Supporting Information

Frequency and Time Domain Nuclear-Electronic Orbital Equation-of-Motion Coupled Cluster Methods: Combination Bands and Electronic-Protonic Double Excitations

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S1.1 Programmable Left Dipole Moment Function at $t = 0$

The left-hand dipole moment function at $t = 0$ is defined as $\langle \tilde{M}_\alpha(0)| = \langle 0^e 0^p|(1+\hat{\Lambda})\bar{\mu}_\alpha$. Its dipole moment amplitudes $\tilde{m}$ are obtained by projecting this equation onto the space of the reference and excited determinants ($|\nu\rangle = \{|0^e 0^p\rangle, |_i^a\rangle\, |_I^A\rangle, |_{ij}^{ab}\rangle, |_{IJ}^{AB}\rangle, |_{iI}^{aA}\rangle\}$). The programmable expressions for $\langle \tilde{M}_\alpha(0)|\nu\rangle$ are:

$$\begin{aligned}
\langle 0^e 0^p|(1+\hat{\Lambda})\bar{\mu}_\alpha|0^e 0^p\rangle = \tilde{m}_0 &= l_{i1}^{a1}\mu_{a1}^{i1} + l_{I1}^{A1}\mu_{A1}^{I1} + \mu_{i1}^{a1}t_{a1}^{i1} - l_{i1}^{a1}\mu_{i2}^{i1}t_{a1}^{i2} + l_{i1}^{a1}\mu_{a1}^{a2}t_{a2}^{i1} \\
&- l_{i1}^{a1}\mu_{i2}^{a2}t_{a1}^{i2}t_{a2}^{i1} + \mu_{I1}^{A1}t_{A1}^{I1} - l_{I1}^{A1}\mu_{I2}^{I1}t_{A1}^{I2} + l_{I1}^{A1}\mu_{A1}^{A2}t_{A2}^{I1} - l_{I1}^{A1}\mu_{I2}^{A2}t_{A1}^{I2}t_{A2}^{I1} + l_{i1}^{a1}\mu_{i2}^{a2}t_{a1a2}^{i1i2} \\
&- \mu_{i1}^{i2}l_{i2i4}^{a1a2}t_{a1a2}^{i1i4}\frac{1}{2} + \mu_{a1}^{a2}l_{i1i2}^{a1a4}t_{a2a4}^{i1i2}\frac{1}{2} + l_{I1}^{A1}\mu_{i1}^{a1}t_{a1A1}^{i1I1} + l_{i1}^{a1}\mu_{I1}^{A1}t_{a1A1}^{i1I1} - \mu_{I1}^{I2}l_{i1I2}^{a1A1}t_{a1A1}^{i1I1} \\
&- \mu_{i1}^{i2}l_{i2I1}^{a1A1}t_{a1A1}^{i1I1} + \mu_{A1}^{A2}l_{i1I1}^{a1A1}t_{a1A2}^{i1I1} + \mu_{a1}^{a2}l_{i1I1}^{a1A1}t_{a2A1}^{i1I1} + l_{I1}^{A1}\mu_{I2}^{A2}t_{A1A2}^{I1I2} - \mu_{I1}^{I2}l_{I2I4}^{A1A2}t_{A1A2}^{I1I4}\frac{1}{2} \\
&+ \mu_{A1}^{A2}l_{I1I2}^{A1A4}t_{A2A4}^{I1I2}\frac{1}{2}
\end{aligned} \tag{S1}$$

$$\begin{aligned}
\langle 0^e 0^p|(1+\hat{\Lambda})\bar{\mu}_\alpha|_i^a\rangle = \tilde{m}_i^a &= l_i^{a1}\mu_{a1}^a + \mu_i^a - l_{i1}^a\mu_i^{i1} + l_i^a\mu_{i1}^{a1}t_{a1}^{i1} - l_i^{a1}\mu_{i1}^a t_{a1}^{i1} - l_{i1}^a\mu_i^{a1}t_{a1}^{i1} \\
&+ l_i^a\mu_{I1}^{A1}t_{A1}^{I1} + \mu_{a1}^{i1}l_{ii1}^{aa1} - \mu_{i2}^{i1}t_{a1}^{i2}l_{ii1}^{aa1} + \mu_{a1}^{a2}t_{a2}^{i1}l_{ii1}^{aa1} - \mu_{i2}^{a2}t_{a1}^{i2}t_{a2}^{i1}l_{ii1}^{aa1} + \mu_{A1}^{I1}l_{iI1}^{aA1} - \mu_{I2}^{I1}t_{A1}^{I2}l_{iI1}^{aA1} \\
&+ \mu_{A1}^{A2}t_{A2}^{I1}l_{iI1}^{aA1} - \mu_{I2}^{A2}t_{A1}^{I2}t_{A2}^{I1}l_{iI1}^{aA1} - \mu_i^{a1}l_{i1i2}^{aa2}t_{a1a2}^{i1i2}\frac{1}{2} + \mu_{i2}^{a2}l_{ii1}^{aa1}t_{a1a2}^{i1i2} - \mu_{i1}^a l_{ii2}^{a1a2}t_{a1a2}^{i1i2}\frac{1}{2} \\
&+ \mu_{I1}^{A1}l_{ii1}^{aa1}t_{a1A1}^{i1I1} - \mu_i^{a1}l_{i1I1}^{aA1}t_{a1A1}^{i1I1} - \mu_{i1}^a l_{iI1}^{a1A1}t_{a1A1}^{i1I1} + \mu_{i1}^{a1}l_{iI1}^{aA1}t_{a1A1}^{i1I1} + \mu_{I2}^{A2}l_{iI1}^{aA1}t_{A1A2}^{I1I2}
\end{aligned} \tag{S2}$$

$$\langle 0^{\mathrm{e}}0^{\mathrm{p}}|(1+\hat{\Lambda})\bar{\mu}_\alpha|_I^A\rangle = \tilde{m}_I^A = l_I^{A1}\mu_{A1}^A + \mu_I^A - l_{I1}^A\mu_I^{I1} + l_I^A\mu_{i1}^{a1}t_{a1}^{i1} + l_I^A\mu_{I1}^{A1}t_{A1}^{I1} \tag{S3}$$
$$- l_I^{A1}\mu_{I1}^A t_{A1}^{I1} - l_{I1}^A\mu_I^{A1}t_{A1}^{I1} + \mu_{a1}^{i1}l_{i1I}^{a1A} - \mu_{i2}^{i1}t_{a1}^{i2}l_{i1I}^{a1A} + \mu_{a1}^{a2}t_{a2}^{i1}l_{i1I}^{a1A} - \mu_{i2}^{a2}t_{a1}^{i2}t_{a2}^{i1}l_{i1I}^{a1A} + \mu_{A1}^{I1}l_{II1}^{AA1}$$
$$- \mu_{I2}^{I1}t_{A1}^{I2}l_{II1}^{AA1} + \mu_{A1}^{A2}t_{A2}^{I1}l_{II1}^{AA1} - \mu_{I2}^{A2}t_{A1}^{I2}t_{A2}^{I1}l_{II1}^{AA1} + \mu_{i2}^{a2}l_{i1I}^{a1A}t_{a1a2}^{i1i2} - \mu_I^{A1}l_{i1I1}^{a1A}t_{a1A1}^{i1I1}$$
$$- \mu_{I1}^A l_{i1I}^{a1A1}t_{a1A1}^{i1I1} + \mu_{I1}^{A1}l_{i1I}^{a1A}t_{a1A1}^{i1I1} + \mu_{i1}^{a1}l_{III1}^{AA1}t_{a1A1}^{i1I1} - \mu_I^{A1}l_{I1I2}^{AA2}t_{A1A2}^{I1I2}\frac{1}{2} + \mu_{I2}^{A2}l_{II1}^{AA1}t_{A1A2}^{I1I2}$$
$$- \mu_{I1}^A l_{II2}^{A1A2}t_{A1A2}^{I1I2}\frac{1}{2}$$

$$\langle 0^{\mathrm{e}}0^{\mathrm{p}}|(1+\hat{\Lambda})\bar{\mu}_\alpha|_{ij}^{ab}\rangle = \tilde{m}_{ij}^{ab} = l_j^b\mu_i^a - l_j^a\mu_i^b - l_i^b\mu_j^a + l_i^a\mu_j^b - \mu_j^{i1}l_{ii1}^{ab} - \mu_j^{a1}t_{a1}^{i1}l_{ii1}^{ab} \tag{S4}$$
$$+ \mu_{a1}^b l_{ij}^{aa1} - \mu_{i1}^b t_{a1}^{i1}l_{ij}^{aa1} + \mu_{i1}^{a1}t_{a1}^{i1}l_{ij}^{ab} + \mu_{I1}^{A1}t_{A1}^{I1}l_{ij}^{ab} - \mu_{a1}^a l_{ij}^{ba1} + \mu_{i1}^a t_{a1}^{i1}l_{ij}^{ba1} + \mu_i^{i1}l_{ji1}^{ab}$$
$$+ \mu_i^{a1}t_{a1}^{i1}l_{ji1}^{ab}$$

$$\langle 0^{\mathrm{e}}0^{\mathrm{p}}|(1+\hat{\Lambda})\bar{\mu}_\alpha|_{IJ}^{AB}\rangle = \tilde{m}_{IJ}^{AB} = l_J^B\mu_I^A - l_J^A\mu_I^B - l_I^B\mu_J^A + l_I^A\mu_J^B - \mu_J^{I1}l_{II2}^{AB} \tag{S5}$$
$$- \mu_J^{A1}t_{A1}^{I1}l_{II2}^{AB} + \mu_{A1}^B l_{IJ}^{AA1} - \mu_{I1}^B t_{A1}^{I1}l_{IJ}^{AA1} + \mu_{i1}^{a1}t_{a1}^{i1}l_{IJ}^{AB} + \mu_{I1}^{A1}t_{A1}^{I1}l_{IJ}^{AB} - \mu_{A1}^A l_{IJ}^{BA1}$$
$$+ \mu_{I1}^A t_{A1}^{I1}l_{IJ}^{BA1} + \mu_I^{I1}l_{JI1}^{AB} + \mu_I^{A1}t_{A1}^{I1}l_{JI1}^{AB}$$

$$\langle 0^{\mathrm{e}}0^{\mathrm{p}}|(1+\hat{\Lambda})\bar{\mu}_\alpha|_{iI}^{aA}\rangle = \tilde{m}_{iI}^{aA} = l_I^A\mu_i^a + l_i^a\mu_I^A - \mu_i^{i1}l_{i1I}^{aA} - \mu_i^{a1}t_{a1}^{i1}l_{i1I}^{aA} - \mu_I^{I1}l_{iI1}^{aA} \tag{S6}$$
$$- \mu_I^{A1}t_{A1}^{I1}l_{iI1}^{aA} + \mu_{a1}^a l_{iI}^{a1A} - \mu_{i1}^a t_{a1}^{i1}l_{iI}^{a1A} + \mu_{A1}^A l_{iI}^{aA1} - \mu_{I1}^A t_{A1}^{I1}l_{iI}^{aA1} + \mu_{i1}^{a1}t_{a1}^{i1}l_{iI}^{aA} + \mu_{I1}^{A1}t_{A1}^{I1}l_{iI}^{aA}$$

