Higher-Metric Symmetry

1. First transform the cell to the proper Niggli reduced cell.
2. Determine the general type of the cell, that is, if the angles are < 90 °, then the cell is type I, and if the angles are ≥ 90 ° then the cell is of type II.
3. Determine the values for *A*, *B*, *C*, *D*, *E*, *F* according to the following: $A = \boldsymbol{a}\cdot\boldsymbol{a}$, $B = \boldsymbol{b}\cdot\boldsymbol{b}$, $C = \boldsymbol{c}\cdot\boldsymbol{c}$, $D = \boldsymbol{b}\cdot\boldsymbol{c}$, $E = \boldsymbol{a}\cdot\boldsymbol{c}$, $F = \boldsymbol{a}\cdot\boldsymbol{b}$.
4. Test the cell type and the conditions on *A*, *B*, *C*, *D*, *E*, *F* in the table below, beginning from the top. When a match is made for the cell type and conditions on *A*, *B*, *C*, *D*, *E*, *F*, then determine the Laue symmetry for the crystal system. If the merging R for the particular crystal system is low (after applying the transform to the *hkl* values of the data), then the proper Bravais lattice for the system has been found. Then apply the transform to both the cell parameters and to the *hkl* values of the data.

Type	*D*	*E*	*F*	Crystal system	Bravais	Transform
A = *B* = *C*						
I	*A*/2	*A*/2	*A*/2	Cubic	*cF*	1 $\bar{1}$1/11 $\bar{1}$/ $\bar{1}$11
I	*D*	*D*	*D*	Trigonal	*hR*	1 $\bar{1}$0/ $\bar{1}$01/ $\bar{1}$ $\bar{1}$ $\bar{1}$
II	0	0	0	Cubic	*cP*	100/010/001
II	-*A*/3	-*A*/3	-*A*/3	Cubic	*cI*	101/110/011
II	*D*	*D*	*D*	Trigonal	*hR*	1 $\bar{1}$0/ $\bar{1}$01/ $\bar{1}$ $\bar{1}$ $\bar{1}$
II	*D**	*D*	*F*	Tetragonal	*tI*	011/101/011
II	*D**	*E*	*E*	Tetragonal	*tI*	101/110/011
II	*D**	*E*	*F*	Orthorhombic	*oI*	$\bar{1}$ $\bar{1}$0/ $\bar{1}$0 $\bar{1}$/0 $\bar{1}$ $\bar{1}$
A = *B*, no conditions on *C*						
I	*A*/2	*A*/2	*A*/2	Trigonal	*hR*	100/ $\bar{1}$10/ $\bar{1}$ $\bar{1}$3
I	*D*	*D*	*F*	Monoclinic	*mC*	110/1 $\bar{1}$0/00 $\bar{1}$
II	0	0	0	Tetragonal	*tP*	100/010/001
II	0	0	-*A*/2	Hexagonal	*hP*	100/010/001
II	0	0	*F*	Orthorhombic	*oC*	110/ $\bar{1}$10/001
II	-*A*/2	-*A*/2	0	Tetragonal	*tI*	100/010/112
II	*D**	*D*	*F*	Orthorhombic	*oF*	$\bar{1}$ $\bar{1}$0/1 $\bar{1}$0/112
II	*D*	*D*	*F*	Monoclinic	*mC*	110/ $\bar{1}$10/001
II	*D**	*E*	*F*	Monoclinic	*mC*	1 $\bar{1}$0/110/ $\bar{1}$0 $\bar{1}$
B = *C*, no conditions on *A*						
I	*A*/4	*A*/2	*A*/2	Tetragonal	*tI*	0 $\bar{1}$1/1 $\bar{1}$ $\bar{1}$/100
I	*D*	*A*/2	*A*/2	Orthorhombic	*oI*	$\bar{1}$00/0 $\bar{1}$1/ $\bar{1}$11
I	*D*	*E*	*E*	Monoclinic	*mC*	011/01 $\bar{1}$/ $\bar{1}$00
II	0	0	0	Tetragonal	*tP*	010/001/100
II	-*B*/2	0	0	Hexagonal	*hP*	010/001/100
II	*D*	0	0	Orthorhombic	*oC*	011/0 $\bar{1}$1/100
II	*D**	-*A*/3	-*A*/3	Trigonal	*hR*	121/0 $\bar{1}$1/100
II	*D*	*E*	*E*	Monoclinic	*mC*	011/0 $\bar{1}$1/100

Type	*D*	*E*	*F*	Crystal System	Bravais	Transform
No conditions on *A, B, C*						
I	*A*/4	*A*/2	*A*/2	Orthorhombic	*oF*	100/ $\bar{1}$20/ $\bar{1}$02
I	*D*	*A*/2	*A*/2	Monoclinic	*mC*	$\bar{1}$20/ $\bar{1}$00/0 $\bar{1}$1
I	*D*	*A*/2	2*D*	Monoclinic	*mC*	$\bar{1}$00/ $\bar{1}$02/010
I	*D*	2*D*	*A*/2	Monoclinic	*mC*	100/1 $\bar{2}$0/00 $\bar{1}$
I	*B*/2	*E*	2*E*	Monoclinic	*mC*	010/01 $\bar{2}$/ $\bar{1}$00
I	*D*	*E*	*F*	Triclinic	*aP*	100/010/001
II	0	0	0	Orthorhombic	*oP*	100/010/001
II	-*B*/2	0	0	Orthorhombic	*oC*	0 $\bar{1}$0/012/ $\bar{1}$00
II	*D*	0	0	Monoclinic	*mP*	0 $\bar{1}$0/ $\bar{1}$00/00 $\bar{1}$
II	0	-*A*/2	0	Orthorhombic	*oC*	100/ $\bar{1}$0 $\bar{2}$/010
II	0	*E*	0	Monoclinic	*mP*	100/010/001
II	0	0	-*A*/2	Orthorhombic	*oC*	$\bar{1}$00/120/00 $\bar{1}$
II	0	0	*F*	Monoclinic	*mP*	$\bar{1}$00/00 $\bar{1}$/0 $\bar{1}$0
II	-*B*/2	-*A*/2	0	Orthorhombic	*oI*	$\bar{1}$00/0 $\bar{1}$0/112
II	-*B*/2	*E*	0	Monoclinic	*mC*	0 $\bar{1}$ $\bar{2}$/0 $\bar{1}$0/ $\bar{1}$00
II	*D*	-*A*/2	0	Monoclinic	*mC*	102/100/010
II	*D*	0	-*A*/2	Monoclinic	*mC*	$\bar{1}$ $\bar{2}$0/ $\bar{1}$00/00 $\bar{1}$
II	*D*§	*E*	*F*	Monoclinic	*mI*	$\bar{1}$00/ $\bar{1}$ 1 $\bar{2}$/0 $\bar{1}$0
II	*D*	*E*	*F*	Triclinic	*aP*	100/010/001

* $2|D + E + F| = A + B$

§ As footnote * plus $|2D + F| = B$