Approximate Symmetry in *P*2 and *C*2 Organic Structures

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The crystal packing in well-determined, organic, $Z^* \geq 1^{\dagger}$ structures in groups #3 (*P*2) and #5 (*C*2/*A*2/*I*2) has been analyzed. The study completes the survey of packing in organic structures archived in the CSD that have $R \leq 0.050$ and that were reported in low- symmetry (SG# ≤ 8), low-frequency (< 5000 entries) space groups. Surveys of the structures described in *P*1[1] and in group #7 (*Pc*/*Pn*/*Pa*)[2] have already been published.

There are only 6 such structures in group #6 (*Pm*) and only 12 in #8 (*Cm*), with a number of those being either suspicious or very inorganic.

In only 2% of the *ca.* 550 *P*2 and *C*2, $Z^* \geq 1$ structures investigated does crystallographic symmetry seem to have been overlooked; for the structures in *P*1 and *Pc* that value was 8%. Approximate periodic symmetry, however, is again found in more than 80% of the structures in which it is possible ($Z' > 1$ or molecular symmetry). The most common categories are approximate translations, mimics of SG #15 (*C*2/*c*, *etc.*), and structures having additional symmetry that is periodic only within layers.

In most cases the distortions that make a translation approximate seem too large to have been the result of cooling through a phase transition. That observation suggests that it may be common for a crystal nucleus to have a smaller (or perhaps more symmetric) unit cell than does the macroscopic crystal.

In another important group of *C*2 structures there are two independent layers related by an approximate rotation perpendicular to the monoclinic axis (*e.g.*, a rotation around **a**) that is paired with a translation that is not close to either 0 or (*e.g.*) **a**/2. That observation suggests slippage of layers during the very early stages of crystal growth.

(†) Z^* is the number of independent formula units. If $Z' = 1$ but both units lie on twofold axes then $Z^* = 2$.

References

*{1} C. P. Brock (2022). Acta Cryst. B**78**, 576-588.*
*{2} C. P. Brock (2023). Helv. Chim. Acta **106**, e202200170.*