U

S

$\mathfrak{G}_j$

$\mathfrak{D}_j$

$\mathfrak{G}_k$

$\mathfrak{D}_k$

$\mathfrak{D}_i$

$\mathfrak{D}_a$

$\mathfrak{D}_r$

$\mathfrak{D}_x$

$\mathfrak{D}_y$

𝔇z

D ||

D

$\mathfrak{D}_{\perp}$

$$\mathfrak{D}_{iso}$$

$\mathfrak{D}_{ratio}$

(

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$$\frac{I_{sat}}{I_{ref}}$$

$$\sqrt{\frac{(\sigma_{sat} \cdot I_{ref})^2 + (\sigma_{ref} \cdot I_{sat})^2}{I_{ref}}}$$

$$\sum_{i=1}^{n}$$

$$\frac{(\mathrm{R}_i - \mathrm{R}_i(\theta))^2}{\sigma_i^2}$$

$$\hat{\theta}$$

$$\frac{1}{4}$$

(

$$\frac{\mu_0}{4\pi}$$

$$\Big)^2$$

$$\frac{(\gamma_H \gamma_X \hbar)^2}{\langle r^6 \rangle}$$

$$\frac{(\omega_X \Delta\sigma)^2}{3}$$

$\hbar$

$$\frac{\gamma_H}{\gamma_X}$$

$$\frac{\sigma_{\mathrm{NOE}}(\theta)}{\mathrm{R}_1(\theta)}$$

$$\frac{2}{5}$$

$$\sum_{i=-k}^{k}$$

(

$$\frac{S^2}{1 + (\omega\tau_i)^2}$$

$$\frac{(1-S^2)(\tau_e+\tau_i)\tau_e}{(\tau_e+\tau_i)^2+(\omega\tau_e\tau_i)^2}$$

)

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$$\frac{1}{5}$$

(

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$$\frac{1}{\mathfrak{R}}$$

[

$$\mathfrak{D}_r)\left(\delta_x^4+2\delta_y^2\delta_z^2\right)+(1-3\mathfrak{D}_r)\left(\delta_y^4+2\delta_x^2\delta_z^2\right)-2\left(\delta_z^4+2\delta_x^2\delta_y^2\right)\Bigg],$$

$$\mathfrak{R} = \sqrt{1 + 3\mathfrak{D}_r^2}.$$

$\mathfrak{D}_{iso}$.

$\mathfrak{F}_i$

$\mathfrak{T}_i$

$\geq$

$$\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1
\end{pmatrix}$$

$$\begin{pmatrix} S^2 \\ S_f^2 \\ S_s^2 \\ \tau_e \\ \tau_f \\ \tau_s \\ R_{ex} \\ r \\ CSA \end{pmatrix}$$

$\geq$

$$\begin{pmatrix} 0 \\ -1 \\ 0 \\ -1 \\ 0 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.9e^{-10} \\ 2e^{-10} \\ 300e^{-6} \\ 0 \end{pmatrix}$$

$\leq$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\begin{pmatrix} \tau_e \\ \tau_f \\ \tau_s \end{pmatrix}$$

$$\begin{pmatrix} -2\tau_m \\ -2\tau_m \\ -2\tau_m \end{pmatrix}$$

$$\begin{pmatrix} 2 & -1 & 0 & 0 \\ 2 & 0 & -1 & 0 \\ 2 & 0 & 0 & -1 \end{pmatrix}$$

$$\begin{pmatrix} \tau_m \\ \tau_e \\ \tau_f \\ \tau_s \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\begin{pmatrix} \tau_m \\ \mathfrak{D}_a \\ \mathfrak{D}_r \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ -200.0e^{-9} \\ 0 \\ 0 \\ -1 \end{pmatrix}$$

$$(1)$$

$$\left(\mathfrak{D}_a\right)$$

(0)

$$(-1)$$

$$
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1e^{-12} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1e^{-12} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1e^{-12} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & (2\pi\omega_H)^{-2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1e^{-10} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1e^{-4}
\end{pmatrix}
$$

$$\begin{pmatrix} 1e^{-12} & 0 & 0 & 0 & 0 & 0 \\ 0 & 1e^{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1e^{-12} & 0 & 0 & 0 \\ 0 & 1e^{7} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$\mathfrak{D}_y + \mathfrak{D}_z)/2$

$\mathfrak{D}_x + \mathfrak{D}_z)/2$

$\mathfrak{D}_x + \mathfrak{D}_y)/2$

Û

F

Û

$$\hat{\theta}$$

$$\left\{ \vphantom{\begin{matrix}a\\b\\c\\d\end{matrix}} \right.$$

$$\mathfrak{S} : \min_{\hat{\theta} \in \mathfrak{U}} \Delta_{\text{K-L}}(\hat{\theta})$$

$\}$

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S

}

$$\frac{U}{\sum_i \mathrm{NOE}^2}$$

$$\frac{d}{dt}$$

[

$$M_A^+(t)$$
$$M_B^+(t)$$

]

[

$$\begin{matrix} -i\Omega_A - \mathrm{R}^0_{2\mathrm{A}} - p_{\mathrm{B}}\mathrm{k}_{\mathrm{ex}} & p_{\mathrm{A}}\mathrm{k}_{\mathrm{ex}} \\ p_{\mathrm{B}}\mathrm{k}_{\mathrm{ex}} & -i\Omega_B - \mathrm{R}^0_{2\mathrm{B}} - p_{\mathrm{A}}\mathrm{k}_{\mathrm{ex}} \end{matrix}$$

]

$\gg$

$\overline{\omega}$

$\overline{\Omega}$

$$\sqrt{\overline{\Omega}^2 + \omega_1^2}$$

(

$$\frac{\omega_1}{\Omega}$$

)

$\approx$

$$\frac{1}{T_{\text{relax}}}$$

(

$$\frac{I_1(\nu_{\mathrm{CPMG}})}{I_0}$$

)

(

$$\frac{I_1(\omega_1)}{I_0}$$

)

$$\sqrt{\left(\frac{\sigma_{I_1}}{I_1(\omega_1)}\right)^2 + \left(\frac{\sigma_{I_0}}{I_0}\right)^2}$$

(

$$\frac{I_1}{I_0}$$

)

(

$$\frac{X}{Y}$$

)

(

)

(

$$\frac{\sigma_A}{A}$$

$$\Big)^2$$

(

$$\frac{\sigma_{I_0}}{I_0}$$

$$\Big)^2$$

(

$$\frac{\sigma_{I_1}}{I_1}$$

$$)^2$$

$$\frac{\sigma_{I_1}}{T_{\text{relax}} I_1(\omega_1)}$$

[

(

$)^{-1}$

]

$$\sum_{i=2}^{n}$$

$$\frac{\Phi_{\mathrm{ex,i}}}{\mathrm{k_i}}$$

(

$$\frac{4\nu_{\mathrm{CPMG}}}{\mathrm{k_i}}$$

(

$$\frac{\mathrm{k_i}}{4\nu_{\mathrm{CPMG}}}$$

)

)

$$\frac{\Phi_{ex}}{k_{ex}}$$

(

$$\frac{4\nu_{\mathrm{CPMG}}}{\mathrm{k_{ex}}}$$

(

$$\frac{k_{ex}}{4\nu_{CPMG}}$$

)

)

$$\sum_{i=2}^{3}$$

$$\frac{1}{2}$$

(

(

)

)

(

$$\frac{\Psi + 2\Delta\omega^2}{\sqrt{\Psi^2 + \zeta^2}}$$

$\Big)$

$$\frac{-3}{2}$$

$$\frac{1}{\nu_{\mathrm{CPMG}}}$$

(

$$\sqrt{\Psi^2 + \zeta^2}$$

$$\Bigg)^{\frac{1}{2}}$$

(

$)^2$

)

$$\frac{k_{ex}}{2}$$

$\sim$

$$\frac{\Phi_{\mathrm{ex}}\tau_{\mathrm{ex}}}{1+\omega_a^2\tau_{\mathrm{ex}}^2}$$

$$\sqrt{\omega_{1\mathrm{eff}}^4 + p_{\mathrm{A}}^2 \Delta\omega^4}$$

$$\sqrt{3}$$

$$\frac{\sin\left(\Delta\omega\cdot\tau_{\mathrm{CPMG}}\right)}{\Delta\omega\cdot\tau_{\mathrm{CPMG}}}$$

(

)

$$\frac{i}{2}$$

(

)

$$\sqrt{\nu_{1c}^2 - 1}$$

$\approx$

$$\frac{2}{3}$$

(

$)^2$

)

(

$$\frac{m_{D+} + m_{Z+}}{2}$$

$$\sqrt{\frac{p_{\mathrm{B}}}{p_{\mathrm{A}}}}$$

)

$$\frac{\imath k_{\mathrm{ex}}\sqrt{p_{\mathrm{A}}p_{\mathrm{B}}}}{d_{\pm}z_{\pm}}$$

