UNIVERSITI TEKNOLOGI MARA

PREDICTION ON INTERACTION OF BIURET MOLECULE ON UREA CRYSTAL BY USING MOLECULAR MODELLING TECHNIQUE

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ABSTRACT

In this study, the morphology of urea as well as its interaction with biuret is the subject of interest. The objectives of this study are to examine the morphology of urea crystal by using molecular modelling (HABIT98) and to assess the surface interaction between urea and biuret molecule on urea faces. By using HABIT 98, the energies of urea crystals, which include lattice energy and attachment energy of urea crystal are calculated. Upon obtaining these values, the morphology of urea crystal is visualized by using SHAPE. Material Studio is also use in order to visualize the functional group of urea for every faces. Systematic Grid-Based Search is then utilized to evaluate the highest interaction energy between urea and biuret molecule to urea faces by taking into account four faces of urea which are (001), (110), (111), and (-1-1-1). From the findings, it can be observed that (001) face is the fastest growing face whereas (110) face is the slowest growing face. The prediction also shows that the interaction of urea and biuret molecule both favor (001) and (-1-1-1) faces.

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INTRODUCTION

1.1 RESEARCH BACKGROUND

Crystallization is a process that is widely being applied in the pharmacology and chemical industry. It is a process occurred when the solubility of a compound in a solvent is low or limited at a certain temperature or pressure and will produces crystals of high purity. However, a compound is able to crystallize in various shapes or may have many polymorphisms. This ability is related to the underlying solid-state physics and chemistry, and dependent upon external parameters such as the level of supersaturation and the type of solvent (Bisker-Leib and Doherty, 2001). Besides that, temperature, pH, and cooling rates will also affect the morphology of the crystals. The study of morphology allows us to have a deeper knowledge on the structure and shape of the crystals. This study is not only important in the nanotechnology, but also in the pharmaceutical industry where it is being applied in the production of medicine (Hammond, et al., 2007). Manipulating the morphology of the crystal in medicine may for instance optimized the targeting of cancer cells. Hence, by understanding the crystal structure, the crystals shape and morphology are able to be predicted and can be manipulated in order to meet the desired performance characteristics of interest.

In this study, urea is the subject of study. It is theoretically known that urea crystals will grown into a needle-like structure when crystallize in water solution. The needle-like structure of the urea crystals are the result of different growth speed of two relevant faces {001} and {110}, which are known to grow fast and slow respectively (Salvalaglio, et al., 2013). The appearances of needle crystals are unwelcome due to the problem that it may create as it is hard to be handled especially during the downstream processes such as solid-liquid filtration and powder flow. However, the growth of the crystal are able to be control either by