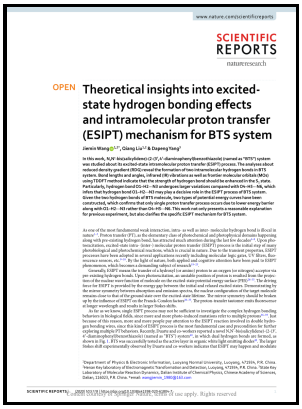
Effect of 4-substitution on some properties of the OH bond in 1-naphthols

- - The Substitution Effect on Reaction Enthalpies of Antioxidant Mechanisms of Juglone and Its Derivatives in Gas and Solution Phase: DFT Study.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Description: -
-effect of 4-substitution on some properties of the OH bond in 1-naphthols
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Notes: Thesis(Ph.D.) - Loughborough University of Technology 1974.
This edition was published in 1974

Tags: #Structural, #spectroscopic #and #NLO #features #of #the #4

The Substitution Effect on Reaction Enthalpies of Antioxidant Mechanisms of Juglone and Its Derivatives in Gas and Solution Phase: DFT Study.

Molecular modeling and pharmacophore approach for structural requirements of some 2-substituted-1-naphthols derivatives as potent 5-lipoxygenase inhibitors. The theoretical infrared spectra also make it possible to examine the relation between the absorption coefficient and the OH-stretching frequency Fig. The best pharmacophore model with hydrophobic, hydrogen bond donor HBD , and aromatic features has root mean square deviation RMSD of 0.

Substitution and torsional effects on the energetics of homolytic N

We also acknowledge previous National Science Foundation support under grant numbers 1246120, 1525057, and 1413739. Based on the results obtained from optimization study and substrate scope, plausible mechanistic insights of both cyclization and acyloxylation reactions have been provided. For the six environments, the substitution by the electron donating groups leads to the reduction of the IP values.

Substitution and torsional effects on the energetics of homolytic N

Our data demonstrate that the three mechanisms analyzed are endothermic but not spontaneous with exception of PT mechanism for benzene, methanol, and water.

Aromatic Compounds with Condensed Nuclei: Naphthalene and Related Compounds

The most stable configuration leads to the closer agreement with the experimental observation in terms of frequency and pleochroism. It is thus noteworthy that the comparison of theoretical and experimental frequencies for the identified configurations follows a well-defined linear trend Fig. Given that oxygen diffuses considerably more slowly than protons in quartz e.

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