

How-to-do : Inverting non-polar Space groups

P 3<sub>2</sub> 2 1 --> P 3<sub>1</sub> 2 1

Change SYMM to

SYMM -Y, X-Y, 0.33333+Z

SYMM Y-X, -X, 0.66667+Z

SYMM Y, X, -Z

SYMM X-Y, -Y, 0.66667-Z

SYMM -X, Y-X, 0.33333-Z

MOVE 1 1 1 -1

P 3<sub>1</sub> 2 1 --> P 3<sub>2</sub> 2 1

Change SYMM to

SYMM -Y, X-Y, 0.66667+Z

SYMM -X+Y, -X, 0.33333+Z

SYMM Y, X, -Z

SYMM X-Y, -Y, 0.33333-Z

SYMM -X, -X+Y, 0.66667-Z

MOVE 1 1 1 -1

P 4<sub>3</sub>2<sub>1</sub>2 --> P 4<sub>1</sub>2<sub>1</sub>2

SYMM -X, -Y, 0.5+Z

SYMM 0.5-Y, 0.5+X, 0.25+Z

SYMM 0.5+Y, 0.5-X, 0.75+Z

SYMM 0.5-X, 0.5+Y, 0.25-Z

SYMM 0.5+X, 0.5-Y, 0.75-Z

SYMM Y, X, -Z

SYMM -Y, -X, 0.5-Z

MOVE 1 1 1 -1

P 4<sub>1</sub>2<sub>1</sub>2 --> p 4<sub>3</sub>2<sub>1</sub>2

SYMM -X, -Y, 0.5+Z

SYMM 0.5-Y, 0.5+X, 0.75+Z

SYMM 0.5+Y, 0.5-X, 0.25+Z

SYMM 0.5-X, 0.5+Y, 0.75-Z

SYMM 0.5+X, 0.5-Y, 0.25-Z

SYMM Y, X, -Z

SYMM -Y, -X, 0.5-Z

MOVE 1 1 1 -1