Electronic Structure of 2,6-Bis{*N*-(2-hydroxyphenyl)iminomethyl}-4-methylphenol

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Schiff Base, Electronic Structure, Polarization Spectrum, X-Ray Data, MO Calculation

The electronic and molecular structure of 2,6-bis{*N*-(2-hydroxyphenyl)iminomethyl}-4-methylphenol (hpimp) is clarified from the measurements of electronic absorption and ^{1}H NMR spectra in various solvents and an X-ray diffraction analysis, together with MO calculations. Electronic absorption bands of hpimp are at 422, 397.9, 359, 341, 294.3, 265.8, and 224 nm in the non-polar solvent cyclohexane. In polar solvents, such as methanol, an additional band which is assigned to a partly formed keto-amine hpimp, is observed at 499 nm. From the ^{1}H NMR spectra it is seen that hpimp exists in the enol-imine form in non-polar solvents, and as an equilibrium mixture of enol-imine and keto-amine forms in polar solvents. Each electronic absorption band of solid hpimp in a KBr disk is broadened compared with the solution state, and an additional band, again assigned to the keto-amine form, appears around 499 nm. An X-ray diffraction analysis shows that hpimp assumes a keto-amine structure in the solid state, and forms a column structure along the *c*-axis. MO calculations suggest that the enol-imine hpimp has a twist structure around the two C–C single bonds, the twist angle being 100° to 120°.