Molecular Crystal Global Phase Diagrams: II. Reference Lattices

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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

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

Reduced Cell

60	60	60	
alpha	beta	gamma	

Normalized Niggli Matrix

1	1	1
0.5	0.5	0.5

Daughter 227a
Ref. Lattice Diamond

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

Character 1 (cF)
Type I
b.bza.a True
c.czb.b True
2|D+E+F| ≤ A+B N/A
|b.c|≤|b.b/2 True
|a.c|≤|a.a/2 True
|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
7/8,3/8,3/8	0.875	0.375	0.375	1
1/8,5/8,5/8	0.125	0.625	0.625	1
7/8,7/8,7/8	0.875	0.875	0.875	1
5/8,1/8,5/8	0.625	0.125	0.625	1
3/8,3/8,7/8	0.375	0.375	0.875	1
5/8,5/8,1/8	0.625	0.625	0.125	1
3/8,7/8,3/8	0.375	0.875	0.375	1

1/8,1/8,1/8 0.125 0.125 0.125 1
7/8,7/8,7/8 -0.125 0.875 0.875 1
1.125 0.125 0.125 1
0.875 0.875 0.875 1
0.125 1.125 0.125 1
0.875 0.875 -0.125 1
0.125 0.125 1.125 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

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

* Very slightly distorted molecules or mislabeled as 197a by authors

8 nearest neighbors
next neighbor 15% farther
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1

a b c
90 90 90

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

Reduced Cell

alpha	beta	gamma	
109.4712206	109.4712206	109.4712206	

Normalized Niggli Matrix

1	1	1
-0.333333333	-0.333333333	-0.333333333

Daughter 217a
Ref. Lattice BCC

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

Character 5 (cI)
Type II
b.bza.a True
c.czb.b True
2|D+E+F| ≤ A+B Equal
|b.c|≤|b.b/2 True
|a.c|≤|a.a/2 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

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

0,0,0 0 0 0 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

* Very slightly distorted molecules or mislabeled as 195a by authors

6 nearest neighbors
next neighbor 41% farther
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1

a b c
1 1 1
90 90 90

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

Reduced Cell

alpha	beta	gamma	
90	90	90	

Normalized Niggli Matrix

1	1	1
0	0	0

Daughter 215a
Ref. Lattice SC

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

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

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

Reduced Cell

alpha	beta	gamma	
90	90	90	

Normalized Niggli Matrix

1	1	1
0	0	0

Daughter 218a,c
Ref. Lattice 223a,c

|G|	Z	|G|/Z	
24	8	3	
48	8	6	
	1	2	
	(size)	(index)	

Character 3 (cP)
Type II
b.bza.a True
c.czb.b True
2|D+E+F| ≤ A+B True
|b.c|≤|b.b/2 True
|a.c|≤|a.a/2 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
next neighbor 55% farther

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

c 2 nearest neighbors
next neighbor 12% farther

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

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

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

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

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

Reduced Cell

alpha	beta	gamma	
90	90	90	

Normalized Niggli Matrix

1	1	1
0	0	0

See #16 and #17 above.

Center of Mass Coordinates

a 12 nearest neighbors
next neighbor 55% farther
distorted icosahedral coordination

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

d -4.. Origin Choice 2

d 2 nearest neighbors
next neighbor 12% farther
pairs of rods in 3 orthogonal directions

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

c -4..

1/2,1/2,1/2 0.5 0.5 0.5 1
0,0,0 1 1 1 1
3/4,1/2,0 0.75 0.5 1 1
1/4,1/2,0 1.25 0.5 1 1
0,3/4,1/2 1 0.75 0.5 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

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

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

1 nearest neighbor
next neighbor 33% farther
dimer packing

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:

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

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

Inverse Transformation
-1 1 1 0
1 -1 1 0
1 1 -1 0
0 0 0 1
Det= 4

Normalized Niggli Matrix
1 1 1
0.5 0.5 0.5

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

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	

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

	|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)

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

Order Parameter = X5+

205c P_a_-3
20 VADRAU

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

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

1 nearest neighbor
next neighbor 25% farther
dimer packing

See #19 above.