(

$$\frac{\sin(z_{\pm}\delta)}{\sin((d_{\pm}+z_{\pm})\delta)}$$

)

干

(

$$\frac{\sin(d_\pm \delta)}{\sin((d_\pm + z_\pm)\delta)}$$

$\Big)$

(

)

(

)

$$\frac{1}{4\nu_{\mathrm{CPMG}}}$$

$$\frac{\mathbf{M}_A(T_{\mathrm{relax}})}{\mathbf{M}_A(0)}$$

(

$)^n$

$$\begin{pmatrix} -\mathrm{k_{AB}} - \mathrm{R}^0_{2\mathrm{A}} & \mathrm{k_{BA}} \\ \mathrm{k_{AB}} & -\mathrm{k_{BA}} \pm \imath\Delta\omega - \mathrm{R}^0_{2\mathrm{B}} \end{pmatrix}$$

$$\frac{1}{T}$$

{

[

$$\frac{0.5}{p_{\mathrm{A}}}$$

$$\begin{pmatrix} 1 & 0 \end{pmatrix}$$

(

)

$$\begin{pmatrix} p_{\mathrm{A}} \\ p_{\mathrm{B}} \end{pmatrix}$$

]

$$\}$$

$$\begin{pmatrix} -\mathrm{k_{AB}} & \mathrm{k_{BA}} & 0 \\ \mathrm{k_{AB}} & -\mathrm{k_{BA}} - \mathrm{k_{BC}} \pm \imath\Delta\omega_{\mathrm{AB}} & \mathrm{k_{CB}} \\ 0 & \mathrm{k_{BC}} & -\mathrm{k_{CB}} \pm \imath\Delta\omega_{\mathrm{AC}} \end{pmatrix}$$

$$\begin{pmatrix} \mathrm{R}_{2\mathrm{A}}^{0} & 0 & 0 \\ 0 & \mathrm{R}_{2\mathrm{B}}^{0} & 0 \\ 0 & 0 & \mathrm{R}_{2\mathrm{C}}^{0} \end{pmatrix}$$

$$\Bigg\{$$

[

$$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} p_{\mathrm{A}} \\ p_{\mathrm{B}} \\ p_{\mathrm{C}} \end{pmatrix}$$

]

$\}$

$$\begin{pmatrix} -\mathrm{k}_{\mathrm{AB}} - \mathrm{k}_{\mathrm{AC}} & \mathrm{k}_{\mathrm{BA}} & \mathrm{k}_{\mathrm{CA}} \\ \mathrm{k}_{\mathrm{AB}} & -\mathrm{k}_{\mathrm{BA}} - \mathrm{k}_{\mathrm{BC}} \pm \imath\Delta\omega_{\mathrm{AB}} & \mathrm{k}_{\mathrm{CB}} \\ \mathrm{k}_{\mathrm{AC}} & \mathrm{k}_{\mathrm{BC}} & -\mathrm{k}_{\mathrm{CB}} - \mathrm{k}_{\mathrm{CA}} \pm \imath\Delta\omega_{\mathrm{AC}} \end{pmatrix}$$

$$\frac{\Phi_{\mathrm{ex}} k_{\mathrm{ex}}}{k_{\mathrm{ex}}^2 + \omega_{\mathrm{e}}^2}$$

$$\frac{p_A^2 p_B \Delta\omega^2 k_{ex}}{k_{ex}^2 + p_A^2 \Delta\omega^2 + \omega_1^2}$$

(

)

$$\frac{\sin^2\theta p_{\mathrm{A}} p_{\mathrm{B}} \Delta\omega^2 \mathrm{k}_{\mathrm{ex}}}{\omega_{\mathrm{Aeff}}^2 \omega_{\mathrm{Beff}}^2 / \omega_{\mathrm{eff}}^2 + \mathrm{k}_{\mathrm{ex}}^2}$$

(

$$\frac{1}{\gamma}$$

)

$$\frac{\sin^2\hat{\theta} p_\mathrm{A} p_\mathrm{B} \Delta\omega^2 \mathrm{k}_\mathrm{ex}}{\hat{\omega}_\mathrm{Aeff}^2 \hat{\omega}_\mathrm{Beff}^2 / \hat{\omega}_\mathrm{eff}^2 + \mathrm{k}_\mathrm{ex}^2 - 2\sin^2\hat{\theta} p_\mathrm{A} p_\mathrm{B} \Delta\omega^2 + (1-\gamma)\omega_1^2}$$

$$\frac{\sin^2\theta p_A p_B \Delta\omega^2 \mathrm{k_{ex}}}{\omega_{\mathrm{Aeff}}^2 \omega_{\mathrm{Beff}}^2/\omega_{\mathrm{eff}}^2 + \mathrm{k_{ex}^2} - \sin^2\theta p_A p_B \Delta\omega^2 \left(1 + \frac{2\mathrm{k_{ex}^2}\left(p_A \omega_{\mathrm{Aeff}}^2 + p_B \omega_{\mathrm{Beff}}^2\right)}{\omega_{\mathrm{Aeff}}^2 \omega_{\mathrm{Beff}}^2 + \omega_{\mathrm{eff}}^2 \mathrm{k_{ex}^2}}\right)}$$

(

)

$$\begin{pmatrix} \sin\theta \\ 0 \\ \cos\theta \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

(

$$\frac{\omega_1}{\Omega_A}$$

)

$$
\begin{pmatrix}
-\mathrm{R}'_{1\rho} - \mathrm{k_{AB}} & -\delta_A & 0 & \mathrm{k_{BA}} & 0 & 0 \\
\delta_A & -\mathrm{R}'_{1\rho} - \mathrm{k_{AB}} & -\omega_1 & 0 & \mathrm{k_{BA}} & 0 \\
0 & \omega_1 & -\mathrm{R_1} - \mathrm{k_{AB}} & 0 & 0 & \mathrm{k_{BA}} \\
\mathrm{k_{AB}} & 0 & 0 & -\mathrm{R}'_{1\rho} - \mathrm{k_{BA}} & -\delta_B & 0 \\
0 & \mathrm{k_{AB}} & 0 & \delta_B & -\mathrm{R}'_{1\rho} - \mathrm{k_{BA}} & -\omega_1 \\
0 & 0 & \mathrm{k_{AB}} & 0 & \omega_1 & -\mathrm{R_1} - \mathrm{k_{BA}}
\end{pmatrix}
$$

$$\begin{pmatrix} \sin\theta \\ 0 \\ \cos\theta \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} -\mathrm{R}'_{1\rho A} - \mathrm{k}_{\mathrm{AB}} - \mathrm{k}_{\mathrm{AC}} & -\delta_A & 0 & \cdots \\ \delta_A & -\mathrm{R}'_{1\rho A} - \mathrm{k}_{\mathrm{AB}} - \mathrm{k}_{\mathrm{AC}} & -\omega_1 & \cdots \\ 0 & \omega_1 & -\mathrm{R}_{1\mathrm{A}} - \mathrm{k}_{\mathrm{AB}} - \mathrm{k}_{\mathrm{AC}} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \iddots \\ \cdots & -\mathrm{R}'_{1\rho B} - \mathrm{k_{BA}} - \mathrm{k_{BC}} & -\delta_B & 0 & \cdots \\ \cdots & \delta_B & -\mathrm{R}'_{1\rho B} - \mathrm{k_{BA}} - \mathrm{k_{BC}} & -\omega_1 & \cdots \\ \cdots & 0 & \omega_1 & -\mathrm{R_{1B}} - \mathrm{k_{BA}} - \mathrm{k_{BC}} & \cdots \\ \iddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\begin{pmatrix} \ddots & \vdots & \vdots & \vdots \\ \cdots & -\mathrm{R}'_{1\rho C} - \mathrm{k_{CA}} - \mathrm{k_{CB}} & -\delta_C & 0 \\ \cdots & \delta_C & -\mathrm{R}'_{1\rho C} - \mathrm{k_{CA}} - \mathrm{k_{CB}} & -\omega_1 \\ \cdots & 0 & \omega_1 & -\mathrm{R_{1C}} - \mathrm{k_{CA}} - \mathrm{k_{CB}} \end{pmatrix}$$

$$
\begin{pmatrix}
 & & & \mathrm{k_{BA}} & 0 & 0 & \cdots \\
 & \ddots & & 0 & \mathrm{k_{BA}} & 0 & \cdots \\
 & & & 0 & 0 & \mathrm{k_{BA}} & \cdots \\
\mathrm{k_{AB}} & 0 & 0 & & & & \\
0 & \mathrm{k_{AB}} & 0 & & \ddots & & \cdots \\
0 & 0 & \mathrm{k_{AB}} & & & & \\
\vdots & \vdots & \vdots & & \vdots & & \ddots
\end{pmatrix}
$$

