Molecular Crystal Global Phase Diagrams: II. Reference Lattices

by R. B. McClurg and J. B. Keith

Notes to Accompany

Table 6: Structure Classification

Sphere Packing

See MEZDIE01 on pages 14 and 15. Notes refer to the hand-written letters on the following pages.

A. CSD entry MEZDIE01 is described using space group 2 with a single molecule in the asymmetric unit with center of mass located at the Wyckoff site i. The Hermann-Mauguin label (P_-1) is provided for convenience.
B. Unit cell parameters from MEZDIE01.cif
C. Non-dimensional unit cell parameters using the a-axis length as the reference length
D. Notes based on the neighbor histogram (separate document) indicating that there are 6 nearly equi-distant neighbors that are not in a single hemisphere. Therefore the structure appears to approximate a sphere packing. The remainder of the entry serves to classify the packing.
E. Matrix representation for the parameters in C above. Euclidean norms of the columns give the desired magnitudes (1, 1.4527186, and 0.9209443). Dot products of the columns yield the product of the column norms and the cosine of the included angle according to the cosine law. The angles have the expected values (90.47694, 111.67244, and 89.98776 degrees). See Appendix A, equation 1.
F. There is a single molecule in the asymmetric unit at Wyckoff site "i" with point symmetry "1".
G. The fractional center-of-mass coordinates are provided for both molecules in the unit cell. See Appendix A, equations 2 and 3.
H. A transformation matrix is provided which halves the volume of the unit cell (Determinant = ½), rotates the unit cell, and shifts the origin. Halving the volume of the cell recognizes that the center-of-mass lattice has a single molecule in the primitive unit cell. [The observed unit cell has two molecules in the unit cell due to orientation of the non-spherical molecules and minor translations of their centers.] See Appendix A, equations 4, 5, 7, and 8.
I. The inverse transformation matrix is calculated for use below.
J. The dot product of the matrix representation (E above) and the upper-left transformation submatrix (H above) yields the transformed matrix representation. See Appendix A, equation 6. Unit cell parameters are calculated using Euclidean norms and the cosine law as described in E above.
K. The Niggli matrix, normalized using the (new) a-axis length is provided.
L. The Niggli matrix conforms to the "Main Conditions" for a Type II reduced unit cell. Comparing the Niggli matrix to tabulated character definitions reveals that the reduced cell is triclinic (character 44), but close to body-centered-cubic (cI, character 5).
M. Transforming the fractional center-of-mass coordinates (G) using the inverse transformation matrix (I) as indicated in the Appendix, equations 9 and 10, yields the indicated coordinates. Both molecules are near the origin (0,0,0) of a unit cell (modulo unity). This is a necessary condition for successful unit cell volume reduction (H). There is one molecule in the reduced unit cell (Z'=1). See Appendix A, equations 9 and 10.
N. The observed unit cell (MEZDIE01), called the daughter, was observed in a space group with two symmetry operations (|G|=2) and two molecules per primitive unit cell (Z=2) yielding a symmetry density of one (|G|/Z=1). The identified BCC reference lattice

(space group 229) has 48 symmetry operations per primitive unit cell (|G|=48) and one molecule per primitive unit cell (Z'=1 as indicated in M above). The ratio yields a symmetry density of 48 for the BCC reference lattice. The ratios of the Z values gives the "size" and ratios of the symmetry densities gives the "index" of the symmetry-breaking transformation in passing from the reference lattice to the daughter cell. Note that the ratios are in opposite senses.

O. The transformation from the reduced basis for character 5 to the conventional basis is tabulated along with the character definitions. See Appendix A, equations 11, 12, and 14.

P. The matrix inverse of the product of the transformation matrices (H and O) yields the overall transformation matrix from the reference lattice (BCC) to the observed structure. The determinant of the transformation is unity since the conventional BCC reference cell and MEZDIE01 each contain two molecules. See Appendix A, equations 15 and 16.

Q. COPL indicates that the overall transformation matrix is consistent with the indicated symmetry-breaking transition with size 2 and index 48 as calculated in N above. The order parameter is coupled.

