**Electrophilic Bromination of Benzaldehyde – Reaction Coordinates**

**Basic problem**: Can computational methods reproduce the experimentally known regiochemical preferences for the electron acceptor substituted benzene system, benzaldehyde?

**Method**: Build and optimize benzaldehyde using a semiempirical 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 benzaldehyde.

- Which is the more stable intermediate in terms of energy?
- Based upon the charge distribution in benzaldehyde, which site is most likely to be attacked by Br+ to give the final bromobenzaldehyde?
- 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 benzaldehyde.