S1.2 Programmable Right Dipole Moment Function at $t = 0$

The right-hand dipole moment function at $t = 0$ is defined as $|M_\alpha(0)\rangle = \bar{\mu}_\alpha|0^e 0^P\rangle$. Its dipole moment amplitudes m are obtained by projecting this equation onto the space of the reference and excited determinants ($|\nu\rangle = \{|0^e 0^P\rangle, |_i^a\rangle\, |_I^A\rangle, |_{ij}^{ab}\rangle, |_{IJ}^{AB}\rangle, |_{iI}^{aA}\rangle\}$). The programmable expressions for $\langle\nu|M_\alpha(0)\rangle$ are:

$$\langle 0^e 0^P|\bar{\mu}_\alpha|0^e 0^P\rangle = m_0 = \mu_{i1}^{a1} t_{a1}^{i1} + \mu_{I1}^{A1} t_{A1}^{I1} \tag{S7}$$

$$\langle {}_i^a|\bar{\mu}_\alpha|0^e 0^P\rangle = m_a^i = \mu_a^i + \mu_a^{a1} t_{a1}^i - \mu_{i1}^i t_a^{i1} - \mu_{i1}^{a1} t_{a1}^i t_a^{i1} + \mu_{i1}^{a1} t_{aa1}^{ii1} + \mu_{I1}^{A1} t_{aA1}^{iI1} \tag{S8}$$

$$\langle {}_I^A|\bar{\mu}_\alpha|0^e 0^P\rangle = m_A^I = \mu_A^I + \mu_A^{A1} t_{A1}^I - \mu_{I1}^I t_A^{I1} - \mu_{I1}^{A1} t_{A1}^I t_A^{I1} + \mu_{i1}^{a1} t_{a1A}^{i1I} + \mu_{I1}^{A1} t_{AA1}^{II1} \tag{S9}$$

$$\langle {}_{ij}^{ab}|\bar{\mu}_\alpha|0^e 0^P\rangle = m_{ab}^{ij} = \mu_b^{a1} t_{aa1}^{ij} - \mu_{i1}^j t_{ab}^{ii1} + \mu_{i1}^i t_{ab}^{ji1} - \mu_a^{a1} t_{ba1}^{ij} \tag{S10}$$

$$\langle {}_{IJ}^{AB}|\bar{\mu}_\alpha|0^e 0^P\rangle = m_{AB}^{IJ} = \mu_B^{A1} t_{AA1}^{IJ} - \mu_{I1}^J t_{AB}^{II1} + \mu_{I1}^I t_{AB}^{JI1} - \mu_A^{A1} t_{BA1}^{IJ} \tag{S11}$$

$$\langle {}_{iI}^{aA}|\bar{\mu}_\alpha|0^e 0^P\rangle = m_{aA}^{iI} = \mu_a^{a1} t_{a1A}^{iI} + \mu_A^{A1} t_{aA1}^{iI} - \mu_{i1}^i t_{aA}^{i1I} - \mu_{I1}^I t_{aA}^{iI1} \tag{S12}$$

S1.3 Programmable Expressions of Time Derivative of m Amplitudes

The time evolution of the dipole moment amplitudes m is governed by the time-dependent NEO Schrödinger equation

$$\frac{\partial}{\partial t}|M_\alpha(t)\rangle = -\mathrm{i}\bar{H}_\mathrm{N}|M_\alpha(t)\rangle \tag{S13}$$

Projecting Eq. S13 onto the space of the reference and excited determinants ($|\nu\rangle = \{|0^\mathrm{e}0^\mathrm{p}\rangle, |^a_i\rangle$ $|^A_I\rangle, |^{ab}_{ij}\rangle, |^{AB}_{IJ}\rangle, |^{aA}_{iI}\rangle\}$) gives

$$\frac{\partial}{\partial t}\langle\nu|M_\alpha(t)\rangle = -\mathrm{i}\langle\nu|\bar{H}_\mathrm{N}|M_\alpha(t)\rangle = -\mathrm{i}\sigma_\nu \tag{S14}$$

The programmable expressions for σ_ν are:

$$\begin{aligned}\sigma_0 &= F^{a1}_{i1}m^{i1}_{a1} + F^{A1}_{I1}m^{I1}_{A1} + m^{i1}_{a1}t^{i4}_{a4}\bar{g}^{a1a4}_{i1i4} - m^{I1}_{A1}t^{i1}_{a1}g^{a1A1}_{i1I1} - m^{i1}_{a1}t^{I1}_{A1}g^{a1A1}_{i1I1} + m^{I1}_{A1}t^{I4}_{A4}\bar{g}^{A1A4}_{I1I4} \\ &+ \bar{g}^{a1a4}_{i1i4}m^{i1i4}_{a1a4}\frac{1}{4} - g^{a1A1}_{i1I1}m^{i1I1}_{a1A1} + \bar{g}^{A1A4}_{I1I4}m^{I1I4}_{A1A4}\frac{1}{4}\end{aligned} \tag{S15}$$

$$\begin{aligned}\sigma^i_a &= F^{a1}_a m^i_{a1} - F^i_{i1}m^{i1}_a - F^{a1}_{i1}m^{i1}_a t^i_{a1} - F^{a1}_{i1}m^i_{a1}t^{i1}_a + m^{i1}_{a2}t^i_{a1}\bar{g}^{a1a2}_{ai1} + m^i_{a1}t^{i1}_{a2}\bar{g}^{a1a2}_{ai1} + m^{i1}_{a1}\bar{g}^{ia1}_{ai1} \\ &- m^{i1}_a t^i_{a1}t^{i2}_{a2}\bar{g}^{a1a2}_{i1i2} - m^{i2}_{a2}t^i_{a1}t^{i1}_a\bar{g}^{a1a2}_{i1i2} - m^i_{a1}t^{i2}_{a2}t^{i1}_a\bar{g}^{a1a2}_{i1i2} - m^{i1}_a t^{i2}_{a1}\bar{g}^{ia1}_{i1i2} - m^{i2}_{a1}t^{i1}_a\bar{g}^{ia1}_{i1i2} \\ &- m^{I1}_{A1}t^i_{a1}g^{a1A1}_{aI1} - m^i_{a1}t^{I1}_{A1}g^{a1A1}_{aI1} - m^{I1}_{A1}g^{iA1}_{aI1} + m^{I1}_{A1}t^i_{a1}t^{i1}_a g^{a1A1}_{i1I1} + m^{i1}_a t^i_{a1}t^{I1}_{A1}g^{a1A1}_{i1I1} \\ &+ m^i_{a1}t^{i1}_a t^{I1}_{A1}g^{a1A1}_{i1I1} + m^{I1}_{A1}t^{i1}_a g^{iA1}_{i1I1} + m^{i1}_a t^{I1}_{A1}g^{iA1}_{i1I1} + \bar{g}^{a1a2}_{ai1}m^{ii1}_{a1a2}\frac{1}{2} - t^{i1}_a\bar{g}^{a1a2}_{i1i2}m^{ii2}_{a1a2}\frac{1}{2} \\ &- \bar{g}^{ia1}_{i1i2}m^{i1i2}_{aa1}\frac{1}{2} + F^{a1}_{i1}m^{ii1}_{aa1} + t^{i2}_{a2}\bar{g}^{a1a2}_{i1i2}m^{ii1}_{aa1} - t^{I1}_{A1}g^{a1A1}_{i1I1}m^{ii1}_{aa1} - t^i_{a1}\bar{g}^{a1a2}_{i1i2}m^{i1i2}_{aa2}\frac{1}{2} - g^{a1A1}_{aI1}m^{iI1}_{a1A1} \\ &+ t^{i1}_a g^{a1A1}_{i1I1}m^{iI1}_{a1A1} + t^i_{a1}g^{a1A1}_{i1I1}m^{i1I1}_{aA1} + g^{iA1}_{i1I1}m^{i1I1}_{aA1} + F^{A1}_{I1}m^{iI1}_{aA1} - t^{i1}_{a1}g^{a1A1}_{i1I1}m^{iI1}_{aA1} + t^{I2}_{A2}\bar{g}^{A1A2}_{I1I2}m^{iI1}_{aA1} \\ &- m^{i1}_a\bar{g}^{a1a2}_{i1i2}t^{ii2}_{a1a2}\frac{1}{2} + m^{i2}_{a2}\bar{g}^{a1a2}_{i1i2}t^{ii1}_{aa1} - m^{I1}_{A1}g^{a1A1}_{i1I1}t^{ii1}_{aa1} - m^i_{a1}\bar{g}^{a1a2}_{i1i2}t^{i1i2}_{aa2}\frac{1}{2} + m^{i1}_a g^{a1A1}_{i1I1}t^{iI1}_{a1A1} \\ &+ m^i_{a1}g^{a1A1}_{i1I1}t^{i1I1}_{aA1} - m^{i1}_{a1}g^{a1A1}_{i1I1}t^{iI1}_{aA1} + m^{I2}_{A2}\bar{g}^{A1A2}_{I1I2}t^{iI1}_{aA1}\end{aligned} \tag{S16}$$

$$\sigma_A^I = F_A^{A1} m_{A1}^I - F_{I1}^I m_A^I - F_{I1}^{A1} m_A^I t_{A1}^I - F_{I1}^{A1} m_{A1}^I t_A^{I1} - m_{A1}^I t_{a1}^{i1} g_{i1A}^{a1A1} - m_{a1}^{i1} t_{A1}^I g_{i1A}^{a1A1} \tag{S17}$$
$$- m_{a1}^{i1} g_{i1A}^{a1I} + m_A^I t_{a1}^{i1} t_{A1}^I g_{i1I1}^{a1A1} + m_{A1}^I t_{a1}^{i1} t_A^{I1} g_{i1I1}^{a1A1} + m_{a1}^{i1} t_{A1}^I t_A^{I1} g_{i1I1}^{a1A1} + m_A^I t_{a1}^{i1} g_{i1I1}^{a1I}$$
$$+ m_{a1}^{i1} t_A^{I1} g_{i1I1}^{a1I} + m_{A2}^{I1} t_{A1}^I \bar{g}_{AI1}^{A1A2} + m_{A1}^I t_{A2}^{I1} \bar{g}_{AI1}^{A1A2} + m_{A1}^{I1} \bar{g}_{AI1}^{IA1} - m_A^I t_{A1}^I t_{A2}^{I2} \bar{g}_{I1I2}^{A1A2}$$
$$- m_{A2}^{I2} t_{A1}^I t_A^{I1} \bar{g}_{I1I2}^{A1A2} - m_{A1}^I t_{A2}^{I2} t_A^{I1} \bar{g}_{I1I2}^{A1A2} - m_A^I t_{A1}^{I2} \bar{g}_{I1I2}^{IA1} - m_{A1}^{I2} t_A^{I1} \bar{g}_{I1I2}^{IA1} - g_{i1A}^{a1A1} m_{a1A1}^{i1I}$$
$$+ t_A^{I1} g_{i1I1}^{a1A1} m_{a1A1}^{i1I} + t_{A1}^I g_{i1I1}^{a1A1} m_{a1A}^{i1I1} + g_{i1I1}^{a1I} m_{a1A}^{i1I1} + F_{i1}^{a1} m_{a1A}^{i1I} + t_{a2}^{i2} \bar{g}_{i1i2}^{a1a2} m_{a1A}^{i1I}$$
$$- t_{A1}^{I1} g_{i1I1}^{a1A1} m_{a1A}^{i1I} + \bar{g}_{AI1}^{A1A2} m_{A1A2}^{II1} \frac{1}{2} - t_A^{I1} \bar{g}_{I1I2}^{A1A2} m_{A1A2}^{II2} \frac{1}{2} - \bar{g}_{I1I2}^{IA1} m_{AA1}^{I1I2} \frac{1}{2} + F_{I1}^{A1} m_{AA1}^{II1}$$
$$- t_{a1}^{i1} g_{i1I1}^{a1A1} m_{AA1}^{II1} + t_{A2}^{I2} \bar{g}_{I1I2}^{A1A2} m_{AA1}^{II1} - t_{A1}^I \bar{g}_{I1I2}^{A1A2} m_{AA2}^{I1I2} \frac{1}{2} + m_A^I g_{i1I1}^{a1A1} t_{a1A1}^{i1I} + m_{A1}^I g_{i1I1}^{a1A1} t_{a1A}^{i1I1}$$
$$+ m_{a2}^{i2} \bar{g}_{i1i2}^{a1a2} t_{a1A}^{i1I} - m_{A1}^{I1} g_{i1I1}^{a1A1} t_{a1A}^{i1I} - m_A^I \bar{g}_{I1I2}^{A1A2} t_{A1A2}^{II2} \frac{1}{2} - m_{a1}^{i1} g_{i1I1}^{a1A1} t_{AA1}^{II1} + m_{A2}^{I2} \bar{g}_{I1I2}^{A1A2} t_{AA1}^{II1}$$
$$- m_{A1}^I \bar{g}_{I1I2}^{A1A2} t_{AA2}^{I1I2} \frac{1}{2}$$

