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表征**O－H**解离能参数的**AM1**计算

张红雨,陈德展

淄博学院生物与化学工程系;山东师范大学化学系.济南(250014)

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摘要　对17种酚类化合物用半经验量子化学方法AM1计算了表征O－H解离能的参数△HOF值，即酚类化合物与其经抽氢反应产生的自由基生成热之差。经过与实验测定的17种酚类化合物的O－H解离能比较，评价了AM1方法在计算△HOF值方面的有效性。发现AM1计算的△HOF值与O－H解离能有很好的相关性(γ=0.9495)，优于经验方法，比如加和规则对O－H解离能的预测。虽然AM1方法在计算间位取代对O－H解离能的贡献方面是无效的，但将用于计算解离能类的参数以预测抗氧化剂活性还是可行的。

关键词　解离能　量子化学　化学键　键参数　键能　半经验方程　酚

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AM1 calculation of a parameter characterizing O－H bond dissociation 11:38 01-5-12energy

Zhang Hongyu,Chen Dezhan

Shandong Normal Univ, Dept Chem.Jinan(250014)

Abstract　The O-H bond dissociation energy (BDE) experimentally determined for 17 phgenols were employed to evaluate the effectiveness of AM1 method used in calculating a parameter characterizing the O-H BDE, the difference of heat of formation between phenol and its free radical generated after H- abstraction reaction (△ HOF). It was found that the AM1 calculated △ HOF correlated well with the O-H BDE (γ=0. 9495), and AM1 was better than empirical method such as additive rule derived from experiments to estimate the O-H BDE. Although AM1 was invalid to characterize the contribution of meta groups to the O- H BDE, it is fairly applicable in calculating BDE-like parameters to predict free radical scavenging activity of phenolic antioxidants.

Key words　QUANTUM CHEMISTRY　CHEMICAL BONDS　BOND PARAMETER　BOND ENERGY　SEMIEMPIRICAL EQUATIONS　PHENOL

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通讯作者