$$\begin{pmatrix} & & & \cdots & \mathrm{k_{CA}} & 0 & 0 \\ & \ddots & & \cdots & 0 & \mathrm{k_{CA}} & 0 \\ & & & \cdots & 0 & 0 & \mathrm{k_{CA}} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \mathrm{k_{AC}} & 0 & 0 & \cdots & & & \\ 0 & \mathrm{k_{AC}} & 0 & \cdots & & \ddots & \\ 0 & 0 & \mathrm{k_{AC}} & \cdots & & & \end{pmatrix}$$

$$
\begin{pmatrix}
\ddots & & \vdots & & \vdots & \vdots & \vdots \\
 & & & & \mathrm{k_{CB}} & 0 & 0 \\
\cdots & & \ddots & & 0 & \mathrm{k_{CB}} & 0 \\
 & & & & 0 & 0 & \mathrm{k_{CB}} \\
\cdots & \mathrm{k_{BC}} & 0 & 0 & & & \\
\cdots & 0 & \mathrm{k_{BC}} & 0 & & \ddots & \\
\cdots & 0 & 0 & \mathrm{k_{BC}} & & &
\end{pmatrix}
$$

$$\begin{pmatrix} -\mathrm{R}'_{1\rho A} - \mathrm{k_{AB}} & -\delta_A & 0 & \cdots \\ \delta_A & -\mathrm{R}'_{1\rho A} - \mathrm{k_{AB}} & -\omega_1 & \cdots \\ 0 & \omega_1 & -\mathrm{R_{1A}} - \mathrm{k_{AB}} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\begin{pmatrix} \ddots & \vdots & \vdots & \vdots \\ \cdots & -\mathrm{R}'_{1\rho C} - \mathrm{k_{CB}} & -\delta_C & 0 \\ \cdots & \delta_C & -\mathrm{R}'_{1\rho C} - \mathrm{k_{CB}} & -\omega_1 \\ \cdots & 0 & \omega_1 & -\mathrm{R_{1C}} - \mathrm{k_{CB}} \end{pmatrix}$$

$$\frac{(\mathrm{R}_{2\mathrm{eff}} - \mathrm{R}_{2\mathrm{eff}}(\theta))^2}{\sigma_i^2}$$

$$\begin{pmatrix} \mathrm{R}_2^0 \\ \mathrm{R}_{2\mathrm{A}}^0 \\ \mathrm{R}_{2\mathrm{B}}^0 \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ -200 \\ 0 \\ -200 \\ 0 \\ -200 \end{pmatrix}$$

$$\begin{pmatrix}1&0&0&0&0&0&0&0&0&0\\0&1&0&0&0&0&0&0&0&0\\0&0&1&0&0&0&0&0&0&0\\0&0&0&1&0&0&0&0&0&0\\0&0&0&0&1&0&0&0&0&0\\0&0&0&0&0&1&0&0&0&0\\0&0&0&0&0&0&1&0&0&0\\0&0&0&0&0&0&0&1&0&0\\0&0&0&0&0&0&0&0&1&0\\0&0&0&0&0&0&0&0&0&1\end{pmatrix}$$

$$\begin{pmatrix} \Phi_{\mathrm{ex}} \\ \Phi_{\mathrm{ex,B}} \\ \Phi_{\mathrm{ex,C}} \\ p_{\mathrm{A}}\Delta\omega^2 \\ \Delta\omega \\ \Delta\omega_{\mathrm{AB}} \\ \Delta\omega_{\mathrm{BC}} \\ \Delta\omega^{\mathrm{H}} \\ \Delta\omega^{\mathrm{H}}_{\mathrm{AB}} \\ \Delta\omega^{\mathrm{H}}_{\mathrm{BC}} \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} -1 & 0 \\ 1 & 0 \\ 1 & 0 \\ -1 & -1 \\ 1 & 2 \end{pmatrix}$$

$$\begin{pmatrix} p_{\mathrm{A}} \\ p_{\mathrm{B}} \end{pmatrix}$$

$$\begin{pmatrix} -1 \\ 0.5 \\ 0.85 \\ -1 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} k_{\mathrm{ex}} \\ k_{\mathrm{ex}}^{\mathrm{AB}} \\ k_{\mathrm{ex}}^{\mathrm{BC}} \\ k_{\mathrm{B}} \\ k_{\mathrm{C}} \\ k_{\mathrm{AB}} \\ \tau_{\mathrm{ex}} \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ -2e^6 \\ 0 \\ -2e^6 \\ 0 \\ -2e^6 \\ 0 \\ -2e^6 \\ 0 \\ -2e^6 \\ 0 \\ -100 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix}
10 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 10 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 10 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1e^4 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1e^4 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1e^4 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 20 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1e^{-4}
\end{pmatrix}$$

[

$]^T$

$$\begin{bmatrix} \delta_x^2 & \delta_x\delta_y & \delta_x\delta_z \\ \delta_y\delta_x & \delta_y^2 & \delta_y\delta_z \\ \delta_z\delta_x & \delta_z\delta_y & \delta_z^2 \end{bmatrix}$$

$$\overline{\delta_i \delta_j}$$

$$\begin{bmatrix} S_{xx}(\infty) & S_{xy}(\infty) & S_{xz}(\infty) \\ S_{yx}(\infty) & S_{yy}(\infty) & S_{yz}(\infty) \\ S_{zx}(\infty) & S_{zy}(\infty) & S_{zz}(\infty) \end{bmatrix}$$

$$\begin{bmatrix} c_{xx} & c_{xy} & c_{xz} \\ c_{yx} & c_{yy} & c_{yz} \\ c_{zx} & c_{zy} & c_{zz} \end{bmatrix}$$

$$\begin{bmatrix} \delta_{xx} & \delta_{xy} & \delta_{xz} \\ \delta_{yx} & \delta_{yy} & \delta_{yz} \\ \delta_{zx} & \delta_{zy} & \delta_{zz} \end{bmatrix}$$

$$\overline{R(t) \otimes R(t)}$$

$$\left[\begin{array}{ccc:ccc:ccc}
\delta_{xx}^2 & \delta_{xx}\delta_{xy} & \delta_{xx}\delta_{xz} & \delta_{xy}\delta_{xx} & \delta_{xy}^2 & \delta_{xy}\delta_{xz} & \delta_{xz}\delta_{xx} & \delta_{xz}\delta_{xy} & \delta_{xz}^2 \\
\delta_{xx}\delta_{yx} & \delta_{xx}\delta_{yy} & \delta_{xx}\delta_{yz} & \delta_{xy}\delta_{yx} & \delta_{xy}\delta_{yy} & \delta_{xy}\delta_{yz} & \delta_{xz}\delta_{yx} & \delta_{xz}\delta_{yy} & \delta_{xz}\delta_{yz} \\
\delta_{xx}\delta_{zx} & \delta_{xx}\delta_{zy} & \delta_{xx}\delta_{zz} & \delta_{xy}\delta_{zx} & \delta_{xy}\delta_{zy} & \delta_{xy}\delta_{zz} & \delta_{xz}\delta_{zx} & \delta_{xz}\delta_{zy} & \delta_{xz}\delta_{zz} \\
\hdashline
\delta_{yx}\delta_{xx} & \delta_{yx}\delta_{xy} & \delta_{yx}\delta_{xz} & \delta_{yy}\delta_{xx} & \delta_{yy}\delta_{xy} & \delta_{yy}\delta_{xz} & \delta_{yz}\delta_{xx} & \delta_{yz}\delta_{xy} & \delta_{yz}\delta_{xz} \\
\delta_{yx}^2 & \delta_{yx}\delta_{yy} & \delta_{yx}\delta_{yz} & \delta_{yy}\delta_{yx} & \delta_{yy}^2 & \delta_{yy}\delta_{yz} & \delta_{yz}\delta_{yx} & \delta_{yz}\delta_{yy} & \delta_{yz}^2 \\
\delta_{yx}\delta_{zx} & \delta_{yx}\delta_{zy} & \delta_{yx}\delta_{zz} & \delta_{yy}\delta_{zx} & \delta_{yy}\delta_{zy} & \delta_{yy}\delta_{zz} & \delta_{yz}\delta_{zx} & \delta_{yz}\delta_{zy} & \delta_{yz}\delta_{zz} \\
\hdashline
\delta_{zx}\delta_{xx} & \delta_{zx}\delta_{xy} & \delta_{zx}\delta_{xz} & \delta_{zy}\delta_{xx} & \delta_{zy}\delta_{xy} & \delta_{zy}\delta_{xz} & \delta_{zz}\delta_{xx} & \delta_{zz}\delta_{xy} & \delta_{zz}\delta_{xz} \\
\delta_{zx}\delta_{yx} & \delta_{zx}\delta_{yy} & \delta_{zx}\delta_{yz} & \delta_{zy}\delta_{yx} & \delta_{zy}\delta_{yy} & \delta_{zy}\delta_{yz} & \delta_{zz}\delta_{yx} & \delta_{zz}\delta_{yy} & \delta_{zz}\delta_{yz} \\
\delta_{zx}^2 & \delta_{zx}\delta_{zy} & \delta_{zx}\delta_{zz} & \delta_{zy}\delta_{zx} & \delta_{zy}^2 & \delta_{zy}\delta_{zz} & \delta_{zz}\delta_{zx} & \delta_{zz}\delta_{zy} & \delta_{zz}^2
\end{array}\right]$$

