

\mathfrak{D}_{ratio}



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

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



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

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







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

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

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

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

$$\frac{\sigma_{\text{NOE}}(\theta)}{R_1(\theta)}$$

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



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

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

















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

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





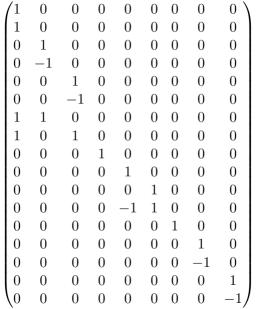






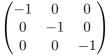






$$\begin{pmatrix} S^2 \\ S_f^2 \\ S_s^2 \\ \tau_e \\ \tau_f \\ \tau_s \\ R_{ex} \\ r \\ CSA \end{pmatrix}$$





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

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



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



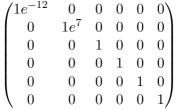




$$\begin{pmatrix} \tau_m \\ \mathfrak{D}_a \\ \mathfrak{D}_r \end{pmatrix}$$



/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	$1e^{-4}$



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





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

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

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





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



$$\frac{U}{\sum_{i} \text{NOE}^2}$$

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



$$M_A^+(t)$$

 $M_B^+(t)$





$$-i\Omega_A - R_{2A}^0 - p_B k_{ex} \qquad p_A k_{ex}$$

$$p_B k_{ex} \qquad -i\Omega_B - R_{2B}^0 - p_A k_{ex}$$



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



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



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



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

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



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





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



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



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

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



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



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



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

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



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



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













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



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



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



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

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

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













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





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

$$\sqrt{rac{p_{
m B}}{p_{
m A}}}$$



$$\frac{i k_{\rm ex} \sqrt{p_{\rm A} p_{\rm B}}}{d_{\pm} z_{\pm}}$$



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



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

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

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

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





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















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

$$\begin{pmatrix} R_{2A}^0 & 0 & 0 \\ 0 & R_{2B}^0 & 0 \\ 0 & 0 & R_{2C}^0 \end{pmatrix}$$





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



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

$$\frac{p_{\rm A}^2 p_{\rm B} \Delta \omega^2 k_{\rm ex}}{k_{\rm ex}^2 + p_{\rm A}^2 \Delta \omega^2 + \omega_1^2}$$





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



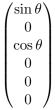


$$\frac{\sin^2\hat{\theta}p_{\rm A}p_{\rm B}\Delta\omega^2k_{\rm ex}}{\hat{\omega}_{\rm Aeff}^2\hat{\omega}_{\rm Beff}^2/\hat{\omega}_{\rm eff}^2+k_{\rm ex}^2-2\sin^2\hat{\theta}p_{\rm A}p_{\rm B}\Delta\omega^2+(1-\gamma)\omega_1^2}$$



$$\frac{\sin^2\theta p_{\rm A}p_{\rm B}\Delta\omega^2 k_{\rm ex}}{\omega_{\rm Aeff}^2\omega_{\rm Beff}^2/\omega_{\rm eff}^2 + k_{\rm ex}^2 - \sin^2\theta p_{\rm A}p_{\rm B}\Delta\omega^2 \left(1 + \frac{2k_{\rm ex}^2(p_{\rm A}\omega_{\rm Aeff}^2 + p_{\rm B}\omega_{\rm Beff}^2)}{\omega_{\rm Aeff}^2\omega_{\rm Beff}^2 + \omega_{\rm eff}^2k_{\rm ex}^2}\right)}$$

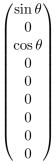






$$\frac{\omega_1}{\Omega_{\rm A}}$$

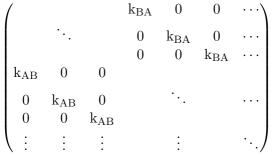
$$\begin{pmatrix} -R'_{1\rho} - k_{AB} & -\delta_A & 0 & k_{BA} & 0 & 0 \\ \delta_A & -R'_{1\rho} - k_{AB} & -\omega_1 & 0 & k_{BA} & 0 \\ 0 & \omega_1 & -R_1 - k_{AB} & 0 & 0 & k_{BA} \\ k_{AB} & 0 & 0 & -R'_{1\rho} - k_{BA} & -\delta_B & 0 \\ 0 & k_{AB} & 0 & \delta_B & -R'_{1\rho} - k_{BA} & -\omega_1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



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

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

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



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

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

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

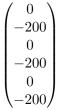
$$\begin{pmatrix}
\cdot & \vdots & \vdots & \vdots \\
\cdot & \cdot & -R'_{1\rho C} - k_{CB} & -\delta_{C} & 0 \\
\cdot & \cdot & \delta_{C} & -R'_{1\rho C} - k_{CB} & -\omega_{1} \\
\cdot & \cdot & 0 & \omega_{1} & -R_{1C} - k_{CB}
\end{pmatrix}$$

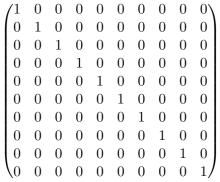
$$\frac{(R_{2eff} - R_{2eff}(\theta))^2}{\sigma_i^2}$$



