

W0120

The Unusual Phases of Anhydrous and Hydrated Pinacol. Carolyn P. Brock, Xiang Hao, Sean Parkin, Dept. of Chemistry, Univ. of Kentucky, Lexington, KY 40506-0055, USA.

Pinacol (2,3-dimethyl-2,3-butanediol) confounds expectations about how molecules should pack. Most small molecules crystallize with $Z' \leq 1$ in centrosymmetric space groups that are monoclinic or triclinic. Hydrates are expected to contain a small number of independent water molecules. Anhydrous pinacol, however, has two conformers (*gauche* and *trans*) located on three kinds of symmetry sites in $C2/c$ (Jeffrey & Robbins, 1978). Also in the Cambridge Structural Database are a tetragonal hexahydrate (Kim & Jeffrey, 1970), and a hexagonal structure that is chiral (Dahlqvist & Sillanpaa, 2000).

Twin refinements of new data for the hexahydrate support the suggestion that it is orthorhombic and twinned; significant diffuse scattering has been found. The hexagonal structure, which contains large channels, seems to have an uncertain composition.

A monohydrate that seems to have been mentioned in the literature as being orthorhombic has been solved and refined as a twinned, monoclinic structure.

The small size of the pinacol molecule and the high density of H-bonding groups are probably responsible for the unusual and varied structures.

Jeffrey & Robbins (1978); *Acta Cryst.* **B34**, 3817-20.

Kim & Jeffrey (1970). *J. Chem. Phys.* **53**, 3610-15.

Dahlqvist & Sillanpaa (2000). *J. Mol. Struct.* **524**, 141-9.