Supplementary Material

Molecular Crystal Global Phase Diagrams: II. Reference Lattices

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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

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

D

E

Matrix Representation

$$\left|\begin{array}{ccc} 1 & 0.0003125 & -0.340105 \\ 0 & 1.4627185 & -0.007593 \\ 0 & 0 & 0.8558094 \end{array}\right|$$

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

H

Transformation to Reduced Cell

$$\left|\begin{array}{ccc|c} 0.5 & 0.5 & 0 & 0.75 \\ 0.5 & -0.5 & 0 & 0.25 \\ 0.5 & 0.5 & -1 & 0.25 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 0.5

Inverse Transformation

$$\left|\begin{array}{ccc|c} 1 & 1 & 0 & -1 \\ 1 & -1 & 0 & -0.5 \\ 1 & 0 & -1 & -0.5 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 2

I

Center of Mass Coordinates

F i 1

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

G

J

Matrix Representation

$$\begin{vmatrix} 0.330103967 & 0.329791489 & 0.340104544 \\ 0.727562585 & -0.735155941 & 0.007593356 \\ 0.427904687 & 0.427904687 & -0.855809373 \end{vmatrix}$$

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

K

Normalized Niggli Matrix

$$\begin{vmatrix} 1 & 1.01327063 & 1.032529194 \\ -0.316067389 & -0.302416346 & -0.295712962 \end{vmatrix}$$

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

M

N

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

L

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

O

Transformation to Conventional Cell

$$\left|\begin{array}{ccc|c} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 2

P

Overall Transformation

$$\left|\begin{array}{ccc|c} 0.5 & -1 & -0.5 & 0 \\ 0.5 & 1 & -0.5 & -0.5 \\ 0.5 & 0 & 0.5 & -0.5 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

Order Parameter = Coupled

Q

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 2nd 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

$$\begin{vmatrix} 1 & 0 & -0.29084 \\ 0 & 1.6109065 & 0 \\ 0 & 0 & 1.0889241 \end{vmatrix}$$

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

H

Transformation to Rod Coordinates

$$\left|\begin{array}{ccc|c} 0 & 0.29084 & 1 & 0.20498 \\ 1 & 0 & 0 & 0.25 \\ 0 & 1 & 0 & 0.219284 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

I

Inverse Transformation

$$\left|\begin{array}{ccc|c} 0 & 1 & 0 & -0.25 \\ 0 & 0 & 1 & -0.219284 \\ 1 & 0 & -0.29084 & -0.141203 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

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			

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

J

rod axis:

1	0	0

rod origin:

0.20498	0.25	0.219284

Transformation to orthogonal axes:
0.29084

K.

Rotation about rod and rescaling:

$$\left|\begin{array}{ccc|c} 0.581364682 & 0.581364682 & 0 & 0 \\ -0.860045365 & 0.860045365 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

Inverse Transformation

$$\left|\begin{array}{ccc|c} 0.860045365 & -0.581364682 & 0 & 0 \\ 0.860045365 & 0.581364682 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

rotation angle:
45 degrees

Rescaling parameter:
0.822173817

L

Matrix Representation

$$\left|\begin{array}{ccc} 0 & 0 & 1 \\ 0.93652412 & 0.93652412 & 0 \\ -0.93652412 & 0.93652412 & 0 \end{array}\right|$$

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

M

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 (size)	4 (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

$$\begin{vmatrix} 1 & 0 & -0.045942 \\ 0 & 1.4133155 & 0 \\ 0 & 0 & 1.6345307 \end{vmatrix}$$

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

F

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

x= 0.1712083
y= 0.0255667
z= 0.2124792

G

Transformation to Planar Coordinates

$$\left|\begin{array}{ccc|c} 0 & 0.045942 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

Inverse Transformation

$$\left|\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & -0.045942 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

plane normal:

1	0	0

plane origin:

0	0	0

Transformation to orthogonal axes:
0.045942

H

Rotation about plane normal and rescaling:

$$\left|\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

Inverse Transformation

$$\left|\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

rotation angle:
0 degrees

I

Matrix Representation

$$\left|\begin{array}{ccc} 8.65761E-17 & 0 & 1 \\ 1.413315495 & 1.02981E-16 & 0 \\ 0 & 1.634530713 & 0 \end{array}\right|$$

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

K

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

		$\lvert G\rvert$	Z	$\lvert G\rvert/Z$
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

Matrix Representation

$$\begin{vmatrix} 1 & 0 & -0.25024 \\ 0 & 0.6348963 & 0 \\ 0 & 0 & 0.9820885 \end{vmatrix}$$

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

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

G

Transformation to Reduced Cell

$$\left|\begin{array}{ccc|c} 0 & -1 & 0 & 1 \\ -1 & 0 & 0 & 1 \\ 0 & 0 & -1 & 1 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

Inverse Transformation

$$\left|\begin{array}{ccc|c} 0 & -1 & 0 & 1 \\ -1 & 0 & 0 & 1 \\ 0 & 0 & -1 & 1 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

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

$$\begin{vmatrix} 0 & -1 & 0.250239959 \\ -0.634896334 & 0 & 0 \\ 0 & 0 & -0.982088534 \end{vmatrix}$$

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

I

Normalized Niggli Matrix

$$\begin{vmatrix} 1 & 2.480814901 & 2.548089455 \\ -0.620799018 & 9.77836E-17 & 9.64841E-17 \end{vmatrix}$$

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	

L

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

M

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

N

Transformation to Reduced Cell

$$\left|\begin{array}{ccc|c} 0 & 0 & -1 & 0 \\ -0.5 & 0.5 & 0 & 0 \\ 0.5 & 0.5 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 0.5

Inverse Transformation

$$\left|\begin{array}{ccc|c} 0 & -1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 2

O

Matrix Representation

$$\begin{vmatrix} -0.125119979 & -0.125119979 & -1 \\ -0.317448167 & 0.317448167 & 0 \\ 0.491044267 & 0.491044267 & 0 \end{vmatrix}$$

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

P

Normalized Niggli Matrix

$$\begin{vmatrix} 1 & 1 & 2.796789577 \\ 0.349934254 & 0.349934254 & 0.436316354 \end{vmatrix}$$

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

R

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)

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

T

Transformation to Conventional Cell

$$\left|\begin{array}{ccc|c} 1 & -1 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 3 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 3

U

Overall Transformation

$$\left|\begin{array}{ccc|c} -0.666667 & 0 & 2 & 0 \\ -0.333333 & 1 & 1 & 0 \\ -0.333333 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

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

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

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

G

Transformation to Reduced Cell

$$\left|\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

Inverse Transformation

$$\left|\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

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

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

H

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

Normalized Niggli Matrix

$$\begin{vmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \end{vmatrix}$$

L

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

I

Transformation to Conventional Cell

K

$$\left|\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

Overall Transformation

L

$$\left|\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right|$$

Det= 1

Order Parameter = GM2-

Molecular Crystal Global Phase Diagrams:
II. Reference Lattices

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

Table 6: Structure Classification

Cubic (Isometric) Crystal Structures (195-230)

227a F_d_3_m

1 ZNOXAC01

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

4 equidistant neighbors
next neighbor 63% farther
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1
a	b	c
1	1	1
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

0	0.5	0.5	0
0.5	0	0.5	0
0.5	0.5	0	0
0	0	0	1

Det= 0.25

Inverse Transformation

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

Det= 4

Matrix Representation

0	0.5	0.5
0.5	0	0.5
0.5	0.5	0
a	b	c
0.707106781	0.707106781	0.707106781
60	60	60
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1
0.5	0.5	0.5

		|G|	Z	|G|/Z
Daughter	227a	48	2	24
Ref. Lattice	Diamond	48	2	24
			1	1
			(size)	(index)

Reduced Cell

Character	1 (cF)		
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

Transformation to Conventional Cell

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

Det= 4

Overall Transformation

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

Det= 1

Center of Mass Coordinates

a -43m	Origin Choice 2								
1/8,1/8,1/8	0.125	0.125	0.125	1	1/8,1/8,1/8	0.125	0.125	0.125	1
7/8,3/8,3/8	0.875	0.375	0.375	1	7/8,7/8,7/8	-0.125	0.875	0.875	1
1/8,5/8,5/8	0.125	0.625	0.625	1		1.125	0.125	0.125	1
7/8,7/8,7/8	0.875	0.875	0.875	1		0.875	0.875	0.875	1
5/8,1/8,5/8	0.625	0.125	0.625	1		0.125	1.125	0.125	1
3/8,3/8,7/8	0.375	0.375	0.875	1		0.875	0.875	-0.125	1
5/8,5/8,1/8	0.625	0.625	0.125	1		0.125	0.125	1.125	1
3/8,7/8,3/8	0.375	0.875	0.375	1		0.875	-0.125	0.875	1

Z' = 2

Order Parameter = GM1+

217a I_-4_3_m

2 DEQPAQ
3 HMGETP *
4 HMSIPA
5 HXMTAM07
6 KELREY
7 MESIAD
8 MPTHOT01
9 NIWMIP
10 POSLOY10
11 TMEPTC
12 YEYQAU
* Very slightly distorted molecules or mislabeled as 197a by authors

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

8 nearest neighbors
next neighbor 15% farther
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1
a	b	c
1	1	1
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

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

Det= 2

Matrix Representation

-0.5	0.5	0.5
0.5	-0.5	0.5
0.5	0.5	-0.5
a	b	c
0.866025404	0.866025404	0.866025404
109.4712206	109.4712206	109.4712206
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1
-0.333333333	-0.333333333	-0.333333333

		|G|	Z	|G|/Z
Daughter	217a	24	1	24
Ref. Lattice	BCC	48	1	48
			1	2
			(size)	(index)

Reduced Cell

Character	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	Equal	|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

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

Det= 1

Center of Mass Coordinates

a -43m	Origin Choice 2								
0,0,0	0	0	0	1	0,0,0	0	0	0	1
1/2,1/2,1/2	0.5	0.5	0.5	1		1	1	1	1

Z' = 1

Order Parameter = GM2-

215a P_-4_3_m

13 FOHCUA
14 FUZVOL
15 JUFWUC *

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

6 nearest neighbors
next neighbor 41% farther
sphere packing
* Very slightly distorted molecules or mislabeled as 195a by authors

Matrix Representation

1	0	0
0	1	0
0	0	1
a	b	c
1	1	1
90	90	90
alpha	beta	gamma

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

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	215a	24	1	24
Ref. Lattice	SC	48	1	48
			1	2
			(size)	(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

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

Center of Mass Coordinates

a -43m	Origin Choice 2								
0,0,0	0	0	0	1	0,0,0	0	0	0	1

Z' = 1

Order Parameter = GM2-

218a,c P_-4_3_n

16 KOXKOX
17 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

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

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	2
			(size)	(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

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

Center of Mass Coordinates

a	12 nearest neighbors	a -43m	Origin Choice 2								
	next neighbor 55% farther	0,0,0	0	0	0	1	0,0,0	0	0	0	1
		1/2,1/2,1/2	0.5	0.5	0.5	1	1/2,1/2,1/2	0.5	0.5	0.5	1
		c -4..	Origin Choice 2								
c	2 nearest neighbors	1/4,1/2,0	0.25	0.5	0	1	1/4,1/2,0	0.25	0.5	0	1
	next neighbor 12% farther	3/4,1/2,0	0.75	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	0,1/4,1/2	0	0.25	0.5	1
		0,3/4,1/2	0	0.75	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	1/2,0,1/4	0.5	0	0.25	1
		1/2,0,3/4	0.5	0	0.75	1	1/2,0,3/4	0.5	0	0.75	1

Z' = 2

Z' = 6

Order Parameter = GM2-

218a,d P_-4_3_n

18 RUQMEV

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

Transformation to Reduced Cell

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

Det= 1

Inverse Transformation

1	0	0	0.5
0	1	0	0.5
0	0	1	0.5
0	0	0	1

Det= 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

See #16 and #17 above.

Center of Mass Coordinates

a	12 nearest neighbors	a -43m	Origin Choice 2				a -43m				
	next neighbor 55% farther	0,0,0	0	0	0	1	1/2,1/2,1/2	0.5	0.5	0.5	1
	distorted icosahedral coordination	1/2,1/2,1/2	0.5	0.5	0.5	1	0,0,0	1	1	1	1
		d -4..	Origin Choice 2				c -4..				
d	2 nearest neighbors	1/4,0,1/2	0.25	0	0.5	1	3/4,1/2,0	0.75	0.5	1	1
	next neighbor 12% farther	3/4,0,1/2	0.75	0	0.5	1	1/4,1/2,0	1.25	0.5	1	1
	pairs of rods in 3 orthogonal directions	1/2,1/4,0	0.5	0.25	0	1	0,3/4,1/2	1	0.75	0.5	1
		1/2,3/4,0	0.5	0.75	0	1	0,1/4,1/2	1	1.25	0.5	1

See above.	0,1/2,1/4	0	0.5	0.25	1	1/2,0,3/4	0.5	1	0.75	1
	0,1/2,3/4	0	0.5	0.75	1	1/2,0,1/4	0.5	1	1.25	1

205c P_a_-3

19 FOJBUB02

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

1 nearest neighbor
next neighbor 33% farther
dimer packing

Matrix Representation

1	0	0
0	1	0
0	0	1
a	b	c
1	1	1
90	90	90
alpha	beta	gamma

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

Matrix Representation

1	0	0
0	1	0
0	0	1
a	b	c
1	1	1
90	90	90
alpha	beta	gamma

Center of Mass Coordinates

	c .3.	Origin Choice 2									
i	x,x,x	0.1220303	0.1220303	0.1220303	1	x,x,x	0.1220303	0.1220303	0.1220303	1	Z' = 8
ii	1/2-x,1-x,1	0.3779697	0.8779697	0.6220303	1		0.3779697	0.8779697	0.6220303	1	
iii	1-x,1/2+x,1	0.8779697	0.6220303	0.3779697	1		0.8779697	0.6220303	0.3779697	1	
iv	1/2+x,1/2-x	0.6220303	0.3779697	0.8779697	1		0.6220303	0.3779697	0.8779697	1	
i	1-x,1-x,1-x	0.8779697	0.8779697	0.8779697	1		0.8779697	0.8779697	0.8779697	1	
ii	1/2+x,x,1/2	0.6220303	0.1220303	0.3779697	1		0.6220303	0.1220303	0.3779697	1	
iii	x,1/2-x,1/2-	0.1220303	0.3779697	0.6220303	1		0.1220303	0.3779697	0.6220303	1	
iv	1/2-x,1/2+x	0.3779697	0.6220303	0.1220303	1		0.3779697	0.6220303	0.1220303	1	
	x=	0.1220303				x=	0.1220303				

dimers:

Dimer Coordinates (a), -3 WP symmetry ensures C3i dimer symmetry
12 nearest neighbors
next neighbor 41% farther
sphere packing (of dimers)

Transformation to Reduced Cell

0	0.5	0.5	0
0.5	0	0.5	0
0.5	0.5	0	0
0	0	0	1

Det= 0.25

Inverse Transformation

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

Det= 4

Matrix Representation

0	0.5	0.5
0.5	0	0.5
0.5	0.5	0
a	b	c
0.707106781	0.707106781	0.707106781
60	60	60
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1
0.5	0.5	0.5

		|G|	Z	|G|/Z
Daughter	205c	24	8	3
C3i Dimers	205a	24	4	6
Ref. Lattice	FCC	48	1	48
			4	8
			(size)	(index)

Reduced Cell

Character	1 (cF)		
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

Transformation to Conventional Cell

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

Det= 4

Overall Transformation

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

Det= 1

Dimer Center of Mass Coordinates

	a .-3.	Origin Choice 2									
i	0,0,0	0	0	0	1	0,0,0	0	0	0	1	Z' = 1
ii	1/2,0,1/2	0.5	1	0.5	1		1	0	1	1	
iii	0,1/2,1/2	1	0.5	0.5	1		0	1	1	1	
iv	1/2,1/2,0	0.5	0.5	1	1		1	1	0	1	

Order Parameter = X5+

205c P_a_-3

20 VADRAU

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

1 nearest neighbor
next neighbor 25% farther
dimer packing

See above.

Matrix Representation

1	0	0
0	1	0
0	0	1
a	b	c
1	1	1
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

1	0	0	0.5
0	1	0	0.5
0	0	1	0.5
0	0	0	1

Det= 1

Inverse Transformation

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

Det= 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

See #19 above.

Center of Mass Coordinates

	c .3.	Origin Choice 2								
i	x,x,x	0.371591	0.371591	0.371591	1		-0.128409	-0.128409	-0.128409	1
ii	1/2-x,1-x,1	0.128409	0.628409	0.871591	1		-0.371591	0.128409	0.371591	1
iii	1-x,1/2+x,1	0.628409	0.871591	0.128409	1		0.128409	0.371591	-0.371591	1
iv	1/2+x,1/2-x	0.871591	0.128409	0.628409	1		0.371591	-0.371591	0.128409	1
i	1-x,1-x,1-x	0.628409	0.628409	0.628409	1	x,x,x	0.128409	0.128409	0.128409	1
ii	1/2+x,x,1/2	0.871591	0.371591	0.128409	1		0.371591	-0.128409	-0.371591	1
iii	x,1/2-x,1/2-	0.371591	0.128409	0.871591	1		-0.128409	-0.371591	0.371591	1
iv	1/2-x,1/2+x	0.128409	0.871591	0.371591	1		-0.371591	0.371591	-0.128409	1
	x=	0.371591				x=	0.128409			

Hexagonal Crystal Structures (168-194)

176h P_63/m

21 CUCZUV

a=	15.7954		
b=	15.7954	b/a=	1
c=	14.0566	c/a=	0.8899173
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	120	gamma=	120

12 neighbors within 15% of nearest
next neighbor 49% farther than nearest
sphere packing

Matrix Representation

1	-0.5	0
0	0.8660254	0
0	0	0.8899173
a	b	c
1	1	0.8899173
90	90	120
alpha	beta	gamma

Transformation to Reduced Cell

0.666667	-0.333333	0	0
0.333333	0.333333	0	0
0	0	1	0.5
0	0	0	1

Det= 0.333333

Inverse Transformation

1	1	0	0
-1	2	0	0
0	0	1	-0.5
0	0	0	1

Det= 3

Matrix Representation

0.5	-0.5	0
0.288675135	0.288675135	0
0	0	0.889917318
a	b	c
0.577350269	0.577350269	0.889917318
90	90	120
alpha	beta	gamma

Normalized Niggli Matrix

1	1	2.375858497
0	0	-0.5

		|G|	Z	|G|/Z
Daughter	176h	12	6	2
Ref. Lattice	HCP	24	2	12
			3	6
			(size)	(index)

Reduced Cell

Character	12 (hP)		
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

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

Det= 1

Overall Transformation

1	1	0	0
-1	2	0	0
0	0	1	-0.5
0	0	0	1

Det= 3

Center of Mass Coordinates

h m..									
x,y,1/4	0.3612963	0.3339991	0.25	1	2/3,1/3,3/4	0.695295357	0.306701964	-0.25	1
1-y,x-y,1/4	0.6660009	0.0272971	0.25	1		0.693298036	-0.611406607	-0.25	1
y-x,1-x,1/4	-0.027297	0.6387038	0.25	1		0.611406607	1.304704643	-0.25	1
1-x,1-y,3/4	0.6387038	0.6660009	0.75	1		1.304704643	0.693298036	0.25	1
y,y-x,3/4	0.3339991	-0.027297	0.75	1		0.306701964	-0.388593393	0.25	1
x-y,x,3/4	0.0272971	0.3612963	0.75	1	1/3,2/3,1/4	0.388593393	0.695295357	0.25	1
x=	0.3612963								
y=	0.3339991				error	0.05526006	0.02862869	0	

Z'= 2

cr/ar= 1.54
cr/ar_ideal= 1.63
slightly compressed vs. ideal HCP

Order Parameter = K4

Trigonal Crystal Structures (143-167)

165d P_-3_c_1

22 DILWIE01

a=	10.442		
b=	10.442	b/a=	1
c=	32.086	c/a=	3.072783
alpha=	90	alpha=	90

Matrix Representation

1	-0.5	0
0	0.8660254	0
0	0	3.072783
a	b	c

Transformation to Reduced Cell

1	0	0	0
0	1	0	0
0	0	0.5	0
0	0	0	1

Det= 0.5

Matrix Representation

1	-0.5	0
0	0.866025404	0
0	0	1.536391496
a	b	c

		|G|	Z	|G|/Z
Daughter	165d	12	4	3
Ref. Lattice	HCP	24	2	12
			2	4
			(size)	(index)

Transformation to Conventional Cell

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

Det= 1

beta=	90	beta=	90
gamma=	120	gamma=	120

1	1	3.072783
90	90	120
alpha	beta	gamma

12 neighbors within 6% of nearest
next neighbor 46% farther than nearest
sphere packing

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	2	0
0	0	0	1

Det= 2

1	1	1.536391496
90	90	120
alpha	beta	gamma

Normalized Niggli Matrix

1	1	2.360498829
0	0	-0.5

Reduced Cell

Character	12 (hP)		
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

Overall Transformation

1	0	0	0
0	1	0	0
0	0	2	0
0	0	0	1

Det= 2

Center of Mass Coordinates
d 3..

