

COMPUTED CRYSTAL ENERGY LANDSCAPES AS AN AID TO UNDERSTANDING POLYMORPHISM

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The fundamental scientific and industrial interest in controlling crystallisation is inspiring the development of methods of predicting which crystal structures are thermodynamically feasible. Frequently, computing this crystal energy landscape will reveal that there are many crystal structures that are approximately equi-energetic compromises between the various intermolecular interactions allowed by the conformational flexibility. Contrasting these crystal energy landscapes with the solid forms found experimentally shows the capacity to rationalise and predict polymorphism, disorder and a propensity for solvate formation. By providing ideas about likely packing motifs, it can help with the solution of crystal structures from powder.

Price SL 2008. Computed crystal energy landscapes for understanding and predicting organic crystal structures and polymorphism. [Accounts Chem Res](#) 2009, 42, 117-126.