

### **Supplementary Information: Higher Order Cartesian Gaussian Multipole Tensors**

Although the AMOEBA force field does not include octopole or hexadecapole moments, future scattering models based on Cartesian Gaussian multipoles may. Therefore, we present the 3<sup>rd</sup>, 4<sup>th</sup> and 5<sup>th</sup> order tensors and the derivatives of the 3<sup>rd</sup> and 4<sup>th</sup> order tensors with respect to both ADP and  $\kappa$  parameters for future convenience.

### Cartesian Gaussian Tensors of 3<sup>rd</sup>, 4<sup>th</sup> and 5<sup>th</sup> Order

$$\begin{aligned}
\nabla_\alpha \nabla_\beta \nabla_\gamma \rho(\mathbf{r}) &= -(2\pi)^{-3/2} \sum_{i=1}^n a_i |\mathbf{U}_i|^{-1/2} e^{-\frac{1}{2} \mathbf{r}' \mathbf{U}_i^{-1} \mathbf{r}} \\
&\quad \times \left[ \begin{aligned} &(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) U_{i,\beta\gamma}^{-1} \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\alpha\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\beta}^{-1} \end{aligned} \right] \\
\nabla_\alpha \nabla_\beta \nabla_\gamma \nabla_\delta \rho(\mathbf{r}) &= (2\pi)^{-3/2} \sum_{i=1}^n a_i |\mathbf{U}_i|^{-1/2} e^{-\frac{1}{2} \mathbf{r}' \mathbf{U}_i^{-1} \mathbf{r}} \\
&\quad \times \left[ \begin{aligned} &(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\gamma\delta}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\beta\delta}^{-1} \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\beta\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\delta}^{-1} \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\beta}^{-1} \\ &+ U_{i,\alpha\beta}^{-1} U_{i,\gamma\delta}^{-1} + U_{i,\alpha\gamma}^{-1} U_{i,\beta\delta}^{-1} + U_{i,\alpha\delta}^{-1} U_{i,\beta\gamma}^{-1} \end{aligned} \right] \\
\nabla_\alpha \nabla_\beta \nabla_\gamma \nabla_\delta \nabla_\varepsilon \rho(\mathbf{r}) &= -(2\pi)^{-3/2} \sum_{i=1}^n a_i |\mathbf{U}_i|^{-1/2} e^{-\frac{1}{2} \mathbf{r}' \mathbf{U}_i^{-1} \mathbf{r}} \\
&\quad \times \left\{ \begin{aligned} &(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\varepsilon) \left[ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) \right. \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\gamma\delta}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\beta\delta}^{-1} \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\beta\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\delta}^{-1} \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\beta}^{-1} \\ &\left. + U_{i,\alpha\beta}^{-1} U_{i,\gamma\delta}^{-1} + U_{i,\alpha\gamma}^{-1} U_{i,\beta\delta}^{-1} + U_{i,\alpha\delta}^{-1} U_{i,\beta\gamma}^{-1} \right] \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{u}'_\varepsilon \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\gamma\varepsilon}^{-1} \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\delta\varepsilon}^{-1} \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\beta\varepsilon}^{-1} \\ &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\varepsilon}^{-1} \\ &+ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) \left[ U_{i,\beta\gamma}^{-1} U_{i,\delta\varepsilon}^{-1} + U_{i,\beta\delta}^{-1} U_{i,\gamma\varepsilon}^{-1} + U_{i,\beta\varepsilon}^{-1} U_{i,\gamma\delta}^{-1} \right] \\ &+ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) \left[ U_{i,\alpha\gamma}^{-1} U_{i,\delta\varepsilon}^{-1} + U_{i,\alpha\delta}^{-1} U_{i,\gamma\varepsilon}^{-1} + U_{i,\alpha\varepsilon}^{-1} U_{i,\gamma\delta}^{-1} \right] \\ &+ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) \left[ U_{i,\alpha\beta}^{-1} U_{i,\delta\varepsilon}^{-1} + U_{i,\alpha\delta}^{-1} U_{i,\beta\varepsilon}^{-1} + U_{i,\alpha\varepsilon}^{-1} U_{i,\beta\delta}^{-1} \right] \\ &+ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) \left[ U_{i,\alpha\beta}^{-1} U_{i,\varepsilon\gamma}^{-1} + U_{i,\alpha\gamma}^{-1} U_{i,\beta\varepsilon}^{-1} + U_{i,\alpha\varepsilon}^{-1} U_{i,\beta\gamma}^{-1} \right] \end{aligned} \right\} \quad (1)
\end{aligned}$$

