Investigation of Major Intermolecular Interactions in 7,8-dihydrobenzo(k)phenanthridin-6(5H)-one Crystal Using Quantum Calculations and Crystallographic Visualization Programs

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Abstract

Currently, tablets and capsules are the most common ways of delivering drugs. The active pharmaceutical ingredients and excipients used to make those tablets and capsules are in their crystalline form generally. However, a single molecule can form multiple different crystal structures because of different packing arrangements of the molecules. These different crystal structures have identical chemical composition but different properties such as solubility, density, stability, etc. This phenomenon is called polymorphism. Occurrence of polymorphism could be a disaster for both patients and pharmaceutical companies, as the drug could lose its efficacy due to changes in properties. Studying intermolecular interactions in crystals can give us a better understanding of how and why molecules pack together in a certain way. In this research, 7,8-dihydrobenzo(k)phenanthridin-6(5H)-one is the molecule investigated. Its crystal data files were obtained from the Cambridge Crystallographic Data Centre. A crystallographic visualization program called Mercury was used to observe all contact modes and measure distances between atoms. Quantum calculations were performed using Density Functional Theory. Then, Fukui functions and electrostatic potentials for both the crystal and the molecule were calculated. These properties were mapped on the molecule's Hirshfeld surface and on molecular slices using OpenDX software to help visualize intermolecular interactions. Comparison between crystals and molecules was performed to observe how these properties change when molecules form crystals. These mapped properties were helpful to analyze major intermolecular interactions, but further analysis on other compounds is needed in order to fully explain molecular packing in crystals and predict crystal structures.