GI-MS48-P11 | PERVASIVE APPROXIMATE SYMMETRY IN P1 AND HIGH-Z' ORGANIC CRYSTALS

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Ca. half (*i.e.*, 750) of the organic crystal structures in space group *P*1 with Z > 1, and *ca.* 300 more with Z' > 4 (Brock, 2016; *Acta Cryst.* B72, 807), have been investigated in detail. Obvious approximate symmetry has been found in well over 50% of them, while overlooked symmetry was identified in only *ca.* 10% of the *P*1 structures and 5% of the *Z'* > 4 structures. Approximate 2_1 screw axes, pseudoinversion centers and pseudotranslations all occur frequently; pseudoglides are less common. A program to find and characterize pseudotranslations (*i.e.*, modulations) has been written (Taylor & Brock, in preparation) and used to find relationships between phases.

The *P*1 structures examined were not chosen randomly; ca. 60% of them have a cell angle in the range 88.5 – 91.5° because such structures are especially likely to have been described in a cell of too-low symmetry. *Ca*. 10% more are kryptoracemates, quasiracemates, and compounds of diastereomers. Another *ca.* 10% were found using the new program that identifies pseudotranslations.

About a quarter of the *P*1, *Z* > 1 structures examined have obvious layers with approximate 2-D symmetry higher than the 3-D symmetry of the crystal. Offsets between adjacent layers account for the symmetry lowering. If interlayer forces are weaker than intralayer forces then deformations during the early stages of crystal growth are more likely between layers than within them. Perhaps the crystal nucleus is often more symmetric than the macroscopic crystal.