# Approximate Symmetry in Organic Structures in Low-Symmetry Space Groups

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A survey of organic P1 structures with R≤0.050 found that approximate symmetry is pervasive when Z=Z'>1. In some cases the P1 structure is clearly the result of cooling a higher symmetry crystal, but 40% of the structures that seem to be distorted forms of structures having smaller asymmetric units were determined at room temperature. That observation suggests that some low-symmetry structures with Z'>1 could be the result of a deformation of a higher-symmetry crystal nucleus, with the symmetry lowering occurring during the early stages of crystal growth. The same seems to be true of P1, Z=1 crystals of symmetric molecules.

To investigate further the prevalence of approximate symmetry other low-symmetry groups were considered. The numbers of organic Z'≥1, R≤0.050 structures in groups P2, Pm, Cm, P2/m, and C2/m are all less than 20; the number in P21/m is not quite 60. There are too many structures in groups P1-bar and P21 to look at individually. That leaves groups #5 (C2, I2), #7 (Pc, Pa, Pn), #9 (Cc, Ia), and # (P2/c).

In this project the organic structures in space group #7 were investigated. The R≤0.050 requirement was again imposed to limit the number of structures and help ensure their reliability. As of November 2019 there were 392 Z'>1 structures that met those requirements and 982 Z'=1 structures, with a substantial fraction of the 982 containing molecules that could lie on a special position.

About 10% of the Pc/Pa/Pn Z'>1 structures should almost certainly have been refined in a smaller and/or higher-symmetry unit cell, and about 20% seem to have no approximate symmetry. Of the remaining structures about a third seem either to be distorted versions of a P21/c cell or to mimic that symmetry (as must be the case if the material is enantiomerically pure). A little more than 10% seem to be derived from or mimic Cc packing. A few have approximate symmetry that points to an orthorhombic group (e.g., Pca21, Pna21, Aea2) or a trigonal or tetragonal group.

In only ca. 60% of the structures that have approximate symmetry is that symmetry periodic in three dimensions. In most of the rest the approximate periodic symmetry is confined to layers but there are also structures in which it is limited to columns of molecules.

The temperature is listed as ≥293 K in about a quarter of the structures having approximate periodic symmetry.