

SHORT COMMUNICATIONS

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Multiplicity of crystal planes belonging to the point group $\bar{4}m2$. Erratum

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Abstract

There is an error in Table 10.2.2 of *International Tables for Crystallography*, Vol. A (Hahn, 1992, 1995). The multiplicity of (00*l*) and (00 \bar{l}) belonging to the point group $\bar{4}m2$ is 2 not 1. The equivalent reflections in the point group $\bar{4}m2$ (Ibers, 1967; Ibers & Hamilton, 1973) are

$$hkl = \bar{h}kl = h\bar{k}l = \bar{h}\bar{k}l = kh\bar{l} = k\bar{h}\bar{l} = k\bar{h}l = \bar{k}\bar{h}l.$$

Substitution of $h = k = 0$ into the above relation results in $00l = 00\bar{l}$. Therefore, the multiplicity of 00*l* or 00 \bar{l} in the point group $\bar{4}m2$ is 2.

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Ab initio molecular packing analysis

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Abstract

A method is presented which, given a molecular structure and an intermolecular force field, can predict observed polymorphic crystal structures and molecular clusters without any prior assumption of space symmetry.

1. Introduction

In molecular-packing calculations, symmetry constraints are often used to simplify the problem. For example, in early benzene molecular-cluster calculations, Williams (1980) assumed inversion symmetry and limited consideration to clusters containing an odd number of molecules. More recently, symmetry constraints were removed and four different energy-minimum structures for the benzene tetramer cluster have been predicted (Williams, 1992). In the earlier work, 13- and 15-molecule clusters showed some resemblance to the structure of crystalline orthorhombic benzene. Of course, the structure of a sufficiently large cluster should become identical to the crystal. However, the molecular-cluster approach to crystal structure prediction can quickly become intractable because each additional molecule contributes six degrees of freedom to the calculation. When one is attempting to predict a crystal

References

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structure, it is computationally expedient to assume lattice symmetry, *i.e.* repetition of unit cells in three-dimensional space.

In the traditional approach to prediction of crystal structure from a known molecular structure, the observed crystal space group is utilized. An early example is the prediction of the dibenzoylmethane (IUPAC name: 3-hydroxy-1,3-diphenyl-2-propen-1-one) crystal structure in *Pbca* (Williams, 1966); in this case, a very approximate force field was used along with the observed cell constants. Very often, development of force-field parameters has utilized molecular-packing calculations where the aim was to minimize the difference between the calculated energy-minimum structure (relaxed structure) and the observed structure. The accuracy of today's available intermolecular force fields reflects heavy dependence on such crystal structure calculations.

In the preceding case, only small deviations are considered from observed crystal structures and the space group is known. But what if only the molecular structure is known and the crystal structure must be predicted from first principles? Gavezzotti (1994) has recently reviewed possible approaches to this question. The overwhelming success of experimental diffraction methods has no doubt removed much of the urgency to develop *ab initio* crystal structure prediction, but successful