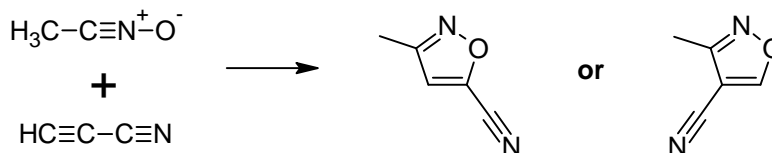


Building Transition State Models & Using ZPE

Reaction



Hypothesis

1. Use FMO theory to predict the kinetic regioisomer
2. Rather than test your prediction with an experiment, you will see whether your prediction is supported by the calculated energies (HF/3-21G) of the regioisomeric transition states

Suggestions

There are three ways to generate trial transition states. I suggest you find a way that works and *only then* add substituents. Options:

1. Build reactants (use **Insert** to start second reactant molecule), define reaction, search database for matching structure
2. Build product, define retro-reaction, search database for matching structure
3. Build product, constrain reacting *single* bonds to likely distances in transition state (2-2.2 Å), perform constrained equilibrium geometry calculation

Supporting Analysis

1. FMO analysis of the reactants: identify dominant interaction (is there one?) and predict regiochemistry
2. Are the transition state *energies* in accord with the FMO prediction?
3. Are the transition state *geometries* in accord with the FMO prediction?
4. Are the transition states *asynchronous*?
5. Are the transition state *geometries* in accord with the Hammond postulate?
6. Is the direction of *electron transfer* in the transition state consistent with the FMO prediction?