$$\sigma_{ab}^{ij} = m_{a2}^j t_{a1}^i \bar{g}_{ab}^{a1a2} - m_{a2}^i t_{a1}^j \bar{g}_{ab}^{a1a2} + m_{a1}^j \bar{g}_{ab}^{ia1} - m_{a1}^i \bar{g}_{ab}^{ja1} - m_b^{i1} t_{a1}^i t_{a2}^j \bar{g}_{ai1}^{a1a2} \tag{S18}$$
$$+ m_{a1}^j t_{a2}^i t_b^{i1} \bar{g}_{ai1}^{a1a2} - m_{a1}^i t_{a2}^j t_b^{i1} \bar{g}_{ai1}^{a1a2} - m_b^{i1} t_{a1}^j \bar{g}_{ai1}^{ia1} - m_{a1}^j t_b^{i1} \bar{g}_{ai1}^{ia1} - m_b^{i1} \bar{g}_{ai1}^{ij} + m_b^{i1} t_{a1}^i \bar{g}_{ai1}^{ja1}$$
$$+ m_{a1}^i t_b^{i1} \bar{g}_{ai1}^{ja1} + m_a^{i1} t_{a1}^i t_{a2}^j \bar{g}_{bi1}^{a1a2} - m_{a1}^j t_{a2}^i t_a^{i1} \bar{g}_{bi1}^{a1a2} + m_{a1}^i t_{a2}^j t_a^{i1} \bar{g}_{bi1}^{a1a2} + m_a^{i1} t_{a1}^j \bar{g}_{bi1}^{ia1}$$
$$+ m_{a1}^j t_a^{i1} \bar{g}_{bi1}^{ia1} + m_a^{i1} \bar{g}_{bi1}^{ij} - m_a^{i1} t_{a1}^i \bar{g}_{bi1}^{ja1} - m_{a1}^i t_a^{i1} \bar{g}_{bi1}^{ja1} - m_b^{i1} t_{a1}^i t_{a2}^j t_a^{i2} \bar{g}_{i1i2}^{a1a2} + m_a^{i1} t_{a1}^i t_{a2}^j t_b^{i2} \bar{g}_{i1i2}^{a1a2}$$
$$- m_{a1}^j t_{a2}^i t_a^{i1} t_b^{i2} \bar{g}_{i1i2}^{a1a2} + m_{a1}^i t_{a2}^j t_a^{i1} t_b^{i2} \bar{g}_{i1i2}^{a1a2} - m_b^{i1} t_{a1}^j t_a^{i2} \bar{g}_{i1i2}^{ia1} + m_a^{i1} t_{a1}^j t_b^{i2} \bar{g}_{i1i2}^{ia1} + m_{a1}^j t_a^{i1} t_b^{i2} \bar{g}_{i1i2}^{ia1}$$
$$+ m_b^{i2} t_a^{i1} \bar{g}_{i1i2}^{ij} - m_a^{i2} t_b^{i1} \bar{g}_{i1i2}^{ij} + m_b^{i1} t_{a1}^i t_a^{i2} \bar{g}_{i1i2}^{ja1} - m_a^{i1} t_{a1}^i t_b^{i2} \bar{g}_{i1i2}^{ja1} - m_{a1}^i t_a^{i1} t_b^{i2} \bar{g}_{i1i2}^{ja1} + \bar{g}_{ab}^{a1a2} m_{a1a2}^{ij} \frac{1}{2}$$
$$- t_b^{i1} \bar{g}_{ai1}^{a1a2} m_{a1a2}^{ij} \frac{1}{2} + t_a^{i1} \bar{g}_{bi1}^{a1a2} m_{a1a2}^{ij} \frac{1}{2} + t_a^{i1} t_b^{i2} \bar{g}_{i1i2}^{a1a2} m_{a1a2}^{ij} \frac{1}{2} - t_{a2}^j \bar{g}_{bi1}^{a1a2} m_{aa1}^{ii1} + \bar{g}_{bi1}^{ja1} m_{aa1}^{ii1}$$
$$- t_{a2}^j t_b^{i2} \bar{g}_{i1i2}^{a1a2} m_{aa1}^{ii1} + t_b^{i2} \bar{g}_{i1i2}^{ja1} m_{aa1}^{ii1} + F_b^{a1} m_{aa1}^{ij} - F_{i1}^{a1} t_b^{i1} m_{aa1}^{ij} + t_{a2}^{i1} \bar{g}_{bi1}^{a1a2} m_{aa1}^{ij} - t_{a2}^{i2} t_b^{i1} \bar{g}_{i1i2}^{a1a2} m_{aa1}^{ij}$$
$$- t_{A1}^{I1} g_{bI1}^{a1A1} m_{aa1}^{ij} + t_b^{i1} t_{A1}^{I1} g_{i1I1}^{a1A1} m_{aa1}^{ij} + t_{a2}^i \bar{g}_{bi1}^{a1a2} m_{aa1}^{ji1} - \bar{g}_{bi1}^{ia1} m_{aa1}^{ji1} + t_{a2}^i t_b^{i2} \bar{g}_{i1i2}^{a1a2} m_{aa1}^{ji1}$$
$$- t_b^{i2} \bar{g}_{i1i2}^{ia1} m_{aa1}^{ji1} + t_{a1}^i t_{a2}^j \bar{g}_{i1i2}^{a1a2} m_{ab}^{i1i2} \frac{1}{2} + t_{a1}^j \bar{g}_{i1i2}^{ia1} m_{ab}^{i1i2} \frac{1}{2} + \bar{g}_{i1i2}^{ij} m_{ab}^{i1i2} \frac{1}{2} - t_{a1}^i \bar{g}_{i1i2}^{ja1} m_{ab}^{i1i2} \frac{1}{2}$$
$$- F_{i1}^j m_{ab}^{ii1} - F_{i1}^{a1} t_{a1}^j m_{ab}^{ii1} - t_{a1}^j t_{a2}^{i2} \bar{g}_{i1i2}^{a1a2} m_{ab}^{ii1} - t_{a1}^{i2} \bar{g}_{i1i2}^{ja1} m_{ab}^{ii1} + t_{a1}^j t_{A1}^{I1} g_{i1I1}^{a1A1} m_{ab}^{ii1} + t_{A1}^{I1} g_{i1I1}^{jA1} m_{ab}^{ii1}$$

