Non-merohedral Twinning in Small Molecule and Protein Crystallography

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In contrast to twinning by merohedry the reciprocal lattices of the different domains of non-merohedral twins do not overlap exactly. If both twin domains are similar in size, there are often problems with the cell determinations and usual automatic indexing programs fail. But nowadays there are several programs that can deal with such kinds of problems [1], [2], [3].

In principle two different integration procedures are possible. The simpler one would be to integrate with all orientation matrices separately in different runs. This leads to three kinds of reflections: the reflections with no overlap, the reflections with an exact overlap, and the reflection with a partial overlap of a reflection of a second domain. A better way of integration is to use all orientation matrices in one step. Then the whole intensity of every reflection is integrated and we only have non- or exactly overlapped reflections [4], [5].

A special program for scaling and absorption correction is necessary to handle such data sets [6].

Refinements with data sets generated by different integration processes will be compared [7].

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