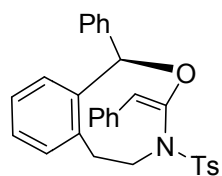
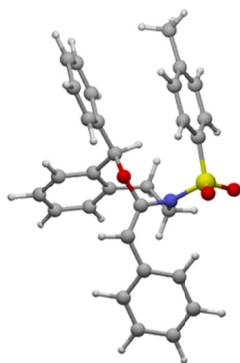


Energy and imaginary vibrational frequency of calculated structures using ω B97XD method.

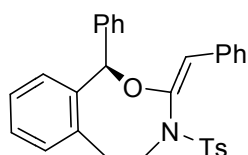


6a

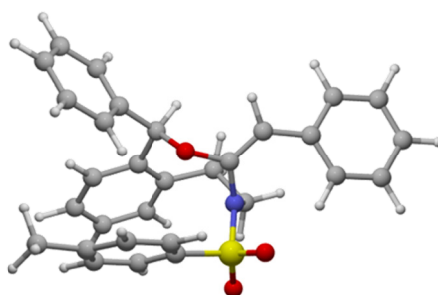


E= -1837.56529 Hartree

E_{SMD}= -1838.150955 Hartree

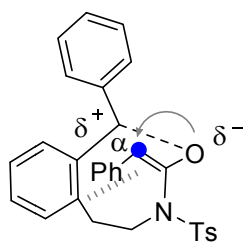


6a_iso

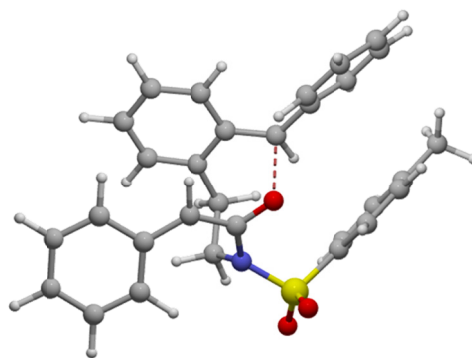


E= -1837.556936 Hartree

E_{SMD}= -1838.142449 Hartree



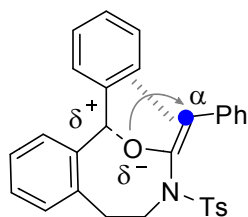
TS_cis



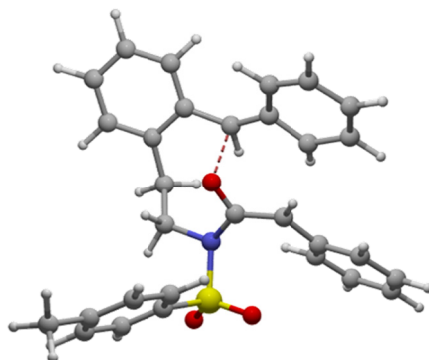
E= -1837.505693 Hartree

E_{SMD}= -1838.093161 Hartree

Frequency= -257.46 cm⁻¹



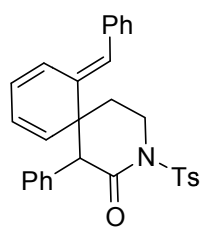
TS_trans



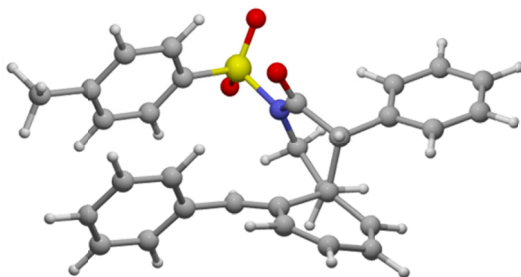
E= -1837.478131 Hartree

E_{SMD}= -1838.071071 Hartree

Frequency= -274.00 cm⁻¹

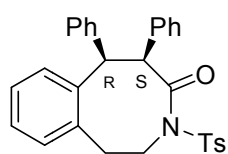


Spiro_Int

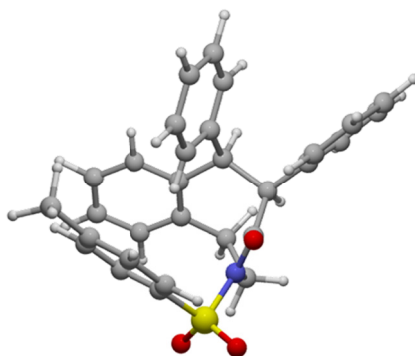


E= -1837.549305 Hartree

E_{SMD}= -1838.135975 Hartree

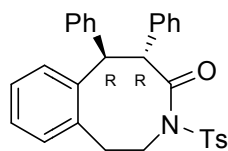


2a_cis

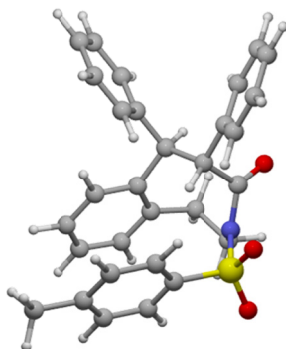


E= -1837.594085 Hartree

E_{SMD}= -1838.178264 Hartree



2a_trans



E= -1837.588939 Hartree

E_{SMD}= -1838.178308 Hartree
