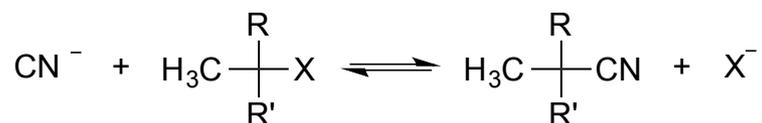


SN₂ NUCLEOPHILIC SUBSTITUTIONS

1/ We consider the SN₂ reaction implying the cyanide ion and the ethyl bromide (X = Br and R = R' = H). Model this reaction at the AM1 level in a solvent (acetone), by using the SM5.2 continuum solvation model.



2/ Impact of the halogen leaving group on the reactivity

Model the reaction above at the AM1 level with R = R' = H and X = Cl, Br and I. Comment on the impact of X on the reactivity.

3/ Steric Effects on SN₂ Reaction Rates

Model the reaction above at the AM1 level with X = Br and:

- i) R = R' = H
- ii) R = H and R' = CH₃
- iii) R = R' = CH₃

Comment on the impact of the steric hindrance on the reactivity.