

Inverting racemic twins for “special” space groups ... From the SHELX-97 manual (page 6-2 to 6-3).

G. Sheldrick 1997

“For most space groups 'inversion' of the structure simply involves inserting an instruction 'MOVE 1 1 1 -1' before the first atom. Where the space group is one of the 11 enantiomorphous pairs [e.g. P31 and P32] the translation parts of the symmetry operators need to be inverted as well to generate the other member of the pair. There are seven cases for which, if the standard setting of the International Tables for Crystallography has been used, inversion in the origin does **not** lead to the inverted absolute structure. This problem was probably first described in print by Parthe & Gelato (1984) and Bernardinelli & Flack (1985), but had been investigated previously by D. Rogers”

The offending space groups and corresponding correct MOVE instructions are:

Fdd2	MOVE	0.25	0.25	1	-1
F4(1)32	MOVE	0.25	0.25	0.25	-1
I4(1)	MOVE	1	0.5	1	-1
I4(1)22	MOVE	1.5	0.25	-1	
I4(1)md	MOVE	1.5	1	-1	
I4(1)cd	MOVE	1.5	1	-1	
I-42d	MOVE	1.5	0.25	-1	