Charge localization and Jahn-Teller distortions in the benzene dimer cation

Piotr A. Pieniazek, Stephen E. Bradforth* and Anna I. Krylov*

Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482

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I. EOM-IP ENERGY EXPRESSIONS

In the matrix form, the EOM-IP/EA-CCSD equations assume the following form:

$$\begin{pmatrix} \bar{H}_{SS} - E_{CC} & \bar{H}_{SD} \\ \bar{H}_{DS} & \bar{H}_{DD} - E_{CC} \end{pmatrix} \begin{pmatrix} R_1(n) \\ R_2(n) \end{pmatrix} = \omega_n \begin{pmatrix} R_1(n) \\ R_2(n) \end{pmatrix} \tag{1}$$

$$\begin{pmatrix} L_1(n) & L_2(n) \end{pmatrix} \begin{pmatrix} \bar{H}_{SS} - E_{CC} & \bar{H}_{SD} \\ \bar{H}_{DS} & \bar{H}_{DD} - E_{CC} \end{pmatrix} = \omega_n \begin{pmatrix} L_1(n) & L_2(n) \end{pmatrix} \tag{2}$$

where the IP/EA superscript is dropped. These equations are usually solved using the Davidson iterative diagonalization procedure [1–3], which requires the computation of the σ-vectors, the products of the Hamiltonian and trial vectors.

For the EOM-IP-CC(2,3) model the matrix equation for the σ vectors assumes the following form:

$$\begin{pmatrix} \bar{H}_{SS} - E_{CC} & \bar{H}_{SD} & \bar{H}_{ST} \\ \bar{H}_{DS} & \bar{H}_{DD} - E_{CC} & \bar{H}_{DT} \\ \bar{H}_{TS} & \bar{H}_{TD} & \bar{H}_{TT} - E_{CC} \end{pmatrix} \begin{pmatrix} R_1 \\ R_2 \\ R_3 \end{pmatrix} = \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix} \tag{3}$$

$$\tag{4}$$

The EOM-IP-CCSD model is recovered by setting $R_3 = 0$. The left eigenvalue problem for EOM-IP-CCSD has the form:

$$\begin{pmatrix} L_1 & L_2 \end{pmatrix} \begin{pmatrix} \bar{H}_{SS} - E_{CC} & \bar{H}_{SD} \\ \bar{H}_{DS} & \bar{H}_{DD} - E_{CC} \end{pmatrix} = \begin{pmatrix} \tilde{\sigma}_1 & \tilde{\sigma}_2 \end{pmatrix} \tag{5}$$

Programmable expressions for the left and right EOM-IP-CCSD σ-vectors, as well as the right EOM-IP-CC(2,3) σ-vectors are given in Sec. III.

II. EOM-IP-CC GRADIENTS

The Hellmann-Feynman theorem states that once the wave function of a system has been fully variationally optimized, the forces on the system in response to a perturbation ξ can be determined by computing the corresponding expectation value using the unperturbed wave function $|\Psi\rangle$:

$$\frac{\partial E}{\partial \xi} = \frac{\partial \langle \Psi | H | \Psi \rangle}{\partial \xi} = \left\langle \Psi \middle| \frac{\partial H}{\partial \xi} \middle| \Psi \right\rangle \tag{6}$$

Using the second-quantized Hamiltonian, the energy of the system can be expressed as:

$$E = \langle \Psi_L | H | \Psi_R \rangle = \sum_{pq} h_{pq} \gamma'_{pq} + \frac{1}{4} \sum_{pqrs} < pq||rs > \Gamma'_{pqrs} \tag{7}$$

$$\gamma'_{pq} = \frac{1}{2} \left\langle \Psi_L \middle| p^+ q + q^+ p \middle| \Psi_R \right\rangle \tag{8}$$

$$\Gamma'_{pqrs} = \frac{1}{2} \left\langle \Psi_L \middle| p^+ q^+ sr + s^+ r^+ pq \middle| \Psi_R \right\rangle \tag{9}$$

where ${\gamma'}_{pq}$ and ${\Gamma'}_{pqrs}$ are the one and two-particle reduced density matrices that do not depend on the perturbation. The derivative is simply:

$$\frac{\partial E}{\partial \xi} = \sum_{pq} h^{\xi}_{pq} \gamma'_{pq} + \frac{1}{4} \sum_{pqrs} < pq||rs >^{\xi} {\Gamma'}_{pqrs} \tag{10}$$

