'_5 a_8}_{i_1 i_2} (\Xi_{12})^{i_7}_{a_8}$$
$$(\xi_8)^{a'_5 a_6}_{i_1 i_2} = +t^{a_6}_{i_7} (\xi_{8,0})^{i_7 a'_5}_{i_1 i_2} + F^{a'_5 a'_7}_{i_1 i_2} (\xi_{8,1})^{a_6}_{a'_7}$$

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TABLE ESI.4.XXVIII: The computational sequence and intermediates for the geminal λ amplitude equation of Λ-CCSDTQ-R12 [Part II]

$$
\begin{aligned}
(\xi_{7,1,0})^{i_3 i_4}_{i_8 a_9} &= -v^{i_3 i_4}_{i_8 a_9} + \tfrac{1}{2}(\Xi_{13})^{i_3 i_4}_{i_8 a_9} \\
(\xi_{7,1})^{i_3 i_4}_{i_7 i_8} &= +P_2 t^{a_9}_{i_7} (\xi_{7,1,0})^{i_3 i_4}_{i_8 a_9} + \tfrac{1}{2} t^{a_9 a_{10}}_{i_7 i_8} v^{i_3 i_4}_{a_9 a_{10}} \\
(\xi_{7,0,0})^{i_4}_{a_8} &= -f^{i_4}_{a_8} - (\Xi_{12})^{i_4}_{a_8} \\
(\xi_{7,0})^{i_4}_{i_7} &= +t^{a_8}_{i_7} (\xi_{7,0,0})^{i_4}_{a_8} - t^{a_8 a_9}_{i_9 i_7} v^{i_4 i_9}_{i_7 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_7 i_{10}} v^{i_4 i_{10}}_{a_8 a_9} - \tfrac{1}{2} t^{i_8 i_9}_{i_7 i_{10}} V^{i_4 i_{10}}_{i_8 i_9} \\
(\xi_7)^{i_3 i_4}_{i_5 i_6} &= +P_2 \lambda^{i_3 i_7}_{i_5 i_6} (\xi_{7,0})^{i_4}_{i_7} + \tfrac{1}{2} \lambda^{i_7 i_8}_{i_5 i_6} (\xi_{7,1})^{i_3 i_4}_{i_7 i_8} \\
(\xi_6)^{i_5 i_6}_{i_1 i_2} &= +B^{i_5 i_6}_{i_1 i_2} + P^{i_5 i_6}_{i_1 i_2} \\
(\xi_{4,1})^{i_7 a_6}_{i_1 i_2} &= -(\Xi_0)^{i_7 a_6}_{i_1 i_2} - (\Xi_{30})^{i_7 a_6}_{i_1 i_2} \\
(\xi_{4,0})^{a_6}_{a'_7} &= -f^{a_6}_{a'_7} + (\Xi_5)^{a_6}_{a'_7} + (\Xi_{10})^{a_6}_{a'_7} - (\Xi_{11})^{a_6}_{a'_7} \\
(\xi_4)^{a_5 a_6}_{i_1 i_2} &= +V^{a_5 a_6}_{i_1 i_2} + P_2 F^{a'_7 a_5}_{i_1 i_2} (\xi_{4,0})^{a_6}_{a'_7} + P_2 t^{a_5}_{i_7} (\xi_{4,1})^{i_7 a_6}_{i_1 i_2} \\
(\xi_3)^{i_4}_{i_5} &= -t^{a_6}_{i_5} \lambda^{i_4}_{a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_5 i_8} \lambda^{i_4 i_8}_{a_6 a_7} \\
&\quad - \tfrac{1}{2} t^{i_6 i_7}_{i_5 i_8} (\Xi_3)^{i_4 i_8}_{i_6 i_7} - \tfrac{1}{12} t^{a_6 a_7 a_8}_{i_5 i_9 i_{10}} \lambda^{i_4 i_9 i_{10}}_{a_6 a_7 a_8} \\
&\quad - \tfrac{1}{144} t^{a_6 a_7 a_8 a_9}_{i_5 i_{10} i_{11} i_{12}} \lambda^{i_4 i_{10} i_{11} i_{12}}_{a_6 a_7 a_8 a_9} \\
(\xi_{2,3})^{a'_5}_{a'_7} &= -(\Xi_{19})^{a'_5}_{a'_7} - (\Xi_{20})^{a'_5}_{a'_7} \\
(\xi_{2,2})^{a_6}_{a'_7} &= -(\Xi_{14})^{a_6}_{a'_7} + (\Xi_{21})^{a_6}_{a'_7} \\
(\xi_{2,1})^{a_6}_{a'_7} &= -\tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} \lambda^{i_9 i_{10}}_{a_7 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} \tilde{\lambda}^{i_9 i_{10}}_{a'_8 a_7} - \tfrac{1}{12} t^{a_6 a_8 a_9}_{i_{10} i_{11} i_{12}} \lambda^{i_{10} i_{11} i_{12}}_{a_7 a_8 a_9} \\
&\quad - \tfrac{1}{144} t^{a_6 a_8 a_9 a_{10}}_{i_{11} i_{12} i_{13} i_{14}} \lambda^{i_{11} i_{12} i_{13} i_{14}}_{a_7 a_8 a_9 a_{10}} \\
(\xi_2)^{a'_5 a_6}_{i_1 i_2} &= -t^{a_6}_{i_7} (\Xi_1)^{i_7 a'_5}_{i_1 i_2} + F^{a'_5 a_7}_{i_1 i_2} (\xi_{2,1})^{a_6}_{a_7} + F^{a'_5 a_7}_{i_1 i_2} (\xi_{2,2})^{a_6}_{a'_7} + F^{a'_7 a_6}_{i_1 i_2} (\xi_{2,3})^{a'_5}_{a'_7} \\
(\xi_{18,0,0})^{i_9 a_8}_{i_5 a'_{10}} &= -(\Xi_7)^{i_9 a_8}_{i_5 a'_{10}} + (\Xi_{17})^{i_9 a_8}_{i_5 a'_{10}} \\
(\xi_{18,0})^{i_9 a_7 a_8}_{i_1 i_2 i_5} &= +P_2 F^{a'_{10} a_7}_{i_1 i_2} (\xi_{18,0,0})^{i_9 a_8}_{i_5 a'_{10}} \\
(\xi_{18})^{a_6 a_7 a_8}_{i_1 i_2 i_5} &= +P_3 t^{a_6}_{i_9} (\xi_{18,0})^{i_9 a_7 a_8}_{i_1 i_2 i_5} \\
(\xi_{17,0})^{a'_6}_{a'_7} &= -(\Xi_{19})^{a'_6}_{a'_7} - (\Xi_{20})^{a'_6}_{a'_7} \\
(\xi_{17})^{a'_5 a'_6}_{i_1 i_2} &= +P_2 F^{a'_5 a'_7}_{i_1 i_2} (\xi_{17,0})^{a'_6}_{a'_7} \\
(\xi_{16})^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} t^{i_5 i_6}_{i_7 i_8} (\Xi_3)^{i_7 i_8}_{i_1 i_2} \\
(\xi_{15,0})^{a_6}_{a'_7} &= +(\Xi_{14})^{a_6}_{a'_7} - (\Xi_{21})^{a_6}_{a'_7} \\
(\xi_{15})^{a_5 a_6}_{i_1 i_2} &= +P_2 F^{a'_7 a_5}_{i_1 i_2} (\xi_{15,0})^{a_6}_{a'_7} \\
(\xi_{14,0})^{i_3 i_4}_{i_6 a_7} &= +\tfrac{1}{2} (\Xi_6)^{i_3 i_4}_{i_6 a_7} + (\Xi_{22})^{i_3 i_4}_{i_6 a_7} + (\Xi_{25})^{i_3 i_4}_{i_6 a_7} \\
(\xi_{14})^{i_3 i_4}_{i_5 i_6} &= +P_2 t^{a_7}_{i_5} (\xi_{14,0})^{i_3 i_4}_{i_6 a_7} + \tfrac{1}{2} t^{a_7 a_8}_{i_5 i_6} \lambda^{i_3 i_4}_{a_7 a_8} + \tfrac{1}{2} t^{i_7 i_8}_{i_5 i_6} (\Xi_3)^{i_3 i_4}_{i_7 i_8} + \tfrac{1}{6} t^{a_7 a_8 a_9}_{i_5 i_6 i_{10}} \lambda^{i_3 i_4 i_{10}}_{a_7 a_8 a_9} \\
&\quad - \tfrac{1}{4} P_2 t^{a_7 a_8}_{i_5 i_9} (\Xi_{26})^{i_3 i_4 i_9}_{i_6 a_7 a_8} + \tfrac{1}{48} t^{a_7 a_8 a_9 a_{10}}_{i_5 i_6 i_{11} i_{12}} \lambda^{i_3 i_4 i_{11} i_{12}}_{a_7 a_8 a_9 a_{10}} \\
(\xi_{12})^{i_3 i_4}_{i_5 a_6} &= +(\Xi_6)^{i_3 i_4}_{i_5 a_6} + (\Xi_{22})^{i_3 i_4}_{i_5 a_6} + (\Xi_{25})^{i_3 i_4}_{i_5 a_6} \\
(\xi_{11,5})^{i_4 a'_8}_{i_7 a'_6} &= +\tilde{t}^{a'_8 a'_9}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_6 a'_9} \\
(\xi_{11,4})^{i_4 a_8}_{i_7 a'_6} &= -(\Xi_{18})^{i_4 a_8}_{i_7 a'_6} + t^{a_8 a_9}_{i_7 i_{10}} \tilde{\lambda}^{i_4 i_{10}}_{a'_6 a_9} \\
(\xi_{11,2})^{a'_7}_{a'_6} &= -(\Xi_8)^{a'_7}_{a'_6} - (\Xi_{15})^{a'_7}_{a'_6} - (\Xi_{16})^{a'_7}_{a'_6} \\
(\xi_{11,1,0})^{i_4 i_9}_{i_7 a'_6} &= -t^{a_{10}}_{i_7} v^{i_4 i_9}_{a'_6 a_{10}} \\
(\xi_{11,1})^{i_4 a_8}_{i_7 a'_6} &= -v^{i_4 a_8}_{i_7 a'_6} + (\Xi_7)^{i_4 a_8}_{i_7 a'_6} - (\Xi_{17})^{i_4 a_8}_{i_7 a'_6} + t^{a_8}_{i_9} (\xi_{11,1,0})^{i_4 i_9}_{i_7 a'_6} \\
(\xi_{11,0})^{i_4 a'_8}_{i_7 a'_6} &= -v^{i_4 a'_8}_{i_7 a'_6} + (\Xi_9)^{i_4 a'_8}_{i_7 a'_6} \\
(\xi_{11})^{i_3 i_4}_{a'_5 a'_6} &= +P_2 P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a'_8} (\xi_{11,0})^{i_4 a'_8}_{i_7 a'_6} + P_2 P_2 \tilde{\lambda}^{i_3 i_7}_{a'_5 a_8} (\xi_{11,1})^{i_4 a_8}_{i_7 a'_6} \\
&\quad + P_2 \tilde{\lambda}^{i_3 i_4}_{a'_5 a'_7} (\xi_{11,2})^{a'_7}_{a'_6} + P_2 P_2 v^{i_3 i_7}_{i_8 a'_5} (\Xi_4)^{i_4 i_8}_{i_7 a'_6} \\
&\quad + P_2 P_2 v^{i_3 i_7}_{a'_5 a_8} (\xi_{11,4})^{i_4 a_8}_{i_7 a'_6} + P_2 P_2 v^{i_3 i_7}_{a'_5 a'_8} (\xi_{11,5})^{i_4 a'_8}_{i_7 a'_6} \\
(\xi_0)^{i_4 a_5}_{i_1 i_2} &= -(\Xi_0)^{i_4 a_5}_{i_1 i_2} - V^{i_4 a_5}_{i_1 i_2} - (\Xi_{30})^{i_4 a_5}_{i_1 i_2} \\
\delta^{i_3 i_4}_{i_1 i_2} &= +V^{i_3 i_4}_{i_1 i_2} + P_2 \lambda^{i_3}_{a_5} (\xi_0)^{i_4 a_5}_{i_1 i_2} + v^{i_3 i_4}_{i_5 a'_6} (\Xi_1)^{i_5 a'_6}_{i_1 i_2} + v^{i_3 i_4}_{a'_5 a_6} (\xi_2)^{a'_5 a_6}_{i_1 i_2} \\
&\quad + P_2 V^{i_3 i_5}_{i_1 i_2} (\xi_3)^{i_4}_{i_5} + \tfrac{1}{2} \lambda^{i_3 i_4}_{a_5 a_6} (\xi_4)^{a_5 a_6}_{i_1 i_2} + P_2 f^{i_3}_{i_5} (\Xi_3)^{i_4 i_5}_{i_1 i_2} + \tfrac{1}{2} \lambda^{i_3 i_4}_{i_5 i_6} (\xi_6)^{i_5 i_6}_{i_1 i_2} \\
&\quad + \tfrac{1}{2} X^{i_5 i_6}_{i_1 i_2} (\xi_7)^{i_3 i_4}_{i_5 i_6} + \tilde{\lambda}^{i_3 i_4}_{a'_5 a_6} (\xi_8)^{a'_5 a_6}_{i_1 i_2} + F^{a'_5 a_6}_{i_1 i_2} (\xi_9)^{i_3 i_4}_{a'_5 a_6} + \tfrac{1}{2} v^{i_3 i_4}_{i_5 i_6} (\Xi_3)^{i_5 i_6}_{i_1 i_2} \\
&\quad + \tfrac{1}{2} F^{a'_5 a'_6}_{i_1 i_2} (\xi_{11})^{i_3 i_4}_{a'_5 a'_6} + V^{i_5 a_6}_{i_1 i_2} (\xi_{12})^{i_3 i_4}_{i_5 a_6} + V^{i_5 a'_6}_{i_1 i_2} (\Xi_4)^{i_3 i_4}_{i_5 a'_6} \\
&\quad + \tfrac{1}{2} V^{i_5 i_6}_{i_1 i_2} (\xi_{14})^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{2} v^{i_3 i_4}_{a_5 a_6} (\xi_{15})^{a_5 a_6}_{i_1 i_2} + \tfrac{1}{2} V^{i_3 i_4}_{i_5 i_6} (\xi_{16})^{i_5 i_6}_{i_1 i_2} \\
&\quad + \tfrac{1}{2} v^{i_3 i_4}_{a'_5 a'_6} (\xi_{17})^{a'_5 a'_6}_{i_1 i_2} + \tfrac{1}{6} \lambda^{i_3 i_4 i_5}_{a_6 a_7 a_8} (\xi_{18})^{a_6 a_7 a_8}_{i_1 i_2 i_5}
\end{aligned}
$$

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G. EOM-CCSD-R12

TABLE ESI.4.XXIX: The computational sequence and intermediates for the R_1 amplitude equation of right-hand EOM-CCSD-R12

$$(\Xi_0)^{i_4}_{a_3} = +t^{a_5}_{i_6} v^{i_4 i_6}_{a_3 a_5}$$
$$(\Xi_1)^{i_4}_{a_3} = +r^{a_5}_{i_6} v^{i_4 i_6}_{a_3 a_5}$$
$$(\xi_9)^{i_4 i_5}_{i_1 a'_3} = -r^{a_6}_{i_1} v^{i_4 i_5}_{a'_3 a_6}$$
$$(\xi_7)^{i_4 i_5}_{i_1 a_3} = +r^{a_6}_{i_1} v^{i_4 i_5}_{a_3 a_6}$$
$$(\xi_6)^{a_2}_{a_3} = -r^{a_4}_{i_5} v^{i_5 a_2}_{a_3 a_4}$$
$$(\xi_4)^{i_4}_{a'_3} = -f^{i_4}_{a'_3} - t^{a_5}_{i_6} v^{i_4 i_6}_{a'_3 a_5}$$
$$(\xi_3)^{i_4}_{a_3} = +f^{i_4}_{a_3} + (\Xi_0)^{i_4}_{a_3}$$
$$(\xi_{2,0})^{i_3}_{a_4} = -f^{i_3}_{a_4} - (\Xi_0)^{i_3}_{a_4}$$
$$(\xi_2)^{i_3}_{i_1} = +r^{a_4}_{i_1}(\xi_{2,0})^{i_3}_{a_4} - r^{a_4}_{i_5} v^{i_3 i_5}_{i_1 a_4} - t^{a_4}_{i_1}(\Xi_1)^{i_3}_{a_4} - \tfrac{1}{2} r^{a_4 a_5}_{i_1 i_6} v^{i_3 i_6}_{a_4 a_5} - \tfrac{1}{2} r^{i_5 i_6}_{i_1 i_4} V^{i_3 i_4}_{i_5 i_6}$$
$$(\xi_{13})^{i_4 i_5}_{i_1 a'_3} = +v^{i_4 i_5}_{i_1 a'_3} - t^{a_6}_{i_1} v^{i_4 i_5}_{a'_3 a_6}$$
$$(\xi_{11})^{i_4 i_5}_{i_1 a_3} = -v^{i_4 i_5}_{i_1 a_3} + t^{a_6}_{i_1} v^{i_4 i_5}_{a_3 a_6}$$
$$(\xi_{10})^{i_4}_{a'_3} = -r^{a_5}_{i_6} v^{i_4 i_6}_{a'_3 a_5}$$
$$(\xi_1)^{a_2}_{a_3} = +f^{a_2}_{a_3} - t^{a_4}_{i_5} v^{i_5 a_2}_{a_3 a_4}$$
$$(\xi_{0,0})^{i_3}_{a_4} = -f^{i_3}_{a_4} - (\Xi_0)^{i_3}_{a_4}$$
$$(\xi_0)^{i_3}_{i_1} = -f^{i_3}_{i_1} + t^{a_4}_{i_1}(\xi_{0,0})^{i_3}_{a_4} - t^{a_4}_{i_5} v^{i_3 i_5}_{i_1 a_4} - \tfrac{1}{2} t^{a_4 a_5}_{i_1 i_6} v^{i_3 i_6}_{a_4 a_5} - \tfrac{1}{2} t^{i_4 i_5}_{i_1 i_6} V^{i_3 i_6}_{i_4 i_5}$$
$$\begin{aligned}\delta^{a_2}_{i_1} = &+r^{a_2}_{i_3}(\xi_0)^{i_3}_{i_1} + r^{a_3}_{i_1}(\xi_1)^{a_2}_{a_3} + t^{a_2}_{i_3}(\xi_2)^{i_3}_{i_1} + r^{a_2 a_3}_{i_1 i_4}(\xi_3)^{i_4}_{a_3} + \tilde{r}^{\,a'_3 a_2}_{i_1 i_4}(\xi_4)^{i_4}_{a'_3} \\ &-r^{a_3}_{i_4} v^{i_4 a_2}_{i_1 a_3} + t^{a_3}_{i_1}(\xi_6)^{a_2}_{a_3} + \tfrac{1}{2} t^{a_2 a_3}_{i_4 i_5}(\xi_7)^{i_4 i_5}_{i_1 a_3} + t^{a_2 a_3}_{i_1 i_4}(\Xi_1)^{i_4}_{a_3} \\ &+\tfrac{1}{2}\tilde{t}^{\,a'_3 a_2}_{i_4 i_5}(\xi_9)^{i_4 i_5}_{i_1 a'_3} + \tilde{t}^{\,a'_3 a_2}_{i_1 i_4}(\xi_{10})^{i_4}_{a'_3} + \tfrac{1}{2} r^{a_2 a_3}_{i_4 i_5}(\xi_{11})^{i_4 i_5}_{i_1 a_3} - \tfrac{1}{2} r^{a_3 a_4}_{i_1 i_5} v^{i_5 a_2}_{a_3 a_4} \\ &+\tfrac{1}{2}\tilde{r}^{\,a'_3 a_2}_{i_4 i_5}(\xi_{13})^{i_4 i_5}_{i_1 a'_3} - \tfrac{1}{2} r^{i_4 i_5}_{i_1 i_3} V^{i_3 a_2}_{i_4 i_5}\end{aligned}$$

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TABLE ESI.4.XXX: The computational sequence and intermediates for the R_2 amplitude equation of right-hand EOM-CCSD-R12

$$
\begin{aligned}
(\Xi_0)^{i_5 i_6}_{i_1 i_2} &= +P_2 t^{a_7}_{i_1} v^{i_5 i_6}_{i_2 a_7} \\
(\Xi_1)^{i_6 a_4}_{i_2 a_5} &= +t^{a_7}_{i_2} v^{i_6 a_4}_{a_5 a_7} \\
(\Xi_2)^{i_5 i_6}_{i_1 i_2} &= +P_2 r^{a_7}_{i_1} v^{i_5 i_6}_{i_2 a_7} \\
(\Xi_3)^{i_6 a_4}_{i_2 a_5} &= +r^{a_7}_{i_2} v^{i_6 a_4}_{a_5 a_7} \\
(\Xi_4)^{i_5 i_7}_{i_2 a_6} &= +t^{a_8}_{i_2} v^{i_5 i_7}_{a_6 a_8} \\
(\Xi_5)^{i_5 i_6}_{i_2 a_7} &= +r^{a_8}_{i_2} v^{i_5 i_6}_{a_7 a_8} \\
(\Xi_6)^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} t^{a_7 a_8}_{i_1 i_2} v^{i_5 i_6}_{a_7 a_8} \\
(\Xi_7)^{i_5}_{a_6} &= +t^{a_7}_{i_8} v^{i_5 i_8}_{a_6 a_7} \\
(\Xi_8)^{i_5}_{a_6} &= +r^{a_7}_{i_8} v^{i_5 i_8}_{a_6 a_7} \\
(\Xi_9)^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} t^{i_7 i_8}_{i_1 i_2} V^{i_5 i_6}_{i_7 i_8} \\
(\Xi_{10})^{i_5 i_7}_{i_2 a'_6} &= +t^{a_8}_{i_2} v^{i_5 i_7}_{a'_6 a_8} \\
(\Xi_{11})^{i_5}_{a'_6} &= +t^{a_7}_{i_8} v^{i_5 i_8}_{a'_6 a_7} \\
(\Xi_{12})^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} r^{a_7 a_8}_{i_1 i_2} v^{i_5 i_6}_{a_7 a_8} \\
(\Xi_{13})^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} V^{i_5 i_6}_{i_7 i_8} r^{i_7 i_8}_{i_1 i_2} \\
(\Xi_{14})^{i_5 i_6}_{i_1 i_2} &= +P_2 t^{a_7}_{i_1} (\Xi_4)^{i_5 i_6}_{i_2 a_7} \\
(\Xi_{15})^{i_5 i_6}_{i_1 i_2} &= +P_2 t^{a_7}_{i_1} (\Xi_5)^{i_5 i_6}_{i_2 a_7} \\
(\xi_9)^{i_6 a_4}_{i_2 a_5} &= +(\Xi_3)^{i_6 a_4}_{i_2 a_5} + r^{a_4 a_7}_{i_2 i_8} v^{i_6 i_8}_{a_5 a_7} + \tilde{r}^{\,a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_7 a_5} \\
(\xi_8)^{i_5 i_6}_{i_1 i_2} &= -(\Xi_2)^{i_5 i_6}_{i_1 i_2} + (\Xi_{15})^{i_5 i_6}_{i_1 i_2} + (\Xi_{12})^{i_5 i_6}_{i_1 i_2} + (\Xi_{13})^{i_5 i_6}_{i_1 i_2} \\
(\xi_7)^{a_3 a_4}_{i_2 a_5} &= +r^{a_6}_{i_2} v^{a_3 a_4}_{a_5 a_6} \\
(\xi_{5,9})^{i_5}_{a'_6} &= -r^{a_7}_{i_8} v^{i_5 i_8}_{a'_6 a_7} \\
(\xi_{5,8})^{i_5 i_7}_{i_2 a'_6} &= +r^{a_8}_{i_2} v^{i_5 i_7}_{a'_6 a_8} \\
(\xi_{5,4})^{i_5 i_6}_{i_1 i_2} &= -(\Xi_2)^{i_5 i_6}_{i_1 i_2} + (\Xi_{15})^{i_5 i_6}_{i_1 i_2} + (\Xi_{12})^{i_5 i_6}_{i_1 i_2} + (\Xi_{13})^{i_5 i_6}_{i_1 i_2} \\
(\xi_{5,2})^{i_5 i_6}_{i_1 i_2} &= +v^{i_5 i_6}_{i_1 i_2} - (\Xi_0)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2}(\Xi_{14})^{i_5 i_6}_{i_1 i_2} + (\Xi_6)^{i_5 i_6}_{i_1 i_2} + (\Xi_9)^{i_5 i_6}_{i_1 i_2} \\
(\xi_{5,12})^{i_5 i_7}_{i_2 a'_6} &= -v^{i_5 i_7}_{i_2 a'_6} + (\Xi_{10})^{i_5 i_7}_{i_2 a'_6} \\
(\xi_{5,10})^{i_5 i_7}_{i_2 a_6} &= +v^{i_5 i_7}_{i_2 a_6} - (\Xi_4)^{i_5 i_7}_{i_2 a_6} \\
(\xi_{5,1})^{i_5}_{a'_6} &= -f^{i_5}_{a'_6} - (\Xi_{11})^{i_5}_{a'_6} \\
(\xi_{5,0})^{i_5}_{a_6} &= +f^{i_5}_{a_6} + (\Xi_7)^{i_5}_{a_6} \\
(\xi_5)^{i_5 a_4}_{i_1 i_2} &= +r^{a_4 a_6}_{i_1 i_2} (\xi_{5,0})^{i_5}_{a_6} + \tilde{r}^{\,a'_6 a_4}_{i_1 i_2} (\xi_{5,1})^{i_5}_{a'_6} + r^{a_4}_{i_6} (\xi_{5,2})^{i_5 i_6}_{i_1 i_2} + P_2 r^{a_6}_{i_1} v^{i_5 a_4}_{i_2 a_6} \\
&\quad + \tfrac{1}{2} t^{a_4}_{i_6} (\xi_{5,4})^{i_5 i_6}_{i_1 i_2} - P_2 t^{a_6}_{i_1} (\Xi_3)^{i_5 a_4}_{i_2 a_6} - P_2 t^{a_4 a_6}_{i_1 i_7} (\Xi_5)^{i_5 i_7}_{i_2 a_6} \\
&\quad + t^{a_4 a_6}_{i_1 i_2} (\Xi_8)^{i_5}_{a_6} + P_2 \tilde{t}^{\,a'_6 a_4}_{i_1 i_7} (\xi_{5,8})^{i_5 i_7}_{i_2 a'_6} + \tilde{t}^{\,a'_6 a_4}_{i_1 i_2} (\xi_{5,9})^{i_5}_{a'_6} \\
&\quad + P_2 r^{a_4 a_6}_{i_1 i_7} (\xi_{5,10})^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} r^{a_6 a_7}_{i_1 i_2} v^{i_5 a_4}_{a_6 a_7} + P_2 \tilde{r}^{\,a'_6 a_4}_{i_1 i_7} (\xi_{5,12})^{i_5 i_7}_{i_2 a'_6} \\
&\quad - \tfrac{1}{2} r^{i_6 i_7}_{i_1 i_2} V^{i_5 a_4}_{i_6 i_7}
\end{aligned}
$$

