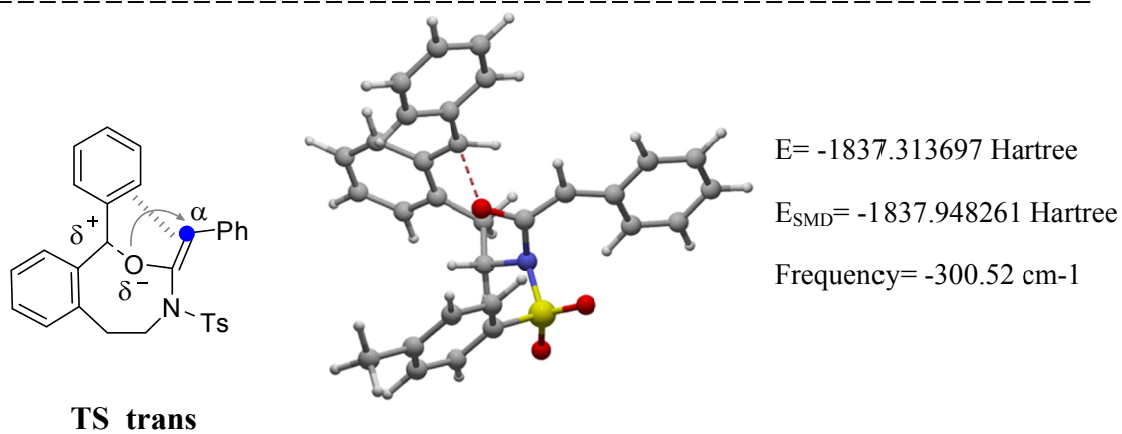
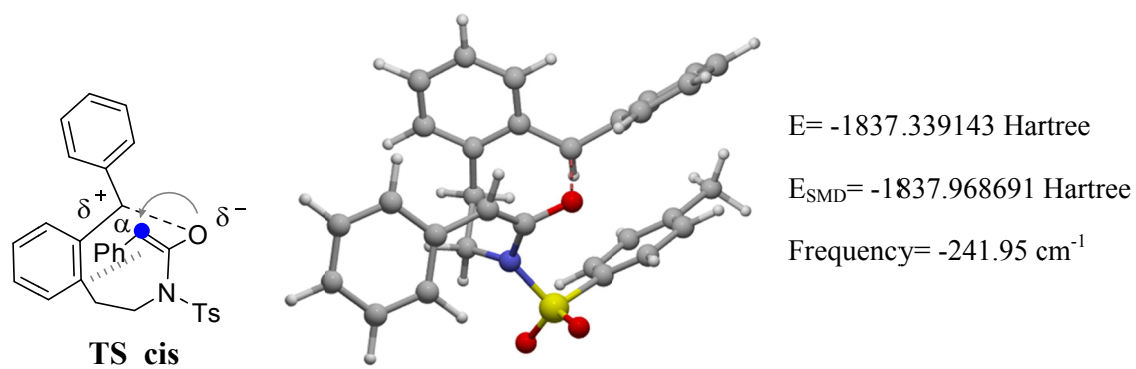
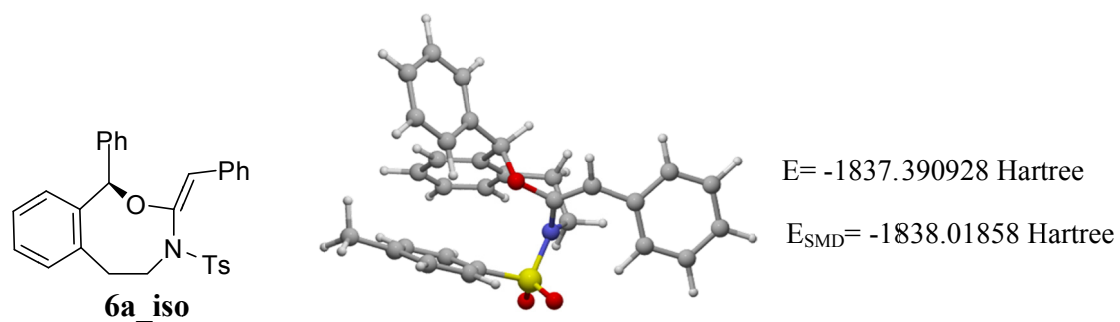
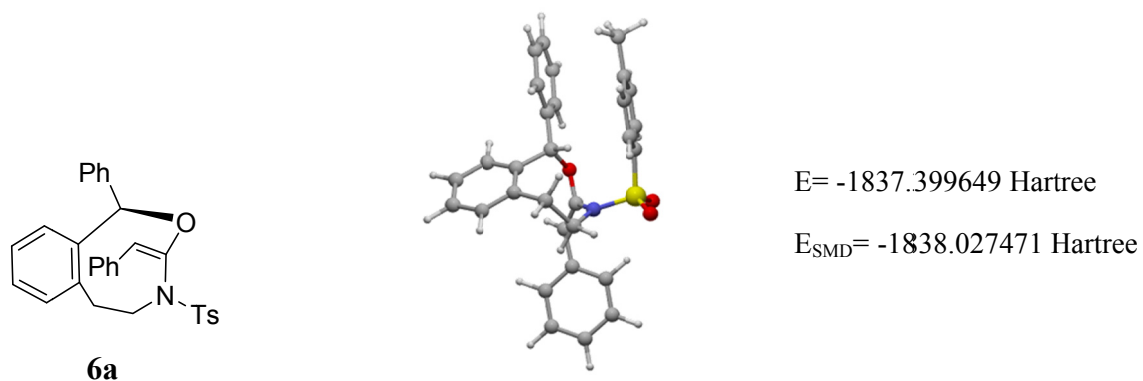
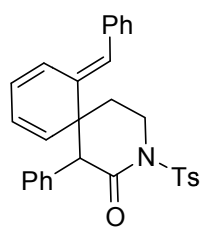
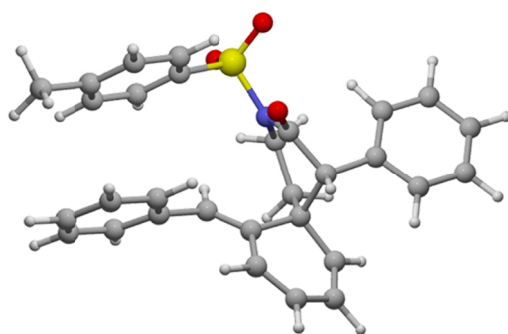