1/3,2/3,z	0.3333333	0.6666667	0.1216413	1
2/3,1/3,1/2	0.6666667	0.3333333	0.3783587	1
2/3,1/3,1-z	0.6666667	0.3333333	0.8783587	1
1/3,2/3,1/2	0.3333333	0.6666667	0.6216413	1
z=	0.1216413			

1/3,2/3,1/4	0.333333333	0.666666667	0.243282667	1
2/3,1/3,3/4	0.666666667	0.333333333	0.756717333	1
	0.666666667	0.333333333	1.756717333	1
	0.333333333	0.666666667	1.243282667	1
error	0	0	-0.006717333	

Z'= 2

Order Parameter = A2

cr/ar= 1.54
cr/ar_ideal= 1.63
slightly compressed vs. ideal HCP

165d	P_-3_c_1		
23 ZEYHIU			
a=	10.7713		
b=	10.7713	b/a=	1
c=	32.7927	c/a=	3.0444515
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	120	gamma=	120

12 neighbors within 10% of nearest
next neighbor 48% farther than nearest
sphere packing

See above.

Matrix Representation

1	-0.5	0
0	0.8660254	0
0	0	3.0444515
a	b	c
1	1	3.0444515
90	90	120
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

-1	0	0	1
0	-1	0	1
0	0	2	0
0	0	0	1

Det= 2

Matrix Representation

-1	0.5	0
0	-0.866025404	0
0	0	1.522225729
a	b	c
1	1	1.522225729
90	90	120
alpha	beta	gamma

Normalized Niggli Matrix

1	1	2.317171172
0	0	-0.5

See #22 above.

Center of Mass Coordinates
d 3..

1/3,2/3,z	0.3333333	0.6666667	0.3835717	1
2/3,1/3,1/2	0.6666667	0.3333333	0.1164283	1
2/3,1/3,1-z	0.6666667	0.3333333	0.6164283	1
1/3,2/3,1/2	0.3333333	0.6666667	0.8835717	1
z=	0.3835717			

2/3,1/3,3/4	0.666666667	0.333333333	0.767143316	1
1/3,2/3,1/4	0.333333333	0.666666667	0.232856684	1
	0.333333333	0.666666667	1.232856684	1
	0.666666667	0.333333333	1.767143316	1
error	0	0	-0.017143316	

Z'= 2

cr/ar= 1.52
cr/ar_ideal= 1.63
slightly compressed vs. ideal HCP

161a	R_3_c		
24 TCYMET			
a=	9.0622		
b=	9.0622	b/a=	1
c=	11.6253	c/a=	1.2828342
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	120.00	gamma=	120

8 neighbors within 5% of nearest
next neighbor 17% farther than nearest
sphere packing

Matrix Representation

1	-0.5	0
0	0.8660254	0
0	0	1.2828342
a	b	c
1	1	1.2828342
90	90	120
alpha	beta	gamma

Transformation to Reduced Cell

0.333333	-0.666667	0.333333	0
0.666667	-0.333333	-0.333333	0
0.166667	0.166667	0.166667	0
0	0	0	1

Det= 0.166667

Inverse Transformation

0	1	2	0
-1	0	2	0
1	-1	2	0
0	0	0	1

Det= 6

Matrix Representation

0	-0.5	0.5
0.577350269	-0.288675135	-0.288675135
0.213805698	0.213805698	0.213805698
a	b	c
0.615667288	0.615667288	0.615667288
108.6085285	108.6085285	108.6085285
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1
-0.319100381	-0.319100381	-0.319100381

		|G|	Z	|G|/Z
Daughter	161a	6	2	3
Ref. Lattice	BCC	48	1	48
			2	16
			(size)	(index)

Reduced Cell

Character	4 (hR)	… but very 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	-1	1	0
1	0	1	0
-1	1	1	0
0	0	0	1

Det= 3

Center of Mass Coordinates
a 3.

0,0,z	0	0	0.0004	1
0,0,1/2+z	0	0	0.5004	1
2/3,1/3,1/3	0.6666667	0.3333333	0.3337	1
2/3,1/3,5/6	0.6666667	0.3333333	0.8337	1
1/3,2/3,2/3	0.3333333	0.6666667	0.6671	1
1/3,2/3,1/6	0.3333333	0.6666667	0.1671	1
z=	0.0004			

0,0,0	0.0008	0.0008	0.0008	1
	1.0008	1.0008	1.0008	1
	1.0008	0.0008	1.0008	1
	2.0008	1.0008	2.0008	1
	2.0008	1.0008	1.0008	1
	1.0008	0.0008	0.0008	1
error	0.0008	0.0008	0.0008	

Z'= 1

Order Parameter = Coupled

147d	P_-3		
25 ZIZHIZ			
a=	9.168711		
b=	9.168711	b/a=	1
c=	13.88732	c/a=	1.514642
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	120	gamma=	120

12 neighbors within 6% of nearest
next neighbor 45% farther than nearest
sphere packing

Matrix Representation

1	-0.5	0
0	0.8660254	0
0	0	1.514642
a	b	c
1	1	1.514642
90	90	120
alpha	beta	gamma

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

Matrix Representation

1	-0.5	0
0	0.866025404	0
0	0	1.514642025
a	b	c
1	1	1.514642025
90	90	120
alpha	beta	gamma

Normalized Niggli Matrix

1	1	2.294140465
0	0	-0.5

		|G|	Z	|G|/Z
Daughter	147d	6	2	3
Ref. Lattice	HCP	24	2	12
			1	4
			(size)	(index)

Reduced Cell

Character	12 (hP)		
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

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

Center of Mass Coordinates
d 3..

1/3,2/3,z	0.3333333	0.6666667	0.2519732	1
2/3,1/3,1-z	0.6666667	0.3333333	0.7480268	1
z=	0.2519732			

1/3,2/3,1/4	0.333333333	0.666666667	0.251973233	1
2/3,1/3,3/4	0.666666667	0.333333333	0.748026767	1
error	0	0	0.001973233	

Z'= 2

Order Parameter = Coupled

cr/ar= 1.51
cr/ar_ideal= 1.63
slightly compressed vs. ideal HCP

152b	P_31_2_1		
26 MTRETC10			
a=	10.071		
b=	10.071	b/a=	1
c=	25.922	c/a=	2.5739251
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	120	gamma=	120

12 neighbors within 8% of nearest
next neighbor 42% farther than nearest
sphere packing

Matrix Representation

1	-0.5	0
0	0.8660254	0
0	0	2.5739251
a	b	c
1	1	2.5739251
90	90	120
alpha	beta	gamma

Transformation to Reduced Cell

-1	0	-0.333333	0
0	1	0.333333	0.666667
0	0	-0.333333	0.166667
0	0	0	1

Det= 0.333333

Inverse Transformation

1	0	-1	0.166667
0	-1	-1	0.833333
0	0	-3	0.5
0	0	0	1

Det= 3

Matrix Representation

-1	-0.5	-0.5
0	0.866025404	0.288675135
0	0	-0.857975044
a	b	c
1	1	1.034144337
61.086313	61.086313	60
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1.069454509
0.5	0.5	0.5

		|G|	Z	|G|/Z
Daughter	152b	6	3	2
Ref. Lattice	FCC	48	1	48
			3	24
			(size)	(index)

Reduced Cell

Character	9 (hR)	… but very close to 1 (cF)	
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

Transformation to Conventional Cell

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

Det= 4

Overall Transformation

0	0.5	-1	-0.166667
-0.5	0	-1	0.166667
-0.5	0.5	1	-0.5
0	0	0	1

Det= 0.75

Center of Mass Coordinates
b .2.

x,0,5/6	0.7146722	0	0.8333333	1
0,x,1/6	0	0.7146722	0.1666667	1
1-x,1-x,1/2	0.2853278	0.2853278	0.5	1
x=	0.7146722			

	0.048005556	0	-2	1
0,0,0	0	-0.048005556	0	1
	-0.048005556	0.048005556	-1	1
error	0	-0.048005556	0	

Z'= 1

Order Parameter = LD3

Tetragonal Crystal Structures (75-142)

141a I_41/a_m_d

27 FUZLUH

a=	14.5613		
b=	14.5613	b/a=	1
c=	10.5074	c/a=	0.7215977
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

4 nearest neighbors
next neighbor 36% farther than nearest
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	0.7215977
a	b	c
1	1	0.7215977
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

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

Det= 2

Matrix Representation

0	-0.5	0.5
0	-0.5	-0.5
0.72159766	0.36079883	0.36079883
a	b	c
0.72159766	0.793836126	0.793836126
78.07854374	62.96720689	62.96720689
alpha	beta	gamma

Normalized Niggli Matrix

1	1.210239954	1.210239954
0.25	0.5	0.5

				|G|	Z	|G|/Z
Daughter	141a			16	2	8
Ref. Lattice	141a			16	2	8
					1	1
					(size)	(index)

Reduced Cell

Character	18 (tI)		
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

Transformation to Conventional Cell

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

Det= 2

Overall Transformation

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

Det= 1

Center of Mass Coordinates

a -4m2 Origin Choice 2

0,3/4,1/8	0	0.75	0.125	1	7/8,1/4,1/4	0.875	0.25	0.25	1
1/2,3/4,3/8	0.5	0.75	0.375	1	1/8,3/4,3/4	1.125	-0.25	0.75	1
1/2,1/4,5/8	0.5	0.25	0.625	1		0.875	0.25	1.25	1
0,1/4,7/8	0	0.25	0.875	1		1.125	0.75	0.75	1
					error	0	0	0	

Z'= 2

Order Parameter = GM1+

c/a_conv= 0.72
c/a_ideal= 1.41
Very distorted diamond cubic.

141a I_41/a_m_d

28 VAFWAA

a=	14.7313		
b=	14.7313	b/a=	1
c=	10.5743	c/a=	0.7178117
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

4 nearest neighbors
next neighbor 35% farther than nearest
sphere packing

See above.

Matrix Representation

1	0	0
0	1	0
0	0	0.7178117
a	b	c
1	1	0.7178117
90	90	90
alpha	beta	gamma

See #27 above.

Center of Mass Coordinates

a -4m2 Origin Choice 2

0,3/4,1/8	0	0.75	0.125	1
1/2,3/4,3/8	0.5	0.75	0.375	1
1/2,1/4,5/8	0.5	0.25	0.625	1
0,1/4,7/8	0	0.25	0.875	1

c/a_conv= 0.72
c/a_ideal= 1.41
Very distorted diamond cubic.

137a P_42/n_m_c

29 FUZTEZ

a=	8.5599		
b=	8.5599	b/a=	1
c=	6.0179	c/a=	0.7030339
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

2 nearest neighbors
next neighbor 13% farther than nearest

Square packing of p-42m rods.

Matrix Representation

1	0	0
0	1	0
0	0	0.7030339
a	b	c
1	1	0.7030339
90	90	90
alpha	beta	gamma

Transformation to Rod Coordinates

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

rod axis:
0 0 1

rod origin:
0 0 0

Transformation to orthogonal axes:
0

Rotation about rod and rescaling:

0.707106781	-0.707106781	0	0
0.707106781	0.707106781	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.707106781	0.707106781	0	0
-0.707106781	0.707106781	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:
-45 degrees

Rescaling parameter:
1

Matrix Representation

0.707106781	-0.707106781	0
0.707106781	0.707106781	0
0	0	0.703034
a	b	c
1	1	0.703034
90	90	90
alpha	beta	gamma

p-42m (#37)
2nd setting

			|G|	Z	|G|/Z
Daughter	137a		16	2	8
Rod	37a		8	1	8
				2	1
				(size)	(index)

Center of Mass Coordinates

a -4m2 (Origin Choice 1)

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

a -42m

Molecular 3-fold axes

h 1

0,y,z	0	0.235	0.233	1
y,0,-z	0.235	0	-0.233	1
0,-y,z	0	-0.235	0.233	1
-y,0,-z	-0.235	0	-0.233	1
y=	0.235			
z=	0.233			

f ..m

x,x,z	0.166170094	0.166170094	0.233	1
x,-x,-z	0.166170094	-0.166170094	-0.233	1
-x,-x,z	-0.166170094	-0.166170094	0.233	1
-x,x,-z	-0.166170094	0.166170094	-0.233	1
x=	0.166170094			
z=	0.233			

121a I_-4_2_m

30 ZZZKDW01

a=	6.4094		
b=	6.4094	b/a=	1
c=	9.5586	c/a=	1.4913408
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

12 neighbors within 3% of nearest
next neighbor 41% farther than nearest
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1.4913408
a	b	c
1	1	1.4913408
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

-1	0	1	0
0	-1	1	0
0	0	2	0
0	0	0	1

Det= 2

Matrix Representation

-1	0	0.5
0	-1	0.5
0	0	0.745670422
a	b	c
1	1	1.027630467
119.1144824	119.1144824	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1.056024378
-0.5	-0.5	0

				|G|	Z	|G|/Z
Daughter	121a			8	1	8
Ref. Lattice	FCC			48	1	48
					1	6
					(size)	(index)

Reduced Cell

Character	15 (tI)	… but close to singularity: 1 (cF)	
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	Equal	|a.b|≤a.a/2	True

Transformation to Conventional Cell

1	1	-1	0
-1	1	-1	0
0	2	0	0
0	0	0	1

Det= 4

Overall Transformation

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

Det= 0.5

Center of Mass Coordinates

a -4m2

0,0,0	0	0	0	1	0,0,0	0	0	0	1
1/2,1/2,1/2	0.5	0.5	0.5	1		0	0	1	1

Z'= 1

Order Parameter = GM5-

142a I_41/a_c_d

31 KUJSIR

a=	14.9351		
b=	14.9351	b/a=	1
c=	30.2202	c/a=	2.0234347
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

12 neighbors within 1% of nearest
next neighbor 41% farther than nearest
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	2.0234347
a	b	c
1	1	2.0234347
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

0.5	-0.5	0	0
0.5	0.5	-0.5	0.25
0	0	0.25	0.375
0	0	0	1

Det= 0.125

Inverse Transformation

1	1	2	-1
-1	1	2	-1
0	0	4	-1.5
0	0	0	1

Det= 8

Matrix Representation

0.5	-0.5	0
0.5	0.5	-0.5
0	0	0.505858682
a	b	c
0.707106781	0.707106781	0.71126156
119.8069547	119.8069547	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1.011786012
-0.5	-0.5	0

				|G|	Z	|G|/Z
Daughter	142a			16	4	4
Ref. Lattice	FCC			48	1	48
					4	12
					(size)	(index)

Reduced Cell

Character	15 (tI)	… but close to singularity: 1 (cF)	
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	Equal	|a.b|≤a.a/2	True

Transformation to Conventional Cell

1	1	-1	0
-1	1	-1	0
0	2	0	0
0	0	0	1

Det= 4

Overall Transformation

1	0	0	0
0	0	2	-0.75
0	-1	0	0.25
0	0	0	1

Det= 2

Center of Mass Coordinates

a -4.. Origin Choice 2

0,1/4,3/8	0	0.25	0.375	1	0,0,0	0	0	0	1
0,3/4,5/8	0	0.75	0.625	1		1	1	1	1
1/2,1/4,5/8	0.5	0.25	0.625	1		1	0	1	1
1/2,3/4,3/8	0.5	0.75	0.375	1		1	0	0	1
1/2,3/4,7/8	0.5	0.75	0.875	1		2	1	2	1
1/2,1/4,1/8	0.5	0.25	0.125	1		0	-1	-1	1
0,3/4,1/8	0	0.75	0.125	1		0	0	-1	1
0,1/4,7/8	0	0.25	0.875	1		1	1	2	1

Z'= 1

Order Parameter = W3

120c I_-4_c_2
32 YEMRIR

a=	9.0991		
b=	9.0991	b/a=	1
c=	13.6601	c/a=	1.5012584
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

6 neighbors within 7% of nearest
next neighbor 41% farther than nearest
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1.5012584
a	b	c
1	1	1.5012584
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.25

Inverse Transformation

1	1	0	-0.5
-1	1	0	-0.5
0	0	2	-0.5
0	0	0	1

Det= 4

Matrix Representation

0.5	-0.5	0
0.5	0.5	0
0	0	0.750629183
a	b	c
0.707106781	0.707106781	0.750629183
90	90	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1.126888341
0	0	0

Daughter	120c	
Ref. Lattice	SC	

|G|	Z	|G|/Z
8	2	4
48	1	48
	2	12
	(size)	(index)

Reduced Cell

Character	11 (tP)	… but close to 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

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	1	0	-0.5
-1	1	0	-0.5
0	0	2	-0.5
0	0	0	1

Det= 4

Center of Mass Coordinates
c -4..

0,1/2,1/4	0	0.5	0.25	1	0,0,0	0	0	0	1
0,1/2,3/4	0	0.5	0.75	1		0	0	1	1
1/2,0,3/4	0.5	0	0.75	1		0	-1	1	1
1/2,0,1/4	0.5	0	0.25	1		0	-1	0	1

Z'= 1

Order Parameter = Coupled

114a P_-4_21_c
33 ADAMAN08

a=	6.6397		
b=	6.6397	b/a=	1
c=	8.9189	c/a=	1.3432685
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

12 neighbors within 3% of nearest
next neighbor 38% farther than nearest
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1.3432685
a	b	c
1	1	1.3432685
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

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

Det= 2

Matrix Representation

0.5	-0.5	0.5
0.5	0.5	-0.5
-0.671634261	0.671634261	0.671634261
a	b	c
0.975239755	0.975239755	0.975239755
92.9475839	118.3130554	118.3130554
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1
-0.051422355	-0.474288823	-0.474288823

Daughter	114a	
Ref. Lattice	FCC	

|G|	Z	|G|/Z
8	2	4
48	1	48
	2	12
	(size)	(index)

Reduced Cell

Character	7 (tI)	… but close to singularity: 1 (cF)	
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	Equal	|a.b|≤a.a/2	True

Transformation to Conventional Cell

0	0	2	0
1	1	1	0
-1	1	1	0
0	0	0	1

Det= 4

Overall Transformation

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

Det= 0.5

Center of Mass Coordinates
a -4..

0,0,0	0	0	0	1	0,0,0	0	0	0	1
1/2,1/2,1/2	0.5	0.5	0.5	1		1	1	1	1

Z'= 1

Order Parameter = Coupled

114b P_-4_21_c
34 GERHOA

a=	10.0441		
b=	10.0441	b/a=	1
c=	12.4722	c/a=	1.2417439
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

12 neighbors within 7% of nearest
next neighbor 32% farther than nearest
sphere packing

See above.

Matrix Representation

1	0	0
0	1	0
0	0	1.2417439
a	b	c
1	1	1.2417439
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

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

Det= 2

Matrix Representation

0.5	-0.5	0.5
0.5	0.5	-0.5
-0.620871955	0.620871955	0.620871955
a	b	c
0.941000523	0.941000523	0.941000523
97.43078797	115.8066616	115.8066616
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1
-0.129328454	-0.435335773	-0.435335773

See #33 above.

Along tetragonal path from FCC to BCC.
Closer to FCC than BCC.

Center of Mass Coordinates
b -4..

0,0,1/2	0	0	0.5	1	0,0,0	0	0	0	1
1/2,1/2,0	0.5	0.5	0	1		1	0	0	1

88a I_41/a
35 KANGUB01

a=	7.1984		
b=	7.1984	b/a=	1
c=	28.582	c/a=	3.9706046
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

8 neighbors within 12% of nearest
next neighbor 41% farther than nearest
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	3.9706046
a	b	c
1	1	3.9706046
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

1	0	1	0
0	1	1	0.5
0	0	2	0
0	0	0	1

Det= 2

Matrix Representation

1	0	-0.5
0	1	-0.5
0	0	1.985302289
a	b	c
1	1	2.107468904
103.7243738	103.7243738	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1	4.44142518
-0.5	-0.5	0

Daughter	88a	
Ref. Lattice	141a	

|G|	Z	|G|/Z
16	4	4
16	2	8
	2	2
	(size)	(index)

Reduced Cell

Character	15 (tI)		
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	Equal	|a.b|≤a.a/2	True

Transformation to Conventional Cell

1	0	1	0
0	1	1	0
0	0	2	0
0	0	0	1

Det= 2

Overall Transformation

1	0	0	0
0	1	0	0.5
0	0	1	0
0	0	0	1

Det= 1

Center of Mass Coordinates
a -4..

0,1/4,1/8	0	0.25	0.125	1	1/8,7/8,1/4	0.125	0.875	0.25	1
1/2,1/4,3/8	0.5	0.25	0.375	1	7/8,1/8,3/4	0.875	1.125	0.75	1
1/2,3/4,5/8	0.5	0.75	0.625	1		1.125	1.875	1.25	1
0,3/4,7/8	0	0.75	0.875	1		0.875	2.125	1.75	1

Z'= 2

Order Parameter = GM3+

c/a_conv= 3.97
c/a_ideal= 1.41
Very distorted diamond cubic.