$$\overline{\delta_{ij}\delta_{kl}}$$

$$\overline{c_{ij} c_{kl}}$$

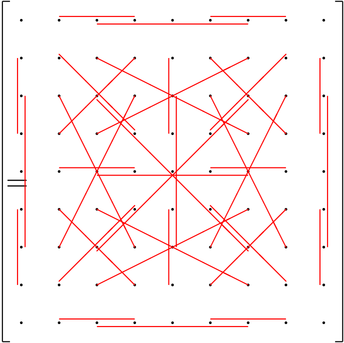
$$
\left[\begin{array}{ccc:ccc:ccc}
\delta_{xx}^2 & \delta_{yx}\delta_{xx} & \delta_{zx}\delta_{xx} & \delta_{xy}\delta_{xx} & \delta_{yy}\delta_{xx} & \delta_{zy}\delta_{xx} & \delta_{xz}\delta_{xx} & \delta_{yz}\delta_{xx} & \delta_{zz}\delta_{xx} \\
\delta_{xx}\delta_{yx} & \delta_{yx}^2 & \delta_{zx}\delta_{yx} & \delta_{xy}\delta_{yx} & \delta_{yy}\delta_{yx} & \delta_{zy}\delta_{yx} & \delta_{xz}\delta_{yx} & \delta_{yz}\delta_{yx} & \delta_{zz}\delta_{yx} \\
\delta_{xx}\delta_{zx} & \delta_{yx}\delta_{zx} & \delta_{zx}^2 & \delta_{xy}\delta_{zx} & \delta_{yy}\delta_{zx} & \delta_{zy}\delta_{zx} & \delta_{xz}\delta_{zx} & \delta_{yz}\delta_{zx} & \delta_{zz}\delta_{zx} \\
\hdashline
\delta_{xx}\delta_{xy} & \delta_{yx}\delta_{xy} & \delta_{zx}\delta_{xy} & \delta_{xy}^2 & \delta_{yy}\delta_{xy} & \delta_{zy}\delta_{xy} & \delta_{xz}\delta_{xy} & \delta_{yz}\delta_{xy} & \delta_{zz}\delta_{xy} \\
\delta_{xx}\delta_{yy} & \delta_{yx}\delta_{yy} & \delta_{zx}\delta_{yy} & \delta_{xy}\delta_{yy} & \delta_{yy}^2 & \delta_{zy}\delta_{yy} & \delta_{xz}\delta_{yy} & \delta_{yz}\delta_{yy} & \delta_{zz}\delta_{yy} \\
\delta_{xx}\delta_{zy} & \delta_{yx}\delta_{zy} & \delta_{zx}\delta_{zy} & \delta_{xy}\delta_{zy} & \delta_{yy}\delta_{zy} & \delta_{zy}^2 & \delta_{xz}\delta_{zy} & \delta_{yz}\delta_{zy} & \delta_{zz}\delta_{zy} \\
\hdashline
\delta_{xx}\delta_{xz} & \delta_{yx}\delta_{xz} & \delta_{zx}\delta_{xz} & \delta_{xy}\delta_{xz} & \delta_{yy}\delta_{xz} & \delta_{zy}\delta_{xz} & \delta_{xz}^2 & \delta_{yz}\delta_{xz} & \delta_{zz}\delta_{xz} \\
\delta_{xx}\delta_{yz} & \delta_{yx}\delta_{yz} & \delta_{zx}\delta_{yz} & \delta_{xy}\delta_{yz} & \delta_{yy}\delta_{yz} & \delta_{zy}\delta_{yz} & \delta_{xz}\delta_{yz} & \delta_{yz}^2 & \delta_{zz}\delta_{yz} \\
\delta_{xx}\delta_{zz} & \delta_{yx}\delta_{zz} & \delta_{zx}\delta_{zz} & \delta_{xy}\delta_{zz} & \delta_{yy}\delta_{zz} & \delta_{zy}\delta_{zz} & \delta_{xz}\delta_{zz} & \delta_{yz}\delta_{zz} & \delta_{zz}^2
\end{array}\right]
$$

$$\begin{bmatrix} \overline{e_x \otimes e_x} & \overline{e_x \otimes e_y} & \overline{e_x \otimes e_z} \\ \overline{e_y \otimes e_x} & \overline{e_y \otimes e_y} & \overline{e_y \otimes e_z} \\ \overline{e_z \otimes e_x} & \overline{e_z \otimes e_y} & \overline{e_z \otimes e_z} \end{bmatrix}$$

$$\overline{e_A \otimes e_B}$$

$$\begin{bmatrix} S_{\mathrm{XX}}(t) & S_{\mathrm{XY}}(t) & S_{\mathrm{XZ}}(t) \\ S_{\mathrm{YX}}(t) & S_{\mathrm{YY}}(t) & S_{\mathrm{YZ}}(t) \\ S_{\mathrm{ZX}}(t) & S_{\mathrm{ZY}}(t) & S_{\mathrm{ZZ}}(t) \end{bmatrix}$$

$$\mathrm{Daeg}^{(2)}(t) =$$



$$\overline{c_{ij} c_{kl}}$$

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\begin{array}{ccc|ccc|ccc}
\overline{\delta_{xx}^2} & \cdot & \cdot & \cdot & \overline{\delta_{xy}^2} & \cdot & \cdot & \cdot & \overline{\delta_{xz}^2} \\
\cdot & \overline{\delta_{xx}\delta_{yy}} & \cdot & \overline{\delta_{xy}\delta_{yx}} & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \overline{\delta_{xx}\delta_{zz}} & \cdot & \cdot & \cdot & \overline{\delta_{xz}\delta_{zx}} & \cdot & \cdot \\
\hline
\cdot & \overline{\delta_{yx}\delta_{xy}} & \cdot & \overline{\delta_{yy}\delta_{xx}} & \cdot & \cdot & \cdot & \cdot & \cdot \\
\overline{\delta_{yx}^2} & \cdot & \cdot & \cdot & \overline{\delta_{yy}^2} & \cdot & \cdot & \cdot & \overline{\delta_{yz}^2} \\
\cdot & \cdot & \cdot & \cdot & \cdot & \overline{\delta_{yy}\delta_{zz}} & \cdot & \overline{\delta_{yz}\delta_{zy}} & \cdot \\
\hline
\cdot & \cdot & \overline{\delta_{zx}\delta_{xz}} & \cdot & \cdot & \cdot & \overline{\delta_{zz}\delta_{xx}} & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \overline{\delta_{zy}\delta_{yz}} & \cdot & \overline{\delta_{zz}\delta_{yy}} & \cdot \\
\overline{\delta_{zx}^2} & \cdot & \cdot & \cdot & \overline{\delta_{zy}^2} & \cdot & \cdot & \cdot & \overline{\delta_{zz}^2}
\end{array}
$$

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$$\frac{1}{3}$$

$\stackrel{\text{def}}{=}$

$$\overline{R^{\otimes n}(t)}$$

$$\overline{R'(t) \otimes R'(t)}$$

$$\overline{A}$$

$$\hat{r}^T$$

$\hat{r}$

$\hat{r}$

$$\frac{3}{2\pi}$$

$$\frac{\gamma_I \gamma_S \hbar}{\langle r \rangle^3}$$

$$\frac{1}{2\pi}$$

$\overline{A}$

$$\frac{15kT}{B_0^2}$$

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$\overline{A}$

$\langle$

$$\int_0^{t_{\max}}$$

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$$\sum_{kl}$$

$$\overline{A_{ij}}$$

$$\overline{c_{ki}c_{lj}}$$

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$$\begin{bmatrix} A_{xx} \\ A_{yy} \\ A_{xy} \\ A_{xz} \\ A_{yz} \end{bmatrix}$$