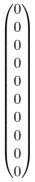








$$\begin{pmatrix} \Phi_{\rm ex} \\ \Phi_{\rm ex,B} \\ \Phi_{\rm ex,C} \\ p_{\rm A}\Delta\omega^2 \\ \Delta\omega \\ \Delta\omega_{\rm AB} \\ \Delta\omega_{\rm BC} \\ \Delta\omega^{\rm H} \\ \Delta\omega_{\rm AB}^{\rm H} \\ \Delta\omega_{\rm AB}^{\rm H} \end{pmatrix}$$





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



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

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



/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
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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
$\int 0$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	$1e^{-4}$





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



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

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

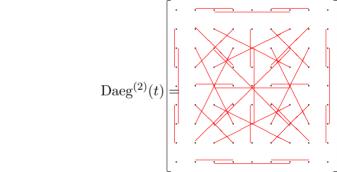
$$\begin{bmatrix} \delta_{xx} & \delta_{xy} & \delta_{xz} \\ \delta_{yx} & \delta_{yy} & \delta_{yz} \\ \delta_{zx} & \delta_{zy} & \delta_{zz} \end{bmatrix}$$

$$\begin{bmatrix} \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} \\ \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_{xx} & \delta_{yz}\delta_{yy} & \delta_{yz}^2 \\ \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}\delta_{yy} & \delta_{zy}\delta_{zz} & \delta_{zz}\delta_{zx} & \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}\delta_{zz} & \delta_{zy}\delta_{zz} & \delta_{zz}\delta_{zx} & \delta_{zz}\delta_{zy} & \delta_{zz}\delta_{zz} \end{bmatrix}$$

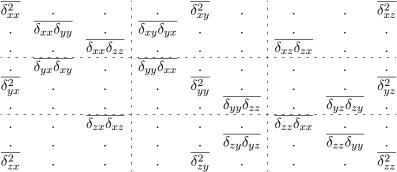
$$\begin{bmatrix} \delta_{xx}^2 & \delta_{yx}\delta_{xx} & \delta_{zx}\delta_{xx} & \delta_{xy}\delta_{xx} & \delta_{yy}\delta_{xx} & \delta_{zy}\delta_{xx} & \delta_{xz}\delta_{xx} & \delta_{yz}\delta_{xx} & \delta_{zz}\delta_{xx} \\ \delta_{xx}\delta_{yx} & \delta_{yx}^2 & \delta_{zx}\delta_{yx} & \delta_{xy}\delta_{yx} & \delta_{yy}\delta_{yx} & \delta_{zy}\delta_{yx} & \delta_{xz}\delta_{yx} & \delta_{yz}\delta_{xx} & \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} \\ \delta_{xx}\delta_{xy} & \delta_{yx}\delta_{xy} & \delta_{zx}\delta_{xy} & \delta_{zy}\delta_{xy} & \delta_{zy}\delta_{xy} & \delta_{zy}\delta_{xy} & \delta_{zz}\delta_{xy} \\ \delta_{xx}\delta_{yy} & \delta_{yx}\delta_{yy} & \delta_{zx}\delta_{yy} & \delta_{xy}\delta_{yy} & \delta_{zy}^2 & \delta_{zy}\delta_{yy} & \delta_{xz}\delta_{yy} & \delta_{yz}\delta_{yy} & \delta_{zz}\delta_{yy} \\ \delta_{xx}\delta_{yy} & \delta_{yx}\delta_{yy} & \delta_{zx}\delta_{zy} & \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_{xz} & \delta_{yx}\delta_{zy} & \delta_{zx}\delta_{zy} & \delta_{xy}\delta_{xz} & \delta_{yy}\delta_{xz} & \delta_{zy}\delta_{xz} & \delta_{xz}\delta_{yz} & \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_{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_{zz}\delta_{zz} & \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_{zz}\delta_{zz} & \delta_{zz}\delta_{zz} \end{bmatrix}$$

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

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





















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



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



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

























$\left\lceil \text{Daeg}_{xxxx} - \text{Daeg}_{zxzx} \right\rceil$	$Daeg_{yxyx} - Daeg_{zxzx}$	$Daeg_{xxyx} + Daeg_{yxxx}$	$Daeg_{xxzx} + Daeg_{zxxx}$	$Daeg_{yxzx} + Daeg_{zxyx}$
		$Daeg_{xyyy} + Daeg_{yyxy}$		
		$Daeg_{xxyy} + Daeg_{yxxy}$		
		$Daeg_{xxyz} + Daeg_{yxxz}$		
				$Daeg_{yyzz} + Daeg_{zyyz}$



$\lceil \text{Daeg}_{00} - \text{Daeg}_{80} \rceil$	$Daeg_{40} - Daeg_{80}$	$Daeg_{10} + Daeg_{30}$	$Daeg_{20} + Daeg_{60}$	$Daeg_{50} + Daeg_{70}$
	$Daeg_{44} - Daeg_{84}$			
	$Daeg_{41} - Daeg_{81}$			
	$Daeg_{42} - Daeg_{82}$			
				$Daeg_{55} + Daeg_{75}$