$$
\begin{aligned}
(\xi_4)^{a_4}_{a'_5} &= -f^{a_4}_{a'_5} + t^{a_6}_{i_7} v^{i_7 a_4}_{a'_5 a_6} + \tfrac{1}{2} t^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a_6} - \tfrac{1}{2} \tilde{t}^{\,a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a'_6} \\
(\xi_3)^{a_4}_{a_5} &= +f^{a_4}_{a_5} - t^{a_6}_{i_7} v^{i_7 a_4}_{a_5 a_6} - \tfrac{1}{2} t^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_5 a_6} - \tfrac{1}{2} \tilde{t}^{\,a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_5} \\
(\xi_{2,0})^{i_5}_{a_6} &= -f^{i_5}_{a_6} - (\Xi_7)^{i_5}_{a_6} \\
(\xi_2)^{i_5}_{i_2} &= -f^{i_5}_{i_2} + t^{a_6}_{i_2} (\xi_{2,0})^{i_5}_{a_6} - t^{a_6}_{i_7} v^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_2 i_8} v^{i_5 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_2 i_8} V^{i_5 i_8}_{i_6 i_7} \\
(\xi_{16})^{i_6 a_4}_{i_2 a'_5} &= +v^{i_6 a_4}_{i_2 a'_5} - t^{a_7}_{i_2} v^{i_6 a_4}_{a'_5 a_7} + \tilde{t}^{\,a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_5 a'_7} \\
(\xi_{14})^{i_6 a_4}_{i_2 a_5} &= -v^{i_6 a_4}_{i_2 a_5} + (\Xi_1)^{i_6 a_4}_{i_2 a_5} + \tilde{t}^{\,a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_7 a_5} \\
(\xi_{13})^{i_5 i_6}_{i_1 i_2} &= +v^{i_5 i_6}_{i_1 i_2} - (\Xi_0)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2}(\Xi_{14})^{i_5 i_6}_{i_1 i_2} + (\Xi_6)^{i_5 i_6}_{i_1 i_2} + (\Xi_9)^{i_5 i_6}_{i_1 i_2} \\
(\xi_{12})^{a_4}_{a'_5} &= +r^{a_6}_{i_7} v^{i_7 a_4}_{a'_5 a_6} + \tfrac{1}{2} r^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a_6} - \tfrac{1}{2} \tilde{r}^{\,a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a'_6} \\
(\xi_{11})^{i_6 a_4}_{i_2 a'_5} &= -r^{a_7}_{i_2} v^{i_6 a_4}_{a'_5 a_7} \\
(\xi_{10})^{a_4}_{a_5} &= -r^{a_6}_{i_7} v^{i_7 a_4}_{a_5 a_6} - \tfrac{1}{2} r^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_5 a_6} - \tfrac{1}{2} \tilde{r}^{\,a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_5} \\
(\xi_{1,0})^{i_5}_{a_6} &= -f^{i_5}_{a_6} - (\Xi_7)^{i_5}_{a_6} \\
(\xi_1)^{i_5}_{i_2} &= +r^{a_6}_{i_2} (\xi_{1,0})^{i_5}_{a_6} - r^{a_6}_{i_7} v^{i_5 i_7}_{i_2 a_6} - t^{a_6}_{i_2} (\Xi_8)^{i_5}_{a_6} - \tfrac{1}{2} r^{a_6 a_7}_{i_2 i_8} v^{i_5 i_8}_{a_6 a_7} - \tfrac{1}{2} r^{i_7 i_8}_{i_2 i_6} V^{i_5 i_6}_{i_7 i_8} \\
(\xi_{0,5})^{i_5 i_7}_{i_2 a'_6} &= -v^{i_5 i_7}_{i_2 a'_6} + (\Xi_{10})^{i_5 i_7}_{i_2 a'_6} \\
(\xi_{0,3})^{i_5 i_7}_{i_2 a_6} &= +v^{i_5 i_7}_{i_2 a_6} - (\Xi_4)^{i_5 i_7}_{i_2 a_6} \\
(\xi_{0,2})^{i_5 a_4}_{i_2 a_6} &= +v^{i_5 a_4}_{i_2 a_6} - \tfrac{1}{2}(\Xi_1)^{i_5 a_4}_{i_2 a_6} \\
(\xi_{0,1})^{i_5}_{a'_6} &= -f^{i_5}_{a'_6} - (\Xi_{11})^{i_5}_{a'_6} \\
(\xi_{0,0})^{i_5}_{a_6} &= +f^{i_5}_{a_6} + (\Xi_7)^{i_5}_{a_6} \\
(\xi_0)^{i_5 a_4}_{i_1 i_2} &= -v^{i_5 a_4}_{i_1 i_2} + t^{a_4 a_6}_{i_1 i_2} (\xi_{0,0})^{i_5}_{a_6} + \tilde{t}^{\,a'_6 a_4}_{i_1 i_2} (\xi_{0,1})^{i_5}_{a'_6} + P_2 t^{a_6}_{i_1} (\xi_{0,2})^{i_5 a_4}_{i_2 a_6} \\
&\quad + P_2 t^{a_4 a_6}_{i_1 i_7} (\xi_{0,3})^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_1 i_2} v^{i_5 a_4}_{a_6 a_7} + P_2 \tilde{t}^{\,a'_6 a_4}_{i_1 i_7} (\xi_{0,5})^{i_5 i_7}_{i_2 a'_6} - \tfrac{1}{2} t^{i_6 i_7}_{i_1 i_2} V^{i_5 a_4}_{i_6 i_7} \\
\delta^{a_3 a_4}_{i_1 i_2} &= +P_2 r^{a_3}_{i_5} (\xi_0)^{i_5 a_4}_{i_1 i_2} + P_2 t^{a_3 a_4}_{i_1 i_5} (\xi_1)^{i_5}_{i_2} + P_2 r^{a_3 a_4}_{i_1 i_5} (\xi_2)^{i_5}_{i_2} + P_2 r^{a_3 a_5}_{i_1 i_2} (\xi_3)^{a_4}_{a_5} \\
&\quad + P_2 \tilde{r}^{\,a'_5 a_3}_{i_1 i_2} (\xi_4)^{a_4}_{a'_5} + P_2 t^{a_3}_{i_5} (\xi_5)^{i_5 a_4}_{i_1 i_2} - P_2 r^{a_5}_{i_1} v^{a_3 a_4}_{i_2 a_5} + P_2 t^{a_5}_{i_1} (\xi_7)^{a_3 a_4}_{i_2 a_5} \\
&\quad + \tfrac{1}{2} t^{a_3 a_4}_{i_5 i_6} (\xi_8)^{i_5 i_6}_{i_1 i_2} + P_2 P_2 t^{a_3 a_5}_{i_1 i_6} (\xi_9)^{i_6 a_4}_{i_2 a_5} + P_2 t^{a_3 a_5}_{i_1 i_2} (\xi_{10})^{a_4}_{a_5} \\
&\quad + P_2 P_2 \tilde{t}^{\,a'_5 a_3}_{i_1 i_6} (\xi_{11})^{i_6 a_4}_{i_2 a'_5} + P_2 \tilde{t}^{\,a'_5 a_3}_{i_1 i_2} (\xi_{12})^{a_4}_{a'_5} + \tfrac{1}{2} r^{a_3 a_4}_{i_5 i_6} (\xi_{13})^{i_5 i_6}_{i_1 i_2} \\
&\quad + P_2 P_2 r^{a_3 a_5}_{i_1 i_6} (\xi_{14})^{i_6 a_4}_{i_2 a_5} + \tfrac{1}{2} r^{a_5 a_6}_{i_1 i_2} v^{a_3 a_4}_{a_5 a_6} \\
&\quad + P_2 P_2 \tilde{r}^{\,a'_5 a_3}_{i_1 i_6} (\xi_{16})^{i_6 a_4}_{i_2 a'_5} + \tfrac{1}{2} r^{i_5 i_6}_{i_1 i_2} V^{a_3 a_4}_{i_5 i_6}
\end{aligned}
$$

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TABLE ESI.4.XXXI: The computational sequence and intermediates for the geminal r amplitude equation of right-hand EOM-CCSD-R12 [Part I]

$$(\Xi_0)^{i_3 i_4}_{i_7 a'_8} = +r^{a_9}_{i_7} F^{i_3 i_4 *}_{a'_8 a_9}$$
$$(\Xi_1)^{i_3 i_4}_{i_7 a'_8} = +t^{a_9}_{i_7} F^{i_3 i_4 *}_{a'_8 a_9}$$
$$(\Xi_2)^{i_8 a'_6}_{i_2 a_7} = +t^{a_9}_{i_2} v^{i_8 a'_6}_{a_7 a_9}$$
$$(\Xi_3)^{i_8 a'_6}_{i_2 a_7} = +r^{a_9}_{i_2} v^{i_8 a'_6}_{a_7 a_9}$$
$$(\Xi_4)^{a'_7}_{a_6} = +r^{a_8}_{i_9} v^{i_9 a'_7}_{a_6 a_8}$$
$$(\Xi_5)^{i_8 a'_5}_{i_2 a'_7} = +r^{a_9}_{i_2} v^{i_8 a'_5}_{a'_7 a_9}$$
$$(\Xi_6)^{a'_5}_{a'_7} = +r^{a_8}_{i_9} v^{i_9 a'_5}_{a'_7 a_8}$$
$$(\Xi_7)^{i_7 i_9}_{i_2 a'_8} = +t^{a_{10}}_{i_2} v^{i_7 i_9}_{a'_8 a_{10}}$$
$$(\Xi_8)^{i_7 i_9}_{i_2 a_8} = +t^{a_{10}}_{i_2} v^{i_7 i_9}_{a_8 a_{10}}$$
$$(\Xi_9)^{i_7}_{a'_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_{10})^{i_7}_{a_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\Xi_{11})^{i_7 i_8}_{i_2 a_9} = +r^{a_{10}}_{i_2} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\Xi_{12})^{i_7}_{a_8} = +r^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\Xi_{13})^{a'_7}_{a_6} = +t^{a_8}_{i_9} v^{i_9 a'_7}_{a_6 a_8}$$
$$(\Xi_{14})^{a'_7}_{a'_5} = +t^{a_8}_{i_9} v^{i_9 a'_7}_{a'_5 a_8}$$
$$(\Xi_{15})^{i_8 a'_5}_{i_2 a'_7} = +t^{a_9}_{i_2} v^{i_8 a'_5}_{a'_7 a_9}$$
$$(\Xi_{16})^{i_8 a'_6}_{i_2 a_7} = +\tilde{r}^{\,a'_6 a'_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\Xi_{17})^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{r}^{\,a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\Xi_{18})^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{r}^{\,a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8}$$
$$(\Xi_{19})^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{t}^{\,a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\Xi_{20})^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{t}^{\,a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8}$$
$$(\Xi_{21})^{i_8 a'_6}_{i_2 a_7} = +\tilde{t}^{\,a'_6 a'_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\Xi_{22})^{a'_7}_{a'_5} = +\tfrac{1}{2}\tilde{t}^{\,a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_5 a'_8}$$
$$(\Xi_{23})^{a'_7}_{a'_5} = +\tfrac{1}{2}\tilde{t}^{\,a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_5 a_8}$$
$$(\Xi_{24})^{a'_5}_{a'_7} = +\tfrac{1}{2}\tilde{r}^{\,a'_5 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{25})^{a'_5}_{a'_7} = +\tfrac{1}{2}\tilde{r}^{\,a'_5 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\xi_{9,1})^{a'_7}_{a_6} = +(\Xi_4)^{a'_7}_{a_6} - (\Xi_{17})^{a'_7}_{a_6} + (\Xi_{18})^{a'_7}_{a_6}$$
$$(\xi_9)^{i_3 i_4}_{a_5 a_6} = +v^{i_7 a'_8}_{a_5 a_6}(\Xi_0)^{i_3 i_4}_{i_7 a'_8} + P_2 F^{i_3 i_4 *}_{a'_7 a_5}(\xi_{9,1})^{a'_7}_{a_6}$$
$$(\xi_8)^{i_3 i_4}_{i_2 a_5} = -v^{i_6 a'_7}_{i_2 a_5}(\Xi_0)^{i_3 i_4}_{i_6 a'_7} + r^{a_6}_{i_2}(V^\dagger)^{i_3 i_4}_{a_5 a_6}$$
$$(\xi_7)^{i_3 i_4}_{i_2 a_5} = -(V^\dagger)^{i_3 i_4}_{i_2 a_5} - v^{i_6 a'_7}_{i_2 a_5}(\Xi_1)^{i_3 i_4}_{i_6 a'_7}$$
$$(\xi_{5,3})^{a_7}_{a_6} = -t^{a_8}_{i_9} v^{i_9 a_7}_{a_6 a_8} - \tfrac{1}{2} t^{a_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8} - \tfrac{1}{2}\tilde{t}^{\,a'_8 a_7}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\xi_{5,2})^{a'_7}_{a_6} = -(\Xi_{13})^{a'_7}_{a_6} + (\Xi_{19})^{a'_7}_{a_6} - (\Xi_{20})^{a'_7}_{a_6}$$
$$(\xi_{5,1})^{a'_7}_{a'_5} = -(\Xi_{14})^{a'_7}_{a'_5} - (\Xi_{22})^{a'_7}_{a'_5} - (\Xi_{23})^{a'_7}_{a'_5}$$
$$(\xi_5)^{i_3 i_4}_{a'_5 a_6} = -f^{i_7}_{a_6}(\Xi_1)^{i_3 i_4}_{i_7 a'_5} + F^{i_3 i_4 *}_{a'_7 a_6}(\xi_{5,1})^{a'_7}_{a'_5} + F^{i_3 i_4 *}_{a'_5 a'_7}(\xi_{5,2})^{a'_7}_{a_6} + F^{i_3 i_4 *}_{a'_5 a_7}(\xi_{5,3})^{a_7}_{a_6}$$
$$(\xi_4)^{i_3 i_4}_{i_5 i_6} = +B^{i_3 i_4}_{i_5 i_6} + P^{i_3 i_4}_{i_5 i_6} + V^{i_7 a'_8}_{i_5 i_6}(\Xi_1)^{i_3 i_4}_{i_7 a'_8}$$
$$(\xi_{3,0})^{a'_7}_{a_6} = -f^{a'_7}_{a_6} + (\Xi_{13})^{a'_7}_{a_6} - (\Xi_{19})^{a'_7}_{a_6} + (\Xi_{20})^{a'_7}_{a_6}$$
$$(\xi_3)^{i_3 i_4}_{a_5 a_6} = +(V^\dagger)^{i_3 i_4}_{a_5 a_6} + P_2 F^{i_3 i_4 *}_{a'_7 a_5}(\xi_{3,0})^{a'_7}_{a_6} + v^{i_7 a'_8}_{a_5 a_6}(\Xi_1)^{i_3 i_4}_{i_7 a'_8}$$

$$(\xi_{2,3,0})^{i_7 i_8}_{i_2 a_9} = -v^{i_7 i_8}_{i_2 a_9} + \tfrac{1}{2}(\Xi_8)^{i_7 i_8}_{i_2 a_9}$$
$$(\xi_{2,3})^{i_7 i_8}_{i_1 i_2} = +P_2 t^{a_9}_{i_1}(\xi_{2,3,0})^{i_7 i_8}_{i_2 a_9} + \tfrac{1}{2} t^{a_9 a_{10}}_{i_1 i_2} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\xi_{2,2})^{i_7 i_8}_{i_1 i_2} = -P_2 r^{a_9}_{i_1} v^{i_7 i_8}_{i_2 a_9} + P_2 t^{a_9}_{i_1}(\Xi_{11})^{i_7 i_8}_{i_2 a_9} + \tfrac{1}{2} r^{a_9 a_{10}}_{i_1 i_2} v^{i_7 i_8}_{a_9 a_{10}} + \tfrac{1}{2} r^{i_9 i_{10}}_{i_1 i_2} V^{i_7 i_8}_{i_9 i_{10}}$$
$$(\xi_{2,1,0})^{i_7}_{a_8} = -f^{i_7}_{a_8} - (\Xi_{10})^{i_7}_{a_8}$$
$$(\xi_{2,1})^{i_7}_{i_2} = -f^{i_7}_{i_2} + t^{a_8}_{i_2}(\xi_{2,1,0})^{i_7}_{a_8} - t^{a_8}_{i_9} v^{i_7 i_9}_{i_2 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_2 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} t^{i_8 i_9}_{i_2 i_{10}} V^{i_7 i_{10}}_{i_8 i_9}$$
$$(\xi_{2,0,0})^{i_7}_{a_8} = -f^{i_7}_{a_8} - (\Xi_{10})^{i_7}_{a_8}$$
$$(\xi_{2,0})^{i_7}_{i_2} = +r^{a_8}_{i_2}(\xi_{2,0,0})^{i_7}_{a_8} - r^{a_8}_{i_9} v^{i_7 i_9}_{i_2 a_8} - t^{a_8}_{i_2}(\Xi_{12})^{i_7}_{a_8} - \tfrac{1}{2} r^{a_8 a_9}_{i_2 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} r^{i_8 i_9}_{i_2 i_{10}} V^{i_7 i_{10}}_{i_8 i_9}$$
$$(\xi_2)^{i_5 i_6}_{i_1 i_2} = +P_2 t^{i_5 i_6}_{i_1 i_7}(\xi_{2,0})^{i_7}_{i_2} + P_2 r^{i_5 i_6}_{i_1 i_7}(\xi_{2,1})^{i_7}_{i_2} + \tfrac{1}{2}\tilde{t}^{\,i_5 i_6}_{i_7 i_8}(\xi_{2,2})^{i_7 i_8}_{i_1 i_2} + \tfrac{1}{2} r^{i_5 i_6}_{i_7 i_8}(\xi_{2,3})^{i_7 i_8}_{i_1 i_2}$$
$$(\xi_{13,0})^{a'_7}_{a'_6} = -(\Xi_{14})^{a'_7}_{a'_6} - (\Xi_{22})^{a'_7}_{a'_6} - (\Xi_{23})^{a'_7}_{a'_6}$$
$$(\xi_{13})^{i_3 i_4}_{a'_5 a'_6} = +P_2 F^{i_3 i_4 *}_{a'_5 a'_7}(\xi_{13,0})^{a'_7}_{a'_6}$$
$$(\xi_{12})^{i_3 i_4}_{i_5 i_6} = +\tfrac{1}{2} r^{i_7 i_8}_{i_5 i_6} X^{i_3 i_4}_{i_7 i_8}$$
$$(\xi_{11,4})^{i_8 a'_6}_{i_2 a_7} = -v^{i_8 a'_6}_{i_2 a_7} + (\Xi_2)^{i_8 a'_6}_{i_2 a_7} - (\Xi_{21})^{i_8 a'_6}_{i_2 a_7} + \tilde{t}^{\,a'_6 a_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a_7 a_9}$$
$$(\xi_{11,3})^{i_8 a'_6}_{i_2 a'_7} = -v^{i_8 a'_6}_{i_2 a'_7} + (\Xi_{15})^{i_8 a'_6}_{i_2 a'_7} + \tilde{t}^{\,a'_6 a'_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_7 a'_9}$$
$$(\xi_{11,2})^{a'_6}_{a'_7} = -(\Xi_6)^{a'_6}_{a'_7} - (\Xi_{24})^{a'_6}_{a'_7} - (\Xi_{25})^{a'_6}_{a'_7}$$
$$(\xi_{11,1})^{i_8 a'_6}_{i_2 a_7} = +(\Xi_3)^{i_8 a'_6}_{i_2 a_7} - (\Xi_{16})^{i_8 a'_6}_{i_2 a_7}$$
$$(\xi_{11})^{a'_5 a'_6}_{i_1 i_2} = +P_2 P_2 \tilde{t}^{\,a'_5 a'_7}_{i_1 i_8}(\Xi_5)^{i_8 a'_6}_{i_2 a'_7} + P_2 P_2 \tilde{t}^{\,a'_5 a_7}_{i_1 i_8}(\xi_{11,1})^{i_8 a'_6}_{i_2 a_7} + P_2 \tilde{t}^{\,a'_5 a'_7}_{i_1 i_2}(\xi_{11,2})^{a'_6}_{a'_7} + P_2 P_2 \tilde{r}^{\,a'_5 a'_7}_{i_1 i_8}(\xi_{11,3})^{i_8 a'_6}_{i_2 a'_7} + P_2 P_2 \tilde{r}^{\,a'_5 a_7}_{i_1 i_8}(\xi_{11,4})^{i_8 a'_6}_{i_2 a_7}$$
$$(\xi_{10,1})^{i_7 i_8}_{i_5 i_6} = +\tfrac{1}{2} r^{i_7 i_8}_{i_9 i_{10}} V^{i_9 i_{10}}_{i_5 i_6}$$
$$(\xi_{10})^{i_3 i_4}_{i_5 i_6} = +V^{i_7 a'_8}_{i_5 i_6}(\Xi_0)^{i_3 i_4}_{i_7 a'_8} + \tfrac{1}{2} X^{i_3 i_4}_{i_7 i_8}(\xi_{10,1})^{i_7 i_8}_{i_5 i_6}$$
$$(\xi_{1,1})^{a'_7}_{a_6} = -(\Xi_4)^{a'_7}_{a_6} + (\Xi_{17})^{a'_7}_{a_6} - (\Xi_{18})^{a'_7}_{a_6}$$
$$(\xi_1)^{i_3 i_4}_{a'_5 a_6} = -f^{i_7}_{a_6}(\Xi_0)^{i_3 i_4}_{i_7 a'_5} + F^{i_3 i_4 *}_{a'_5 a'_7}(\xi_{1,1})^{a'_7}_{a_6}$$
$$(\xi_{0,9})^{i_8 a'_5}_{i_2 a'_7} = +v^{i_8 a'_5}_{i_2 a'_7} - (\Xi_2)^{i_8 a'_5}_{i_2 a'_7} + (\Xi_{21})^{i_8 a'_5}_{i_2 a'_7}$$
$$(\xi_{0,8})^{a_6}_{a'_7} = -r^{a_8}_{i_9} v^{i_9 a_6}_{a'_7 a_8} - \tfrac{1}{2} r^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8} - \tfrac{1}{2}\tilde{r}^{\,a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a'_7}$$
$$(\xi_{0,7})^{a'_5}_{a'_7} = -(\Xi_6)^{a'_5}_{a'_7} - (\Xi_{24})^{a'_5}_{a'_7} - (\Xi_{25})^{a'_5}_{a'_7}$$
$$(\xi_{0,6})^{a_6}_{a'_7} = -r^{a_8}_{i_9} v^{i_9 a_6}_{a'_7 a_8} - \tfrac{1}{2} r^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8} + \tfrac{1}{2}\tilde{r}^{\,a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\xi_{0,5})^{i_8 a_6}_{i_2 a_7} = +r^{a_9}_{i_2} v^{i_8 a_6}_{a_7 a_9} + r^{a_6 a_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a_7 a_9} + \tilde{r}^{\,a'_9 a_6}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\xi_{0,3})^{i_8 a_6}_{i_2 a'_7} = +r^{a_9}_{i_2} v^{i_8 a_6}_{a'_7 a_9} - \tilde{r}^{\,a'_9 a_6}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_7 a'_9}$$
$$(\xi_{0,2})^{i_8 a'_5}_{i_2 a_7} = -(\Xi_3)^{i_8 a'_5}_{i_2 a_7} + (\Xi_{16})^{i_8 a'_5}_{i_2 a_7}$$
$$(\xi_{0,13})^{a_6}_{a'_7} = -t^{a_8}_{i_9} v^{i_9 a_6}_{a'_7 a_8} - \tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8} + \tfrac{1}{2}\tilde{t}^{\,a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\xi_{0,12})^{i_8 a_6}_{i_2 a_7} = -v^{i_8 a_6}_{i_2 a_7} + t^{a_9}_{i_2} v^{i_8 a_6}_{a_7 a_9} + t^{a_6 a_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a_7 a_9} + \tilde{t}^{\,a'_9 a_6}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\xi_{0,11})^{i_8 a'_5}_{i_2 a'_7} = -v^{i_8 a'_5}_{i_2 a'_7} + (\Xi_{15})^{i_8 a'_5}_{i_2 a'_7}$$
$$(\xi_{0,10})^{i_8 a_6}_{i_2 a'_7} = -v^{i_8 a_6}_{i_2 a'_7} + t^{a_9}_{i_2} v^{i_8 a_6}_{a'_7 a_9} - \tilde{t}^{\,a'_9 a_6}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_7 a'_9}$$
$$(\xi_{0,1,7})^{i_7 i_9}_{i_2 a_8} = -v^{i_7 i_9}_{i_2 a_8} + (\Xi_8)^{i_7 i_9}_{i_2 a_8}$$
$$(\xi_{0,1,6})^{i_7 i_9}_{i_2 a'_8} = -v^{i_7 i_9}_{i_2 a'_8} + (\Xi_7)^{i_7 i_9}_{i_2 a'_8}$$
$$(\xi_{0,1,4})^{i_7}_{a'_8} = -r^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\xi_{0,1,2})^{i_7 i_9}_{i_2 a'_8} = +r^{a_{10}}_{i_2} v^{i_7 i_9}_{a'_8 a_{10}}$$
$$(\xi_{0,1,0})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - (\Xi_9)^{i_7}_{a'_8}$$

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TABLE ESI.4.XXXII: The computational sequence and intermediates for the geminal r amplitude equation of right-hand EOM-CCSD-R12 [Part II]

$$
\begin{aligned}
(\xi_{0,1,0})^{i_7}_{a'_8} &= -f^{i_7}_{a'_8} - (\Xi_9)^{i_7}_{a'_8} \\
(\xi_{0,1})^{i_7 a'_5}_{i_1 i_2} &= +\tilde{r}^{a'_5 a'_8}_{i_1 i_2}(\xi_{0,1,0})^{i_7}_{a'_8} + P_2 t^{a_8}_{i_1}(\Xi_3)^{i_7 a'_5}_{i_2 a_8} + P_2 \tilde{t}^{a'_5 a'_8}_{i_1 i_9}(\xi_{0,1,2})^{i_7 i_9}_{i_2 a'_8} \\
&\quad + P_2 \tilde{t}^{a'_5 a_8}_{i_1 i_9}(\Xi_{11})^{i_7 i_9}_{i_2 a_8} + \tilde{t}^{a'_5 a'_8}_{i_1 i_2}(\xi_{0,1,4})^{i_7}_{a'_8} - \tilde{t}^{a'_5 a_8}_{i_1 i_2}(\Xi_{12})^{i_7}_{a_8} \\
&\quad + P_2 \tilde{r}^{a'_5 a'_8}_{i_1 i_9}(\xi_{0,1,6})^{i_7 i_9}_{i_2 a'_8} + P_2 \tilde{r}^{a'_5 a_8}_{i_1 i_9}(\xi_{0,1,7})^{i_7 i_9}_{i_2 a_8} - \tilde{r}^{a'_5 a_8}_{i_1 i_2}(\Xi_{10})^{i_7}_{a_8} \\
(\xi_{0,0,3})^{i_7 i_9}_{i_2 a_8} &= -v^{i_7 i_9}_{i_2 a_8} + (\Xi_8)^{i_7 i_9}_{i_2 a_8} \\
(\xi_{0,0,2})^{i_7 i_9}_{i_2 a'_8} &= -v^{i_7 i_9}_{i_2 a'_8} + (\Xi_7)^{i_7 i_9}_{i_2 a'_8} \\
(\xi_{0,0,0})^{i_7}_{a'_8} &= -f^{i_7}_{a'_8} - (\Xi_9)^{i_7}_{a'_8} \\
(\xi_{0,0})^{i_7 a'_5}_{i_1 i_2} &= +\tilde{t}^{a'_5 a'_8}_{i_1 i_2}(\xi_{0,0,0})^{i_7}_{a'_8} + \tfrac{1}{2} P_2 t^{a_8}_{i_1}(\Xi_2)^{i_7 a'_5}_{i_2 a_8} + P_2 \tilde{t}^{a'_5 a'_8}_{i_1 i_9}(\xi_{0,0,2})^{i_7 i_9}_{i_2 a'_8} \\
&\quad + P_2 \tilde{t}^{a'_5 a_8}_{i_1 i_9}(\xi_{0,0,3})^{i_7 i_9}_{i_2 a_8} - \tilde{t}^{a'_5 a_8}_{i_1 i_2}(\Xi_{10})^{i_7}_{a_8}
\end{aligned}
$$

$$
\begin{aligned}
(\xi_0)^{a'_5 a_6}_{i_1 i_2} &= +r^{a_6}_{i_7}(\xi_{0,0})^{i_7 a'_5}_{i_1 i_2} + t^{a_6}_{i_7}(\xi_{0,1})^{i_7 a'_5}_{i_1 i_2} + P_2 t^{a_6 a_7}_{i_1 i_8}(\xi_{0,2})^{i_8 a'_5}_{i_2 a_7} \\
&\quad + P_2 \tilde{t}^{a'_5 a'_7}_{i_1 i_8}(\xi_{0,3})^{i_8 a_6}_{i_2 a'_7} + P_2 \tilde{t}^{a'_7 a_6}_{i_1 i_8}(\Xi_5)^{i_8 a'_5}_{i_2 a'_7} + P_2 \tilde{t}^{a'_5 a_7}_{i_1 i_8}(\xi_{0,5})^{i_8 a_6}_{i_2 a_7} \\
&\quad + \tilde{t}^{a'_5 a'_7}_{i_1 i_2}(\xi_{0,6})^{a_6}_{a'_7} + \tilde{t}^{a'_7 a_6}_{i_1 i_2}(\xi_{0,7})^{a'_5}_{a'_7} + \tilde{t}^{a'_5 a_7}_{i_1 i_2}(\xi_{0,8})^{a_6}_{a_7} \\
&\quad + P_2 r^{a_6 a_7}_{i_1 i_8}(\xi_{0,9})^{i_8 a'_5}_{i_2 a_7} + P_2 \tilde{r}^{a'_5 a'_7}_{i_1 i_8}(\xi_{0,10})^{i_8 a_6}_{i_2 a'_7} + P_2 \tilde{r}^{a'_7 a_6}_{i_1 i_8}(\xi_{0,11})^{i_8 a'_5}_{i_2 a'_7} \\
&\quad + P_2 \tilde{r}^{a'_5 a_7}_{i_1 i_8}(\xi_{0,12})^{i_8 a_6}_{i_2 a_7} + \tilde{r}^{a'_5 a'_7}_{i_1 i_2}(\xi_{0,13})^{a_6}_{a'_7} \\
\delta^{i_3 i_4}_{i_1 i_2} &= +F^{i_3 i_4 *}_{a'_5 a_6}(\xi_0)^{a'_5 a_6}_{i_1 i_2} + \tilde{t}^{a'_5 a_6}_{i_1 i_2}(\xi_1)^{i_3 i_4}_{a'_5 a_6} + \tfrac{1}{2} X^{i_3 i_4}_{i_5 i_6}(\xi_2)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} r^{a_5 a_6}_{i_1 i_2}(\xi_3)^{i_3 i_4}_{a_5 a_6} \\
&\quad + \tfrac{1}{2} r^{i_5 i_6}_{i_1 i_2}(\xi_4)^{i_3 i_4}_{i_5 i_6} + \tilde{r}^{a'_5 a_6}_{i_1 i_2}(\xi_5)^{i_3 i_4}_{a'_5 a_6} + v^{i_5 a'_6}_{i_1 i_2}(\Xi_0)^{i_3 i_4}_{i_5 a'_6} + P_2 r^{a_5}_{i_1}(\xi_7)^{i_3 i_4}_{i_2 a_5} \\
&\quad + P_2 t^{a_5}_{i_1}(\xi_8)^{i_3 i_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_5 a_6}_{i_1 i_2}(\xi_9)^{i_3 i_4}_{a_5 a_6} + \tfrac{1}{2} t^{i_5 i_6}_{i_1 i_2}(\xi_{10})^{i_3 i_4}_{i_5 i_6} \\
&\quad + \tfrac{1}{2} F^{i_3 i_4 *}_{a'_5 a'_6}(\xi_{11})^{a'_5 a'_6}_{i_1 i_2} + \tfrac{1}{2} v^{i_5 i_6}_{i_1 i_2}(\xi_{12})^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{2} \tilde{r}^{a'_5 a'_6}_{i_1 i_2}(\xi_{13})^{i_3 i_4}_{a'_5 a'_6}
\end{aligned}
$$

