QUANTUM CHEMICAL STUDIES ON ACIDITY-BASICITY BEHAVIOURS OF SOME SUBSTITUTED PYRIDINE DERIVATIVES

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Due to existence of pyridine ring in the structure of many biologically active compounds like herbicides such as nicosulfuron; pesticides such as ivin; insecticides such as anabasine, nicotine and imidacloprid; fungicides such as ethidium bromide; cardiovascular drugs such as nifedipine; analgesics such as nictetamide; sulfadrugs such as sulfapyridine; synthetic alcoloids such as chloroquine and plasmocid; antiseptics such as proflavine, ethacine and isoniazid; natural alcoloids such as quinine, emetine and papavarine; vitamin B5, nicotinic acid, nicotinamide vitamin B6, pyridoxal and pyridoxamine; nicotinamide adenine dinucleotide the pyridine ring has been studied extensively both experimentally1,2 and theoretically3-6. However, we believe that the potentially active pyridine derivatives deserve more detailed and systematic theoretical studies using updated computer programs and knowledge on structure activity relations.

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\begin{align*}
3,5-\text{Dichloro pyridine} \\
2,3-\text{Dichloro pyridine} \\
2,6-\text{Dichloro pyridine} \\
2,3,5-6-\text{Tetrachloro pyridine} \\
Pentachloro Pyridine \\
3,4,5-\text{Tribromo pyridine} \\
2,3,4-\text{Tribromo pyridine} \\
2,4,6-\text{Tribromo pyridine} \\
3,4,5-\text{Tribromo pyridine} \\
2,3,6-\text{Tribromo pyridine} \\
2,3,4,5-\text{Tetrabromo pyridine} \\
2,3,5,6-\text{Tribromo pyridine} \\
Pentabromo pyridine
\end{align*}
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Scheme1: Protonation pattern for pyridine derivatives

In this work, the acidity–basicity behaviours of some chloro- and bromo- substituted pyridine derivatives were investigated using HF and DFT methods. The calculated acidity constants, nucleophilicities, electronic charges and substituent constants were compared with the experimental pK\textsubscript{a} values\textsuperscript{5} and an acceptable correlation was observed.

References