$$
\begin{aligned}
&+ F^{i}_{i1} m^{ji1}_{ab} + F^{a1}_{i1} t^{i}_{a1} m^{ji1}_{ab} + t^{i}_{a1} t^{i2}_{a2} \bar{g}^{a1a2}_{i1i2} m^{ji1}_{ab} + t^{i2}_{a1} \bar{g}^{ia1}_{i1i2} m^{ji1}_{ab} - t^{i}_{a1} t^{I1}_{A1} g^{a1A1}_{i1I1} m^{ji1}_{ab} - t^{I1}_{A1} g^{iA1}_{i1I1} m^{ji1}_{ab} \\
&+ t^{j}_{a2} \bar{g}^{a1a2}_{ai1} m^{ii1}_{ba1} - \bar{g}^{ja1}_{ai1} m^{ii1}_{ba1} + t^{j}_{a2} t^{i2}_{a} \bar{g}^{a1a2}_{i1i2} m^{ii1}_{ba1} - t^{i2}_{a} \bar{g}^{ja1}_{i1i2} m^{ii1}_{ba1} - F^{a1}_{a} m^{ij}_{ba1} + F^{a1}_{i1} t^{i1}_{a} m^{ij}_{ba1} \\
&- t^{i1}_{a2} \bar{g}^{a1a2}_{ai1} m^{ij}_{ba1} + t^{i2}_{a2} t^{i1}_{a} \bar{g}^{a1a2}_{i1i2} m^{ij}_{ba1} + t^{I1}_{A1} g^{a1A1}_{aI1} m^{ij}_{ba1} - t^{i1}_{a} t^{I1}_{A1} g^{a1A1}_{i1I1} m^{ij}_{ba1} - t^{i}_{a2} \bar{g}^{a1a2}_{ai1} m^{ji1}_{ba1} \\
&+ \bar{g}^{ia1}_{ai1} m^{ji1}_{ba1} - t^{i}_{a2} t^{i2}_{a} \bar{g}^{a1a2}_{i1i2} m^{ji1}_{ba1} + t^{i2}_{a} \bar{g}^{ia1}_{i1i2} m^{ji1}_{ba1} - t^{j}_{a1} g^{a1A1}_{bI1} m^{iI1}_{aA1} - g^{jA1}_{bI1} m^{iI1}_{aA1} + t^{j}_{a1} t^{i1}_{b} g^{a1A1}_{i1I1} m^{iI1}_{aA1} \\
&+ t^{i1}_{b} g^{jA1}_{i1I1} m^{iI1}_{aA1} + t^{i}_{a1} g^{a1A1}_{bI1} m^{jI1}_{aA1} + g^{iA1}_{bI1} m^{jI1}_{aA1} - t^{i}_{a1} t^{i1}_{b} g^{a1A1}_{i1I1} m^{jI1}_{aA1} - t^{i1}_{b} g^{iA1}_{i1I1} m^{jI1}_{aA1} + t^{j}_{a1} g^{a1A1}_{aI1} m^{iI1}_{bA1} \\
&+ g^{jA1}_{aI1} m^{iI1}_{bA1} - t^{j}_{a1} t^{i1}_{a} g^{a1A1}_{i1I1} m^{iI1}_{bA1} - t^{i1}_{a} g^{jA1}_{i1I1} m^{iI1}_{bA1} - t^{i}_{a1} g^{a1A1}_{aI1} m^{jI1}_{bA1} - g^{iA1}_{aI1} m^{jI1}_{bA1} + t^{i}_{a1} t^{i1}_{a} g^{a1A1}_{i1I1} m^{jI1}_{bA1} \\
&+ t^{i1}_{a} g^{iA1}_{i1I1} m^{jI1}_{bA1} + \bar{g}^{a1a2}_{i1i2} m^{ji1}_{ab} t^{ii2}_{a1a2} \frac{1}{2} - m^{i1}_{b} \bar{g}^{a1a2}_{ai1} t^{ij}_{a1a2} \frac{1}{2} + m^{i1}_{a} \bar{g}^{a1a2}_{bi1} t^{ij}_{a1a2} \frac{1}{2} - m^{i1}_{b} t^{i2}_{a} \bar{g}^{a1a2}_{i1i2} t^{ij}_{a1a2} \frac{1}{2} \\
&+ m^{i1}_{a} t^{i2}_{b} \bar{g}^{a1a2}_{i1i2} t^{ij}_{a1a2} \frac{1}{2} + \bar{g}^{a1a2}_{i1i2} m^{i1i2}_{ab} t^{ij}_{a1a2} \frac{1}{4} - \bar{g}^{a1a2}_{i1i2} m^{ii1}_{ab} t^{ji2}_{a1a2} \frac{1}{2} - m^{j}_{a2} \bar{g}^{a1a2}_{bi1} t^{ii1}_{aa1} - m^{i2}_{b} t^{j}_{a2} \bar{g}^{a1a2}_{i1i2} t^{ii1}_{aa1} \\
&- m^{j}_{a2} t^{i2}_{b} \bar{g}^{a1a2}_{i1i2} t^{ii1}_{aa1} + m^{i2}_{b} \bar{g}^{ja1}_{i1i2} t^{ii1}_{aa1} - g^{a1A1}_{i1I1} m^{jI1}_{bA1} t^{ii1}_{aa1} - F^{a1}_{i1} m^{i1}_{b} t^{ij}_{aa1} + m^{i1}_{a2} \bar{g}^{a1a2}_{bi1} t^{ij}_{aa1} - m^{i1}_{b} t^{i2}_{a2} \bar{g}^{a1a2}_{i1i2} t^{ij}_{aa1} \\
&- m^{i2}_{a2} t^{i1}_{b} \bar{g}^{a1a2}_{i1i2} t^{ij}_{aa1} - m^{I1}_{A1} g^{a1A1}_{bI1} t^{ij}_{aa1} + m^{I1}_{A1} t^{i1}_{b} g^{a1A1}_{i1I1} t^{ij}_{aa1} + m^{i1}_{b} t^{I1}_{A1} g^{a1A1}_{i1I1} t^{ij}_{aa1} - \bar{g}^{a1a2}_{i1i2} m^{i1i2}_{ba2} t^{ij}_{aa1} \frac{1}{2} \\
&+ g^{a1A1}_{i1I1} m^{i1I1}_{bA1} t^{ij}_{aa1} + m^{i}_{a2} \bar{g}^{a1a2}_{bi1} t^{ji1}_{aa1} + m^{i2}_{b} t^{i}_{a2} \bar{g}^{a1a2}_{i1i2} t^{ji1}_{aa1} + m^{i}_{a2} t^{i2}_{b} \bar{g}^{a1a2}_{i1i2} t^{ji1}_{aa1} - m^{i2}_{b} \bar{g}^{ia1}_{i1i2} t^{ji1}_{aa1} \\
&+ g^{a1A1}_{i1I1} m^{iI1}_{bA1} t^{ji1}_{aa1} + \bar{g}^{a1a2}_{i1i2} m^{ij}_{ba1} t^{i1i2}_{aa2} \frac{1}{2} + \bar{g}^{a1a2}_{i1i2} m^{ji1}_{ba1} t^{ii2}_{aa2} - \bar{g}^{a1a2}_{i1i2} m^{ii1}_{ba1} t^{ji2}_{aa2} \\
&- m^{j}_{a1} t^{i}_{a2} \bar{g}^{a1a2}_{i1i2} t^{i1i2}_{ab} \frac{1}{2} + m^{i}_{a1} t^{j}_{a2} \bar{g}^{a1a2}_{i1i2} t^{i1i2}_{ab} \frac{1}{2} + m^{j}_{a1} \bar{g}^{ia1}_{i1i2} t^{i1i2}_{ab} \frac{1}{2} - m^{i}_{a1} \bar{g}^{ja1}_{i1i2} t^{i1i2}_{ab} \frac{1}{2} + \bar{g}^{a1a2}_{i1i2} m^{ij}_{a1a2} t^{i1i2}_{ab} \frac{1}{4} \\
&- F^{a1}_{i1} m^{j}_{a1} t^{ii1}_{ab} - m^{i2}_{a2} t^{j}_{a1} \bar{g}^{a1a2}_{i1i2} t^{ii1}_{ab} - m^{j}_{a1} t^{i2}_{a2} \bar{g}^{a1a2}_{i1i2} t^{ii1}_{ab} - m^{i2}_{a1} \bar{g}^{ja1}_{i1i2} t^{ii1}_{ab} + m^{I1}_{A1} t^{j}_{a1} g^{a1A1}_{i1I1} t^{ii1}_{ab} + m^{j}_{a1} t^{I1}_{A1} g^{a1A1}_{i1I1} t^{ii1}_{ab} \\
&+ m^{I1}_{A1} g^{jA1}_{i1I1} t^{ii1}_{ab} - \bar{g}^{a1a2}_{i1i2} m^{ji2}_{a1a2} t^{ii1}_{ab} \frac{1}{2} + g^{a1A1}_{i1I1} m^{jI1}_{a1A1} t^{ii1}_{ab} + F^{a1}_{i1} m^{i}_{a1} t^{ji1}_{ab} + m^{i2}_{a2} t^{i}_{a1} \bar{g}^{a1a2}_{i1i2} t^{ji1}_{ab} + m^{i}_{a1} t^{i2}_{a2} \bar{g}^{a1a2}_{i1i2} t^{ji1}_{ab} \\
&+ m^{i2}_{a1} \bar{g}^{ia1}_{i1i2} t^{ji1}_{ab} - m^{I1}_{A1} t^{i}_{a1} g^{a1A1}_{i1I1} t^{ji1}_{ab} - m^{i}_{a1} t^{I1}_{A1} g^{a1A1}_{i1I1} t^{ji1}_{ab} - m^{I1}_{A1} g^{iA1}_{i1I1} t^{ji1}_{ab} + \bar{g}^{a1a2}_{i1i2} m^{ii2}_{a1a2} t^{ji1}_{ab} \frac{1}{2} \\
&- g^{a1A1}_{i1I1} m^{iI1}_{a1A1} t^{ji1}_{ab} + m^{j}_{a2} \bar{g}^{a1a2}_{ai1} t^{ii1}_{ba1} + m^{i2}_{a} t^{j}_{a2} \bar{g}^{a1a2}_{i1i2} t^{ii1}_{ba1} + m^{j}_{a2} t^{i2}_{a} \bar{g}^{a1a2}_{i1i2} t^{ii1}_{ba1} - m^{i2}_{a} \bar{g}^{ja1}_{i1i2} t^{ii1}_{ba1} + g^{a1A1}_{i1I1} m^{jI1}_{aA1} t^{ii1}_{ba1} \\
&+ F^{a1}_{i1} m^{i1}_{a} t^{ij}_{ba1} - m^{i1}_{a2} \bar{g}^{a1a2}_{ai1} t^{ij}_{ba1} + m^{i1}_{a} t^{i2}_{a2} \bar{g}^{a1a2}_{i1i2} t^{ij}_{ba1} + m^{i2}_{a2} t^{i1}_{a} \bar{g}^{a1a2}_{i1i2} t^{ij}_{ba1} + m^{I1}_{A1} g^{a1A1}_{aI1} t^{ij}_{ba1} - m^{I1}_{A1} t^{i1}_{a} g^{a1A1}_{i1I1} t^{ij}_{ba1} \\
&- m^{i1}_{a} t^{I1}_{A1} g^{a1A1}_{i1I1} t^{ij}_{ba1} + \bar{g}^{a1a2}_{i1i2} m^{i1i2}_{aa2} t^{ij}_{ba1} \frac{1}{2} - g^{a1A1}_{i1I1} m^{i1I1}_{aA1} t^{ij}_{ba1} - m^{i}_{a2} \bar{g}^{a1a2}_{ai1} t^{ji1}_{ba1} - m^{i2}_{a} t^{i}_{a2} \bar{g}^{a1a2}_{i1i2} t^{ji1}_{ba1} \\
&- m^{i}_{a2} t^{i2}_{a} \bar{g}^{a1a2}_{i1i2} t^{ji1}_{ba1} + m^{i2}_{a} \bar{g}^{ia1}_{i1i2} t^{ji1}_{ba1} - g^{a1A1}_{i1I1} m^{iI1}_{aA1} t^{ji1}_{ba1} - \bar{g}^{a1a2}_{i1i2} m^{ij}_{aa1} t^{i1i2}_{ba2} \frac{1}{2} - \bar{g}^{a1a2}_{i1i2} m^{ji1}_{aa1} t^{ii2}_{ba2} + \bar{g}^{a1a2}_{i1i2} m^{ii1}_{aa1} t^{ji2}_{ba2} \\
&- g^{a1A1}_{i1I1} m^{ji1}_{ab} t^{iI1}_{a1A1} + g^{a1A1}_{i1I1} m^{ii1}_{ab} t^{jI1}_{a1A1} - g^{a1A1}_{i1I1} m^{ij}_{ba1} t^{i1I1}_{aA1} - m^{j}_{a1} g^{a1A1}_{bI1} t^{iI1}_{aA1} + m^{i1}_{b} t^{j}_{a1} g^{a1A1}_{i1I1} t^{iI1}_{aA1} \\
&+ m^{j}_{a1} t^{i1}_{b} g^{a1A1}_{i1I1} t^{iI1}_{aA1} + m^{i1}_{b} g^{jA1}_{i1I1} t^{iI1}_{aA1} - g^{a1A1}_{i1I1} m^{ji1}_{ba1} t^{iI1}_{aA1} + m^{i}_{a1} g^{a1A1}_{bI1} t^{jI1}_{aA1} - m^{i1}_{b} t^{i}_{a1} g^{a1A1}_{i1I1} t^{jI1}_{aA1} \\
&- m^{i}_{a1} t^{i1}_{b} g^{a1A1}_{i1I1} t^{jI1}_{aA1} - m^{i1}_{b} g^{iA1}_{i1I1} t^{jI1}_{aA1} + g^{a1A1}_{i1I1} m^{ii1}_{ba1} t^{jI1}_{aA1} + \bar{g}^{A1A2}_{I1I2} m^{jI1}_{bA1} t^{iI2}_{aA2} - \bar{g}^{A1A2}_{I1I2} m^{iI1}_{bA1} t^{jI2}_{aA2}
\end{aligned}
$$

$$+ g^{a1A1}_{i1I1} m^{ij}_{aa1} t^{i1I1}_{bA1} + m^{j}_{a1} g^{a1A1}_{aI1} t^{iI1}_{bA1} - m^{i1}_{a} t^{j}_{a1} g^{a1A1}_{i1I1} t^{iI1}_{bA1} - m^{j}_{a1} t^{i1}_{a} g^{a1A1}_{i1I1} t^{iI1}_{bA1} - m^{i1}_{a} g^{jA1}_{i1I1} t^{iI1}_{bA1}$$
$$+ g^{a1A1}_{i1I1} m^{ji1}_{aa1} t^{iI1}_{bA1} - m^{i}_{a1} g^{a1A1}_{aI1} t^{jI1}_{bA1} + m^{i1}_{a} t^{i}_{a1} g^{a1A1}_{i1I1} t^{jI1}_{bA1} + m^{i}_{a1} t^{i1}_{a} g^{a1A1}_{i1I1} t^{jI1}_{bA1} + m^{i1}_{a} g^{iA1}_{i1I1} t^{jI1}_{bA1}$$
$$- g^{a1A1}_{i1I1} m^{ii1}_{aa1} t^{jI1}_{bA1} - \bar{g}^{A1A2}_{I1I2} m^{jI1}_{aA1} t^{iI2}_{bA2} + \bar{g}^{A1A2}_{I1I2} m^{iI1}_{aA1} t^{jI2}_{bA2}$$

