NMR技术在苯基-2′, 3′, 4′-三羟基苯基酮分子内活泼质子动态特性研究中的应用

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摘 要:本文通过一维(ID)、二维(2D)核磁共振波谱法确定了苯基-2',3',4'——三羟基苯基酮分子结构,利用二维交换谱(2D EXSY)研究了该分子内活泼质子在二甲亚砜(DMSO)溶液中的动态特性,建立了活泼质子与溶液中水分子间的化学交换网络,并定量计算了化学交换的速率常数。实验结果表明:酚羟基氧形成分子内氢键使得它与自身的羟基氢的共价键被削弱,该活泼质子酸性增强,更容易发生反应。 关键词:

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Investigating the dynamic properties of labile protons in salicylic aldehyde thiosemicarbazone using two dimensional exchange spectroscopy

Abstract: The structure of phenyl-2, 3, 4-trihydroxyphenone has been concluded through 1D, 2D NMR test. The dynamic properties of labile protons in phenyl-2, 3, 4-trihydroxyphenone have been studied in DMSO using two dimensional exchange spectroscopy (EXSY). The network of chemical exchange has been built and the exchange rate constants have also been calculated. The results show that its acidity changes since the formation of intramolecular hydrogen-bond between hydroxyl groups on the phenol; so that the che

Key words:

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