See 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

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

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

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	Z'= 2
	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	cr/ar= 1.54
	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	cr/ar_ideal= 1.63
	x=	0.3612963									slightly compressed vs. ideal HCP
	y=	0.3339991				error	0.05526006	0.02862869	0		

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

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

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

Order Parameter = K4

Trigonal Crystal Structures (143-167)

165d P_-3_c_1
22 DILWIE01

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

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

	|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 1 1 3.072783
gamma= 120 gamma= 120 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

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 1 1.536391496
90 90 120
alpha beta gamma

Normalized Niggli Matrix

1	1	2.360498829
0	0	-0.5

2|D+E+F| ≤ A+B: True

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

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

Z'= 2

Order Parameter = A2

cr/ar= 1.54
error 0 0 -0.006717333 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

Matrix Representation

1	-0.5	0	
0	0.8660254	0	
0	0	3.0444515	

a b c
1 1 3.0444515

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.

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

See 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

Z'= 2

cr/ar= 1.52
error 0 0 -0.017143316 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

Matrix Representation

1	-0.5	0	
0	0.8660254	0	
0	0	1.2828342	

a b c
1 1 1.2828342

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

90 90 120
alpha beta gamma

Normalized Niggli Matrix

1	1	1
-0.319100381	-0.319100381	-0.319100381

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

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

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

Z'= 1

Order Parameter = Coupled

error 0.0008 0.0008 0.0008

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

Matrix Representation

1	-0.5	0	
0	0.8660254	0	
0	0	1.514642	

a b c
1 1 1.514642

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

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

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

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

Z'= 2

Order Parameter = Coupled

error 0 0 0.001973233

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

Matrix Representation

1	-0.5	0	
0	0.8660254	0	
0	0	2.5739251	

a b c
1 1 2.5739251

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

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

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

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

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

Z'= 1

Order Parameter = LD3

error 0 -0.048005556 0

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

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

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

7/8,1/4,1/4	0.875	0.25	0.25	1
1/8,3/4,3/4	1.125	-0.25	0.75	1
	0.875	0.25	1.25	1
	1.125	0.75	0.75	1
error	0	0	0	

Daughter 141a
Ref. Lattice 141a

	|G|	Z	|G|/Z
	16	2	8
	16	2	8
		1	1
		(size)	(index)

Reduced Cell
Character 18 (tI)
Type I
b.b≥a.a True
c.c≥b.b True
2\|D+E+F\| ≤ A+B N/A

|b.c|≤b.b/2 True
|a.c|≤a.a/2 True
|a.b|≤a.a/2 True

Z'= 2

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

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

Order Parameter = GM1+

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

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.

See 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

Center of Mass Coordinates

a -4m2 (Origin Choice 1)

0,0,0	0	0	0	1

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			

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

a -42m

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

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			

Daughter 137a
Rod 37a

	|G|	Z	|G|/Z
	16	2	8
	8	1	8
		2	1
		(size)	(index)

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

Center of Mass Coordinates

a -4m2

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

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

0,0,0	0	0	0	1
	0	0	1	1

Z'= 1

Daughter 121a
Ref. Lattice FCC

	|G|	Z	|G|/Z
	8	1	8
	48	1	48
		1	6
		(size)	(index)

Reduced Cell
Character 15 (tI)
Type II
b.b≥a.a True
c.c≥b.b True
2\|D+E+F\| ≤ A+B Equal

… but close to singularity: 1 (cF)

|b.c|≤b.b/2 True
|a.c|≤a.a/2 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	0	0
0	0	1	0
0.5	0.5	0	0
0	0	0	1

Det= 0.5

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

Center of Mass Coordinates

a -4..

