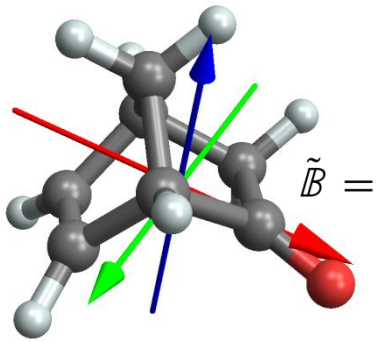
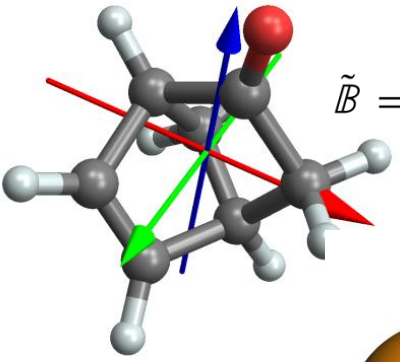


$$\tilde{\mathbb{B}} = \begin{pmatrix} -2.64 & -2.83 & 0.22 \\ -2.83 & -5.09 & 1.39 \\ 0.22 & 1.39 & -4.48 \end{pmatrix}$$

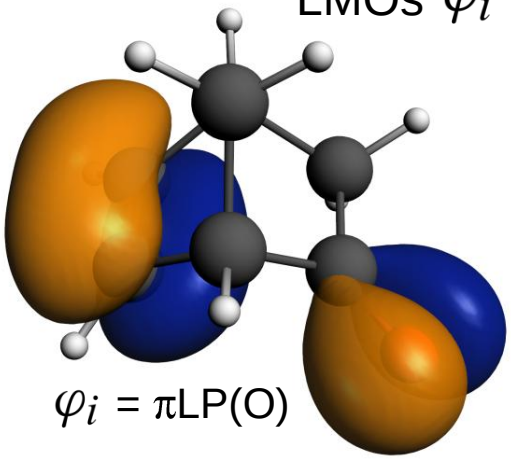
Determine chiroptical response tensor for standard orientation, origin at CNC.



$$\tilde{\mathbb{B}} = \begin{pmatrix} -6.84 & 0.00 & 0.00 \\ 0.00 & -3.66 & 0.00 \\ 0.00 & 0.00 & 3.57 \end{pmatrix}$$

Rotation of molecule into PAS (chiroptical response tensor diagonal).

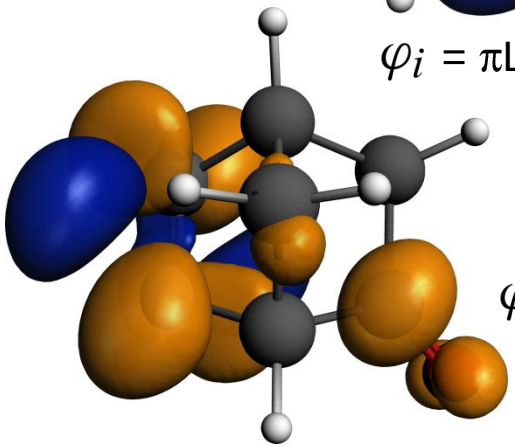
LMOs φ_i



φ_i = π(C$_3$-C$_4$)

φ_i = πLP(O)

Analyze xx, yy, and zz components of OR chiroptical response tensor in the PAS.



$\beta^i_{33}(\boldsymbol{r})$

φ_i = π(C$_3$-C$_4$)

Examine contributions from localized molecular orbitals (LMOs), canonical molecular orbitals (CMOs), electric-/magnetic-field perturbed orbitals, and their products [integrand of Eq. (1)].