Derivative with respect to ADPs of 3<sup>rd</sup> and 4<sup>th</sup> Order Cartesian Gaussian Tensors

$$\begin{aligned}
 \frac{\partial [\nabla_\alpha \nabla_\beta \nabla_\gamma \rho(\mathbf{r})]}{\partial U_{\tau\nu}} &= -(2\pi)^{-3/2} \sum_{i=1}^n a_i |\mathbf{U}_i|^{-1/2} e^{-\frac{1}{2} \mathbf{r}' \mathbf{U}_i^{-1} \mathbf{r}} \\
 &\times \left\{ \begin{aligned}
 &\frac{1}{2} [\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{r} - U_{i,\tau\nu}^{-1} (2 - \delta_{\tau\nu})] [(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) \\
 &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) U_{i,\beta\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\alpha\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\beta}^{-1}] \\
 &+ (\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) \\
 &+ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\gamma) - (\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\alpha) U_{i,\beta\gamma}^{-1} - (\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\beta) U_{i,\alpha\gamma}^{-1} \\
 &- (\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\gamma) U_{i,\alpha\beta}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) J_{i,\beta\gamma}^{(\tau\nu)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) J_{i,\alpha\gamma}^{(\tau\nu)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) J_{i,\alpha\beta}^{(\tau\nu)}
 \end{aligned} \right\} \\
 \frac{\partial [\nabla_\alpha \nabla_\beta \nabla_\gamma \nabla_\delta \rho(\mathbf{r})]}{\partial U_{\tau\nu}} &= (2\pi)^{-3/2} \sum_{i=1}^n a_i |\mathbf{U}_i|^{-1/2} e^{-\frac{1}{2} \mathbf{r}' \mathbf{U}_i^{-1} \mathbf{r}} \\
 &\times \left\{ \begin{aligned}
 &\frac{1}{2} [\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{r} - U_{i,\tau\nu}^{-1} (2 - \delta_{\tau\nu})] \\
 &\times \left[ \begin{aligned}
 &(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) \\
 &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\gamma\delta}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\beta\delta}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\beta\gamma}^{-1} \\
 &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\delta}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\beta}^{-1} \\
 &+ U_{i,\alpha\beta}^{-1} U_{i,\gamma\delta}^{-1} + U_{i,\alpha\gamma}^{-1} U_{i,\beta\delta}^{-1} + U_{i,\alpha\delta}^{-1} U_{i,\beta\gamma}^{-1}
 \end{aligned} \right] \\
 &+ (\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) \\
 &+ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\delta) \\
 &\times \left[ \begin{aligned}
 &-(\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\alpha) [(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\gamma\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\beta\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\beta\gamma}^{-1}] \\
 &-(\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\beta) [(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) U_{i,\gamma\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\gamma}^{-1}] \\
 &-(\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\gamma) [(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) U_{i,\beta\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\alpha\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\beta}^{-1}] \\
 &-(\mathbf{r}' \mathbf{J}_i^{(\tau\nu)} \mathbf{u}_\delta) [(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) U_{i,\beta\gamma}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\alpha\gamma}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\beta}^{-1}] \\
 &-(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) J_{i,\gamma\delta}^{(\tau\nu)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) J_{i,\beta\delta}^{(\tau\nu)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) J_{i,\beta\gamma}^{(\tau\nu)} \\
 &-(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) J_{i,\alpha\delta}^{(\tau\nu)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) J_{i,\alpha\gamma}^{(\tau\nu)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma)(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) J_{i,\alpha\beta}^{(\tau\nu)} \\
 &+ J_{i,\alpha\beta}^{(\tau\nu)} U_{i,\gamma\delta}^{-1} + J_{i,\alpha\gamma}^{(\tau\nu)} U_{i,\beta\delta}^{-1} + J_{i,\alpha\delta}^{(\tau\nu)} U_{i,\beta\gamma}^{-1} \\
 &+ J_{i,\beta\delta}^{(\tau\nu)} U_{i,\alpha\gamma}^{-1} + J_{i,\beta\gamma}^{(\tau\nu)} U_{i,\alpha\delta}^{-1} + J_{i,\gamma\delta}^{(\tau\nu)} U_{i,\alpha\beta}^{-1}
 \end{aligned} \right]
 \end{aligned} \right\} \quad (2)
 \end{aligned}$$