$$\sigma^{IJ}_{AB} = m^{J}_{A2} t^{I}_{A1} \bar{g}^{A1A2}_{AB} - m^{I}_{A2} t^{J}_{A1} \bar{g}^{A1A2}_{AB} + m^{J}_{A1} \bar{g}^{IA1}_{AB} - m^{I}_{A1} \bar{g}^{JA1}_{AB} - m^{I1}_{B} t^{I}_{A1} t^{J}_{A2} \bar{g}^{A1A2}_{AI1} \tag{S19}$$
$$+ m^{J}_{A1} t^{I}_{A2} t^{I1}_{B} \bar{g}^{A1A2}_{AI1} - m^{I}_{A1} t^{J}_{A2} t^{I1}_{B} \bar{g}^{A1A2}_{AI1} - m^{I1}_{B} t^{J}_{A1} \bar{g}^{IA1}_{AI1} - m^{J}_{A1} t^{I1}_{B} \bar{g}^{IA1}_{AI1} - m^{I1}_{B} \bar{g}^{IJ}_{AI1} + m^{I1}_{B} t^{I}_{A1} \bar{g}^{JA1}_{AI1}$$
$$+ m^{I}_{A1} t^{I1}_{B} \bar{g}^{JA1}_{AI1} + m^{I}_{A} t^{I}_{A1} t^{J}_{A2} \bar{g}^{A1A2}_{BI1} - m^{J}_{A1} t^{I}_{A2} t^{I1}_{A} \bar{g}^{A1A2}_{BI1} + m^{I}_{A1} t^{J}_{A2} t^{I1}_{A} \bar{g}^{A1A2}_{BI1} + m^{I}_{A} t^{J}_{A1} \bar{g}^{IA1}_{BI1}$$
$$+ m^{J}_{A1} t^{I1}_{A} \bar{g}^{IA1}_{BI1} + m^{I}_{A} \bar{g}^{IJ}_{BI1} - m^{I}_{A} t^{I}_{A1} \bar{g}^{JA1}_{BI1} - m^{I}_{A1} t^{I1}_{A} \bar{g}^{JA1}_{BI1} - m^{I1}_{B} t^{I}_{A1} t^{J}_{A2} t^{I2}_{A} \bar{g}^{A1A2}_{I1I2} + m^{I}_{A} t^{I}_{A1} t^{J}_{A2} t^{I2}_{B} \bar{g}^{A1A2}_{I1I2}$$
$$- m^{J}_{A1} t^{I}_{A2} t^{I1}_{A} t^{I2}_{B} \bar{g}^{A1A2}_{I1I2} + m^{I}_{A1} t^{J}_{A2} t^{I1}_{A} t^{I2}_{B} \bar{g}^{A1A2}_{I1I2} - m^{I1}_{B} t^{J}_{A1} t^{I2}_{A} \bar{g}^{IA1}_{I1I2} + m^{I}_{A} t^{J}_{A1} t^{I2}_{B} \bar{g}^{IA1}_{I1I2} + m^{J}_{A1} t^{I1}_{A} t^{I2}_{B} \bar{g}^{IA1}_{I1I2}$$
$$+ m^{I2}_{B} t^{I1}_{A} \bar{g}^{IJ}_{I1I2} - m^{I2}_{A} t^{I1}_{B} \bar{g}^{IJ}_{I1I2} + m^{I1}_{B} t^{I}_{A1} t^{I2}_{A} \bar{g}^{JA1}_{I1I2} - m^{I}_{A} t^{I}_{A1} t^{I2}_{B} \bar{g}^{JA1}_{I1I2} - m^{I}_{A1} t^{I1}_{A} t^{I2}_{B} \bar{g}^{JA1}_{I1I2} - t^{J}_{A1} g^{a1A1}_{i1B} m^{i1I}_{a1A}$$
$$- g^{a1J}_{i1B} m^{i1I}_{a1A} + t^{J}_{A1} t^{I1}_{B} g^{a1A1}_{i1I1} m^{i1I}_{a1A} + t^{I1}_{B} g^{a1J}_{i1I1} m^{i1I}_{a1A} + t^{I}_{A1} g^{a1A1}_{i1B} m^{i1J}_{a1A} + g^{a1I}_{i1B} m^{i1J}_{a1A} - t^{I}_{A1} t^{I1}_{B} g^{a1A1}_{i1I1} m^{i1J}_{a1A}$$
$$- t^{I1}_{B} g^{a1I}_{i1I1} m^{i1J}_{a1A} + t^{J}_{A1} g^{a1A1}_{i1A} m^{i1J}_{a1B} + g^{a1J}_{i1A} m^{i1J}_{a1B} - t^{J}_{A1} t^{I1}_{A} g^{a1A1}_{i1I1} m^{i1J}_{a1B} - t^{I1}_{A} g^{a1J}_{i1I1} m^{i1J}_{a1B} - t^{I}_{A1} g^{a1A1}_{i1A} m^{i1J}_{a1B}$$
$$- g^{a1I}_{i1A} m^{i1J}_{a1B} + t^{I}_{A1} t^{I1}_{A} g^{a1A1}_{i1I1} m^{i1J}_{a1B} + t^{I1}_{A} g^{a1I}_{i1I1} m^{i1J}_{a1B} + \bar{g}^{A1A2}_{AB} m^{IJ}_{A1A2} \frac{1}{2} - t^{I1}_{B} \bar{g}^{A1A2}_{AI1} m^{IJ}_{A1A2} \frac{1}{2}$$
$$+ t^{I1}_{A} \bar{g}^{A1A2}_{BI1} m^{IJ}_{A1A2} \frac{1}{2} + t^{I1}_{A} t^{I2}_{B} \bar{g}^{A1A2}_{I1I2} m^{IJ}_{A1A2} \frac{1}{2} - t^{J}_{A2} \bar{g}^{A1A2}_{BI1} m^{II1}_{AA1} + \bar{g}^{JA1}_{BI1} m^{II1}_{AA1} - t^{J}_{A2} t^{I2}_{B} \bar{g}^{A1A2}_{I1I2} m^{II1}_{AA1}$$
$$+ t^{I2}_{B} \bar{g}^{JA1}_{I1I2} m^{II1}_{AA1} + F^{A1}_{B} m^{IJ}_{AA1} - F^{A1}_{I1} t^{I1}_{B} m^{IJ}_{AA1} - t^{i1}_{a1} g^{a1A1}_{i1B} m^{IJ}_{AA1} + t^{i1}_{a1} t^{I1}_{B} g^{a1A1}_{i1I1} m^{IJ}_{AA1} + t^{I1}_{A2} \bar{g}^{A1A2}_{BI1} m^{IJ}_{AA1}$$
$$- t^{I2}_{A2} t^{I1}_{B} \bar{g}^{A1A2}_{I1I2} m^{IJ}_{AA1} + t^{I}_{A2} \bar{g}^{A1A2}_{BI1} m^{JI1}_{AA1} - \bar{g}^{IA1}_{BI1} m^{JI1}_{AA1} + t^{I}_{A2} t^{I2}_{B} \bar{g}^{A1A2}_{I1I2} m^{JI1}_{AA1} - t^{I2}_{B} \bar{g}^{IA1}_{I1I2} m^{JI1}_{AA1}$$
$$+ t^{I}_{A1} t^{J}_{A2} \bar{g}^{A1A2}_{I1I2} m^{I1I2}_{AB} \frac{1}{2} + t^{J}_{A1} \bar{g}^{IA1}_{I1I2} m^{I1I2}_{AB} \frac{1}{2} + \bar{g}^{IJ}_{I1I2} m^{I1I2}_{AB} \frac{1}{2} - t^{I}_{A1} \bar{g}^{JA1}_{I1I2} m^{I1I2}_{AB} \frac{1}{2} - F^{J}_{I1} m^{II1}_{AB} - F^{A1}_{I1} t^{J}_{A1} m^{II1}_{AB}$$
$$+ t^{i1}_{a1} t^{J}_{A1} g^{a1A1}_{i1I1} m^{II1}_{AB} + t^{i1}_{a1} g^{a1J}_{i1I1} m^{II1}_{AB} - t^{J}_{A1} t^{I2}_{A2} \bar{g}^{A1A2}_{I1I2} m^{II1}_{AB} - t^{I2}_{A1} \bar{g}^{JA1}_{I1I2} m^{II1}_{AB} + F^{I}_{I1} m^{JI1}_{AB} + F^{A1}_{I1} t^{I}_{A1} m^{JI1}_{AB}$$
$$- t^{i1}_{a1} t^{I}_{A1} g^{a1A1}_{i1I1} m^{JI1}_{AB} - t^{i1}_{a1} g^{a1I}_{i1I1} m^{JI1}_{AB} + t^{I}_{A1} t^{I2}_{A2} \bar{g}^{A1A2}_{I1I2} m^{JI1}_{AB} + t^{I2}_{A1} \bar{g}^{IA1}_{I1I2} m^{JI1}_{AB} + t^{J}_{A2} \bar{g}^{A1A2}_{AI1} m^{II1}_{BA1}$$
$$- \bar{g}^{JA1}_{AI1} m^{II1}_{BA1} + t^{J}_{A2} t^{I2}_{A} \bar{g}^{A1A2}_{I1I2} m^{II1}_{BA1} - t^{I2}_{A} \bar{g}^{JA1}_{I1I2} m^{II1}_{BA1} - F^{A1}_{A} m^{IJ}_{BA1} + F^{A1}_{I1} t^{I1}_{A} m^{IJ}_{BA1} + t^{i1}_{a1} g^{a1A1}_{i1A} m^{IJ}_{BA1}$$
$$- t^{i1}_{a1} t^{I1}_{A} g^{a1A1}_{i1I1} m^{IJ}_{BA1} - t^{I1}_{A2} \bar{g}^{A1A2}_{AI1} m^{IJ}_{BA1} + t^{I2}_{A2} t^{I1}_{A} \bar{g}^{A1A2}_{I1I2} m^{IJ}_{BA1} - t^{I}_{A2} \bar{g}^{A1A2}_{AI1} m^{JI1}_{BA1} + \bar{g}^{IA1}_{AI1} m^{JI1}_{BA1}$$
$$- t^{I}_{A2} t^{I2}_{A} \bar{g}^{A1A2}_{I1I2} m^{JI1}_{BA1} + t^{I2}_{A} \bar{g}^{IA1}_{I1I2} m^{JI1}_{BA1} - g^{a1A1}_{i1I1} m^{JI1}_{AB} t^{i1I}_{a1A1} + g^{a1A1}_{i1I1} m^{II1}_{AB} t^{i1J}_{a1A1} - g^{a1A1}_{i1I1} m^{IJ}_{BA1} t^{i1I1}_{a1A}$$

