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Crystal Engineering of Ibuprofen Compounds: From Molecule to Crystal Structure to  
Morphology Prediction by Computational Simulation and Experimental Study

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**ABSTRACT:**

We selected the crystal structures of ibuprofen with seven common space groups ( $Cc$ ,  $P2_1/c$ ,  $P2_12_12_1$ ,  $P2_1$ ,  $Pbca$ ,  $Pna2_1$ , and  $Pbcn$ ), which was generated from ibuprofen molecule by molecular simulation. The predicted crystal structures of ibuprofen with space group  $P2_1/c$  has the lowest total energy and the largest density, which is nearly indistinguishable with experimental result. In addition, the XRD

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