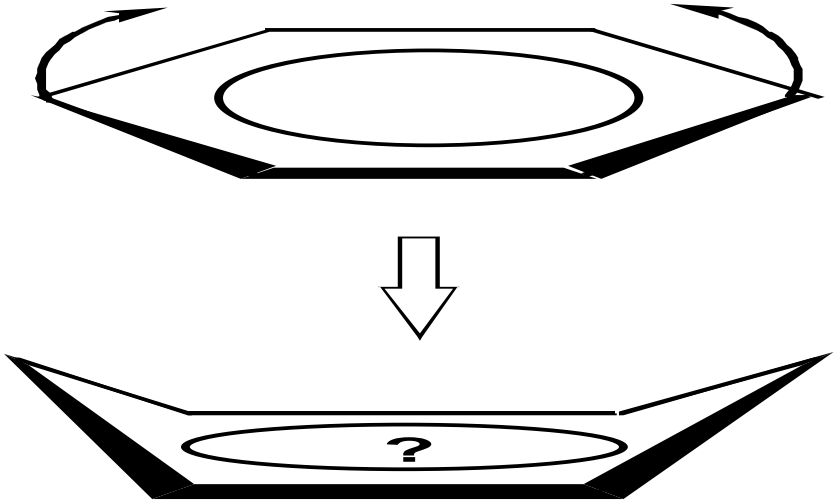
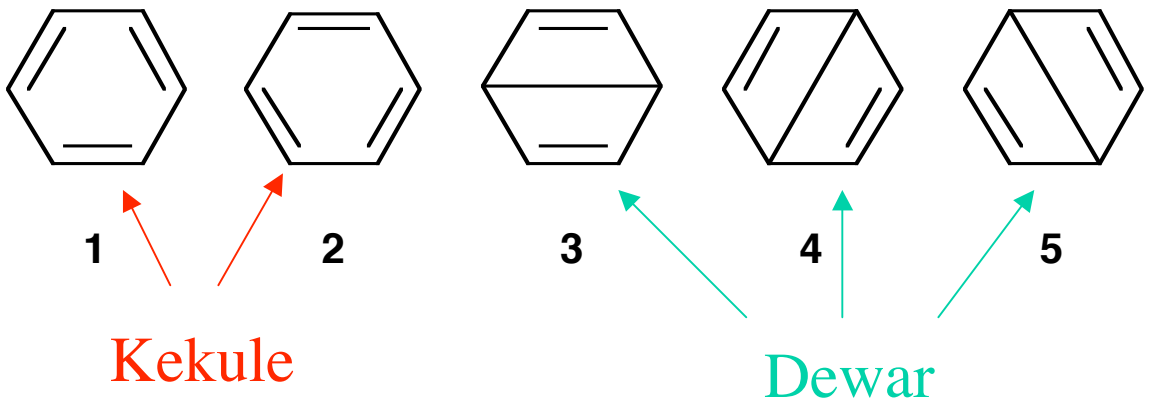
VB calculations on bent π-systems

