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The Role of Solvent Hydroxyl Functional Groups on the Interaction Energy and Growth of Form i Paracetamol Crystal Facets

Shahrir, Nurshahzanani[a]; Anuar, Nornizar[a] ✉; Abdul Muttalib, Nur Aisyah[a]; Yusop, Siti Nurul'Ain[a]; Abu Bakar, Mohd. Rushdi[b]; Adam, Fatmawati[c]; Ibrahim, Siti Fatimah[d]

Save all to author list

[a] School of Chemical Engineering, College of Engineering, Universiti Teknologi MARA, Shah Alam, 40450, Malaysia

[b] Department of Pharmaceutical Technology, Kulliyyah of Pharmacy, International Islamic University Malaysia, Bandar Indera Mahkota, Kuantan, Pahang, 25200, Malaysia

[c] Faculty of Chemical and Process Engineering Technology, Universiti Malaysia Pahang, Lebuhraya Tun Razak, Kuantan, Pahang, 26300, Malaysia

[d] Malaysian Institute of Chemical and Bioengineering Technology, Universiti Kuala Lumpur, Lot 1988, Kawasan Perindustrian Bandar Vendor, Simpang Ampat, Alor Gajah, 78000, Malaysia

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Abstract

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Abstract

The morphology of a crystal grown in a solvent can change depending on the solvent used during the crystallization process. Modification of the morphology of a crystal can be engineered based on information conferred by the functional groups of the facets of interest and the functional

groups of the solvent . This study aims to predict the effect of the alcoholic functional group of amyl alcohol, benzyl alcohol, and phenol on the {002}, {011}, and {110} facets of Form I paracetamol . Prediction and simulation studies were carried out using an embedded tool available in Material Studio. The interaction between the solvents (phenol, benzyl alcohol, and amyl alcohol) and the surfaces used in this study revealed that the {011} facet had the most negative nonbonded energy , followed by the {110} and {002} facets . Overall, the nonbonded interactions between the solvents and the facets were dominated by Coulombic interactions, accounting for more than 90% of the energies, which is within the range from -2566 to -3613 kcal/mol. The binding energy for amyl and benzyl alcohols on the facets of the crystal , ranked from the strongest to the weakest, was in the order {002} > {110} > {011}, while for phenol, the rank was {002} > {011} > {110}. This result is in line with the observed crystal morphology of Form I paracetamol crystallized in a polar protic solvent , in which the most favorable solvent binding on the {002} facets delayed the growth of the elongated hexagonal morphology along the c-axis and formed prismatic-like morphology. Using benzyl alcohol as a case study, an assessment of synthon formation on facets {002} and {011} showed that synthon B is an important synthon for the growth of units of these facets , while synthon F is an important building block synthon for the {110} facet . © 2022 American Chemical Society.

Author keywords

binding energy ; crystal facet ; functional group ; nonbonded interactions; solvent effect; synthons

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Anuar, N.; School of Chemical Engineering, College of Engineering, Universiti Teknologi MARA, Shah Alam, Malaysia; email:nornizar@uitm.edu.my

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