

Electrophilic Bromination of Phenol – Reaction Coordinates

Basic problem: Can computational methods reproduce the experimentally known regiochemical preferences for the electron donor substituted benzene system, phenol?

Method: Build and optimize phenol using the semiempirical AM1 method. Record the enthalpy of formation of the molecule and the charge distribution on the aromatic ring carbons. Build and optimize the cationic sigma-complex formed by *para* and for *meta* attack of Br⁺ upon phenol.

- Which is the more stable intermediate?
- Based upon the charge distribution in phenol, which site is most likely to be attacked by Br⁺ to give the final bromophenol?
- Based upon the relative stabilities of the sigma-complexes, which would be the most stable product to form?
- Do your answers for the preceding questions agree?

Literature: You may use any standard organic chemistry text for background data on electrophilic substitution on phenol.