where the superscript ξ denotes the derivative of the respective integrals. However, this holds true only for wave functions optimized variationally w.r.t all their parameters. The wave functions obtained by electronic structure methods (including EOM-CC) are subject to constraints, and their response to perturbation ξ must be accounted for through the additional terms:

$$\frac{\partial E}{\partial \xi} = \left\langle \Psi \middle| \frac{\partial H}{\partial \xi} \middle| \Psi \right\rangle + \left\langle \frac{\partial \Psi}{\partial \xi} \middle| H \middle| \Psi \right\rangle + \left\langle \Psi \middle| \frac{\partial H}{\partial \xi} \middle| \frac{\partial \Psi}{\partial \xi} \right\rangle \tag{11}$$

The direct determination of these terms is inefficient, and the Z-vector [4] and the Lagrangian [5–10] techniques have been developed to compute additional wave function response terms. Below we summarize the Lagrangian-based derivation of the EOM-IP-CCSD gradients following the presentation in Ref. [10].

The Lagrangian is constructed to incorporate the constraints on the wave function as variational parameters through the undetermined multipliers. In the case of EOM-IP-CCSD, the constraints are: (i) the CC equations are satisfied; (ii) the orbitals are eigenfunctions of

the Fock operator; (iii) the orbitals are orthonormal. Thus, for unrestricted/restricted HF references, the EOM-CC Lagrangian assumes the following form:

$$\mathcal{L}(L,R,T,C,Z,\Lambda,\Omega) = \frac{<\Phi_0 L|\bar{H}|R\Phi_0>}{<\Phi_0 L|R\Phi_0>} + \sum_{\mu=1}^{n} z_\mu <\Phi_\mu|\bar{H}-E|\Phi_0> + \frac{1}{2}\sum_{pq}\lambda_{pq}(f_{pq}-\delta_{pq}) + \sum_{pq}\omega_{pq}(S_{pq}-\delta_{pq}), \quad (12)$$

where $Z \equiv \{z_\mu\}$, $\Lambda \equiv \{\lambda_{pq}\}$, and $\Omega \equiv \{\omega_{pq}\}$ are the undetermined Lagrange multipliers, and f and S are the Fock and MO overlap matrices, respectively:

$$f_{pq} =< p|h|q > + \sum_j < pj||qj > \quad (13)$$

$$S_{pq} =< \phi_p|\phi_q > \quad (14)$$

C is the MO matrix and is implicit in the integrals and the MO overlap matrix. The value of the Lagrangian is the same as the energy (if the constraints are satisfied) and its derivative w.r.t. perturbation ξ is the same as the respective derivative of the Lagrangian:

$$\frac{dE}{d\xi} = \frac{d\mathcal{L}}{d\xi} = \frac{\partial\mathcal{L}}{\partial\xi} + \frac{\partial\mathcal{L}}{\partial L}\frac{dL}{d\xi} + \frac{\partial\mathcal{L}}{\partial R}\frac{dR}{d\xi} + \frac{\partial\mathcal{L}}{\partial T}\frac{dT}{d\xi} + \frac{\partial\mathcal{L}}{\partial C}\frac{dC}{d\xi} + \frac{\partial\mathcal{L}}{\partial Z}\frac{dC}{d\xi} + \frac{\partial\mathcal{L}}{\partial\Lambda}\frac{dC}{d\xi} + \frac{\partial\mathcal{L}}{\partial\Omega}\frac{dC}{d\xi} \quad (15)$$

The first term describes the explicit dependence of the Hamiltonian on the perturbation. The second and third terms are zero, because the EOM-CC energy functional is stationary w.r.t the L and R vectors. The last three terms also vanish by virtue of the Lagrangian construction. Finally, the multipliers are defined by requiring that $\frac{\partial\mathcal{L}}{\partial T}$ and $\frac{\partial\mathcal{L}}{\partial C}$ are zero. This yields the amplitude and the orbital response equations that need to be solved for the gradient evaluation. Once the Lagrange multipliers Z, Λ, and Ω are computed, the derivative of the energy w.r.t. ξ is:

$$\frac{dE}{d\xi} = \frac{\partial\mathcal{L}}{\partial\xi} = \quad (16)$$

$$\left\langle \Phi_0 L e^{-T}\left|\frac{\partial H}{\partial\xi}\right|e^T R\Phi_0\right\rangle + \left\langle \Phi_0 Z e^{-T}\left|\frac{\partial H}{\partial\xi}\right|e^T\Phi_0\right\rangle + \frac{1}{2}\sum_{pq}\lambda_{pq}\frac{\partial f_{pq}}{\partial\xi} + \sum_{pq}\omega_{pq}\frac{\partial S_{pq}}{\partial\xi} =$$

$$\sum_{pq} h^\xi_{pq}\rho_{pq} + \frac{1}{4}\sum_{pqrs} < pq||rs >^\xi \Pi_{pqrs} + \sum_{pq}\omega_{pq}S^\xi_{pq} \quad (17)$$

where ρ and Π are the effective one- and two-particle density matrices, respectively, including wave function response terms, and the h^ξ_{pq}, $\langle pq|\,|rs\rangle^\xi$, and S^ξ_{pq} are the derivatives of the respective integrals. The programmable expressions for the Lagrange multipliers {Z,Λ,Ω} and the density matrices are given in the next section.

III. PROGRAMMABLE EXPRESSIONS

The starting point for deriving programmable expressions for σ-vectors is this:

$$
\begin{aligned}
\sigma_1 = \sigma_i &= ([\bar{H}_{SS} - E_{CC}]R_1)_i + (\bar{H}_{SD}R_2)_i + (\bar{H}_{ST}R_3)_i \\
\sigma_2 = \sigma_{ij}^a &= (\bar{H}_{DS}R_1)_{ij}^a + ([\bar{H}_{DD} - E_{CC}]R_2)_{ij}^a + (\bar{H}_{DT}R_3)_{ij}^a \\
\sigma_3 = \sigma_{ijk}^{ab} &= (\bar{H}_{TS}R_1)_{ijk}^{ab} + (\bar{H}_{TD}R_2)_{ijk}^{ab} + ([\bar{H}_{TT} - E_{CC}]R_3)_{ijk}^{ab} \\
\tilde{\sigma}_1 = \tilde{\sigma}_i &= (L_1[\bar{H}_{SS} - E_{CC}])_i + (L_2\bar{H}_{DS})_i \\
\tilde{\sigma}_2 = \tilde{\sigma}_{ij}^a &= (L_1\bar{H}_{SD})_{ij}^a + (L_2[\bar{H}_{DD} - E_{CC}])_{ij}^a
\end{aligned}
$$

Tables I-III contain EOM-IP-CCSD and EOM-IP-CC(2,3) energy expressions. Density matrices are given in Table IV-VII following Ref. [10].

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TABLE I: Programmable expressions for the right σ-vectors in EOM-IP-CC(2,3) model.

σ_i
$([\bar{H}_{SS} - E_{CC}]R_1)_i = -\sum_j r_j F_{ij}$
$(\bar{H}_{SD}R_2)_i = \sum_{jb} r^b_{ij} F_{jb} + \frac{1}{2}\sum_{jkb} r^b_{jk} I^6_{kjib}$
$(\bar{H}_{ST}R_3)_i = \frac{1}{4}\sum_{jkab} \langle jk\|\|ab\rangle r^{ab}_{ijk}$
σ^a_{ij}
$(\bar{H}_{DS}R_1)^a_{ij} = \sum_k r_k I^2_{ijka}$
$([\bar{H}_{DD} - E_{CC}]R_2)^a_{ij} = P(ij)\sum_k r^a_{jk} F_{ik} + \sum_b r^b_{ij} F_{ab}$ $-P(ij)\sum_{kb} r^b_{ik} I^1_{jbka} + \sum_{kl} r^a_{kl} I^4_{ijkl} + \sum_b T^4_b t^{ab}_{ij}$
$(\bar{H}_{DT}R_3)^a_{ij} = \sum_{kb} F_{kb} r^{ab}_{ijk} + \frac{1}{2}P(ij)\sum_{klb} I^6_{klib} r^{ab}_{klj} - \frac{1}{2}\sum_{kbc} I^7_{kabc} r^{bc}_{ijk}$
σ^{ab}_{ijk}
$(\bar{H}_{TS}R_1)^{ab}_{ijk} = P(ij\|k)\left[\sum_l t^{ab}_{kl} H^2_{ijl} - P(ab)\sum_d t^{ac}_{ij} H^3_{kcb}\right]$
$(\bar{H}_{TD}R_2)^{ab}_{ijk} = P(ij\|k)[-\sum_c r^c_{ij} I^3_{kcba} + \sum_l t^{ab}_{kl} H^4_{ijl}$ $-P(ab)\sum_l r^b_{kl} I^2_{ijla} + P(ab)\sum_c t^{ac}_{ij} H^5_{kcb}$
$([\bar{H}_{TT} - E_{CC}]R_3)^{ab}_{ijk} = P(ij\|k)\left[-\sum_l F_{kl} r^{ab}_{ijl} + \sum_{lm} I^4_{ijlm} r^{ab}_{lmk}\right] +$ $P(ab)\sum_c F_{bc} r^{ac}_{ijk} + \sum_{cd} I^5_{abcd} r^{cd}_{ijk} - P(ab)P(i\|jk)\sum_{cl} I^1_{icla} r^{cb}_{ljk} +$ $P(ij\|k)\left[\sum_l H^6_{ijl} t^{ab}_{kl} - P(ab)\sum_c H^7_{kbc} t^{ac}_{ij}\right]$