$$
\begin{aligned}
&- m^{J}_{A1} g^{a1A1}_{i1B} t^{i1I}_{a1A} + m^{I1}_{B} t^{J}_{A1} g^{a1A1}_{i1I1} t^{i1I}_{a1A} + m^{J}_{A1} t^{I1}_{B} g^{a1A1}_{i1I1} t^{i1I}_{a1A} + m^{I1}_{B} g^{a1J}_{i1I1} t^{i1I}_{a1A} - g^{a1A1}_{i1I1} m^{JI1}_{BA1} t^{i1I}_{a1A} \\
&+ m^{I}_{A1} g^{a1A1}_{i1B} t^{i1J}_{a1A} - m^{I1}_{B} t^{I}_{A1} g^{a1A1}_{i1I1} t^{i1J}_{a1A} - m^{I}_{A1} t^{I1}_{B} g^{a1A1}_{i1I1} t^{i1J}_{a1A} - m^{I1}_{B} g^{a1I}_{i1I1} t^{i1J}_{a1A} + g^{a1A1}_{i1I1} m^{II1}_{BA1} t^{i1J}_{a1A} \\
&+ g^{a1A1}_{i1I1} m^{IJ}_{AA1} t^{i1I1}_{a1B} + m^{J}_{A1} g^{a1A1}_{i1A} t^{i1I}_{a1B} - m^{I}_{A} t^{J}_{A1} g^{a1A1}_{i1I1} t^{i1I}_{a1B} - m^{J}_{A1} t^{I1}_{A} g^{a1A1}_{i1I1} t^{i1I}_{a1B} - m^{I}_{A} g^{a1J}_{i1I1} t^{i1I}_{a1B} \\
&+ g^{a1A1}_{i1I1} m^{JI1}_{AA1} t^{i1I}_{a1B} - m^{I}_{A1} g^{a1A1}_{i1A} t^{i1J}_{a1B} + m^{I}_{A} t^{I}_{A1} g^{a1A1}_{i1I1} t^{i1J}_{a1B} + m^{I}_{A1} t^{I1}_{A} g^{a1A1}_{i1I1} t^{i1J}_{a1B} + m^{I}_{A} g^{a1I}_{i1I1} t^{i1J}_{a1B} \\
&- g^{a1A1}_{i1I1} m^{II1}_{AA1} t^{i1J}_{a1B} + \bar{g}^{a1a2}_{i1i2} m^{i1J}_{a1B} t^{i2I}_{a2A} - \bar{g}^{a1a2}_{i1i2} m^{i1J}_{a1B} t^{i2J}_{a2A} - \bar{g}^{a1a2}_{i1i2} m^{i1J}_{a1A} t^{i2I}_{a2B} + \bar{g}^{a1a2}_{i1i2} m^{i1I}_{a1A} t^{i2J}_{a2B} \\
&+ \bar{g}^{A1A2}_{I1I2} m^{JI1}_{AB} t^{II2}_{A1A2} \frac{1}{2} - m^{I1}_{B} \bar{g}^{A1A2}_{AI1} t^{IJ}_{A1A2} \frac{1}{2} + m^{I}_{A} \bar{g}^{A1A2}_{BI1} t^{IJ}_{A1A2} \frac{1}{2} - m^{I1}_{B} t^{I2}_{A} \bar{g}^{A1A2}_{I1I2} t^{IJ}_{A1A2} \frac{1}{2} \\
&+ m^{I}_{A} t^{I2}_{B} \bar{g}^{A1A2}_{I1I2} t^{IJ}_{A1A2} \frac{1}{2} + \bar{g}^{A1A2}_{I1I2} m^{I1I2}_{AB} t^{IJ}_{A1A2} \frac{1}{4} - \bar{g}^{A1A2}_{I1I2} m^{II1}_{AB} t^{JI2}_{A1A2} \frac{1}{2} - m^{J}_{A2} \bar{g}^{A1A2}_{BI1} t^{II1}_{AA1} \\
&- m^{I2}_{B} t^{J}_{A2} \bar{g}^{A1A2}_{I1I2} t^{II1}_{AA1} - m^{J}_{A2} t^{I2}_{B} \bar{g}^{A1A2}_{I1I2} t^{II1}_{AA1} + m^{I2}_{B} \bar{g}^{JA1}_{I1I2} t^{II1}_{AA1} - g^{a1A1}_{i1I1} m^{i1J}_{a1B} t^{II1}_{AA1} - F^{A1}_{I1} m^{I1}_{B} t^{IJ}_{AA1} \\
&- m^{i1}_{a1} g^{a1A1}_{i1B} t^{IJ}_{AA1} + m^{I1}_{B} t^{i1}_{a1} g^{a1A1}_{i1I1} t^{IJ}_{AA1} + m^{i1}_{a1} t^{I1}_{B} g^{a1A1}_{i1I1} t^{IJ}_{AA1} + m^{I1}_{A2} \bar{g}^{A1A2}_{BI1} t^{IJ}_{AA1} - m^{I1}_{B} t^{I2}_{A2} \bar{g}^{A1A2}_{I1I2} t^{IJ}_{AA1} \\
&- m^{I2}_{A2} t^{I1}_{B} \bar{g}^{A1A2}_{I1I2} t^{IJ}_{AA1} + g^{a1A1}_{i1I1} m^{i1I1}_{a1B} t^{IJ}_{AA1} - \bar{g}^{A1A2}_{I1I2} m^{I1I2}_{BA2} t^{IJ}_{AA1} \frac{1}{2} + m^{I}_{A2} \bar{g}^{A1A2}_{BI1} t^{JI1}_{AA1} + m^{I2}_{B} t^{I}_{A2} \bar{g}^{A1A2}_{I1I2} t^{JI1}_{AA1} \\
&+ m^{I}_{A2} t^{I2}_{B} \bar{g}^{A1A2}_{I1I2} t^{JI1}_{AA1} - m^{I2}_{B} \bar{g}^{IA1}_{I1I2} t^{JI1}_{AA1} + g^{a1A1}_{i1I1} m^{i1J}_{a1B} t^{JI1}_{AA1} + \bar{g}^{A1A2}_{I1I2} m^{IJ}_{BA1} t^{I1I2}_{AA2} \frac{1}{2} + \bar{g}^{A1A2}_{I1I2} m^{JI1}_{BA1} t^{II2}_{AA2} \\
&- \bar{g}^{A1A2}_{I1I2} m^{II1}_{BA1} t^{JI2}_{AA2} - m^{J}_{A1} t^{I}_{A2} \bar{g}^{A1A2}_{I1I2} t^{I1I2}_{AB} \frac{1}{2} + m^{I}_{A1} t^{J}_{A2} \bar{g}^{A1A2}_{I1I2} t^{I1I2}_{AB} \frac{1}{2} + m^{J}_{A1} \bar{g}^{IA1}_{I1I2} t^{I1I2}_{AB} \frac{1}{2} \\
&- m^{I}_{A1} \bar{g}^{JA1}_{I1I2} t^{I1I2}_{AB} \frac{1}{2} + \bar{g}^{A1A2}_{I1I2} m^{IJ}_{A1A2} t^{I1I2}_{AB} \frac{1}{4} - F^{A1}_{I1} m^{J}_{A1} t^{II1}_{AB} + m^{J}_{A1} t^{i1}_{a1} g^{a1A1}_{i1I1} t^{II1}_{AB} + m^{i1}_{a1} t^{J}_{A1} g^{a1A1}_{i1I1} t^{II1}_{AB} \\
&+ m^{i1}_{a1} g^{a1J}_{i1I1} t^{II1}_{AB} - m^{I2}_{A2} t^{J}_{A1} \bar{g}^{A1A2}_{I1I2} t^{II1}_{AB} - m^{J}_{A1} t^{I2}_{A2} \bar{g}^{A1A2}_{I1I2} t^{II1}_{AB} - m^{I2}_{A1} \bar{g}^{JA1}_{I1I2} t^{II1}_{AB} + g^{a1A1}_{i1I1} m^{i1J}_{a1A1} t^{II1}_{AB} \\
&- \bar{g}^{A1A2}_{I1I2} m^{JI2}_{A1A2} t^{II1}_{AB} \frac{1}{2} + F^{A1}_{I1} m^{I}_{A1} t^{JI1}_{AB} - m^{I}_{A1} t^{i1}_{a1} g^{a1A1}_{i1I1} t^{JI1}_{AB} - m^{i1}_{a1} t^{I}_{A1} g^{a1A1}_{i1I1} t^{JI1}_{AB} - m^{i1}_{a1} g^{a1I}_{i1I1} t^{JI1}_{AB} \\
&+ m^{I2}_{A2} t^{I}_{A1} \bar{g}^{A1A2}_{I1I2} t^{JI1}_{AB} + m^{I}_{A1} t^{I2}_{A2} \bar{g}^{A1A2}_{I1I2} t^{JI1}_{AB} + m^{I2}_{A1} \bar{g}^{IA1}_{I1I2} t^{JI1}_{AB} - g^{a1A1}_{i1I1} m^{i1I}_{a1A1} t^{JI1}_{AB} + \bar{g}^{A1A2}_{I1I2} m^{II2}_{A1A2} t^{JI1}_{AB} \frac{1}{2} \\
&+ m^{J}_{A2} \bar{g}^{A1A2}_{AI1} t^{II1}_{BA1} + m^{I2}_{A} t^{J}_{A2} \bar{g}^{A1A2}_{I1I2} t^{II1}_{BA1} + m^{J}_{A2} t^{I2}_{A} \bar{g}^{A1A2}_{I1I2} t^{II1}_{BA1} - m^{I2}_{A} \bar{g}^{JA1}_{I1I2} t^{II1}_{BA1} + g^{a1A1}_{i1I1} m^{i1J}_{a1A} t^{II1}_{BA1} \\
&+ F^{A1}_{I1} m^{I}_{A} t^{IJ}_{BA1} + m^{i1}_{a1} g^{a1A1}_{i1A} t^{IJ}_{BA1} - m^{I}_{A} t^{i1}_{a1} g^{a1A1}_{i1I1} t^{IJ}_{BA1} - m^{i1}_{a1} t^{I1}_{A} g^{a1A1}_{i1I1} t^{IJ}_{BA1} - m^{I1}_{A2} \bar{g}^{A1A2}_{AI1} t^{IJ}_{BA1} \\
&+ m^{I}_{A} t^{I2}_{A2} \bar{g}^{A1A2}_{I1I2} t^{IJ}_{BA1} + m^{I2}_{A2} t^{I1}_{A} \bar{g}^{A1A2}_{I1I2} t^{IJ}_{BA1} - g^{a1A1}_{i1I1} m^{i1I1}_{a1A} t^{IJ}_{BA1} + \bar{g}^{A1A2}_{I1I2} m^{I1I2}_{AA2} t^{IJ}_{BA1} \frac{1}{2} - m^{I}_{A2} \bar{g}^{A1A2}_{AI1} t^{JI1}_{BA1} \\
&- m^{I2}_{A} t^{I}_{A2} \bar{g}^{A1A2}_{I1I2} t^{JI1}_{BA1} - m^{I}_{A2} t^{I2}_{A} \bar{g}^{A1A2}_{I1I2} t^{JI1}_{BA1} + m^{I2}_{A} \bar{g}^{IA1}_{I1I2} t^{JI1}_{BA1} - g^{a1A1}_{i1I1} m^{i1I}_{a1A} t^{JI1}_{BA1} \\
&- \bar{g}^{A1A2}_{I1I2} m^{IJ}_{AA1} t^{I1I2}_{BA2} \frac{1}{2} - \bar{g}^{A1A2}_{I1I2} m^{JI1}_{AA1} t^{II2}_{BA2} + \bar{g}^{A1A2}_{I1I2} m^{II1}_{AA1} t^{JI2}_{BA2}
\end{aligned}
$$

$$\sigma_{aA}^{iI} = -m_{A1}^{I} t_{a1}^{i} g_{aA}^{a1A1} - m_{a1}^{i} t_{A1}^{I} g_{aA}^{a1A1} - m_{a1}^{i} g_{aA}^{a1I} - m_{A1}^{I} g_{aA}^{iA1} + m_{A}^{I} t_{a1}^{i} t_{A1}^{I} g_{aA}^{a1A1} \tag{S20}$$

$$+ m_{A1}^{I} t_{a1}^{i} t_{A}^{I1} g_{aI1}^{a1A1} + m_{a1}^{i} t_{A1}^{I} t_{A}^{I1} g_{aI1}^{a1A1} + m_{A}^{I} t_{a1}^{i} g_{aI1}^{a1I} + m_{a1}^{i} t_{A}^{I1} g_{aI1}^{a1I} + m_{A}^{I} t_{A1}^{I} g_{aI1}^{iA1} + m_{A1}^{I} t_{A}^{I1} g_{aI1}^{iA1}$$

$$+ m_{A}^{I} g_{aI1}^{iI} + m_{A1}^{I} t_{a1}^{i} t_{a}^{i1} g_{i1A}^{a1A1} + m_{a}^{i1} t_{a1}^{i} t_{A1}^{I} g_{i1A}^{a1A1} + m_{a1}^{i} t_{a}^{i1} t_{A1}^{I} g_{i1A}^{a1A1} + m_{a}^{i1} t_{a1}^{i} g_{i1A}^{a1I} + m_{a1}^{i} t_{a}^{i1} g_{i1A}^{a1I}$$

$$+ m_{A1}^{I} t_{a}^{i1} g_{i1A}^{iA1} + m_{a}^{i1} t_{A1}^{I} g_{i1A}^{iA1} + m_{a}^{i1} g_{i1A}^{iI} - m_{A}^{I} t_{a1}^{i} t_{a}^{i1} t_{A1}^{I} g_{i1I1}^{a1A1} - m_{A1}^{I} t_{a1}^{i} t_{a}^{i1} t_{A}^{I1} g_{i1I1}^{a1A1}$$

$$- m_{a}^{i1} t_{a1}^{i} t_{A1}^{I} t_{A}^{I1} g_{i1I1}^{a1A1} - m_{a1}^{i} t_{a}^{i1} t_{A1}^{I} t_{A}^{I1} g_{i1I1}^{a1A1} - m_{A}^{I} t_{a1}^{i} t_{a}^{i1} g_{i1I1}^{a1I} - m_{a}^{i1} t_{a1}^{i} t_{A}^{I1} g_{i1I1}^{a1I} - m_{a1}^{i} t_{a}^{i1} t_{A}^{I1} g_{i1I1}^{a1I}$$

