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Interrelation of crystal morphology and intermolecular contacts in a new thiophosphoramide structure: an energy framework analysis

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The morphology of the crystal structures is an influencing factor on some physical properties. Particularly, morphology affects the dissolution rate, tabletibility, and stability of pharmaceuticals [1,2]. In a crystal lattice, the morphological feature originates from the intermolecular interactions [3,4]. Understanding the interplay of "intermolecular interactions" and "morphological features" can help to provide insight into changing the properties. Herein, the synthesis, characterization, and crystal structure of a new thiophosphorylated thiourea with the formula $(C_2H_5O)_2P(S)(NHC(S)NHCH_2(C_4H_7O))$ is reported. The N—H···S═C and C—H···S═C hydrogen bonds are the strongest intermolecular interactions, which appear as red spots on the Hirshfeld surface map and propagate the molecular assembly along the *b*-axis. The energy frameworks, calculated using CE-B3LYP/6-31G(d,p) method, show that these interactions take part in the most potent molecular pairs (with the energy values of –57.2 and –48.8 kJ/mol) in the structure. Interaction energies in two other directions are remarkably weaker. The combinations of the interactions in the *b*-direction with some weaker interactions lead to the formation of plates parallel to the *ab*-plane. The plates (with a thickness of about 1 nm) are stacked together with the weakest interactions. This feature reduces the ability of the crystal to grow in the *c*-direction compared to the *a*- and *b*- directions.

Keywords: Thiophosphoramide, Morphology, Interactions, Energy framework, DFT

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