88f I_41/a
36 LUFYEQ

a=	15.66931		
b=	15.66931	b/a=	1
c=	19.5592	c/a=	1.2482486
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

1 nearest neighbor
next neighbor 33% farther than nearest
dimer packing

Matrix Representation

1	0	0
0	1	0
0	0	1.2482486
a	b	c
1	1	1.2482486
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

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

Det= 2

Matrix Representation

0.5	0.5	-0.5
0.5	-0.5	0.5
0.624124324	-0.624124324	-0.624124324
a	b	c
0.943149602	0.943149602	0.943149602
97.13384882	115.9703615	115.9703615
alpha	beta	gamma

Center of Mass Coordinates
f 1

a	x,y,z	0.0519571	0.0932353	0.3109161	1		-0.3548076	-0.258959	-0.21768084	1
b	1/2-x,1-y,1.	0.4480429	0.9067647	0.8109161	1		0.8548076	-0.36287324	0.0958486	1
c	3/4-y,1/4+x	0.6567647	0.3019571	0.5609161	1		0.45872184	0.0958486	-0.258959	1
d	3/4+y,3/4-x	0.8432353	0.6980429	1.0609161	1		1.04127816	-0.21768084	-0.36287324	1
e	1-x,1-y,1-z	0.9480429	0.9067647	0.6890839	1		1.3548076	0.258959	0.21768084	1
f	1/2+x,y,1/2	0.5519571	0.0932353	0.1890839	1		0.1451924	0.36287324	-0.0958486	1
g	1/4+y,3/4-x	0.3432353	0.6980429	0.4390839	1		0.54127816	-0.0958486	0.258959	1
h	1/4-y,1/4+x	0.1567647	0.3019571	-0.060916	1		-0.04127816	0.21768084	0.36287324	1
b	1/2+x,1/2+	0.5519571	0.5932353	0.8109161	1		0.6451924	-0.258959	-0.21768084	1
a	1-x,1/2-y,z	0.9480429	0.4067647	0.3109161	1		0.8548076	0.63712676	0.0958486	1
d	1/4-y,3/4+x	0.1567647	0.8019571	1.0609161	1		0.45872184	-0.9041514	-0.258959	1
c	1/4+y,1/4-x	0.3432353	0.1980429	0.5609161	1		0.04127816	-0.21768084	-0.36287324	1
f	1/2-x,1/2-y	0.4480429	0.4067647	0.1890839	1	x,y,z	0.3548076	0.258959	0.21768084	1
e	x,1/2+y,1-z	0.0519571	0.5932353	0.6890839	1		0.1451924	-0.63712676	-0.0958486	1
h	3/4+y,1/4-x	0.8432353	0.1980429	-0.060916	1		0.54127816	0.9041514	0.258959	1
g	3/4-y,3/4+x	0.6567647	0.8019571	0.4390839	1		0.95872184	0.21768084	0.36287324	1

Z'= 8

x= 0.0519571
y= 0.0932353
z= 0.3109161

dimers:

Dimer Coordinates (e), 2.. WP Symmetry ensures C2 dimer symmetry
Slightly distorted C2v dimers

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

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

Det= 2

Matrix Representation

0.5	0.5	-0.5
0.5	-0.5	0.5
0.624124324	-0.624124324	-0.624124324

a	b	c
0.943149602	0.943149602	0.943149602
97.13384882	115.9703615	115.9703615
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1
-0.124187698	-0.437906151	-0.437906151

		|G|	Z	|G|/Z
Daughter	88f	8	8	1
C2 Dimers	88e	8	4	2
Ref. Lattice	141e	16	4	4
			1	2
			(size)	(index)

Reduced Cell

Character	7 (tl)		
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	Equal	|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	0	-1	0.25
0	1	0	-0.25
1	0	0	-0.25
0	0	0	1

Det= 1

Dimer Center of Mass Coordinates

e 2..		Origin Choice 2								
a	0,1/4,z	0	0.25	0.3109161	1		-0.25	-0.31091612	-0.06091612	1
b		0.5	0.75	0.8109161	1	3/4,2/3,11/	0.75	-0.31091612	-0.06091612	1
c		0.5	0.25	0.5609161	1	1/4,11/12,2	0.25	-0.06091612	-0.31091612	1
d		0	0.75	1.0609161	1		0.25	-1.06091612	-0.31091612	1
e		0	0.75	0.6890839	1		0.25	-0.68908388	0.06091612	1
f		0.5	0.25	0.1890839	1	1/4,1/3,1/1	0.25	0.31091612	0.06091612	1
g		0.5	0.75	0.4390839	1	3/4,1/12,1/	0.75	0.06091612	0.31091612	1
h		0	0.25	-0.060916	1		-0.25	0.06091612	0.31091612	1

z= 0.3109161

error 0 0.022417213 -0.022417213

Z' = 4

Order Parameter = X5+

quads:

Quadramer Coordinates (a), -4.. WP Symmetry ensures S4 quadramer symmetry

4 equidistant nearest neighbors
next neighbor >60% further
sphere packing (of quadramers)

Quadramer Center of Mass Coordinates

a -4..		Origin Choice 2			
ah	0,1/4,1/8	0	0.25	0.125	1
bg	1/2,3/4,5/8	0.5	0.75	0.625	1
cf	1/2,1/4,3/8	0.5	0.25	0.375	1
de	0,3/4,7/8	0	0.75	0.875	1

		|G|	Z	|G|/Z
Daughter	88f	8	8	1
C2 Dimers	88e	8	4	2
S4 Quadramers	88a	8	2	4
Ref. Lattice	227a	48	2	24
			1	6
			(size)	(index)

c/a_conv= 1.25
c/a_ideal= 1.41
Somewhat compressed diamond cubic.

Overall Transformation

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

Det= 1

Order Parameter = GM4+

Orthorhombic Crystal Structures (16-74)

62c P_n_m_a
37 GUTCED

a=	11.47068		
b=	12.64188	b/a=	1.1021038
c=	12.51698	c/a=	1.0912152
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

2 nearest neighbors
next neighbor 10% farther than nearest

Square packing of p1121/m rods.

Matrix Representation

1	0	0
0	1.1021038	0
0	0	1.0912152

a	b	c
1	1.1021038	1.0912152
90	90	90
alpha	beta	gamma

Transformation to Rod Coordinates

0	1	0	0.5
0	0	1	0
1	0	0	0
0	0	0	1

Det= 1

Inverse Transformation

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

Det= 1

Rotation about rod and rescaling:

0.957292823	0	0	0
0	1.044612449	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1.044612449	0	0	0
0	0.957292823	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

0	1.044612449	0
0	0	1.102104
1.044612449	0	0

a	b	c
1.044612449	1.044612449	1.102104
90	90	90
alpha	beta	gamma

p1121/m (#12)

		|G|	Z	|G|/Z
Daughter	62c	8	4	2
Rod	12b	4	2	2
			2	1
			(size)	(index)

Center of Mass Coordinates

	c .m.				
i	x,1/4,z	0.3286569	0.25	-0.013779	1
ii	1-x,3/4,1-z	0.6713431	0.75	1.013779	1
	1/2-x,3/4,1	0.1713431	0.75	0.486221	1
	1/2+x,1/4,1	0.8286569	0.25	0.513779	1

x= 0.3286569
z= -0.013779

rod axis: 0 1 0

rod origin: 0.5 0 0

Transformation to orthogonal axes:
0

rotation angle:
0 degrees

Rescaling parameter:
0.957292823

b m				
x,y,1/4	-0.014393677	-0.164025564	0.25	1
-x,-y,3/4	1.059006126	0.164025564	0.75	1
	0.507912547	-0.314620847	0.75	1
	0.536699901	0.314620847	0.25	1

Z'= 2

error 0 0 0

Molecular 3-fold axes

c .m.				
i	0.4309	0.25	-0.2415	1
i	0.5287	0.25	0.1508	1
d 1				
i	0.177	0.4492	0.018	1
i	0.177	0.0508	0.018	1
c .m.				
ii	0.4713	0.75	-0.1508	1
ii	0.5691	0.75	0.2415	1
d 1				
ii	0.823	0.5508	-0.018	1
ii	0.823	0.9492	-0.018	1

b m				
	-0.252273906	-0.066148934	0.25	1
x,y,1/4	0.157527557	0.027474304	0.25	1

b m				
-x,-y,3/4	-0.157527557	-0.027474304	0.75	1
	0.252273906	0.066148934	0.75	1

62c P_n_m_a
38 JEYSEL

a=	10.0621		
b=	16.3473	b/a=	1.624641
c=	18.0792	c/a=	1.7967621
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

2 nearest neighbors
next neighbor 12% farther than nearest

See above.

Matrix Representation

1	0	0
0	1.624641	0
0	0	1.7967621

a	b	c
1	1.624641	1.7967621
90	90	90
alpha	beta	gamma

Transformation to Rod Coordinates

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

Det= 1

Inverse Transformation

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

Det= 1

Rotation about rod and rescaling:

0.746027282	0	0	0
0	1.340433552	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1.340433552	0	0	0
0	0.746027282	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

0	1.340433552	0
0	0	1.624641
1.340433552	0	0

a	b	c
1.340433552	1.340433552	1.624641
90	90	90
alpha	beta	gamma

p1121/m (#12)

See # 37 above.

Center of Mass Coordinates

	c .m.				
i	x,1/4,z	-0.06938	0.25	-0.030205	1
	1/2-x,3/4,1	0.5693802	0.75	0.469795	1
ii	1-x,3/4,1-z	1.0693802	0.75	1.030205	1
	1/2+x,1/4,1	0.4306198	0.25	0.530205	1

x= -0.06938
z= -0.030205

rod axis: 0 1 0

rod origin: 0 0 0

Transformation to orthogonal axes:
0

rotation angle:
0 degrees

Rescaling parameter:
0.746027282

b m				
x,y,1/4	-0.040487816	-0.051759486	0.25	1
-x,-y,3/4	0.62972896	0.424773127	0.75	1
	1.380921368	0.797786768	0.75	1
	0.710704592	0.321254155	0.25	1

Z'= 2

error 0 0 0

Molecular 3-fold axes

c .m.				
i	0.3077	0.25	-0.0354	1
i	-0.1829	0.25	0.1574	1
d 1				
i	-0.1771	0.0646	-0.1282	1
i	-0.1771	0.4354	-0.1282	1
c .m.				
ii	-0.3077	0.75	0.0354	1

b m				
	-0.047451348	0.229552595	0.25	1
x,y,1/4	0.210984241	-0.13644839	0.25	1

b m				
	0.047451348	-0.229552595	0.75	1

ii		0.1829	0.75	-0.1574	1
	d 1				
ii		0.1771	0.9354	0.1282	1
ii		0.1771	0.5646	0.1282	1

-x,-y,3/4	-0.210984241	0.13644839	0.75	1

62c P_n_m_a
39 RIMMOP

a=	10.33609		
b=	15.0811	b/a=	1.459072
c=	16.6321	c/a=	1.6091288
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

2 nearest neighbors
next nearest neighbors are not coplanar
next neighbor 17% farther than nearest

See above.

Matrix Representation

1	0	0
0	1.459072	0
0	0	1.6091288
a	b	c
1	1.459072	1.6091288
90	90	90
alpha	beta	gamma

Center of Mass Coordinates

	c .m.				
i	x,1/4,z	0.1867586	0.25	0.4677994	1
	1/2-x,3/4,1.	0.3132414	0.75	0.9677994	1
ii	1-x,3/4,1-z	0.8132414	0.75	0.5322006	1
	1/2+x,1/4,1	0.6867586	0.25	0.0322006	1
	x=	0.1867586			
	z=	0.4677994			

Molecular 3-fold axes

	c .m.				
i	x,1/4,z	0.0266	0.25	0.4729	1
ii	1-x,3/4,1-z	-0.0266	0.75	0.5271	1
	c .m.				
i	x,1/4,z	0.2488	0.25	0.5612	1
ii	1-x,3/4,1-z	0.7512	0.75	0.4388	1
	d 1				
i	x,y,z	0.2371	0.1593	0.4189	1
i	x,1/2-y,z	0.2371	0.3407	0.4189	1
ii	1-x,1/2+y,1	0.7629	0.6593	0.5811	1
ii	1-x,1-y,1-z	0.7629	0.8407	0.5811	1

Transformation to Rod Coordinates

0	1	0	0.5
0	0	1	0
1	0	0	0
0	0	0	1

Det= 1

Inverse Transformation

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

Det= 1

rod axis:
0 1 0

rod origin:
0.5 0 0

Transformation to orthogonal axes:
0

Rotation about rod and rescaling:

0.788323726	0	0	0
0	1.268514403	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1.268514403	0	0	0
0	0.788323726	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:
0 degrees

Rescaling parameter:
0.788323726

Matrix Representation

0	1.268514403	0
0	0	1.459072
1.268514403	0	0
a	b	c
1.268514403	1.268514403	1.459072
90	90	90
alpha	beta	gamma

See # 37 above.

p1121/m (#12)

b	m			
x,y,1/4	0.593410245	-0.246935632	0.25	1
	1.227667446	-0.14722623	0.75	1
-x,1-y,3/4	0.675104158	0.246935632	0.75	1
	0.040846957	0.14722623	0.25	1

Z'= 2

b	m			
	0.599880461	-0.373192452	0.25	1
	0.668633942	-0.415131274	0.75	1
b	m			
	0.711890283	-0.19802692	0.25	1
	0.55662412	0.19802692	0.75	1

64d,f C_m_c_a Renamed Cmce
40 METHANEiii

a=	11.7079		
b=	8.1893	b/a=	0.6994679
c=	8.1842	c/a=	0.6990323
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

Not from the CSD. See Neuman '03

Matrix Representation

1	0	0
0	0.6994679	0
0	0	0.6990323
a	b	c
1	0.6994679	0.6990323
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.0625

Inverse Transformation

2	0	2	-0.5
2	-2	0	-0.5
4	0	0	-1
0	0	0	1

Det= 16

Matrix Representation

0	0	0.25
0	-0.34973394	0.17486697
0.349516139	0	-0.174758069
a	b	c
0.349516139	0.34973394	0.35159471
119.8250837	119.8046299	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1.001246692	1.01192936
-0.500623346	-0.5	0

Daughter	64d,f
Ref. Lattice	FCC

	|G|	Z	|G|/Z
Daughter	8	8	1
Ref. Lattice	48	1	48
		8	48
		(size)	(index)

Reduced Cell

Character	42 (oI)	… but close to singularity: 1 (cF)	
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	Equal	|a.b|≤a.a/2	True

sphere packing

Transformation to Conventional Cell

1	1	-1	0
-1	1	-1	0
0	2	0	0
0	0	0	1

Det= 4

Overall Transformation

0	1	1	0
2	0	0	-0.5
0	1	-1	0
0	0	0	1

Det= 4

Order Parameter = Coupled

Center of Mass Coordinates

d: 2 nearest neighbors
12 neighbors within 9%
next neighbor >46% further

d 2..									
x,0,0	0.24982	0	0	1	0,0,0	-0.00036	-0.00036	-0.00072	1
1-x,1/2,1/2	0.75018	0.5	0.5	1		2.00036	0.00036	2.00072	1
1-x,0,0	0.75018	0	0	1		1.00036	1.00036	2.00072	1
x,1/2,1/2	0.24982	0.5	0.5	1		0.99964	-1.00036	-0.00072	1
1/2+x,1/2,0	0.74982	0.5	0	1		0.99964	-0.00036	1.99928	1
1/2-x,0,1/2	0.25018	0	0.5	1		1.00036	0.00036	0.00072	1
1/2-x,1/2,0	0.25018	0.5	0	1		0.00036	-0.99964	0.00072	1
1/2+x,0,1/2	0.74982	0	0.5	1		1.99964	0.99964	1.99928	1
x=	0.24982								
					error	0.00036	0.00036	0.00072	

Z'= 1

f: 2 nearest neighbors
12 neighbors within 9%
next neighbor >34% further

Sphere packing

f m..									
0,y,z	0	0.22962	0.26968	1		0.03936	-0.95924	-1	1
0,1/2-y,1/2	0	0.27038	0.76968	1		1.03936	-1.04076	-1	1
0,1/2+y,1/2	0	0.72962	0.23032	1		-0.03936	-1.95924	-1	1
0,1-y,1-z	0	0.77038	0.73032	1		0.96064	-2.04076	-1	1
1/2,1/2+y,z	0.5	0.72962	0.26968	1		1.03936	-0.95924	1	1
1/2,1-y,1/2	0.5	0.77038	0.76968	1		2.03936	-1.04076	1	1
1/2,y,1/2-z	0.5	0.22962	0.23032	1		0.96064	0.04076	1	1
1/2,1/2-y,1	0.5	0.27038	0.73032	1		1.96064	-0.04076	1	1
y=	0.22962								
z=	0.26968				error	0.03936	0.04076	0	

19a P_21_21_21
41 MZNMOX10

a=	7.48115		
b=	7.67315	b/a=	1.0256645
c=	29.425	c/a=	3.9332188
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

4 neighbors within 3% of nearest (coplanar)
next neighbor 13% farther than nearest
planar packing

Matrix Representation

1	0	0
0	1.0256645	0
0	0	3.9332188
a	b	c
1	1.0256645	3.9332188
90	90	90
alpha	beta	gamma

Center of Mass Coordinates

	a 1				
i	x,y,z	-0.065579	0.0674563	0.1228419	1
	1/2-x,1-y,1.	0.5655794	0.9325438	0.6228419	1
	1-x,1/2+y,1	1.0655794	0.5674563	0.3771581	1
	1/2+x,1/2-y	0.4344206	0.4325438	0.8771581	1
	x=	-0.065579			
	y=	0.0674563			
	z=	0.1228419			

Molecular 3-fold axes

	a 1				
i	x,y,z	-0.2792	0.0041	0.0955	1
i	x,y,z	0.0764	0.2022	0.0815	1
i	x,y,z	-0.1107	0.2066	0.175	1
i	x,y,z	0.0653	-0.132	0.1403	1

Transformation to Planar Coordinates

1	0	0	-0.065579
0	1	0	0.067456
0	0	1	0.122842
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0.065579
0	1	0	-0.067456
0	0	1	-0.122842
0	0	0	1

Det= 1

plane normal:
0 0 1

plane origin:
-0.065579 0.067456 0.122842

Transformation to orthogonal axes:
0

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

Rescaling parameter:
1 1.012750958

Matrix Representation

1	6.28296E-17	0
0	1.025664503	0
0	0	3.933219
a	b	c
1	1.025664503	3.933219
90	90	90
alpha	beta	gamma

p1 (#1)
distorted p4mm (#11)
S4 (-4) when accounting for 3rd dimension

0,0,0	0	0	0	1
x,y,z	-0.213620625	-0.06335625	-0.027342	1
x,y,z	0.141979375	0.13474375	-0.041342	1
x,y,z	-0.045120625	0.13914375	0.052158	1
x,y,z	0.130879375	-0.19945625	0.017458	1

Z'= 1

		|G|	Z	|G|/Z
Daughter	P_21_21_2	4	4	1
Plane	p1	1	1	1
			4	1
			(size)	(index)

60c,d P_b_c_n
42 YIMWEW

a=	24.4809		
b=	10.9912	b/a=	0.4489704
c=	11.2429	c/a=	0.4592519
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

Matrix Representation

1	0	0
0	0.4489704	0
0	0	0.4592519
a	b	c
1	0.4489704	0.4592519
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

0.166667	0.166667	-0.166667	0
0.5	-0.5	0	-0.25
0	0	-0.5	0.25
0	0	0	1

Det= 0.083333

Inverse Transformation

3	1	-1	0.5
3	-1	-1	0
0	0	-2	0.5
0	0	0	1

Det= 12

Matrix Representation

0.166666667	0.166666667	-0.166666667
0.224485211	-0.224485211	0
0	0	-0.229625953
a	b	c
0.279591466	0.279591466	0.283735539
110.4967722	110.4967722	106.8167033
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1.029863465
-0.355344565	-0.355344565	-0.289310869

Daughter	60c,d	|G|	Z	|G|/Z	
Ref. Lattice	BCC	8	12	0.666667	
		48	1	48	
			12	72	
			(size)	(index)	

Reduced Cell

Character	16 (oF)	… 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	Equal	|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	-1	-1	0
0	1	-1	0.5
3	0	0	0
0	0	0	1

Det= 6

Center of Mass Coordinates

c 2 nearest neighbors
8 neighbors within 5% of nearest
next neighbor 11% farther than nearest

c .2.									
0,y,1/4	0	-0.187538	0.25	1	0,0,0	0.062462	-0.062462	0	1
1/2,1/2-y,3	0.5	0.687538	0.75	1		1.937538	0.062462	-1	1
0,1-y,3/4	0	1.187538	0.75	1		0.937538	-1.937538	-1	1
1/2,1/2+y,1	0.5	0.312462	0.25	1		2.062462	0.937538	0	1
y=	-0.187538								

Z'= 1

Order Parameter = Coupled

d 1 nearest neighbor
7 neighbors within 5% of nearest
9 neighbors within 8% of nearest
next neighbor >11% farther than nearest

Sphere packing

d 1								
x,y,z	0.1688182	0.2974947	0.206184	1	1.097765367	0.002776033	0.087632	1
1/2-x,1/2-y	0.3311818	0.2025053	0.706184	1	0.989866633	0.084855967	-0.912368	1
1-x,y,1/2-z	0.8311818	0.2974947	0.293816	1	2.997223967	1.902234633	-0.087632	1
1/2+x,1/2-y	0.6688182	0.2025053	0.793816	1	1.915144033	1.010133367	-1.087632	1
1-x,1-y,1-z	0.8311818	0.7025053	0.793816	1	2.902234633	0.997223967	-1.087632	1
1/2+x,1/2+	0.6688182	0.7974947	0.293816	1	3.010133367	0.915144033	-0.087632	1
x,1-y,1/2+z	0.1688182	0.7025053	0.706184	1	1.002776033	-0.902234633	-0.912368	1
1/2-x,1/2+y	0.3311818	0.7974947	0.206184	1	2.084855967	-0.010133367	0.087632	1
x=	0.1688182							
y=	0.2974947							
z=	0.206184							

Monoclinic Crystal Structures (3-15)

15e *A2/a*
43 BOGMEP

a=	19.4179		
b=	9.7886	b/a=	0.5041019
c=	22.7929	c/a=	1.1738087
alpha=	90	alpha=	90
beta=	116.083	beta=	116.083
gamma=	90	gamma=	90

2 nearest neighbors
next neighbor 10.5% farther than nearest

Hexagonal packing of p-4m2 rods.

