

Nuclear magnetic resonance spectroscopic studies on self-association of 2-tert-butylphenol and a mixed association of 2-tert-butylphenol with dioxane in carbon tetrachloride. Strohbusch, Frank; Zimmermann, Herbert. Univ. Munich, Munich, Fed. Rep. Ger. Berichte der Bunsen-Gesellschaft (1967), 71(7), 679-84. CODEN: BBPCAX ISSN: 0940-483X. Journal written in German. CAN 68:7903 AN 1968:7903 CAPLUS (Copyright (C) 2008 ACS on SciFinder (R))

Abstract

The chem. shift of the OH signal from 2-tert-butylphenol (I) was measured in CCl₄, and in mixts. of dioxane and CCl₄ as a function of the mole fraction. The const. for the equil. between monomers and assocd. mols. were detd. In the system I/CCl₄ the I monomers are in equil. with dimers only. The const. of assocn. is $K_d = 0.53 \text{ mole fraction}^{-1}$. In the system I/dioxane/CCl₄ both self-assocn. and mixed assocn. occur. In the mixed associates both O atoms of the dioxane form H bonds with I almost independently. Therefore, complexes of molar compn. I:dioxane = 1:1 and 2:1, resp., coexist in the solns. The mean const. of association of a I mol. and an O atom of dioxane is $K_x = 13.4 \text{ mole fraction}^{-1}$. Some restricting conditions for the calcn. of assocn. const. from N.M.R. data are discussed.