

Remark on "Torsional Coordinate in the Book of Wilson, Decius and Cross"

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The note by Cyvin and Brunvoll¹ with the above title needs a correction. The given equations^{1,2} for the \mathbf{s} vectors are fortunately correct, and so are the rules for the direction of movement for the atoms during a torsional displacement. The discussion for the special planar case of $\tau = \pi$ is however wrong.

By virtue of the relation (in usual notation¹⁻³)

$$\frac{\mathbf{e}_{12} \times \mathbf{e}_{23}}{\sin \varphi_2} \cos \tau + \mathbf{e}_{23} \times \left(\frac{\mathbf{e}_{12} \times \mathbf{e}_{23}}{\sin \varphi_2} \right) \times \sin \tau = - \frac{\mathbf{e}_{43} \times \mathbf{e}_{32}}{\sin \varphi_3} \quad (1)$$

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it is seen that the expression for \mathbf{s}_{i2} of Refs. 1, 2 reduces to that of Wilson, Decius and Cross,³ with a minor correction of a rather typographic nature;

$$\mathbf{s}_{i2} = \frac{r_{23} - r_{12} \cos \varphi_2}{r_{23} r_{12} \sin \varphi_2} \frac{\mathbf{e}_{12} \times \mathbf{e}_{23}}{\sin \varphi_2} + \frac{\cos \varphi_2}{r_{23} \sin \varphi_3} \frac{\mathbf{e}_{43} \times \mathbf{e}_{32}}{\sin \varphi_3} \quad (2)$$

Eqn. (1) explains the way in which the dihedral angle τ enters *implicitly* into eqn. (2).

One of the writers (S.J.C.) regrets to have added to the confusion by publishing the previous note.¹

1. Cyvin, S. J. and Brunvoll, J. *Acta Chem. Scand.* **18** (1964) 1028.
2. Decius, J. C. *J. Chem. Phys.* **16** (1948) 1025.
3. Wilson, E. B., Jr., Decius, J. C. and Cross, P. C. *Molecular Vibrations*, McGraw-Hill Book Co., New York 1955, p. 61.

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