Matrix Representation

1	0	-0.516092
0	0.5041019	0
0	0	1.0542658
a	b	c
1	0.5041019	1.1738087
90	116.083	90
alpha	beta	gamma

Transformation to Rod Coordinates

1	-0.516081	0	0.25
0	0	1	0.25689
0	-1	0	0.5
0	0	0	1

Det= 1

Inverse Transformation

1	0	-0.516081	0.008041
0	0	-1	0.5
0	1	0	-0.25689
0	0	0	1

Det= 1

rod axis:

0	1	0

rod origin:

0.25	0.25689	0.5

Transformation to orthogonal axes:
-0.516081

Rotation about rod and rescaling:

1.026221172	-0.032039118	0	0
0.030393135	0.973499922	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.973499922	0.032039118	0	0
-0.030393135	1.026221172	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:
-1.788220892 degrees

Rescaling parameter:
1.026721188

Matrix Representation

1.026221494	-0.032028812	0
0	0	0.504102
-0.032042441	-1.026327633	0
a	b	c
1.026721614	1.026827276	0.504102
90	90	90
alpha	beta	gamma

p112 (#8)
… but close to p-4m2 (#37)

Daughter	15e	|G|	Z	|G|/Z
Rod	37a	4	2	2
		8	1	8
			2	4
			(size)	(index)

Center of Mass Coordinates

	e 2						a -4m2				
i	1/4,y,1/2	0.25	0.2568903	0.5	1	0,0,0	0	0	0	1	Z'= 1
	1/4,1/2+y,0	0.25	0.7568903	0	1		0.267221992	0.505267925	0.5	1	
	3/4,1/2-y,0	0.75	0.2431097	0	1		0.753971953	0.490071358	-0.013781	1	
	3/4,1-y,1/2	0.75	0.7431097	0.5	1		0.486749961	-0.015196567	0.486219	1	
	y=	0.2568903									
						error	0	0	0		

Molecular 3-fold axes

	f 1						f m				
i	1/2-x,y,1-z	0.3347	0.1504	0.5517	1	x,-x,-z	0.054824689	-0.054819002	-0.10649	1
i	x,y,z	0.1653	0.1504	0.4483	1	-x,x,-z	-0.054824689	0.054819002	-0.10649	1
i		0.2219	0.3791	0.5538	1	-x,-x,z	-0.056108434	-0.053512782	0.12221	1
i		0.2781	0.3791	0.4462	1	x,x,z	0.056108434	0.053512782	0.12221	1
						x=	0.054816227			
						z=	0.11435			
						error	0.001292207	-0.001303445	0.00786	

15e C2/c
44 MSISUL10

a=	9.3821		
b=	16.5132	b/a=	1.760075
c=	10.58411	c/a=	1.1281174
alpha=	90	alpha=	90
beta=	107.1717	beta=	107.1717
gamma=	90	gamma=	90

2 nearest neighbors
next neighbor 19% farther than nearest

Hexagonal packing of pmcm rods.

Matrix Representation

1	0	-0.333061
0	1.760075	0
0	0	1.0778308
a	b	c
1	1.760075	1.1281174
90	107.1717	90
alpha	beta	gamma

Transformation to Rod Coordinates

1	0	0	0
0	1	0	0.5
0.261707	0	1	0.5
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	-0.5
-0.261707	0	1	-0.5
0	0	0	1

Det= 1

rod axis:

0	0	1

rod origin:

0	0.5	0.5

Transformation to orthogonal axes:
0.261707

Rotation about rod and rescaling:

1.357273748	0	0	0
0	0.736771047	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.736771047	0	0	0
0	1.357273748	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:
0 degrees

Rescaling parameter:
1.357273748

Matrix Representation

1.238967834	0	-0.333061
0	1.296772327	0
0.382853985	0	1.077831
a	b	c
1.296772327	1.296772327	1.128117
90	90	90
alpha	beta	gamma

pmcm (#22)

Daughter	15e	|G|	Z	|G|/Z
Rod	22b	4	2	2
		8	2	4
			1	2
			(size)	(index)

Center of Mass Coordinates

	e 2						b m2m				
	0,y,1/4	0	0.8926227	0.25	1	0,-y,3/4	0	0.532896473	-0.25	1	Z'= 2
i	0,1-y,3/4	0	0.1073773	0.75	1	0,y,1/4	0	-0.532896473	0.25	1	
	1/2,1/2+y,1	0.5	0.3926227	0.25	1		0.368385523	-0.145740401	-0.380853	1	
	1/2,1/2-y,3	0.5	0.6073773	0.75	1		0.368385523	0.145740401	0.119147	1	
	y=	0.8926227									

Molecular 3-fold axes

	f 1				
i		-0.0026	0.1801	0.9088	1
i		0.0026	0.1801	0.5912	1
	f 1				
i		-0.1872	0.0356	0.6989	1
i		0.1872	0.0356	0.8011	1

d m				
0,y,1/2-z	-0.001915605	-0.434191872	0.40948	1
0,y,z	0.001915605	-0.434191872	0.09052	1
error	0.001915605	0	0	

e m				
-x,y,1/4	-0.13792354	-0.630317929	0.247892	1
x,y,1/4	0.13792354	-0.630317929	0.252108	1
error	0	0	0.002108	

15e C2/c
45 TMGEHS10

a=	9.4225		
b=	16.7798	b/a=	1.7808225
c=	10.7085	c/a=	1.1364818
alpha=	90	alpha=	90
beta=	107.943	beta=	107.943
gamma=	90	gamma=	90

2 nearest neighbors

Matrix Representation

1	0	-0.350117
0	1.7808225	0
0	0	1.0812073
a	b	c
1	1.7808225	1.1364818
90	107.943	90
alpha	beta	gamma

See #44 above.

next neighbor 19% farther than nearest
rod packing

See above.

Center of Mass Coordinates

e 2

0,y,1/4	0	0.8945	0.25	1
0,1-y,3/4	0	0.1055	0.75	1
1/2,1/2+y,1	0.5	0.3945	0.25	1
1/2,1/2-y,3	0.5	0.6055	0.75	1
y=	0.8945			

15e C2/c

46 TMSNHS10

a=	9.7726		
b=	17.3516	b/a=	1.7755357
c=	10.9585	c/a=	1.1213495
alpha=	90	alpha=	90
beta=	108.984	beta=	108.984
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.36478
0	1.7755357	0
0	0	1.0603587
a	b	c
1	1.7755357	1.1213495
90	108.984	90
alpha	beta	gamma

See #44 above.

2 nearest neighbors
next neighbor 21% farther than nearest
rod packing

See above.

Center of Mass Coordinates

e 2

0,y,1/4	0	0.1023143	0.25	1
0,1-y,3/4	0	0.8976857	0.75	1
1/2,1/2+y,1	0.5	0.6023143	0.25	1
1/2,1/2-y,3	0.5	0.3976857	0.75	1
y=	0.1023143			

15e C2/c

47 RASDOE

a=	20.0104		
b=	10.1162	b/a=	0.5055471
c=	19.3224	c/a=	0.9656179
alpha=	90	alpha=	90
beta=	120.132	beta=	120.132
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.484734
0	0.5055471	0
0	0	0.8351351
a	b	c
1	0.5055471	0.9656179
90	120.132	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

1	-1	0	0.5
-2	0	1	0
0	0	-1	0.5
0	0	0	1

Det= 2

Matrix Representation

0	-0.5	-0.015265763
-0.505547115	-0.252773558	-0.252773558
0	0	-0.835135083
a	b	c
0.505547115	0.560262859	0.872684434
81.58784777	73.16296173	63.18125235
alpha	beta	gamma

Normalized Niggli Matrix

1	1.228175397	2.979827926
0.279865187	0.5	0.5

Daughter 15e
Ref. Lattice 70a

|G|	Z	|G|/Z
4	2	2
8	2	4
	1	2
	(size)	(index)

Reduced Cell

Character	27 (mC)	… but close to 26 (oF)	
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

Transformation to Conventional Cell

1	-1	-1	0
0	2	0	0
0	0	2	0
0	0	0	1

Det= 4

Overall Transformation

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

Det= 0.5

2 nearest neighbors
6 neighbors within 2% of nearest
10 neighbors within 13% of nearest
next neighbor 24% farther than nearest
sphere packing

Center of Mass Coordinates

e 2

0,y,1/4	0	0.377	0.25	1	x,1/4,1/4	0.123	0.25	0.25	1
0,1-y,3/4	0	0.623	0.75	1	1-x,3/4,3/4	-0.123	0.75	-0.25	1
1/2,1/2+y,1	0.5	0.877	0.25	1		0.123	-0.75	0.25	1
1/2,1/2-y,3	0.5	0.123	0.75	1		0.877	-0.25	-0.25	1
y=	0.377								

Z'= 2

Order Parameter = GM3+

Very distorted diamond cubic.
Close to particular distortion w/ 10 nearest neighbors.

15e *C2/n*

48 TFMETH02

a=	8.40982		
b=	4.30221	b/a=	0.5115698
c=	8.35062	c/a=	0.9929606
alpha=	90	alpha=	90
beta=	119.5881	beta=	119.5881
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.490285
0	0.5115698	0
0	0	0.8634761
a	b	c
1	0.5115698	0.9929606
90	119.5881	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

1	-1	0	0
-2	0	1	0
0	0	-1	1
0	0	0	1

Det= 2

Matrix Representation

0	-0.5	-0.009714511
-0.511569808	-0.255784904	-0.255784904
0	0	-0.863476064
a	b	c
0.511569808	0.561627917	0.900617123
82.01283561	73.50027726	62.90708582
alpha	beta	gamma

Normalized Niggli Matrix

1	1.20527893	3.099349763
0.268560135	0.5	0.5

See #47 above.

6 neighbors within 6% of nearest
10 neighbors within 12% of nearest
next neighbor 20% farther than nearest
sphere packing

See above.

Center of Mass Coordinates

e 2

1/4,y,1/4	0.25	0.32562	0.25	1	-x,3/4,3/4	-0.07562	-0.25	0.75	1
1/4,1/2-y,3	0.25	0.17438	0.75	1	x,1/4,1/4	0.07562	0.25	0.25	1
3/4,1/2+y,1	0.75	0.82562	0.25	1		-0.07562	-1.25	0.75	1
3/4,1-y,3/4	0.75	0.67438	0.75	1		0.07562	-0.75	0.25	1
y=	0.32562								

15e C2/c

49 REKYUB

a=	19.8721		
b=	9.49968	b/a=	0.4780411
c=	19.7822	c/a=	0.9954761
alpha=	90	alpha=	90
beta=	123.4156	beta=	123.4156
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.548217
0	0.4780411	0
0	0	0.8309218
a	b	c
1	0.4780411	0.9954761
90	123.4156	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.25

Inverse Transformation

1	-1	0	0.5
2	0	-2	0.5
2	0	0	0
0	0	0	1

Det= 4

Matrix Representation

0	0.27410833	0.22589167
-0.478041073	0	0.239020536
0	-0.415460918	0.415460918
a	b	c
0.478041073	0.497738035	0.529873228
114.8151994	116.8136414	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1.084104714	1.228608542
-0.484366374	-0.5	6.37814E-17

Daughter 15e
Ref. Lattice FCC

|G|	Z	|G|/Z
4	2	2
48	1	48
	2	24
	(size)	(index)

Reduced Cell

Character	37 (mC)	… but close to singularity: 1 (cF)	
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

1	1	-1	0
-1	1	-1	0
0	2	0	0
0	0	0	1

Det= 4

Overall Transformation

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

Det= 1

12 neighbors within 16% of nearest
next neighbor 41% farther than nearest

sphere packing

Center of Mass Coordinates

e 2

0,y,1/4	0	0.5238033	0.25	1	0,0,0	-0.023803333	0	0	1
0,1-y,3/4	0	0.4761967	0.75	1		0.023803333	-1	0	1
1/2,1/2+y,1	0.5	0.0238033	0.25	1		0.976196667	1	1	1
1/2,1/2-y,3	0.5	0.9761967	0.75	1		0.023803333	0	1	1
y=	0.5238033								
					error	-0.023803333	0	0	

Z'= 1

Order Parameter = Coupled

12i C2/m

50 MECKOU

a=	15.7928		
b=	11.5117	b/a=	0.7289208
c=	18.4079	c/a=	1.1655881
alpha=	90	alpha=	90
beta=	109.736	beta=	109.736
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.393604
0	0.7289208	0
0	0	1.0971198
a	b	c
1	0.7289208	1.1655881
90	109.736	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.25

Inverse Transformation

1	-1	-1	0
1	1	-1	0
0	0	2	-0.5
0	0	0	1

Det= 4

Matrix Representation

0.5	0.5	0.303198177
-0.364460387	0.364460387	0
0	0	0.548559893
a	b	c
0.618733686	0.618733686	0.626775152
66.98862618	66.98862618	72.17816954
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1.026162217
0.395994422	0.395994422	0.306058057

Daughter 12i
Ref. Lattice FCC

|G|	Z	|G|/Z
4	2	2
48	1	48
	2	24
	(size)	(index)

Reduced Cell

Character	14 (mC)	along rhom path from FCC to BCC	
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

Transformation to Conventional Cell

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

Det= 4

Overall Transformation

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

Det= 1

5 neighbors within 0.5% of nearest
8 neighbors within 9% of nearest
12 neighbors within 19% of nearest
next neighbor 40% farther than nearest

Center of Mass Coordinates

sphere packing

i m

x,0,z	0.2535	0	0.2411	1
1-x,1,1-z	0.7465	1	0.7589	1
1/2+x,1/2,z	0.7535	0.5	0.2411	1
1/2-x,1/2,1·	0.2465	0.5	0.7589	1
x=	0.2535			
z=	0.2411			

0,0,0	0.0124	0.0124	-0.0178	1
	-1.0124	0.9876	1.0178	1
	0.0124	1.0124	-0.0178	1
	-1.0124	-0.0124	1.0178	1
error	0.0124	0.0124	-0.0178	

Z'= 1

Order Parameter = Coupled

11e P_21/m

51 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

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

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

Inverse Transformation

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

Det= 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

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

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

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			

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

rod axis: 1 0 0

rod origin: 0.20498 0.25 0.219284

Transformation to orthogonal axes:
0.29084

rotation angle:
45 degrees

Rescaling parameter:
0.822173817

a m2m

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

Z'= 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			

14e P_21/c

52 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

Inverse Transformation

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

Det= 1

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

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

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

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
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

rotation angle:
0 degrees

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	

Z'= 4

14e P_21/c

53 VAVYAS

a=	9.6783		
b=	14.3654	b/a=	1.4842896
c=	17.0195	c/a=	1.7585216
alpha=	90	alpha=	90
beta=	92.242	beta=	92.242
gamma=	90	gamma=	90

3 neighbors within 4% of nearest
next neighbor 27% farther than nearest
planar packing

See above.

Matrix Representation

1	0	-0.068794
0	1.4842896	0
0	0	1.7571755
a	b	c
1	1.4842896	1.7585216
90	92.242	90
alpha	beta	gamma

See #52 above.

Center of Mass Coordinates

e 1

x,y,z	0.3443616	0.5277806	0.2914611	1
1-x,1/2+y,1	0.6556384	0.0277806	0.2085389	1
1-x,1-y,1-z	0.6556384	0.4722194	0.7085389	1
x,1/2-y,1/2·	0.3443616	0.9722194	0.7914611	1
x=	0.3443616			
y=	0.5277806			
z=	0.2914611			

14e P_21/c

54 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

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

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

Normalized Niggli Matrix

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

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

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			

0.933	0.752	0.843	1
0.433	0.248	0.657	1
0.067	0.248	0.157	1
0.567	0.752	0.343	1

Z'= 4

dimers:

Transformation to Reduced Cell

0	0	-1	0

Matrix Representation

-0.125119979	-0.125119979	-1

|G|	Z	|G|/Z

Transformation to Conventional Cell

1	-1	-1	0

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

-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

-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

Normalized Niggli Matrix

1	1	2.796789577
0.349934254	0.349934254	0.436316354

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

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

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

Dimer Center of Mass Coordinates

a -1

i	0,0,0	0	0	0	1	0,0,0	0	0	0	1	Z' = 1
ii	0,1/2,1/2	0	0.5	0.5	1		0	1	0	1	

Order Parameter = F2+

14e P_21/c
55 QUGBOJ

a=	16.1133		
b=	9.5502	b/a=	0.5926905
c=	17.0133	c/a=	1.0558545
alpha=	90	alpha=	90
beta=	104.893	beta=	104.893
gamma=	90	gamma=	90

4 neighbors within 2% of nearest
next neighbor 10% farther than nearest

Hexagonal packing of pc11 rods

Matrix Representation

1	0	-0.27137
0	0.5926905	0
0	0	1.0203857

a	b	c
1	0.5926905	1.0558545
90	104.893	90
alpha	beta	gamma

Center of Mass Coordinates

e 1

x,y,z	0.2324831	0.8707496	0.4302323	1
1-x,1/2+y,1	0.7675169	0.3707496	0.0697677	1
1-x,1-y,1-z	0.7675169	0.1292504	0.5697677	1
x,1/2-y,1/2·	0.2324831	0.6292504	0.9302323	1

x= 0.2324831
y= 0.8707496
z= 0.4302323

Transformation to Rod Coordinates

0	1	0	0.25
-1	0	0	0.75
0	0.243414	1	0
0	0	0	1

Det= 1

Inverse Transformation

0	-1	0	0.75
1	0	0	-0.25
-0.243414	0	1	0.060854
0	0	0	1

Det= 1

rod axis:
0 0 1

rod origin:
0.25 0.75 0

Transformation to orthogonal axes:
0.243414

Rotation about rod and rescaling:

1.276927253	0	0	0
0	0.783129969	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.783129969	0	0	0
0	1.276927253	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:
0

Rescaling parameter:
1.276927253 1

Matrix Representation

-4.6361E-17	0.731400026	0
-1	0	8.13E-17
0	0.194511051	1.020386

a	b	c
0.756822665	0.756822665	1.055854
90.00027569	90	90
alpha	beta	gamma

pc11 (#5)

a 1

x,y,z	-0.094562635	-0.0223678	0.434496	1	Z'= 2
	0.29700235	0.660831427	-0.056203	1	
	0.486127619	0.660831427	0.443797	1	
-x,y,z+1/2	0.094562635	-0.0223678	0.934496	1	

		|G|	Z	|G|/Z
Daughter	14e	4	4	1
Rod	5a	2	2	1
			2	1
			(size)	(index)

14e P_21/n
56 DOCNIS

a=	8.4595		
b=	12.2587	b/a=	1.4491046
c=	13.1488	c/a=	1.5543235
alpha=	90	alpha=	90
beta=	93.285	beta=	93.285
gamma=	90	gamma=	90

2 neighbors within 3% of nearest
next neighbor 10% farther than nearest

Hexagonal packing of p-1 rods

Matrix Representation

1	0	-0.089067
0	1.4491046	0
0	0	1.5517696

a	b	c
1	1.4491046	1.5543235
90	93.285	90
alpha	beta	gamma

Center of Mass Coordinates

e 1

i	x,y,z	0.3257927	0.254875	0.4281235	1
ii	1-x,1-y,1-z	0.6742073	0.745125	0.5718765	1
	1/2-x,1/2+y	0.1742073	0.754875	0.0718765	1
	1/2+x,1/2-y	0.8257927	0.245125	0.9281235	1

x= 0.3257927
y= 0.254875
z= 0.4281235

Molecular 3-fold axes

e 1

i	x,y,z	0.4285	0.3111	0.534	1
ii	x,y,z	0.5715	0.6889	0.466	1

x= 0.4285
y= 0.3111
z= 0.534

Transformation to Rod Coordinates

0	1	0	0.5
0	0	1	0
1	0.036867	0	0.5
0	0	0	1

Det= 1

Inverse Transformation

-0.036867	0	1	-0.481567
1	0	0	-0.5
0	1	0	0
0	0	0	1

Det= 1

rod axis:
0 1 0

rod origin:
0.5 0 0.5

Transformation to orthogonal axes:
0.036867

Rotation about rod and rescaling:

0.801442168	0	0	0
0	1.247750667	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1.247750667	0	0	0
0	0.801442168	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:
0

Rescaling parameter:
0.801442168

Matrix Representation

-0.071381948	1.243653563	0
0	0	1.449105
1.24365356	0.07138189	0

a	b	c
1.245700429	1.245700429	1.449105
90	90	90
alpha	beta	gamma

p-1 (#2)

c 1

x,y,z	-0.081670409	-0.139617052	0.254875	1	Z'= 1
-x,-y,-z	0.081670409	0.139617052	0.745125	1	

c 1

x,y,z	0.045712545	-0.057303115	0.3111	1
-x,-y,-z	-0.045712545	0.057303115	0.6889	1

		|G|	Z	|G|/Z
Daughter	14e	4	4	1
Rod	2c	2	2	1
			2	1
			(size)	(index)

14e P_21/c
57 TMSIAD

a=	8.8592		
b=	9.8442	b/a=	1.1111839
c=	18.3163	c/a=	2.0674892
alpha=	90	alpha=	90
beta=	91.073	beta=	91.073
gamma=	90	gamma=	90

2 neighbors within 4% of nearest
next neighbor 24% farther than nearest

Square packing of p-1 rods

Matrix Representation

1	0	-0.038716
0	1.1111839	0
0	0	2.0671266

a	b	c
1	1.1111839	2.0674892
90	91.073	90
alpha	beta	gamma

Center of Mass Coordinates

e 1

i	x,y,z	-0.169642	0.2582289	0.0914053	1
ii	1-x,1-y,1-z	0.1696421	0.7417711	-0.091405	1
	1-x,1/2+y,1	0.1696421	0.7582289	0.4085947	1
	x,1/2-y,1/2·	-0.169642	0.2417711	0.5914053	1

x= -0.169642
y= 0.2582289
z= 0.0914053

Molecular 3-fold axes

e 1

i	x,y,z	-0.2308	0.4381	0.1222	1
ii	x,y,z	0.2308	0.5619	-0.1222	1

x= -0.2308
y= 0.4381
z= 0.1222

Transformation to Rod Coordinates

0	1	0	0
0	0	1	0
1	0.009057	0	0
0	0	0	1

Det= 1

Inverse Transformation

-0.009057	0	1	0
1	0	0	0
0	1	0	0
0	0	0	1

Det= 1

rod axis:
0 1 0

rod origin:
0 0 0

Transformation to orthogonal axes:
0.009057

Rotation about rod and rescaling:

0.521466571	0.46007203	0	0
-0.95136076	1.078315571	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1.078315571	-0.46007203	0	0
0.95136076	0.521466571	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:
41.42085259

Rescaling parameter:
0.695408986

Matrix Representation

-0.971216454	1.060125106	0
0	0	1.111184
1.060125296	0.97121623	0

a	b	c
1.437750689	1.437750398	1.111184
90	90	90
alpha	beta	gamma

p-1 (#2)

c 1

x,y,z	0.178268157	-4.15243E-05	0.258229	1	Z'= 1
-x,-y,-z	-0.178268157	4.15243E-05	0.741771	1	

c 1

x,y,z	0.240208951	-0.002109429	0.4381	1
-x,-y,-z	-0.240208951	0.002109429	0.5619	1

		|G|	Z	|G|/Z
Daughter	14e	4	2	2
Rod	2c	2	1	2
			2	1
			(size)	(index)

14e P_21/n
58 MECKUA

a=	16.7235		
b=	11.1082	b/a=	0.664227
c=	19.1055	c/a=	1.1424343
alpha=	90	alpha=	90
beta=	112.703	beta=	112.703
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.440927
0	0.664227	0
0	0	1.0539161

a	b	c
1	0.664227	1.1424343
90	112.703	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.25

Inverse Transformation

0	0	-2	0.5

Matrix Representation

-0.279536259	-0.5	-0.5
0	-0.332113493	0.332113493
-0.526958035	0	0

a	b	c
0.596510931	0.600249425	0.600249425
67.1863708	67.02350771	67.02350771
alpha	beta	gamma

		|G|	Z	|G|/Z
Daughter	14e	4	4	1
Ref. Lattice	FCC	48	1	48
			4	48
			(size)	(index)

Reduced Cell
Character 20 (mC) …but close to 1 (cF)

Transformation to Conventional Cell

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

Det= 4

Overall Transformation

12 neighbors within 14% of nearest
next neighbor 45% farther than nearest
sphere packing

Center of Mass Coordinates

	e 1			
x,y,z	0.0013148	0.2747839	0.2493133	1
1-x,1-y,1-z	0.9986852	0.7252161	0.7506867	1
1/2-x,1/2+y	0.4986852	0.7747839	0.2506867	1
1/2+x,1/2-y	0.5013148	0.2252161	0.7493133	1

x= 0.0013148
y= 0.2747839
z= 0.2493133

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

Det= 4

Normalized Niggli Matrix

1	1.012573816	1.012573816
0.39261017	0.392799874	0.392799874

0,0,0	0.001373469	-0.026785469	0.022782313	1
	-1.001373469	-0.973214531	-0.022782313	1
	-0.001373469	-1.022782313	0.026785469	1
	-0.998626531	0.022782313	-0.026785469	1
error	0.001373469	-0.026785469	0.022782313	

Z'= 1

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

Along Rhom. Path from FCC to BCC

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

Det= 1

Order Parameter = Coupled

14e P_21/c
59 TOHSUE

a=	10.4005		
b=	10.5225	b/a=	1.0117302
c=	28.7446	c/a=	2.763771
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

Matrix Representation

1	0	0
0	1.0117302	0
0	0	2.763771
a	b	c
1	1.0117302	2.763771
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

-0.5	-0.5	0.5	0.25
-0.5	0.5	-0.5	0.75
0.25	-0.25	-0.25	0.125
0	0	0	1

Det= 0.25

Inverse Transformation

-1	-1	0	1
-1	0	-2	0.5
0	-1	-2	1
0	0	0	1

Det= 4

Matrix Representation

-0.5	-0.5	0.5
-0.505865103	0.505865103	-0.505865103
0.690942743	-0.690942743	-0.690942743
a	b	c
0.991615539	0.991615539	0.991615539
91.66075478	118.653373	119.4398054
alpha	beta	gamma

Daughter 14e
Ref. Lattice FCC

|G|	Z	|G|/Z
4	4	1
48	1	48
	4	48
	(size)	(index)

Transformation to Conventional Cell

0	0	2	0
1	1	1	0
-1	1	1	0
0	0	0	1

Det= 4

12 neighbors within 3% of nearest
next neighbor 40% farther than nearest
sphere packing

Normalized Niggli Matrix

1	1	1
-0.02898158	-0.479509521	-0.491508898

Reduced Cell
Character 8 (oI) … but close to singularity: 1 (cF)

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	Equal	|a.b|≤a.a/2	True

Overall Transformation

-0.5	0.5	0	-0.25
0	0	-2	0.25
-0.5	-0.5	0	0.5
0	0	0	1

Det= 1

Center of Mass Coordinates

	e 1			
x,y,z	0.2504837	0.7448743	0.1256666	1
1-x,1/2+y,1	0.7495163	0.2448743	0.3743334	1
1-x,1-y,1-z	0.7495163	0.2551257	0.8743334	1
x,1/2-y,1/2·	0.2504837	0.7551257	0.6256666	1

x= 0.2504837
y= 0.7448743
z= 0.1256666

0,0,0	0.004641935	-0.001816854	0.003792581	1
	0.005609435	-0.998183146	0.00645879	1
	-0.004641935	-1.998183146	-1.003792581	1
	-0.005609435	-1.001816854	-1.00645879	1
error	0.004641935	-0.001816854	0.003792581	

Z'= 1

Order Parameter = Coupled

14ee P_21/n
60 CANFIG

a=	18.2286		
b=	16.7496	b/a=	0.9188638
c=	8.7652	c/a=	0.4808488
alpha=	90	alpha=	90
beta=	90.694	beta=	90.694
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.005824
0	0.9188638	0
0	0	0.4808135
a	b	c
1	0.9188638	0.4808488
90	90.694	90
alpha	beta	gamma

Transformation to Planar Coordinates

0.005824	0	1	0.25
0	1	0	0
1	0	0	0.25
0	0	0	1

Det= -1

Inverse Transformation

0	0	1	-0.25
0	1	0	0
1	0	-0.005824	-0.248544
0	0	0	1

Det= -1

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

Matrix Representation

-5.7798E-08	5.62872E-17	1
2.98123E-17	0.918863764	0
0.480813503	0	0
a	b	c
0.480813503	0.918863764	1
90	90.00000689	90
alpha	beta	gamma

pg (#4) in projection
distorted p6mm (#17) - puckered honeycomb
2_1 when accounting for 3rd dimension

		|G|	Z	|G|/Z
Daughter	14ee	4	8	0.5
Plane	2_1	2	4	0.5
			2	1
			(size)	(index)

e: 3 neighbors within 6% of nearest
next neighbor 28% farther than nearest

e: 3 neighbors within 6% of nearest
next neighbor 30% farther than ne

planar

Center of Mass Coordinates

	e 1			
x,y,z	0.2987978	0.5073711	-0.02555	1
1-x,1-y,1-z	0.7012022	0.4926289	1.02555	1
1/2-x,1/2+y	0.2012022	0.0073711	0.52555	1
1/2+x,1/2-y	0.7987978	0.9926289	0.47445	1

x= 0.2987978
y= 0.5073711
z= -0.02555

	e 1			
x,y,z	0.37146	0.17384	0.0347222	1
1-x,1-y,1-z	0.62854	0.82616	0.9652778	1
1/2-x,1/2+y	0.12854	0.67384	0.4652778	1
1/2+x,1/2-y	0.87146	0.32616	0.5347222	1

x= 0.37146
y= 0.17384
z= 0.0347222

plane normal:

1	0	0

plane origin:

0.25	0	0.25

Transformation to orthogonal axes:
0.005824

rotation angle:
0 degrees

-x,1/2+y,-z	-0.27555	0.507371111	0.050403	1
	0.77555	0.492628889	0.446685	1
x,y,z	0.27555	0.007371111	-0.050403	1
	0.22445	0.992628889	0.547491	1

Z'= 4

x= 0.27555
y= 0.007371111
z= 0.050402614

x,y,z	-0.215277778	0.17384	0.122714	1
	0.715277778	0.82616	0.374374	1
-x,1/2+y,-z	0.215277778	0.67384	-0.122714	1
	0.284722222	0.32616	0.619802	1

x= -0.215277778
y= 0.17384
z= 0.122713804

14ee P_21/a
61 MXSNOX

a=	18.3874		
b=	18.5194	b/a=	1.0071788
c=	10.5433	c/a=	0.5733981
alpha=	90	alpha=	90
beta=	104.742	beta=	104.742
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.145911
0	1.0071788	0
0	0	0.5545227
a	b	c
1	1.0071788	0.5733981
90	104.742	90
alpha	beta	gamma

Transformation to Rod Coordinates

1	0	0	0.071518
0	1	0	0.274913
0.443769	0	1	0.158782
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	-0.071518
0	1	0	-0.274913
-0.443769	0	1	-0.127045
0	0	0	1

Det= 1

Rotation about rod and rescaling:

0.809124867	0.62191573	0	0
-0.597156301	0.776912352	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.776912352	-0.62191573	0	0
0.597156301	0.809124867	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

0.756733494	0.581646273	0
-1	1	4.41E-17
0.199109283	0.153040897	0.554523
a	b	c
0.986926538	0.986926538	0.573398
90.00039009	90.00050751	90
alpha	beta	gamma

p11c (#5)
… but nearly pmcm (#22)

		|G|	Z	|G|/Z
Daughter	14ee	4	8	0.5
Rod	22b	8	2	4
			4	8
			(size)	(index)

Center of Mass Coordinates

e: 1 nearest neighbor
next neighbor less than 1% farther
next neighbor 4% farther than nearest

	e 1			
x,y,z	0.9989317	0.8207	0.1219222	1
1-x,1-y,1-z	0.0010683	0.1793	0.8780778	1
1/2-x,1/2+y	0.5010683	0.3207	0.8780778	1
1/2+x,1/2-y	0.4989317	0.6793	0.1219222	1

x= 0.9989317
y= 0.8207
z= 0.1219222

e: 1 nearest neighbor
next neighbor less than 1% farther
next neighbor 4% farther than nearest

	e 1			
x,y,z	0.8550967	0.6405294	0.5592111	1
1-x,1-y,1-z	0.1449033	0.3594706	0.4407889	1
1/2-x,1/2+y	0.6449033	0.1405294	0.4407889	1
1/2+x,1/2-y	0.3550967	0.8594706	0.5592111	1

x= 0.8550967
y= 0.6405294
z= 0.5592111

rod axis:

0	0	1

rod origin:

0.071518	0.274913	0.158782

Transformation to orthogonal axes:
0.443769

rotation angle:
37.546875

Rescaling parameter:
1.020520566

b m2m

	0.381085562	0.995420431	-0.448417	1
0,-y,3/4	0.004729961	-0.119432636	0.750559	1
	0.305247253	0.293555771	0.528675	1
	0.08056827	0.582432024	-0.226533	1

Z'= 2

b m2m

	0.381389276	0.763747978	0.052701	1
0,y,1/4	0.004426247	0.112239818	0.249441	1
	0.529045344	0.233667271	0.027556	1
	-0.143229821	0.642320525	0.274586	1

y= 0.115836227

error= 0.004426247 -0.003596409 -0.000559

13efg P_2/c
62 RIMNAC

a=	18.3422		
b=	9.51838	b/a=	0.5189334
c=	33.8124	c/a=	1.8434212
alpha=	90	alpha=	90
beta=	94.3008	beta=	94.3008
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.138243
0	0.5189334	0
0	0	1.8382303
a	b	c
1	0.5189334	1.8434212
90	94.3008	90
alpha	beta	gamma

Transformation to Rod Coordinates

1	-0.138243	0	0
0	0	1	0.481138
0	-1	0	0.25
0	0	0	1

Det= 1

Inverse Transformation

1	0	-0.138243	0.034561
0	0	-1	0.25
0	1	0	-0.481138

Rotation about rod and rescaling:

1.354553635	-0.058435591	0	0
0.031789048	0.736879192	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.736879192	0.058435591	0	0
-0.031789048	1.354553635	0	0
0	0	1	0

Matrix Representation

1.354553635	-0.058435588	0
-3.85892E-18	-8.9451E-17	1
-0.058435591	-1.354553635	0
a	b	c
1.355813508	1.355813507	0.518933
90	90	90
alpha	beta	gamma

p-42m (#37)

		|G|	Z	|G|/Z
Daughter	13efg	4	8	0.5
Rod	37a	8	1	8
			8	16
			(size)	(index)

0	0	0	1

Det= 1

0	0	0	1

Det= 1

2nd setting

Center of Mass Coordinates

e: 2 nearest neighbors
4 neighbors within 2% of nearest
next neighbor 5% farther than nearest

e 2	Unique axis b, Cell Choice 1			
0,y,1/4	0	0.4811384	0.25	1
0,1-y,3/4	0	0.5188616	0.75	1
y=	0.4811384			

f: 2 nearest neighbors
4 neighbors within 2% of nearest
next neighbor 3% farther than nearest

f 2	Unique axis b, Cell Choice 1			
1/2,y,1/4	0.5	0.8131861	0.25	1
1/2,1-y,3/4	0.5	0.1868139	0.75	1
y=	0.8131861			

g: 1 nearest neighbor
3 neighbors within 1% of nearest
next neighbor 4% farther than nearest

Hexagonal packing of p-42m rods
with 3 independent orientations

g 1	Unique axis b, Cell Choice 1			
x,y,z	0.2557004	0.1578597	0.0006353	1
1-x,y,1/2-z	0.7442996	0.1578597	0.4993647	1
1-x,1-y,1-z	0.7442996	0.8421403	0.9993647	1
x,1-y,1/2+z	0.2557004	0.8421403	0.5006353	1
x=	0.2557004			
y=	0.1578597			
z=	0.0006353			

Molecular 3-fold axes

g 1				
x,y,z	0.0585	0.5809	0.277	1
	-0.0585	0.5809	0.223	1
	-0.0463	0.3787	0.2794	1
	0.0463	0.3787	0.2206	1

rod axis:

0	1	0

rod origin:

0	0.481138	0.25	(e)
0.5	0.813186	0.25	(f)
0.25	0.15786	0	(g)

Transformation to orthogonal axes:
-0.138243

rotation angle:
-2.470214495 degrees

Rescaling parameter:
1.355813508

a	-42m				
0,0,0	0	0	0	1	Z'= ?
f	..m				
x,-x,z	0.038779225	-0.038313953	0.099762	1	
-x,x,z	-0.038779225	0.038313953	0.099762	1	
-x,-x,-z	-0.038830444	-0.038222842	-0.102438	1	
x,x,-z	0.038830444	0.038222842	-0.102438	1	
x=	0.038536616				
z=	0.1011				
error=	0.000242609	0.000222663	-0.001338		
	-0.000242609	-0.000222663	-0.001338		
	-0.000293828	0.000313774	-0.001338		
	0.000293828	-0.000313774	-0.001338		

15ffff C2/c
63 CTBROM

a=	21.434		
b=	12.122	b/a=	0.5655501
c=	21.024	c/a=	0.9808715
alpha=	90	alpha=	90
beta=	110.883	beta=	110.883
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.349642
0	0.5655501	0
0	0	0.9164383
a	b	c
1	0.5655501	0.9808715
90	110.883	90
alpha	beta	gamma

Transformation to Reduced Cell

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

Det= 0.5

Inverse Transformation

-1	-1	0	1
2	0	-1	0
0	0	1	0
0	0	0	1

Det= 2

Matrix Representation

-3.46441E-17	1	0.150357756
-1	-0.28277503	-0.28277503
0	0	0.916438337
a	b	c
0.565550061	0.574422943	0.970787514
73.84672292	73.06514726	60.50966745
alpha	beta	gamma

Normalized Niggli Matrix

1	1.031624029	2.946498726
0.485046471	0.5	0.5

Daughter	15ffff	
Ref. Lattice	FCC	

|G|	Z	|G|/Z
4	16	0.25
48	1	48
	16	192
	(size)	(index)

Reduced Cell

Character	41 (mC)	… but close to singularity: 1 (cF)	
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

Transformation to Conventional Cell

1	1	-1	0
-1	1	-1	0
0	2	0	0
0	0	0	1

Det= 4

Overall Transformation

-1.5	-0.5	0.5	0.5
0	0	0.5	0
-0.5	0.5	1	-0.5
0	0	0	1

Det= 0.5

f: 1 nearest neighbor
12 neighbors within 25% of nearest
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of neare Center of Mass Coordinates
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of nearest
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of nearest
next neighbors >40% of nearest
sphere packing

Z'= 1

Order Parameter = Coupled

f 1									
x,y,z	0.0961	0.0316	0.3782	1	0,0,0	0.8723	-0.186	0.3782	1
1-x,y,1/2-z	0.9039	0.0316	0.1218	1		0.0645	1.686	0.1218	1
1-x,1-y,1-z	0.9039	0.9684	0.6218	1		-0.8723	1.186	0.6218	1
x,1-y,1/2+z	0.0961	0.9684	0.8782	1		-0.0645	-0.686	0.8782	1
1/2+x,1/2+	0.5961	0.5316	0.3782	1		-0.1277	0.814	0.3782	1
1/2-x,1/2+y	0.4039	0.5316	0.1218	1		0.0645	0.686	0.1218	1
1/2-x,1/2-y	0.4039	0.4684	0.6218	1		0.1277	0.186	0.6218	1
1/2+x,1/2-y	0.5961	0.4684	0.8782	1		-0.0645	0.314	0.8782	1
x=	0.0961								
y=	0.0316								
z=	0.3782								

f 1								
x,y,z	0.3792	0.0597	0.1201	1	0.5611	0.6383	0.1201	1
1-x,y,1/2-z	0.6208	0.0597	0.3799	1	0.3195	0.8617	0.3799	1
1-x,1-y,1-z	0.6208	0.9403	0.8799	1	-0.5611	0.3617	0.8799	1
x,1-y,1/2+z	0.3792	0.9403	0.6201	1	-0.3195	0.1383	0.6201	1
1/2+x,1/2+	0.8792	0.5597	0.1201	1	-0.4389	1.6383	0.1201	1
1/2-x,1/2+y	0.1208	0.5597	0.3799	1	0.3195	-0.1383	0.3799	1
1/2-x,1/2-y	0.1208	0.4403	0.8799	1	0.4389	-0.6383	0.8799	1
1/2+x,1/2-y	0.8792	0.4403	0.6201	1	-0.3195	1.1383	0.6201	1
x=	0.3792							
y=	0.0597							
z=	0.1201							

f 1								
x,y,z	0.1261	0.3158	0.1232	1	0.5581	0.129	0.1232	1
1-x,y,1/2-z	0.8739	0.3158	0.3768	1	-0.1897	1.371	0.3768	1
1-x,1-y,1-z	0.8739	0.6842	0.8768	1	-0.5581	0.871	0.8768	1
x,1-y,1/2+z	0.1261	0.6842	0.6232	1	0.1897	-0.371	0.6232	1
1/2+x,1/2+	0.6261	0.8158	0.1232	1	-0.4419	1.129	0.1232	1
1/2-x,1/2+y	0.3739	0.8158	0.3768	1	-0.1897	0.371	0.3768	1
1/2-x,1/2-y	0.3739	0.1842	0.8768	1	0.4419	-0.129	0.8768	1
1/2+x,1/2-y	0.6261	0.1842	0.6232	1	0.1897	0.629	0.6232	1
x=	0.1261							
y=	0.3158							
z=	0.1232							

f 1								
x,y,z	0.3452	0.2907	0.3713	1	0.3641	0.3191	0.3713	1
1-x,y,1/2-z	0.6548	0.2907	0.1287	1	0.0545	1.1809	0.1287	1
1-x,1-y,1-z	0.6548	0.7093	0.6287	1	-0.3641	0.6809	0.6287	1
x,1-y,1/2+z	0.3452	0.7093	0.8713	1	-0.0545	-0.1809	0.8713	1
1/2+x,1/2+	0.8452	0.7907	0.3713	1	-0.6359	1.3191	0.3713	1
1/2-x,1/2+y	0.1548	0.7907	0.1287	1	0.0545	0.1809	0.1287	1
1/2-x,1/2-y	0.1548	0.2093	0.6287	1	0.6359	-0.3191	0.6287	1
1/2+x,1/2-y	0.8452	0.2093	0.8713	1	-0.0545	0.8191	0.8713	1
x=	0.3452							
y=	0.2907							
z=	0.3713							

15ffff C2/c
64 CARBTC07

a=	20.1818		
b=	11.3504	b/a=	0.5624077
c=	19.7616	c/a=	0.9791793
alpha=	90	alpha=	90
beta=	111.463	beta=	111.463
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.358282
0	0.5624077	0
0	0	0.9112771
a	b	c
1	0.5624077	0.9791793
90	111.463	90
alpha	beta	gamma

See #63 above.

f: 1 nearest neighbor
12 neighbors within 25% of nearest
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of neare Center of Mass Coordinates
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of nearest
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of nearest

f 1				
x,y,z	0.0948	0.0343	0.3766	1
1-x,y,1/2-z	0.9052	0.0343	0.1234	1
1-x,1-y,1-z	0.9052	0.9657	0.6234	1
x,1-y,1/2+z	0.0948	0.9657	0.8766	1
1/2+x,1/2+	0.5948	0.5343	0.3766	1

next neighbors >40% of nearest
sphere packing

See above.

