



Showcasing research from Professor Yukihiro Ozaki, Kwansai Gakuin University, Professor Mirosław Czarnecki, University of Wrocław, and Professor Yusuke Morisawa, Kindai University.

Solvent effect on the competition between weak and strong interactions in phenol solutions studied by near-infrared spectroscopy and DFT calculations

Phenol has interactions like $\text{OH}\cdots\text{OH}$ and $\text{OH}\cdots\pi$. NIR spectroscopy was used to investigate them. In aromatic solvents the $\text{OH}\cdots\pi$ interactions play an important role. Depending on the concentration, in cyclohexane solutions free OH and OH in the $\text{OH}\cdots\text{OH}$ interactions are present. In the aromatic solvents the $\text{OH}\cdots\text{OH}$ interactions compete with the $\text{OH}\cdots\pi$. Consequently, the associates of phenol in aromatic solvents are shorter compared with those in non-aromatic ones.

As featured in:



See Mirosław Antoni Czarnecki, Yusuke Morisawa, Yukihiro Ozaki *et al.*, *Phys. Chem. Chem. Phys.*, 2021, 23, 19188.