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H. EOM-CCSDT-R12

TABLE ESI.4.XXXIII: The computational sequence and intermediates for the R_1 amplitude equation of right-hand EOM-CCSDT-R12 and higher-order EOM-CC-R12

$$(\Xi_0)^{i_4}_{a_3} = +t^{a_5}_{i_6} v^{i_4 i_6}_{a_3 a_5}$$
$$(\Xi_1)^{i_4}_{a_3} = +r^{a_5}_{i_6} v^{i_4 i_6}_{a_3 a_5}$$
$$(\xi_9)^{i_4 i_5}_{i_1 a'_3} = -r^{a_6}_{i_1} v^{i_4 i_5}_{a'_3 a_6}$$
$$(\xi_7)^{i_4 i_5}_{i_1 a_3} = +r^{a_6}_{i_1} v^{i_4 i_5}_{a_3 a_6}$$
$$(\xi_6)^{a_2}_{a_3} = -r^{a_4}_{i_5} v^{i_5 a_2}_{a_3 a_4}$$
$$(\xi_4)^{i_4}_{a'_3} = -f^{i_4}_{a'_3} - t^{a_5}_{i_6} v^{i_4 i_6}_{a'_3 a_5}$$
$$(\xi_3)^{i_4}_{a_3} = +f^{i_4}_{a_3} + (\Xi_0)^{i_4}_{a_3}$$
$$(\xi_{2,0})^{i_3}_{a_4} = -f^{i_3}_{a_4} - (\Xi_0)^{i_3}_{a_4}$$
$$(\xi_2)^{i_3}_{i_1} = +r^{a_4}_{i_1}(\xi_{2,0})^{i_3}_{a_4} - r^{a_4}_{i_5} v^{i_3 i_5}_{i_1 a_4} - t^{a_4}_{i_1}(\Xi_1)^{i_3}_{a_4} - \tfrac{1}{2} r^{a_4 a_5}_{i_1 i_6} v^{i_3 i_6}_{a_4 a_5} - \tfrac{1}{2} r^{i_5 i_6}_{i_1 i_4} V^{i_3 i_4}_{i_5 i_6}$$
$$(\xi_{13})^{i_4 i_5}_{i_1 a'_3} = +v^{i_4 i_5}_{i_1 a'_3} - t^{a_6}_{i_1} v^{i_4 i_5}_{a'_3 a_6}$$
$$(\xi_{11})^{i_4 i_5}_{i_1 a_3} = -v^{i_4 i_5}_{i_1 a_3} + t^{a_6}_{i_1} v^{i_4 i_5}_{a_3 a_6}$$
$$(\xi_{10})^{i_4}_{a'_3} = -r^{a_5}_{i_6} v^{i_4 i_6}_{a'_3 a_5}$$
$$(\xi_1)^{a_2}_{a_3} = +f^{a_2}_{a_3} - t^{a_4}_{i_5} v^{i_5 a_2}_{a_3 a_4}$$
$$(\xi_{0,0})^{i_3}_{a_4} = -f^{i_3}_{a_4} - (\Xi_0)^{i_3}_{a_4}$$
$$(\xi_0)^{i_3}_{i_1} = -f^{i_3}_{i_1} + t^{a_4}_{i_1}(\xi_{0,0})^{i_3}_{a_4} - t^{a_4}_{i_5} v^{i_3 i_5}_{i_1 a_4} - \tfrac{1}{2} t^{a_4 a_5}_{i_1 i_6} v^{i_3 i_6}_{a_4 a_5} - \tfrac{1}{2} t^{i_4 i_5}_{i_1 i_6} V^{i_3 i_6}_{i_4 i_5}$$
$$\begin{aligned}\delta^{a_2}_{i_1} = &+r^{a_2}_{i_3}(\xi_0)^{i_3}_{i_1} + r^{a_3}_{i_1}(\xi_1)^{a_2}_{a_3} + t^{a_2}_{i_3}(\xi_2)^{i_3}_{i_1} + r^{a_2 a_3}_{i_1 i_4}(\xi_3)^{i_4}_{a_3} + \tilde{r}^{\,a'_3 a_2}_{i_1 i_4}(\xi_4)^{i_4}_{a'_3} \\ &-r^{a_3}_{i_4} v^{i_4 a_2}_{i_1 a_3} + t^{a_3}_{i_1}(\xi_6)^{a_2}_{a_3} + \tfrac{1}{2} t^{a_2 a_3}_{i_4 i_5}(\xi_7)^{i_4 i_5}_{i_1 a_3} + t^{a_2 a_3}_{i_1 i_4}(\Xi_1)^{i_4}_{a_3} \\ &+\tfrac{1}{2}\tilde{t}^{\,a'_3 a_2}_{i_4 i_5}(\xi_9)^{i_4 i_5}_{i_1 a'_3} + \tilde{t}^{\,a'_3 a_2}_{i_1 i_4}(\xi_{10})^{i_4}_{a'_3} + \tfrac{1}{2} r^{a_2 a_3}_{i_4 i_5}(\xi_{11})^{i_4 i_5}_{i_1 a_3} \\ &-\tfrac{1}{2} r^{a_3 a_4}_{i_1 i_5} v^{i_5 a_2}_{a_3 a_4} + \tfrac{1}{2}\tilde{r}^{\,a'_3 a_2}_{i_4 i_5}(\xi_{13})^{i_4 i_5}_{i_1 a'_3} - \tfrac{1}{2} r^{i_4 i_5}_{i_1 i_3} V^{i_3 a_2}_{i_4 i_5} + \tfrac{1}{4} r^{a_2 a_3 a_4}_{i_1 i_5 i_6} v^{i_5 i_6}_{a_3 a_4}\end{aligned}$$

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TABLE ESI.4.XXXIV: The computational sequence and intermediates for the R_2 amplitude equation of right-hand EOM-CCSDT-R12

$$
\begin{aligned}
(\Xi_0)^{i_5 i_6}_{i_1 i_2} &= +P_2 t^{a_7}_{i_1} v^{i_5 i_6}_{i_2 a_7} \\
(\Xi_1)^{i_6 a_4}_{i_2 a_5} &= +t^{a_7}_{i_2} v^{i_6 a_4}_{a_5 a_7} \\
(\Xi_2)^{i_5 i_6}_{i_1 i_2} &= +P_2 r^{a_7}_{i_1} v^{i_5 i_6}_{i_2 a_7} \\
(\Xi_3)^{i_6 a_4}_{i_2 a_5} &= +r^{a_7}_{i_2} v^{i_6 a_4}_{a_5 a_7} \\
(\Xi_4)^{i_6 i_7}_{i_2 a_5} &= +t^{a_8}_{i_2} v^{i_6 i_7}_{a_5 a_8} \\
(\Xi_5)^{i_6 i_7}_{i_2 a_5} &= +r^{a_8}_{i_2} v^{i_6 i_7}_{a_5 a_8} \\
(\Xi_6)^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} t^{a_7 a_8}_{i_1 i_2} v^{i_5 i_6}_{a_7 a_8} \\
(\Xi_7)^{i_6}_{a_5} &= +t^{a_7}_{i_8} v^{i_6 i_8}_{a_5 a_7} \\
(\Xi_8)^{i_6}_{a_5} &= +r^{a_7}_{i_8} v^{i_6 i_8}_{a_5 a_7} \\
(\Xi_9)^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} t^{i_7 i_8}_{i_1 i_2} V^{i_5 i_6}_{i_7 i_8} \\
(\Xi_{10})^{i_5 i_7}_{i_2 a'_6} &= +t^{a_8}_{i_2} v^{i_5 i_7}_{a'_6 a_8} \\
(\Xi_{11})^{i_5}_{a'_6} &= +t^{a_7}_{i_8} v^{i_5 i_8}_{a'_6 a_7} \\
(\Xi_{12})^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} r^{a_7 a_8}_{i_1 i_2} v^{i_5 i_6}_{a_7 a_8} \\
(\Xi_{13})^{i_5 i_6}_{i_1 i_2} &= +\tfrac{1}{2} V^{i_5 i_6}_{i_7 i_8} r^{i_7 i_8}_{i_1 i_2} \\
(\Xi_{14})^{i_5 i_6}_{i_1 i_2} &= +P_2 t^{a_7}_{i_1} (\Xi_4)^{i_5 i_6}_{i_2 a_7} \\
(\Xi_{15})^{i_5 i_6}_{i_1 i_2} &= +P_2 t^{a_7}_{i_1} (\Xi_5)^{i_5 i_6}_{i_2 a_7} \\
(\xi_9)^{i_5 i_6}_{i_1 i_2} &= -(\Xi_2)^{i_5 i_6}_{i_1 i_2} + (\Xi_{15})^{i_5 i_6}_{i_1 i_2} + (\Xi_{12})^{i_5 i_6}_{i_1 i_2} + (\Xi_{13})^{i_5 i_6}_{i_1 i_2} \\
(\xi_8)^{a_3 a_4}_{i_2 a_5} &= +r^{a_6}_{i_2} v^{a_3 a_4}_{a_5 a_6} \\
(\xi_6)^{i_6}_{a_5} &= +f^{i_6}_{a_5} + (\Xi_7)^{i_6}_{a_5} \\
(\xi_{5,9})^{i_5}_{a'_6} &= -r^{a_7}_{i_8} v^{i_5 i_8}_{a'_6 a_7} \\
(\xi_{5,8})^{i_5 i_7}_{i_2 a'_6} &= +r^{a_8}_{i_2} v^{i_5 i_7}_{a'_6 a_8} \\
(\xi_{5,4})^{i_5 i_6}_{i_1 i_2} &= -(\Xi_2)^{i_5 i_6}_{i_1 i_2} + (\Xi_{15})^{i_5 i_6}_{i_1 i_2} + (\Xi_{12})^{i_5 i_6}_{i_1 i_2} + (\Xi_{13})^{i_5 i_6}_{i_1 i_2} \\
(\xi_{5,2})^{i_5 i_6}_{i_1 i_2} &= +v^{i_5 i_6}_{i_1 i_2} - (\Xi_0)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2}(\Xi_{14})^{i_5 i_6}_{i_1 i_2} + (\Xi_6)^{i_5 i_6}_{i_1 i_2} + (\Xi_9)^{i_5 i_6}_{i_1 i_2} \\
(\xi_{5,12})^{i_5 i_7}_{i_2 a'_6} &= -v^{i_5 i_7}_{i_2 a'_6} + (\Xi_{10})^{i_5 i_7}_{i_2 a'_6} \\
(\xi_{5,10})^{i_5 i_7}_{i_2 a_6} &= +v^{i_5 i_7}_{i_2 a_6} - (\Xi_4)^{i_5 i_7}_{i_2 a_6} \\
(\xi_{5,1})^{i_5}_{a'_6} &= -f^{i_5}_{a'_6} - (\Xi_{11})^{i_5}_{a'_6} \\
(\xi_{5,0})^{i_5}_{a_6} &= +f^{i_5}_{a_6} + (\Xi_7)^{i_5}_{a_6} \\
(\xi_5)^{i_5 a_4}_{i_1 i_2} &= +r^{a_4 a_6}_{i_1 i_2} (\xi_{5,0})^{i_5}_{a_6} + \tilde{r}^{a'_6 a_4}_{i_1 i_2} (\xi_{5,1})^{i_5}_{a'_6} + r^{a_4}_{i_6} (\xi_{5,2})^{i_5 i_6}_{i_1 i_2} \\
&\quad + P_2 r^{a_6}_{i_1} v^{i_5 a_4}_{i_2 a_6} + \tfrac{1}{2} t^{a_4}_{i_6} (\xi_{5,4})^{i_5 i_6}_{i_1 i_2} - P_2 t^{a_6}_{i_1} (\Xi_3)^{i_5 a_4}_{i_2 a_6} \\
&\quad - P_2 t^{a_4 a_6}_{i_1 i_7} (\Xi_5)^{i_5 i_7}_{i_2 a_6} + t^{a_4 a_6}_{i_1 i_2} (\Xi_8)^{i_5}_{a_6} + P_2 \tilde{t}^{a'_6 a_4}_{i_1 i_7} (\xi_{5,8})^{i_5 i_7}_{i_2 a'_6} \\
&\quad + \tilde{t}^{a'_6 a_4}_{i_1 i_2} (\xi_{5,9})^{i_5}_{a'_6} + P_2 r^{a_4 a_6}_{i_1 i_7} (\xi_{5,10})^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} r^{a_6 a_7}_{i_1 i_2} v^{i_5 a_4}_{a_6 a_7} \\
&\quad + P_2 \tilde{r}^{a'_6 a_4}_{i_1 i_7} (\xi_{5,12})^{i_5 i_7}_{i_2 a'_6} - \tfrac{1}{2} r^{i_6 i_7}_{i_1 i_2} V^{i_5 a_4}_{i_6 i_7} + \tfrac{1}{2} r^{a_4 a_6 a_7}_{i_1 i_2 i_8} v^{i_5 i_8}_{a_6 a_7} \\
(\xi_4)^{a_4}_{a'_5} &= -f^{a_4}_{a'_5} + t^{a_6}_{i_7} v^{i_7 a_4}_{a'_5 a_6} + \tfrac{1}{2} t^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a'_6} \\
(\xi_3)^{a_4}_{a_5} &= +f^{a_4}_{a_5} - t^{a_6}_{i_7} v^{i_7 a_4}_{a_5 a_6} - \tfrac{1}{2} t^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_5 a_6} - \tfrac{1}{2} \tilde{t}^{a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_5} \\
(\xi_{21})^{i_6 i_7}_{i_2 a_5} &= -v^{i_6 i_7}_{i_2 a_5} + (\Xi_4)^{i_6 i_7}_{i_2 a_5} \\
(\xi_{2,0})^{i_5}_{a_6} &= -f^{i_5}_{a_6} - (\Xi_7)^{i_5}_{a_6} \\
(\xi_2)^{i_5}_{i_2} &= -f^{i_5}_{i_2} + t^{a_6}_{i_2} (\xi_{2,0})^{i_5}_{a_6} - t^{a_6}_{i_7} v^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_2 i_8} v^{i_5 i_8}_{a_6 a_7} - \tfrac{1}{2} t^{i_6 i_7}_{i_2 i_8} V^{i_5 i_8}_{i_6 i_7} \\
(\xi_{19})^{i_6 a_4}_{i_2 a'_5} &= +v^{i_6 a_4}_{i_2 a'_5} - t^{a_7}_{i_2} v^{i_6 a_4}_{a'_5 a_7} + \tilde{t}^{a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_5 a'_7} \\
(\xi_{17})^{i_6 a_4}_{i_2 a_5} &= -v^{i_6 a_4}_{i_2 a_5} + (\Xi_1)^{i_6 a_4}_{i_2 a_5} + \tilde{t}^{a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_7 a_5} \\
(\xi_{16})^{i_5 i_6}_{i_1 i_2} &= +v^{i_5 i_6}_{i_1 i_2} - (\Xi_0)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2}(\Xi_{14})^{i_5 i_6}_{i_1 i_2} + (\Xi_6)^{i_5 i_6}_{i_1 i_2} + (\Xi_9)^{i_5 i_6}_{i_1 i_2} \\
(\xi_{13})^{a_4}_{a'_5} &= +r^{a_6}_{i_7} v^{i_7 a_4}_{a'_5 a_6} + \tfrac{1}{2} r^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a_6} - \tfrac{1}{2} \tilde{r}^{a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_5 a'_6} \\
(\xi_{12})^{i_6 a_4}_{i_2 a'_5} &= -r^{a_7}_{i_2} v^{i_6 a_4}_{a'_5 a_7} \\
(\xi_{11})^{a_4}_{a_5} &= -r^{a_6}_{i_7} v^{i_7 a_4}_{a_5 a_6} - \tfrac{1}{2} r^{a_4 a_6}_{i_7 i_8} v^{i_7 i_8}_{a_5 a_6} - \tfrac{1}{2} \tilde{r}^{a'_6 a_4}_{i_7 i_8} v^{i_7 i_8}_{a'_6 a_5} \\
(\xi_{10})^{i_6 a_4}_{i_2 a_5} &= +(\Xi_3)^{i_6 a_4}_{i_2 a_5} + r^{a_4 a_7}_{i_2 i_8} v^{i_6 i_8}_{a_5 a_7} + \tilde{r}^{a'_7 a_4}_{i_2 i_8} v^{i_6 i_8}_{a'_7 a_5} \\
(\xi_{1,0})^{i_5}_{a_6} &= -f^{i_5}_{a_6} - (\Xi_7)^{i_5}_{a_6} \\
(\xi_1)^{i_5}_{i_2} &= +r^{a_6}_{i_2} (\xi_{1,0})^{i_5}_{a_6} - r^{a_6}_{i_7} v^{i_5 i_7}_{i_2 a_6} - t^{a_6}_{i_2} (\Xi_8)^{i_5}_{a_6} - \tfrac{1}{2} r^{a_6 a_7}_{i_2 i_8} v^{i_5 i_8}_{a_6 a_7} \\
&\quad - \tfrac{1}{2} r^{i_7 i_8}_{i_2 i_6} V^{i_5 i_6}_{i_7 i_8} \\
(\xi_{0,5})^{i_5 i_7}_{i_2 a'_6} &= -v^{i_5 i_7}_{i_2 a'_6} + (\Xi_{10})^{i_5 i_7}_{i_2 a'_6} \\
(\xi_{0,3})^{i_5 i_7}_{i_2 a_6} &= +v^{i_5 i_7}_{i_2 a_6} - (\Xi_4)^{i_5 i_7}_{i_2 a_6} \\
(\xi_{0,2})^{i_5 a_4}_{i_2 a_6} &= +v^{i_5 a_4}_{i_2 a_6} - \tfrac{1}{2} (\Xi_1)^{i_5 a_4}_{i_2 a_6} \\
(\xi_{0,1})^{i_5}_{a'_6} &= -f^{i_5}_{a'_6} - (\Xi_{11})^{i_5}_{a'_6} \\
(\xi_{0,0})^{i_5}_{a_6} &= +f^{i_5}_{a_6} + (\Xi_7)^{i_5}_{a_6} \\
(\xi_0)^{i_5 a_4}_{i_1 i_2} &= -v^{i_5 a_4}_{i_1 i_2} + t^{a_4 a_6}_{i_1 i_2} (\xi_{0,0})^{i_5}_{a_6} + \tilde{t}^{a'_6 a_4}_{i_1 i_2} (\xi_{0,1})^{i_5}_{a'_6} + P_2 t^{a_6}_{i_1} (\xi_{0,2})^{i_5 a_4}_{i_2 a_6} \\
&\quad + P_2 t^{a_4 a_6}_{i_1 i_7} (\xi_{0,3})^{i_5 i_7}_{i_2 a_6} - \tfrac{1}{2} t^{a_6 a_7}_{i_1 i_2} v^{i_5 a_4}_{a_6 a_7} + P_2 \tilde{t}^{a'_6 a_4}_{i_1 i_7} (\xi_{0,5})^{i_5 i_7}_{i_2 a'_6} \\
&\quad - \tfrac{1}{2} t^{i_6 i_7}_{i_1 i_2} V^{i_5 a_4}_{i_6 i_7} + \tfrac{1}{2} t^{a_4 a_6 a_7}_{i_1 i_2 i_8} v^{i_5 i_8}_{a_6 a_7} \\
\delta^{a_3 a_4}_{i_1 i_2} &= +P_2 r^{a_3}_{i_5} (\xi_0)^{i_5 a_4}_{i_1 i_2} + P_2 t^{a_3 a_4}_{i_1 i_5} (\xi_1)^{i_5}_{i_2} + P_2 r^{a_3 a_4}_{i_1 i_5} (\xi_2)^{i_5}_{i_2} + P_2 r^{a_3 a_5}_{i_1 i_2} (\xi_3)^{a_4}_{a_5} \\
&\quad + P_2 \tilde{r}^{a'_5 a_3}_{i_1 i_2} (\xi_4)^{a_4}_{a'_5} + P_2 t^{a_3}_{i_5} (\xi_5)^{i_5 a_4}_{i_1 i_2} + r^{a_3 a_4 a_5}_{i_1 i_2 i_6} (\xi_6)^{i_6}_{a_5} - P_2 r^{a_5}_{i_1} v^{a_3 a_4}_{i_2 a_5} \\
&\quad + P_2 t^{a_5}_{i_1} (\xi_8)^{a_3 a_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_3 a_4}_{i_5 i_6} (\xi_9)^{i_5 i_6}_{i_1 i_2} + P_2 P_2 t^{a_3 a_5}_{i_1 i_6} (\xi_{10})^{i_6 a_4}_{i_2 a_5} \\
&\quad + P_2 t^{a_3 a_5}_{i_1 i_2} (\xi_{11})^{a_4}_{a_5} + P_2 P_2 \tilde{t}^{a'_5 a_3}_{i_1 i_6} (\xi_{12})^{i_6 a_4}_{i_2 a'_5} + P_2 \tilde{t}^{a'_5 a_3}_{i_1 i_2} (\xi_{13})^{a_4}_{a'_5} \\
&\quad + \tfrac{1}{2} P_2 t^{a_3 a_4 a_5}_{i_1 i_6 i_7} (\Xi_5)^{i_6 i_7}_{i_2 a_5} + t^{a_3 a_4 a_5}_{i_1 i_2 i_6} (\Xi_8)^{i_6}_{a_5} + \tfrac{1}{2} r^{a_3 a_4}_{i_5 i_6} (\xi_{16})^{i_5 i_6}_{i_1 i_2} \\
&\quad + P_2 P_2 r^{a_3 a_5}_{i_1 i_6} (\xi_{17})^{i_6 a_4}_{i_2 a_5} + \tfrac{1}{2} r^{a_5 a_6}_{i_1 i_2} v^{a_3 a_4}_{a_5 a_6} + P_2 P_2 \tilde{r}^{a'_5 a_3}_{i_1 i_6} (\xi_{19})^{i_6 a_4}_{i_2 a'_5} \\
&\quad + \tfrac{1}{2} r^{i_5 i_6}_{i_1 i_2} V^{a_3 a_4}_{i_5 i_6} + \tfrac{1}{2} P_2 r^{a_3 a_4 a_5}_{i_1 i_6 i_7} (\xi_{21})^{i_6 i_7}_{i_2 a_5} - \tfrac{1}{2} P_2 r^{a_3 a_5 a_6}_{i_1 i_2 i_7} v^{i_7 a_4}_{a_5 a_6}
\end{aligned}
$$