1/2-x,1/2+y	0.4052	0.5343	0.1234	1
1/2-x,1/2-y	0.4052	0.4657	0.6234	1
1/2+x,1/2-y	0.5948	0.4657	0.8766	1
x=	0.0948			
y=	0.0343			
z=	0.3766			

f 1

x,y,z	0.3793	0.0648	0.1221	1
1-x,y,1/2-z	0.6207	0.0648	0.3779	1
1-x,1-y,1-z	0.6207	0.9352	0.8779	1
x,1-y,1/2+z	0.3793	0.9352	0.6221	1
1/2+x,1/2+	0.8793	0.5648	0.1221	1
1/2-x,1/2+y	0.1207	0.5648	0.3779	1
1/2-x,1/2-y	0.1207	0.4352	0.8779	1
1/2+x,1/2-y	0.8793	0.4352	0.6221	1
x=	0.3793			
y=	0.0648			
z=	0.1221			

f 1

x,y,z	0.1267	0.3131	0.1231	1
1-x,y,1/2-z	0.8733	0.3131	0.3769	1
1-x,1-y,1-z	0.8733	0.6869	0.8769	1
x,1-y,1/2+z	0.1267	0.6869	0.6231	1
1/2+x,1/2+	0.6267	0.8131	0.1231	1
1/2-x,1/2+y	0.3733	0.8131	0.3769	1
1/2-x,1/2-y	0.3733	0.1869	0.8769	1
1/2+x,1/2-y	0.6267	0.1869	0.6231	1
x=	0.1267			
y=	0.3131			
z=	0.1231			

f 1

x,y,z	0.3418	0.285	0.3745	1
1-x,y,1/2-z	0.6582	0.285	0.1255	1
1-x,1-y,1-z	0.6582	0.715	0.6255	1
x,1-y,1/2+z	0.3418	0.715	0.8745	1
1/2+x,1/2+	0.8418	0.785	0.3745	1
1/2-x,1/2+y	0.1582	0.785	0.1255	1
1/2-x,1/2-y	0.1582	0.215	0.6255	1
1/2+x,1/2-y	0.8418	0.215	0.8745	1
x=	0.3418			
y=	0.285			
z=	0.3745			

Triclinic Crystal Structures (1-2)

2i P_-1
65 BASXOI

a=	9.1472		
b=	10.4952	b/a=	1.1473675
c=	10.5082	c/a=	1.1487887
alpha=	85.60	alpha=	85.602
beta=	89.83	beta=	89.832
gamma=	65.71	gamma=	65.713

2 neighbors within 1% of nearest
next neighbor 14% farther than nearest

Square packing of p-1 rods.

Matrix Representation

1	0.4719209	0.0033684
0	1.0458216	0.0951276
0	0	1.1448384
a	b	c
1	1.1473675	1.1487887
85.602	89.832	65.713
alpha	beta	gamma

Transformation to Rod Coordinates

0.615286	0.071184	1	0
0.384714	-0.071184	-1	0.5
0	1	0	1
0	0	0	1

Det= 1

Inverse Transformation

1	1	0	-0.5
0	0	1	-1
0.384714	-0.615286	-0.071184	0.378827
0	0	0	1

Det= 1

rod axis:
1 -1 0

rod origin:
0 0.5 1

Transformation to monoclinic axes:
-0.384714
0.071184

Transformation to Orthogonal Coordinates

1	-0.051402326	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0.051402326	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Transformation to orthogonal axes:
-0.051402326

Rotation about rod and rescaling:

0.385523889	1.064837859	0	0
-0.830277535	0.300601469	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.300601469	-1.064837859	0	0
0.830277535	0.385523889	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:
70.09724248 degrees

Rescaling parameter:
1.132478845

Matrix Representation

0.307201	0.8485059	0.528079
0.155112	0.428429472	-1.045822
-0.950534	0.344140092	0
a	b	c
1.010914	1.010913685	1.171585
89.99916	89.99963973	90
alpha	beta	gamma

p-1 (#2)

Daughter	2i		
Rod	2c		

|G|	Z	|G|/Z
2	2	1
2	1	2
	2	2
	(size)	(index)

Center of Mass Coordinates
i 1

i	x,y,z	0.2974607	0.3063664	0.7986807	1
ii	1-x,1-y,1-z	-0.297461	0.6936336	1.2013193	1
	x=	0.2974607			
	y=	0.3063664			
	z=	0.7986807			

c 1

x,y,z	0.242472	6.36615E-09	0.247908	1
-x,-y,-z	-0.242472	-6.36615E-09	-0.247908	1

Z'= 1

c 1

x,y,z	0.142336	-0.230276221	0.307522	1
-x,-y,-z	-0.142336	0.230276221	-0.307522	1

Molecular 3-fold axes
i 1

i	x,y,z	0.183	0.1363	0.8126	1
ii	x,y,z	-0.183	0.8637	1.1874	1
	x=	0.183			
	y=	0.1363			
	z=	0.8126			

2i P_-1
66 XAGXAE

a=	9.007214		
b=	9.208015	b/a=	1.0222934
c=	9.1952	c/a=	1.0208706
alpha=	92.502	alpha=	92.502
beta=	100.722	beta=	100.722
gamma=	109.8421	gamma=	109.84211

2 neighbors within 6% of nearest
next neighbor 11% farther than nearest

Oblique packing of p-1 rods.

Matrix Representation

1	-0.346996	-0.189927
0	0.9616014	-0.115914
0	0	0.9963276
a	b	c
1	1.0222934	1.0208706
92.502	100.722	109.84211
alpha	beta	gamma

Transformation to Rod Coordinates

0	1	0	0
0.043593	0.332027	1	0
1	0	0	0
0	0	0	1

Det= 1

Inverse Transformation

0	0	1	0
1	0	0	0
-0.332027	1	-0.043593	0
0	0	0	1

Det= 1

rod axis:
0 1 0

rod origin:
0 0 0

Transformation to monoclinic axes:
0.332027
0.043593

Transformation to Orthogonal Coordinates

1	0.197125158	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	-0.197125158	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Transformation to orthogonal axes:
0.197125158

Rotation about rod and rescaling:

-0.796749907	-0.51590333	0	0
0.5726109	-0.884327847	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

-0.884327847	0.51590333	0	0
-0.5726109	-0.796749907	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:
-147.0765496

Rescaling parameter:
0.949192636

Matrix Representation

0.64687	-0.640909051	-0.346996
0.233425	-0.231273599	0.961601
-0.681362	-0.687691794	0
a	b	c
0.968082	0.968076387	1.022293
89.99999	90.00000241	90.00014
alpha	beta	gamma

p-1 (#2)

Daughter	2i		
Rod	2c		

|G|	Z	|G|/Z
4	2	2
2	1	2
	2	1
	(size)	(index)

Center of Mass Coordinates
i 1

i	x,y,z	0.1543118	0.2575931	-0.184303	1
ii	1-x,1-y,1-z	-0.154312	0.7424069	0.1843034	1
	x=	0.1543118			
	y=	0.2575931			
	z=	-0.184303			

c 1

x,y,z	0.269495	4.31622E-06	0.214392	1
-x,-y,-z	-0.269495	-4.31622E-06	0.785608	1

Z'= 1

c 1

x,y,z	0.346219	-0.072542055	0.010215	1
-x,-y,-z	-0.346219	0.072542055	0.989785	1

Molecular 3-fold axes
i 1

i	x,y,z	0.2624	0.0892	-0.1867	1
ii	x,y,z	-0.2624	0.9108	0.1867	1
	x=	0.2624			
	y=	0.0892			
	z=	-0.1867			

2i P_-1
67 MEZDIE01

a=	9.920097		
b=	14.51031	b/a=	1.4627186
c=	9.135857	c/a=	0.9209443
alpha=	90.47694	alpha=	90.47694
beta=	111.6724	beta=	111.67244

Matrix Representation

1	0.0003125	-0.340105
0	1.4627185	-0.007593
0	0	0.8558094
a	b	c
1	1.4627186	0.9209443

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

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

Daughter	2i		
Ref. Lattice	BCC		

|G|	Z	|G|/Z
2	2	1
48	1	48
	2	48
	(size)	(index)

Transformation to Conventional Cell

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

Det= 2

```
gamma=  89.98776  gamma=  89.98776      90.47694  111.67244  89.98776     Inverse Transformation                      107.9992896   107.3143809   107.0838036     Reduced Cell
                                          alpha      beta      gamma       |   1      1      0  |   -1  |              alpha          beta          gamma          Character  44 (aP)     ... but close to 5 (cl)          Overall Transformation
  6 neighbors within 3% of nearest                                         |   1     -1      0  |  -0.5 |                                                          Type       II                                          |  0.5    -1    -0.5 |   0  |
  next neighbor 11% farther than nearest                                   |   1      0     -1  |  -0.5 |          Normalized Niggli Matrix                        b.b≥a.a    True        |b.c|≤b.b/2   True          |  0.5     1    -0.5 | -0.5 |
  sphere packing                                                           |   0      0      0  |   1   |         |  1             1.01327063    1.032529194  |      c.c≥b.b    True        |a.c|≤a.a/2   True          |  0.5     0     0.5 | -0.5 |
                                                                                            Det= 2              | -0.316067389  -0.302416346  -0.295712962  |      2|D+E+F|   True        |a.b|≤a.a/2   True          |  0       0     0   |   1  |
                                                                                                                                                                    ≤ A+B                                                                    Det= 1
                              Center of Mass Coordinates
                                    i 1
                                     x,y,z       0.7605859  0.2506235    0.24179    1                     0,0,0     0.011209412   0.009962353   0.018795882     1      Z'= 1                                              Order Parameter =  Coupled
                                     1-x,1-y,1-z 0.2394141  0.7493765    0.75821    1                              -0.011209412  -1.009962353  -1.018795882     1
                                              x= 0.7605859
                                              y= 0.2506235
                                              z=    0.24179
```

```
   2i          P_-1                              Matrix Representation
68 MEZDOK01                                      |  1    -0.000126  -0.341044 |
        a=  9.944575                             |  0    1.4610255  -0.008613 |
        b=  14.52928        b/a= 1.4610255       |  0        0      0.8556222 |
        c=  9.160215        c/a= 0.9211268
   alpha=  90.53393     alpha=   90.53393             a          b          c
    beta=  111.7308      beta=  111.73083             1      1.4610255  0.9211268         See #67 above.
   gamma=  90.00494     gamma=   90.00494         90.53393   111.73083   90.00494
                                                    alpha       beta       gamma
  6 neighbors within 3% of nearest
  next neighbor 11% farther than nearest
  sphere packing

  See above.                   Center of Mass Coordinates
                                     i 1
                                      x,y,z       0.7617465  0.2495818  0.2417818    1
                                      1-x,1-y,1-z 0.2382535  0.7504182  0.7582182    1
                                               x= 0.7617465
                                               y= 0.2495818
                                               z= 0.2417818
```

```
   2i          P_-1
69 XUWROW                                  Thin Film Crystal w/ Large Voids
                   a=      9.6802
                   b=     17.9373       b/a= 1.852989
                   c=     28.0315       c/a= 2.895756
               alpha=      96.622
                beta=      99.962
               gamma=     105.681

             i 1
              0.041217   0.745871  0.4152899 x,y,z
              0.958783   0.254129  0.5847101 1-x,1-y,1-z

                     x=  0.041217
                     y=  0.745871
                     z=   0.41529

             Molecules clustered near c=(n+1)/2 and large c/a lead to unrealistically large gaps between layers.
```

```
   2iii        P_-1                              Matrix Representation                   Transformation to Reduced Cell                          Matrix Representation                                                                          |G|      Z       |G|/Z           Transformation to Conventional Cell
70 OHABEE                                        |  1    0.0018522  0.0015842 |          | -0.333333  -0.333333  -0.333333 | 0.333333 |       | -0.333861416  -0.332143174  -0.33399541  |     Daughter      2iii           2        6     0.333333          |  0     1     1 |  0 |
        a=   9.79238                             |  0    1.4884328  0.0017618 |          |     0         0.5       -0.5    |  -0.25   |       | -0.000587265   0.744510039  -0.743922774 |     Ref. Lattice  BCC           48        1       48               |  1     0     1 |  0 |
        b=  14.57531      b/a= 1.488434          |  0        0      2.5714065 |          | -0.333333   0.166667   0.166667 | 0.083333 |       | -0.857135491   0.428567745   0.428567745 |                                         6      144               |  1     1     0 |  0 |
        c=   25.1802      c/a= 2.5714076                                                 |     0          0          0     |    1     |                                                                                                (size)  (index)            |  0     0     0 |  1 |
   alpha=   89.9607    alpha=    89.9607              a          b          c                                    Det= -0.166667               a              b              c                                                                                              Det= 2
    beta=   89.9647     beta=    89.9647              1       1.488434  2.5714076                                                       0.919861424    0.921023669    0.921218943
   gamma=   89.9287    gamma=    89.9287           89.9607    89.9647    89.9287      Inverse Transformation                               107.7916146    107.5410774    107.6508078       Reduced Cell
                                                    alpha       beta      gamma      |  -1     1     1 |  -0.5 |                          alpha          beta           gamma          Character  44 (aP)     ... but close to 5 (cl)          Overall Transformation
                                                                                     |  -1     0    -2 |   1.5 |                                                                       Type       II                                          | -0.5    0     2 |  0  |
                                                                                     |  -1    -1     1 |   0   |          Normalized Niggli Matrix                                     b.b≥a.a    True        |b.c|≤b.b/2   True          | -0.5   -1    -1 |  0  |
                                                                                     |   0     0     0 |   1   |         |  1            1.002528597    1.00295375   |                   c.c≥b.b    True        |a.c|≤a.a/2   True          | -0.5    1    -1 | 0.5 |
                                                                                                    Det= 6               | -0.30639353  -0.301834263  -0.303598139  |                   2|D+E+F|   True        |a.b|≤a.a/2   True          |  0     0     0 |  1  |
                              Center of Mass Coordinates                                                                                                                                    ≤ A+B                                                                   Det= -3
  i: 1 nearest neighbor              i 1
    8 neighbors within 10% of nearest  x,y,z       0.3198117  0.2466519  0.5851674    1                 0,0,0     0.012007596   0.009853611   0.018703811     1      Z'=          1                                   Order Parameter =  Coupled
    next neighbor 16% farther than nearest 1-x,1-y,1-z 0.6801883 0.7533481 0.4148326  1                          -0.012007596  -0.009853611  -1.018703811     1
                                            x= 0.3198117
                                            y= 0.2466519                                                 error     0.012007596   0.009853611   0.018703811
                                            z= 0.5851674
  i: 1 nearest neighbor              i
    8 neighbors within 10% of nearest  x,y,z        0.016409  0.2535574  0.2500246    1                          -0.012827038   0.983541861  -0.019941823     1
    next neighbor 18% farther than nearest 1-x,1-y,1-z 0.983591 0.7464426 0.7499754   1                           0.012827038  -0.983541861  -0.980058177     1
                                            x=  0.016409
                                            y= 0.2535574                                                 error    -0.012827038  -0.016458139  -0.019941823
                                            z= 0.2500246
  i: 2 nearest neighbors             i
    8 neighbors within 10% of nearest  x,y,z       0.3180757  0.7535794  0.0817532    1                           0.017256975   1.018417871  -0.989901882     1
    next neighbor 15% farther than nearest 1-x,1-y,1-z 0.6819243 0.2464206 0.9182468  1                          -0.017256975  -1.018417871  -0.010098118     1
                                            x= 0.3180757
    sphere packing                          y= 0.7535794                                                 error     0.017256975   0.018417871   0.010098118
                                            z= 0.0817532
```

```
   2iiii       P_-1                              Matrix Representation                   Transformation to Planar Coordinates           Rotation about plane normal and rescaling:              Matrix Representation
71 CANFOM                                        |  1    0.0307136  -0.006985 |          | 0.006985  -0.030726     1     |  0.25  |    |  1     0     0 |  0 |                              | -3.90214E-08  -1.29356E-05    1 |                                         |G|      Z      |G|/Z
        a=   18.4086                             |  0    0.9181114  0.0164553 |          |    0         1         0     |   0    |    |  0     1     0 |  0 |                              |  0.0164553    0.918111404     0 |     Daughter     2iiii          2        8      0.25
        b=   16.9106      b/a= 0.918625          |  0        0      0.4795676 |          |    1         0         0     |  0.25  |    |  0     0     1 |  0 |                              |  0.479567629       0          0 |     Plane        2_1            2        4      0.5
        c=    8.8343      c/a= 0.4799007                                                 |    0         0         0     |   1    |    |  0     0     0 |  1 |                                                                                                         2        2
   alpha=    88.064    alpha=     88.064              a          b          c                            Det= -1                                   Det= 1                         a              b             c                                         (size)  (index)
    beta=    90.834     beta=     90.834              1       0.918625  0.4799007                                                                                                0.479849859    0.918111404      1
   gamma=    88.084    gamma=     88.084            88.064     90.834     88.084      Inverse Transformation                          Inverse Transformation                        90.00080726    90.00000466   88.03479
                                                    alpha       beta      gamma      |  0       0         1      | -0.25    |    |  1     0     0 |  0 |                            alpha          beta          gamma
  i: 1 nearest neighbor                                                              |  0       1         0      |   0      |    |  0     1     0 |  0 |
    3 neighbors within 8% of nearest                                                 |  1   0.030726  -0.006985  | -0.248254|    |  0     0     1 |  0 |                         pg (#4) in projection
    next neighbor 26% farther than nearest                                           |  0       0         0      |   1      |    |  0     0     0 |  1 |                         distorted p6mm (#17) - puckered honeycomb
  i: 1 nearest neighbor                                                                                 Det= -1                                   Det= 1                         2_1 when accounting for 3rd dimension
    3 neighbors within 8% of nearest  Center of Mass Coordinates
    next neighbor 29% farther than ne  i 1                                           plane normal:                                  rotation angle:
  i: 1 nearest neighbor                x,y,z       0.1987578  0.0060756  0.5133267    1      1        0        0                            0  degrees              1/4,0,-z     0.263326667   0.006075556  -0.052895     1      Z'=        4
    3 neighbors within 7% of nearest   1-x,1-y,1-z 0.8012422  0.9939244  0.4866733    1                                                                                                  0.236673333   0.993924444   0.580129     1
    next neighbor 33% farther than nearest      x= 0.1987578                         plane origin:
  i: 1 nearest neighbor                         y= 0.0060756                           0.25     0      0.25                                                    3/4,1/2,z    0.720098889   0.506314444   0.060231     1
    3 neighbors within 9% of nearest            z= 0.5133267                                                                                                                -0.220098889   0.493685556   0.467003     1
    next neighbor 32% farther than ne  i 1                                           Transformation to orthogonal axes:
                                       x,y,z       0.2997033  0.5063144  0.9700989    1    0.006985                                                                        z=           0.056562756
    planar                             1-x,1-y,1-z 0.7002967  0.4936856  0.0299011    1   -0.030726                                                                        error=       0.013326667   0.006075556   0.003668
```

x=	0.2997033			
y=	0.5063144			
z=	0.9700989			
i 1				
x,y,z	0.12601	0.6773511	0.4547744	1
1-x,1-y,1-z	0.87399	0.3226489	0.5452256	1
x=	0.12601			
y=	0.6773511			
z=	0.4547744			
i 1				
x,y,z	0.3692444	0.1746478	0.0148856	1
1-x,1-y,1-z	0.6307556	0.8253522	0.9851144	1
x=	0.3692444			
y=	0.1746478			
z=	0.0148856			