Energy and imaginary vibrational frequency of calculated structures using M062X method.



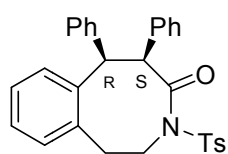


Spiro_Int

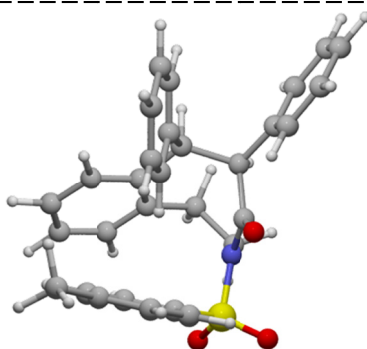


E= -1837.381669 Hartree

E_{SMD}= -1838.009498 Hartree

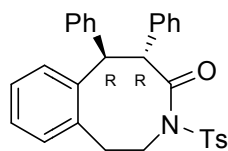


2a_cis

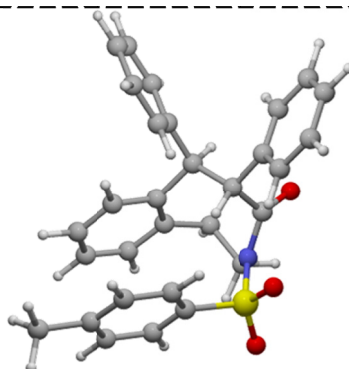


E= -1837.424244 Hartree

E_{SMD}= -1838.050336 Hartree



2a_trans



E= -1837.419198 Hartree

E_{SMD}= -1838.050075 Hartree