What is a π-system

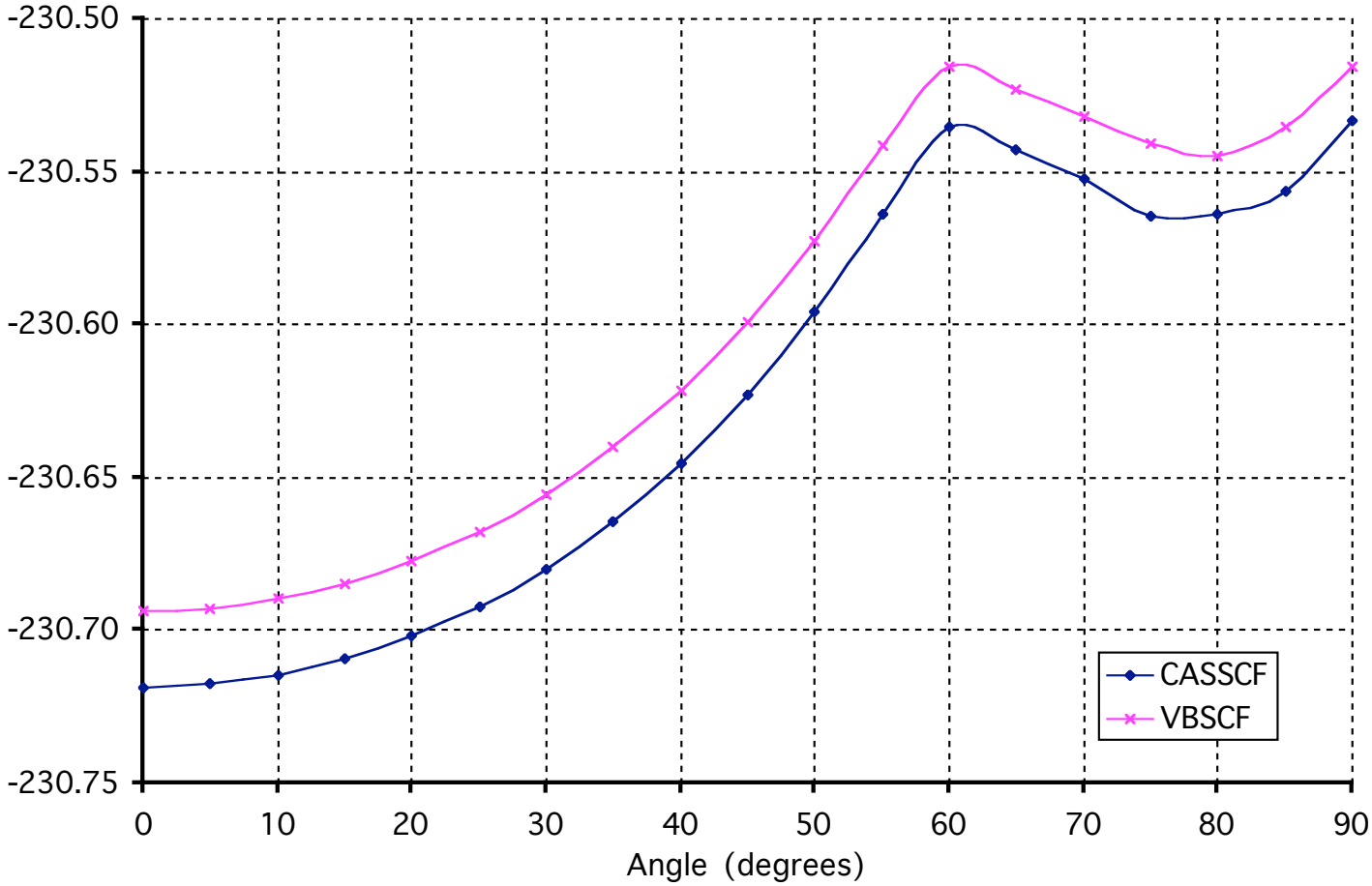


Definition of π-system

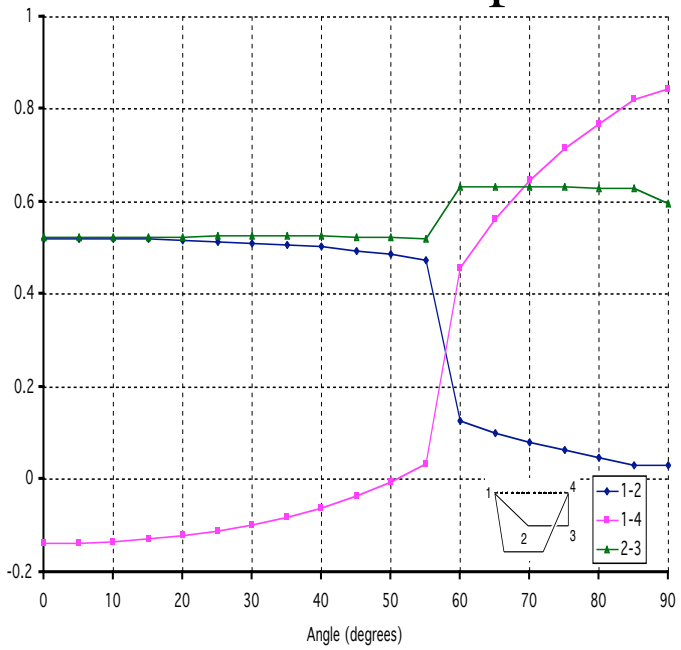


- 6-31G basis
- Geometries from 10*10 CASSCF
- Orthogonal σ-core
- p-orbitals atomic (delocalised)
- All orbitals optimised

