



Original Research Article

The prediction of thermo physical, vibrational spectroscopy, chemical reactivity, biological properties of morpholinium borate, phosphate, chloride and bromide Ionic Liquid: A DFT Study

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ABSTRACT

In the light of computational chemistry, based on morpholinium cation-based Ionic Liquid, their different types of physical, chemical, and biological properties is highlighted. The physical properties are evaluated through the Density Functional Theory (DFT) of Molecular Mechanics and also examine the chemical and biological properties. The difference between Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) is starting from 11.19 to 4.00, which means that their chemical reactions change as soon as an anion change is done. Biological activity of predictions given by QSAR calculation is forecasted. Where the value of all the LogP that is available is positive, which indicates hydrophobic, on the other hand, PIC50 calculations are found that all the values below 5 are biologically active. To identify these molecules, computational data is used to determine the vibrational spectrum and electronic spectrum.

Keywords: HOMO, LUMO, Vibrational spectroscopy, QSAR, and UV visible spectrum

Introduction

At present, morpholine is widely used in rubber and color industries as additive materials (1). The second use area in chemical industries as solvents for their low polar nature and low cost. The great deal is as solvents in synthetic process in solvent in organic synthesis, reactions and chemical industry research (2-4). It is also used in the manufacture of paper, glass, soap, detergent, dye and synthetic fiber (5). Morpholine is colorless and free of suspended matter. In recent time, it is finding as target additive molecule in both fossil fuel and nuclear power plant steam systems due to have pH adjustment (6, 7). The another key point of morpholine is a heterocyclic chemical compound containing both of nitrogen and oxygen atoms, which indicates amine and ether functional groups and focusing the amine groups becoming as morpholinium salt. Morpholine is a base due to the presence of the amine showing nucleophilic character typical of secondary amines (8). On the other hand, in the medical sciences, new discoveries of scientists have to be searched for new drugs day by day. The reason is that side effects of these medicines on human body and searching more effective medicines developed from rows. In medical science, about 20 drugs contain the morpholine moiety which was approved by FDA, although it is often metabolically labile. Morpholine-based analogues may advantageously alter important pharmacokinetic properties such as lipophilicity and metabolic stability (9). It was grafted into molecular scaffolds in previous case. The overall pharmacokinetics, it was inactive in experimental models of systemic mycoses. In reason strong protein binding and/or rapid metabolism and toxicity considerations have so far not allowed the further development of systemically active morpholines based drugs. If we go into our body after using morpholine as a drug, it may lead to headaches, stomach problems, respiratory problems, lightheadedness, kidney problems, and obstruction of blood circulation. Again, as an alternative to morpholine, scientists are trying to detect any other drug. On the other hand, since 2007, Ionic Liquid has played an important role in liquid drug discovery. Another quality of the third generation of Ionic liquid is bio active and they are called designer molecule. For these reasons it is very easy to invent new drugs by Ionic Liquid (10-12) for its tunable physical and chemical properties. During last five years, some researchers added different types of anion with morpholine to synthesize some morpholinium based ionic liquids for different purposes. Some ammonium carboxylate anion based ionic liquids were established as bioactive molecules by M. Ismail and A. Kumer 2017, 2018 (13-16). Some of which are biologically active and toxic much less than it parent molecule. It is extremely important for its anti-microbial activity to use one of the ingredients as a drug. If anti-microbial activity