Origin Choice 2

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

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

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

Z'= 1

Daughter 142a
Ref. Lattice FCC

	|G|	Z	|G|/Z
	16	4	4
	48	1	48
		4	12
		(size)	(index)

Reduced Cell
Character 15 (tI)
Type II
b.b≥a.a True
c.c≥b.b True
2\|D+E+F\| ≤ A+B Equal

… but close to singularity: 1 (cF)

|b.c|≤b.b/2 True
|a.c|≤a.a/2 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

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

Det= 2

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

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

	|G|	Z	|G|/Z
Daughter 120c	8	2	4
Ref. Lattice SC	48	1	48
		2	12
		(size)	(index)

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	Z'= 1	Order Parameter = Coupled
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		

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

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

	|G|	Z	|G|/Z
Daughter 114a	8	2	4
Ref. Lattice FCC	48	1	48
		2	12
		(size)	(index)

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	Z'= 1	Order Parameter = Coupled
1/2,1/2,1/2	0.5	0.5	0.5	1		1	1	1	1		

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	
103.7243738	103.7243738	90	
alpha	beta	gamma	

Normalized Niggli Matrix

1	1	4.44142518
-0.5	-0.5	0

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

	|G|	Z	|G|/Z
Daughter 88a	16	4	4
Ref. Lattice 141a	16	2	8
		2	2
		(size)	(index)

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	Z'= 2	Order Parameter = GM3+
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		

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	Z'= 8
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	

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	1	2
			(size)	(index)

Reduced Cell

Character	7 (tI)
Type	II
b.b≥a.a	True
c.c≥b.b	True
2|D+E+F| ≤ A+B	Equal

|b.c|≤b.b/2	True	
|a.c|≤a.a/2	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	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	
b		0.5	0.75	0.8109161	1	
c		0.5	0.25	0.5609161	1	
d		0	0.75	1.0609161	1	
e		0	0.75	0.6890839	1	
f		0.5	0.25	0.1890839	1	
g		0.5	0.75	0.4390839	1	
h		0	0.25	-0.060916	1	
		z= 0.3109161				

	-0.25	-0.31091612	-0.06091612	1
3/4,2/3,11/	0.75	-0.31091612	-0.06091612	1
1/4,11/12,2	0.25	-0.06091612	-0.31091612	1
	0.25	-1.06091612	-0.31091612	1
	0.25	-0.68908388	0.06091612	1
1/4,1/3,1/1:	0.25	0.31091612	0.06091612	1
3/4,1/12,1/	0.75	0.06091612	0.31091612	1
	-0.25	0.06091612	0.31091612	1
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	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

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

2 nearest neighbors
next neighbor 10% farther than nearest

Square packing of p1121/m rods.

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	1.04612449	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	Z'= 2
-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	
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

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

2 nearest neighbors
next neighbor 12% farther than nearest

See above.

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	Z'= 2
-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	
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 -x,-y,3/4 -0.210984241 0.13644839 0.75 1
d 1
ii 0.1771 0.9354 0.1282 1
ii 0.1771 0.5646 0.1282 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

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:

0.788323726	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

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)

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			

rod axis: 0 1 0
rod origin: 0.5 0 0
Transformation to orthogonal axes:
0

rotation angle:
0 degrees
Rescaling parameter:
0.788323726

b	m				
x,y,1/4	0.593410245	-0.246935632	0.25	1	Z'= 2
	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	

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

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	|G|	Z	|G|/Z
Ref. Lattice	FCC	8	8	1
		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

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

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

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

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

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			

plane normal: 0 0 1
plane origin: -0.065579 0.067456 0.122842
Transformation to orthogonal axes:
0

rotation angle:
0 degrees
Rescaling parameter:
1 1.012750958

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

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

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
Ref. Lattice BCC

	|G|	Z	|G|/Z
	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 — c .2.

8 neighbors within 5% of nearest	0,y,1/4	0	-0.187538	0.25	1
next neighbor 11% farther than nearest	1/2,1/2-y,3.	0.5	0.687538	0.75	1
	0,1-y,3/4	0	1.187538	0.75	1
	1/2,1/2+y,1	0.5	0.312462	0.25	1

y= -0.187538

d 1 nearest neighbor — d 1

7 neighbors within 5% of nearest	x,y,z	0.1688182	0.2974947	0.206184	1
9 neighbors within 8% of nearest	1/2-x,1/2-y	0.3311818	0.2025053	0.706184	1
next neighbor >11% farther than nearest	1-x,y,1/2-z	0.8311818	0.2974947	0.293816	1
	1/2+x,1/2-y	0.6688182	0.2025053	0.793816	1
	1-x,1-y,1-z	0.8311818	0.7025053	0.793816	1
Sphere packing	1/2+x,1/2+	0.6688182	0.7974947	0.293816	1
	x,1-y,1/2+z	0.1688182	0.7025053	0.706184	1
	1/2-x,1/2+y	0.3311818	0.7974947	0.206184	1