$$\begin{bmatrix} \mathrm{Daeg}_{xxxx} - \mathrm{Daeg}_{zxzx} & \mathrm{Daeg}_{yxyx} - \mathrm{Daeg}_{zxzx} & \mathrm{Daeg}_{xxyx} + \mathrm{Daeg}_{yxxx} & \mathrm{Daeg}_{xxzx} + \mathrm{Daeg}_{zxxx} & \mathrm{Daeg}_{yxzx} + \mathrm{Daeg}_{zxyx} \\ \mathrm{Daeg}_{xyxy} - \mathrm{Daeg}_{zyzy} & \mathrm{Daeg}_{yyyy} - \mathrm{Daeg}_{zyzy} & \mathrm{Daeg}_{xyyy} + \mathrm{Daeg}_{yyxy} & \mathrm{Daeg}_{xyzy} + \mathrm{Daeg}_{zyxy} & \mathrm{Daeg}_{yyzy} + \mathrm{Daeg}_{zyyy} \\ \mathrm{Daeg}_{xxxy} - \mathrm{Daeg}_{zxzy} & \mathrm{Daeg}_{yxyy} - \mathrm{Daeg}_{zxzy} & \mathrm{Daeg}_{xxyy} + \mathrm{Daeg}_{yxxy} & \mathrm{Daeg}_{xxzy} + \mathrm{Daeg}_{zxxy} & \mathrm{Daeg}_{yxzy} + \mathrm{Daeg}_{zxyy} \\ \mathrm{Daeg}_{xxxz} - \mathrm{Daeg}_{zxzz} & \mathrm{Daeg}_{yxyz} - \mathrm{Daeg}_{zxzz} & \mathrm{Daeg}_{xxyz} + \mathrm{Daeg}_{yxxz} & \mathrm{Daeg}_{xxzz} + \mathrm{Daeg}_{zxxz} & \mathrm{Daeg}_{yxzz} + \mathrm{Daeg}_{zxyz} \\ \mathrm{Daeg}_{xyxz} - \mathrm{Daeg}_{zyzz} & \mathrm{Daeg}_{yyyz} - \mathrm{Daeg}_{zyzz} & \mathrm{Daeg}_{xyyz} + \mathrm{Daeg}_{yyxz} & \mathrm{Daeg}_{xyzz} + \mathrm{Daeg}_{zyxz} & \mathrm{Daeg}_{yyzz} + \mathrm{Daeg}_{zyyz} \end{bmatrix}$$

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$$\begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix}$$

$$\begin{bmatrix} \mathrm{Daeg}_{00} - \mathrm{Daeg}_{80} & \mathrm{Daeg}_{40} - \mathrm{Daeg}_{80} & \mathrm{Daeg}_{10} + \mathrm{Daeg}_{30} & \mathrm{Daeg}_{20} + \mathrm{Daeg}_{60} & \mathrm{Daeg}_{50} + \mathrm{Daeg}_{70} \\ \mathrm{Daeg}_{04} - \mathrm{Daeg}_{84} & \mathrm{Daeg}_{44} - \mathrm{Daeg}_{84} & \mathrm{Daeg}_{14} + \mathrm{Daeg}_{34} & \mathrm{Daeg}_{24} + \mathrm{Daeg}_{64} & \mathrm{Daeg}_{54} + \mathrm{Daeg}_{74} \\ \mathrm{Daeg}_{01} - \mathrm{Daeg}_{81} & \mathrm{Daeg}_{41} - \mathrm{Daeg}_{81} & \mathrm{Daeg}_{11} + \mathrm{Daeg}_{31} & \mathrm{Daeg}_{21} + \mathrm{Daeg}_{61} & \mathrm{Daeg}_{51} + \mathrm{Daeg}_{71} \\ \mathrm{Daeg}_{02} - \mathrm{Daeg}_{82} & \mathrm{Daeg}_{42} - \mathrm{Daeg}_{82} & \mathrm{Daeg}_{12} + \mathrm{Daeg}_{32} & \mathrm{Daeg}_{22} + \mathrm{Daeg}_{62} & \mathrm{Daeg}_{52} + \mathrm{Daeg}_{72} \\ \mathrm{Daeg}_{05} - \mathrm{Daeg}_{85} & \mathrm{Daeg}_{45} - \mathrm{Daeg}_{85} & \mathrm{Daeg}_{15} + \mathrm{Daeg}_{35} & \mathrm{Daeg}_{25} + \mathrm{Daeg}_{65} & \mathrm{Daeg}_{55} + \mathrm{Daeg}_{75} \end{bmatrix}$$

$$\begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix}$$

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$$\frac{c}{|r_i|^5}$$

$$\overline{c_{jj}c_{kk}}$$

$$\overline{c_{jk}c_{kj}}$$

$\mathfrak{D}_i + \mathfrak{D}_j + \mathfrak{D}_k)t$

$$\overline{c_{ii}^2}$$

$$\frac{1}{6}$$

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$$\mathfrak{D}_{iso} - \sqrt{\mathfrak{D}_{iso}^2 - \mathfrak{L}^2}$$

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$$\mathfrak{D}_{iso}+\sqrt{\mathfrak{D}_{iso}^2-\mathfrak{L}^2}$$

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$$\overline{c_{jk}^2}$$

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$$\frac{\mathfrak{D}_i - \mathfrak{D}_{iso}}{\sqrt{\mathfrak{D}_{iso}^2 - \mathfrak{L}^2}}$$

$$\mathfrak{D}_{iso} = \frac{1}{3} \sum_i \mathfrak{D}_i,$$

$$\mathfrak{L}^2 = \frac{1}{3} \sum_{i<j} \mathfrak{D}_i \mathfrak{D}_j,$$

$\mathfrak{D}_i$

$$\frac{\theta'_x + \theta'_y}{2}$$

Condition	Permutation name	Cone half-angles $[\theta'_x, \theta'_y, \sigma'_{\max}]$	Axes $[x', y', z']$
$\theta_x \leq \theta_y \leq \sigma_{\max}$	Self[1]	$[\theta_x, \theta_y, \sigma_{\max}]$	$[x, y, z]$
	A	$[\theta_x, \sigma_{\max}, \theta_y]$	$[-z, y, x]$
	B	$[\theta_y, \sigma_{\max}, \theta_x]$	$[z, x, y]$
$\theta_x \leq \sigma_{\max} \leq \theta_y$	Self[1]	$[\theta_x, \theta_y, \sigma_{\max}]$	$[x, y, z]$
	A	$[\theta_x, \sigma_{\max}, \theta_y]$	$[-z, y, x]$
	B	$[\sigma_{\max}, \theta_y, \theta_x]$	$[x, -z, y]$
$\sigma_{\max} \leq \theta_x \leq \theta_y$	Self[1]	$[\theta_x, \theta_y, \sigma_{\max}]$	$[x, y, z]$
	A	$[\sigma_{\max}, \theta_x, \theta_y]$	$[y, z, x]$
	B	$[\sigma_{\max}, \theta_y, \theta_x]$	$[x, -z, y]$

[1] The first optimised solution.

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\begin{pmatrix} P_x \\ P_y \\ P_z \\ p_x \\ p_y \\ p_z \end{pmatrix}$$

$$\begin{pmatrix} -500 \\ -500 \\ -500 \\ -500 \\ -500 \\ -500 \\ -999 \\ -999 \\ -999 \\ -999 \\ -999 \\ -999 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\begin{pmatrix} \theta \\ \theta_x \\ \theta_y \\ \sigma_{\max} \\ \sigma_{\max,2} \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ -\pi \\ 0 \\ -\pi \\ 0 \\ 0 \\ -\pi \\ 0 \\ -\pi \\ 0 \\ -\pi \end{pmatrix}$$

$$\int$$

$$\sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{N}}$$

$\overline{\delta}$

$$\int_S$$

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$$\mathfrak{T} = \{P_x, P_y, P_z\},$$

$$\mathfrak{O} = \{P_\alpha, P_\beta, P_\gamma\}\,.$$

$$\mathfrak{S} = \{\theta, \theta_x, \theta_y, \sigma_{\max}, \sigma_{\max,2}\} .$$

images/cam_iq_abc_whole_structural_noise-eps-converted-to.pdf

$\mathbb{R}$

$$\min_{\theta}$$

$$\frac{(y_i - y_i(\theta))^2}{\sigma_i^2}$$

$$\begin{pmatrix} \dfrac{\partial}{\partial \theta_1} \\ \dfrac{\partial}{\partial \theta_2} \\ \vdots \\ \dfrac{\partial}{\partial \theta_n} \end{pmatrix}$$

$$\frac{1}{2}$$

$$\begin{pmatrix} \frac{\partial^2}{\partial {\theta_1}^2} & \frac{\partial^2}{\partial \theta_1 \cdot \partial \theta_2} & \cdots & \frac{\partial^2}{\partial \theta_1 \cdot \partial \theta_n} \\ \frac{\partial^2}{\partial \theta_2 \cdot \partial \theta_1} & \frac{\partial^2}{\partial {\theta_2}^2} & \cdots & \frac{\partial^2}{\partial \theta_2 \cdot \partial \theta_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2}{\partial \theta_n \cdot \partial \theta_1} & \frac{\partial^2}{\partial \theta_n \cdot \partial \theta_2} & \cdots & \frac{\partial^2}{\partial {\theta_n}^2} \end{pmatrix}$$

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$$\min_{p \in \mathbb{R}^n}$$