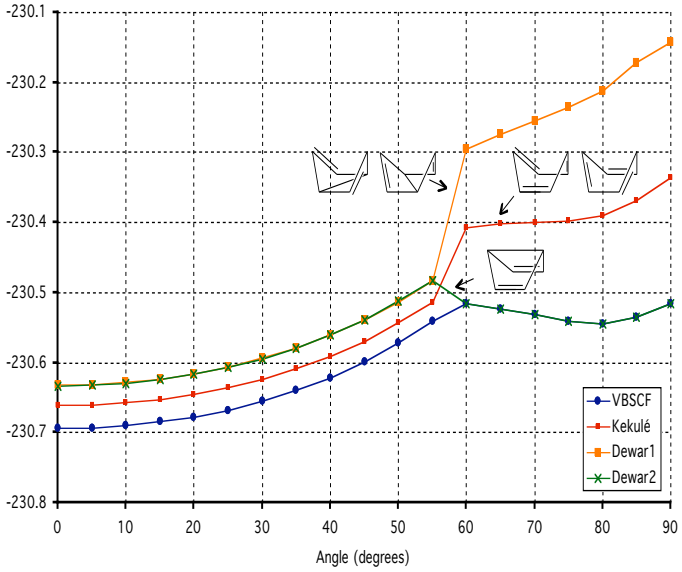
Energy curves for VBSCF/CASSCF



Orbital overlaps

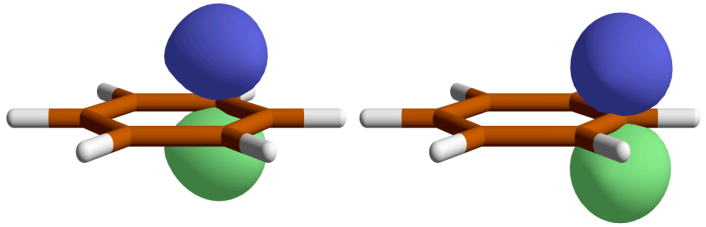


Structure energies

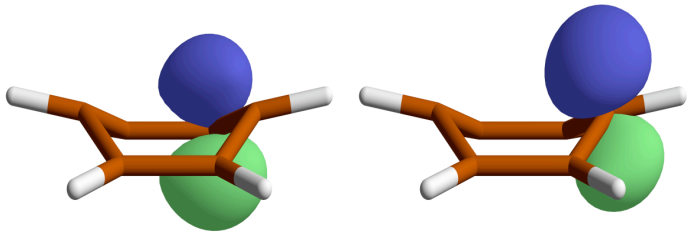


π-orbitals for atoms 3,4