x= 0.1688182
y= 0.2974947
z= 0.206184

0,0,0

0.062462	-0.062462	0	1	Z'= 1
1.937538	0.062462	-1	1	
0.937538	-1.937538	-1	1	
2.062462	0.937538	0	1	
1.097765367	0.002776033	0.087632	1	
0.989866633	0.084855967	-0.912368	1	
2.997223967	1.902234633	-0.087632	1	
1.915144033	1.010133367	-1.087632	1	
2.902234633	0.997223967	-1.087632	1	
3.010133367	0.915144033	-0.087632	1	
1.002776033	-0.902234633	-0.912368	1	
2.084855967	-0.010133367	0.087632	1	

Order Parameter = Coupled

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

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

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

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	

Daughter 15e
Rod 37a

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

2 nearest neighbors
next neighbor 10.5% farther than nearest

p112 (#8)
… but close to p-4m2 (#37)

Hexagonal packing of p-4m2 rods.

Center of Mass Coordinates

e 2

i	1/4,y,1/2	0.25	0.2568903	0.5	1
	1/4,1/2+y,(	0.25	0.7568903	0	1
	3/4,1/2-y,0	0.75	0.2431097	0	1
	3/4,1-y,1/2	0.75	0.7431097	0.5	1

y= 0.2568903

rod axis: 0 1 0

rod origin: 0.25 0.25689 0.5

Transformation to orthogonal axes:
-0.516081

rotation angle:
-1.788220892 degrees

Rescaling parameter:
1.026721188

a -4m2

0,0,0	0	0	0	1	Z'= 1
	0.267221992	0.505267925	0.5	1	
	0.753971953	0.490071358	-0.013781	1	
	0.486749961	-0.015196567	0.486219	1	
error	0	0	0		

Molecular 3-fold axes

f 1

i	1/2-x,y,1-z	0.3347	0.1504	0.5517	1
i	x,y,z	0.1653	0.1504	0.4483	1
i		0.2219	0.3791	0.5538	1
i		0.2781	0.3791	0.4462	1

f m

x,-x,-z	0.054824689	-0.054819002	-0.10649	1
-x,x,-z	-0.054824689	0.054819002	-0.10649	1
-x,-x,z	-0.056108434	-0.053512782	0.12221	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

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

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

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	

Daughter 15e
Rod 22b

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

2 nearest neighbors
next neighbor 19% farther than nearest

pmcm (#22)

Hexagonal packing of pmcm rods.

Center of Mass Coordinates

e 2

	0,y,1/4	0	0.8926227	0.25	1
i	0,1-y,3/4	0	0.1073773	0.75	1
	1/2,1/2+y,1	0.5	0.3926227	0.25	1
	1/2,1/2-y,3.	0.5	0.6073773	0.75	1

y= 0.8926227

rod axis: 0 0 1

rod origin: 0 0.5 0.5

Transformation to orthogonal axes:
0.261707

rotation angle:
0 degrees

Rescaling parameter:
1.357273748

b m2m

0,-y,3/4	0	0.532896473	-0.25	1	Z'= 2
0,y,1/4	0	-0.532896473	0.25	1	
	0.368385523	-0.145740401	-0.380853	1	
	0.368385523	0.145740401	0.119147	1	

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

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.

2 nearest neighbors

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,3/4	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,3/4	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,3/4	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

Center of Mass Coordinates

See above.

		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,3/4	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,3/4	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

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	Z'= 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

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

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	
-0.936524 12	0.93652412	0	

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

p-42m (#37)
2nd setting

Daughter	11e	4	2	2
Rod	37a	8	1	8
			2	4
			(size)	(index)

Hexagonal packing of p-42m rods

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	Z'= 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

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

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

Daughter	14e	4	4	1
Plane	2_1/c	4	4	1
			1	1
			(size)	(index)

planar packing

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	Z'= 4
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

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

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.