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TABLE ESI.4.XXXV: The computational sequence and intermediates for the R_3 amplitude equation of right-hand EOM-CCSDT-R12 [Part I]

$$(\Xi_0)^{i_7 i_8}_{i_2 i_3} = +P_2 t^{a_9}_{i_2} v^{i_7 i_8}_{i_3 a_9}$$
$$(\Xi_1)^{i_8 a_6}_{i_3 a_7} = +t^{a_9}_{i_3} v^{i_8 a_6}_{a_7 a_9}$$
$$(\Xi_2)^{i_7 i_8}_{i_2 i_3} = +P_2 r^{a_9}_{i_2} v^{i_7 i_8}_{i_3 a_9}$$
$$(\Xi_3)^{i_8 a_6}_{i_3 a_7} = +r^{a_9}_{i_3} v^{i_8 a_6}_{a_7 a_9}$$
$$(\Xi_4)^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +P_3 \tilde{t}^{a'_9 a_6}_{i_1 i_2} v^{i_7 i_8}_{i_3 a'_9}$$
$$(\Xi_5)^{i_7 a_6}_{i_3 a'_8} = +t^{a_9}_{i_3} v^{i_7 a_6}_{a'_8 a_9}$$
$$(\Xi_6)^{i_7 i_9}_{i_3 a_8} = +t^{a_{10}}_{i_3} v^{i_7 i_9}_{a_8 a_{10}}$$
$$(\Xi_7)^{i_7 i_9}_{i_3 a_8} = +r^{a_{10}}_{i_3} v^{i_7 i_9}_{a_8 a_{10}}$$
$$(\Xi_8)^{i_7 i_8}_{i_3 a'_9} = +t^{a_{10}}_{i_3} v^{i_7 i_8}_{a'_9 a_{10}}$$
$$(\Xi_9)^{i_7 i_8}_{i_3 a'_9} = +r^{a_{10}}_{i_3} v^{i_7 i_8}_{a'_9 a_{10}}$$
$$(\Xi_{10})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +\tfrac{1}{2} t^{a_6 a_9 a_{10}}_{i_1 i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\Xi_{11})^{i_7}_{a_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\Xi_{12})^{i_7}_{a_8} = +r^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\Xi_{13})^{i_8 a_6}_{i_3 a_7} = +t^{a_6 a_9}_{i_3 i_{10}} v^{i_8 i_{10}}_{a_7 a_9}$$
$$(\Xi_{14})^{i_7 i_8}_{i_2 i_3} = +\tfrac{1}{2} t^{a_9 a_{10}}_{i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\Xi_{15})^{i_7 i_8}_{i_2 i_3} = +\tfrac{1}{2} t^{i_9 i_{10}}_{i_2 i_3} V^{i_7 i_8}_{i_9 i_{10}}$$
$$(\Xi_{16})^{i_8 a_6}_{i_3 a_7} = +\tilde{t}^{a'_9 a_6}_{i_3 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\Xi_{17})^{i_7 a_6}_{i_3 a'_8} = +t^{a_6 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_{18})^{i_7 a_6}_{i_3 a'_8} = +\tilde{t}^{a'_9 a_6}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a'_9}$$
$$(\Xi_{19})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +P_3 \tilde{r}^{a'_9 a_6}_{i_1 i_2} v^{i_7 i_8}_{i_3 a'_9}$$
$$(\Xi_{20})^{i_8 a_6}_{i_3 a_7} = +r^{a_6 a_9}_{i_3 i_{10}} v^{i_8 i_{10}}_{a_7 a_9}$$
$$(\Xi_{21})^{i_7 i_8}_{i_2 i_3} = +\tfrac{1}{2} r^{a_9 a_{10}}_{i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\Xi_{22})^{i_7}_{a'_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_{23})^{i_8 a_6}_{i_3 a_7} = +\tilde{r}^{a'_9 a_6}_{i_3 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\Xi_{24})^{i_7 i_8}_{i_2 i_3} = +\tfrac{1}{2} V^{i_7 i_8}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_2 i_3}$$
$$(\Xi_{25})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +\tfrac{1}{2} r^{a_6 a_9 a_{10}}_{i_1 i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\Xi_{26})^{i_7 i_8}_{i_2 i_3} = +P_2 t^{a_9}_{i_2} (\Xi_6)^{i_7 i_8}_{i_3 a_9}$$
$$(\Xi_{27})^{i_7 i_8}_{i_2 i_3} = +P_2 t^{a_9}_{i_2} (\Xi_7)^{i_7 i_8}_{i_3 a_9}$$
$$(\Xi_{28})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +P_3 \tilde{t}^{a'_9 a_6}_{i_1 i_2} (\Xi_8)^{i_7 i_8}_{i_3 a'_9}$$
$$(\Xi_{29})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +P_3 \tilde{t}^{a'_9 a_6}_{i_1 i_2} (\Xi_9)^{i_7 i_8}_{i_3 a'_9}$$
$$(\Xi_{30})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +P_3 \tilde{r}^{a'_9 a_6}_{i_1 i_2} (\Xi_8)^{i_7 i_8}_{i_3 a'_9}$$
$$(\xi_9)^{i_7 i_8}_{i_2 i_3} = -(\Xi_2)^{i_7 i_8}_{i_2 i_3} + (\Xi_{27})^{i_7 i_8}_{i_2 i_3} + (\Xi_{21})^{i_7 i_8}_{i_2 i_3} + (\Xi_{24})^{i_7 i_8}_{i_2 i_3}$$
$$(\xi_8)^{a_5 a_6}_{i_3 a'_7} = -r^{a_8}_{i_3} v^{a_5 a_6}_{a'_7 a_8} - P_2 r^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a_8} + P_2 \tilde{r}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a'_8} - \tfrac{1}{2} r^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\xi_{7,2})^{i_8 i_9}_{i_3 a_7} = -v^{i_8 i_9}_{i_3 a_7} + (\Xi_6)^{i_8 i_9}_{i_3 a_7}$$
$$(\xi_7)^{a_5 a_6}_{i_3 a_7} = +r^{a_8}_{i_3} v^{a_5 a_6}_{a_7 a_8} + \tfrac{1}{2} t^{a_5 a_6}_{i_8 i_9} (\Xi_7)^{i_8 i_9}_{i_3 a_7} + \tfrac{1}{2} r^{a_5 a_6}_{i_8 i_9} (\xi_{7,2})^{i_8 i_9}_{i_3 a_7} + P_2 r^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a_7 a_8} + P_2 \tilde{r}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_8 a_7} + \tfrac{1}{2} r^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8}$$
$$(\xi_{6,9})^{i_7 i_9}_{i_3 a_8} = -v^{i_7 i_9}_{i_3 a_8} + (\Xi_6)^{i_7 i_9}_{i_3 a_8}$$
$$(\xi_{6,8})^{i_7 a_6}_{i_3 a'_8} = +v^{i_7 a_6}_{i_3 a'_8} - (\Xi_5)^{i_7 a_6}_{i_3 a'_8} - (\Xi_{17})^{i_7 a_6}_{i_3 a'_8} + (\Xi_{18})^{i_7 a_6}_{i_3 a'_8}$$
$$(\xi_{6,7})^{i_7 a_6}_{i_3 a_8} = -v^{i_7 a_6}_{i_3 a_8} + (\Xi_1)^{i_7 a_6}_{i_3 a_8} + (\Xi_{13})^{i_7 a_6}_{i_3 a_8} + (\Xi_{16})^{i_7 a_6}_{i_3 a_8}$$
$$(\xi_{6,4,1})^{i_7 i_8}_{i_3 a_9} = -v^{i_7 i_8}_{i_3 a_9} + (\Xi_6)^{i_7 i_8}_{i_3 a_9}$$
$$(\xi_{6,4})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = -(\Xi_{29})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{19})^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{30})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{25})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 t^{a_6 a_9}_{i_1 i_2} (\Xi_7)^{i_7 i_8}_{i_3 a_9} + P_3 r^{a_6 a_9}_{i_1 i_2} (\xi_{6,4,1})^{i_7 i_8}_{i_3 a_9}$$
$$(\xi_{6,3})^{i_7 a_6}_{i_3 a'_8} = -r^{a_9}_{i_3} v^{i_7 a_6}_{a'_8 a_9} - r^{a_6 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a_9} + \tilde{r}^{a'_9 a_6}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a'_9}$$
$$(\xi_{6,2})^{i_7 a_6}_{i_3 a_8} = +(\Xi_3)^{i_7 a_6}_{i_3 a_8} + (\Xi_{20})^{i_7 a_6}_{i_3 a_8} + (\Xi_{23})^{i_7 a_6}_{i_3 a_8}$$
$$(\xi_{6,1,0})^{i_7 i_8}_{i_3 a_9} = -v^{i_7 i_8}_{i_3 a_9} + (\Xi_6)^{i_7 i_8}_{i_3 a_9}$$
$$(\xi_{6,1})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +(\Xi_4)^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{28})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{10})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 t^{a_6 a_9}_{i_1 i_2} (\xi_{6,1,0})^{i_7 i_8}_{i_3 a_9}$$
$$(\xi_{6,0})^{i_7}_{a_8} = -f^{i_7}_{a_8} - (\Xi_{11})^{i_7}_{a_8}$$
$$(\xi_6)^{i_7 a_5 a_6}_{i_1 i_2 i_3} = +r^{a_5 a_6 a_8}_{i_1 i_2 i_3} (\xi_{6,0})^{i_7}_{a_8} + P_2 r^{a_5}_{i_8} (\xi_{6,1})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_2 P_3 t^{a_5 a_8}_{i_1 i_2} (\xi_{6,2})^{i_7 a_6}_{i_3 a_8} + P_2 P_3 \tilde{t}^{a'_8 a_5}_{i_1 i_2} (\xi_{6,3})^{i_7 a_6}_{i_3 a'_8} + \tfrac{1}{2} P_2 t^{a_5}_{i_8} (\xi_{6,4})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 t^{a_5 a_6 a_8}_{i_1 i_2 i_9} (\Xi_7)^{i_7 i_9}_{i_3 a_8} - t^{a_5 a_6 a_8}_{i_1 i_2 i_3} (\Xi_{12})^{i_7}_{a_8} + P_2 P_3 r^{a_5 a_8}_{i_1 i_2} (\xi_{6,7})^{i_7 a_6}_{i_3 a_8} + P_2 P_3 \tilde{r}^{a'_8 a_5}_{i_1 i_2} (\xi_{6,8})^{i_7 a_6}_{i_3 a'_8} + P_3 r^{a_5 a_6 a_8}_{i_1 i_2 i_9} (\xi_{6,9})^{i_7 i_9}_{i_3 a_8} + \tfrac{1}{2} P_2 r^{a_5 a_8 a_9}_{i_1 i_2 i_3} v^{i_7 a_6}_{a_8 a_9}$$
$$(\xi_5)^{a_6}_{a_7} = +f^{a_6}_{a_7} - t^{a_8}_{i_9} v^{i_9 a_6}_{a_7 a_8} - \tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_7}$$
$$(\xi_{4,0})^{i_7}_{a_8} = -f^{i_7}_{a_8} - (\Xi_{11})^{i_7}_{a_8}$$
$$(\xi_4)^{i_7}_{i_3} = -f^{i_7}_{i_3} + t^{a_8}_{i_3} (\xi_{4,0})^{i_7}_{a_8} - t^{a_8}_{i_9} v^{i_7 i_9}_{i_3 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} t^{i_8 i_9}_{i_3 i_{10}} V^{i_7 i_{10}}_{i_8 i_9}$$
$$(\xi_{3,9})^{i_7}_{a'_8} = -r^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\xi_{3,4})^{i_7 i_8}_{i_2 i_3} = -(\Xi_2)^{i_7 i_8}_{i_2 i_3} + (\Xi_{27})^{i_7 i_8}_{i_2 i_3} + (\Xi_{21})^{i_7 i_8}_{i_2 i_3} + (\Xi_{24})^{i_7 i_8}_{i_2 i_3}$$
$$(\xi_{3,2})^{i_7 i_8}_{i_2 i_3} = +v^{i_7 i_8}_{i_2 i_3} - (\Xi_0)^{i_7 i_8}_{i_2 i_3} + \tfrac{1}{2} (\Xi_{26})^{i_7 i_8}_{i_2 i_3} + (\Xi_{14})^{i_7 i_8}_{i_2 i_3} + (\Xi_{15})^{i_7 i_8}_{i_2 i_3}$$
$$(\xi_{3,12})^{i_7 i_9}_{i_3 a'_8} = -v^{i_7 i_9}_{i_3 a'_8} + (\Xi_8)^{i_7 i_9}_{i_3 a'_8}$$
$$(\xi_{3,10})^{i_7 i_9}_{i_3 a_8} = +v^{i_7 i_9}_{i_3 a_8} - (\Xi_6)^{i_7 i_9}_{i_3 a_8}$$
$$(\xi_{3,1})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - (\Xi_{22})^{i_7}_{a'_8}$$
$$(\xi_{3,0})^{i_7}_{a_8} = +f^{i_7}_{a_8} + (\Xi_{11})^{i_7}_{a_8}$$
$$(\xi_3)^{i_7 a_6}_{i_2 i_3} = +r^{a_6 a_8}_{i_2 i_3} (\xi_{3,0})^{i_7}_{a_8} + \tilde{r}^{a'_8 a_6}_{i_2 i_3} (\xi_{3,1})^{i_7}_{a'_8} + r^{a_6}_{i_8} (\xi_{3,2})^{i_7 i_8}_{i_2 i_3} + P_2 r^{a_8}_{i_2} v^{i_7 a_6}_{i_3 a_8} + t^{a_6}_{i_8} (\xi_{3,4})^{i_7 i_8}_{i_2 i_3} - P_2 t^{a_8}_{i_2} (\Xi_3)^{i_7 a_6}_{i_3 a_8} - P_2 t^{a_6 a_8}_{i_2 i_9} (\Xi_7)^{i_7 i_9}_{i_3 a_8} + t^{a_6 a_8}_{i_2 i_3} (\Xi_{12})^{i_7}_{a_8} + P_2 \tilde{t}^{a'_8 a_6}_{i_2 i_9} (\Xi_9)^{i_7 i_9}_{i_3 a'_8} + \tilde{t}^{a'_8 a_6}_{i_2 i_3} (\xi_{3,9})^{i_7}_{a'_8} + P_2 r^{a_6 a_8}_{i_2 i_9} (\xi_{3,10})^{i_7 i_9}_{i_3 a_8} - \tfrac{1}{2} r^{a_8 a_9}_{i_2 i_3} v^{i_7 a_6}_{a_8 a_9} + P_2 \tilde{r}^{a'_8 a_6}_{i_2 i_9} (\xi_{3,12})^{i_7 i_9}_{i_3 a'_8} - \tfrac{1}{2} r^{i_8 i_9}_{i_2 i_3} V^{i_7 a_6}_{i_8 i_9} + \tfrac{1}{2} r^{a_6 a_8 a_9}_{i_2 i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\xi_{2,6})^{i_7 i_9}_{i_3 a'_8} = -v^{i_7 i_9}_{i_3 a'_8} + (\Xi_8)^{i_7 i_9}_{i_3 a'_8}$$
$$(\xi_{2,4})^{i_7 i_9}_{i_3 a_8} = +v^{i_7 i_9}_{i_3 a_8} - (\Xi_6)^{i_7 i_9}_{i_3 a_8}$$
$$(\xi_{2,3})^{i_7 a_6}_{i_3 a_8} = +v^{i_7 a_6}_{i_3 a_8} - \tfrac{1}{2} (\Xi_1)^{i_7 a_6}_{i_3 a_8}$$
$$(\xi_{2,2})^{i_7 i_8}_{i_2 i_3} = +v^{i_7 i_8}_{i_2 i_3} - (\Xi_0)^{i_7 i_8}_{i_2 i_3} + \tfrac{1}{2} (\Xi_{26})^{i_7 i_8}_{i_2 i_3} + (\Xi_{14})^{i_7 i_8}_{i_2 i_3} + (\Xi_{15})^{i_7 i_8}_{i_2 i_3}$$
$$(\xi_{2,1})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - (\Xi_{22})^{i_7}_{a'_8}$$
$$(\xi_{2,0})^{i_7}_{a_8} = +f^{i_7}_{a_8} + (\Xi_{11})^{i_7}_{a_8}$$
$$(\xi_2)^{i_7 a_6}_{i_2 i_3} = -v^{i_7 a_6}_{i_2 i_3} + t^{a_6 a_8}_{i_2 i_3} (\xi_{2,0})^{i_7}_{a_8} + \tilde{t}^{a'_8 a_6}_{i_2 i_3} (\xi_{2,1})^{i_7}_{a'_8} + t^{a_6}_{i_8} (\xi_{2,2})^{i_7 i_8}_{i_2 i_3} + P_2 t^{a_8}_{i_2} (\xi_{2,3})^{i_7 a_6}_{i_3 a_8} + P_2 t^{a_6 a_8}_{i_2 i_9} (\xi_{2,4})^{i_7 i_9}_{i_3 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_2 i_3} v^{i_7 a_6}_{a_8 a_9} + P_2 \tilde{t}^{a'_8 a_6}_{i_2 i_9} (\xi_{2,6})^{i_7 i_9}_{i_3 a'_8} - \tfrac{1}{2} t^{i_8 i_9}_{i_2 i_3} V^{i_7 a_6}_{i_8 i_9} + \tfrac{1}{2} t^{a_6 a_8 a_9}_{i_2 i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\xi_{17})^{i_8 a_6}_{i_3 a_7} = -v^{i_8 a_6}_{i_3 a_7} + (\Xi_1)^{i_8 a_6}_{i_3 a_7} + (\Xi_{13})^{i_8 a_6}_{i_3 a_7} + (\Xi_{16})^{i_8 a_6}_{i_3 a_7}$$
$$(\xi_{16})^{i_7 i_8}_{i_2 i_3} = +v^{i_7 i_8}_{i_2 i_3} - (\Xi_0)^{i_7 i_8}_{i_2 i_3} + \tfrac{1}{2} (\Xi_{26})^{i_7 i_8}_{i_2 i_3} + (\Xi_{14})^{i_7 i_8}_{i_2 i_3} + (\Xi_{15})^{i_7 i_8}_{i_2 i_3}$$
$$(\xi_{15})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +(\Xi_4)^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{28})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{10})^{i_7 i_8 a_6}_{i_1 i_2 i_3}$$
$$(\xi_{14})^{a_5 a_6}_{i_3 a'_7} = +v^{a_5 a_6}_{i_3 a'_7} - t^{a_8}_{i_3} v^{a_5 a_6}_{a'_7 a_8} - P_2 t^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a_8} + P_2 \tilde{t}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a'_8} - \tfrac{1}{2} t^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\xi_{13,1})^{i_8 i_9}_{i_3 a_7} = -v^{i_8 i_9}_{i_3 a_7} + (\Xi_6)^{i_8 i_9}_{i_3 a_7}$$
$$(\xi_{13})^{a_5 a_6}_{i_3 a_7} = -v^{a_5 a_6}_{i_3 a_7} + t^{a_8}_{i_3} v^{a_5 a_6}_{a_7 a_8} + \tfrac{1}{2} t^{a_5 a_6}_{i_8 i_9} (\xi_{13,1})^{i_8 i_9}_{i_3 a_7} + P_2 t^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a_7 a_8} + P_2 \tilde{t}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_8 a_7} + \tfrac{1}{2} t^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8}$$
$$(\xi_{12})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = -(\Xi_{29})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{19})^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{30})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{25})^{i_7 i_8 a_6}_{i_1 i_2 i_3}$$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.4.XXXVI: The computational sequence and intermediates for the R_3 amplitude equation of right-hand EOM-CCSDT-R12 [Part II]

$$
\begin{aligned}
(\xi_{11})^{a_6}_{a_7} &= -r^{a_8}_{i_9} v^{i_9 a_6}_{a_7 a_8} - \tfrac{1}{2} r^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8} - \tfrac{1}{2} \tilde{r}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_7} \\
(\xi_{10})^{i_8 a_6}_{i_3 a_7} &= +(\Xi_3)^{i_8 a_6}_{i_3 a_7} + (\Xi_{20})^{i_8 a_6}_{i_3 a_7} + (\Xi_{23})^{i_8 a_6}_{i_3 a_7} \\
(\xi_{1,0})^{i_7}_{a_8} &= -f^{i_7}_{a_8} - (\Xi_{11})^{i_7}_{a_8} \\
(\xi_1)^{i_7}_{i_3} &= +r^{a_8}_{i_3} (\xi_{1,0})^{i_7}_{a_8} - r^{a_8}_{i_9} v^{i_7 i_9}_{i_3 a_8} - t^{a_8}_{i_3} (\Xi_{12})^{i_7}_{a_8} - \tfrac{1}{2} r^{a_8 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} r^{i_9 i_{10}}_{i_3 i_8} V^{i_7 i_8}_{i_9 i_{10}} \\
(\xi_{0,3})^{i_7 i_9}_{i_3 a_8} &= -v^{i_7 i_9}_{i_3 a_8} + (\Xi_6)^{i_7 i_9}_{i_3 a_8} \\
(\xi_{0,2})^{i_7 a_6}_{i_3 a'_8} &= +v^{i_7 a_6}_{i_3 a'_8} - (\Xi_5)^{i_7 a_6}_{i_3 a'_8} - (\Xi_{17})^{i_7 a_6}_{i_3 a'_8} + (\Xi_{18})^{i_7 a_6}_{i_3 a'_8} \\
(\xi_{0,1})^{i_7 a_6}_{i_3 a_8} &= -v^{i_7 a_6}_{i_3 a_8} + (\Xi_1)^{i_7 a_6}_{i_3 a_8} + (\Xi_{13})^{i_7 a_6}_{i_3 a_8} + (\Xi_{16})^{i_7 a_6}_{i_3 a_8} \\
(\xi_{0,0})^{i_7}_{a_8} &= -f^{i_7}_{a_8} - (\Xi_{11})^{i_7}_{a_8} \\
(\xi_0)^{i_7 a_5 a_6}_{i_1 i_2 i_3} &= +t^{a_5 a_6 a_8}_{i_1 i_2 i_3} (\xi_{0,0})^{i_7}_{a_8} + P_2 P_3 t^{a_5 a_8}_{i_1 i_2} (\xi_{0,1})^{i_7 a_6}_{i_3 a_8} + P_2 P_3 \tilde{t}^{a'_8 a_5}_{i_1 i_2} (\xi_{0,2})^{i_7 a_6}_{i_3 a'_8} \\
&\quad + P_3 t^{a_5 a_6 a_8}_{i_1 i_2 i_9} (\xi_{0,3})^{i_7 i_9}_{i_3 a_8} + \tfrac{1}{2} P_2 t^{a_5 a_8 a_9}_{i_1 i_2 i_3} v^{i_7 a_6}_{a_8 a_9}
\end{aligned}
$$

$$
\begin{aligned}
\delta^{a_4 a_5 a_6}_{i_1 i_2 i_3} &= +P_3 r^{a_4}_{i_7} (\xi_0)^{i_7 a_5 a_6}_{i_1 i_2 i_3} + P_3 t^{a_4 a_5 a_6}_{i_1 i_2 i_7} (\xi_1)^{i_7}_{i_3} + P_3 P_3 r^{a_4 a_5}_{i_1 i_7} (\xi_2)^{i_7 a_6}_{i_2 i_3} \\
&\quad + P_3 P_3 t^{a_4 a_5}_{i_1 i_7} (\xi_3)^{i_7 a_6}_{i_2 i_3} + P_3 r^{a_4 a_5 a_6}_{i_1 i_2 i_7} (\xi_4)^{i_7}_{i_3} + P_3 r^{a_4 a_5 a_7}_{i_1 i_2 i_3} (\xi_5)^{a_6}_{a_7} \\
&\quad + P_3 t^{a_4}_{i_7} (\xi_6)^{i_7 a_5 a_6}_{i_1 i_2 i_3} + P_3 P_3 t^{a_4 a_7}_{i_1 i_2} (\xi_7)^{a_5 a_6}_{i_3 a_7} + P_3 P_3 \tilde{t}^{a'_7 a_4}_{i_1 i_2} (\xi_8)^{a_5 a_6}_{i_3 a'_7} \\
&\quad + \tfrac{1}{2} P_3 t^{a_4 a_5 a_6}_{i_1 i_7 i_8} (\xi_9)^{i_7 i_8}_{i_2 i_3} + P_3 P_3 t^{a_4 a_5 a_7}_{i_1 i_2 i_8} (\xi_{10})^{i_8 a_6}_{i_3 a_7} + P_3 t^{a_4 a_5 a_7}_{i_1 i_2 i_3} (\xi_{11})^{a_6}_{a_7} \\
&\quad + \tfrac{1}{2} P_3 t^{a_4 a_5}_{i_7 i_8} (\xi_{12})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 P_3 r^{a_4 a_7}_{i_1 i_2} (\xi_{13})^{a_5 a_6}_{i_3 a_7} \\
&\quad + P_3 P_3 \tilde{r}^{a'_7 a_4}_{i_1 i_2} (\xi_{14})^{a_5 a_6}_{i_3 a'_7} + \tfrac{1}{2} P_3 r^{a_4 a_5}_{i_7 i_8} (\xi_{15})^{i_7 i_8 a_6}_{i_1 i_2 i_3} \\
&\quad + \tfrac{1}{2} P_3 r^{a_4 a_5 a_6}_{i_1 i_7 i_8} (\xi_{16})^{i_7 i_8}_{i_2 i_3} + P_3 P_3 r^{a_4 a_5 a_7}_{i_1 i_2 i_8} (\xi_{17})^{i_8 a_6}_{i_3 a_7} + \tfrac{1}{2} P_3 r^{a_4 a_7 a_8}_{i_1 i_2 i_3} v^{a_5 a_6}_{a_7 a_8}
\end{aligned}
$$

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TABLE ESI.4.XXXVII: The computational sequence and intermediates for the geminal r amplitude equation of right-hand EOM-CCSDT-R12 and higher-order EOM-CC-R12 [Part I]

$$(\Xi_0)^{i_3 i_4}_{i_7 a'_8} = +r^{a_9}_{i_7} F^{i_3 i_4 *}_{a'_8 a_9}$$
$$(\Xi_1)^{i_3 i_4}_{i_7 a'_8} = +t^{a_9}_{i_7} F^{i_3 i_4 *}_{a'_8 a_9}$$
$$(\Xi_2)^{i_8 a'_6}_{i_2 a_7} = +t^{a_9}_{i_2} v^{i_8 a'_6}_{a_7 a_9}$$
$$(\Xi_3)^{i_8 a'_6}_{i_2 a_7} = +r^{a_9}_{i_2} v^{i_8 a'_6}_{a_7 a_9}$$
$$(\Xi_4)^{a'_7}_{a_6} = +r^{a_8}_{i_9} v^{i_9 a'_7}_{a_6 a_8}$$
$$(\Xi_5)^{i_8 a'_5}_{i_2 a'_7} = +r^{a_9}_{i_2} v^{i_8 a'_5}_{a'_7 a_9}$$
$$(\Xi_6)^{a'_5}_{a'_7} = +r^{a_8}_{i_9} v^{i_9 a'_5}_{a'_7 a_8}$$
$$(\Xi_7)^{i_7 i_9}_{i_2 a'_8} = +t^{a_{10}}_{i_2} v^{i_7 i_9}_{a'_8 a_{10}}$$
$$(\Xi_8)^{i_7 i_9}_{i_2 a_8} = +t^{a_{10}}_{i_2} v^{i_7 i_9}_{a_8 a_{10}}$$
$$(\Xi_9)^{i_7}_{a'_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_{10})^{i_7}_{a_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\Xi_{11})^{i_7 i_8}_{i_2 a_9} = +r^{a_{10}}_{i_2} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\Xi_{12})^{i_7}_{a_8} = +r^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\Xi_{13})^{a'_7}_{a_6} = +t^{a_8}_{i_9} v^{i_9 a'_7}_{a_6 a_8}$$
$$(\Xi_{14})^{a'_7}_{a'_5} = +t^{a_8}_{i_9} v^{i_9 a'_7}_{a'_5 a_8}$$
$$(\Xi_{15})^{i_8 a'_5}_{i_2 a'_7} = +t^{a_9}_{i_2} v^{i_8 a'_5}_{a'_7 a_9}$$
$$(\Xi_{16})^{i_8 a'_6}_{i_2 a_7} = +\tilde{r}^{\,a'_6 a_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\Xi_{17})^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{r}^{\,a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\Xi_{18})^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{r}^{\,a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8}$$
$$(\Xi_{19})^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{t}^{\,a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\Xi_{20})^{a'_7}_{a_6} = +\tfrac{1}{2}\tilde{t}^{\,a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8}$$
$$(\Xi_{21})^{i_8 a'_6}_{i_2 a_7} = +\tilde{t}^{\,a'_6 a'_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\Xi_{22})^{a'_7}_{a'_5} = +\tfrac{1}{2}\tilde{t}^{\,a'_7 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_5 a'_8}$$
$$(\Xi_{23})^{a'_7}_{a'_5} = +\tfrac{1}{2}\tilde{t}^{\,a'_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_5 a_8}$$
$$(\Xi_{24})^{a'_5}_{a'_7} = +\tfrac{1}{2}\tilde{r}^{\,a'_5 a'_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\Xi_{25})^{a'_5}_{a'_7} = +\tfrac{1}{2}\tilde{r}^{\,a'_5 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\xi_{9,1})^{a'_7}_{a_6} = +(\Xi_4)^{a'_7}_{a_6} - (\Xi_{17})^{a'_7}_{a_6} + (\Xi_{18})^{a'_7}_{a_6}$$
$$(\xi_9)^{i_3 i_4}_{a_5 a_6} = +v^{i_7 a'_8}_{a_5 a_6}(\Xi_0)^{i_3 i_4}_{i_7 a'_8} + P_2 F^{i_3 i_4 *}_{a'_7 a_5}(\xi_{9,1})^{a'_7}_{a_6}$$
$$(\xi_8)^{i_3 i_4}_{i_2 a_5} = -v^{i_6 a'_7}_{i_2 a_5}(\Xi_0)^{i_3 i_4}_{i_6 a'_7} + r^{a_6}_{i_2}(V^\dagger)^{i_3 i_4}_{a_5 a_6}$$
$$(\xi_7)^{i_3 i_4}_{i_2 a_5} = -(V^\dagger)^{i_3 i_4}_{i_2 a_5} - v^{i_6 a'_7}_{i_2 a_5}(\Xi_1)^{i_3 i_4}_{i_6 a'_7}$$
$$(\xi_{5,3})^{a_7}_{a_6} = -t^{a_8}_{i_9} v^{i_9 a_7}_{a_6 a_8} - \tfrac{1}{2} t^{a_7 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_6 a_8} - \tfrac{1}{2}\tilde{t}^{\,a'_8 a_7}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_6}$$
$$(\xi_{5,2})^{a'_7}_{a_6} = -(\Xi_{13})^{a'_7}_{a_6} + (\Xi_{19})^{a'_7}_{a_6} - (\Xi_{20})^{a'_7}_{a_6}$$
$$(\xi_{5,1})^{a'_7}_{a'_5} = -(\Xi_{14})^{a'_7}_{a'_5} - (\Xi_{22})^{a'_7}_{a'_5} - (\Xi_{23})^{a'_7}_{a'_5}$$
$$(\xi_5)^{i_3 i_4}_{a'_5 a_6} = -f^{i_7}_{a_6}(\Xi_1)^{i_3 i_4}_{i_7 a'_5} + F^{i_3 i_4 *}_{a'_7 a_6}(\xi_{5,1})^{a'_7}_{a'_5} + F^{i_3 i_4 *}_{a'_5 a'_7}(\xi_{5,2})^{a'_7}_{a_6} + F^{i_3 i_4 *}_{a'_5 a_7}(\xi_{5,3})^{a_7}_{a_6}$$
$$(\xi_4)^{i_3 i_4}_{i_5 i_6} = +B^{i_3 i_4}_{i_5 i_6} + P^{i_3 i_4}_{i_5 i_6} + V^{i_7 a'_8}_{i_5 i_6}(\Xi_1)^{i_3 i_4}_{i_7 a'_8}$$
$$(\xi_{3,0})^{a'_7}_{a_6} = -f^{a'_7}_{a_6} + (\Xi_{13})^{a'_7}_{a_6} - (\Xi_{19})^{a'_7}_{a_6} + (\Xi_{20})^{a'_7}_{a_6}$$
$$(\xi_3)^{i_3 i_4}_{a_5 a_6} = +(V^\dagger)^{i_3 i_4}_{a_5 a_6} + P_2 F^{i_3 i_4 *}_{a'_7 a_5}(\xi_{3,0})^{a'_7}_{a_6} + v^{i_7 a'_8}_{a_5 a_6}(\Xi_1)^{i_3 i_4}_{i_7 a'_8}$$

