

Cool Structures: Unique/Problem Structures in the Daily Life of a Staff Crystallographer

Michael R. Gau

University of Pennsylvania, Philadelphia, PA 19104, USA, gaum@sas.upenn.edu

A variety of small molecule crystal structures will be presented that display interesting and challenging problems. As a staff crystallographer at the X-ray crystallography facility at the University of Pennsylvania (U Penn), we encounter multiple structures with issues such as whole molecule disorder, disorder on a special position, twinning, desolvation and compositional disorder to name a few. A step-by-step manner will be presented that describes our thought process and of how we are able to successfully model the molecular structures. The structures presented include organic compounds, as well as, inorganic complexes that have been grown by various research groups at U Penn and collected on our Bruker APEXII DUO or D8 Quest.