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













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



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



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

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

$$\mathfrak{D}_{iso} = \frac{1}{3} \sum_{i} \mathfrak{D}_{i},$$

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







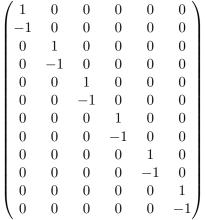
$$\frac{x}{2}$$

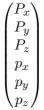
Condition	Permutation name	Cone half-angles	Axes
		$[heta_x', heta_y',\sigma_{ ext{max}}']$	[x', y', z']
$\theta_x \le \theta_y \le \sigma_{\max}$	Self^1	$[\theta_x, \theta_y, \sigma_{\max}]$	[x, y, z]
	\mathbf{A}	$[heta_x, \sigma_{ ext{max}}, heta_y]$	[-z, y, x]
	В	$[heta_y, \sigma_{ ext{max}}, heta_x]$	[z, x, y]
$\theta_x \le \sigma_{\max} \le \theta_y$	Self^1	$[\theta_x, \theta_y, \sigma_{\max}]$	[x,y,z]
	\mathbf{A}	$[\theta_x, \sigma_{\max}, \theta_y]$	[-z, y, x]
	В	$[\sigma_{ ext{max}}, heta_y, heta_x]$	[x, -z, y]
$\sigma_{\max} \le \theta_x \le \theta_y$	$\mathrm{Self^1}$	$[heta_x, heta_y, \sigma_{ ext{max}}]$	[x,y,z]
	\mathbf{A}	$[\sigma_{ ext{max}}, heta_x, heta_y]$	[y,z,x]
	В	$[\sigma_{\max}, heta_y, heta_x]$	[x,-z,y]
¹ The first optimised solution.			





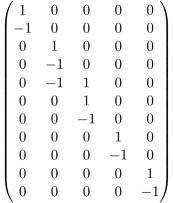




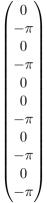


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$$\begin{pmatrix} \theta \\ \theta_x \\ \theta_y \\ \sigma_{\text{max}} \\ \sigma_{\text{max},2} \end{pmatrix}$$



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









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

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







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



images/cam_iq_abc_whole_structural_noise-eps-converted-to.pd





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

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

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



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

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

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

$$\mathfrak{L}_{A}(\theta, \lambda^{k}; \mu_{k}) = \nabla^{2} f(\theta) + \sum_{i \in \mathfrak{I} | c_{i}(\theta) \leqslant \mu_{k} \lambda_{i}^{k}} \left[\frac{1}{\mu_{k}} \nabla c_{i}^{2}(\theta) - \left(\lambda_{i}^{k} - \frac{c_{i}(\theta)}{\mu_{k}} \right) \nabla^{2} c_{i}(\theta) \right].$$

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



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

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

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

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

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

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

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

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

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

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



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

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





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







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

$$\frac{\left(\gamma_H \gamma_X \hbar\right)^2}{\langle r^7 \rangle}$$

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

$$\frac{\left(\gamma_H \gamma_X \hbar\right)^2}{\langle r^8 \rangle}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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



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

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



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

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

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

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

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

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

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









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

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

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

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

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

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

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

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



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

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

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

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

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

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

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















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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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





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

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

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

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

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

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



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

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

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



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



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

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



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



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

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









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

$$\frac{1}{\Re^3}$$

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











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

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



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

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



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

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





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



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

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











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

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













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

$$\frac{1}{\Re^5}$$

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

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

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



















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

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

















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

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

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

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

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



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

$$rac{\partial}{\partial \mathfrak{O}_j}$$



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

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









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

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

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











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

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



$$\frac{\partial \widehat{\mathfrak{D}_{\parallel}}}{\partial \mathfrak{D}_{i}}$$

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



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

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



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

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







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



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





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



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

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

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

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

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

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

images/pseudo_elliptic_cone-eps-converted-



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



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

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





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





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

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

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

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

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

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

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

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





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



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





images/pec_y-eps-converted-to.

images/pec_diag-eps-converted-



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









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

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







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



Data type	String	Description
S^2 .	's2'	The standard model-free order parameter, equal to S_f^2 .S2s for the two timescale models. The default colour gradient starts at 'yellow' and ends at 'red'.
S_f^2 .	'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_s^2 .	's2s'	The order parameter of the slower of two internal motions. This functions exactly as S_f^2
Amplitude of fast motions.	'amp_fast'	except that S_s^2 is plotted instead. 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_f^2 . However, for residues described by mod-
Amplitude of slow motions.	'amp_slow'	els 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 . 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 .
$ au_e$.	'te'	The correlation time, τ_e . The default colour gradient starts at 'turquoise' and ends at 'blue'.
$ au_f$.	'tf'	The correlation time, τ_f . The default colour gradient is the same as that of τ_e .
$ au_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.