$$(\xi_{2,3,0})^{i_7 i_8}_{i_2 a_9} = -v^{i_7 i_8}_{i_2 a_9} + \tfrac{1}{2}(\Xi_8)^{i_7 i_8}_{i_2 a_9}$$
$$(\xi_{2,3})^{i_7 i_8}_{i_1 i_2} = +P_2 t^{a_9}_{i_1}(\xi_{2,3,0})^{i_7 i_8}_{i_2 a_9} + \tfrac{1}{2} t^{a_9 a_{10}}_{i_1 i_2} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\xi_{2,2})^{i_7 i_8}_{i_1 i_2} = -P_2 r^{a_9}_{i_1} v^{i_7 i_8}_{i_2 a_9} + P_2 t^{a_9}_{i_1}(\Xi_{11})^{i_7 i_8}_{i_2 a_9} + \tfrac{1}{2} r^{a_9 a_{10}}_{i_1 i_2} v^{i_7 i_8}_{a_9 a_{10}} + \tfrac{1}{2} r^{i_9 i_{10}}_{i_1 i_2} V^{i_7 i_8}_{i_9 i_{10}}$$
$$(\xi_{2,1,0})^{i_7}_{a_8} = -f^{i_7}_{a_8} - (\Xi_{10})^{i_7}_{a_8}$$
$$(\xi_{2,1})^{i_7}_{i_2} = -f^{i_7}_{i_2} + t^{a_8}_{i_2}(\xi_{2,1,0})^{i_7}_{a_8} - t^{a_8}_{i_9} v^{i_7 i_9}_{i_2 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_2 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} t^{i_8 i_9}_{i_2 i_{10}} V^{i_7 i_{10}}_{i_8 i_9}$$
$$(\xi_{2,0,0})^{i_7}_{a_8} = -f^{i_7}_{a_8} - (\Xi_{10})^{i_7}_{a_8}$$
$$(\xi_{2,0})^{i_7}_{i_2} = +r^{a_8}_{i_2}(\xi_{2,0,0})^{i_7}_{a_8} - r^{a_8}_{i_9} v^{i_7 i_9}_{i_2 a_8} - t^{a_8}_{i_2}(\Xi_{12})^{i_7}_{a_8} - \tfrac{1}{2} r^{a_8 a_9}_{i_2 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} r^{i_8 i_9}_{i_2 i_{10}} V^{i_7 i_{10}}_{i_8 i_9}$$
$$(\xi_2)^{i_5 i_6}_{i_1 i_2} = +P_2 t^{i_5 i_6}_{i_1 i_7}(\xi_{2,0})^{i_7}_{i_2} + P_2 r^{i_5 i_6}_{i_1 i_7}(\xi_{2,1})^{i_7}_{i_2} + \tfrac{1}{2} t^{i_5 i_6}_{i_7 i_8}(\xi_{2,2})^{i_7 i_8}_{i_1 i_2} + \tfrac{1}{2} r^{i_5 i_6}_{i_7 i_8}(\xi_{2,3})^{i_7 i_8}_{i_1 i_2}$$
$$(\xi_{13,0})^{a'_7}_{a'_6} = -(\Xi_{14})^{a'_7}_{a'_6} - (\Xi_{22})^{a'_7}_{a'_6} - (\Xi_{23})^{a'_7}_{a'_6}$$
$$(\xi_{13})^{i_3 i_4}_{a'_5 a'_6} = +P_2 F^{i_3 i_4 *}_{a'_5 a'_7}(\xi_{13,0})^{a'_7}_{a'_6}$$
$$(\xi_{12})^{i_3 i_4}_{i_5 i_6} = +\tfrac{1}{2} r^{i_7 i_8}_{i_5 i_6} X^{i_3 i_4}_{i_7 i_8}$$
$$(\xi_{11,4})^{i_8 a'_6}_{i_2 a_7} = -v^{i_8 a'_6}_{i_2 a_7} + (\Xi_2)^{i_8 a'_6}_{i_2 a_7} - (\Xi_{21})^{i_8 a'_6}_{i_2 a_7} + \tilde{t}^{\,a'_6 a_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a_7 a_9}$$
$$(\xi_{11,3})^{i_8 a'_6}_{i_2 a'_7} = -v^{i_8 a'_6}_{i_2 a'_7} + (\Xi_{15})^{i_8 a'_6}_{i_2 a'_7} + \tilde{t}^{\,a'_6 a'_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_7 a'_9}$$
$$(\xi_{11,2})^{a'_6}_{a'_7} = -(\Xi_6)^{a'_6}_{a'_7} - (\Xi_{24})^{a'_6}_{a'_7} - (\Xi_{25})^{a'_6}_{a'_7}$$
$$(\xi_{11,1})^{i_8 a'_6}_{i_2 a_7} = +(\Xi_3)^{i_8 a'_6}_{i_2 a_7} - (\Xi_{16})^{i_8 a'_6}_{i_2 a_7}$$
$$(\xi_{11})^{a'_5 a'_6}_{i_1 i_2} = +P_2 P_2 \tilde{t}^{\,a'_5 a'_7}_{i_1 i_8}(\Xi_5)^{i_8 a'_6}_{i_2 a'_7} + P_2 P_2 \tilde{t}^{\,a'_5 a_7}_{i_1 i_8}(\xi_{11,1})^{i_8 a'_6}_{i_2 a_7} + P_2 \tilde{t}^{\,a'_5 a'_7}_{i_1 i_2}(\xi_{11,2})^{a'_6}_{a'_7} + P_2 P_2 \tilde{r}^{\,a'_5 a'_7}_{i_1 i_8}(\xi_{11,3})^{i_8 a'_6}_{i_2 a'_7} + P_2 P_2 \tilde{r}^{\,a'_5 a_7}_{i_1 i_8}(\xi_{11,4})^{i_8 a'_6}_{i_2 a_7}$$
$$(\xi_{10,1})^{i_7 i_8}_{i_5 i_6} = +\tfrac{1}{2} r^{i_7 i_8}_{i_9 i_{10}} V^{i_9 i_{10}}_{i_5 i_6}$$
$$(\xi_{10})^{i_3 i_4}_{i_5 i_6} = +V^{i_7 a'_8}_{i_5 i_6}(\Xi_0)^{i_3 i_4}_{i_7 a'_8} + \tfrac{1}{2} X^{i_3 i_4}_{i_7 i_8}(\xi_{10,1})^{i_7 i_8}_{i_5 i_6}$$
$$(\xi_{1,1})^{a'_7}_{a_6} = -(\Xi_4)^{a'_7}_{a_6} + (\Xi_{17})^{a'_7}_{a_6} - (\Xi_{18})^{a'_7}_{a_6}$$
$$(\xi_1)^{i_3 i_4}_{a'_5 a_6} = -f^{i_7}_{a_6}(\Xi_0)^{i_3 i_4}_{i_7 a'_5} + F^{i_3 i_4 *}_{a'_5 a'_7}(\xi_{1,1})^{a'_7}_{a_6}$$
$$(\xi_{0,9})^{i_8 a'_5}_{i_2 a'_7} = +v^{i_8 a'_5}_{i_2 a'_7} - (\Xi_2)^{i_8 a'_5}_{i_2 a'_7} + (\Xi_{21})^{i_8 a'_5}_{i_2 a'_7}$$
$$(\xi_{0,8})^{a_6}_{a'_7} = -r^{a_8}_{i_9} v^{i_9 a_6}_{a'_7 a_8} - \tfrac{1}{2} r^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8} - \tfrac{1}{2}\tilde{r}^{\,a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a'_7}$$
$$(\xi_{0,7})^{a'_5}_{a'_7} = -(\Xi_6)^{a'_5}_{a'_7} - (\Xi_{24})^{a'_5}_{a'_7} - (\Xi_{25})^{a'_5}_{a'_7}$$
$$(\xi_{0,6})^{a_6}_{a'_7} = -r^{a_8}_{i_9} v^{i_9 a_6}_{a'_7 a_8} - \tfrac{1}{2} r^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8} + \tfrac{1}{2}\tilde{r}^{\,a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\xi_{0,5})^{i_8 a_6}_{i_2 a_7} = +r^{a_9}_{i_2} v^{i_8 a_6}_{a_7 a_9} + r^{a_6 a_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a_7 a_9} + \tilde{r}^{\,a'_9 a_6}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\xi_{0,3})^{i_8 a_6}_{i_2 a'_7} = +r^{a_9}_{i_2} v^{i_8 a_6}_{a'_7 a_9} - \tilde{r}^{\,a'_9 a_6}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_7 a'_9}$$
$$(\xi_{0,2})^{i_8 a'_5}_{i_2 a_7} = -(\Xi_3)^{i_8 a'_5}_{i_2 a_7} + (\Xi_{16})^{i_8 a'_5}_{i_2 a_7}$$
$$(\xi_{0,13})^{a_6}_{a'_7} = -t^{a_8}_{i_9} v^{i_9 a_6}_{a'_7 a_8} - \tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8} + \tfrac{1}{2}\tilde{t}^{\,a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a'_8}$$
$$(\xi_{0,12})^{i_8 a_6}_{i_2 a_7} = -v^{i_8 a_6}_{i_2 a_7} + t^{a_9}_{i_2} v^{i_8 a_6}_{a_7 a_9} + t^{a_6 a_9}_{i_2 i_{10}} v^{i_8 i_{10}}_{a_7 a_9} + \tilde{t}^{\,a'_9 a_6}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\xi_{0,11})^{i_8 a'_5}_{i_2 a'_7} = -v^{i_8 a'_5}_{i_2 a'_7} + (\Xi_{15})^{i_8 a'_5}_{i_2 a'_7}$$
$$(\xi_{0,10})^{i_8 a_6}_{i_2 a'_7} = -v^{i_8 a_6}_{i_2 a'_7} + t^{a_9}_{i_2} v^{i_8 a_6}_{a'_7 a_9} - \tilde{t}^{\,a'_9 a_6}_{i_2 i_{10}} v^{i_8 i_{10}}_{a'_7 a'_9}$$
$$(\xi_{0,1,7})^{i_7 i_9}_{i_2 a_8} = -v^{i_7 i_9}_{i_2 a_8} + (\Xi_8)^{i_7 i_9}_{i_2 a_8}$$
$$(\xi_{0,1,6})^{i_7 i_9}_{i_2 a'_8} = -v^{i_7 i_9}_{i_2 a'_8} + (\Xi_7)^{i_7 i_9}_{i_2 a'_8}$$
$$(\xi_{0,1,4})^{i_7}_{a'_8} = -r^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\xi_{0,1,2})^{i_7 i_9}_{i_2 a'_8} = +r^{a_{10}}_{i_2} v^{i_7 i_9}_{a'_8 a_{10}}$$
$$(\xi_{0,1,0})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - (\Xi_9)^{i_7}_{a'_8}$$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.4.XXXVIII: The computational sequence and intermediates for the geminal r amplitude equation of right-hand EOM-CCSDT-R12 and higher-order EOM-CC-R12 [Part II]

$$
\begin{aligned}
(\xi_{0,1})^{i_7 a'_5}_{i_1 i_2} &= +\tilde{r}^{a'_5 a'_8}_{i_1 i_2}(\xi_{0,1,0})^{i_7}_{a'_8} + P_2 t^{a_8}_{i_1}(\Xi_3)^{i_7 a'_5}_{i_2 a_8} + P_2 \tilde{t}^{a'_5 a'_8}_{i_1 i_9}(\xi_{0,1,2})^{i_7 i_9}_{i_2 a'_8} \\
&\quad + P_2 \tilde{t}^{a'_5 a_8}_{i_1 i_9}(\Xi_{11})^{i_7 i_9}_{i_2 a_8} + \tilde{t}^{a'_5 a'_8}_{i_1 i_2}(\xi_{0,1,4})^{i_7}_{a'_8} - \tilde{t}^{a'_5 a_8}_{i_1 i_2}(\Xi_{12})^{i_7}_{a_8} \\
&\quad + P_2 \tilde{r}^{a'_5 a'_8}_{i_1 i_9}(\xi_{0,1,6})^{i_7 i_9}_{i_2 a'_8} + P_2 \tilde{r}^{a'_5 a_8}_{i_1 i_9}(\xi_{0,1,7})^{i_7 i_9}_{i_2 a_8} - \tilde{r}^{a'_5 a_8}_{i_1 i_2}(\Xi_{10})^{i_7}_{a_8} \\
(\xi_{0,0,3})^{i_7 i_9}_{i_2 a_8} &= -v^{i_7 i_9}_{i_2 a_8} + (\Xi_8)^{i_7 i_9}_{i_2 a_8} \\
(\xi_{0,0,2})^{i_7 i_9}_{i_2 a'_8} &= -v^{i_7 i_9}_{i_2 a'_8} + (\Xi_7)^{i_7 i_9}_{i_2 a'_8} \\
(\xi_{0,0,0})^{i_7}_{a'_8} &= -f^{i_7}_{a'_8} - (\Xi_9)^{i_7}_{a'_8} \\
(\xi_{0,0})^{i_7 a'_5}_{i_1 i_2} &= +\tilde{t}^{a'_5 a'_8}_{i_1 i_2}(\xi_{0,0,0})^{i_7}_{a'_8} + \tfrac{1}{2} P_2 t^{a_8}_{i_1}(\Xi_2)^{i_7 a'_5}_{i_2 a_8} + P_2 \tilde{t}^{a'_5 a'_8}_{i_1 i_9}(\xi_{0,0,2})^{i_7 i_9}_{i_2 a'_8} \\
&\quad + P_2 \tilde{t}^{a'_5 a_8}_{i_1 i_9}(\xi_{0,0,3})^{i_7 i_9}_{i_2 a_8} - \tilde{t}^{a'_5 a_8}_{i_1 i_2}(\Xi_{10})^{i_7}_{a_8}
\end{aligned}
$$

$$
\begin{aligned}
(\xi_0)^{a'_5 a_6}_{i_1 i_2} &= +r^{a_6}_{i_7}(\xi_{0,0})^{i_7 a'_5}_{i_1 i_2} + t^{a_6}_{i_7}(\xi_{0,1})^{i_7 a'_5}_{i_1 i_2} + P_2 t^{a_6 a_7}_{i_1 i_8}(\xi_{0,2})^{i_8 a'_5}_{i_2 a_7} \\
&\quad + P_2 \tilde{t}^{a'_5 a'_7}_{i_1 i_8}(\xi_{0,3})^{i_8 a_6}_{i_2 a'_7} + P_2 \tilde{t}^{a'_7 a_6}_{i_1 i_8}(\Xi_5)^{i_8 a'_5}_{i_2 a'_7} + P_2 \tilde{t}^{a'_5 a_7}_{i_1 i_8}(\xi_{0,5})^{i_8 a_6}_{i_2 a_7} \\
&\quad + \tilde{t}^{a'_5 a'_7}_{i_1 i_2}(\xi_{0,6})^{a_6}_{a'_7} + \tilde{t}^{a'_7 a_6}_{i_1 i_2}(\xi_{0,7})^{a'_5}_{a'_7} + \tilde{t}^{a'_5 a_7}_{i_1 i_2}(\xi_{0,8})^{a_6}_{a_7} \\
&\quad + P_2 r^{a_6 a_7}_{i_1 i_8}(\xi_{0,9})^{i_8 a'_5}_{i_2 a_7} + P_2 \tilde{r}^{a'_5 a'_7}_{i_1 i_8}(\xi_{0,10})^{i_8 a_6}_{i_2 a'_7} + P_2 \tilde{r}^{a'_7 a_6}_{i_1 i_8}(\xi_{0,11})^{i_8 a'_5}_{i_2 a'_7} \\
&\quad + P_2 \tilde{r}^{a'_5 a_7}_{i_1 i_8}(\xi_{0,12})^{i_8 a_6}_{i_2 a_7} + \tilde{r}^{a'_5 a'_7}_{i_1 i_2}(\xi_{0,13})^{a_6}_{a'_7} + \tfrac{1}{2} r^{a_6 a_7 a_8}_{i_1 i_2 i_9} v^{i_9 a'_5}_{a_7 a_8} \\
\delta^{i_3 i_4}_{i_1 i_2} &= +F^{i_3 i_4 *}_{a'_5 a_6}(\xi_0)^{a'_5 a_6}_{i_1 i_2} + \tilde{t}^{a'_5 a_6}_{i_1 i_2}(\xi_1)^{i_3 i_4}_{a'_5 a_6} + \tfrac{1}{2} X^{i_3 i_4}_{i_5 i_6}(\xi_2)^{i_5 i_6}_{i_1 i_2} + \tfrac{1}{2} r^{a_5 a_6}_{i_1 i_2}(\xi_3)^{i_3 i_4}_{a_5 a_6} \\
&\quad + \tfrac{1}{2} r^{i_5 i_6}_{i_1 i_2}(\xi_4)^{i_3 i_4}_{i_5 i_6} + \tilde{r}^{a'_5 a_6}_{i_1 i_2}(\xi_5)^{i_3 i_4}_{a'_5 a_6} + v^{i_5 a'_6}_{i_1 i_2}(\Xi_0)^{i_3 i_4}_{i_5 a'_6} + P_2 r^{a_5}_{i_1}(\xi_7)^{i_3 i_4}_{i_2 a_5} \\
&\quad + P_2 t^{a_5}_{i_1}(\xi_8)^{i_3 i_4}_{i_2 a_5} + \tfrac{1}{2} t^{a_5 a_6}_{i_1 i_2}(\xi_9)^{i_3 i_4}_{a_5 a_6} + \tfrac{1}{2} t^{i_5 i_6}_{i_1 i_2}(\xi_{10})^{i_3 i_4}_{i_5 i_6} \\
&\quad + \tfrac{1}{2} F^{i_3 i_4 *}_{a'_5 a'_6}(\xi_{11})^{a'_5 a'_6}_{i_1 i_2} + \tfrac{1}{2} v^{i_5 i_6}_{i_1 i_2}(\xi_{12})^{i_3 i_4}_{i_5 i_6} + \tfrac{1}{2} \tilde{r}^{a'_5 a'_6}_{i_1 i_2}(\xi_{13})^{i_3 i_4}_{a'_5 a'_6}
\end{aligned}
$$

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I. EOM-CCSDTQ-R12

TABLE ESI.4.XXXIX: The computational sequence and intermediates for the R_2 amplitude equation of right-hand EOM-CCSDTQ-R12

$$
\begin{aligned}
(\Xi_0)^{i_5i_6}_{i_1i_2} &= +P_2 t^{a_7}_{i_1} v^{i_5i_6}_{i_2a_7} \\
(\Xi_1)^{i_6a_4}_{i_2a_5} &= +t^{a_7}_{i_2} v^{i_6a_4}_{a_5a_7} \\
(\Xi_2)^{i_5i_6}_{i_1i_2} &= +P_2 r^{a_7}_{i_1} v^{i_5i_6}_{i_2a_7} \\
(\Xi_3)^{i_6a_4}_{i_2a_5} &= +r^{a_7}_{i_2} v^{i_6a_4}_{a_5a_7} \\
(\Xi_4)^{i_6i_7}_{i_2a_5} &= +t^{a_8}_{i_2} v^{i_6i_7}_{a_5a_8} \\
(\Xi_5)^{i_6i_7}_{i_2a_5} &= +r^{a_8}_{i_2} v^{i_6i_7}_{a_5a_8} \\
(\Xi_6)^{i_5i_6}_{i_1i_2} &= +\tfrac{1}{2} t^{i_7i_8}_{i_1i_2} V^{i_5i_6}_{i_7i_8} \\
(\Xi_7)^{i_5i_7}_{i_2a'_6} &= +t^{a_8}_{i_2} v^{i_5i_7}_{a'_6a_8} \\
(\Xi_8)^{i_5}_{a'_6} &= +t^{a_7}_{i_8} v^{i_5i_8}_{a'_6a_7} \\
(\Xi_9)^{i_6}_{a_5} &= +t^{a_7}_{i_8} v^{i_6i_8}_{a_5a_7} \\
(\Xi_{10})^{i_5i_6}_{i_1i_2} &= +\tfrac{1}{2} t^{a_7a_8}_{i_1i_2} v^{i_5i_6}_{a_7a_8} \\
(\Xi_{11})^{i_6}_{a_5} &= +r^{a_7}_{i_8} v^{i_6i_8}_{a_5a_7} \\
(\Xi_{12})^{i_5i_6}_{i_1i_2} &= +\tfrac{1}{2} r^{a_7a_8}_{i_1i_2} v^{i_5i_6}_{a_7a_8} \\
(\Xi_{13})^{i_5i_6}_{i_1i_2} &= +\tfrac{1}{2} V^{i_5i_6}_{i_7i_8} r^{i_7i_8}_{i_1i_2} \\
(\Xi_{14})^{i_5i_6}_{i_1i_2} &= +P_2 t^{a_7}_{i_1} (\Xi_4)^{i_5i_6}_{i_2a_7} \\
(\Xi_{15})^{i_5i_6}_{i_1i_2} &= +P_2 t^{a_7}_{i_1} (\Xi_5)^{i_5i_6}_{i_2a_7} \\
(\xi_9)^{i_5i_6}_{i_1i_2} &= -(\Xi_2)^{i_5i_6}_{i_1i_2} + (\Xi_{15})^{i_5i_6}_{i_1i_2} + (\Xi_{12})^{i_5i_6}_{i_1i_2} + (\Xi_{13})^{i_5i_6}_{i_1i_2} \\
(\xi_8)^{a_3a_4}_{i_2a_5} &= +r^{a_6}_{i_2} v^{a_3a_4}_{a_5a_6} \\
(\xi_6)^{i_6}_{a_5} &= +f^{i_6}_{a_5} + (\Xi_9)^{i_6}_{a_5} \\
(\xi_{5,7})^{i_5}_{a'_6} &= -r^{a_7}_{i_8} v^{i_5i_8}_{a'_6a_7} \\
(\xi_{5,6})^{i_5i_7}_{i_2a'_6} &= +r^{a_8}_{i_2} v^{i_5i_7}_{a'_6a_8} \\
(\xi_{5,4})^{i_5i_6}_{i_1i_2} &= -(\Xi_2)^{i_5i_6}_{i_1i_2} + (\Xi_{15})^{i_5i_6}_{i_1i_2} + (\Xi_{12})^{i_5i_6}_{i_1i_2} + (\Xi_{13})^{i_5i_6}_{i_1i_2} \\
(\xi_{5,2})^{i_5i_6}_{i_1i_2} &= +v^{i_5i_6}_{i_1i_2} - (\Xi_0)^{i_5i_6}_{i_1i_2} + \tfrac{1}{2}(\Xi_{14})^{i_5i_6}_{i_1i_2} + (\Xi_6)^{i_5i_6}_{i_1i_2} + (\Xi_{10})^{i_5i_6}_{i_1i_2} \\
(\xi_{5,12})^{i_5i_7}_{i_2a'_6} &= -v^{i_5i_7}_{i_2a'_6} + (\Xi_7)^{i_5i_7}_{i_2a'_6} \\
(\xi_{5,10})^{i_5i_7}_{i_2a_6} &= +v^{i_5i_7}_{i_2a_6} - (\Xi_4)^{i_5i_7}_{i_2a_6} \\
(\xi_{5,1})^{i_5}_{a'_6} &= -f^{i_5}_{a'_6} - (\Xi_8)^{i_5}_{a'_6} \\
(\xi_{5,0})^{i_5}_{a_6} &= +f^{i_5}_{a_6} + (\Xi_9)^{i_5}_{a_6} \\
(\xi_5)^{i_5a_4}_{i_1i_2} &= +r^{a_4a_6}_{i_1i_2} (\xi_{5,0})^{i_5}_{a_6} + \tilde{r}^{a'_6a_4}_{i_1i_2} (\xi_{5,1})^{i_5}_{a'_6} + r^{a_4}_{i_6} (\xi_{5,2})^{i_5i_6}_{i_1i_2} + P_2 r^{a_6}_{i_1} v^{i_5a_4}_{i_2a_6} \\
&\quad + \tfrac{1}{2} t^{a_4}_{i_6} (\xi_{5,4})^{i_5i_6}_{i_1i_2} - P_2 t^{a_6}_{i_1} (\Xi_3)^{i_5a_4}_{i_2a_6} + P_2 \tilde{t}^{a'_6a_4}_{i_1i_7} (\xi_{5,6})^{i_5i_7}_{i_2a'_6} \\
&\quad + \tilde{t}^{a'_6a_4}_{i_1i_2} (\xi_{5,7})^{i_5}_{a'_6} - P_2 t^{a_4a_6}_{i_1i_7} (\Xi_5)^{i_5i_7}_{i_2a_6} + t^{a_4a_6}_{i_1i_2} (\Xi_{11})^{i_5}_{a_6} \\
&\quad + P_2 r^{a_4a_6}_{i_1i_7} (\xi_{5,10})^{i_5i_7}_{i_2a_6} - \tfrac{1}{2} r^{a_6a_7}_{i_1i_2} v^{i_5a_4}_{a_6a_7} + P_2 \tilde{r}^{a'_6a_4}_{i_1i_7} (\xi_{5,12})^{i_5i_7}_{i_2a'_6} \\
&\quad - \tfrac{1}{2} r^{i_6i_7}_{i_1i_2} V^{i_5a_4}_{i_6i_7} + \tfrac{1}{2} r^{a_4a_6a_7}_{i_1i_2i_8} v^{i_5i_8}_{a_6a_7} \\
(\xi_4)^{a_4}_{a'_5} &= -f^{a_4}_{a'_5} + t^{a_6}_{i_7} v^{i_7a_4}_{a'_5a_6} + \tfrac{1}{2} t^{a_4a_6}_{i_7i_8} v^{i_7i_8}_{a'_5a_6} - \tfrac{1}{2} \tilde{t}^{a'_6a_4}_{i_7i_8} v^{i_7i_8}_{a'_5a'_6} \\
(\xi_3)^{a_4}_{a_5} &= +f^{a_4}_{a_5} - t^{a_6}_{i_7} v^{i_7a_4}_{a_5a_6} - \tfrac{1}{2} t^{a_4a_6}_{i_7i_8} v^{i_7i_8}_{a_5a_6} - \tfrac{1}{2} \tilde{t}^{a'_6a_4}_{i_7i_8} v^{i_7i_8}_{a'_6a_5} \\
(\xi_{21})^{i_6i_7}_{i_2a_5} &= -v^{i_6i_7}_{i_2a_5} + (\Xi_4)^{i_6i_7}_{i_2a_5} \\
(\xi_{2,0})^{i_5}_{a_6} &= -f^{i_5}_{a_6} - (\Xi_9)^{i_5}_{a_6} \\
(\xi_2)^{i_5}_{i_2} &= -f^{i_5}_{i_2} + t^{a_6}_{i_2} (\xi_{2,0})^{i_5}_{a_6} - t^{a_6}_{i_7} v^{i_5i_7}_{i_2a_6} - \tfrac{1}{2} t^{a_6a_7}_{i_2i_8} v^{i_5i_8}_{a_6a_7} - \tfrac{1}{2} t^{i_6i_7}_{i_2i_8} V^{i_5i_8}_{i_6i_7} \\
(\xi_{19})^{i_6a_4}_{i_2a'_5} &= +v^{i_6a_4}_{i_2a'_5} - t^{a_7}_{i_2} v^{i_6a_4}_{a'_5a_7} + \tilde{t}^{a'_7a_4}_{i_2i_8} v^{i_6i_8}_{a'_5a'_7} \\
(\xi_{17})^{i_6a_4}_{i_2a_5} &= -v^{i_6a_4}_{i_2a_5} + (\Xi_1)^{i_6a_4}_{i_2a_5} + \tilde{t}^{a'_7a_4}_{i_2i_8} v^{i_6i_8}_{a'_7a_5} \\
(\xi_{16})^{i_5i_6}_{i_1i_2} &= +v^{i_5i_6}_{i_1i_2} - (\Xi_0)^{i_5i_6}_{i_1i_2} + \tfrac{1}{2}(\Xi_{14})^{i_5i_6}_{i_1i_2} + (\Xi_{10})^{i_5i_6}_{i_1i_2} + (\Xi_6)^{i_5i_6}_{i_1i_2} \\
(\xi_{13})^{a_4}_{a'_5} &= +r^{a_6}_{i_7} v^{i_7a_4}_{a'_5a_6} + \tfrac{1}{2} r^{a_4a_6}_{i_7i_8} v^{i_7i_8}_{a'_5a_6} - \tfrac{1}{2} \tilde{r}^{a'_6a_4}_{i_7i_8} v^{i_7i_8}_{a'_5a'_6} \\
(\xi_{12})^{i_6a_4}_{i_2a'_5} &= -r^{a_7}_{i_2} v^{i_6a_4}_{a'_5a_7} \\
(\xi_{11})^{a_4}_{a_5} &= -r^{a_6}_{i_7} v^{i_7a_4}_{a_5a_6} - \tfrac{1}{2} r^{a_4a_6}_{i_7i_8} v^{i_7i_8}_{a_5a_6} - \tfrac{1}{2} \tilde{r}^{a'_6a_4}_{i_7i_8} v^{i_7i_8}_{a'_6a_5} \\
(\xi_{10})^{i_6a_4}_{i_2a_5} &= +(\Xi_3)^{i_6a_4}_{i_2a_5} + r^{a_4a_7}_{i_2i_8} v^{i_6i_8}_{a_5a_7} + \tilde{r}^{a'_7a_4}_{i_2i_8} v^{i_6i_8}_{a'_7a_5} \\
(\xi_{1,0})^{i_5}_{a_6} &= -f^{i_5}_{a_6} - (\Xi_9)^{i_5}_{a_6} \\
(\xi_1)^{i_5}_{i_2} &= +r^{a_6}_{i_2} (\xi_{1,0})^{i_5}_{a_6} - r^{a_6}_{i_7} v^{i_5i_7}_{i_2a_6} - t^{a_6}_{i_2} (\Xi_{11})^{i_5}_{a_6} - \tfrac{1}{2} r^{a_6a_7}_{i_2i_8} v^{i_5i_8}_{a_6a_7} - \tfrac{1}{2} r^{i_7i_8}_{i_2i_6} V^{i_5i_6}_{i_7i_8} \\
(\xi_{0,5})^{i_5i_7}_{i_2a'_6} &= -v^{i_5i_7}_{i_2a'_6} + (\Xi_7)^{i_5i_7}_{i_2a'_6} \\
(\xi_{0,3})^{i_5i_7}_{i_2a_6} &= +v^{i_5i_7}_{i_2a_6} - (\Xi_4)^{i_5i_7}_{i_2a_6} \\
(\xi_{0,2})^{i_5a_4}_{i_2a_6} &= +v^{i_5a_4}_{i_2a_6} - \tfrac{1}{2}(\Xi_1)^{i_5a_4}_{i_2a_6} \\
(\xi_{0,1})^{i_5}_{a'_6} &= -f^{i_5}_{a'_6} - (\Xi_8)^{i_5}_{a'_6} \\
(\xi_{0,0})^{i_5}_{a_6} &= +f^{i_5}_{a_6} + (\Xi_9)^{i_5}_{a_6} \\
(\xi_0)^{i_5a_4}_{i_1i_2} &= -v^{i_5a_4}_{i_1i_2} + t^{a_4a_6}_{i_1i_2} (\xi_{0,0})^{i_5}_{a_6} + \tilde{t}^{a'_6a_4}_{i_1i_2} (\xi_{0,1})^{i_5}_{a'_6} + P_2 t^{a_6}_{i_1} (\xi_{0,2})^{i_5a_4}_{i_2a_6} \\
&\quad + P_2 t^{a_4a_6}_{i_1i_7} (\xi_{0,3})^{i_5i_7}_{i_2a_6} - \tfrac{1}{2} t^{a_6a_7}_{i_1i_2} v^{i_5a_4}_{a_6a_7} + P_2 \tilde{t}^{a'_6a_4}_{i_1i_7} (\xi_{0,5})^{i_5i_7}_{i_2a'_6} - \tfrac{1}{2} t^{i_6i_7}_{i_1i_2} V^{i_5a_4}_{i_6i_7} \\
&\quad + \tfrac{1}{2} t^{a_4a_6a_7}_{i_1i_2i_8} v^{i_5i_8}_{a_6a_7} \\
\delta^{a_3a_4}_{i_1i_2} &= +P_2 r^{a_3}_{i_5} (\xi_0)^{i_5a_4}_{i_1i_2} + P_2 t^{a_3a_4}_{i_1i_5} (\xi_1)^{i_5}_{i_2} + P_2 r^{a_3a_4}_{i_1i_5} (\xi_2)^{i_5}_{i_2} + P_2 r^{a_3a_5}_{i_1i_2} (\xi_3)^{a_4}_{a_5} \\
&\quad + P_2 \tilde{r}^{a'_5a_3}_{i_1i_2} (\xi_4)^{a_4}_{a'_5} + P_2 t^{a_3}_{i_5} (\xi_5)^{i_5a_4}_{i_1i_2} + r^{a_3a_4a_5}_{i_1i_2i_6} (\xi_6)^{i_6}_{a_5} - P_2 r^{a_5}_{i_1} v^{a_3a_4}_{i_2a_5} \\
&\quad + P_2 t^{a_5}_{i_1} (\xi_8)^{a_3a_4}_{i_2a_5} + \tfrac{1}{2} t^{a_3a_4}_{i_5i_6} (\xi_9)^{i_5i_6}_{i_1i_2} + P_2 P_2 t^{a_3a_5}_{i_1i_6} (\xi_{10})^{i_6a_4}_{i_2a_5} \\
&\quad + P_2 t^{a_3a_5}_{i_1i_2} (\xi_{11})^{a_4}_{a_5} + P_2 P_2 \tilde{t}^{a'_5a_3}_{i_1i_6} (\xi_{12})^{i_6a_4}_{i_2a'_5} + P_2 \tilde{t}^{a'_5a_3}_{i_1i_2} (\xi_{13})^{a_4}_{a'_5} \\
&\quad + \tfrac{1}{2} P_2 t^{a_3a_4a_5}_{i_1i_6i_7} (\Xi_5)^{i_6i_7}_{i_2a_5} + t^{a_3a_4a_5}_{i_1i_2i_6} (\Xi_{11})^{i_6}_{a_5} + \tfrac{1}{2} r^{a_3a_4}_{i_5i_6} (\xi_{16})^{i_5i_6}_{i_1i_2} \\
&\quad + P_2 P_2 r^{a_3a_5}_{i_1i_6} (\xi_{17})^{i_6a_4}_{i_2a_5} + \tfrac{1}{2} r^{a_5a_6}_{i_1i_2} v^{a_3a_4}_{a_5a_6} + P_2 P_2 \tilde{r}^{a'_5a_3}_{i_1i_6} (\xi_{19})^{i_6a_4}_{i_2a'_5} \\
&\quad + \tfrac{1}{2} r^{i_5i_6}_{i_1i_2} V^{a_3a_4}_{i_5i_6} + \tfrac{1}{2} P_2 r^{a_3a_4a_5}_{i_1i_6i_7} (\xi_{21})^{i_6i_7}_{i_2a_5} \\
&\quad - \tfrac{1}{2} P_2 r^{a_3a_5a_6}_{i_1i_2i_7} v^{i_7a_4}_{a_5a_6} + \tfrac{1}{4} r^{a_3a_4a_5a_6}_{i_1i_2i_7i_8} v^{i_7i_8}_{a_5a_6}
\end{aligned}
$$