TABLE II: R-independenet intermediates used in the energy EOM-IP-CCSD and EOM-IP-CC(2,3) expressions.

$$F_{ia} = f_{ia} + \sum_{jb} t_j^b < ij||ab >$$

$$F_{ij} = f_{ij} + \sum_a t_i^a f_{ja} + \sum_{ka} t_k^a < jk||ia > + \sum_{kab} t_i^a t_k^b < jk||ab > + \frac{1}{2} \sum_{kbc} t_{ik}^{bc} < jk||bc >$$

$$F_{ab} = f_{ab} - \sum_i t_i^a f_{ib} - \sum_{ic} t_i^c < ia||bc > + \sum_{ijc} t_i^c t_j^a < ij||bc > - \frac{1}{2} \sum_{jkc} t_{jk}^{ac} < jk||bc >$$

$$I^1_{iajb} =< ia||jb > - \sum_k t_k^b < jk||ia > - \sum_c t_i^c < jb||ac > + \sum_{kc} t_i^c t_k^b < jk||ac > - \sum_{kc} t_{ik}^{bc} < jk||ac >$$

$$I^2_{ijka} = - < ij||ka > + 2 \sum_l t_l^a I^4_{ijkl} + P(ij) \sum_b \left(t_i^b (< jb||ka > - \sum_{lc} t_{jl}^{ac} < kl||bc >) \right) - \sum_{bc} t_i^b t_j^c < ka||bc > - \sum_{lbc} t_l^b t_{ij}^{ac} < kl||bc > + \sum_c t_{ij}^{bc} f_{kc} - \frac{1}{2} \sum_{cd} t_{ij}^{cd} < kb||cd > + P(ij) \sum_{lc} t_{il}^{bc} < jc||kl >$$

$$I^3_{icab} = - < ic||ab > + 2 \sum_d t_i^d I^5_{bcad} + P(bc) \sum_j \left(t_j^b (< ia||jc > - \sum_{kd} t_{ik}^{cd} < jk||ad >) \right) - \sum_{jk} t_j^b t_k^c < jk||ia > - \sum_{jkd} t_j^d t_{ik}^{bc} < jk||ad > + \sum_k t_{ik}^{ab} f_{kc} - \frac{1}{2} \sum_{kl} t_{kl}^{ab} < ic||kl > + P(ab) \sum_{kd} t_{ik}^{ad} < kb||cd >$$

$$I^4_{ijkl} = \frac{1}{2} < ij||kl > - \frac{1}{2} P(ij) \sum_a t_i^a < kl||ja > + \frac{1}{2} \sum_{ab} t_i^a t_j^b < kl||ab > + \frac{1}{4} \sum_{cd} t_{ij}^{cd} < kl||cd >$$

$$I^6_{ijka} =< ij||ka > - \sum_c t_k^c < ij||ac >$$

$$I^7_{iabc} =< ia||bc > - \sum_j t_j^a < ij||bc >$$

TABLE III: R-dependent intermediates used in the energy EOM-IP-CCSD and EOM-IP-CC(2,3) expressions.

