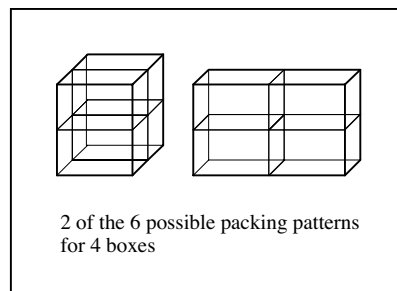


W0025

A New, Simple Description of Crystal Packing. E. Pidcock, W.D.S. Motherwell, Cambridge Crystallographic Data Centre, 12 Union Rd., Cambridge, CB2 1EZ. UK.

A new model of crystal packing has been proposed that describes unit cells and their contents in terms of “packing patterns”.¹ These packing patterns were derived from a consideration of the ways in which boxes of unequal dimensions can be stacked with faces touching and edges aligned. For example, there are six ways of stacking four boxes in a “close-packed” manner, two of which are shown. The resulting arrays of boxes have the same total volume but different surface areas. An examination of thousands of experimental structures contained within the Cambridge Structural Database² has shown that these packing patterns are a viable description of crystal structures and that molecular dimensions relate to unit cell dimensions in a systematic way. The packing patterns are not populated equally by experimental structures; packing patterns characterised by low surface area and most equal dimensions are preferred. Correlations are found between broadly-defined molecular shapes and the packing pattern utilised. In addition the position of the molecule in the unit cell is restrained by the packing pattern. Applications of the new model to the fields of crystal structure prediction and polymorphism will be discussed.



1. E. Pidcock & W.D.S. Motherwell. **2003**. *Chem. Comm.* 3028
2. Allen, F.H. **2002**. *Acta Cryst.* B58, 380