Supplementary data for Phys. Chem. Chem. Phys.

TABLE ESI.4.XL: The computational sequence and intermediates for the R_3 amplitude equation of right-hand EOM-CCSDTQ-R12 [Part I]

$$(\Xi_0)^{i_7 i_8}_{i_2 i_3} = +P_2 t^{a_9}_{i_2} v^{i_7 i_8}_{i_3 a_9}$$
$$(\Xi_1)^{i_8 a_6}_{i_3 a_7} = +t^{a_9}_{i_3} v^{i_8 a_6}_{a_7 a_9}$$
$$(\Xi_2)^{i_7 i_8}_{i_2 i_3} = +P_2 r^{a_9}_{i_2} v^{i_7 i_8}_{i_3 a_9}$$
$$(\Xi_3)^{i_8 a_6}_{i_3 a_7} = +r^{a_9}_{i_3} v^{i_8 a_6}_{a_7 a_9}$$
$$(\Xi_4)^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +P_3 \tilde{t}^{a'_9 a_6}_{i_1 i_2} v^{i_7 i_8}_{i_3 a'_9}$$
$$(\Xi_5)^{i_7 a_6}_{i_3 a'_8} = +t^{a_9}_{i_3} v^{i_7 a_6}_{a'_8 a_9}$$
$$(\Xi_6)^{i_8 i_9}_{i_3 a_7} = +t^{a_{10}}_{i_3} v^{i_8 i_9}_{a_7 a_{10}}$$
$$(\Xi_7)^{i_8 i_9}_{i_3 a_7} = +r^{a_{10}}_{i_3} v^{i_8 i_9}_{a_7 a_{10}}$$
$$(\Xi_8)^{i_7 i_8}_{i_3 a'_9} = +t^{a_{10}}_{i_3} v^{i_7 i_8}_{a'_9 a_{10}}$$
$$(\Xi_9)^{i_7 i_8}_{i_3 a'_9} = +r^{a_{10}}_{i_3} v^{i_7 i_8}_{a'_9 a_{10}}$$
$$(\Xi_{10})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +\tfrac{1}{2} t^{a_6 a_9 a_{10}}_{i_1 i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\Xi_{11})^{i_8}_{a_7} = +t^{a_9}_{i_{10}} v^{i_8 i_{10}}_{a_7 a_9}$$
$$(\Xi_{12})^{i_8}_{a_7} = +r^{a_9}_{i_{10}} v^{i_8 i_{10}}_{a_7 a_9}$$
$$(\Xi_{13})^{i_8 a_6}_{i_3 a_7} = +t^{a_6 a_9}_{i_3 i_{10}} v^{i_8 i_{10}}_{a_7 a_9}$$
$$(\Xi_{14})^{i_7 i_8}_{i_2 i_3} = +\tfrac{1}{2} t^{a_9 a_{10}}_{i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\Xi_{15})^{i_7 i_8}_{i_2 i_3} = +\tfrac{1}{2} t^{i_9 i_{10}}_{i_2 i_3} V^{i_7 i_8}_{i_9 i_{10}}$$
$$(\Xi_{16})^{i_8 a_6}_{i_3 a_7} = +\tilde{t}^{a'_9 a_6}_{i_3 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\Xi_{17})^{i_7 a_6}_{i_3 a'_8} = +t^{a_6 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_{18})^{i_7 a_6}_{i_3 a'_8} = +\tilde{t}^{a'_9 a_6}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a'_9}$$
$$(\Xi_{19})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +P_3 \tilde{r}^{a'_9 a_6}_{i_1 i_2} v^{i_7 i_8}_{i_3 a'_9}$$
$$(\Xi_{20})^{i_8 a_6}_{i_3 a_7} = +r^{a_6 a_9}_{i_3 i_{10}} v^{i_8 i_{10}}_{a_7 a_9}$$
$$(\Xi_{21})^{i_7 i_8}_{i_2 i_3} = +\tfrac{1}{2} r^{a_9 a_{10}}_{i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\Xi_{22})^{i_7}_{a'_8} = +t^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\Xi_{23})^{i_8 a_6}_{i_3 a_7} = +\tilde{r}^{a'_9 a_6}_{i_3 i_{10}} v^{i_8 i_{10}}_{a'_9 a_7}$$
$$(\Xi_{24})^{i_7 i_8}_{i_2 i_3} = +\tfrac{1}{2} V^{i_7 i_8}_{i_9 i_{10}} r^{i_9 i_{10}}_{i_2 i_3}$$
$$(\Xi_{25})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +\tfrac{1}{2} r^{a_6 a_9 a_{10}}_{i_1 i_2 i_3} v^{i_7 i_8}_{a_9 a_{10}}$$
$$(\Xi_{26})^{i_7 i_8}_{i_2 i_3} = +P_2 t^{a_9}_{i_2} (\Xi_6)^{i_7 i_8}_{i_3 a_9}$$
$$(\Xi_{27})^{i_7 i_8}_{i_2 i_3} = +P_2 t^{a_9}_{i_2} (\Xi_7)^{i_7 i_8}_{i_3 a_9}$$
$$(\Xi_{28})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +P_3 \tilde{t}^{a'_9 a_6}_{i_1 i_2} (\Xi_8)^{i_7 i_8}_{i_3 a'_9}$$
$$(\Xi_{29})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +P_3 \tilde{t}^{a'_9 a_6}_{i_1 i_2} (\Xi_9)^{i_7 i_8}_{i_3 a'_9}$$
$$(\Xi_{30})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +P_3 \tilde{r}^{a'_9 a_6}_{i_1 i_2} (\Xi_8)^{i_7 i_8}_{i_3 a'_9}$$
$$(\xi_9)^{a_5 a_6}_{i_3 a'_7} = -r^{a_8}_{i_3} v^{a_5 a_6}_{a'_7 a_8} - P_2 r^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a_8} + P_2 \tilde{r}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a'_8} - \tfrac{1}{2} r^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8}$$
$$(\xi_{8,2})^{i_8 i_9}_{i_3 a_7} = -v^{i_8 i_9}_{i_3 a_7} + (\Xi_6)^{i_8 i_9}_{i_3 a_7}$$
$$(\xi_8)^{a_5 a_6}_{i_3 a_7} = +r^{a_8}_{i_3} v^{a_5 a_6}_{a_7 a_8} + \tfrac{1}{2} t^{a_5 a_6}_{i_8 i_9} (\Xi_7)^{i_8 i_9}_{i_3 a_7} + \tfrac{1}{2} r^{a_5 a_6}_{i_8 i_9} (\xi_{8,2})^{i_8 i_9}_{i_3 a_7} + P_2 r^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a_7 a_8} + P_2 \tilde{r}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_8 a_7} + \tfrac{1}{2} r^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8}$$
$$(\xi_7)^{i_8}_{a_7} = +f^{i_8}_{a_7} + (\Xi_{11})^{i_8}_{a_7}$$
$$(\xi_{6,9})^{i_7 i_9}_{i_3 a_8} = -v^{i_7 i_9}_{i_3 a_8} + (\Xi_6)^{i_7 i_9}_{i_3 a_8}$$
$$(\xi_{6,8})^{i_7 a_6}_{i_3 a'_8} = +v^{i_7 a_6}_{i_3 a'_8} - (\Xi_5)^{i_7 a_6}_{i_3 a'_8} - (\Xi_{17})^{i_7 a_6}_{i_3 a'_8} + (\Xi_{18})^{i_7 a_6}_{i_3 a'_8}$$
$$(\xi_{6,7})^{i_7 a_6}_{i_3 a_8} = -v^{i_7 a_6}_{i_3 a_8} + (\Xi_1)^{i_7 a_6}_{i_3 a_8} + (\Xi_{13})^{i_7 a_6}_{i_3 a_8} + (\Xi_{16})^{i_7 a_6}_{i_3 a_8}$$
$$(\xi_{6,4,1})^{i_7 i_8}_{i_3 a_9} = -v^{i_7 i_8}_{i_3 a_9} + (\Xi_6)^{i_7 i_8}_{i_3 a_9}$$
$$(\xi_{6,4})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = -(\Xi_{29})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{19})^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{30})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{25})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 t^{a_6 a_9}_{i_1 i_2} (\Xi_7)^{i_7 i_8}_{i_3 a_9} + P_3 r^{a_6 a_9}_{i_1 i_2} (\xi_{6,4,1})^{i_7 i_8}_{i_3 a_9}$$
$$(\xi_{6,3})^{i_7 a_6}_{i_3 a'_8} = -r^{a_9}_{i_3} v^{i_7 a_6}_{a'_8 a_9} - r^{a_6 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a_9} + \tilde{r}^{a'_9 a_6}_{i_3 i_{10}} v^{i_7 i_{10}}_{a'_8 a'_9}$$
$$(\xi_{6,2})^{i_7 a_6}_{i_3 a_8} = +(\Xi_3)^{i_7 a_6}_{i_3 a_8} + (\Xi_{20})^{i_7 a_6}_{i_3 a_8} + (\Xi_{23})^{i_7 a_6}_{i_3 a_8}$$
$$(\xi_{6,1,0})^{i_7 i_8}_{i_3 a_9} = -v^{i_7 i_8}_{i_3 a_9} + (\Xi_6)^{i_7 i_8}_{i_3 a_9}$$
$$(\xi_{6,1})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +(\Xi_4)^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{28})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{10})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 t^{a_6 a_9}_{i_1 i_2} (\xi_{6,1,0})^{i_7 i_8}_{i_3 a_9}$$
$$(\xi_{6,0})^{i_7}_{a_8} = -f^{i_7}_{a_8} - (\Xi_{11})^{i_7}_{a_8}$$
$$(\xi_6)^{i_7 a_5 a_6}_{i_1 i_2 i_3} = +r^{a_5 a_6 a_8}_{i_1 i_2 i_3} (\xi_{6,0})^{i_7}_{a_8} + P_2 r^{a_5}_{i_8} (\xi_{6,1})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_2 P_3 t^{a_5 a_8}_{i_1 i_2} (\xi_{6,2})^{i_7 a_6}_{i_3 a_8} + P_2 P_3 \tilde{t}^{a'_8 a_5}_{i_1 i_2} (\xi_{6,3})^{i_7 a_6}_{i_3 a'_8} + \tfrac{1}{2} P_2 t^{a_5}_{i_8} (\xi_{6,4})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + P_3 t^{a_5 a_6 a_8}_{i_1 i_2 i_9} (\Xi_7)^{i_7 i_9}_{i_3 a_8} - t^{a_5 a_6 a_8}_{i_1 i_2 i_3} (\Xi_{12})^{i_7}_{a_8} + P_2 P_3 r^{a_5 a_8}_{i_1 i_2} (\xi_{6,7})^{i_7 a_6}_{i_3 a_8} + P_2 P_3 \tilde{r}^{a'_8 a_5}_{i_1 i_2} (\xi_{6,8})^{i_7 a_6}_{i_3 a'_8} + P_3 r^{a_5 a_6 a_8}_{i_1 i_2 i_9} (\xi_{6,9})^{i_7 i_9}_{i_3 a_8} + \tfrac{1}{2} P_2 r^{a_5 a_8 a_9}_{i_1 i_2 i_3} v^{i_7 a_6}_{a_8 a_9} - \tfrac{1}{2} r^{a_5 a_6 a_8 a_9}_{i_1 i_2 i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\xi_5)^{a_6}_{a_7} = +f^{a_6}_{a_7} - t^{a_8}_{i_9} v^{i_9 a_6}_{a_7 a_8} - \tfrac{1}{2} t^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8} - \tfrac{1}{2} \tilde{t}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_7}$$
$$(\xi_{4,0})^{i_7}_{a_8} = -f^{i_7}_{a_8} - (\Xi_{11})^{i_7}_{a_8}$$
$$(\xi_4)^{i_7}_{i_3} = -f^{i_7}_{i_3} + t^{a_8}_{i_3} (\xi_{4,0})^{i_7}_{a_8} - t^{a_8}_{i_9} v^{i_7 i_9}_{i_3 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} t^{i_8 i_9}_{i_3 i_{10}} V^{i_7 i_{10}}_{i_8 i_9}$$
$$(\xi_{3,9})^{i_7}_{a'_8} = -r^{a_9}_{i_{10}} v^{i_7 i_{10}}_{a'_8 a_9}$$
$$(\xi_{3,4})^{i_7 i_8}_{i_2 i_3} = -(\Xi_2)^{i_7 i_8}_{i_2 i_3} + (\Xi_{27})^{i_7 i_8}_{i_2 i_3} + (\Xi_{21})^{i_7 i_8}_{i_2 i_3} + (\Xi_{24})^{i_7 i_8}_{i_2 i_3}$$
$$(\xi_{3,2})^{i_7 i_8}_{i_2 i_3} = +v^{i_7 i_8}_{i_2 i_3} - (\Xi_0)^{i_7 i_8}_{i_2 i_3} + \tfrac{1}{2} (\Xi_{26})^{i_7 i_8}_{i_2 i_3} + (\Xi_{14})^{i_7 i_8}_{i_2 i_3} + (\Xi_{15})^{i_7 i_8}_{i_2 i_3}$$
$$(\xi_{3,12})^{i_7 i_9}_{i_3 a'_8} = -v^{i_7 i_9}_{i_3 a'_8} + (\Xi_8)^{i_7 i_9}_{i_3 a'_8}$$
$$(\xi_{3,10})^{i_7 i_9}_{i_3 a_8} = +v^{i_7 i_9}_{i_3 a_8} - (\Xi_6)^{i_7 i_9}_{i_3 a_8}$$
$$(\xi_{3,1})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - (\Xi_{22})^{i_7}_{a'_8}$$
$$(\xi_{3,0})^{i_7}_{a_8} = +f^{i_7}_{a_8} + (\Xi_{11})^{i_7}_{a_8}$$
$$(\xi_3)^{i_7 a_6}_{i_2 i_3} = +r^{a_6 a_8}_{i_2 i_3} (\xi_{3,0})^{i_7}_{a_8} + \tilde{r}^{a'_8 a_6}_{i_2 i_3} (\xi_{3,1})^{i_7}_{a'_8} + r^{a_6}_{i_8} (\xi_{3,2})^{i_7 i_8}_{i_2 i_3} + P_2 r^{a_8}_{i_2} v^{i_7 a_6}_{i_3 a_8} + t^{a_6}_{i_8} (\xi_{3,4})^{i_7 i_8}_{i_2 i_3} - P_2 t^{a_8}_{i_2} (\Xi_3)^{i_7 a_6}_{i_3 a_8} - P_2 t^{a_6 a_8}_{i_2 i_9} (\Xi_7)^{i_7 i_9}_{i_3 a_8} + t^{a_6 a_8}_{i_2 i_3} (\Xi_{12})^{i_7}_{a_8} + P_2 \tilde{t}^{a'_8 a_6}_{i_2 i_9} (\Xi_9)^{i_7 i_9}_{i_3 a'_8} + \tilde{t}^{a'_8 a_6}_{i_2 i_3} (\xi_{3,9})^{i_7}_{a'_8} + P_2 r^{a_6 a_8}_{i_2 i_9} (\xi_{3,10})^{i_7 i_9}_{i_3 a_8} - \tfrac{1}{2} r^{a_8 a_9}_{i_2 i_3} v^{i_7 a_6}_{a_8 a_9} + P_2 \tilde{r}^{a'_8 a_6}_{i_2 i_9} (\xi_{3,12})^{i_7 i_9}_{i_3 a'_8} - \tfrac{1}{2} r^{i_8 i_9}_{i_2 i_3} V^{i_7 a_6}_{i_8 i_9} + \tfrac{1}{2} r^{a_6 a_8 a_9}_{i_2 i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\xi_{22})^{i_8 i_9}_{i_3 a_7} = -v^{i_8 i_9}_{i_3 a_7} + (\Xi_6)^{i_8 i_9}_{i_3 a_7}$$
$$(\xi_{20})^{i_8 a_6}_{i_3 a_7} = -v^{i_8 a_6}_{i_3 a_7} + (\Xi_1)^{i_8 a_6}_{i_3 a_7} + (\Xi_{13})^{i_8 a_6}_{i_3 a_7} + (\Xi_{16})^{i_8 a_6}_{i_3 a_7}$$
$$(\xi_{2,6})^{i_7 i_9}_{i_3 a'_8} = -v^{i_7 i_9}_{i_3 a'_8} + (\Xi_8)^{i_7 i_9}_{i_3 a'_8}$$
$$(\xi_{2,4})^{i_7 i_9}_{i_3 a_8} = +v^{i_7 i_9}_{i_3 a_8} - (\Xi_6)^{i_7 i_9}_{i_3 a_8}$$
$$(\xi_{2,3})^{i_7 a_6}_{i_3 a_8} = +v^{i_7 a_6}_{i_3 a_8} - \tfrac{1}{2} (\Xi_1)^{i_7 a_6}_{i_3 a_8}$$
$$(\xi_{2,2})^{i_7 i_8}_{i_2 i_3} = +v^{i_7 i_8}_{i_2 i_3} - (\Xi_0)^{i_7 i_8}_{i_2 i_3} + \tfrac{1}{2} (\Xi_{26})^{i_7 i_8}_{i_2 i_3} + (\Xi_{14})^{i_7 i_8}_{i_2 i_3} + (\Xi_{15})^{i_7 i_8}_{i_2 i_3}$$
$$(\xi_{2,1})^{i_7}_{a'_8} = -f^{i_7}_{a'_8} - (\Xi_{22})^{i_7}_{a'_8}$$
$$(\xi_{2,0})^{i_7}_{a_8} = +f^{i_7}_{a_8} + (\Xi_{11})^{i_7}_{a_8}$$
$$(\xi_2)^{i_7 a_6}_{i_2 i_3} = -v^{i_7 a_6}_{i_2 i_3} + t^{a_6 a_8}_{i_2 i_3} (\xi_{2,0})^{i_7}_{a_8} + \tilde{t}^{a'_8 a_6}_{i_2 i_3} (\xi_{2,1})^{i_7}_{a'_8} + t^{a_6}_{i_8} (\xi_{2,2})^{i_7 i_8}_{i_2 i_3} + P_2 t^{a_8}_{i_2} (\xi_{2,3})^{i_7 a_6}_{i_3 a_8} + P_2 t^{a_6 a_8}_{i_2 i_9} (\xi_{2,4})^{i_7 i_9}_{i_3 a_8} - \tfrac{1}{2} t^{a_8 a_9}_{i_2 i_3} v^{i_7 a_6}_{a_8 a_9} + P_2 \tilde{t}^{a'_8 a_6}_{i_2 i_9} (\xi_{2,6})^{i_7 i_9}_{i_3 a'_8} - \tfrac{1}{2} t^{i_8 i_9}_{i_2 i_3} V^{i_7 a_6}_{i_8 i_9} + \tfrac{1}{2} t^{a_6 a_8 a_9}_{i_2 i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9}$$
$$(\xi_{19})^{i_7 i_8}_{i_2 i_3} = +v^{i_7 i_8}_{i_2 i_3} - (\Xi_0)^{i_7 i_8}_{i_2 i_3} + \tfrac{1}{2} (\Xi_{26})^{i_7 i_8}_{i_2 i_3} + (\Xi_{14})^{i_7 i_8}_{i_2 i_3} + (\Xi_{15})^{i_7 i_8}_{i_2 i_3}$$
$$(\xi_{18})^{i_7 i_8 a_6}_{i_1 i_2 i_3} = +(\Xi_4)^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{28})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{10})^{i_7 i_8 a_6}_{i_1 i_2 i_3}$$
$$(\xi_{17})^{a_5 a_6}_{i_3 a'_7} = +v^{a_5 a_6}_{i_3 a'_7} - t^{a_8}_{i_3} v^{a_5 a_6}_{a'_7 a_8} - P_2 t^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a_8} + P_2 \tilde{t}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_7 a'_8} - \tfrac{1}{2} t^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a'_7 a_8}$$