$$- m_{A}^{I} t_{a}^{i1} t_{A1}^{I} g_{i1I1}^{iA1} - m_{A1}^{I} t_{a}^{i1} t_{A}^{I1} g_{i1I1}^{iA1} - m_{a}^{i1} t_{A1}^{I} t_{A}^{I1} g_{i1I1}^{iA1} - m_{A}^{I} t_{a}^{i1} g_{i1I1}^{iI} - m_{a}^{i1} t_{A}^{I1} g_{i1I1}^{iI} - t_{A1}^{I} g_{i1A}^{a1A1} m_{aa1}^{ii1}$$

$$- g_{i1A}^{a1I} m_{aa1}^{ii1} + t_{A1}^{I} t_{A}^{I1} g_{i1I1}^{a1A1} m_{aa1}^{ii1} + t_{A}^{I1} g_{i1I1}^{a1I} m_{aa1}^{ii1} - g_{aA}^{a1A1} m_{a1A1}^{iI} + t_{A}^{I1} g_{aI1}^{a1A1} m_{a1A1}^{iI} + t_{a}^{i1} g_{i1A}^{a1A1} m_{a1A1}^{iI}$$

$$- t_{a}^{i1} t_{A}^{I1} g_{i1I1}^{a1A1} m_{a1A1}^{iI} - t_{a2}^{i} \bar{g}_{ai1}^{a1a2} m_{a1A}^{i1I} + \bar{g}_{ai1}^{ia1} m_{a1A}^{i1I} - t_{a2}^{i} t_{a}^{i2} \bar{g}_{i1i2}^{a1a2} m_{a1A}^{i1I} + t_{a}^{i2} \bar{g}_{i1i2}^{ia1} m_{a1A}^{i1I} + t_{A1}^{I} g_{aI1}^{a1A1} m_{a1A}^{iI1}$$

$$+ g_{aI1}^{a1I} m_{a1A}^{iI1} - t_{a}^{i1} t_{A1}^{I} g_{i1I1}^{a1A1} m_{a1A}^{iI1} - t_{a}^{i1} g_{i1I1}^{a1I} m_{a1A}^{iI1} + F_{a}^{a1} m_{a1A}^{iI} - F_{i1}^{a1} t_{a}^{i1} m_{a1A}^{iI} + t_{a2}^{i1} \bar{g}_{ai1}^{a1a2} m_{a1A}^{iI}$$

$$- t_{a2}^{i2} t_{a}^{i1} \bar{g}_{i1i2}^{a1a2} m_{a1A}^{iI} - t_{A1}^{I1} g_{aI1}^{a1A1} m_{a1A}^{iI} + t_{a}^{i1} t_{A1}^{I1} g_{i1I1}^{a1A1} m_{a1A}^{iI} + t_{a1}^{i} g_{i1A}^{a1A1} m_{aA1}^{i1I} + g_{i1A}^{iA1} m_{aA1}^{i1I}$$

$$- t_{a1}^{i} t_{A}^{I1} g_{i1I1}^{a1A1} m_{aA1}^{i1I} - t_{A}^{I1} g_{i1I1}^{iA1} m_{aA1}^{i1I} - t_{A2}^{I} \bar{g}_{AI1}^{A1A2} m_{aA1}^{iI1} + \bar{g}_{AI1}^{IA1} m_{aA1}^{iI1} - t_{A2}^{I} t_{A}^{I2} \bar{g}_{I1I2}^{A1A2} m_{aA1}^{iI1}$$

$$+ t_{A}^{I2} \bar{g}_{I1I2}^{IA1} m_{aA1}^{iI1} + F_{A}^{A1} m_{aA1}^{iI} - F_{I1}^{A1} t_{A}^{I1} m_{aA1}^{iI} - t_{a1}^{i1} g_{i1A}^{a1A1} m_{aA1}^{iI} + t_{a1}^{i1} t_{A}^{I1} g_{i1I1}^{a1A1} m_{aA1}^{iI} + t_{A2}^{I1} \bar{g}_{AI1}^{A1A2} m_{aA1}^{iI}$$

$$- t_{A2}^{I2} t_{A}^{I1} \bar{g}_{I1I2}^{A1A2} m_{aA1}^{iI} - t_{a1}^{i} t_{A1}^{I} g_{i1I1}^{a1A1} m_{aA}^{i1I1} - t_{a1}^{i} g_{i1I1}^{a1I} m_{aA}^{i1I1} - t_{A1}^{I} g_{i1I1}^{iA1} m_{aA}^{i1I1} - g_{i1I1}^{iI} m_{aA}^{i1I1} - F_{i1}^{i} m_{aA}^{i1I}$$

$$- F_{i1}^{a1} t_{a1}^{i} m_{aA}^{i1I} - t_{a1}^{i} t_{a2}^{i2} \bar{g}_{i1i2}^{a1a2} m_{aA}^{i1I} - t_{a1}^{i2} \bar{g}_{i1i2}^{ia1} m_{aA}^{i1I} + t_{a1}^{i} t_{A1}^{I1} g_{i1I1}^{a1A1} m_{aA}^{i1I} + t_{A1}^{I1} g_{i1I1}^{iA1} m_{aA}^{i1I} - F_{I1}^{I} m_{aA}^{iI1}$$

$$- F_{I1}^{A1} t_{A1}^{I} m_{aA}^{iI1} + t_{a1}^{i1} t_{A1}^{I} g_{i1I1}^{a1A1} m_{aA}^{iI1} + t_{a1}^{i1} g_{i1I1}^{a1I} m_{aA}^{iI1} - t_{A1}^{I} t_{A2}^{I2} \bar{g}_{I1I2}^{A1A2} m_{aA}^{iI1} - t_{A1}^{I2} \bar{g}_{I1I2}^{IA1} m_{aA}^{iI1}$$

$$- t_{a1}^{i} g_{aI1}^{a1A1} m_{AA1}^{II1} - g_{aI1}^{iA1} m_{AA1}^{II1} + t_{a1}^{i} t_{a}^{i1} g_{i1I1}^{a1A1} m_{AA1}^{II1} + t_{a}^{i1} g_{i1I1}^{iA1} m_{AA1}^{II1} - \bar{g}_{i1i2}^{a1a2} m_{aA}^{i1I} t_{a1a2}^{ii2} \frac{1}{2}$$

$$- m_{A1}^{I} g_{i1A}^{a1A1} t_{aa1}^{ii1} + m_{A}^{I} t_{A1}^{I} g_{i1I1}^{a1A1} t_{aa1}^{ii1} + m_{A1}^{I} t_{A}^{I1} g_{i1I1}^{a1A1} t_{aa1}^{ii1} + m_{A}^{I} g_{i1I1}^{a1I} t_{aa1}^{ii1} - g_{i1I1}^{a1A1} m_{AA1}^{II1} t_{aa1}^{ii1}$$

$$- \bar{g}_{i1i2}^{a1a2} m_{a1A}^{iI} t_{aa2}^{i1i2} \frac{1}{2} + \bar{g}_{i1i2}^{a1a2} m_{a1A}^{i1I} t_{aa2}^{ii2} + g_{i1I1}^{a1A1} m_{aA}^{iI1} t_{a1A1}^{i1I} + g_{i1I1}^{a1A1} m_{aA}^{i1I} t_{a1A1}^{iI1} + m_{A}^{I} g_{aI1}^{a1A1} t_{a1A1}^{iI}$$

$$+ m_{a}^{i1} g_{i1A}^{a1A1} t_{a1A1}^{iI} - m_{A}^{I} t_{a}^{i1} g_{i1I1}^{a1A1} t_{a1A1}^{iI} - m_{a}^{i1} t_{A}^{I1} g_{i1I1}^{a1A1} t_{a1A1}^{iI} - g_{i1I1}^{a1A1} m_{aA}^{i1I1} t_{a1A1}^{iI} + g_{i1I1}^{a1A1} m_{aA1}^{iI} t_{a1A}^{i1I1}$$

$$- m_{a2}^{i} \bar{g}_{ai1}^{a1a2} t_{a1A}^{i1I} - m_{a}^{i2} t_{a2}^{i} \bar{g}_{i1i2}^{a1a2} t_{a1A}^{i1I} - m_{a2}^{i} t_{a}^{i2} \bar{g}_{i1i2}^{a1a2} t_{a1A}^{i1I} + m_{a}^{i2} \bar{g}_{i1i2}^{ia1} t_{a1A}^{i1I} - g_{i1I1}^{a1A1} m_{aA1}^{iI1} t_{a1A}^{i1I}$$

$$+ m_{A1}^{I} g_{aI1}^{a1A1} t_{a1A}^{iI1} - m_{A1}^{I} t_{a}^{i1} g_{i1I1}^{a1A1} t_{a1A}^{iI1} - m_{a}^{i1} t_{A1}^{I} g_{i1I1}^{a1A1} t_{a1A}^{iI1} - m_{a}^{i1} g_{i1I1}^{a1I} t_{a1A}^{iI1} - g_{i1I1}^{a1A1} m_{aA1}^{i1I} t_{a1A}^{iI1}$$

$$- F_{i1}^{a1} m_{a}^{i1} t_{a1A}^{iI} + m_{a2}^{i1} \bar{g}_{ai1}^{a1a2} t_{a1A}^{iI} - m_{a}^{i1} t_{a2}^{i2} \bar{g}_{i1i2}^{a1a2} t_{a1A}^{iI} - m_{a2}^{i2} t_{a}^{i1} \bar{g}_{i1i2}^{a1a2} t_{a1A}^{iI} - m_{A1}^{I1} g_{aI1}^{a1A1} t_{a1A}^{iI}$$

