MS28-1-4 RESI, steady, go! Using the RESI tool in SHELX to help refine high Z' structures.
#MS28-1-4

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Abstract
Crystal structures with more than one molecule in the asymmetric unit have been of interest in recent years, for example via collating projects run by Prof. Jon Steed at Durham University in the UK. In this work, new polymorphs or entirely new structures with moderate to high Z' values will be presented.
The Z' = 1 structure of trimellitic acid appears twice in the CSD, in both cases from the early 1970's and measured at room temperature [1,2 & Fig 1 (left)]. Here, new polymorphs with Z' = 6 and 10 will be discussed. Intriguingly, these both originate from crystallisations in the presence of lanthanide salts.
There is also a Z' = 1 entry in the CSD for 4-(methoxycarbonyl)benzoic acid, which is mono-methylated terephthalic acid. [3 & Fig 1 (right)] Here, a new polymorph with Z' = 3 is discussed.
The last structure is a new Pd-phosphine complex incorporating a long C_{18} chain and having a remarkable Z' = 20. Crystallising compounds with long greasy chains is often troublesome, but has been achieved for this and several similar compounds.
Clearly, the mechanics of refining such high Z' structures is a challenge. This starts with atom labelling to incorporating H atoms, and then analysing geometrical features, etc, and so the RESI command in SHELX has been explored to see how it might help in such cases. As a novice user of this command, even after nearly 30 years in crystallography, some discussion with more experienced users of RESI would be welcomed.

References
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Figure 1.