Essentials of Tensor Transformation and Vectorization

General objective: Build a toolkit for tensor manipulation and inversion.

$$\vec{\beta}'^{new} = \boldsymbol{R}_{\phi} \cdot \vec{\beta}'^{old}$$

Specific Objectives:

1. Introduce several useful theorems for tensor manipulation
2. Derive an expression for the molecular tensor in a rotated reference frame.
3. Derive an expression for the vectorized molecular tensor in a rotated reference frame.

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Note: Citations to the contents of these slides should reference the following textbook:
Simpson, Garth J. (2017) *Nonlinear Optical Polarization Analysis in Chemistry and Biology* (Cambridge University Press, ISBN 978-0-521-51908-3).

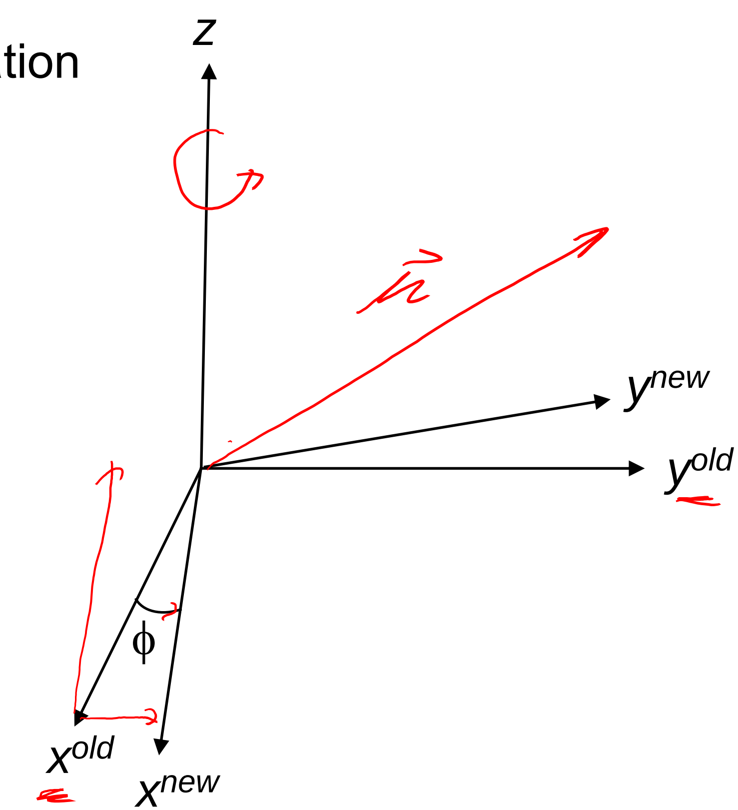
Vector Properties

Let’s introduce a general toolkit by considering a specific problem. How de we describe our molecular tensor in a new coordinate system?

We’ll start by considering azimuthal rotation of a vector.*

$$\vec{\mu}^{new} = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \vec{\mu}^{old}$$

$$\vec{\mu}^{new} = R_\phi \cdot \vec{\mu}^{old}$$



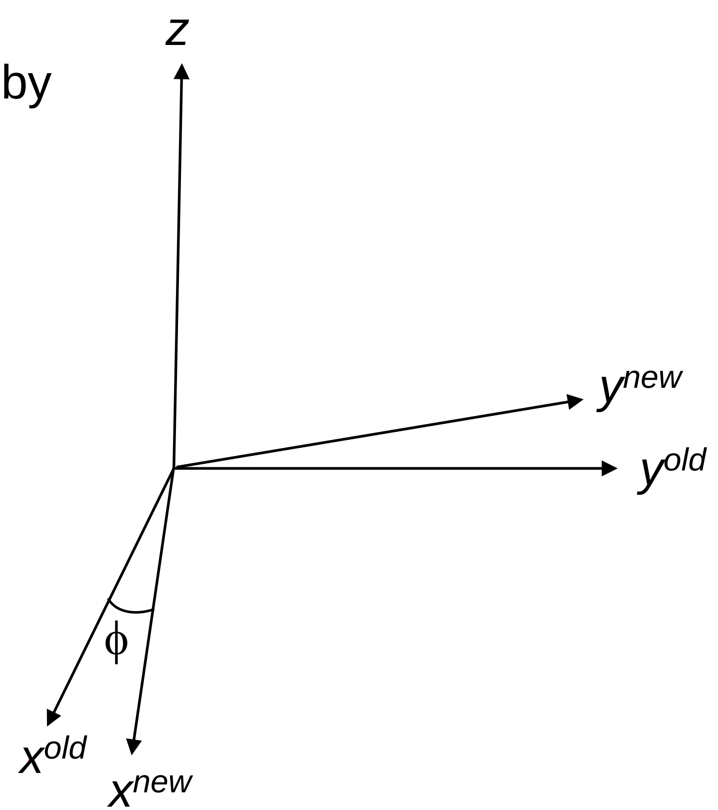
*Note – this particular selection of rotation matrices is consistent with an external rotation, corresponding to projection of the old coordinates onto the new ones.