$H^2_{ijk} = 2\sum_l r_l I^4_{ijkl}$
$H^3_{iab} = \sum_l r_j I^1_{iajb}$
$H^4_{ijk} = P(ij)\sum_{al} r^a_{il} I^6_{klja}$
$H^5_{iab} = \frac{1}{2}\sum_{jk} r^b_{jk} I^6_{jkia} + \sum_{jc} r^c_{ij} I^7_{jbca}$
$H^6_{ijk} = \frac{1}{2}\sum_{abl} r^{ab}_{ijl} \langle kl\|\|ab\rangle$
$H^7_{iab} = \frac{1}{2}\sum_{ckj} r^{ac}_{kji} \langle kj\|\|bc\rangle$
$T^4_a = -\frac{1}{2}\sum_{klb} r^b_{kl} < kl\|\|ab >$
$T^6_a = \frac{1}{2}\sum_{ijb} l^b_{ij} t^{ab}_{ij}$

TABLE IV: Programmable expressions for unrelaxed EOM-IP-CCSD density matrices.

$$\gamma'_{ij} = \tilde{\gamma}_{ij} + \delta_{ij}$$

$$\tilde{\gamma}_{ij} = \tfrac{1}{2} P_+(ij)[-l_i r_j - \tilde{l}_{ij} + \textstyle\sum_a Y^1_{ia} t^a_j]$$

$$\gamma'_{ab} = \tfrac{1}{2} P_+(ab)[\tilde{l}^{ab} - \textstyle\sum_i Y^1_{ia} t^b_i]$$

$$\gamma'_{ia} = \tfrac{1}{2}[-Y^1_{ia} - \textstyle\sum_j l_j (r^a_{ij} + r_i t^a_j) - \sum_{jb} Y^1_{jb}(t^{ab}_{ij} - t^a_j t^b_i)$$
$$-r_i \tilde{\bar{l}}^a - \textstyle\sum_j \tilde{l}_{ji} t^a_j - \sum_b \tilde{l}^{ba} t^b_i + t^a_i]$$

$$\Gamma'_{ijkl} = \tilde{\Gamma}_{ijkl} - \delta_{li}\delta_{kj} + \delta_{ki}\delta_{lj} - \delta_{li}\tilde{\gamma}_{jk} + \delta_{ki}\tilde{\gamma}_{jl} + \delta_{lj}\tilde{\gamma}_{ik} - \delta_{kj}\tilde{\gamma}_{il}$$
$$\tilde{\Gamma}_{ijkl} = \tfrac{1}{2} \textstyle\sum_a (l^a_{kl} \bar{r}^a_{ij} + l^a_{ij} \bar{r}^a_{kl})$$

$$\Gamma'_{abcd} = 0$$

$$\Gamma'_{ijka} = \tilde{\Gamma}_{ijka} - \delta_{kj}\gamma_{ia} + \delta_{ki}\gamma_{ja}$$
$$\tilde{\Gamma}_{ijka} = -\tfrac{1}{2}[l^a_{ij} r_k + l_k \bar{r}^a_{ij} + \textstyle\sum_b Y^1_{kb} \tilde{t}^{ab}_{ij}$$
$$-P(ij)\tilde{l}_{kj} t^a_i - \textstyle\sum_{lb} l^b_{kl}(\bar{r}^b_{ij} t^a_l - P(ij) t^b_i r^a_{jl} - P(ij) t^{ab}_{il} r_j)]$$

$$\Gamma'_{iajb} = \tilde{\Gamma}_{iajb} + \delta_{ji}\gamma_{ab}$$
$$\tilde{\Gamma}_{iajb} = \tfrac{1}{2}[(Y^1_{ja} t^b_i + Y^1_{ib} t^a_j) - \textstyle\sum_k (l^b_{ik} r^a_{jk} + l^a_{jk} r^b_{ik}) - \sum_k (l^a_{jk} t^b_k r_i + l^b_{ik} t^a_k r_j)]$$

$$\Gamma'_{iabc} = -\tfrac{1}{2}[\textstyle\sum_j Y^1_{ja} \tilde{t}^{bc}_{ij} - P(bc) t^b_i \tilde{l}^{ac} + \sum_{jk} l^a_{jk} \tilde{t}^{bc}_{jk} r_i - P(bc) \sum_{jk} l^a_{jk} t^c_j r^b_{ik}]$$