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$$\mathfrak{L}_A(\theta, \lambda^k; \mu_k) \stackrel{\text{def}}{=} f(\theta) + \sum_{i \in \mathfrak{I}} \Psi(c_i(\theta), \lambda_i^k; \mu_k),$$

$$\begin{cases} -\lambda^k c_i(\theta) + \frac{1}{2\mu_k} c_i^2(\theta) & \text{if } c_i(\theta) - \mu_k \lambda^k \leqslant 0, \\ -\frac{\mu_k}{2}(\lambda^k)^2 & \text{otherwise.} \end{cases}$$

$\mathfrak{L}_A$

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$$\mathfrak{L}_A(\theta, \lambda^k; \mu_k) = \nabla f(\theta) - \sum_{i \in \mathfrak{I} | c_i(\theta) \leqslant \mu_k \lambda_i^k} \left(\lambda_i^k - \frac{c_i(\theta)}{\mu_k} \right) \nabla c_i(\theta),$$

$$\mathfrak{L}_A(\theta, \lambda^k; \mu_k) = \nabla^2 f(\theta) + \sum_{i \in \mathfrak{I} | c_i(\theta) \leqslant \mu_k \lambda_i^k} \left[\frac{1}{\mu_k} \nabla c_i^2(\theta) - \left(\lambda_i^k - \frac{c_i(\theta)}{\mu_k} \right) \nabla^2 c_i(\theta) \right].$$

$$\begin{pmatrix} S^2 \\ \tau_e \\ R_{ex} \end{pmatrix}$$

$$\begin{pmatrix} 1 \\ \infty \\ \infty \end{pmatrix}$$

$$\begin{cases} \epsilon \sum_{i=1}^{m} -\log(b_i - A_i^T \theta) & \text{if } A \cdot \theta < b, \\ +\infty & \text{otherwise.} \end{cases}$$

$$\mathfrak{F}_i = k \leqslant 5$$

$$\mathfrak{T}_i = \mathfrak{D}_i \cup \mathfrak{F}_i.$$

$$\mathfrak{T}_i = 1 + k \leqslant 6,$$

$$\mathfrak{G} = \{\mathfrak{D}_{iso}, \mathfrak{D}_a, \mathfrak{D}_r\}$$

D

$$\mathfrak{D} = \mathfrak{G} \cup \mathfrak{O}.$$

$$\mathfrak{D} = 1, \qquad \dim \mathfrak{D} = 4, \qquad \dim \mathfrak{D} = 6,$$

$$\mathfrak{S} = \mathfrak{D} \cup \left(\bigcup_{i=1}^{l} \mathfrak{F}_i \right),$$

$$\mathfrak{S} = \dim \mathfrak{D} + \sum_{i=1}^{l} k_i \leqslant 6 + 5l,$$

$$\sum_{i=1}^{l}$$

$\mathfrak{D}_j$

$$\mathfrak{F}_i^j$$

$\mathfrak{F}_j$

$$\sum_{i=1}^{l}$$

S,

$$\frac{\partial \chi_i^2}{\partial \theta_j}$$

D.

$\mathfrak{D}_k$

$$\mathfrak{F}_i^k$$

$$\mathfrak{F}_l^j$$

$$\mathfrak{F}_l^k$$

$$\frac{1}{\sigma_i^2}$$

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$$\frac{(\gamma_H \gamma_X \hbar)^2}{< r^6 >}$$

$$\frac{\mathrm{d}d}{\mathrm{d}r}$$

$$\frac{3}{2}$$

$$\frac{(\gamma_H \gamma_X \hbar)^2}{< r^7 >}$$

$$\frac{\mathrm{d}^2 d}{\mathrm{d}r^2}$$

$$\frac{21}{2}$$

$$\frac{(\gamma_H \gamma_X \hbar)^2}{< r^8 >}$$

$$\frac{(\omega_X \cdot \Delta\sigma)^2}{3}$$

$$\frac{\mathrm{d}c}{\mathrm{d}\Delta\sigma}$$

$$\frac{2\omega_X^2 \cdot \Delta\sigma}{3}$$

$$\frac{\mathrm{d}^2 c}{\mathrm{d}\Delta\sigma^2}$$

$$\frac{2\omega_X^2}{3}$$

$$\frac{\mathrm{d}R_{ex}}{\mathrm{d}\rho_{ex}}$$

$$\frac{\mathrm{d}^2 R_{ex}}{\mathrm{d}\rho_{ex}^2}$$

$$\frac{\partial J_d^{\mathrm{R}_1}}{\partial \theta_j}$$

$$\frac{\partial J(\omega_H - \omega_X)}{\partial \theta_j}$$

$$\frac{\partial J(\omega_X)}{\partial \theta_j}$$

$$\frac{\partial J(\omega_H + \omega_X)}{\partial \theta_j}$$

$$\frac{\partial^2 J_d^{\mathrm{R}_1}}{\partial\theta_j \cdot \partial\theta_k}$$

$$\frac{\partial^2 J(\omega_H - \omega_X)}{\partial \theta_j \cdot \partial \theta_k}$$

$$\frac{\partial^2 J(\omega_X)}{\partial \theta_j \cdot \partial \theta_k}$$

$$\frac{\partial^2 J(\omega_H + \omega_X)}{\partial \theta_j \cdot \partial \theta_k}$$

$$\frac{\partial J_c^{\mathrm{R}_1}}{\partial \theta_j}$$

$$\frac{\partial^2 J_c^{\mathrm{R}_1}}{\partial\theta_j.\partial\theta_k}$$

$$\frac{\partial J_d^{\mathrm{R}_2}}{\partial \theta_j}$$

$$\frac{\partial J(0)}{\partial \theta_j}$$

$$\frac{\partial J(\omega_H)}{\partial \theta_j}$$

$$\frac{\partial J_c^{\mathrm{R}_2}}{\partial \theta_j}$$

$$\frac{\partial^2 J_c^{\mathrm{R}_2}}{\partial\theta_j \cdot \partial\theta_k}$$

$$\frac{\partial^2 J(0)}{\partial \theta_j \cdot \partial \theta_k}$$

$$\frac{\partial J_d^{\sigma_{\mathrm{NOE}}}}{\partial \theta_j}$$

$$\frac{\partial^2 J_d^{\sigma_{\mathrm{NOE}}}}{\partial \theta_j \cdot \partial \theta_k}$$

$$\frac{(1 - S_f^2)(\tau_f + \tau_i)\tau_f}{(\tau_f + \tau_i)^2 + (\omega \tau_f \tau_i)^2}$$

$$\frac{(S_f^2 - S^2)(\tau_s + \tau_i)\tau_s}{(\tau_s + \tau_i)^2 + (\omega\tau_s\tau_i)^2}$$

$\mathfrak{G}_i$

$$\frac{\partial J(\omega)}{\partial \mathfrak{D}_j}$$

$$\frac{\partial c_i}{\partial \mathfrak{D}_j}$$

$$\frac{\partial J(\omega)}{\partial S^2}$$

$$\frac{1}{1+(\omega\tau_i)^2}$$

$$\frac{(\tau_e + \tau_i)\tau_e}{(\tau_e + \tau_i)^2 + (\omega \tau_e \tau_i)^2}$$

$$\frac{\partial J(\omega)}{\partial \tau_e}$$

$$\frac{(\tau_e + \tau_i)^2 - (\omega \tau_e \tau_i)^2}{\left((\tau_e + \tau_i)^2 + (\omega \tau_e \tau_i)^2\right)^2}$$

$$\frac{\partial^2 J(\omega)}{\partial \mathfrak{D}_j \cdot \partial \mathfrak{D}_k}$$

$$\frac{\partial^2 c_i}{\partial \mathfrak{D}_j \cdot \partial \mathfrak{D}_k}$$

$$\frac{\partial^2 J(\omega)}{\partial \mathfrak{O}_j \cdot \partial S^2}$$

$$\frac{\partial^2 J(\omega)}{\partial \mathfrak{D}_j \cdot \partial \tau_e}$$

$$\frac{\partial^2 J(\omega)}{(\partial S^2)^2}$$

$$\frac{\partial^2 J(\omega)}{\partial S^2 \cdot \partial \tau_e}$$

$$\frac{\partial^2 J(\omega)}{\partial {\tau_e}^2}$$

$$\frac{4}{5}$$

$$\frac{(\tau_e+\tau_i)^3+3\omega^2\tau_i^3\tau_e(\tau_e+\tau_i)-(\omega\tau_i)^4\tau_e^3}{\left((\tau_e+\tau_i)^2+(\omega\tau_e\tau_i)^2\right)^3}$$

$$\frac{(\tau_s + \tau_i)\tau_s}{(\tau_s + \tau_i)^2 + (\omega \tau_s \tau_i)^2}$$

$$\frac{\partial J(\omega)}{\partial S_f^2}$$

$$\frac{(\tau_f + \tau_i)\tau_f}{(\tau_f + \tau_i)^2 + (\omega \tau_f \tau_i)^2}$$

$$\frac{\partial J(\omega)}{\partial \tau_f}$$

$$\frac{(\tau_f + \tau_i)^2 - (\omega \tau_f \tau_i)^2}{\left((\tau_f + \tau_i)^2 + (\omega \tau_f \tau_i)^2\right)^2}$$