$$
\begin{aligned}
&+ m^{I1}_{A1} t^{i1}_{a} g^{a1A1}_{i1I1} t^{iI}_{a1A} + m^{i1}_{a} t^{I1}_{A1} g^{a1A1}_{i1I1} t^{iI}_{a1A} - \bar{g}^{a1a2}_{i1i2} m^{i1i2}_{aa2} t^{iI}_{a1A} \frac{1}{2} + g^{a1A1}_{i1I1} m^{i1I1}_{aA1} t^{iI}_{a1A} + \bar{g}^{a1a2}_{i1i2} m^{ii1}_{aa1} t^{i2I}_{a2A} \\
&+ g^{a1A1}_{i1I1} m^{iI}_{a1A} t^{i1I1}_{aA1} + m^{i}_{a1} g^{a1A1}_{i1A} t^{i1I}_{aA1} - m^{I}_{A} t^{i}_{a1} g^{a1A1}_{i1I1} t^{i1I}_{aA1} - m^{i}_{a1} t^{I1}_{A} g^{a1A1}_{i1I1} t^{i1I}_{aA1} - m^{I}_{A} g^{iA1}_{i1I1} t^{i1I}_{aA1} \\
&- g^{a1A1}_{i1I1} m^{iI1}_{a1A} t^{i1I}_{aA1} - m^{I}_{A2} \bar{g}^{A1A2}_{AI1} t^{iI1}_{aA1} - m^{I2}_{A} t^{I}_{A2} \bar{g}^{A1A2}_{I1I2} t^{iI1}_{aA1} - m^{I}_{A2} t^{I2}_{A} \bar{g}^{A1A2}_{I1I2} t^{iI1}_{aA1} + m^{I2}_{A} \bar{g}^{IA1}_{I1I2} t^{iI1}_{aA1} \\
&- g^{a1A1}_{i1I1} m^{i1I}_{a1A} t^{iI1}_{aA1} - F^{A1}_{I1} m^{I}_{A} t^{iI}_{aA1} - m^{i1}_{a1} g^{a1A1}_{i1A} t^{iI}_{aA1} + m^{I}_{A} t^{i1}_{a1} g^{a1A1}_{i1I1} t^{iI}_{aA1} + m^{i1}_{a1} t^{I1}_{A} g^{a1A1}_{i1I1} t^{iI}_{aA1} \\
&+ m^{I1}_{A2} \bar{g}^{A1A2}_{AI1} t^{iI}_{aA1} - m^{I}_{A} t^{I2}_{A2} \bar{g}^{A1A2}_{I1I2} t^{iI}_{aA1} - m^{I2}_{A2} t^{I1}_{A} \bar{g}^{A1A2}_{I1I2} t^{iI}_{aA1} + g^{a1A1}_{i1I1} m^{i1I1}_{a1A} t^{iI}_{aA1} \\
&- \bar{g}^{A1A2}_{I1I2} m^{I1I2}_{AA2} t^{iI}_{aA1} \frac{1}{2} + \bar{g}^{A1A2}_{I1I2} m^{II1}_{AA1} t^{iI2}_{aA2} - m^{I}_{A1} t^{i}_{a1} g^{a1A1}_{i1I1} t^{i1I1}_{aA} - m^{i}_{a1} t^{I}_{A1} g^{a1A1}_{i1I1} t^{i1I1}_{aA} \\
&- m^{i}_{a1} g^{a1I}_{i1I1} t^{i1I1}_{aA} - m^{I}_{A1} g^{iA1}_{i1I1} t^{i1I1}_{aA} - g^{a1A1}_{i1I1} m^{iI}_{a1A1} t^{i1I1}_{aA} - F^{a1}_{i1} m^{i}_{a1} t^{i1I}_{aA} - m^{i2}_{a2} t^{i}_{a1} \bar{g}^{a1a2}_{i1i2} t^{i1I}_{aA} \\
&- m^{i}_{a1} t^{i2}_{a2} \bar{g}^{a1a2}_{i1i2} t^{i1I}_{aA} - m^{i2}_{a1} \bar{g}^{ia1}_{i1i2} t^{i1I}_{aA} + m^{I1}_{A1} t^{i}_{a1} g^{a1A1}_{i1I1} t^{i1I}_{aA} + m^{i}_{a1} t^{I1}_{A1} g^{a1A1}_{i1I1} t^{i1I}_{aA} + m^{I1}_{A1} g^{iA1}_{i1I1} t^{i1I}_{aA} \\
&- \bar{g}^{a1a2}_{i1i2} m^{ii2}_{a1a2} t^{i1I}_{aA} \frac{1}{2} + g^{a1A1}_{i1I1} m^{iI1}_{a1A1} t^{i1I}_{aA} - F^{A1}_{I1} m^{I}_{A1} t^{iI1}_{aA} + m^{I}_{A1} t^{i1}_{a1} g^{a1A1}_{i1I1} t^{iI1}_{aA} + m^{i1}_{a1} t^{I}_{A1} g^{a1A1}_{i1I1} t^{iI1}_{aA} \\
&+ m^{i1}_{a1} g^{a1I}_{i1I1} t^{iI1}_{aA} - m^{I2}_{A2} t^{I}_{A1} \bar{g}^{A1A2}_{I1I2} t^{iI1}_{aA} - m^{I}_{A1} t^{I2}_{A2} \bar{g}^{A1A2}_{I1I2} t^{iI1}_{aA} - m^{I2}_{A1} \bar{g}^{IA1}_{I1I2} t^{iI1}_{aA} + g^{a1A1}_{i1I1} m^{i1I}_{a1A1} t^{iI1}_{aA} \\
&- \bar{g}^{A1A2}_{I1I2} m^{II2}_{A1A2} t^{iI1}_{aA} \frac{1}{2} - \bar{g}^{A1A2}_{I1I2} m^{iI1}_{aA} t^{II2}_{A1A2} \frac{1}{2} - m^{i}_{a1} g^{a1A1}_{aI1} t^{II1}_{AA1} + m^{i1}_{a} t^{i}_{a1} g^{a1A1}_{i1I1} t^{II1}_{AA1} \\
&+ m^{i}_{a1} t^{i1}_{a} g^{a1A1}_{i1I1} t^{II1}_{AA1} + m^{i1}_{a} g^{iA1}_{i1I1} t^{II1}_{AA1} - g^{a1A1}_{i1I1} m^{ii1}_{aa1} t^{II1}_{AA1} - \bar{g}^{A1A2}_{I1I2} m^{iI}_{aA1} t^{I1I2}_{AA2} \frac{1}{2} + \bar{g}^{A1A2}_{I1I2} m^{iI1}_{aA1} t^{II2}_{AA2}
\end{aligned}
$$

S1.4 Programmable Expression of $\langle \tilde{M}_\alpha(0) | M_\alpha(t) \rangle$

$$
\langle \tilde{M}_\alpha(0) | M_\alpha(t) \rangle = \tilde{m}_0 m_0 + \tilde{m}^{a1}_{i1} m^{i1}_{a1} + \tilde{m}^{A1}_{I1} m^{I1}_{A1} + \tilde{m}^{a1a2}_{i1i2} m^{i1i2}_{a1a2} \frac{1}{4} + \tilde{m}^{A1A2}_{I1I2} m^{I1I2}_{A1A2} \frac{1}{4} + \tilde{m}^{a1A1}_{i1I1} m^{i1I1}_{a1A1} \tag{S21}
$$

S2 Time Evolution of Dipole Moment Autocorrelation Function

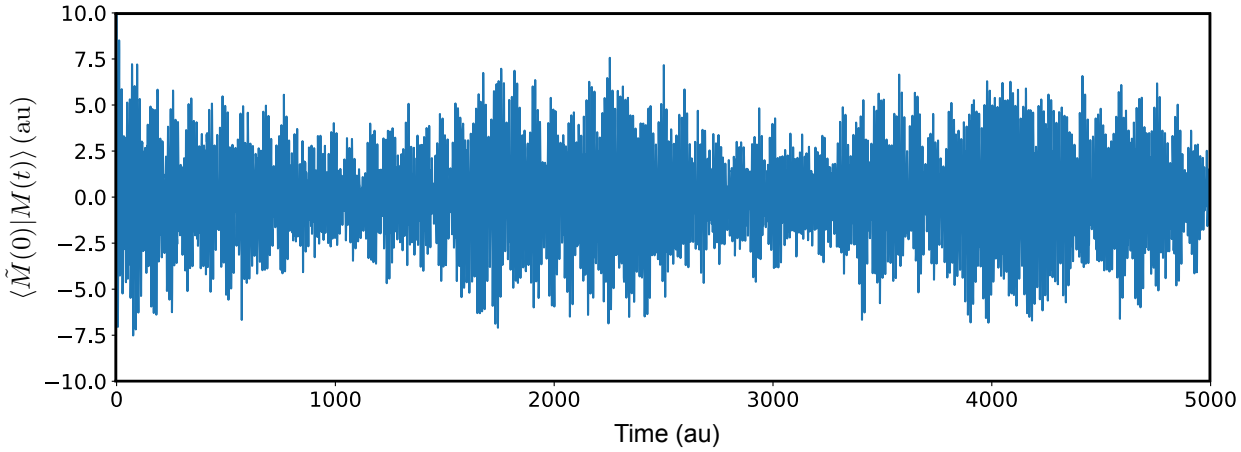

Figure S1: The time evolution of the dipole moment autocorrelation function obtained with the RT-NEO-EOM-CCSD method using the cc-pVDZ electronic basis set and the PB4-F2-a′ nuclear basis set. The total simulation time is 5000 a.u., and the time step is 0.05 a.u.

S3 Definition of the Nuclear Basis Set

Table S1: Exponent Parameters for the PB4-F2-a′ (4s3p2d2f) Nuclear Basis Set.[a]

basis function	exponent
s	3.569
s	10.345
s	18.179
s	29.582
p	5.714
p	17.975
p	35.437
d	9.289
d	20.595
f	11.518
f	22.134

[a] d and f functions are using Gaussians in the Cartesian form.

S4 NEO-TDHF Protonic Transition Densities

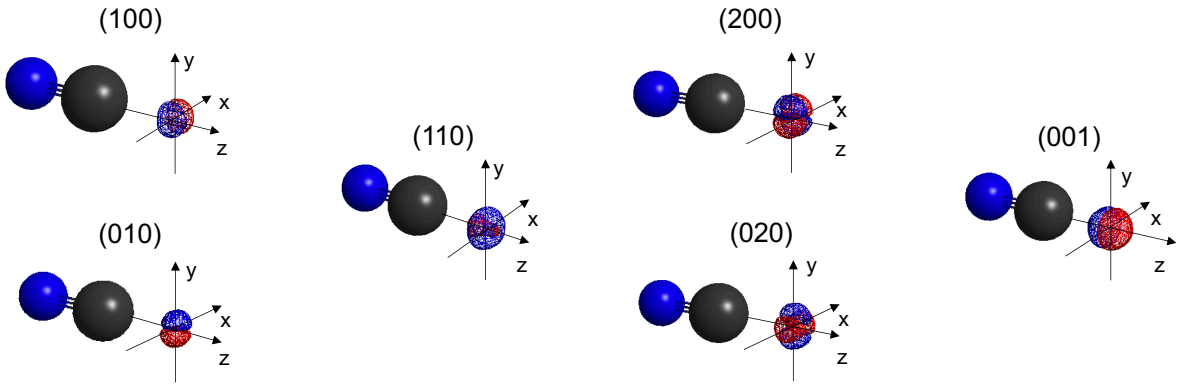

Figure S2: Transition densities for six selected proton vibrational states of the HCN molecule calculated with the NEO-TDHF method employing the cc-pVDZ electronic basis set and the PB4-F2-a′ nuclear basis set.

S5 Excitation Energies and Oscillator Strengths for NEO-TDDFT Methods

Table S2: Excitation Energies (cm^{-1}) and Oscillator Strengths (au) of the Six Selected Proton Vibrational States for the HCN Molecule Calculated with NEO-TDDFT Methods and Different Basis Sets.[a]

	NEO-TDDFT/no-epc[b]				NEO-TDDFT/epc17-2[c]			
	DZ/QZ		DZ/6Z		DZ/QZ		DZ/6Z	
$(\nu_1\nu_2\nu_3)$	ω	f	ω	f	ω	f	ω	f
(100)[d]	1991	0.33	812	0.33	1268	0.34	594	0.34
(110)	9617	7e-03	9470	4e-04	5798	7e-03	5762	4e-03
(200)[d]	10070	0.00	9903	0.00	8004	0.00	7837	0.00
(001)	3605	0.33	3151	0.33	3401	0.35	3243	0.35

[a]The NEO calculations used the PB4-F2-a′ nuclear basis set in conjunction with the cc-pVDZ electronic basis set for C and N and the cc-pVQZ, or cc-pV6Z electronic basis set for H, denoted DZ/QZ, and DZ/6Z, respectively.

[b]B3LYP electronic exchange-correlation functional without any electron-proton correlation functional.

[c]B3LYP electronic exchange-correlation functional with the epc17-2 electron-proton correlation functional.

[d](100) and (010) are degenerate, and (200) and (020) are degenerate.

S6 TD-NEO-EOM-CCSD Excitation Energies with 8s8p8d8f Nuclear Basis Set

Table S3: Excitation Energies (cm^{-1}) of the Six Selected Proton Vibrational States for the HCN Molecule Calculated with the TD-NEO-EOM-CCSD Method and the 8s8p8d8f Nuclear Basis Set.[a]

	TD-NEO-EOM-CCSD	
$(\nu_1\nu_2\nu_3)$	DZ/DZ	DZ/QZ
(100)[b]	3011	1716
(110)	5592	3362
(200)[b]	-	-
(001)	4361	3722

[a]The NEO calculations used the 8s8p8d8f nuclear basis set in conjunction with the cc-pVDZ electronic basis set for C and N and the cc-pVDZ, or cc-pVQZ electronic basis set for H, denoted DZ/DZ, and DZ/QZ, respectively. The 8s8p8d8f basis set is an even tempered basis set with exponents spanning the range from $2\sqrt{2}$ to 32.
[b](100) and (010) are degenerate, and (200) and (020) are degenerate.