Theoretical study of lithium?fluoride and lithium?chloride ion pairs in aqueous solution. An SCF?CNDO/2 approach including continuum solvent effects

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SCF?CNDO/2 calculations, including solvent effects via an extended version of the Generalized Born Formula (GBF), have been performed for LiX(H2O) species (n = 1,2; X = F, Cl). Several minima in the free energy surface, representing intimate and solvent?separated ion pair structures, have been analyzed. Qualitative results show a preferential stabilization of the intimate forms with respect to the solvent?separated ones. The results are discussed on the basis of a convenient partition of the total solute?solvent free energy. The interaction of the ionic species with the bulk solvent neglected in previous studies appears to be responsible for the preferential stability of the intimate forms.