	-0.029901111	0.006314444	0.003668	
1/4,2/3,z	0.204774444	0.677351111	-0.104608	1
	0.295225556	0.322648889	0.631842	1
3/4,1/6,-z	-0.235114444	0.174647778	0.126253	1
	0.735114444	0.825352222	0.400981	1
z=	0.115430415			
error=	-0.045225556	0.010684444	0.010823	
	0.014885556	0.007981111	0.010823	

Molecular Crystal Global Phase Diagrams:
II. Reference Lattices

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

Table 7: Neighbor Histogram

Neighbor distances scaled to the nearest neighbor distance
Red entries highlight large steps in the histogram

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Dimers																		
	205c	FOJBUB02																
monomer	c	1.000	1.329	1.329	1.329	1.329	1.329	1.329	1.449	1.449	1.449	1.449	1.449	1.449	1.966	1.966	1.966	2.121
dimer	a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.414	1.414	1.414	1.414	1.414
	205c	VADRAU																
monomer	c	1.000	1.250	1.250	1.250	1.250	1.250	1.250	1.377	1.377	1.377	1.377	1.377	1.377	1.860	1.860	1.860	2.039
dimer	a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.414	1.414	1.414	1.414	1.414
	88f	LUFYEQ																
monomer	f	1.000	1.331	1.331	1.563	1.563	1.568	1.573	1.573	1.582	1.582	1.597	1.650	1.650	2.082	2.082	2.089	2.089
dimer	e	1.000	1.126	1.126	1.270	1.270	1.270	1.270	1.482	1.482	1.562	1.562	1.562	1.562	1.689	1.989	1.989	2.032
quatramer	a	1.000	1.000	1.000	1.000	1.600	1.600	1.600	1.600	1.600	1.600	1.600	1.600	1.697	1.697	1.697	1.697	1.801
	14e	CARBTC																
monomer	e	1.000	1.060	1.060	1.114	1.114	1.207	1.207	1.231	1.231	1.245	1.245	1.264	1.438	1.438	1.632	1.688	1.727
dimer	a	1.000	1.000	1.000	1.000	1.062	1.062	1.672	1.672	1.695	1.695	1.760	1.760	1.760	1.760	1.804	1.804	1.981
Rods																		
	137a	FUZTEZ																
	a	1.000	1.000	1.123	1.123	1.123	1.123	1.123	1.123	1.123	1.123	1.422	1.422	1.422	1.422	1.739	1.739	1.739
	62c	GUTCED																
	c	1.000	1.000	1.106	1.106	1.174	1.174	1.218	1.218	1.218	1.218	1.321	1.321	1.539	1.539	1.680	1.680	1.697
	62c	JEYSEL																
	c	1.000	1.000	1.125	1.125	1.203	1.203	1.353	1.353	1.430	1.430	1.521	1.521	1.521	1.521	1.647	1.647	1.647
	62c	RIMMOP																
	c	1.000	1.000	1.042	1.042	1.171	1.171	1.210	1.210	1.255	1.255	1.324	1.324	1.324	1.324	1.687	1.687	1.687
	15e	BOGMEP																
	e	1.000	1.000	1.105	1.105	1.117	1.117	1.151	1.151	1.267	1.267	1.267	1.267	1.515	1.515	1.533	1.533	1.787
	15e	MSISUL10																
	e	1.000	1.000	1.191	1.191	1.463	1.463	1.473	1.473	1.491	1.491	1.491	1.491	1.564	1.564	1.661	1.661	1.867
	15e	TMGEHS10																
	e	1.000	1.000	1.195	1.195	1.468	1.468	1.477	1.477	1.499	1.499	1.499	1.499	1.549	1.549	1.668	1.668	1.852
	15e	TMSNHS10																
	e	1.000	1.000	1.213	1.213	1.497	1.497	1.513	1.513	1.525	1.525	1.525	1.525	1.557	1.557	1.678	1.678	1.850
	14e	DOCNIS																
	e	1.000	1.030	1.102	1.102	1.125	1.125	1.161	1.161	1.222	1.224	1.224	1.247	1.532	1.532	1.551	1.551	1.768
	14e	TMSIAD																
	e	1.000	1.036	1.238	1.238	1.248	1.277	1.347	1.347	1.392	1.392	1.470	1.470	1.496	1.496	1.919	1.919	1.955
	2i	BASXOI																
	i	1.000	1.010	1.144	1.147	1.270	1.294	1.316	1.316	1.509	1.509	1.511	1.511	1.531	1.541	1.541	1.735	1.777
	11e	MECKIO																
	e	1.000	1.000	1.022	1.022	1.122	1.122	1.152	1.152	1.188	1.188	1.206	1.206	1.329	1.329	1.624	1.624	1.647
	13efg	RIMNAC																
	e	1.000	1.000	1.019	1.019	1.049	1.049	1.094	1.094	1.172	1.172	1.174	1.174	1.245	1.245	1.644	1.644	1.660
	f	1.000	1.000	1.019	1.019	1.031	1.031	1.038	1.038	1.172	1.172	1.172	1.172	1.421	1.421	1.461	1.461	1.644
	g	1.000	1.007	1.007	1.038	1.041	1.045	1.056	1.102	1.172	1.180	1.182	1.207	1.254	1.431	1.471	1.629	1.655
	14ee	MXSNOX																
	e	1.000	1.003	1.043	1.155	1.384	1.473	1.483	1.483	1.484	1.492	1.492	1.524	1.566	1.566	1.582	1.604	1.758
	e	1.000	1.003	1.043	1.058	1.384	1.420	1.473	1.484	1.524	1.540	1.566	1.566	1.582	1.758	1.767	1.805	1.805
	2i	XAGXAE																
	i	1.000	1.058	1.112	1.149	1.324	1.467	1.467	1.498	1.498	1.500	1.500	1.514	1.539	1.706	1.706	1.829	1.853
	14e	QUGBOJ																
	e	1.000	1.010	1.014	1.014	1.099	1.099	1.109	1.109	1.258	1.266	1.286	1.286	1.464	1.464	1.488	1.488	1.679
Planes																		
	19a	MZNMOX10																
	a	1.000	1.000	1.026	1.026	1.132	1.132	1.151	1.151	1.268	1.268	1.421	1.421	1.432	1.432	1.432	1.432	1.595
	14e	CAMPOV																
	e	1.000	1.035	1.035	1.262	1.262	1.264	1.300	1.300	1.316	1.345	1.345	1.468	1.468	1.475	1.837	1.837	1.850

14e	VAVYAS																
e	1.000	1.038	1.038	1.266	1.266	1.290	1.290	1.303	1.375	1.392	1.392	1.526	1.526	1.539	1.852	1.852	1.873
14ee	CANFIG																
e	1.000	1.044	1.055	1.275	1.395	1.521	1.521	1.590	1.633	1.633	1.690	1.707	1.707	1.744	1.893	1.893	1.936
e	1.000	1.044	1.055	1.302	1.395	1.521	1.521	1.590	1.690	1.744	1.773	1.773	1.818	1.818	1.853	1.853	1.893
2iiii	CANFOM																
i	1.000	1.056	1.072	1.264	1.363	1.523	1.523	1.604	1.614	1.676	1.679	1.695	1.721	1.723	1.913	1.918	1.961
i	1.000	1.071	1.073	1.293	1.449	1.547	1.547	1.631	1.639	1.702	1.721	1.739	1.750	1.814	1.870	1.937	1.960
i	1.000	1.054	1.056	1.333	1.363	1.523	1.523	1.606	1.712	1.721	1.752	1.781	1.789	1.815	1.823	1.824	1.854
i	1.000	1.073	1.089	1.315	1.449	1.547	1.547	1.629	1.705	1.780	1.809	1.814	1.817	1.843	1.852	1.852	1.852
Sphere Packings																	
227a	ZNOXAC01																
a	1.000	1.000	1.000	1.000	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.915
217a	DEQPAQ																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	HMSIPA																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	HXMTAM07																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	KELREY																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	MESIAD																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	MPTHOT01																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	NIWMIP																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	POSLOY10																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	TMEPTC																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	YEYQAU																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a*	HMGETP																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
215a	FOHCUA																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414
215a	FUZVOL																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414
215a*	JUFWUC																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414
176h	CUCZUV																
h	1.000	1.000	1.022	1.022	1.067	1.067	1.067	1.067	1.137	1.137	1.140	1.140	1.492	1.492	1.492	1.492	1.562
165d	DILWIE01																
d	1.000	1.000	1.000	1.035	1.035	1.035	1.059	1.059	1.059	1.059	1.059	1.059	1.456	1.456	1.456	1.481	1.481
165d	ZEYHIU																
d	1.000	1.000	1.000	1.091	1.091	1.091	1.094	1.094	1.094	1.094	1.094	1.094	1.482	1.482	1.482	1.545	1.545
161a	TCYMET																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.042	1.042	1.167	1.167	1.167	1.167	1.167	1.167	1.624	1.624	1.624
147d	ZIZHIZ																
d	1.000	1.000	1.000	1.010	1.010	1.010	1.055	1.055	1.055	1.055	1.055	1.055	1.454	1.454	1.454	1.461	1.461
152b	MTRETC10																
b	1.000	1.000	1.010	1.010	1.010	1.010	1.010	1.010	1.071	1.071	1.071	1.071	1.421	1.421	1.421	1.421	1.521
141a	FUZLUH																
a	1.000	1.000	1.000	1.000	1.358	1.358	1.386	1.386	1.386	1.386	1.493	1.493	1.493	1.493	1.493	1.493	1.493
141a	VAFWAA																
a	1.000	1.000	1.000	1.000	1.351	1.351	1.383	1.383	1.383	1.383	1.493	1.493	1.493	1.493	1.493	1.493	1.493
121a	ZZZKDW01																
a	1.000	1.000	1.000	1.000	1.028	1.028	1.028	1.028	1.028	1.028	1.028	1.028	1.414	1.414	1.414	1.414	1.491
142a	KUJSIR																

	a	1.000	1.000	1.000	1.000	1.006	1.006	1.006	1.006	1.006	1.006	1.006	1.006	1.414	1.414	1.414	1.414	1.431
	120b	YEMRIR																
	b	1.000	1.000	1.000	1.000	1.062	1.062	1.414	1.414	1.414	1.414	1.458	1.458	1.458	1.458	1.458	1.458	1.458
	114a	ADAMAN08																
	a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.025	1.025	1.025	1.025	1.377	1.377	1.450	1.450	1.450
	114a	GERHOA																
	a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.063	1.063	1.063	1.063	1.320	1.320	1.503	1.503	1.503
	88a	KANGUB01																
	a	1.000	1.000	1.000	1.000	1.111	1.111	1.111	1.111	1.414	1.414	1.414	1.414	1.495	1.495	1.495	1.495	1.495
	64d,f	Methane																
	d	1.000	1.000	1.034	1.034	1.034	1.034	1.040	1.040	1.042	1.042	1.082	1.082	1.462	1.462	1.462	1.462	1.478
	f	1.000	1.000	1.037	1.037	1.038	1.038	1.040	1.040	1.042	1.042	1.082	1.082	1.345	1.465	1.469	1.481	1.481
	60c,d	YIMWEW																
	c	1.000	1.000	1.010	1.010	1.041	1.041	1.049	1.049	1.117	1.117	1.213	1.213	1.325	1.325	1.569	1.569	1.641
	d	1.000	1.010	1.013	1.013	1.040	1.040	1.049	1.071	1.071	1.117	1.213	1.243	1.288	1.288	1.564	1.569	1.641
	15e	RASDOE																
	e	1.000	1.000	1.014	1.014	1.018	1.018	1.124	1.124	1.124	1.124	1.235	1.235	1.241	1.241	1.592	1.592	1.609
	15e	TFMETH02																
	e	1.000	1.000	1.018	1.018	1.059	1.059	1.118	1.118	1.118	1.118	1.198	1.198	1.313	1.313	1.533	1.533	1.697
	15e	REKYUB																
	e	1.000	1.000	1.042	1.042	1.088	1.088	1.131	1.131	1.159	1.159	1.159	1.159	1.411	1.411	1.477	1.477	1.750
	12i	MECKOU																
	i	1.000	1.003	1.003	1.003	1.003	1.034	1.083	1.083	1.146	1.146	1.182	1.182	1.400	1.475	1.548	1.548	1.570
	14e	MECKUA																
	e	1.000	1.000	1.000	1.000	1.009	1.009	1.076	1.083	1.112	1.112	1.131	1.138	1.454	1.454	1.495	1.495	1.536
	14e	TOHSUE																
	e	1.000	1.000	1.000	1.001	1.001	1.001	1.011	1.012	1.012	1.012	1.024	1.024	1.398	1.398	1.439	1.439	1.439
	15ffff	CARBTC07																
	f	1.000	1.005	1.062	1.086	1.141	1.155	1.198	1.212	1.213	1.220	1.220	1.237	1.439	1.492	1.592	1.594	1.737
	f	1.000	1.071	1.100	1.119	1.150	1.166	1.167	1.174	1.209	1.223	1.226	1.228	1.411	1.505	1.606	1.630	1.747
	f	1.000	1.056	1.079	1.096	1.150	1.166	1.167	1.206	1.223	1.229	1.231	1.231	1.409	1.599	1.599	1.652	1.675
	f	1.000	1.046	1.069	1.090	1.141	1.155	1.164	1.195	1.215	1.217	1.219	1.237	1.436	1.495	1.495	1.611	1.732
	15ffff	CTBROM																
	f	1.000	1.016	1.062	1.085	1.123	1.154	1.188	1.197	1.203	1.203	1.205	1.219	1.418	1.500	1.588	1.591	1.727
	f	1.000	1.085	1.108	1.141	1.141	1.169	1.179	1.184	1.213	1.223	1.224	1.241	1.432	1.532	1.614	1.625	1.763
	f	1.000	1.066	1.093	1.108	1.141	1.169	1.184	1.207	1.228	1.230	1.242	1.245	1.414	1.616	1.616	1.659	1.670
	f	1.000	1.044	1.070	1.085	1.124	1.154	1.155	1.182	1.199	1.203	1.216	1.216	1.464	1.486	1.486	1.585	1.727
	2i	MEZDIE01																
	i	1.000	1.010	1.010	1.014	1.021	1.021	1.108	1.108	1.172	1.175	1.198	1.198	1.218	1.227	1.619	1.621	1.621
	2i	MEZDOK01																
	i	1.000	1.006	1.007	1.016	1.021	1.021	1.108	1.108	1.167	1.175	1.197	1.197	1.221	1.225	1.615	1.619	1.619
	2i	XUWROW																
	i	1.000	1.000	1.041	1.074	1.114	1.413	1.521	1.711	1.843	1.853	1.853	1.853	1.853	2.000	2.000	2.330	2.330
	2iii	OHABEE																
	i	1.000	1.006	1.007	1.015	1.018	1.033	1.094	1.094	1.168	1.169	1.183	1.185	1.186	1.212	1.611	1.623	1.629
	i	1.000	1.002	1.002	1.005	1.008	1.009	1.096	1.096	1.186	1.188	1.189	1.215	1.215	1.216	1.623	1.624	1.632
	i	1.000	1.000	1.005	1.009	1.020	1.028	1.096	1.096	1.160	1.171	1.178	1.186	1.215	1.216	1.614	1.627	1.632
Mixed																		
	218ac	KOXKOX																
	a	1.000	1.000	1.118	1.118	1.118	1.118	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.803	1.803	1.803
	c	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.549	1.549	1.549	1.549	1.549
	218ac	RUQMEV																
	a	1.000	1.000	1.118	1.118	1.118	1.118	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.803	1.803	1.803
	c	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.549	1.549	1.549	1.549	1.549
	218ac	SENLAY																
	a	1.000	1.000	1.118	1.118	1.118	1.118	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.803	1.803	1.803
	c	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.549	1.549	1.549	1.549	1.549

Molecular Crystal Global Phase Diagrams:
II. Reference Lattices

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

Table 8: Order Parameters

Order Parameters Calculated Using:

```
      COPL as found on:
      H.T.Stokes and D.M.Hatch, (2002).  ISOTROPY, stokes.byu.edu/isotropy.html.
```

Sphere Packings:

ZNOXAC01

```
   Parent: 227 Oh-7, Fd-3m, F4_1/d-32/m, origin choice 2
   Subgroup: 227 Oh-7, Fd-3m, F4_1/d-32/m, origin choice 2
   Lattice vectors:
   1 0 0
   0 1 0
   0 0 1
   origin: 0 0 0

   Irrep Dir  Subgroup   Size
   GM1+  (a)  227 Fd-3m    1

   GM1+ is the primary OP.
```

DEQPAQ, et al.

```
   Parent: 229 Oh-9, Im-3m, I4/m-32/m
   Subgroup: 217 Td-3, I-43m, I-43m
   Lattice vectors:
   1 0 0
   0 1 0
   0 0 1
   origin: 0 0 0

   Irrep Dir  Subgroup   Size
   GM1+  (a)  229 Im-3m    1
   GM2-  (a)  217 I-43m    1

   GM2- is the primary OP.
```

FOHCUA, et al.

```
   Parent: 221 Oh-1, Pm-3m, P4/m-32/m
   Subgroup: 215 Td-1, P-43m, P-43m
   Lattice vectors:
   1 0 0
   0 1 0
   0 0 1
   origin: 0 0 0

   Irrep Dir  Subgroup   Size
   GM1+  (a)  221 Pm-3m    1
   GM2-  (a)  215 P-43m    1

   GM2- is the primary OP.
```

CUCZUV

```
   Parent: 194 D6h-4, P6_3/mmc, P6_3/m2/m2/c
   Subgroup: 176 C6h-2, P6_3/m, P6_3/m
   Lattice vectors:
   1 -1 0
   1 2 0
   0 0 1
   origin: 0 0 1/2

   Irrep Dir    Subgroup      Size
   GM1+  (a)    194 P6_3/mmc    1
   GM2+  (a)    176 P6_3/m      1
   K1    (a,0)  193 P6_3/mcm    3
   K4    (a,0)  176 P6_3/m      3

   K4 is the primary OP.
```

DILWIE01 & ZEYHIU

```
Parent: 194 D6h-4, P6_3/mmc, P6_3/m2/m2/c
Subgroup: 165 D3d-4, P-3c1, P-32/c1
Lattice vectors:
1 0 0
0 1 0
0 0 2
origin: 0 0 0

Irrep Dir    Subgroup      Size
GM1+  (a)    194 P6_3/mmc    1
GM3+  (a)    164 P-3m1       1
A2    (a,a)  165 P-3c1       2
```

A2 is the primary OP.

TCYMET

```
Parent: 229 Oh-9, Im-3m, I4/m-32/m
Subgroup: 161 C3v-6, R3c, R3c, hexangonal axes
Lattice vectors:
0 1 -1
-1 0 1
1 1 1
origin: 0 0 0

Irrep Dir      Subgroup   Size
GM1+  (a)      229 Im-3m    1
GM5+  (a,a,a)  166 R-3m     1
GM2-  (a)      217 I-43m    1
GM4-  (a,a,a)  160 R3m      1
H2+   (a)      223 Pm-3n    2
H4+   (a,a,a)  167 R-3c     2
H1-   (a)      222 Pn-3n    2
H5-   (a,a,a)  167 R-3c     2
```

Coupled OP.

ZIZHIZ

```
Parent: 194 D6h-4, P6_3/mmc, P6_3/m2/m2/c
Subgroup: 147 C3i-1, P-3, P-3
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 0 0

Irrep Dir  Subgroup      Size
GM1+  (a)  194 P6_3/mmc    1
GM2+  (a)  176 P6_3/m      1
GM3+  (a)  164 P-3m1       1
GM4+  (a)  163 P-31c       1
```

Coupled OP.

