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Theoretical study on Alcohols: Phenol, p-methylphenol and p-nitrophenol

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The acetylation of alcohols is one of the most frequently used transformations in organic synthesis as it provides an efficient and inexpensive means for protecting hydroxyl groups in a multistep synthetic process. Geometric parameters of reactants: phenol, p-methyl phenol,p-nitro phenol were performed in the gas phase using the DFT/B3LYP density functional quantum mechanical method and was adopted the 6-31+G* basis set. Enthalpies of formation were determined using the AM1 method. The table lists the energies, lengths and angles values obtained.

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