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

dimers:

Transformation to Reduced Cell

0	0	-1	0

Matrix Representation

-0.125119979	-0.125119979	-1

	|G|	Z	|G|/Z
Daughter	14e	4	4	1
Plane	2_1/c	4	4	1
		1	1	

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

-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

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

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

Det= 3

Inverse Transformation

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

Det= 2

Normalized Niggli Matrix

1	1	2.796789577
0.349934254	0.349934254	0.436316354

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

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			Order Parameter = F2+
ii	0,1/2,1/2	0	0.5	0.5	1		0	1	0	1				

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

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

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

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

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)

Daughter	14e	4	4	1
Rod	5a	2	2	1
			2	1
			(size)	(index)

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

Hexagonal packing of pc11 rods

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				

rod axis:

0	0	1

rod origin:

0.25	0.75	0

Transformation to orthogonal axes:
0.243414

rotation angle:
0

Rescaling parameter:
1.276927253 1

a 1

x,y,z	-0.094562635	-0.0223678	0.434496	1
	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

Z' = 2

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

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

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

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

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)

Daughter	14e	4	4	1
Rod	2c	2	2	1
			2	1
			(size)	(index)

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

Hexagonal packing of p-1 rods

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			

rod axis:

0	1	0

rod origin:

0.5	0	0.5

Transformation to orthogonal axes:
0.036867

rotation angle:
0

Rescaling parameter:
0.801442168

c 1

x,y,z	-0.081670409	-0.139617052	0.254875	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

Z' = 1

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			

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

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

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

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

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)

Daughter	14e	4	4	2
Rod	2c	2	1	2
			2	1
			(size)	(index)

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

Square packing of p-1 rods

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			

rod axis:

0	1	0

rod origin:

0	0	0

Transformation to orthogonal axes:
0.009057

rotation angle:
41.42085259

Rescaling parameter:
0.695408986

c 1

x,y,z	0.178268157	-4.15243E-05	0.258229	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

Z' = 1

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			

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

Reduced Cell

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

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

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

-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

Type I
b.b≥a.a True
c.c≥b.b True
2|D+E+F| ≤ A+B N/A

|b.c|≤b.b/2 True
|a.c|≤a.a/2 True
|a.b|≤a.a/2 True

-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

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

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

Along Rhom. Path from FCC to BCC

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

Reduced Cell
Character 8 (oI) … but close to singularity: 1 (cF)
Type II
b.b≥a.a True
c.c≥b.b True
2|D+E+F| ≤ A+B Equal

|b.c|≤b.b/2 True
|a.c|≤a.a/2 True
|a.b|≤a.a/2 True

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

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

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

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

Daughter 14ee
Plane 2_1

|G|	Z	|G|/Z
4	8	0.5
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

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

x= 0.27555
y= 0.007371111
z= 0.050402614

Z'= 4

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

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)

Daughter 14ee
Rod 22b

|G|	Z	|G|/Z
4	8	0.5
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

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

Z'= 2

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

b m2m

0,y,1/4	0.381389276	0.763747978	0.052701	1
	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	-8.94451E-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)

Daughter 13efg
Rod 37a

|G|	Z	|G|/Z
4	8	0.5
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	e 2	Unique axis b, Cell Choice 1				
4 neighbors within 2% of nearest	0,y,1/4	0	0.4811384	0.25	1
next neighbor 5% farther than nearest	0,1-y,3/4	0	0.5188616	0.75	1
	y=	0.4811384				
f: 2 nearest neighbors	f 2	Unique axis b, Cell Choice 1				
4 neighbors within 2% of nearest	1/2,y,1/4	0.5	0.8131861	0.25	1
next neighbor 3% farther than nearest	1/2,1-y,3/4	0.5	0.1868139	0.75	1
	y=	0.8131861				
g: 1 nearest neighbor	g 1	Unique axis b, Cell Choice 1				
3 neighbors within 1% of nearest	x,y,z	0.2557004	0.1578597	0.0006353	1
next neighbor 4% farther than nearest	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
Hexagonal packing of p-42m rods	x,1-y,1/2+z	0.2557004	0.8421403	0.5006353	1
with 3 independent orientations	x=	0.2557004				
	y=	0.1578597				
	z=	0.0006353				

