1 Spiro-atom angle modeling

The cross-angle in a spiro-atom is expliticly modeled if the disjoint cycles are both small, i.e. of size ≤ 5. Only then is the additional variance when calculating cross-angle bounds particularly harmful for the overall 3D structure.
We define:

$$\vec{a} = R_z\left(\frac{\alpha}{2}\right)\begin{pmatrix}1\\0\\0\end{pmatrix} = \begin{pmatrix}\cos\frac{\alpha}{2}\\\sin\frac{\alpha}{2}\\0\end{pmatrix} \tag{1}$$

$$\vec{b} = R_y\left(\frac{\beta}{2}\right)\begin{pmatrix}-1\\0\\0\end{pmatrix} = \begin{pmatrix}-\cos\frac{\beta}{2}\\0\\\sin\frac{\beta}{2}\end{pmatrix} \tag{2}$$

Where R_y and R_z are the standard three-dimensional rotation matrices, α is the cycle internal angle for the first cycle at the spiro-atom, and β is the cycle internal angle for the second cycle at the spiro-atom.

The angle between these vectors ϕ is then:

$$\vec{a}\vec{b} = ||\vec{a}||\,||\vec{b}||\cos\phi \tag{3}$$

$$\phi = \arccos\left\{\left(\cos\frac{\alpha}{2}\right)\left(-\cos\frac{\beta}{2}\right)\right\} \tag{4}$$