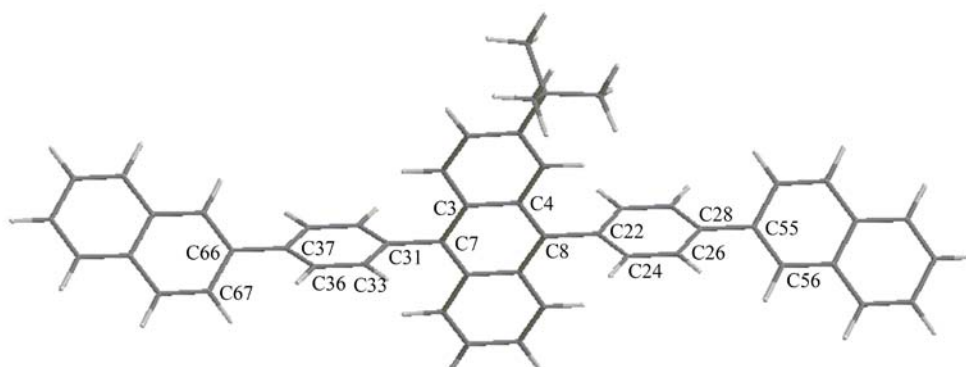


### Calculated stereostructure and frontier orbitals of TBDNPA



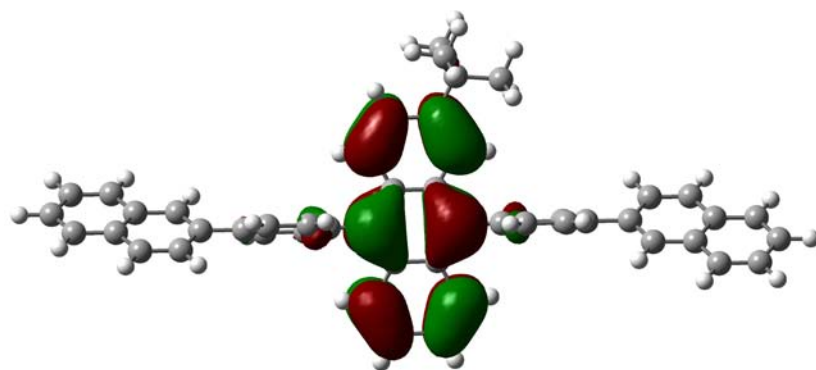
Dihedral angles:

$$C67-C66-C37-C36 = 37.2^\circ$$

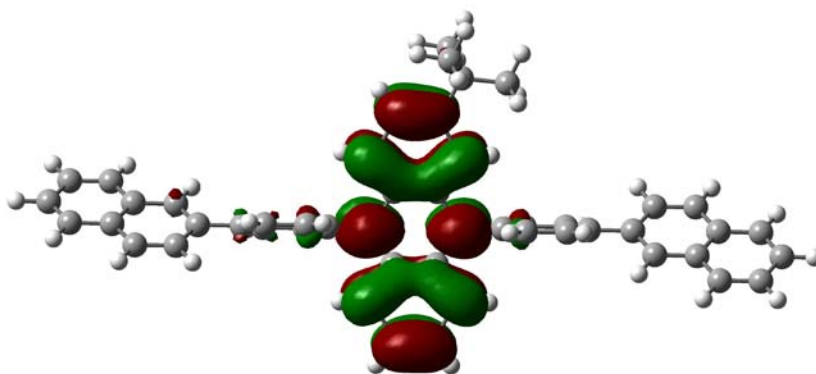
$$C33-C31-C7-C3 = 77.5^\circ$$

$$C24-C22-C8-C4 = 78.4^\circ$$

$$C26-C28-C55-C56 = 37.3^\circ$$



HOMO



LUMO