Solvent and substituent effects on the intramolecular amide hydrolysis of N-methylmaleamic acid

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Abstract
Intramolecular amide hydrolysis of N-methylmaleamic acid is revisited at the B3LYP/6-311G(2df,p)//B3LYP/6-31G(d,p)+ZVPE level, including solvent effects at the CPCM-B3LYP/6-311G(2df,p)//Onsager-B3LYP/6-31G(d,p)+ZPVE level. The concerted reaction mechanism is energetically favorable over stepwise reaction mechanisms in both the gas phase and solution. The calculated reaction barriers are significantly lower in solution than in the gas phase. In addition, it is concluded that the substituents of the four N-methylmaleamic acid derivatives considered herein have a significant effect on the gas-phase reaction barriers but a smaller, or little, effect on the barriers in solution.

References