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TABLE ESI.4.XLI: The computational sequence and intermediates for the R_3 amplitude equation of right-hand EOM-CCSDTQ-R12 [Part II]

$$
\begin{aligned}
(\xi_{16,1})^{i_8 i_9}_{i_3 a_7} &= -v^{i_8 i_9}_{i_3 a_7} + (\Xi_6)^{i_8 i_9}_{i_3 a_7} \\
(\xi_{16})^{a_5 a_6}_{i_3 a_7} &= -v^{a_5 a_6}_{i_3 a_7} + t^{a_8}_{i_3} v^{a_5 a_6}_{a_7 a_8} + \tfrac{1}{2} t^{a_5 a_6}_{i_8 i_9} (\xi_{16,1})^{i_8 i_9}_{i_3 a_7} + P_2 t^{a_5 a_8}_{i_3 i_9} v^{i_9 a_6}_{a_7 a_8} \\
&\quad + P_2 \tilde{t}^{a'_8 a_5}_{i_3 i_9} v^{i_9 a_6}_{a'_8 a_7} + \tfrac{1}{2} t^{a_5 a_6 a_8}_{i_3 i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8} \\
(\xi_{13})^{i_7 i_8 a_6}_{i_1 i_2 i_3} &= -(\Xi_{29})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{19})^{i_7 i_8 a_6}_{i_1 i_2 i_3} - (\Xi_{30})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + (\Xi_{25})^{i_7 i_8 a_6}_{i_1 i_2 i_3} \\
(\xi_{12})^{a_6}_{a_7} &= -r^{a_8}_{i_9} v^{i_9 a_6}_{a_7 a_8} - \tfrac{1}{2} r^{a_6 a_8}_{i_9 i_{10}} v^{i_9 i_{10}}_{a_7 a_8} - \tfrac{1}{2} \tilde{r}^{a'_8 a_6}_{i_9 i_{10}} v^{i_9 i_{10}}_{a'_8 a_7} \\
(\xi_{11})^{i_8 a_6}_{i_3 a_7} &= +(\Xi_3)^{i_8 a_6}_{i_3 a_7} + (\Xi_{20})^{i_8 a_6}_{i_3 a_7} + (\Xi_{23})^{i_8 a_6}_{i_3 a_7} \\
(\xi_{10})^{i_7 i_8}_{i_2 i_3} &= -(\Xi_2)^{i_7 i_8}_{i_2 i_3} + (\Xi_{27})^{i_7 i_8}_{i_2 i_3} + (\Xi_{21})^{i_7 i_8}_{i_2 i_3} + (\Xi_{24})^{i_7 i_8}_{i_2 i_3} \\
(\xi_{1,0})^{i_7}_{a_8} &= -f^{i_7}_{a_8} - (\Xi_{11})^{i_7}_{a_8} \\
(\xi_1)^{i_7}_{i_3} &= +r^{a_8}_{i_3} (\xi_{1,0})^{i_7}_{a_8} - r^{a_8}_{i_9} v^{i_7 i_9}_{i_3 a_8} - t^{a_8}_{i_3} (\Xi_{12})^{i_7}_{a_8} - \tfrac{1}{2} r^{a_8 a_9}_{i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} - \tfrac{1}{2} r^{i_9 i_{10}}_{i_3 i_8} V^{i_7 i_8}_{i_9 i_{10}} \\
(\xi_{0,3})^{i_7 i_9}_{i_3 a_8} &= -v^{i_7 i_9}_{i_3 a_8} + (\Xi_6)^{i_7 i_9}_{i_3 a_8} \\
(\xi_{0,2})^{i_7 a_6}_{i_3 a'_8} &= +v^{i_7 a_6}_{i_3 a'_8} - (\Xi_5)^{i_7 a_6}_{i_3 a'_8} - (\Xi_{17})^{i_7 a_6}_{i_3 a'_8} + (\Xi_{18})^{i_7 a_6}_{i_3 a'_8} \\
(\xi_{0,1})^{i_7 a_6}_{i_3 a_8} &= -v^{i_7 a_6}_{i_3 a_8} + (\Xi_1)^{i_7 a_6}_{i_3 a_8} + (\Xi_{13})^{i_7 a_6}_{i_3 a_8} + (\Xi_{16})^{i_7 a_6}_{i_3 a_8} \\
(\xi_{0,0})^{i_7}_{a_8} &= -f^{i_7}_{a_8} - (\Xi_{11})^{i_7}_{a_8}
\end{aligned}
$$

$$
\begin{aligned}
(\xi_0)^{i_7 a_5 a_6}_{i_1 i_2 i_3} &= +t^{a_5 a_6 a_8}_{i_1 i_2 i_3} (\xi_{0,0})^{i_7}_{a_8} + P_2 P_3 t^{a_5 a_8}_{i_1 i_2} (\xi_{0,1})^{i_7 a_6}_{i_3 a_8} + P_2 P_3 \tilde{t}^{a'_8 a_5}_{i_1 i_2} (\xi_{0,2})^{i_7 a_6}_{i_3 a'_8} \\
&\quad + P_3 t^{a_5 a_6 a_8}_{i_1 i_2 i_9} (\xi_{0,3})^{i_7 i_9}_{i_3 a_8} + \tfrac{1}{2} P_2 t^{a_5 a_8 a_9}_{i_1 i_2 i_3} v^{i_7 a_6}_{a_8 a_9} - \tfrac{1}{2} t^{a_5 a_6 a_8 a_9}_{i_1 i_2 i_3 i_{10}} v^{i_7 i_{10}}_{a_8 a_9} \\
\delta^{a_4 a_5 a_6}_{i_1 i_2 i_3} &= +P_3 r^{a_4}_{i_7} (\xi_0)^{i_7 a_5 a_6}_{i_1 i_2 i_3} + P_3 t^{a_4 a_5 a_6}_{i_1 i_2 i_7} (\xi_1)^{i_7}_{i_3} + P_3 P_3 r^{a_4 a_5}_{i_1 i_7} (\xi_2)^{i_7 a_6}_{i_2 i_3} \\
&\quad + P_3 P_3 t^{a_4 a_5}_{i_1 i_7} (\xi_3)^{i_7 a_6}_{i_2 i_3} + P_3 r^{a_4 a_5 a_6}_{i_1 i_2 i_7} (\xi_4)^{i_7}_{i_3} + P_3 r^{a_4 a_5 a_7}_{i_1 i_2 i_3} (\xi_5)^{a_6}_{a_7} \\
&\quad + P_3 t^{a_4}_{i_7} (\xi_6)^{i_7 a_5 a_6}_{i_1 i_2 i_3} + r^{a_4 a_5 a_6 a_7}_{i_1 i_2 i_3 i_8} (\xi_7)^{i_8}_{a_7} + P_3 P_3 t^{a_4 a_7}_{i_1 i_2} (\xi_8)^{a_5 a_6}_{i_3 a_7} \\
&\quad + P_3 P_3 \tilde{t}^{a'_7 a_4}_{i_1 i_2} (\xi_9)^{a_5 a_6}_{i_3 a'_7} + \tfrac{1}{2} P_3 t^{a_4 a_5 a_6}_{i_1 i_7 i_8} (\xi_{10})^{i_7 i_8}_{i_2 i_3} \\
&\quad + P_3 P_3 t^{a_4 a_5 a_7}_{i_1 i_2 i_8} (\xi_{11})^{i_8 a_6}_{i_3 a_7} + P_3 t^{a_4 a_5 a_7}_{i_1 i_2 i_3} (\xi_{12})^{a_6}_{a_7} + \tfrac{1}{2} P_3 t^{a_4 a_5}_{i_7 i_8} (\xi_{13})^{i_7 i_8 a_6}_{i_1 i_2 i_3} \\
&\quad + \tfrac{1}{2} P_3 t^{a_4 a_5 a_6 a_7}_{i_1 i_2 i_8 i_9} (\Xi_7)^{i_8 i_9}_{i_3 a_7} + t^{a_4 a_5 a_6 a_7}_{i_1 i_2 i_3 i_8} (\Xi_{12})^{i_8}_{a_7} \\
&\quad + P_3 P_3 r^{a_4 a_7}_{i_1 i_2} (\xi_{16})^{a_5 a_6}_{i_3 a_7} + P_3 P_3 \tilde{r}^{a'_7 a_4}_{i_1 i_2} (\xi_{17})^{a_5 a_6}_{i_3 a'_7} \\
&\quad + \tfrac{1}{2} P_3 r^{a_4 a_5}_{i_7 i_8} (\xi_{18})^{i_7 i_8 a_6}_{i_1 i_2 i_3} + \tfrac{1}{2} P_3 r^{a_4 a_5 a_6}_{i_1 i_7 i_8} (\xi_{19})^{i_7 i_8}_{i_2 i_3} \\
&\quad + P_3 P_3 r^{a_4 a_5 a_7}_{i_1 i_2 i_8} (\xi_{20})^{i_8 a_6}_{i_3 a_7} + \tfrac{1}{2} P_3 r^{a_4 a_7 a_8}_{i_1 i_2 i_3} v^{a_5 a_6}_{a_7 a_8} \\
&\quad + \tfrac{1}{2} P_3 r^{a_4 a_5 a_6 a_7}_{i_1 i_2 i_8 i_9} (\xi_{22})^{i_8 i_9}_{i_3 a_7} - \tfrac{1}{2} P_3 r^{a_4 a_5 a_7 a_8}_{i_1 i_2 i_3 i_9} v^{i_9 a_6}_{a_7 a_8}
\end{aligned}
$$

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TABLE ESI.4.XLII: The computational sequence and intermediates for the R_4 amplitude equation of right-hand EOM-CCSDTQ-R12 [Part I]

$$(\Xi_0)^{i_9 i_{10}}_{i_3 i_4} = +P_2 t^{a_{11}}_{i_3} v^{i_9 i_{10}}_{i_4 a_{11}}$$
$$(\Xi_1)^{i_{10} a_8}_{i_4 a_9} = +t^{a_{11}}_{i_4} v^{i_{10} a_8}_{a_9 a_{11}}$$
$$(\Xi_2)^{i_9 i_{10}}_{i_3 i_4} = +P_2 r^{a_{11}}_{i_3} v^{i_9 i_{10}}_{i_4 a_{11}}$$
$$(\Xi_3)^{i_{10} a_8}_{i_4 a_9} = +r^{a_{11}}_{i_4} v^{i_{10} a_8}_{a_9 a_{11}}$$
$$(\Xi_4)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} = +P_3 t^{a_8 a_{11}}_{i_2 i_3} v^{i_9 i_{10}}_{i_4 a_{11}}$$
$$(\Xi_5)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} = +P_3 \tilde{r}^{a'_{11} a_8}_{i_2 i_3} v^{i_9 i_{10}}_{i_4 a'_{11}}$$
$$(\Xi_6)^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} = +P_2 \tilde{t}^{a'_{11} a_7}_{i_3 i_4} v^{i_9 a_8}_{a'_{11} a_{10}}$$
$$(\Xi_7)^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} = +P_2 \tilde{t}^{a'_{11} a_7}_{i_3 i_4} v^{i_9 a_8}_{a'_{10} a'_{11}}$$
$$(\Xi_8)^{i_9 i_{11}}_{i_4 a_{10}} = +t^{a_{12}}_{i_4} v^{i_9 i_{11}}_{a_{10} a_{12}}$$
$$(\Xi_9)^{i_9 i_{11}}_{i_4 a_{10}} = +r^{a_{12}}_{i_4} v^{i_9 i_{11}}_{a_{10} a_{12}}$$
$$(\Xi_{10})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} = +\tfrac{1}{2} t^{a_7 a_8 a_{11} a_{12}}_{i_1 i_2 i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}}$$
$$(\Xi_{11})^{i_9}_{a_{10}} = +t^{a_{11}}_{i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}}$$
$$(\Xi_{12})^{i_9}_{a_{10}} = +r^{a_{11}}_{i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}}$$
$$(\Xi_{13})^{i_9 i_{10} a_8}_{i_3 i_4 a'_{11}} = +\tilde{t}^{a'_{12} a_8}_{i_3 i_4} v^{i_9 i_{10}}_{a'_{11} a'_{12}}$$
$$(\Xi_{14})^{i_9 i_{10}}_{i_4 a'_{11}} = +t^{a_{12}}_{i_4} v^{i_9 i_{10}}_{a'_{11} a_{12}}$$
$$(\Xi_{15})^{i_{10} i_{11} a_8}_{i_3 i_4 a_9} = +\tilde{t}^{a'_{12} a_8}_{i_3 i_4} v^{i_{10} i_{11}}_{a'_{12} a_9}$$
$$(\Xi_{16})^{i_9 i_{11}}_{i_4 a'_{10}} = +r^{a_{12}}_{i_4} v^{i_9 i_{11}}_{a'_{10} a_{12}}$$
$$(\Xi_{17})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} = +\tfrac{1}{2} t^{a_8 a_{11} a_{12}}_{i_2 i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}}$$
$$(\Xi_{18})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} = +t^{a_7 a_8 a_{11}}_{i_3 i_4 i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}}$$
$$(\Xi_{19})^{i_{10} a_8}_{i_4 a_9} = +t^{a_8 a_{11}}_{i_4 i_{12}} v^{i_{10} i_{12}}_{a_9 a_{11}}$$
$$(\Xi_{20})^{i_9 i_{10}}_{i_3 i_4} = +\tfrac{1}{2} t^{a_{11} a_{12}}_{i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}}$$
$$(\Xi_{21})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} = +t^{a_7 a_8 a_{11}}_{i_3 i_4 i_{12}} v^{i_9 i_{12}}_{a'_{10} a_{11}}$$
$$(\Xi_{22})^{i_{10} a_8}_{i_4 a_9} = +\tilde{t}^{a'_{11} a_8}_{i_4 i_{12}} v^{i_{10} i_{12}}_{a'_{11} a_9}$$
$$(\Xi_{23})^{i_9 i_{10}}_{i_3 i_4} = +\tfrac{1}{2} t^{i_{11} i_{12}}_{i_3 i_4} V^{i_9 i_{10}}_{i_{11} i_{12}}$$
$$(\Xi_{24})^{i_9 a_8}_{i_4 a'_{10}} = +t^{a_{11}}_{i_4} v^{i_9 a_8}_{a'_{10} a_{11}}$$
$$(\Xi_{25})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} = +P_3 \tilde{r}^{a'_{11} a_8}_{i_2 i_3} v^{i_9 i_{10}}_{i_4 a'_{11}}$$
$$(\Xi_{26})^{i_{10} a_8}_{i_4 a_9} = +r^{a_8 a_{11}}_{i_4 i_{12}} v^{i_{10} i_{12}}_{a_9 a_{11}}$$
$$(\Xi_{27})^{i_9 i_{10}}_{i_3 i_4} = +\tfrac{1}{2} r^{a_{11} a_{12}}_{i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}}$$
$$(\Xi_{28})^{i_9}_{a'_{10}} = +t^{a_{11}}_{i_{12}} v^{i_9 i_{12}}_{a'_{10} a_{11}}$$
$$(\Xi_{29})^{i_{10} a_8}_{i_4 a_9} = +\tilde{r}^{a'_{11} a_8}_{i_4 i_{12}} v^{i_{10} i_{12}}_{a'_{11} a_9}$$
$$(\Xi_{30})^{i_9 i_{10}}_{i_3 i_4} = +\tfrac{1}{2} V^{i_9 i_{10}}_{i_{11} i_{12}} r^{i_{11} i_{12}}_{i_3 i_4}$$
$$(\Xi_{31})^{i_{10} i_{11} a_8}_{i_3 i_4 a_9} = +\tilde{r}^{a'_{12} a_8}_{i_3 i_4} v^{i_{10} i_{11}}_{a'_{12} a_9}$$
$$(\Xi_{32})^{i_9 a_8}_{i_4 a'_{10}} = +t^{a_8 a_{11}}_{i_4 i_{12}} v^{i_9 i_{12}}_{a'_{10} a_{11}}$$
$$(\Xi_{33})^{i_9 a_8}_{i_4 a'_{10}} = +\tilde{t}^{a'_{11} a_8}_{i_4 i_{12}} v^{i_9 i_{12}}_{a'_{10} a'_{11}}$$
$$(\Xi_{34})^{i_{10} a_7 a_8}_{i_3 i_4 a_9} = +r^{a_7 a_8 a_{11}}_{i_3 i_4 i_{12}} v^{i_{10} i_{12}}_{a_9 a_{11}}$$
$$(\Xi_{35})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} = +\tfrac{1}{2} r^{a_8 a_{11} a_{12}}_{i_2 i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}}$$
$$(\Xi_{36})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} = +\tfrac{1}{2} r^{a_7 a_8 a_{11} a_{12}}_{i_1 i_2 i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}}$$
$$(\Xi_{37})^{i_9 i_{10}}_{i_3 i_4} = +P_2 t^{a_{11}}_{i_3} (\Xi_8)^{i_9 i_{10}}_{i_4 a_{11}}$$
$$(\Xi_{38})^{i_9 i_{10}}_{i_3 i_4} = +P_2 t^{a_{11}}_{i_3} (\Xi_9)^{i_9 i_{10}}_{i_4 a_{11}}$$
$$(\Xi_{39})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} = +P_2 P_4 \tilde{t}^{a'_{11} a_7}_{i_1 i_2} (\Xi_{13})^{i_9 i_{10} a_8}_{i_3 i_4 a'_{11}}$$
$$(\Xi_{40})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} = +P_3 \tilde{t}^{a'_{11} a_8}_{i_2 i_3} (\Xi_{14})^{i_9 i_{10}}_{i_4 a'_{11}}$$
$$(\Xi_{41})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} = +P_3 \tilde{t}^{a'_{11} a_8}_{i_2 i_3} (\Xi_{16})^{i_9 i_{10}}_{i_4 a'_{11}}$$
$$(\Xi_{42})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} = +P_3 t^{a_8 a_{11}}_{i_2 i_3} (\Xi_8)^{i_9 i_{10}}_{i_4 a_{11}}$$
$$(\Xi_{43})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} = +P_2 P_4 \tilde{r}^{a'_{11} a_7}_{i_1 i_2} (\Xi_{13})^{i_9 i_{10} a_8}_{i_3 i_4 a'_{11}}$$
$$(\Xi_{44})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} = +P_3 \tilde{r}^{a'_{11} a_8}_{i_2 i_3} (\Xi_{14})^{i_9 i_{10}}_{i_4 a'_{11}}$$
$$(\xi_{9,2})^{i_{10} i_{11}}_{i_4 a_9} = -v^{i_{10} i_{11}}_{i_4 a_9} + (\Xi_8)^{i_{10} i_{11}}_{i_4 a_9}$$
$$\begin{aligned}(\xi_9)^{a_7 a_8}_{i_4 a_9} &= +r^{a_{10}}_{i_4} v^{a_7 a_8}_{a_9 a_{10}} + \tfrac{1}{2} t^{a_7 a_8}_{i_{10} i_{11}} (\Xi_9)^{i_{10} i_{11}}_{i_4 a_9} + \tfrac{1}{2} r^{a_7 a_8}_{i_{10} i_{11}} (\xi_{9,2})^{i_{10} i_{11}}_{i_4 a_9} \\ &\quad + P_2 r^{a_7 a_{10}}_{i_4 i_{11}} v^{i_{11} a_8}_{a_9 a_{10}} + P_2 \tilde{r}^{a'_{10} a_7}_{i_4 i_{11}} v^{i_{11} a_8}_{a'_{10} a_9} + \tfrac{1}{2} r^{a_7 a_8 a_{10}}_{i_4 i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}}\end{aligned}$$
$$(\xi_{8,9})^{i_9 a_8}_{i_4 a_{10}} = +v^{i_9 a_8}_{i_4 a_{10}} - (\Xi_1)^{i_9 a_8}_{i_4 a_{10}} - (\Xi_{22})^{i_9 a_8}_{i_4 a_{10}} - (\Xi_{19})^{i_9 a_8}_{i_4 a_{10}}$$
$$(\xi_{8,8})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} = +(\Xi_{34})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} + P_2 r^{a_7 a_{11}}_{i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} + P_2 \tilde{r}^{a'_{11} a_7}_{i_3 i_4} v^{i_9 a_8}_{a'_{11} a_{10}}$$
$$(\xi_{8,7})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} = +(\Xi_7)^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} - (\Xi_{21})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}}$$
$$(\xi_{8,6})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} = +(\Xi_6)^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} + (\Xi_{18})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}}$$
$$(\xi_{8,3,3})^{i_9 i_{10}}_{i_4 a_{11}} = -v^{i_9 i_{10}}_{i_4 a_{11}} + (\Xi_8)^{i_9 i_{10}}_{i_4 a_{11}}$$
$$(\xi_{8,3,2})^{i_9 i_{10} a_8}_{i_3 i_4 a_{11}} = -(\Xi_{31})^{i_9 i_{10} a_8}_{i_3 i_4 a_{11}} - r^{a_8 a_{12}}_{i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}}$$
$$\begin{aligned}(\xi_{8,3})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} &= -(\Xi_{43})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} + (\Xi_{36})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} \\ &\quad + P_4 t^{a_7 a_8 a_{11}}_{i_1 i_2 i_3} (\Xi_9)^{i_9 i_{10}}_{i_4 a_{11}} - P_2 P_4 r^{a_7 a_{11}}_{i_1 i_2} (\Xi_{15})^{i_9 i_{10} a_8}_{i_3 i_4 a_{11}} \\ &\quad + P_2 P_4 t^{a_7 a_{11}}_{i_1 i_2} (\xi_{8,3,2})^{i_9 i_{10} a_8}_{i_3 i_4 a_{11}} + P_4 r^{a_7 a_8 a_{11}}_{i_1 i_2 i_3} (\xi_{8,3,3})^{i_9 i_{10}}_{i_4 a_{11}}\end{aligned}$$
$$(\xi_{8,2})^{i_9 a_8}_{i_4 a_{10}} = -(\Xi_3)^{i_9 a_8}_{i_4 a_{10}} - (\Xi_{26})^{i_9 a_8}_{i_4 a_{10}} - (\Xi_{29})^{i_9 a_8}_{i_4 a_{10}}$$
$$(\xi_{8,11})^{i_9 i_{11}}_{i_4 a_{10}} = +v^{i_9 i_{11}}_{i_4 a_{10}} - (\Xi_8)^{i_9 i_{11}}_{i_4 a_{10}}$$
$$(\xi_{8,10})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} = -r^{a_7 a_8 a_{11}}_{i_3 i_4 i_{12}} v^{i_9 i_{12}}_{a'_{10} a_{11}}$$
$$(\xi_{8,1,1})^{i_9 i_{10} a_8}_{i_3 i_4 a_{11}} = -(\Xi_{15})^{i_9 i_{10} a_8}_{i_3 i_4 a_{11}} - \tfrac{1}{2} t^{a_8 a_{12}}_{i_3 i_4} v^{i_9 i_{10}}_{a_{11} a_{12}}$$
$$(\xi_{8,1,0})^{i_9 i_{10}}_{i_4 a_{11}} = -v^{i_9 i_{10}}_{i_4 a_{11}} + (\Xi_8)^{i_9 i_{10}}_{i_4 a_{11}}$$
$$\begin{aligned}(\xi_{8,1})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} &= +(\Xi_{10})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} - \tfrac{1}{2} (\Xi_{39})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} \\ &\quad + P_4 t^{a_7 a_8 a_{11}}_{i_1 i_2 i_3} (\xi_{8,1,0})^{i_9 i_{10}}_{i_4 a_{11}} + P_2 P_4 t^{a_7 a_{11}}_{i_1 i_2} (\xi_{8,1,1})^{i_9 i_{10} a_8}_{i_3 i_4 a_{11}}\end{aligned}$$
$$(\xi_{8,0})^{i_9}_{a_{10}} = +f^{i_9}_{a_{10}} + (\Xi_{11})^{i_9}_{a_{10}}$$
$$\begin{aligned}(\xi_8)^{i_9 a_6 a_7 a_8}_{i_1 i_2 i_3 i_4} &= +r^{a_6 a_7 a_8 a_{10}}_{i_1 i_2 i_3 i_4} (\xi_{8,0})^{i_9}_{a_{10}} + P_3 r^{a_6}_{i_{10}} (\xi_{8,1})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} \\ &\quad + P_3 P_4 t^{a_6 a_7 a_{10}}_{i_1 i_2 i_3} (\xi_{8,2})^{i_9 a_8}_{i_4 a_{10}} + \tfrac{1}{2} P_3 t^{a_6}_{i_{10}} (\xi_{8,3})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} \\ &\quad - P_4 t^{a_6 a_7 a_8 a_{10}}_{i_1 i_2 i_3 i_{11}} (\Xi_9)^{i_9 i_{11}}_{i_4 a_{10}} + t^{a_6 a_7 a_8 a_{10}}_{i_1 i_2 i_3 i_4} (\Xi_{12})^{i_9}_{a_{10}} \\ &\quad + P_3 P_4 r^{a_6 a_{10}}_{i_1 i_2} (\xi_{8,6})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} + P_3 P_4 \tilde{r}^{a'_{10} a_6}_{i_1 i_2} (\xi_{8,7})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} \\ &\quad + P_3 P_4 t^{a_6 a_{10}}_{i_1 i_2} (\xi_{8,8})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} + P_3 P_4 r^{a_6 a_7 a_{10}}_{i_1 i_2 i_3} (\xi_{8,9})^{i_9 a_8}_{i_4 a_{10}} \\ &\quad + P_3 P_4 \tilde{t}^{a'_{10} a_6}_{i_1 i_2} (\xi_{8,10})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} + P_4 r^{a_6 a_7 a_8 a_{10}}_{i_1 i_2 i_3 i_{11}} (\xi_{8,11})^{i_9 i_{11}}_{i_4 a_{10}} \\ &\quad - \tfrac{1}{2} P_3 r^{a_6 a_7 a_{10} a_{11}}_{i_1 i_2 i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}}\end{aligned}$$
$$(\xi_7)^{a_8}_{a_9} = +f^{a_8}_{a_9} - t^{a_{10}}_{i_{11}} v^{i_{11} a_8}_{a_9 a_{10}} - \tfrac{1}{2} t^{a_8 a_{10}}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} - \tfrac{1}{2} \tilde{t}^{a'_{10} a_8}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a'_{10} a_9}$$
$$(\xi_{6,0})^{i_9}_{a_{10}} = -f^{i_9}_{a_{10}} - (\Xi_{11})^{i_9}_{a_{10}}$$
$$(\xi_6)^{i_9}_{i_4} = -f^{i_9}_{i_4} + t^{a_{10}}_{i_4} (\xi_{6,0})^{i_9}_{a_{10}} - t^{a_{10} a_{11}}_{i_{11}} v^{i_9 i_{11}}_{i_4 a_{10}} - \tfrac{1}{2} t^{a_{10} a_{11}}_{i_4 i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}} - \tfrac{1}{2} t^{i_{10} i_{11}}_{i_4 i_{12}} V^{i_9 i_{12}}_{i_{10} i_{11}}$$
$$(\xi_{5,9})^{i_9 a_8}_{i_4 a_{10}} = -v^{i_9 a_8}_{i_4 a_{10}} + (\Xi_1)^{i_9 a_8}_{i_4 a_{10}} + (\Xi_{19})^{i_9 a_8}_{i_4 a_{10}} + (\Xi_{22})^{i_9 a_8}_{i_4 a_{10}}$$
$$(\xi_{5,8})^{i_9 i_{10}}_{i_3 i_4} = -v^{i_9 i_{10}}_{i_3 i_4} + (\Xi_0)^{i_9 i_{10}}_{i_3 i_4} - \tfrac{1}{2} (\Xi_{37})^{i_9 i_{10}}_{i_3 i_4} - (\Xi_{20})^{i_9 i_{10}}_{i_3 i_4} - (\Xi_{23})^{i_9 i_{10}}_{i_3 i_4}$$
$$(\xi_{5,5,1})^{i_9 i_{10}}_{i_4 a_{11}} = -v^{i_9 i_{10}}_{i_4 a_{11}} + (\Xi_8)^{i_9 i_{10}}_{i_4 a_{11}}$$
$$\begin{aligned}(\xi_{5,5})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} &= -(\Xi_{41})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + (\Xi_{25})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} - (\Xi_{44})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + (\Xi_{35})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\ &\quad + P_3 t^{a_8 a_{11}}_{i_2 i_3} (\Xi_9)^{i_9 i_{10}}_{i_4 a_{11}} + P_3 r^{a_8 a_{11}}_{i_2 i_3} (\xi_{5,5,1})^{i_9 i_{10}}_{i_4 a_{11}}\end{aligned}$$
$$(\xi_{5,4})^{i_9 a_8}_{i_4 a'_{10}} = -r^{a_{11}}_{i_4} v^{i_9 a_8}_{a'_{10} a_{11}} - r^{a_8 a_{11}}_{i_4 i_{12}} v^{i_9 i_{12}}_{a'_{10} a_{11}} + \tilde{r}^{a'_{11} a_8}_{i_4 i_{12}} v^{i_9 i_{12}}_{a'_{10} a'_{11}}$$
$$(\xi_{5,3})^{i_9 a_8}_{i_4 a_{10}} = +(\Xi_3)^{i_9 a_8}_{i_4 a_{10}} + (\Xi_{26})^{i_9 a_8}_{i_4 a_{10}} + (\Xi_{29})^{i_9 a_8}_{i_4 a_{10}}$$
$$(\xi_{5,2})^{i_9 i_{10}}_{i_3 i_4} = +(\Xi_2)^{i_9 i_{10}}_{i_3 i_4} - (\Xi_{38})^{i_9 i_{10}}_{i_3 i_4} - (\Xi_{27})^{i_9 i_{10}}_{i_3 i_4} - (\Xi_{30})^{i_9 i_{10}}_{i_3 i_4}$$
$$(\xi_{5,11})^{i_9 i_{11}}_{i_4 a_{10}} = -v^{i_9 i_{11}}_{i_4 a_{10}} + (\Xi_8)^{i_9 i_{11}}_{i_4 a_{10}}$$
$$(\xi_{5,10})^{i_9 a_8}_{i_4 a'_{10}} = +v^{i_9 a_8}_{i_4 a'_{10}} - (\Xi_{24})^{i_9 a_8}_{i_4 a'_{10}} - (\Xi_{32})^{i_9 a_8}_{i_4 a'_{10}} + (\Xi_{33})^{i_9 a_8}_{i_4 a'_{10}}$$