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		

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

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

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					0.5611	0.6383	0.1201	1
z=	0.3782					0.3195	0.8617	0.3799	1
f 1						-0.5611	0.3617	0.8799	1
x,y,z	0.3792	0.0597	0.1201	1		-0.3195	0.1383	0.6201	1
1-x,y,1/2-z	0.6208	0.0597	0.3799	1		-0.4389	1.6383	0.1201	1
1-x,1-y,1-z	0.6208	0.9403	0.8799	1		0.3195	-0.1383	0.3799	1
x,1-y,1/2+z	0.3792	0.9403	0.6201	1		0.4389	-0.6383	0.8799	1
1/2+x,1/2+	0.8792	0.5597	0.1201	1		-0.3195	1.1383	0.6201	1
1/2-x,1/2+y	0.1208	0.5597	0.3799	1					
1/2-x,1/2-y	0.1208	0.4403	0.8799	1		0.5581	0.129	0.1232	1
1/2+x,1/2-y	0.8792	0.4403	0.6201	1		-0.1897	1.371	0.3768	1
x=	0.3792					-0.5581	0.871	0.8768	1
y=	0.0597					0.1897	-0.371	0.6232	1
z=	0.1201					-0.4419	1.129	0.1232	1
f 1						-0.1897	0.371	0.3768	1
x,y,z	0.1261	0.3158	0.1232	1		0.4419	-0.129	0.8768	1
1-x,y,1/2-z	0.8739	0.3158	0.3768	1		0.1897	0.629	0.6232	1
1-x,1-y,1-z	0.8739	0.6842	0.8768	1					
x,1-y,1/2+z	0.1261	0.6842	0.6232	1		0.3641	0.3191	0.3713	1
1/2+x,1/2+	0.6261	0.8158	0.1232	1		0.0545	1.1809	0.1287	1
1/2-x,1/2+y	0.3739	0.8158	0.3768	1		-0.3641	0.6809	0.6287	1
1/2-x,1/2-y	0.3739	0.1842	0.8768	1		-0.0545	-0.1809	0.8713	1
1/2+x,1/2-y	0.6261	0.1842	0.6232	1		-0.6359	1.3191	0.3713	1
x=	0.1261					0.0545	0.1809	0.1287	1
y=	0.3158					0.6359	-0.3191	0.6287	1
z=	0.1232					-0.0545	0.8191	0.8713	1
f 1									
x,y,z	0.3452	0.2907	0.3713	1					
1-x,y,1/2-z	0.6548	0.2907	0.1287	1					
1-x,1-y,1-z	0.6548	0.7093	0.6287	1					
x,1-y,1/2+z	0.3452	0.7093	0.8713	1					
1/2+x,1/2+	0.8452	0.7907	0.3713	1					
1/2-x,1/2+y	0.1548	0.7907	0.1287	1					
1/2-x,1/2-y	0.1548	0.2093	0.6287	1					
1/2+x,1/2-y	0.8452	0.2093	0.8713	1					
x=	0.3452								
y=	0.2907								
z=	0.3713								

Z'= 1

Order Parameter = Coupled

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	1/2-x,1/2+y	0.4052	0.5343	0.1234	1
sphere packing	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
See above.	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+y	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+y	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+y	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

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			

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			

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)

c 1

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

c 1

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

Z'= 1

	|G|	Z	|G|/Z	
Daughter 2i	2	2	1	
Rod 2c	2	1	2	
		2	2	
		(size)	(index)	

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

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			

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			

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)

c 1

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

c 1

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

Z'= 1

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

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

		|G|	Z	|G|/Z
Daughter	2i	2	2	1
Ref. Lattice	BCC	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
alpha beta gamma

