

Chem. 1460: HW #6 Assigned March 1, due March 21.

1. Optimize the geometry of tetramethyleneethane in its singlet and triplet states assuming a planar structure and using the becke3lyp/6-31G(d) method. What do you get for the singlet triplet separation?

You will probably want to build the geometry using a z-matrix, and to use opt=z-matrix. Also, for the triplet state you will need to set the spin multiplicity=3.

2. consider two H₂ molecules approaching parallel to one another, going through a square intermediate, breaking the two original HH bonds and forming the two perpendicular HH bonds, and proceeding to 2 H₂.

Is this reaction symmetry allowed or forbidden? Explain.

Using the CAS(2,2)/3-21G method calculate the activation energy for this exchange process.