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TABLE ESI.4.XLIII: The computational sequence and intermediates for the R_4 amplitude equation of right-hand EOM-CCSDTQ-R12 [Part II]

$$
\begin{aligned}
(\xi_{5,1})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} &= -(\Xi_4)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + (\Xi_5)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} - (\Xi_{40})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + (\Xi_{42})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
&\quad +(\Xi_{17})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
(\xi_{5,0})^{i_9}_{a_{10}} &= -f^{i_9}_{a_{10}} - (\Xi_{11})^{i_9}_{a_{10}} \\
(\xi_5)^{i_9 a_7 a_8}_{i_2 i_3 i_4} &= +r^{a_7 a_8 a_{10}}_{i_2 i_3 i_4} (\xi_{5,0})^{i_9}_{a_{10}} + P_2 r^{a_7}_{i_{10}} (\xi_{5,1})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
&\quad +\tfrac{1}{2} P_3 t^{a_7 a_8}_{i_2 i_{10}} (\xi_{5,2})^{i_9 i_{10}}_{i_3 i_4} + P_2 P_3 t^{a_7 a_{10}}_{i_2 i_3} (\xi_{5,3})^{i_9 a_8}_{i_4 a_{10}} \\
&\quad +P_2 P_3 \tilde{t}^{a'_{10} a_7}_{i_2 i_3} (\xi_{5,4})^{i_9 a_8}_{i_4 a'_{10}} + P_2 t^{a_7}_{i_{10}} (\xi_{5,5})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
&\quad +P_3 t^{a_7 a_8 a_{10}}_{i_2 i_3 i_{11}} (\Xi_9)^{i_9 i_{11}}_{i_4 a_{10}} - t^{a_7 a_8 a_{10}}_{i_2 i_3 i_4} (\Xi_{12})^{i_9}_{a_{10}} \\
&\quad +P_3 r^{a_7 a_8}_{i_2 i_{10}} (\xi_{5,8})^{i_9 i_{10}}_{i_3 i_4} + P_2 P_3 r^{a_7 a_{10}}_{i_2 i_3} (\xi_{5,9})^{i_9 a_8}_{i_4 a_{10}} \\
&\quad +P_2 P_3 \tilde{r}^{a'_{10} a_7}_{i_2 i_3} (\xi_{5,10})^{i_9 a_8}_{i_4 a'_{10}} + P_3 r^{a_7 a_8 a_{10}}_{i_2 i_3 i_{11}} (\xi_{5,11})^{i_9 i_{11}}_{i_4 a_{10}} \\
&\quad +\tfrac{1}{2} P_2 r^{a_7 a_{10} a_{11}}_{i_2 i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} - \tfrac{1}{2} r^{a_7 a_8 a_{10} a_{11}}_{i_2 i_3 i_4 i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}} \\
(\xi_{4,6})^{i_9 i_{11}}_{i_4 a'_{10}} &= -v^{i_9 i_{11}}_{i_4 a'_{10}} + (\Xi_{14})^{i_9 i_{11}}_{i_4 a'_{10}} \\
(\xi_{4,4})^{i_9 i_{11}}_{i_4 a_{10}} &= +v^{i_9 i_{11}}_{i_4 a_{10}} - (\Xi_8)^{i_9 i_{11}}_{i_4 a_{10}} \\
(\xi_{4,3})^{i_9 a_8}_{i_4 a_{10}} &= +v^{i_9 a_8}_{i_4 a_{10}} - \tfrac{1}{2} (\Xi_1)^{i_9 a_8}_{i_4 a_{10}} \\
(\xi_{4,2})^{i_9 i_{10}}_{i_3 i_4} &= +v^{i_9 i_{10}}_{i_3 i_4} - (\Xi_0)^{i_9 i_{10}}_{i_3 i_4} + \tfrac{1}{2} (\Xi_{37})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{23})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{20})^{i_9 i_{10}}_{i_3 i_4} \\
(\xi_{4,1})^{i_9}_{a'_{10}} &= -f^{i_9}_{a'_{10}} - (\Xi_{28})^{i_9}_{a'_{10}} \\
(\xi_{4,0})^{i_9}_{a_{10}} &= +f^{i_9}_{a_{10}} + (\Xi_{11})^{i_9}_{a_{10}} \\
(\xi_4)^{i_9 a_8}_{i_3 i_4} &= -v^{i_9 a_8}_{i_3 i_4} + t^{a_8 a_{10}}_{i_3 i_4} (\xi_{4,0})^{i_9}_{a_{10}} + \tilde{t}^{a'_{10} a_8}_{i_3 i_4} (\xi_{4,1})^{i_9}_{a'_{10}} + t^{a_8}_{i_{10}} (\xi_{4,2})^{i_9 i_{10}}_{i_3 i_4} \\
&\quad +P_2 t^{a_{10}}_{i_3} (\xi_{4,3})^{i_9 a_8}_{i_4 a_{10}} + P_2 t^{a_8 a_{10}}_{i_3 i_{11}} (\xi_{4,4})^{i_9 i_{11}}_{i_4 a_{10}} - \tfrac{1}{2} t^{a_{10} a_{11}}_{i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} \\
&\quad +P_2 \tilde{t}^{a'_{10} a_8}_{i_3 i_{11}} (\xi_{4,6})^{i_9 i_{11}}_{i_4 a'_{10}} - \tfrac{1}{2} t^{i_{10} i_{11}}_{i_3 i_4} V^{i_9 a_8}_{i_{10} i_{11}} + \tfrac{1}{2} t^{a_8 a_{10} a_{11}}_{i_3 i_4 i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}} \\
(\xi_{3,9})^{i_9}_{a'_{10}} &= -r^{a_{11}}_{i_{12}} v^{i_9 i_{12}}_{a'_{10} a_{11}} \\
(\xi_{3,4})^{i_9 i_{10}}_{i_3 i_4} &= -(\Xi_2)^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{38})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{27})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{30})^{i_9 i_{10}}_{i_3 i_4} \\
(\xi_{3,2})^{i_9 i_{10}}_{i_3 i_4} &= +v^{i_9 i_{10}}_{i_3 i_4} - (\Xi_0)^{i_9 i_{10}}_{i_3 i_4} + \tfrac{1}{2} (\Xi_{37})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{20})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{23})^{i_9 i_{10}}_{i_3 i_4} \\
(\xi_{3,12})^{i_9 i_{11}}_{i_4 a'_{10}} &= -v^{i_9 i_{11}}_{i_4 a'_{10}} + (\Xi_{14})^{i_9 i_{11}}_{i_4 a'_{10}} \\
(\xi_{3,10})^{i_9 i_{11}}_{i_4 a_{10}} &= +v^{i_9 i_{11}}_{i_4 a_{10}} - (\Xi_8)^{i_9 i_{11}}_{i_4 a_{10}} \\
(\xi_{3,1})^{i_9}_{a'_{10}} &= -f^{i_9}_{a'_{10}} - (\Xi_{28})^{i_9}_{a'_{10}} \\
(\xi_{3,0})^{i_9}_{a_{10}} &= +f^{i_9}_{a_{10}} + (\Xi_{11})^{i_9}_{a_{10}} \\
(\xi_3)^{i_9 a_8}_{i_3 i_4} &= +r^{a_8 a_{10}}_{i_3 i_4} (\xi_{3,0})^{i_9}_{a_{10}} + \tilde{r}^{a'_{10} a_8}_{i_3 i_4} (\xi_{3,1})^{i_9}_{a'_{10}} + r^{a_8}_{i_{10}} (\xi_{3,2})^{i_9 i_{10}}_{i_3 i_4} \\
&\quad +P_2 r^{a_{10}}_{i_3} v^{i_9 a_8}_{i_4 a_{10}} + t^{a_8}_{i_{10}} (\xi_{3,4})^{i_9 i_{10}}_{i_3 i_4} - P_2 t^{a_{10}}_{i_3} (\Xi_3)^{i_9 a_8}_{i_4 a_{10}} \\
&\quad -P_2 t^{a_8 a_{10}}_{i_3 i_{11}} (\Xi_9)^{i_9 i_{11}}_{i_4 a_{10}} + t^{a_8 a_{10}}_{i_3 i_4} (\Xi_{12})^{i_9}_{a_{10}} + P_2 \tilde{t}^{a'_{10} a_8}_{i_3 i_{11}} (\Xi_{16})^{i_9 i_{11}}_{i_4 a'_{10}} \\
&\quad +\tilde{t}^{a'_{10} a_8}_{i_3 i_4} (\xi_{3,9})^{i_9}_{a'_{10}} + P_2 r^{a_8 a_{10}}_{i_3 i_{11}} (\xi_{3,10})^{i_9 i_{11}}_{i_4 a_{10}} - \tfrac{1}{2} r^{a_{10} a_{11}}_{i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} \\
&\quad +P_2 \tilde{r}^{a'_{10} a_8}_{i_3 i_{11}} (\xi_{3,12})^{i_9 i_{11}}_{i_4 a'_{10}} - \tfrac{1}{2} r^{i_{10} i_{11}}_{i_3 i_4} V^{i_9 a_8}_{i_{10} i_{11}} + \tfrac{1}{2} r^{a_8 a_{10} a_{11}}_{i_3 i_4 i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}} \\
(\xi_{24})^{i_{10} a_8}_{i_4 a_9} &= -v^{i_{10} a_8}_{i_4 a_9} + (\Xi_1)^{i_{10} a_8}_{i_4 a_9} + (\Xi_{19})^{i_{10} a_8}_{i_4 a_9} + (\Xi_{22})^{i_{10} a_8}_{i_4 a_9} \\
(\xi_{23})^{i_9 i_{10}}_{i_3 i_4} &= +v^{i_9 i_{10}}_{i_3 i_4} - (\Xi_0)^{i_9 i_{10}}_{i_3 i_4} + \tfrac{1}{2} (\Xi_{37})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{20})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{23})^{i_9 i_{10}}_{i_3 i_4} \\
(\xi_{21})^{a_6 a_7 a_8}_{i_3 i_4 a'_9} &= +P_3 r^{a_6 a_7 a_{10}}_{i_3 i_4 i_{11}} v^{i_{11} a_8}_{a'_9 a_{10}} + \tfrac{1}{2} r^{a_6 a_7 a_8 a_{10}}_{i_3 i_4 i_{11} i_{12}} v^{i_{11} i_{12}}_{a'_9 a_{10}} \\
(\xi_{20})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} &= +(\Xi_5)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} - (\Xi_{40})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + (\Xi_{17})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
(\xi_{2,4})^{i_9 i_{11}}_{i_4 a_{10}} &= -v^{i_9 i_{11}}_{i_4 a_{10}} + (\Xi_8)^{i_9 i_{11}}_{i_4 a_{10}} \\
(\xi_{2,3})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} &= +(\Xi_5)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} - (\Xi_4)^{i_9 i_{10} a_8}_{i_2 i_3 i_4} - (\Xi_{40})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + (\Xi_{17})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
&\quad +(\Xi_{42})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
(\xi_{2,2})^{i_9 a_8}_{i_4 a'_{10}} &= +v^{i_9 a_8}_{i_4 a'_{10}} - (\Xi_{24})^{i_9 a_8}_{i_4 a'_{10}} - (\Xi_{32})^{i_9 a_8}_{i_4 a'_{10}} + (\Xi_{33})^{i_9 a_8}_{i_4 a'_{10}} \\
(\xi_{2,1})^{i_9 a_8}_{i_4 a_{10}} &= -v^{i_9 a_8}_{i_4 a_{10}} + (\Xi_1)^{i_9 a_8}_{i_4 a_{10}} + (\Xi_{19})^{i_9 a_8}_{i_4 a_{10}} + (\Xi_{22})^{i_9 a_8}_{i_4 a_{10}} \\
(\xi_{2,0})^{i_9}_{a_{10}} &= -f^{i_9}_{a_{10}} - (\Xi_{11})^{i_9}_{a_{10}} \\
(\xi_2)^{i_9 a_7 a_8}_{i_2 i_3 i_4} &= +t^{a_7 a_8 a_{10}}_{i_2 i_3 i_4} (\xi_{2,0})^{i_9}_{a_{10}} + P_2 P_3 t^{a_7 a_{10}}_{i_2 i_3} (\xi_{2,1})^{i_9 a_8}_{i_4 a_{10}} \\
&\quad +P_2 P_3 \tilde{t}^{a'_{10} a_7}_{i_2 i_3} (\xi_{2,2})^{i_9 a_8}_{i_4 a'_{10}} + P_2 t^{a_7}_{i_{10}} (\xi_{2,3})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
&\quad +P_3 t^{a_7 a_8 a_{10}}_{i_2 i_3 i_{11}} (\xi_{2,4})^{i_9 i_{11}}_{i_4 a_{10}} + \tfrac{1}{2} P_2 t^{a_7 a_{10} a_{11}}_{i_2 i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} \\
&\quad -\tfrac{1}{2} t^{a_7 a_8 a_{10} a_{11}}_{i_2 i_3 i_4 i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}} \\
(\xi_{19,1})^{i_{10} i_{11}}_{i_4 a_9} &= -v^{i_{10} i_{11}}_{i_4 a_9} + (\Xi_8)^{i_{10} i_{11}}_{i_4 a_9} \\
(\xi_{19})^{a_7 a_8}_{i_4 a_9} &= -v^{a_7 a_8}_{i_4 a_9} + t^{a_{10}}_{i_4} v^{a_7 a_8}_{a_9 a_{10}} + \tfrac{1}{2} t^{a_7 a_8}_{i_{10} i_{11}} (\xi_{19,1})^{i_{10} i_{11}}_{i_4 a_9} + P_2 t^{a_7 a_{10}}_{i_4 i_{11}} v^{i_{11} a_8}_{a_9 a_{10}} \\
&\quad +P_2 \tilde{t}^{a'_{10} a_7}_{i_4 i_{11}} v^{i_{11} a_8}_{a'_{10} a_9} + \tfrac{1}{2} t^{a_7 a_8 a_{10}}_{i_4 i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} \\
(\xi_{18})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} &= +(\Xi_{10})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} - \tfrac{1}{2} (\Xi_{39})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} \\
(\xi_{17})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} &= -(\Xi_{43})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} + (\Xi_{36})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} \\
(\xi_{16})^{a_6 a_7 a_8}_{i_3 i_4 a'_9} &= -P_3 \tilde{t}^{a'_{10} a_6}_{i_3 i_4} v^{a_7 a_8}_{a'_9 a'_{10}} + P_3 t^{a_6 a_7 a_{10}}_{i_3 i_4 i_{11}} v^{i_{11} a_8}_{a'_9 a_{10}} + \tfrac{1}{2} t^{a_6 a_7 a_8 a_{10}}_{i_3 i_4 i_{11} i_{12}} v^{i_{11} i_{12}}_{a'_9 a_{10}} \\
(\xi_{15,1})^{i_{10} i_{11}}_{i_4 a_9} &= +v^{i_{10} i_{11}}_{i_4 a_9} - (\Xi_8)^{i_{10} i_{11}}_{i_4 a_9} \\
(\xi_{15})^{a_6 a_7 a_8}_{i_3 i_4 a_9} &= -P_3 \tilde{t}^{a'_{10} a_6}_{i_3 i_4} v^{a_7 a_8}_{a'_{10} a_9} + \tfrac{1}{2} P_2 t^{a_6 a_7 a_8}_{i_3 i_{10} i_{11}} (\xi_{15,1})^{i_{10} i_{11}}_{i_4 a_9} \\
&\quad -P_3 t^{a_6 a_7 a_{10}}_{i_3 i_4 i_{11}} v^{i_{11} a_8}_{a_9 a_{10}} - \tfrac{1}{2} P_3 t^{a_6 a_7}_{i_{10} i_{11}} (\Xi_{15})^{i_{10} i_{11} a_8}_{i_3 i_4 a_9} - \tfrac{1}{2} t^{a_6 a_7 a_8 a_{10}}_{i_3 i_4 i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} \\
(\xi_{14})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} &= -(\Xi_{41})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + (\Xi_{25})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} - (\Xi_{44})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + (\Xi_{35})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} \\
(\xi_{13,6})^{i_{10} i_{11}}_{i_4 a_9} &= +v^{i_{10} i_{11}}_{i_4 a_9} - (\Xi_8)^{i_{10} i_{11}}_{i_4 a_9} \\
(\xi_{13,3})^{a_7 a_8}_{a_9 a_{10}} &= -\tfrac{1}{2} r^{a_7 a_8}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} \\
(\xi_{13,1})^{a_7 a_8}_{a_9 a_{10}} &= -v^{a_7 a_8}_{a_9 a_{10}} - \tfrac{1}{2} t^{a_7 a_8}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} \\
(\xi_{13})^{a_6 a_7 a_8}_{i_3 i_4 a_9} &= -\tfrac{1}{2} P_2 t^{a_6 a_7 a_8}_{i_3 i_{10} i_{11}} (\Xi_9)^{i_{10} i_{11}}_{i_4 a_9} + P_3 r^{a_6 a_{10}}_{i_3 i_4} (\xi_{13,1})^{a_7 a_8}_{a_9 a_{10}} \\
&\quad -P_3 \tilde{r}^{a'_{10} a_6}_{i_3 i_4} v^{a_7 a_8}_{a'_{10} a_9} + \tfrac{1}{2} P_3 t^{a_6 a_{10}}_{i_3 i_4} (\xi_{13,3})^{a_7 a_8}_{a_9 a_{10}} \\
&\quad -\tfrac{1}{2} P_3 t^{a_6 a_7}_{i_{10} i_{11}} (\Xi_{31})^{i_{10} i_{11} a_8}_{i_3 i_4 a_9} - \tfrac{1}{2} P_3 r^{a_6 a_7}_{i_{10} i_{11}} (\Xi_{15})^{i_{10} i_{11} a_8}_{i_3 i_4 a_9} \\
&\quad +\tfrac{1}{2} P_2 r^{a_6 a_7 a_8}_{i_3 i_{10} i_{11}} (\xi_{13,6})^{i_{10} i_{11}}_{i_4 a_9} - P_3 r^{a_6 a_7 a_{10}}_{i_3 i_4 i_{11}} v^{i_{11} a_8}_{a_9 a_{10}} - \tfrac{1}{2} r^{a_6 a_7 a_8 a_{10}}_{i_3 i_4 i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} \\
(\xi_{12})^{a_8}_{a_9} &= -r^{a_{10}}_{i_{11}} v^{i_{11} a_8}_{a_9 a_{10}} - \tfrac{1}{2} r^{a_8 a_{10}}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a_9 a_{10}} - \tfrac{1}{2} \tilde{r}^{a'_{10} a_8}_{i_{11} i_{12}} v^{i_{11} i_{12}}_{a'_{10} a_9} \\
(\xi_{11})^{i_{10} a_8}_{i_4 a_9} &= +(\Xi_3)^{i_{10} a_8}_{i_4 a_9} + (\Xi_{26})^{i_{10} a_8}_{i_4 a_9} + (\Xi_{29})^{i_{10} a_8}_{i_4 a_9} \\
(\xi_{10})^{i_9 i_{10}}_{i_3 i_4} &= -(\Xi_2)^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{38})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{27})^{i_9 i_{10}}_{i_3 i_4} + (\Xi_{30})^{i_9 i_{10}}_{i_3 i_4} \\
(\xi_{1,0})^{i_9}_{a_{10}} &= -f^{i_9}_{a_{10}} - (\Xi_{11})^{i_9}_{a_{10}} \\
(\xi_1)^{i_9}_{i_4} &= +r^{a_{10}}_{i_4} (\xi_{1,0})^{i_9}_{a_{10}} - r^{a_{10}}_{i_{11}} v^{i_9 i_{11}}_{i_4 a_{10}} - t^{a_{10}}_{i_4} (\Xi_{12})^{i_9}_{a_{10}} - \tfrac{1}{2} r^{a_{10} a_{11}}_{i_4 i_{12}} v^{i_9 i_{12}}_{a_{10} a_{11}} \\
&\quad -\tfrac{1}{2} r^{i_{11} i_{12}}_{i_4 i_{10}} V^{i_9 i_{10}}_{i_{11} i_{12}} \\
(\xi_{0,5})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} &= +\tfrac{1}{2} (\Xi_7)^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} - (\Xi_{21})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} \\
(\xi_{0,3})^{i_9 i_{11}}_{i_4 a_{10}} &= +v^{i_9 i_{11}}_{i_4 a_{10}} - (\Xi_8)^{i_9 i_{11}}_{i_4 a_{10}} \\
(\xi_{0,2})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} &= +(\Xi_6)^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} + (\Xi_{18})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} + \tfrac{1}{2} P_2 t^{a_7 a_{11}}_{i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} \\
(\xi_{0,1})^{i_9 a_8}_{i_4 a_{10}} &= +v^{i_9 a_8}_{i_4 a_{10}} - (\Xi_1)^{i_9 a_8}_{i_4 a_{10}} - (\Xi_{19})^{i_9 a_8}_{i_4 a_{10}} - (\Xi_{22})^{i_9 a_8}_{i_4 a_{10}} \\
(\xi_{0,0})^{i_9}_{a_{10}} &= +f^{i_9}_{a_{10}} + (\Xi_{11})^{i_9}_{a_{10}} \\
(\xi_0)^{i_9 a_6 a_7 a_8}_{i_1 i_2 i_3 i_4} &= +t^{a_6 a_7 a_8 a_{10}}_{i_1 i_2 i_3 i_4} (\xi_{0,0})^{i_9}_{a_{10}} + P_3 P_4 t^{a_6 a_7 a_{10}}_{i_1 i_2 i_3} (\xi_{0,1})^{i_9 a_8}_{i_4 a_{10}} \\
&\quad +P_3 P_4 t^{a_6 a_{10}}_{i_1 i_2} (\xi_{0,2})^{i_9 a_7 a_8}_{i_3 i_4 a_{10}} + P_4 t^{a_6 a_7 a_8 a_{10}}_{i_1 i_2 i_3 i_{11}} (\xi_{0,3})^{i_9 i_{11}}_{i_4 a_{10}} \\
&\quad -\tfrac{1}{2} P_3 t^{a_6 a_7 a_{10} a_{11}}_{i_1 i_2 i_3 i_4} v^{i_9 a_8}_{a_{10} a_{11}} + P_3 P_4 \tilde{t}^{a'_{10} a_6}_{i_1 i_2} (\xi_{0,5})^{i_9 a_7 a_8}_{i_3 i_4 a'_{10}} \\
\delta^{a_5 a_6 a_7 a_8}_{i_1 i_2 i_3 i_4} &= +P_4 r^{a_5}_{i_9} (\xi_0)^{i_9 a_6 a_7 a_8}_{i_1 i_2 i_3 i_4} + P_4 t^{a_5 a_6 a_7 a_8}_{i_1 i_2 i_3 i_9} (\xi_1)^{i_9}_{i_4} \\
&\quad +P_4 P_4 r^{a_5 a_6}_{i_1 i_9} (\xi_2)^{i_9 a_7 a_8}_{i_2 i_3 i_4} + P_4 P_4 t^{a_5 a_6 a_7}_{i_1 i_2 i_9} (\xi_3)^{i_9 a_8}_{i_3 i_4} \\
&\quad +P_4 P_4 r^{a_5 a_6 a_7}_{i_1 i_2 i_9} (\xi_4)^{i_9 a_8}_{i_3 i_4} + P_4 P_4 t^{a_5 a_6}_{i_1 i_9} (\xi_5)^{i_9 a_7 a_8}_{i_2 i_3 i_4} \\
&\quad +P_4 r^{a_5 a_6 a_7 a_8}_{i_1 i_2 i_3 i_9} (\xi_6)^{i_9}_{i_4} + P_4 r^{a_5 a_6 a_7 a_9}_{i_1 i_2 i_3 i_4} (\xi_7)^{a_8}_{a_9} \\
&\quad +P_4 t^{a_5}_{i_9} (\xi_8)^{i_9 a_6 a_7 a_8}_{i_1 i_2 i_3 i_4} + P_4 P_4 t^{a_5 a_6 a_9}_{i_1 i_2 i_3} (\xi_9)^{a_7 a_8}_{i_4 a_9} \\
&\quad +\tfrac{1}{2} P_4 t^{a_5 a_6 a_7 a_8}_{i_1 i_2 i_9 i_{10}} (\xi_{10})^{i_9 i_{10}}_{i_3 i_4} + P_4 P_4 t^{a_5 a_6 a_7 a_9}_{i_1 i_2 i_3 i_{10}} (\xi_{11})^{i_{10} a_8}_{i_4 a_9} \\
&\quad +P_4 t^{a_5 a_6 a_7 a_9}_{i_1 i_2 i_3 i_4} (\xi_{12})^{a_8}_{a_9} + P_4 P_4 t^{a_5 a_9}_{i_1 i_2} (\xi_{13})^{a_6 a_7 a_8}_{i_3 i_4 a_9} \\
&\quad +\tfrac{1}{2} P_4 P_4 t^{a_5 a_6 a_7}_{i_1 i_9 i_{10}} (\xi_{14})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + P_4 P_4 r^{a_5 a_9}_{i_1 i_2} (\xi_{15})^{a_6 a_7 a_8}_{i_3 i_4 a_9} \\
&\quad +P_4 P_4 \tilde{r}^{a'_9 a_5}_{i_1 i_2} (\xi_{16})^{a_6 a_7 a_8}_{i_3 i_4 a'_9} + \tfrac{1}{2} P_4 t^{a_5 a_6}_{i_9 i_{10}} (\xi_{17})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} \\
&\quad +\tfrac{1}{2} P_4 r^{a_5 a_6}_{i_9 i_{10}} (\xi_{18})^{i_9 i_{10} a_7 a_8}_{i_1 i_2 i_3 i_4} + P_4 P_4 r^{a_5 a_6 a_9}_{i_1 i_2 i_3} (\xi_{19})^{a_7 a_8}_{i_4 a_9} \\
&\quad +\tfrac{1}{2} P_4 P_4 t^{a_5 a_6 a_7}_{i_1 i_9 i_{10}} (\xi_{20})^{i_9 i_{10} a_8}_{i_2 i_3 i_4} + P_4 P_4 \tilde{t}^{a'_9 a_5}_{i_1 i_2} (\xi_{21})^{a_6 a_7 a_8}_{i_3 i_4 a'_9} \\
&\quad +P_4 P_4 t^{a_5 a_6 a_9}_{i_1 i_2 i_{10}} (\Xi_{34})^{i_{10} a_7 a_8}_{i_3 i_4 a_9} + \tfrac{1}{2} P_4 r^{a_5 a_6 a_7 a_8}_{i_1 i_2 i_9 i_{10}} (\xi_{23})^{i_9 i_{10}}_{i_3 i_4} \\
&\quad +P_4 P_4 r^{a_5 a_6 a_7 a_9}_{i_1 i_2 i_3 i_{10}} (\xi_{24})^{i_{10} a_8}_{i_4 a_9} + \tfrac{1}{2} P_4 r^{a_5 a_6 a_9 a_{10}}_{i_1 i_2 i_3 i_4} v^{a_7 a_8}_{a_9 a_{10}}
\end{aligned}
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Supplementary data for Phys. Chem. Chem. Phys.

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