吡啶酮系偶氮染料解离平衡的^15NNMR和IR波谱

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摘要 报道了四个富氮-15吡啶酮偶氮染料的氮-15核磁共振中β-氮原子的化学位移,研究了氮-15原子和pH值之间的关联.当样品溶液从酸性转成碱性,β-氮-15原子的化学位移从366-380PPM移到500PPM,相应于从腺型到偶氮阴离子结构.根据各种pH值的化学位移可计算腺结构的含量,用IR证实了这一系列化合物的酸碱离解平衡.在酸性或中性条件下,固态化合物的二个羰基吸收,在碱性条件下变成只有一个羰基吸收峰,其它官能团的吸收峰表明了与平衡的位移的相应变化. 关键词 红外分光光度法 碳13核磁共振谱法 苯偶氮化合物 化学位移 吡啶酮 P 腺 偶氮染料 氮15核磁共振谱

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Investigation on dissociation equilibrium of pyridone azo dyes by ^15N NMR and ir spectroscopy

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Abstract The chem. shifts of b-nitrogen atom in 15N-NMR spectra of four 15N-enriched pyridone azo dyes were reported and the correlation between the chem. shifts of 15N atom and the pH values was studied. When the solution changed from acidic to basic, the chem. shifts of b-15N atom shifted from 366-380 ppm to ~500 ppm, corresponding to an equilibrium shift from hydrazone form to azo anion structure of the dyes. The relative content of hydrazone structure was calculated based on the chem. shifts at different pH values. The acid-base dissociation equilibrium of these compounds was confirmed by IR spectra. The two carbonyl absorptions of the compounds in solid state under acid or neutral conditions changed to one carbonyl band under basic condition. The absorption bands of other functional groups showed corresponding change with the shift of equilibrium

Key words INFRARED SPECTROPHOTOMETRY C13 NMR SPECTROMETRY BENZENE AZO COMPOUNDS CHEMICAL SHIFT PYRIDINONE P GLAND AZO DYES

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