

A theoretical study of solvent effects on the relative thermodynamic stabilities of the allyl⁺/F⁻ and allyl⁻/Li⁺ ion pairs in polar media

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The relative thermodynamic stabilities of several ion-pair structures, including intimate and solvent-separated forms, in solution have been studied for the allyl⁺/F⁻ and allyl⁻/Li⁺ model systems. The electrostatic part of the solvent effects was modelled through the self-consistent reaction field (SCRF) theory and an extension of it including desolvation effects (SCRF/D theory). Specific solvent effects were also analysed by explicitly incorporating a solvent molecule, via the supermolecule (SM) approach. It is shown that a more complete thermodynamic description of these systems is attained by using mixed continuum-SM schemes. This last approach allows qualitative separation of the individual contributions of the electrostatic and hydrogen-bonding effects, which are particularly relevant to a discussion of the relative stabilities of intimate and solvent-separated ion pairs in these systems. © 1990.