Investigating the Molecular Formation Properties of 4-(2-Oxobenzothiazolin-3-YL) Butanoic Acid using PM3, AM1, MNDO Methods

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In this study in order to the geometry optimization of the 4-(2-oxobenzothiazolin-3-yl) butanoic acid crystal, which is used for forming analgesic and antienflamatuar medicine and of which crystal structure was determined using x-ray diffraction method, PM3 (Parametric Model 3), AM1 (Austin Model 1) and MNDO (Modified Neglect of Diatomic Overlap) semi emprical molecular orbital methods found in the HyperChem program were used. By the geometry optimization geometric parameters of the molecules having the minimum energy were found. These values which were theoretically obtained were compared with the emprical values obtained by x-ray diffraction method. These results showed that for the $C_{11}H_{11}NO_3S$ crystal, in bond lengths AM1 method and in bond angles MNDO method was found to be consistent with the emprical x-ray diffraction data. By geometry optimization using PM3, AM1 and MNDO methods relevant energy values of the molecular structure were calculated.

Keywords: semi emprical molecular orbital methods, PM3 AM1 MNDO, oxobenzothiazolin butanoic acid