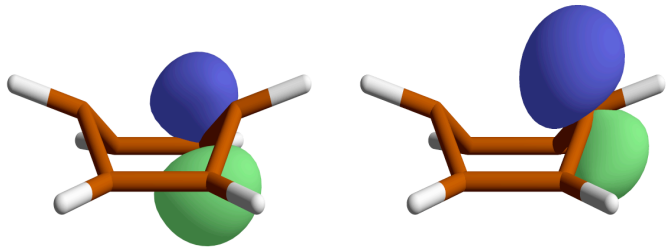
0°



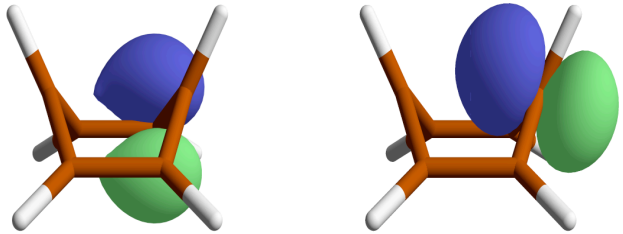
35°



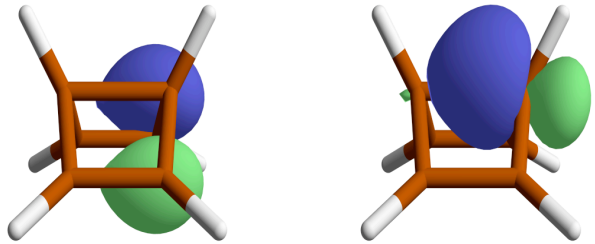
55°



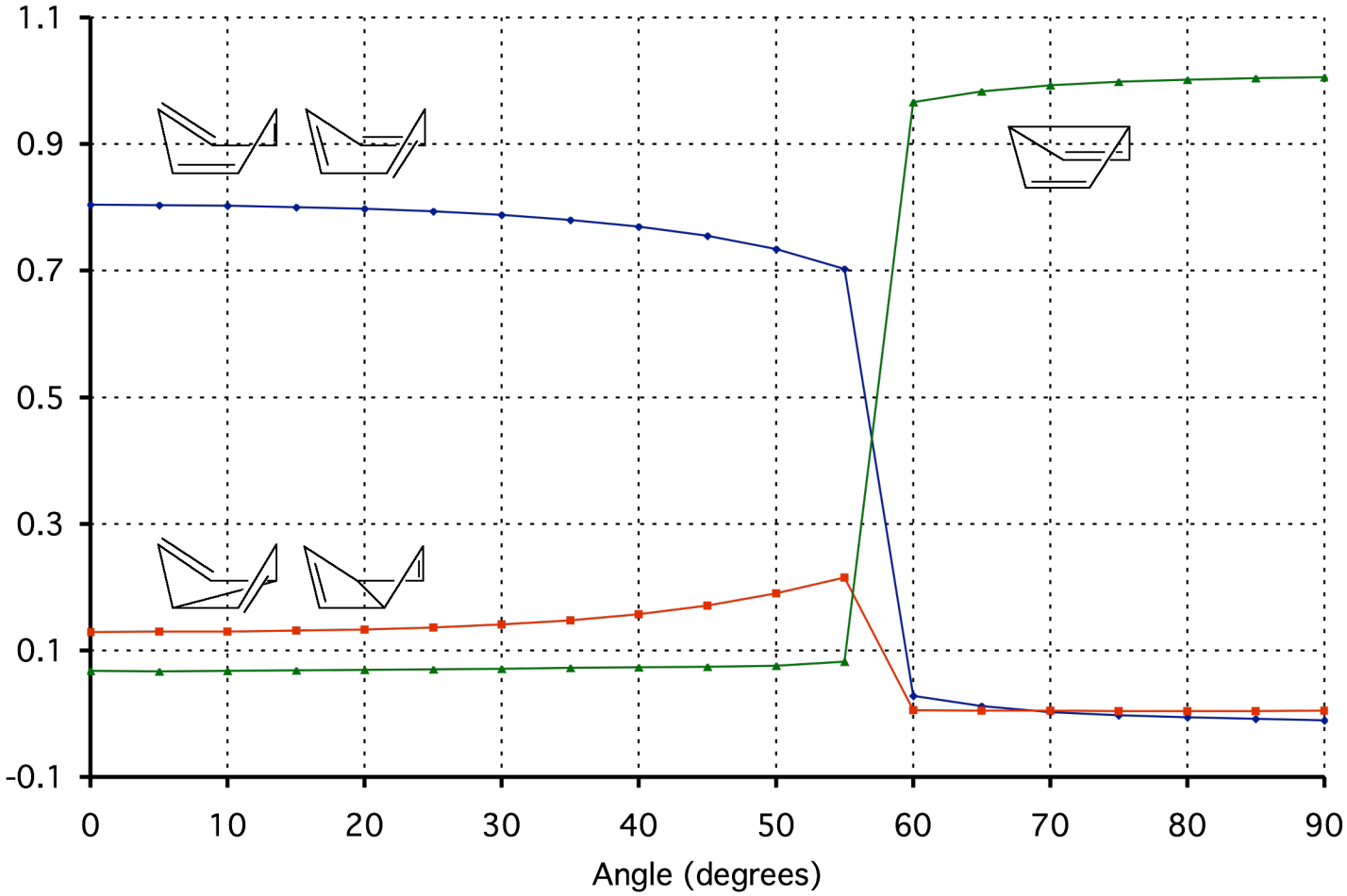
60°



80°



Structure weights



$$W_j = \sum_i c_i c_j S_{ij}$$