Matrix Properties

Let's introduce a general toolkit by considering a specific problem. How de we describe our molecular tensor in a new coordinate system?

Extension to a 3×3 matrix α can be done by sandwiching.

$$\alpha^{new} = R_{\phi} \cdot \alpha^{old} \cdot R_{-\phi}$$

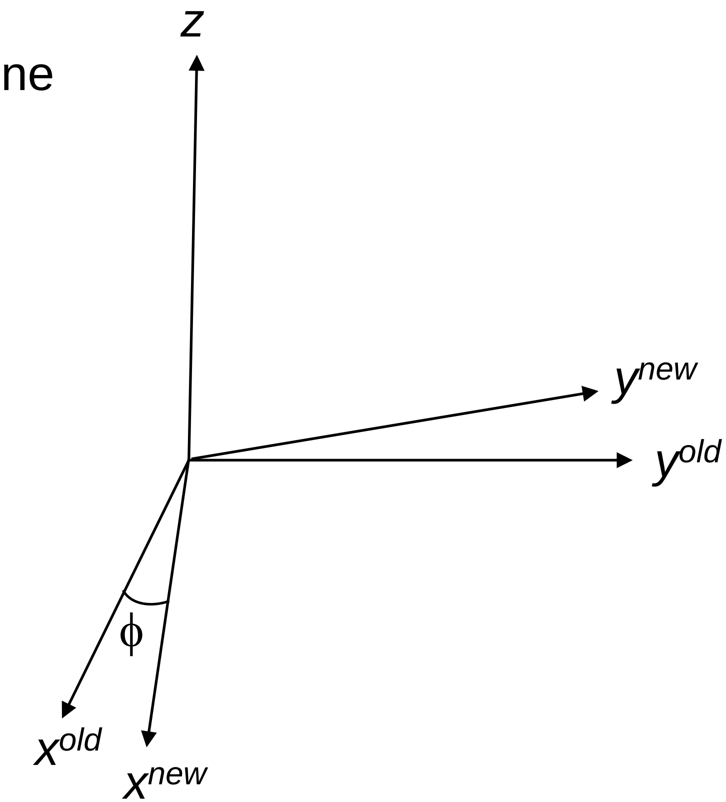


Garth J. Simpson

Let's introduce a general toolkit by considering a specific problem. How de we describe our molecular tensor in a new coordinate system?

Extension to a 3×3×3 tensor β can be done by generalizing the approach taken for matrices.*

$$\beta^{new} = R_{\phi} \cdot \beta^{old} : R_{-\phi} R_{-\phi}$$



*(*submitted*)

Matrix Properties - Revisited

In practice, it is often more convenient to use vectorized tensors.

$\alpha_{xx}, \alpha_{xy}, \alpha_{xz}$

α_{yx}

α_{zx}

$$vec(\alpha) = \begin{bmatrix} \alpha_{xx} \\ \alpha_{yx} \\ \alpha_{zx} \\ \alpha_{xy} \\ \alpha_{yy} \\ \alpha_{zy} \\ \alpha_{xz} \\ \alpha_{yz} \\ \alpha_{zz} \end{bmatrix} \qquad \vec{\alpha} = \underline{asc}(\alpha) = \begin{bmatrix} \alpha_{xx} \\ \alpha_{xy} \\ \alpha_{xz} \\ \alpha_{yx} \\ \alpha_{yy} \\ \alpha_{yz} \\ \alpha_{zx} \\ \alpha_{zy} \\ \alpha_{zz} \end{bmatrix} = vec(\alpha^T)$$

Matrix Properties - Revisited

In practice, it is often more convenient to use vectorized tensors.

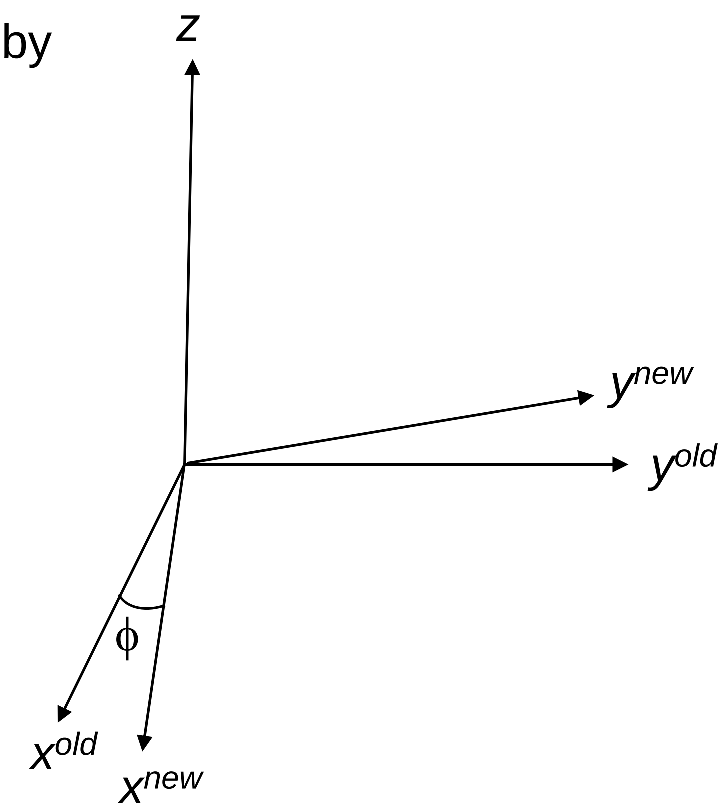
Extension to a 3×3 matrix α can be done by vectorization.

