Poster

Synthesis, crystal structure, biological properties and theoretical calculations of 2-(2-aminophenyl)-1H-benzimidazol-3-ium dichloride

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Heterocyclic compounds such as benzoglyoxalines or benzimidazoles, better known as benzimidazoles, exhibit a wide range of physical properties [1] and pharmacological activities [2], making them useful for therapeutic purposes [3-5]. In the context of our research work, we synthesized the dichloride of 2-(2-aminophenyl)-1H- benzimidazol-3-ium, a hybrid compound derived from benzimidazoles. This compound is described as a benzimidazole linked to an aniline ring, containing two chloride ions Fig. 1. Both strong and weak hydrogen bonds have been observed between the different entities. The hybrid compound was characterized by infrared and UV-visible spectroscopy as well as single-crystal X-ray diffraction, revealing a structure that crystallizes in space group P-1 of the triclinic system. To better understand molecular interaction, a Hirshfeld surface analysis was also conducted. Moreover, biological properties, as well as theoretical calculations, have been conducted.

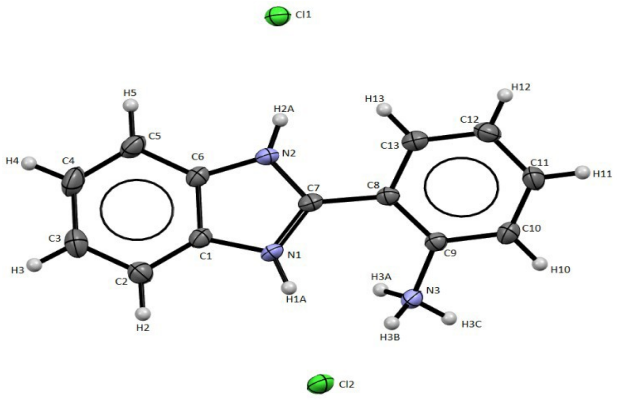

Figure 1 : Ortep [1] of 2-(2-aminophenyl)-1H-benzimidazol-3-ium dichloride

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