



Corrigendum

A new approach for applying residual dipolar couplings as restraints in structure elucidation

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Several errors occurred in Equations 3 and 4 of this paper. The correct equations are printed below:

$$\cos \varphi^{ij} = \begin{pmatrix} \cos \alpha^i \sin \beta^i \\ \sin \alpha^i \sin \beta^i \\ \cos \beta^i \end{pmatrix}^T \begin{pmatrix} \cos \alpha^j \sin \beta^j \\ \sin \alpha^j \sin \beta^j \\ \cos \beta^j \end{pmatrix} \quad (3)$$

Applying Equation 2 to Equation 3 one can eliminate two angles β^i , β^j and arrive at:

$$\begin{aligned} \cos \varphi^{ij} = & \frac{2(3D^i - 2D_{zz} + D_{xx} + D_{yy})}{\sqrt{3(\frac{3}{2}(D_{xx} - D_{yy}) \cos \alpha^i - 2D_{zz} + D_{xx} + D_{yy})}} \\ & \frac{2(3D^j - 2D_{zz} + D_{xx} + D_{yy})}{\sqrt{3(\frac{3}{2}(D_{xx} - D_{yy}) \cos \alpha^j - 2D_{zz} + D_{xx} + D_{yy})}} \\ & \cos(\alpha^j \pm \alpha^i) \quad (4) \\ \pm & \sqrt{1 - \frac{2(3D^i - 2D_{zz} + D_{xx} + D_{yy})}{3(\frac{3}{2}(D_{xx} - D_{yy}) \cos \alpha^i - 2D_{zz} + D_{xx} + D_{yy})}} \\ & \sqrt{1 - \frac{2(3D^j - 2D_{zz} + D_{xx} + D_{yy})}{3(\frac{3}{2}(D_{xx} - D_{yy}) \cos \alpha^j - 2D_{zz} + D_{xx} + D_{yy})}} \end{aligned}$$