$$\vec{\alpha}^{new} = \left[R_{\phi} \otimes \left(R_{-\phi} \right)^{T} \right] \cdot \vec{\alpha}^{old}$$

$$\vec{\alpha}^{new} = \left[R_{\phi} \otimes R_{\phi} \right] \cdot \vec{\alpha}^{old}$$

vs.

$$\alpha^{new} = R_{\phi} \cdot \alpha^{old} \cdot R_{-\phi}$$



Tensor Properties - Revisited

In practice, it is often more convenient to use vectorized tensors.

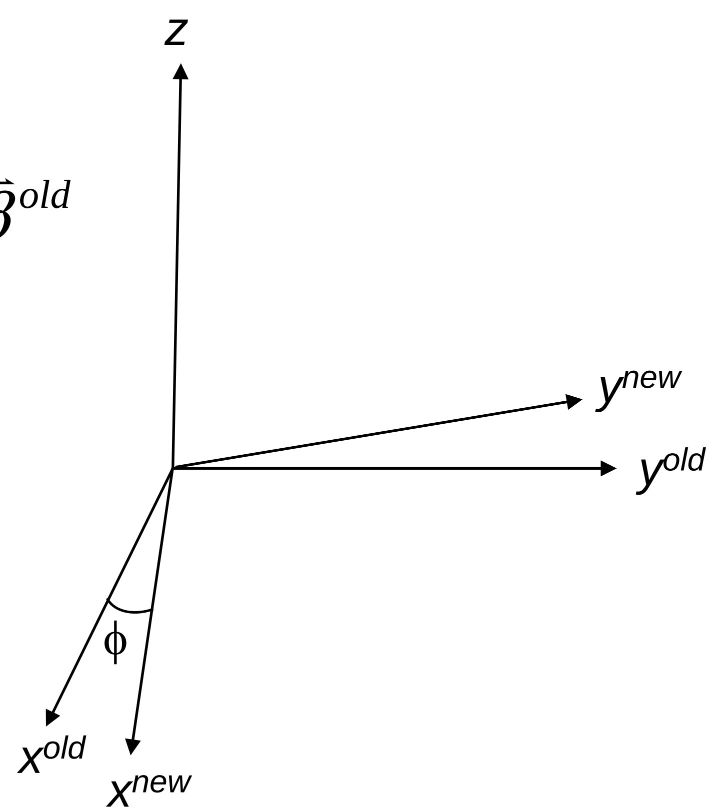
Extension to a 3×3×3 tensor by vectorization.

$$\vec{\beta}^{new} = \left[R_{\phi} \otimes \left(R_{-\phi} \right)^{T} \otimes \left(R_{-\phi} \right)^{T} \right] \cdot \vec{\beta}^{old}$$

$$\boxed{\vec{\beta}^{new} = \left[R_{\phi} \otimes R_{\phi} \otimes R_{\phi} \right] \cdot \vec{\beta}^{old}}$$

vs.

$$\beta^{new} = R_{\phi} \cdot \beta^{old} : R_{-\phi} R_{-\phi}$$



Compendium of Useful Identities

Matrices

$$vec(A\cdot B\cdot C)=(C^T\otimes A)vec(B)$$

$$asc(A\cdot B\cdot C)=(A\otimes C^T)asc(B)$$

$R_\phi \alpha (R_{-\phi})^T$

$$vec(A\cdot B)=[I_n\otimes A]\cdot vec(B)$$

$$=[B^T\otimes I_k]\cdot vec(A)$$

$$asc(AB)=(I_m\otimes B^T)\cdot asc(A)$$

$$=(A\otimes I_k)\cdot asc(B)$$

$$asc(A\cdot B\cdot C)=[I_n\otimes(C^T\cdot B^T)]\cdot asc(A)$$

$$=[(A^T\cdot B^T)\otimes I_k]\cdot asc(C)$$

$$vec(A\cdot B\cdot C)=[I_n\otimes(A\cdot B)]\cdot vec(C)$$

$$=[(C^T\cdot B^T)\otimes I_k]\cdot vec(A)$$

Tensors

$$asc(A\cdot B^{(2)}:CD)=(A\otimes C^T\otimes D^T)\cdot asc(B^{(2)})$$

$$asc(B^{(2)}:CD)=(I_m\otimes C^T\otimes D^T)\cdot asc(B^{(2)})$$

$$B^{(2)}:(C\cdot D)(E\cdot F)=(B^{(2)}:CE)^{(2)}:DF$$

$$(B^{(2)}:CD)\otimes(E^{(2)}:FG)=(B^{(2)}\otimes E^{(2)}):(C\otimes F)(D\otimes G)$$