### Derivative with respect to the Width of 3<sup>rd</sup> and 4<sup>th</sup> Order Cartesian Gaussian Tensors

$$\begin{aligned}
 \frac{\partial [\nabla_\alpha \nabla_\beta \nabla_\gamma \rho(\mathbf{r})]}{\partial \kappa} &= -(2\pi)^{-3/2} \sum_{i=1}^n a_i |\mathbf{U}_i|^{-1/2} e^{-\frac{1}{2} \mathbf{r}' \mathbf{U}_i^{-1} \mathbf{r}} \\
 &\times \left\{ \begin{aligned}
 &\frac{1}{2} \left( -\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{r} - |\mathbf{U}_i|^{-1} \frac{\partial |\mathbf{U}_i|}{\partial \kappa} \right) \left[ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) \right. \\
 &\quad \left. - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) U_{i,\beta\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\alpha\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\beta}^{-1} \right] \\
 &+ (\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) \\
 &+ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\gamma) - (\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\alpha) U_{i,\beta\gamma}^{-1} - (\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\beta) U_{i,\alpha\gamma}^{-1} \\
 &\quad \left. - (\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\gamma) U_{i,\alpha\beta}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) J_{i,\beta\gamma}^{(\kappa)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) J_{i,\alpha\gamma}^{(\kappa)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) J_{i,\alpha\beta}^{(\kappa)} \right\} \\
 \frac{\partial [\nabla_\alpha \nabla_\beta \nabla_\gamma \nabla_\delta \rho(\mathbf{r})]}{\partial \kappa} &= (2\pi)^{-3/2} \sum_{i=1}^n a_i |\mathbf{U}_i|^{-1/2} e^{-\frac{1}{2} \mathbf{r}' \mathbf{U}_i^{-1} \mathbf{r}} \\
 &\times \left\{ \begin{aligned}
 &\frac{1}{2} \left( -\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{r} - |\mathbf{U}_i|^{-1} \frac{\partial |\mathbf{U}_i|}{\partial \kappa} \right) \\
 &\times \left[ \begin{aligned}
 &(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) \\
 &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\gamma\delta}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\beta\delta}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\beta\gamma}^{-1} \\
 &- (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\delta}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\gamma}^{-1} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\beta}^{-1} \\
 &\quad + U_{i,\alpha\beta}^{-1} U_{i,\gamma\delta}^{-1} + U_{i,\alpha\gamma}^{-1} U_{i,\beta\delta}^{-1} + U_{i,\alpha\delta}^{-1} U_{i,\beta\gamma}^{-1}
 \end{aligned} \right] \\
 &+ (\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) \\
 &+ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\gamma) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) (\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\delta) \\
 &\times \left[ \begin{aligned}
 &-(\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\alpha) \left[ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\gamma\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\beta\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\beta\gamma}^{-1} \right] \\
 &-(\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\beta) \left[ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) U_{i,\gamma\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\gamma}^{-1} \right] \\
 &-(\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\gamma) \left[ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) U_{i,\beta\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\alpha\delta}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) U_{i,\alpha\beta}^{-1} \right] \\
 &-(\mathbf{r}' \mathbf{J}_i^{(\kappa)} \mathbf{u}_\delta) \left[ (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) U_{i,\beta\gamma}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) U_{i,\alpha\gamma}^{-1} + (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) U_{i,\alpha\beta}^{-1} \right] \\
 &-(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) J_{i,\gamma\delta}^{(\kappa)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) J_{i,\beta\delta}^{(\kappa)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\alpha) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) J_{i,\beta\gamma}^{(\kappa)} \\
 &-(\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) J_{i,\alpha\delta}^{(\kappa)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\beta) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) J_{i,\alpha\gamma}^{(\kappa)} - (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\gamma) (\mathbf{r}' \mathbf{U}_i^{-1} \mathbf{u}_\delta) J_{i,\alpha\beta}^{(\kappa)} \\
 &+ J_{i,\alpha\beta}^{(\kappa)} U_{i,\gamma\delta}^{-1} + J_{i,\alpha\gamma}^{(\kappa)} U_{i,\beta\delta}^{-1} + J_{i,\alpha\delta}^{(\kappa)} U_{i,\beta\gamma}^{-1} \\
 &+ J_{i,\beta\delta}^{(\kappa)} U_{i,\alpha\gamma}^{-1} + J_{i,\beta\gamma}^{(\kappa)} U_{i,\alpha\delta}^{-1} + J_{i,\gamma\delta}^{(\kappa)} U_{i,\alpha\beta}^{-1}
 \end{aligned} \right]
 \end{aligned} \right\} \quad (3)
 \end{aligned}$$