A

2i P_-1
MEZDIE01

B

a=	9.920097
b=	14.51031
c=	9.135857
alpha=	90.47694
beta=	111.6724
gamma=	89.98776

C

b/a=	1.4627186
c/a=	0.9209443
alpha=	90.47694
beta=	111.67244
gamma=	89.98776

D

6 neighbors within 3% of nearest
next neighbor 11% farther than nearest
sphere packing

E

Matrix Representation

1	0.0003125	-0.340105
0	1.4627185	-0.007593
0	0	0.8558094

a	b	c
1	1.4627186	0.9209443
90.47694	111.67244	89.98776
alpha	beta	gamma

F

i 1

G

Center of Mass Coordinates

x,y,z	0.7605859	0.2506235	0.24179	1
1-x,1-y,1-z	0.2394141	0.7493765	0.75821	1
x=	0.7605859			
y=	0.2506235			
z=	0.24179			

H

Transformation to Reduced Cell

0.5	0.5	0	0.75
0.5	-0.5	0	0.25
0.5	0.5	-1	0.25
0	0	0	1

Det= 0.5

I

Inverse Transformation

1	1	0	-1
1	-1	0	-0.5
1	0	-1	-0.5
0	0	0	1

Det= 2

Matrix Representation

0.330103967	0.329791489	0.340104544
0.727562585	-0.735155941	0.007593356
0.427904687	0.427904687	-0.855809373

a	b	c
0.906321337	0.912315244	0.920944321
107.9992896	107.3143809	107.0838036
alpha	beta	gamma

Normalized Niggli Matrix

1	1.01327063	1.032529194
-0.316067389	-0.302416346	-0.295712962

0,0,0	0.011209412	0.009962353	0.018795882	1	Z'= 1
	-0.011209412	-1.009962353	-1.018795882	1	

	|G|	Z	|G|/Z
Daughter	2	2	1
Ref. Lattice	48	1	48
		2	48
		(size)	(index)

Reduced Cell

Character	44 (aP)	... but close to 5 (cI)	
Type	II		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤a.a/2	True

Transformation to Conventional Cell

0	1	1	0
1	0	1	0
1	1	0	0
0	0	0	1

Det= 2

Overall Transformation

0.5	-1	-0.5	0
0.5	1	-0.5	-0.5
0.5	0	0.5	-0.5
0	0	0	1

Det= 1

Order Parameter = Coupled

Rod Packing

See MECKIO on page 10. Notes refer to the hand-written letters on the following pages.

A-D. See corresponding notes for MEZDIE01. For this structure, the histogram indicates that each molecule has two nearest neighbors forming rods. The rods are shown to have p-42m rod symmetry and pack in a nearly hexagonal arrangement.

E. The indicated matrix transformation is analogous to that for MEZDIE01 above. See Appendix B, equation 19.

F. The molecular centers-of-mass reside at Wyckoff point e with point symmetry m. The fractional coordinates are provided. See Appendix B, equations 20 and 21.

G. Four sites on the 3-fold rotation axes of the molecule are indicated. They are used to determine the rod symmetry below.

H. The indicated transformation matrix puts the rod axis along the x-axis, makes the y- and z-axes perpendicular to the rod axis, and shifts the origin to the center-of-mass of a selected molecule. See Appendix B, equations 22 and 23.

I. The inverse of the transformation matrix is provided for use in transforming fractional coordinates.

J. The rod axis, rod origin, and adjustable parameter in H are extracted from H for convenience.

K. A second transformation rotates the rod about its axis to place the rod in standard orientation and rescales the coordinates perpendicular to the rod axis to make them equal in magnitude. See Appendix B, equations 24 and 25.

L. The unit cell matrix representation (E) transformed by H and K yield the matrix representation L. The unit cell is tetragonal by design.

M. The center-of-mass of the reference molecule is at the origin by design. The three-fold axes of the molecule very closely follow the Wyckoff orbit f of a p-42m rod symmetry in the 2^{nd} setting.

N. There is one molecule in the rod unit cell.

O. The symmetry-breaking transformation from rods to the observed structure has size 2 and index 4. See the analogous note N for MEZDIE01 above.

