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:

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

A more precise definition of these terms is given by

$$\gamma_n^{(1)} = \mathrm{sgn}[(\hat{b}_n \times \hat{t}_n^{(1)}) \cdot \hat{t}_n] \arccos(\hat{b}_n \cdot \hat{t}_n^{(1)})$$
$$\gamma_n^{(2)} = \mathrm{sgn}[(\hat{b}_n \times \hat{t}_{n+1}^{(1)}) \cdot \hat{t}_{n+1}] \arccos(\hat{b}_n \cdot \hat{t}_{n+1}^{(1)}) \tag{2}$$

where $\gamma_n^{(1)}$ and $\gamma_n^{(2)}$ are the angles of the nth 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,

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

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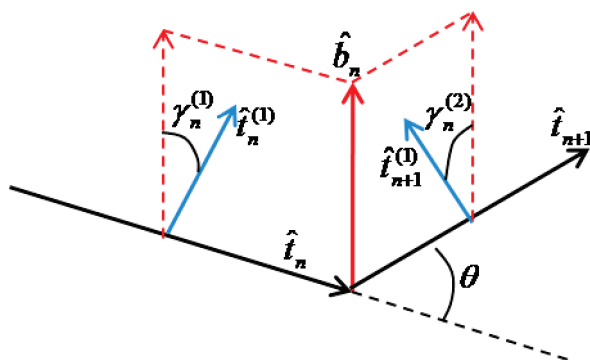
Note that, although in principle $|\gamma_n|$ may be higher than π, this definition is unique and not degenerate only in the range $[-\pi, \pi]$.

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