$$\frac{\partial J(\omega)}{\partial \tau_s}$$

$$\frac{(\tau_s+\tau_i)^2-(\omega\tau_s\tau_i)^2}{\left((\tau_s+\tau_i)^2+(\omega\tau_s\tau_i)^2\right)^2}$$

$$\frac{\partial^2 J(\omega)}{\partial \mathfrak{D}_j \cdot \partial S_f^2}$$

$$\frac{\partial^2 J(\omega)}{\partial \mathfrak{D}_j \cdot \partial \tau_f}$$

$$\frac{\partial^2 J(\omega)}{\partial \mathfrak{D}_j \cdot \partial \tau_s}$$

$$\frac{\partial^2 J(\omega)}{\partial S^2 \cdot \partial S_f^2}$$

$$\frac{\partial^2 J(\omega)}{\partial S^2 \cdot \partial \tau_f}$$

$$\frac{\partial^2 J(\omega)}{\partial S^2 \cdot \partial \tau_s}$$

$$\frac{\partial^2 J(\omega)}{(\partial S_f^2)^2}$$

$$\frac{\partial^2 J(\omega)}{\partial S_f^2 \cdot \partial \tau_f}$$

$$\frac{\partial^2 J(\omega)}{\partial S_f^2 \cdot \partial \tau_s}$$

$$\frac{\partial^2 J(\omega)}{\partial {\tau_f}^2}$$

$$\frac{(\tau_f+\tau_i)^3+3\omega^2\tau_i^3\tau_f(\tau_f+\tau_i)-(\omega\tau_i)^4\tau_f^3}{\left((\tau_f+\tau_i)^2+(\omega\tau_f\tau_i)^2\right)^3}$$

$$\frac{\partial^2 J(\omega)}{\partial \tau_f \cdot \partial \tau_s}$$

$$\frac{\partial^2 J(\omega)}{\partial {\tau_s}^2}$$

$$\frac{(\tau_s+\tau_i)^3+3\omega^2\tau_i^3\tau_s(\tau_s+\tau_i)-(\omega\tau_i)^4\tau_s^3}{\left((\tau_s+\tau_i)^2+(\omega\tau_s\tau_i)^2\right)^3}$$

$$\frac{S_f^2 \cdot S_s^2}{1 + (\omega \tau_i)^2}$$

$$\frac{S_f^2(1 - S_s^2)(\tau_s + \tau_i)\tau_s}{(\tau_s + \tau_i)^2 + (\omega\tau_s\tau_i)^2}$$

$$\frac{S_s^2}{1 + (\omega \tau_i)^2}$$

$$\frac{(1 - S_s^2)(\tau_s + \tau_i)\tau_s}{(\tau_s + \tau_i)^2 + (\omega \tau_s \tau_i)^2}$$

$$\frac{\partial J(\omega)}{\partial S_s^2}$$

$$\frac{\partial^2 J(\omega)}{\partial \mathfrak{D}_j \cdot \partial S_s^2}$$

$$\frac{\partial^2 J(\omega)}{\partial S_f^2 \cdot \partial S_s^2}$$

$$\frac{\partial^2 J(\omega)}{(\partial S_s^2)^2}$$

$$\frac{\partial^2 J(\omega)}{\partial S_s^2 \cdot \partial \tau_f}$$

$$\frac{\partial^2 J(\omega)}{\partial S_s^2 \cdot \partial \tau_s}$$

$$\sum_{i=-2}^{2}$$

$$\frac{\tau}{\tau_i}$$

$$\mathfrak{G} = \{\mathfrak{D}_{iso}, \mathfrak{D}_a, \mathfrak{D}_r\},$$

$$\mathfrak{O} = \{\alpha, \beta, \gamma\}.$$

$$\mathfrak{D}_r)\left(\delta_x^4+2\delta_y^2\delta_z^2\right)+\left(1-3\mathfrak{D}_r\right)\left(\delta_y^4+2\delta_x^2\delta_z^2\right)-2\left(\delta_z^4+2\delta_x^2\delta_y^2\right)\Bigg].$$

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$$\frac{\partial e}{\partial \mathfrak{D}_i}$$

[

$$\mathfrak{D}_r)\left(\delta_x^3\frac{\partial\delta_x}{\partial\mathfrak{O}_i}+\delta_y\delta_z\left(\delta_y\frac{\partial\delta_z}{\partial\mathfrak{O}_i}+\delta_z\frac{\partial\delta_y}{\partial\mathfrak{O}_i}\right)\right)$$

$$\mathfrak{D}_r)\left(\delta_y^3\frac{\partial\delta_y}{\partial\mathfrak{O}_i}+\delta_x\delta_z\left(\delta_x\frac{\partial\delta_z}{\partial\mathfrak{O}_i}+\delta_z\frac{\partial\delta_x}{\partial\mathfrak{O}_i}\right)\right)$$

(

$$\frac{\partial \delta_z}{\partial \mathfrak{D}_i}$$

(

$$\frac{\partial \delta_y}{\partial \mathfrak{D}_i}$$

$$\frac{\partial \delta_x}{\partial \mathfrak{D}_i}$$

)

)

]

$$\frac{\partial e}{\partial \mathfrak{D}_r}$$

$$\frac{1}{\mathfrak{R}^3}$$

$$\mathfrak{D}_r)\left(\delta_x^4+2\delta_y^2\delta_z^2\right)-(1+\mathfrak{D}_r)\left(\delta_y^4+2\delta_x^2\delta_z^2\right)+2\mathfrak{D}_r\left(\delta_z^4+2\delta_x^2\delta_y^2\right)\Bigg].$$

$$\frac{\partial^2 e}{\partial \mathfrak{D}_i \cdot \partial \mathfrak{D}_j}$$

$$\mathfrak{D}_r)\left(\delta_x^2\left(\delta_x\frac{\partial^2\delta_x}{\partial\mathfrak{O}_i\cdot\partial\mathfrak{O}_j}+3\frac{\partial\delta_x}{\partial\mathfrak{O}_i}\cdot\frac{\partial\delta_x}{\partial\mathfrak{O}_j}\right)\right.$$

(

$$\frac{\partial^2 \delta_z}{\partial \mathfrak{D}_i \cdot \partial \mathfrak{D}_j}$$

$$\frac{\partial \delta_z}{\partial \mathfrak{D}_j}$$

)

(

$$\frac{\partial^2 \delta_y}{\partial \mathfrak{D}_i \cdot \partial \mathfrak{D}_j}$$

$$\frac{\partial \delta_y}{\partial \mathfrak{D}_j}$$

)

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$$\mathfrak{D}_r)\left(\delta_y^2\left(\delta_y\frac{\partial^2\delta_y}{\partial\mathfrak{D}_i\cdot\partial\mathfrak{D}_j}+3\frac{\partial\delta_y}{\partial\mathfrak{D}_i}\cdot\frac{\partial\delta_y}{\partial\mathfrak{D}_j}\right)\right.$$

$\Bigg($

$$\frac{\partial^2 \delta_x}{\partial \mathfrak{D}_i \cdot \partial \mathfrak{D}_j}$$

$$\frac{\partial \delta_x}{\partial \mathfrak{D}_j}$$

$\Big)$

$\Bigg($

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$$\frac{\partial^2 e}{\partial \mathfrak{D}_i \cdot \partial \mathfrak{D}_r}$$

$$\mathfrak{D}_r \left(\delta_z^3 \frac{\partial \delta_z}{\partial \mathfrak{D}_i} + \delta_x \delta_y \left(\delta_x \frac{\partial \delta_y}{\partial \mathfrak{D}_i} + \delta_y \frac{\partial \delta_x}{\partial \mathfrak{D}_i} \right) \right)$$

$$\frac{\partial^2 e}{\partial \mathfrak{D}_r^2}$$

$$\frac{1}{\mathfrak{R}^5}$$

$$\mathfrak{D}_r^2 - 9\mathfrak{D}_r - 1)\left(\delta_x^4 + 2\delta_y^2\delta_z^2\right)$$

$$\mathfrak{D}_r^2 + 9\mathfrak{D}_r - 1)\left(\delta_y^4 + 2\delta_x^2\delta_z^2\right)$$

$$\mathfrak{D}_r^2 - 1)\left(\delta_z^4 + 2\delta_x^2\delta_y^2\right)$$

]