A-D

11e P_21/m
MECKIO

a=	9.5283		
b=	15.3492	b/a=	1.6109065
c=	10.7393	c/a=	1.1270951
alpha=	90	alpha=	90
beta=	104.954	beta=	104.954
gamma=	90	gamma=	90

2 nearest neighbors
2 next neighbors not coplanar

Hexagonal packing of p-42m rods

E

Matrix Representation

1	0	-0.29084
0	1.6109065	0
0	0	1.0889241

a	b	c
1	1.6109065	1.1270951
90	104.954	90
alpha	beta	gamma

H

Transformation to Rod Coordinates

0	0.29084	1	0.20498
1	0	0	0.25
0	1	0	0.219284
0	0	0	1

Det= 1

I

Inverse Transformation

0	1	0	-0.25
0	0	1	-0.219284
1	0	-0.29084	-0.141203
0	0	0	1

Det= 1

F

Center of Mass Coordinates

	e m				
i	x,1/4,z	0.2049796	0.25	0.2192841	1
	1-x,3/4,1-z	0.7950204	0.75	0.7807159	1
	x=	0.2049796			
	z=	0.2192841			

J

rod axis:

1	0	0

rod origin:

0.20498	0.25	0.219284

Transformation to orthogonal axes:
0.29084

G

Molecular 3-fold axes

	f 1				
i	x,y,z	0.0917	0.1478	0.2244	1
i	x,1/2-y,z	0.0917	0.3522	0.2244	1
	e m				
i	x,1/4,z	0.2782	0.25	0.0701	1
i		0.3715	0.25	0.3735	1

Rotation about rod and rescaling:

0.581364682	0.581364682	0	0
-0.860045365	0.860045365	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.860045365	-0.581364682	0	0
0.860045365	0.581364682	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:

45 degrees

Rescaling parameter:

0.822173817

Matrix Representation

0	0	1
0.93652412	0.93652412	0
-0.93652412	0.93652412	0

a	b	c
1.324445112	1.324445112	1
89.99999743	90.00000257	90
alpha	beta	gamma

p-42m (#37)
2nd setting

a m2m

0,0,0	0	0	0	1
	0.103626103	0.756419262	0.426754	1

f m

-x,-x,z	-0.09087082	-0.084922453	-0.114767	1
x,x,z	0.084922453	0.09087082	-0.114767	1
x,-x,-z	0.086730387	-0.086730387	0.116609	1
-x,x,-z	-0.089655658	0.089655658	0.121668	1
error	-0.003122377	0.002825991	0.002186	

x= 0.088044829
z= -0.116953091

		|G|	Z	|G|/Z
Daughter	11e	4	2	2
Rod	37a	8	1	8
			2	4
			(size)	(index)

Z'= 1

Planar Packing

See CAMPOV on page 10. Notes refer to the hand-written letters on the following pages.

A-E. See corresponding notes for MEZDIE01. For this structure, the histogram indicates that each molecule has three nearest neighbors forming two-dimensional planes. The planes are shown to have p2gg projection symmetry.

F. The molecular centers-of-mass reside at Wyckoff point e with point symmetry 1. Fractional coordinates are provided.

G. The indicated transformation matrix puts the plane into orthogonal axes. The inverse transformation is used to compute fractional center-of-mass coordinates in the transformed frame.

H. No rotation nor any rescaling of axes are needed to put the plane into standard orientation.

I. The matrix representation of the unit cell (E), after the indicated transformations (G and H), is an orthorhombic cell.

J. Transforming the fractional center-of-mass coordinates (F) using the inverse transformation matrix (G) yields the coordinates indicated. There are four molecules in the primitive cell.

K. The fractional coordinates (J) are consistent with p2gg projection symmetry (neglecting the z-coordinate) and $2_1/c$ symmetry when considering the third dimension.

L. The symmetry-breaking transformation from planes to the observed structure has size 1 and index 1. See the analogous note N for MEZDIE above.