$$\Gamma'_{ijab} = \tfrac{1}{2}[\tilde{t}^{ab}_{ij} - \textstyle\sum_k l_k (P(ij) t^{ab}_{ik} r_j - P(ab) \bar{r}^a_{ij} t^b_k + P(ij)P(ab) t^a_i r^b_{jk}) + P(ab) \tilde{\bar{l}}^b r^a_{ij}$$
$$+ \textstyle\sum_{kc} Y^1_{kc} (P(ab) t^b_k \tilde{t}^{ac}_{ij} - P(ij) t^c_i t^{ab}_{jk} - P(ij)P(ab) t^b_j t^{ac}_{ik})$$
$$+P(ij)P(ab) \tilde{\bar{l}}^b t^a_j r_i - P(ij)P(ab) \textstyle\sum_c \tilde{l}^{cb} t^c_j t^a_i$$
$$+ \textstyle\sum_{klc} l^c_{kl} (-\tfrac{1}{2} P(ab) t^{ac}_{ij} r^b_{kl} + \tfrac{1}{2} t^{ab}_{kl} r^c_{ij} - \tfrac{1}{2} P(ij) t^{ab}_{jk} r^c_{il} + P(ij)P(ab) t^{ac}_{ik} r^b_{jl}$$
$$+P(ij)P(ab) t^b_k t^{ac}_{jl} r_i - \tfrac{1}{2} P(ij) t^c_i t^{ab}_{kl} r_j - \tfrac{1}{2} P(ab) t^b_k t^a_l \bar{r}^c_{ij} + P(ij)P(ab) t^b_k t^c_i r^a_{jl})$$

TABLE V: Intermediates used in the unrealxed EOM-IP-CCSD density matrices calculation.

$$Y^1_{ia} = \sum_j l^a_{ij} r_j$$
$$\tilde{l}_{ij} = \sum_{ka} l^a_{ik} r^a_{jk}$$
$$\tilde{l}^{ab} = \tfrac{1}{2} \sum_{ij} l^a_{ij} r^b_{ij}$$
$$\tilde{\tilde{l}}^a = \tfrac{1}{2} \sum_{ijb} l^b_{ij} t^{ab}_{ij}$$
$$\bar{r}^a_{ij} = r^a_{ij} + P(ij) r_i t^a_j$$
$$\tilde{t}^{ab}_{ij} = t^{ab}_{ij} + \tfrac{1}{2} P(ij) P(ab) t^a_i t^b_j$$

TABLE VI: EOM-IP-CCSD amplitude response ξ-vector programmable expressions.

$$\xi^a_i = F_{ia}(1 - \sum_j r_j l_j) + T^4_a l_i - \sum_{jkb} l_k r^b_{jk} < ij||ab > +$$
$$-\tfrac{1}{2} \sum_b Y^2_{ab} F_{ib} + \tfrac{1}{2} \sum_{bc} Y^2_{bc} I^7_{ibac}$$
$$- \sum_j Y^3_{ij} F_{ja} + \sum_{jk} Y^3_{jk} I^6_{ikja}$$
$$+\tfrac{1}{2} \sum_{jklc} l^a_{ij} r^c_{kl} I^6_{kljc}$$
$$+ \sum_{jb} Y^4_{iajb} F_{jb} - \sum_{jkb} Y^4_{jakb} I^6_{ikjb} - \sum_{jbc} Y^4_{icjb} I^7_{jcab}$$
$$+\tfrac{1}{2} \sum_{jkl} Y^5_{ijkl} I^6_{lkja}$$

$$\xi^{ab}_{ij} =< ij||ab > +\tfrac{1}{2} \sum_{kl} Y^5_{ijkl} < kl||ab > - \sum_{kc} r_k l^c_{ij} I^7_{kcab} +$$
$$+P(ij)[\sum_c Y^1_{ic} I^7_{jcab} + \sum_k (X^2_{ik} + Y^3_{ik}) < jk||ab >] +$$
$$-P(ab)[\sum_c Y^2_{bc} < ij||ac > + \sum_k I^6_{ijka} Y^1_{kb}] +$$
$$+P(ij)P(ab)[\sum_{kc} Y^4_{iakc} < jk||bc > -Y^1_{ia} F_{jb} - \sum_{klc} r_l l^a_{ik} I^6_{jlkb}]$$

TABLE VII: Intermediates used in the ξ-vector calculation.

$X^2_{ij} = l_i r_j$
$Y^2_{ab} = \sum_{ijc} l^a_{ij} r^b_{ij}$
$Y^3_{ij} = \sum_{ka} l^a_{ik} r^a_{jk}$
$Y^4_{iajb} = \sum_{kc} l^a_{ik} r^b_{jk}$
$Y^5_{ijkl} = \sum_{a} l^a_{ij} r^a_{kl}$