

# Poster Presentations

## [MS11-P01] A 1:1 Twinned Structure Described Equally Well in Space Groups P-1 and P21 .A. David Rae,

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The commensurately modulated structure of bis(acetylacetonato)(s-trans-1,4di-tert-butylbuta-1,3diene)ruthenium(II) [1] can be refined as a 1:1 twin with intensities  $[|F(hkl)|^2 + |F(h-kl)|^2]/2$  to give good quality refinements using either the space group  $P2_1$  or the space group  $P-1$ . In both instances the asymmetric unit consists of 8 pseudo- glide related molecules. It is the equal twinning that allows the dual solutions. An equal 4-fold twin of  $P1$  symmetry is also a possible model but this would double the size of the asymmetric unit. The structure can be described as a displacive modulation of a  $P2_1/n$  parent structure with a first order modulation wave described by  $\mathbf{q} = 0.75 \mathbf{c}^*$  where  $\mathbf{a}^*$ ,  $\mathbf{b}^*$ ,  $\mathbf{c}^*$  are the vectors describing the reciprocal lattice of the parent structure. This allows reflexions to be re-indexed in (3+1) dimensions with alternative indexing for  $h,k,l,m$ . The structure was initially solved as untwinned  $P2_1$  but shown to be 1:1 twinned. It was then shown that it was possible to initiate the refinement of the alternative structure with sufficient accuracy by simply moving the origin of the asymmetric unit when both space group options are in their standard settings and the pseudo glide planes are at  $y = \pm 1/4$ . Understanding the reasons why the structures are semi equivalent and why the initiation of the alternative structure works requires (3+1)-dimensional crystallography. However the refinements themselves can be carried out using 3-dimensional crystallography. A glide plane cannot be a symmetry element of the 3-dimensional structures. 3 comparative refinements were carried out for each space group. The first used the same local coordinates for each pseudo glide related ligand and these

were refined with respect to separately refined orthonormal axial systems and also used separate  $TLX$  rigid body parameters for each molecule. The second removed the constraints on positions and the third also removed the constraints on anisotropic atom displacement parameters. It was found that although the extra parameters improved the goodness of fit it also increased the standard errors compared to assuming the constraints were exact. It could be concluded that changes created by the extra parameters were not significant and that the average molecule was well determined by the most constrained refinements.

[1] Hänel, Hopf, Jones, Bennett, Hockless & Rae, (to be published)

**Keywords:** modulated structure, twinning, refinement.