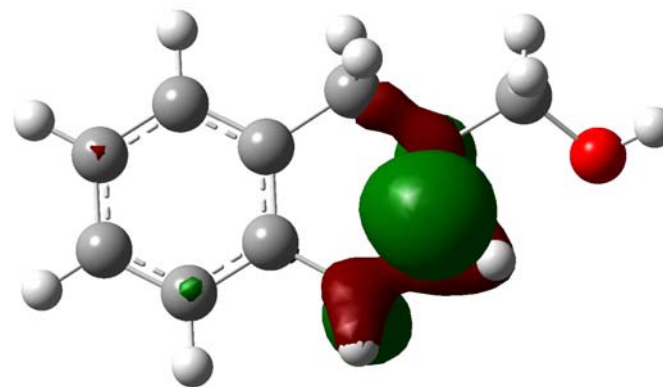
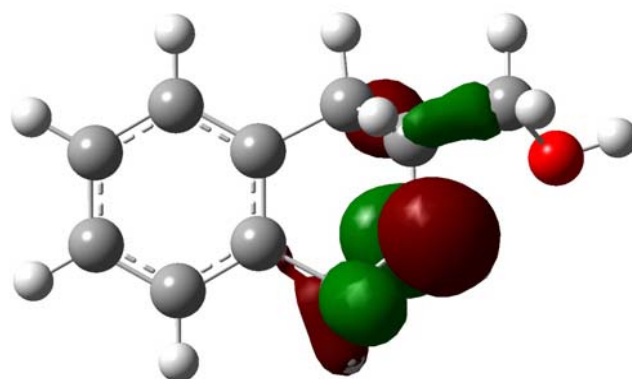


Conformer I



Conformer II



Cation

HOMO Orbitals of neutral Conformers I and II and the ion of THIQM, as obtained at the MP2 6-31++G(d, p) level of theory.