$$\sum_{i=-1}^{1}$$

$$\widehat{XH}$$

$\widehat{\mathfrak{D}}_z$

$$\mathfrak{G} = \{\mathfrak{D}_{iso}, \mathfrak{D}_a\},$$

$$\mathfrak{D} = \{\theta, \phi\}.$$

$$\frac{\tau}{\tau_m}$$

$$\sum_{i=0}^{0}$$

$$\mathfrak{D} = \{\tau_m\}.$$

$$\frac{\partial c_0}{\partial \tau_m}$$

$$\frac{\partial^2 c_0}{\partial {\tau_m}^2}$$

$$\frac{\partial \tau_0}{\partial \tau_m}$$

$$\frac{\partial^2 \tau_0}{\partial {\tau_m}^2}$$

$$\widehat{\mathfrak{D}}_i$$

$$\widehat{XH}$$

$$\widehat{\mathfrak{D}}_i$$

$$\frac{\partial \delta_i}{\partial \mathfrak{D}_j}$$

$$\frac{\partial}{\partial \mathfrak{D}_j}$$

(

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$$\frac{\partial \widehat{\mathfrak{D}_i}}{\partial \mathfrak{D}_j}$$

$$\frac{\partial \widehat{XH}}{\partial \mathfrak{O}_j}$$

$$\widehat{\mathfrak{D}}_x$$

$$\widehat{\mathfrak{D}}_y$$

$\widehat{\mathfrak{D}}_z$

$$\frac{\partial^2 \delta_i}{\partial \mathfrak{D}_j \cdot \partial \mathfrak{D}_k}$$

$$\frac{\partial^2}{\partial \mathfrak{D}_j \cdot \partial \mathfrak{D}_k}$$

$$\frac{\partial^2 \widehat{\mathfrak{D}_i}}{\partial \mathfrak{D}_j \cdot \partial \mathfrak{D}_k}$$

$\widehat{\mathfrak{D}}_{\|}$

$$\widehat{\mathfrak{D}}_{\|}$$

$$\begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}$$

$$\frac{\partial}{\partial \mathfrak{D}_i}$$

(

)

$$\frac{\partial \widehat{\mathfrak{D}_{\parallel}}}{\partial \mathfrak{O}_i}$$

$$\frac{\partial \widehat{XH}}{\partial \mathfrak{O}_i}$$

$$\frac{\partial^2}{\partial \mathfrak{D}_i \cdot \partial \mathfrak{D}_j}$$

$$\frac{\partial^2 \widehat{\mathfrak{D}_\parallel}}{\partial \mathfrak{D}_i \cdot \partial \mathfrak{D}_j}$$

$$\mathfrak{M} = \mathfrak{P} = \{P_x, P_y, P_z, P_\alpha, P_\beta, P_\gamma\},$$

$$\begin{pmatrix} 1 & . & . \\ . & 1 & . \\ . & . & 1 \end{pmatrix}$$

$\{$

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$$\mathfrak{p}_1 = \{p_x, p_y, p_z\}$$

$\mathfrak{p}_1$

$$\hat{r}_{ax}$$

|

$$\hat{r}_{\mathrm{CoM}-\mathfrak{p}_1}$$

$\hat{z}$

$$\hat{r}_{ax}$$

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$$\begin{pmatrix} \cos\sigma & -\sin\sigma & 0 \\ \sin\sigma & \cos\sigma & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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$$\begin{pmatrix}
\frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \cdot \\
\cdot & \frac{1}{2} & \cdot & -\frac{1}{2} & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & -\frac{1}{2} & \cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \cdot & \cdot \\
\frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1
\end{pmatrix}$$

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$$\frac{x^2}{a^2}$$

$$\frac{y^2}{b^2}$$

$$\frac{z^2}{c^2}$$

$$\frac{1}{\theta_{\max}^2}$$

$$\frac{\cos^2 \phi}{\theta_x^2}$$

$$\frac{\sin^2 \phi}{\theta_y^2}$$

images/pseudo_elliptic_cone-eps-converted-

$$\int_{-\sigma_{\max}}^{\sigma_{\max}}$$

$$\int_{-\pi}^{\pi}$$

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$$\int_{-\sigma_{\max}}^{\sigma_{\max}}$$

$$\int_{-\pi}^{\pi}$$

$\Bigg($

(

$$\frac{1}{\sqrt{\frac{\cos^2\phi}{\theta_x^2}+\frac{\sin^2\phi}{\theta_y^2}}}$$

$\Bigg)$

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$$\frac{{\theta_{\max}}^2}{2!}$$

$$\frac{{\theta_{\max}}^4}{4!}$$

$$\frac{{\theta_{\max}}^6}{6!}$$

$$\frac{{\theta_{\max}}^{8}}{8!}$$

$$\frac{{\theta_{\max}}^{10}}{10!}$$

$$\sum_{n=0}^{\infty}$$

$$\frac{(-1)^n}{(2n)!}$$

$$\frac{\pi \theta_x \theta_y}{24}$$

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$$\frac{\pi\theta_x\theta_y}{2880}$$

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$$\frac{\pi\theta_x\theta_y}{322560}$$

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$$\frac{\pi \theta_x \theta_y}{232243200}$$

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images/pec_y-eps-converted-to.

images/pec_diag-eps-converted-

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$$\begin{pmatrix} \cos^2\phi\cos\theta + \sin^2\phi & \cos\phi\sin\phi\cos\theta - \cos\phi\sin\phi & \cos\phi\sin\theta \\ \cos\phi\sin\phi\cos\theta - \cos\phi\sin\phi & \sin^2\phi\cos\theta + \cos^2\phi & \sin\phi\sin\theta \\ -\cos\phi\sin\theta & -\sin\phi\sin\theta & \cos\theta \end{pmatrix}$$

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$$\int_{-\sigma_{\max,2}}^{\sigma_{\max,2}}$$

$$\int_{-\sigma_{\max,1}}^{\sigma_{\max,1}}$$

$$\begin{pmatrix} \operatorname{sinc}\sigma_{\max,1} & . & . \\ . & \operatorname{sinc}\sigma_{\max,2} & . \\ . & . & \operatorname{sinc}\sigma_{\max,1}\operatorname{sinc}\sigma_{\max,2} \end{pmatrix}$$

Data type	String	Description
S^2.	's2'	The standard model-free order parameter, equal to S^2_f.S2s for the two timescale models. The default colour gradient starts at 'yellow' and ends at 'red'.
S^2_f.	's2f'	The order parameter of the faster of two internal motions. Residues which are described by model-free models m1 to m4, the single timescale models, are illustrated as white neon bonds. The default colour gradient is the same as that for the S^2 data type.
S^2_s.	's2s'	The order parameter of the slower of two internal motions. This functions exactly as S^2_f except that S^2_s is plotted instead.
Amplitude of fast motions.	'amp_fast'	Model independent display of the amplite of fast motions. For residues described by model-free models m5 to m8, the value plotted is that of S^2_f. However, for residues described by models m1 to m4, what is shown is dependent on the timescale of the motions. This is because these single timescale models can, at times, be perfect approximations to the more complex two timescale models. Hence if τ_e is less than 200 ps, S^2 is plotted. Otherwise the peptide bond is coloured white. The default colour gradient is the same as that for S^2.
Amplitude of slow motions.	'amp_slow'	Model independent display of the amplite of slow motions, arbitrarily defined as motions slower than 200 ps. For residues described by model-free models m5 to m8, the order parameter S^2 is plotted if $\tau_s > 200$ ps. For models m1 to m4, S^2 is plotted if $\tau_e > 200$ ps. The default colour gradient is the same as that for S^2.
τ_e.	'te'	The correlation time, τ_e. The default colour gradient starts at 'turquoise' and ends at 'blue'.
τ_f.	'tf'	The correlation time, τ_f. The default colour gradient is the same as that of τ_e.
τ_s.	'ts'	The correlation time, τ_s. The default colour gradient starts at 'blue' and ends at 'black'.
Timescale of fast motions	'time_fast'	Model independent display of the timescale of fast motions. For models m5 to m8, only the parameter τ_f is plotted. For models m2 and m4, the parameter τ_e is plotted only if it is less than 200 ps. All other residues are assumed to have a correlation time of zero. The default colour gradient is the same as that of τ_e.
Timescale of slow motions	'time_slow'	Model independent display of the timescale of slow motions. For models m5 to m8, only the parameter τ_s is plotted. For models m2 and m4, the parameter τ_e is plotted only if it is greater than 200 ps. All other residues are coloured white. The default colour gradient is the same as that of τ_s.
Chemical exchange	'rex'	The chemical exchange, R_{ex}. Residues which experience no chemical exchange are coloured white. The default colour gradient starts at 'yellow' and finishes at 'red'.

Value	Param	Description
None	None	This case is used to set the model parameters prior to minimisation or calculation. The model parameters are set to the default values.
1	None	Invalid combination.
n	None	This case is used to set the model parameters prior to minimisation or calculation. The length of the val array must be equal to the number of model parameters. The parameters will be set to the corresponding number.
None	1	The parameter matching the string will be set to the default value.
1	1	The parameter matching the string will be set to the supplied number.
n	1	Invalid combination.
None	n	Each parameter matching the strings will be set to the default values.
1	n	Each parameter matching the strings will be set to the supplied number.
n	n	Each parameter matching the strings will be set to the corresponding number. Both arrays must be of equal length.