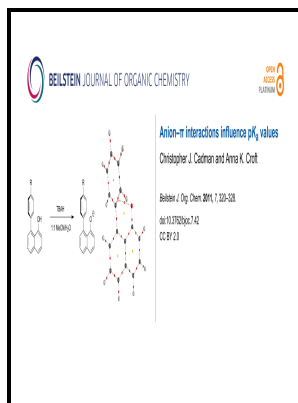


Effect of 4-substitution on some properties of the OH bond in 1-naphthols

- - 6.6: Reactions of Complexes



Description: -

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Applications of NIR/MIR to Determine Site Occupancy in Smectites

The various derivatives of naphthalene which form the core area of interest include alkyl- and aralkyl-naphthalenes, alkylnaphthalenes with substituents in the side-chain, phenylnaphthalenes, halogenonaphthalenes, naphthalenesulfonic acids and naphthalenesulfinic acids, naphthalenemonosulfonic acids, naphthalene di-, tri- and tetra-sulfonic acids, nitronaphthalenes, nitrosonaphthalenes and naphthylhydroxylamines, naphthylamines, azonaphthalenes and their derivatives. The theoretical infrared spectra also make it possible to examine the relation between the absorption coefficient and the OH-stretching frequency Fig.

Chiral hypervalent iodine mediated enantioselective oxidative dearomatization of naphthols

Figure 1: Numbering system used to designate specific atom of juglone and its derivatives followed by specification of electron donating or withdrawing substituent used.

Structural, spectroscopic and NLO features of the 4

The properties of OH defects were theoretically investigated within the density functional theory DFT framework using the PWscf code of the Quantum Espresso package Giannozzi et al. From Table 1, it is noticeable that, for electron withdrawing substituents J14-18, the IP values obtained are higher than those of classical antioxidants selected. The average differences between ETE in the gas phase and different solvent are 83.

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The second part of this thesis unravels the spiroetherification of naphtholic alcohols, thereby yielding spiroethers both in racemic and chiral form. Table 2 Inter-atomic distances and stretching frequencies of OH defects with double Si—O—Si bridges. Strong evidence a 4H Si × defect exists in olivine is provided both by the theoretical modeling of its infrared spectrum Balan et al.

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The binaphthyls are of interest for a number of reasons. Figure 3 showed that the solvation of molecules provokes a diminution of BDE values with the exception of J15 in methanol and acetonitrile. The reaction free energies of reactions 1 - 5 , ordinary denoted BDFE bond dissociation free energy , IPFE ionization potential free energy , PDFE proton dissociation free energy , PAFE proton affinity free energy , and ETFE electron transfer free energy are, respectively, calculated according to relations 6 - 10.

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