

Intrinsically Chiral Aromaticity. Rules Incorporating Linking Number, Twist, and Writhe for Higher-Twist Möbius Annulenes [*J. Am. Chem. Soc.* **2008**, *130*, 7613–7619]. Shay M. Rappaport and Henry S. Rzepa*

Page 7616. The rotation angle, defined in the original article as eq 13 and used in eq 12, is calculated as the difference between two angles:

$$\gamma_n = \gamma_n^{(2)} - \gamma_n^{(1)} \quad (1)$$

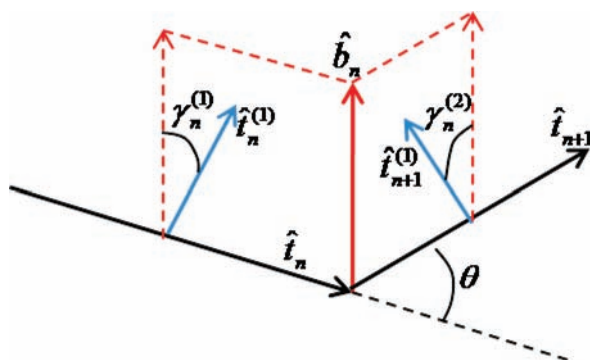
A more precise definition of these terms is given by

$$\begin{aligned} \gamma_n^{(1)} &= \text{sgn}[(\hat{b}_n \times \hat{t}_n^{(1)}) \cdot \hat{t}_n] \arccos(\hat{b}_n \cdot \hat{t}_n^{(1)}) \\ \gamma_n^{(2)} &= \text{sgn}[(\hat{b}_n \times \hat{t}_{n+1}^{(1)}) \cdot \hat{t}_{n+1}] \arccos(\hat{b}_n \cdot \hat{t}_{n+1}^{(1)}) \end{aligned} \quad (2)$$

where $\gamma_n^{(1)}$ and $\gamma_n^{(2)}$ are the angles of the n th and $(n + 1)$ th rod's $\hat{t}^{(1)}$ vectors relative to the rotation plane (i.e., the plane defined by the two successive segments), represented by the binormal,

$$\hat{b}_n = \frac{\hat{t}_n \times \hat{t}_{n+1}}{|\hat{t}_n \times \hat{t}_{n+1}|} \quad (3)$$

The rod's vector must be orthogonal to the curve (i.e., to the tangent vector) and is defined as $\hat{t}_n^{(1)} = (\hat{t}_n \times \hat{\rho}_n) |\hat{t}_n \times \hat{\rho}_n|^{-1}$, where $\hat{\rho}_n$ is the orbital orientation to the n th carbon.



Note that, although in principle $|\gamma_n|$ may be higher than π , this definition is unique and not degenerate only in the range $[-\pi, \pi]$.

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