A-E

14e P_21/c
CAMPOV

a=	10.3894		
b=	14.6835	b/a=	1.4133155
c=	16.9885	c/a=	1.6351762
alpha=	90	alpha=	90
beta=	91.61	beta=	91.61
gamma=	90	gamma=	90

3 neighbors within 4% of nearest
next neighbor 26% farther than nearest

planar packing

Matrix Representation

1	0	-0.045942
0	1.4133155	0
0	0	1.6345307

a	b	c
1	1.4133155	1.6351762
90	91.61	90
alpha	beta	gamma

Transformation to Planar Coordinates

0	0.045942	1	0
1	0	0	0
0	1	0	0
0	0	0	1

Det= 1

G

Inverse Transformation

0	1	0	0
0	0	1	0
1	0	-0.045942	0
0	0	0	1

Det= 1

Center of Mass Coordinates

e 1

x,y,z	0.1712083	0.0255667	0.2124792	1
1-x,1/2+y,1	0.8287917	0.5255667	0.2875208	1
1-x,1-y,1-z	0.8287917	0.9744333	0.7875208	1
x,1/2-y,1/2+	0.1712083	0.4744333	0.7124792	1

F

x= 0.1712083
y= 0.0255667
z= 0.2124792

plane normal:

1	0	0

plane origin:

0	0	0

Transformation to orthogonal axes:
0.045942

H

Rotation about plane normal and rescaling:

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:

0 degrees

I

Matrix Representation

8.65761E-17	0	1
1.413315495	1.02981E-16	0
0	1.634530713	0

a	b	c
1.413315495	1.634530713	1
90	90	90
alpha	beta	gamma

p2gg (#8) in projection

$2_1/c$ when accounting for 3rd dimension

J

x,y,z	0.025566667	0.212479167	0.161447	1
1/2+x,1/2-y,-z	0.525566667	0.287520833	0.815582	1
-x,-y,-z	0.974433333	0.787520833	0.792611	1
1/2-x,1/2+y,z	0.474433333	0.712479167	0.138476	1
x=	0.025566667			
y=	0.212479167			
z=	0.161446598			
error=	0	0	0	

		|G|	Z	|G|/Z
Daughter	14e	4	4	1
Plane	$2_1/c$	4	4	1
			1 (size)	1 (index)

Z'= 4

Dimer Packing

See CARBTC on pages 10 and 11. Notes refer to the hand-written letters on the following pages.

A-E. See corresponding notes for MEZDIE01. For this structure, the histogram indicates that each molecule has a single nearest neighbor. Therefore, the molecules form dimers with Cs point group symmetry.

F. The molecular centers-of-mass reside at Wyckoff point e with point symmetry 1. Fractional coordinates are provided.

G. The indicated transformation sorts the unit cell lengths in order to conform to reduced basis conventions. The inverse transformation is used to compute fractional center-of-mass coordinates in the transformed frame.

H. The dot product of the matrix representation (E above) and the upper-left transformation submatrix (G above) yields the transformed matrix representation. Unit cell parameters are calculated using Euclidean norms and the cosine law.

I. The Niggli matrix, normalized using the (new) a-axis length is provided.

J. The Niggli matrix conforms to the "Main Conditions" for a Type II reduced unit cell. Comparing the Niggli matrix to tabulated character definitions reveals that the reduced cell is monoclinic (character 35), but close to C-centered-orthorhombic (oC, character 23).

K. Transforming the fractional center-of-mass coordinates (F) using the inverse transformation matrix (G) yields the indicated coordinates. There are four distinct molecules in the primitive cell (Z'=4).

L. Since cell reduction (G-K) did not yield a simpler reference lattice, and recognizing the single nearest neighbor, consider the centers-of-mass for dimers.

M. The dimer centers-of-mass reside at Wyckoff point a with point symmetry -1. Fractional coordinates are provided.

N. The indicated transformation halves the volume of the original unit cell (with matrix representation provided in E above) and rotates the unit cell. No origin shift is necessary in this case. Halving the volume of the cell recognizes that the center-of-mass lattice has a single dimer in the primitive unit cell.

O. Applying the upper-left submatrix of the transformation to the original matrix representation yields the transformed matrix representation. Unit cell parameters are calculated using Euclidean norms and the cosine law.

