Theoretical study of solvent effects in the 1,3 rearrangement in the allyl?fluoride system in polar media

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The influence of electrostatic solvent effects on the barrier for the internal return rearrangement in the allyl?fluoride model system has been analyzed. The solvent was modeled through the self?consistent reaction field (SCRF) theory. It is shown that there exists a significant solvent effect operating in favor of the 1,3 fluoride migration. The results are compared with previous theoretical studies based on a supermolecule scheme of calculation, which reported no solvent influence on the barrier for the internal return process in this system. Finally, the effect of acid catalysis is reinterpreted on the basis of the results obtained and discussed in connection with experimental data in related systems.