MTRETC10

```
Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 152 D3-4, P3_121, P3_121
Lattice vectors:
0 -1/2 -1/2
1/2 0 1/2
-1 -1 1
origin: -1/6 1/6 -1/2

Irrep k params  Dir                                      Subgroup    Size
GM1+            (a)                                      225 Fm-3m     1
GM5+            (a,-a,-a)                                166 R-3m      1
GM1-            (a)                                      209 F432      1
GM5-            (a,-a,-a)                                155 R32       1
LD3   2/3       (0,0,0,0,0,0,a,0,0,0,0,0,0,0,-1.732a,0)  152 P3_121    3
```

```
LD3 is the primary OP.
```

FUZLUH & VAFWAA

```
Parent: 227 Oh-7, Fd-3m, F4_1/d-32/m, origin choice 2
Subgroup: 141 D4h-19, I4_1/amd, I4_1/a2/m2/d, origin choice 2
Lattice vectors:
1/2 -1/2 0
1/2 1/2 0
0 0 1
origin: 1/4 1/4 0

Irrep Dir    Subgroup      Size
GM1+  (a)    227 Fd-3m       1
GM3+  (a,0)  141 I4_1/amd    1

GM3+ is the primary OP.
```

ZZZKNW01

```
Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 121 D2d-11, I-42m, I-42m
Lattice vectors:
-1/2 0 1/2
1/2 0 1/2
0 1 0
origin: 0 0 0

Irrep Dir          Subgroup    Size
GM1+  (a)          225 Fm-3m     1
GM3+  (a,-1.732a)  139 I4/mmm    1
GM5-  (0,0,a)      121 I-42m     1

GM5- is the primary OP.
```

KUJSIR

```
Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 142 D4h-20, I4_1/acd, I4_1/a2/c2/d, origin choice 2
Lattice vectors:
1 0 0
0 0 -1
0 2 0
origin: 0 1/4 1/4

Irrep Dir             Subgroup      Size
GM1+  (a)             225 Fm-3m       1
GM3+  (a,-1.732a)     139 I4/mmm      1
X4-   (a,0,0)         134 P4_2/nnm    2
W3    (0,0,a,a,0,0)   142 I4_1/acd    4

W3 is the primary OP.
```

YEMRIR

```
Parent: 221 Oh-1, Pm-3m, P4/m-32/m
Subgroup: 120 D2d-10, I-4c2, I-4c2
Lattice vectors:
1 -1 0
1 1 0
0 0 2
origin: -1/2 -1/2 -1/2

Irrep Dir      Subgroup    Size
GM1+  (a)      221 Pm-3m     1
GM3+  (a,0)    123 P4/mmm    1
GM2-  (a)      215 P-43m     1
GM3-  (a,0)    111 P-42m     1
R4+   (a,0,0)  140 I4/mcm    2
R5-   (a,0,0)  140 I4/mcm    2

Coupled OP.
```

ADAMAN08 & GERHOA

```
   Parent: 225 Oh-5, Fm-3m, F4/m-32/m
   Subgroup: 114 D2d-4, P-42_1c, P-42_1c
   Lattice vectors:
   -1/2 0 1/2
   1/2 0 1/2
   0 1 0
   origin: 0 0 0

   Irrep Dir           Subgroup      Size
   GM1+  (a)           225 Fm-3m       1
   GM3+  (a,-1.732a)   139 I4/mmm      1
   GM5-  (0,0,a)       121 I-42m       1
   X3+   (a,0,0)       128 P4/mnc      2
   X2-   (a,0,0)       137 P4_2/nmc    2

   Coupled OP.
```

KANGUB01

```
   Parent: 141 D4h-19, I4_1/amd, I4_1/a2/m2/d, origin choice 2
   Subgroup:  88 C4h-6, I4_1/a, I4_1/a, origin choice 2
   Lattice vectors:
   1 0 0
   0 1 0
   0 0 1
   origin: 0 1/2 0

   Irrep Dir  Subgroup      Size
   GM1+  (a)  141 I4_1/amd    1
   GM3+  (a)   88 I4_1/a      1

   GM3+ is the primary OP.
```

(methane III)

```
   Parent: 225 Oh-5, Fm-3m, F4/m-32/m
   Subgroup:  64 D2h-18, Cmca, C2/m2/c2_1/a
   Lattice vectors:
   2 0 0
   0 1 1
   0 -1 1
   origin: 1/2 0 0

   Irrep k params  Dir                          Subgroup      Size
   GM1+            (a)                          225 Fm-3m       1
   GM3+            (a,1.732a)                   139 I4/mmm      1
   GM5+            (0,a,0)                       71 Immm        1
   SM2   1/4       (0,0,0,0,0,0,0,0,0,0,a,0)     51 Pmma        4
   L1-             (a,0,a,0)                     67 Cmma        4
   L3-             (a,0.268a,0,0,a,0.268a,0,0)   67 Cmma        4
   X1+             (0,0,a)                      123 P4/mmm      2
   X4+             (0,0,a)                      131 P4_2/mmc    2
   W2              (a,0,0,0,0,0)                139 I4/mmm      4
   W3              (0,a,0,0,0,0)                140 I4/mcm      4

   Coupled OP.
```

YIMWEW

```
   Parent: 229 Oh-9, Im-3m, I4/m-32/m
   Subgroup:  60 D2h-14, Pbcn, P2_1/b2/c2_1/n
   Lattice vectors:
   0 3 0
   -1 0 1
   1 0 1
   origin: -1/2 0 0

   Irrep k params  Dir                         Subgroup    Size
   GM1+            (a)                         229 Im-3m     1
   GM3+            (a,-1.732a)                 139 I4/mmm    1
   GM5+            (0,0,a)                      69 Fmmm      1
   DT5   5/6       (a,-a,a,a,0,0,0,0,0,0,0,0)   64 Cmca      6
   DT1   1/3       (a,0,0,0,0,0)               139 I4/mmm    3
   DT3   1/3       (0,a,0,0,0,0)                69 Fmmm      3
   H4+             (a,-a,0)                     64 Cmca      2
   H5+             (a,a,0)                      64 Cmca      2
   N1-             (0,0,a,0,0,0)                68 Ccca      2
   N4-             (0,0,a,0,0,0)                63 Cmcm      2
   D2    1/6       (0,0,a,0,0,0,0,0,0,0,0,0)    68 Ccca      6
   D3    1/6       (0,0,0,0,0,0,0,0,0,a,0,0)    63 Cmcm      6

   Coupled OP.
```

RASDOE & TFMETH02

```
   Parent:  70 D2h-24, Fddd, F2/d2/d2/d, origin choice 2
   Subgroup:  15 C2h-6, C2/c, C12/c1, unique axis b, cell choice 1
   Lattice vectors:
   0 -1 0
   -1 0 0
   0 1/2 -1/2
   origin: 1/4 0 1/4

   Irrep Dir  Subgroup  Size
   GM1+  (a)   70 Fddd    1
   GM3+  (a)   15 C2/c    1

   GM3+ is the primary OP.
```

REKYUB

```
   Parent: 225 Oh-5, Fm-3m, F4/m-32/m
   Subgroup:  15 C2h-6, C2/c, C12/c1, unique axis b, cell choice 1
   Lattice vectors:
   -1/2 1 -1/2
   -1/2 0 1/2
   1 0 1
   origin: -1/4 0 -1/4

   Irrep Dir                        Subgroup    Size
   GM1+  (a)                        225 Fm-3m     1
   GM3+  (a,-1.732a)                139 I4/mmm    1
   GM4+  (a,0,-a)                    12 C2/m      1
   GM5+  (a,a,b)                     12 C2/m      1
   L1-   (a,0,0,0)                  167 R-3c      2
   L3-   (a,3.732a,0,0,0,0,0,0)      15 C2/c      2

   L3- is the primary OP.
```

MECKOU

```
   Parent: 225 Oh-5, Fm-3m, F4/m-32/m
   Subgroup:  12 C2h-3, C2/m, C12/m1, unique axis b, cell choice 1
   Lattice vectors:
   1/2 -1/2 -1
   1/2 1/2 0
   1/2 -1/2 1
   origin: -1/4 1/4 0

   Irrep Dir                  Subgroup    Size
   GM1+  (a)                  225 Fm-3m     1
   GM3+  (a,0)                139 I4/mmm    1
   GM4+  (a,a,0)               12 C2/m      1
   GM5+  (a,b,-b)              12 C2/m      1
   L2-   (0,0,0,a)            166 R-3m      2
   L3-   (0,0,0,0,0,0,a,a)     12 C2/m      2

   L3- is the primary OP.
```

MECKUA

```
   Parent: 225 Oh-5, Fm-3m, F4/m-32/m
   Subgroup:  14 C2h-5, P2_1/c, P12_1/c1, unique axis b, cell choice 1
   Lattice vectors:
   1/2 1 -1/2
```

```
1/2 0 1/2
1 0 -1
origin: -1/2 -1/4 1/4

Irrep Dir                     Subgroup      Size
GM1+  (a)                     225 Fm-3m       1
GM3+  (a,-1.732a)             139 I4/mmm      1
GM4+  (a,0,a)                  12 C2/m        1
GM5+  (a,-a,b)                 12 C2/m        1
L2+   (0,a,0,0)               167 R-3c        2
L3+   (0,0,a,3.732a,0,0,0,0)   15 C2/c        2
L1-   (0,0,a,0)               167 R-3c        2
L3-   (0,0,0,0,a,3.732a,0,0)   15 C2/c        2
X2-   (a,0,0)                 137 P4_2/nmc    2
X3-   (a,0,0)                 129 P4/nmm      2
X5-   (a,0,0,0,0,0)            59 Pmmn        2

Coupled OP.
```

TOHSUE

```
Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup:  14 C2h-5, P2_1/c, P12_1/c1, unique axis b, cell choice 1
Lattice vectors:
-1/2 0 1/2
1/2 0 1/2
0 2 0
origin: 0 -1/4 -1/4

Irrep k params  Dir                         Subgroup      Size
GM1+            (a)                         225 Fm-3m       1
GM3+            (a,-1.732a)                 139 I4/mmm      1
GM4+            (a,0,a)                      12 C2/m        1
GM5+            (a,-a,b)                     12 C2/m        1
DT2   3/4       (a,-a,0,0,0,0)              138 P4_2/ncm    4
DT4   3/4       (a,a,0,0,0,0)               130 P4/ncc      4
DT5   3/4       (0,a,-a,0,0,0,0,0,0,0,0,0)   62 Pnma        4
X2-             (a,0,0)                     137 P4_2/nmc    2
X3-             (a,0,0)                     129 P4/nmm      2
X5-             (a,0,0,0,0,0)                59 Pmmn        2

Coupled OP.
```

CARBTC07 & CTBROM

```
Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup:  15 C2h-6, C2/c, C12/c1, unique axis b, cell choice 1
Lattice vectors:
-2 -1 -1
0 1 -1
2 -1 -1
origin: -1/2 1/2 1/2

Irrep k params  Dir                                                    Subgroup      Size
GM1+            (a)                                                    225 Fm-3m       1
GM3+            (a,1.732a)                                             139 I4/mmm      1
GM4+            (0,a,-a)                                                12 C2/m        1
GM5+            (a,b,a)                                                 12 C2/m        1
LD2   3/4       (0,a,0,0,0,-a,0,0)                                     167 R-3c        4
LD3   3/4       (0,0,a,0.268a,0,0,0,0,0,0,0.268a,a,0,0,0,0)             15 C2/c        4
L1-             (0,a,0,a)                                               67 Cmma        4
L2-             (a,b,c,-b)                                              12 C2/m        8
L3-             (a,-3.732a,b,c,d,-3.732d,0.866b+0.500c,0.500b-0.866c)   12 C2/m        8
X1+             (a,-a,b)                                               123 P4/mmm      4
X2+             (a,a,0)                                                123 P4/mmm      4
X3+             (a,a,0)                                                134 P4_2/nnm    4
X4+             (a,-a,b)                                               134 P4_2/nnm    4
X5+             (a,b,-b,a,0,c)                                          12 C2/m        4
C1    1/2,1/4   (0,0,a,0,0,0,0,a,0,0,0,0,0,0,a,0,0,0,0,a,0,0,0,0)       12 C2/m        8
C2    1/2,1/4   (0,0,a,0,0,0,0,-a,b,0,0,0,0,0,-a,0,0,0,0,a,-b,0,0,0)    15 C2/c       16

C2 is the primary OP.
```

MEZDIE01 & MEZDOK01

```
Parent: 229 Oh-9, Im-3m, I4/m-32/m
Subgroup:   2 Ci-1, P-1, P-1
Lattice vectors:
1/2 1/2 1/2
1 0 -1
-1/2 1/2 -1/2
origin: -1/4 -1/4 1/4

Irrep Dir            Subgroup   Size
GM1+  (a)            229 Im-3m    1
GM2+  (a)            204 Im-3     1
GM3+  (a,b)           71 Immm     1
GM4+  (a,b,c)          2 P-1      1
GM5+  (a,b,c)          2 P-1      1
N1-   (0,0,a,0,0,0)   68 Ccca     2
N2-   (0,0,0,a,0,0)   63 Cmcm     2
N3-   (0,0,a,0,0,0)   67 Cmma     2
N4-   (0,0,0,a,0,0)   63 Cmcm     2

Coupled OP.
```

OHABEE

```
Parent: 229 Oh-9, Im-3m, I4/m-32/m
Subgroup:   2 Ci-1, P-1, P-1
Lattice vectors:
1/2 1/2 1/2
1 -1 0
1 1 -2
origin: -1 -1/2 1

Irrep k params  Dir                                                          Subgroup    Size
GM1+            (a)                                                          229 Im-3m     1
GM2+            (a)                                                          204 Im-3      1
GM3+            (a,b)                                                         71 Immm      1
GM4+            (a,b,c)                                                        2 P-1       1
GM5+            (a,b,c)                                                        2 P-1       1
LD1   1/3       (a,0,0,0,-1.732a,0,0,0)                                      164 P-3m1     3
LD2   1/3       (a,0,0,0,0.577a,0,0,0)                                       147 P-3       3
LD3   1/3       (a,b,0,0,0,0,0,0,-0.577a-1.155b,-1.155a-0.577b,0,0,0,0,0,0)    2 P-1       3
N1-             (0,0,0,0,a,0)                                                 68 Ccca      2
N2-             (0,0,0,0,0,a)                                                 63 Cmcm      2
N3-             (0,0,0,0,a,0)                                                 67 Cmma      2
N4-             (0,0,0,0,0,a)                                                 63 Cmcm      2
C1    1/6,2/3   (a,0,0,0,0,0,0,0,0,0,0,0,-0.577a,0,0,0,0,0,0,0,0,0,0,0)       11 P2_1/m    6
C2    1/6,2/3   (a,0,0,0,0,0,0,0,0,0,0,0,1.732a,0,0,0,0,0,0,0,0,0,0,0)        13 P2/c      6

Coupled OP.
```

Dimer Packings:

FOJBUB & VADRAU

```
Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 205 Th-6, Pa-3, P2_1/a-3
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 0 0

Irrep Dir            Subgroup   Size
GM1+  (a)            225 Fm-3m    1
GM2+  (a)            202 Fm-3     1
X5+   (a,a,a,a,a,a)  205 Pa-3     4
```

X5+ is the primary OP.

LUFYEQ

```
Parent: 141 D4h-19, I4_1/amd, I4_1/a2/m2/d, origin choice 2
Subgroup:  88 C4h-6, I4_1/a, I4_1/a, origin choice 2
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 1/2 0

Irrep Dir  Subgroup      Size
GM1+  (a)  141 I4_1/amd    1
GM3+  (a)   88 I4_1/a      1
```

GM3+ is the primary OP.

CARBTC

```
Parent: 166 D3d-5, R-3m, R-32/m, hexangonal axes
Subgroup:  14 C2h-5, P2_1/c, P12_1/c1, unique axis b, cell choice 1
Lattice vectors:
-2/3 -1/3 -1/3
0 1 0
2 1 0
origin: 0 0 0

Irrep Dir      Subgroup    Size
GM1+  (a)      166 R-3m      1
GM3+  (a,0)     12 C2/m      1
F2+   (0,a,0)   14 P2_1/c    2
```

F2+ is the primary OP.

Mixed

KOXKOX, RUQMEV, & SENLAY

```
Parent: 223 Oh-3, Pm-3n, P4_2/m-32/n
Subgroup: 218 Td-4, P-43n, P-43n
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 0 0

Irrep Dir  Subgroup   Size
GM1+  (a)  223 Pm-3n    1
GM2-  (a)  218 P-43n    1

GM2- is the primary OP.
```

Table 9. Identifiers, chemical formulas, and assigned frameworks of the tetrahedral data set. The adamantane and cubane molecular frameworks are substituted derivatives of these molecules, while MX_4 molecules have a central atom (denoted M) with four identical X groups.

Identifier	formula	framework
ADAMAN08	C10 H16	adamantane
BASXOI	C4 H12 Se6 Sn4	adamantane
BOGMEP	C24 H48 Cl6 Cu4 N16 O1	other
CAMPOV	C16 H36 N4 Sn4	cubane
CANFIG	C4 H24 B4 U1	MX_4
CANFOM	C4 H24 B4 Th1	MX_4
CARBTC	C1 Cl4	MX_4
CARBTC07	C1 Cl4	MX_4
CTBROM	C1 Br4	MX_4
CUCZUV	C20 H36	tetrahedrane
DEQPAQ	C36 H100 B4 N12 Na4	other
DILWIE01	C16 H48 Pt4 S4	cubane
DOCNIS	C8 H12 S6	adamantane
FOHCUA	C12 Ni4 O18 P4	adamantane
FOJBUB02	C4 Ni1 O4	MX_4
FUZLUH	C12 Co4 O12 Sb4	cubane
FUZTEZ	H16 B4 Np1	MX_4
FUZVOL	H16 B4 Hf1	MX_4
GERHOA	C4 H12 Cl12 N4 Sb4	cubane
GUTCED	C26 H32	other
HMGETP	C12 H36 Ge6 P4	adamantane
HMSIPA	C12 H36 P4 Si6	adamantane
HXMTAM07	C6 H12 N4	adamantane
JEYSEL	C18 H36 Ni4 O6 P4	tetrahedrane
JUFWUC	C12 H40 Cs4 N4 Si4	cubane
KANGUB01	C10 H12 I4	adamantane
KELREY	C12 H36 Cl4 Ti4	cubane
KOXKOX	C16 H36 Ga4 Se4	cubane
KUJSIR	C20 H48 O4 Zn4	cubane
LUFYEQ	C12 H12 Si1	MX_4
MECKIO	C16 H36 Cl4 In4 N4	cubane
MECKOU	C16 H36 Br4 In4 N4	cubane
MECKUA	C16 H36 I4 In4 N4	cubane
MESIAD	C12 H36 As4 Si6	adamantane
MEZDIE01	C12 H36 Si1 Sn4	MX_4
MEZDOK01	C12 H36 Ge1 Sn4	MX_4
MPTHOT01	C12 H40 O4 Pt4	cubane
MSISUL10	C4 H12 S6 Si4	adamantane
MTRETC10	C16 H12 O12 Re4 S4	cubane
MXSNOX	C4 H12 O8 Sn6	other
MZNMOX10	C8 H24 O4 Zn4	cubane
NIWMIP	C12 H36 Al4 N4 S6	adamantane
OHABEE	C16 H36 Si4	tetrahedrane
POSLOY10	C12 Cl4 O12 Tc4	cubane
QUGBOJ	C16 O16 Rh6	other
RASDOE	C16 H48 Ga4 N4 Si4	cubane
REKYUB	C16 H36 Ga4 S4	cubane
RIMMOP	C16 H40 Al4 N4	cubane
RIMNAC	C20 H48 Al4 N4	cubane
RUQMEV	C12 H36 Cu4 I4 N4	cubane
SENLAY	C16 H36 P4 Si4	cubane
TCYMET	C5 N4	MX_4
TFMETH02	C1 F4	MX_4
TMEPTC	C12 H36 Cl4 Pt4	cubane
TMGEHS10	C4 H12 Ge4 S6	adamantane
TMSIAD	C10 H24 Si4	adamantane
TMSNHS10	C4 H12 S6 Sn4	adamantane
TOHSUE	C16 F12 O12 P4 Ru4	cubane
VADRAU	C4 H12 Pb1	MX_4
VAFWAA	C12 Bi4 Co4 O12	cubane
VAVYAS	C20 H36 P4	cubane
XAGXAE	P4 S10	adamantane
XUWROW	C20 H48 Mg4 O4	cubane
YEMRIR	O6 P4 S4	adamantane
YEYQAU	C12 O12 Ru4 Se4	cubane
YIMWEW	C10 H16 O4	adamantane
ZEYHIU	C20 H48 Cd4 O4	cubane
ZIZHIZ	C12 H4 Mn4 O16	cubane
ZNOXAC01	C12 H18 O13 Zn4	other
ZZZKDW01	C1 I4	MX_4