P. The Niggli matrix, normalized using the (new) a-axis length is provided.

Q. The Niggli matrix conforms to the "Main Conditions" for a Type I reduced unit cell. Comparing the Niggli matrix to tabulated character definitions reveals that the reduced cell is C-centered monoclinic (character 10), but close to rhombohedral (hR, character 9).

R. Transforming the fractional center-of-mass coordinates for the dimers (M) using the inverse transformation matrix (N) yields the indicated coordinates. There is one dimer in the primitive cell (Z'=1). The dimer center-of-mass is located at Wyckoff point a of rhombohedral space group R-3m (no 166).

S. The symmetry-breaking transformation from the reference lattice containing orientationally disordered dimers to a monoclinic cell with disordered dimers has size one

and index 3. Orientationally ordering the dimers is a subsequent transformation with size 4 and index 4.

T. The tabulated transformation from a reduced basis in character 9 to the conventional cell (using the hexagonal setting for the rhombohedral cell) is indicated.

U. The transformation from the reference lattice to the observed cell is given by the inverse of the product of the transformations in N and T above. This overall transformation matrix is provided. COPL indicates that the overall transformation matrix is consistent with the indicated symmetry-breaking transition with order parameter F2+.

A-E

14e P_21/c
CARBTC

a=	9.07912		
b=	5.7643	b/a=	0.6348963
c=	9.2014	c/a=	1.0134683
alpha=	90	alpha=	90
beta=	104.295	beta=	104.295
gamma=	90	gamma=	90

1 nearest neighbor
3 neighbors within 6% of nearest
next neighbor 11% farther than nearest

Matrix Representation

1	0	-0.25024
0	0.6348963	0
0	0	0.9820885

a	b	c
1	0.6348963	1.0134683
90	104.295	90
alpha	beta	gamma

G

Transformation to Reduced Cell

0	-1	0	1
-1	0	0	1
0	0	-1	1
0	0	0	1

Det= 1

Inverse Transformation

0	-1	0	1
-1	0	0	1
0	0	-1	1
0	0	0	1

Det= 1

F

Center of Mass Coordinates

e 1

i	x,y,z	0.248	0.067	0.157	1
ii	1-x,1/2+y,1	0.752	0.567	0.343	1
i	1-x,1-y,1-z	0.752	0.933	0.843	1
ii	x,1/2-y,1/2+	0.248	0.433	0.657	1
	x=	0.248			
	y=	0.067			
	z=	0.157			

H

Matrix Representation

0	-1	0.250239959
-0.634896334	0	0
0	0	-0.982088534

a	b	c
0.634896334	1	1.013468266
104.295	90	90
alpha	beta	gamma

I

Normalized Niggli Matrix

1	2.480814901	2.548089455
-0.620799018	9.77836E-17	9.64841E-17

J

Reduced Cell

Character	35 (mP)	... but close to 23 (oC)	
Type	II		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤a.a/2	True

K

0.933	0.752	0.843	1	Z'= 4
0.433	0.248	0.657	1	
0.067	0.248	0.157	1	
0.567	0.752	0.343	1	

dimers:

Dimer Coordinates (a), -1 WP symmetry ensures Cs dimer symmetry
4 nearest neighbors, all coplanar (bc-plane)
next neighbor 6% farther, also co-planar
next neighbor 67% farther than nearest
packing of dimers

Transformation to Reduced Cell

0	0	-1	0
-0.5	0.5	0	0
0.5	0.5	0	0
0	0	0	1

Det= 0.5

Inverse Transformation

0	-1	1	0
0	1	1	0
-1	0	0	0
0	0	0	1

Det= 2

Dimer Center of Mass Coordinates

	a -1				
i	0,0,0	0	0	0	1
ii	0,1/2,1/2	0	0.5	0.5	1

O

Matrix Representation

-0.125119979	-0.125119979	-1
-0.317448167	0.317448167	0
0.491044267	0.491044267	0

a	b	c
0.597957206	0.597957206	1
77.92184748	77.92184748	64.13091485
alpha	beta	gamma

S

		|G|	Z	|G|/Z
Daughter	14e	4	4	1
Cs Dimers	12a	4	1	4
Ref. Lattice	166a	12	1	12
			1 (size)	3 (index)

P

Normalized Niggli Matrix

1	1	2.796789577
0.349934254	0.349934254	0.436316354

Q

Reduced Cell

Character	10 (mC)	... but close to 9 (hR)	
Type	I		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	N/A	|a.b|≤a.a/2	True

R

0,0,0	0	0	0	1	Z' = 1
	0	1	0	1	

Transformation to Conventional Cell

1	-1	-1	0
0	1	-1	0
0	0	3	0
0	0	0	1

Det= 3

Overall Transformation

-0.666667	0	2	0
-0.333333	1	1	0
-0.333333	0	0	0
0	0	0	1

Det= 0.666667

Order Parameter = F2+

Mixed Packing

See KOXKOX and SENLAY on page 1. Notes refer to the hand-written letters on the following pages.

A-E. See corresponding notes for MEZDIE01. For this structure, the histogram indicates that each molecule has three nearest neighbors forming two-dimensional planes. The planes are shown to have p2gg projection symmetry.

F. Two molecules in the unit cell reside at Wyckoff point a with point symmetry -43m. These molecules have 12 nearest neighbors. The remaining six molecules in the unit cell reside at Wyckoff point c with point symmetry -4. They have 2 nearest neighbors. Fractional coordinates are provided.

G. Since the unit cell is already a reduced basis, there is no need for an additional transformation. The Identity matrix leaves the cell and the center-of-mass coordinates unchanged.

H. The cell is a cube which belongs to primitive cubic (cP) character 3.

I. The center-of-mass coordinates are consistent with Wyckoff orbits a and c of space group 223. In this case, the reference lattice has a higher symmetry than the observed structure solely due to the orientations of the molecules. There is no deformation of the cell nor translation of the centers-of-mass within the cell.

J. The symmetry breaking transition in passing from the reference lattice to the observed (daughter) cell has size 1 and index 2.

K. There is no transformation needed for character 3.

L. The overall transformation matrix from observed cell to conventional reference lattice is the identity since the component transformations (G and K) are identities. COPL indicates that the overall transformation matrix is consistent with the indicated symmetry-breaking transition with size 1 and index 2 as calculated in J above. The order parameter is at the gamma point of the Brillioun zone (GM2-).

A-E

218a,c P_-4_3_n
KOXKOX
SENLAY

b/a=	1
c/a=	1
alpha=	90
beta=	90
gamma=	90

Matrix Representation

1	0	0
0	1	0
0	0	1

a	b	c
1	1	1
90	90	90
alpha	beta	gamma

G

Transformation to Reduced Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

F

12 nearest neighbors
next neighbor 55% farther

2 nearest neighbors
next neighbor 12% farther

Center of Mass Coordinates

a -43m	Origin Choice 2			
0,0,0	0	0	0	1
1/2,1/2,1/2	0.5	0.5	0.5	1
c -4..	Origin Choice 2			
1/4,1/2,0	0.25	0.5	0	1
3/4,1/2,0	0.75	0.5	0	1
0,1/4,1/2	0	0.25	0.5	1
0,3/4,1/2	0	0.75	0.5	1
1/2,0,1/4	0.5	0	0.25	1
1/2,0,3/4	0.5	0	0.75	1

Matrix Representation

1	0	0
0	1	0
0	0	1

a	b	c
1	1	1
90	90	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1
0	0	0

	|G|	Z	|G|/Z
Daughter	218a,c	24	8	3
Ref. Lattice	223a,c	48	8	6
			1 (size)	2 (index)

Reduced Cell

Character	3 (cP)		
Type	II		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤a.a/2	True

0,0,0	0	0	0	1	Z' = 2
1/2,1/2,1/2	0.5	0.5	0.5	1	
1/4,1/2,0	0.25	0.5	0	1	Z' = 6
3/4,1/2,0	0.75	0.5	0	1	
0,1/4,1/2	0	0.25	0.5	1	
0,3/4,1/2	0	0.75	0.5	1	
1/2,0,1/4	0.5	0	0.25	1	
1/2,0,3/4	0.5	0	0.75	1	

Transformation to Conventional Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Overall Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Order Parameter = GM2-