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

Inverse Transformation

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

Det= 2

107.9992896 107.3143809 107.0838036
alpha beta gamma

Normalized Niggli Matrix

1	1.01327063	1.032529194
-0.316067389	-0.302416346	-0.295712962

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

Overall Transformation

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

Det= 1

Center of Mass Coordinates

i	1			
x,y,z	0.7605859	0.2506235	0.24179	1
1-x,1-y,1-z	0.2394141	0.7493765	0.7582	1

x= 0.7605859
y= 0.2506235
z= 0.24179

0,0,0 0.011209412 0.009962353 0.018795882 1
-0.011209412 -1.009962353 -1.018795882 1

Z'= 1

Order Parameter = Coupled

2i P_-1

Matrix Representation

1	-0.000126	-0.341044
0	1.4610255	-0.008613
0	0	0.8556222

68 MEZDOK01
a= 9.944575
b= 14.52928 b/a= 1.4610255
c= 9.160215 c/a= 0.9211268
alpha= 90.53393 alpha= 90.53393
beta= 111.7308 beta= 111.73083
gamma= 90.00494 gamma= 90.00494

a	b	c
1	1.4610255	0.9211268
90.53393	111.73083	90.00494
alpha	beta	gamma

See #67 above.

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

1	0.0018522	0.0015842
0	1.4884328	0.0017618
0	0	2.5714065

70 OHABEE
a= 9.79238
b= 14.57531 b/a= 1.488434
c= 25.1802 c/a= 2.5714076
alpha= 89.9607 alpha= 89.9607
beta= 89.9647 beta= 89.9647
gamma= 89.9287 gamma= 89.9287

a	b	c	
1	1.488434	2.5714076	
89.9607	89.9647	89.9287	
alpha	beta	gamma	

Transformation to Reduced Cell

-0.333333	-0.333333	-0.333333	0.333333
0	0.5	-0.5	-0.25
-0.333333	0.166667	0.166667	0.083333
0	0	0	1

Det= -0.166667

Inverse Transformation

-1	1	1	-0.5
-1	0	-2	1.5
-1	-1	1	0
0	0	0	1

Det= 6

Matrix Representation

-0.333861416	-0.332143174	-0.33399541
-0.000587265	0.744510039	-0.743922774
-0.857135491	0.428567745	0.428567745

a	b	c		
0.919861424	0.921023669	0.921218943		
107.7916146	107.5410774	107.6508078		
alpha	beta	gamma		
Daughter	2iii	2	6	0.333333
Ref. Lattice	BCC	48	1	48
			6	144
			(size)	(index)

Reduced Cell

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

Transformation to Conventional Cell

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

Det= 2

Overall Transformation

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

Det= -3

Center of Mass Coordinates

i: 1 nearest neighbor
8 neighbors within 10% of nearest
next neighbor 16% farther than nearest

i	1			
x,y,z	0.3198117	0.2466519	0.5851674	1
1-x,1-y,1-z	0.6801883	0.7533481	0.4148326	1

x= 0.3198117
y= 0.2466519
z= 0.5851674

0,0,0 0.012007596 0.009853611 0.018703811 1
-0.012007596 -0.009853611 -1.018703811 1

Z'= 1

Order Parameter = Coupled

error 0.012007596 0.009853611 0.018703811

i: 1 nearest neighbor
8 neighbors within 10% of nearest
next neighbor 18% farther than nearest

i				
x,y,z	0.016409	0.2535574	0.2500246	1
1-x,1-y,1-z	0.983591	0.7464426	0.7499754	1

x= 0.016409
y= 0.2535574
z= 0.2500246

-0.012827038 0.983541861 -0.019941823 1
0.012827038 -0.983541861 -0.980058177 1

error -0.012827038 -0.016458139 -0.019941823

i: 2 nearest neighbors
8 neighbors within 10% of nearest
next neighbor 15% farther than nearest
sphere packing

i				
x,y,z	0.3180757	0.7535794	0.0817532	1
1-x,1-y,1-z	0.6819243	0.2464206	0.9182468	1

x= 0.3180757
y= 0.7535794
z= 0.0817532

0.017256975 1.018417871 -0.989901882 1
-0.017256975 -1.018417871 -0.010098118 1

error 0.017256975 0.018417871 0.010098118

2iii P_-1

Matrix Representation

1	0.0307136	-0.006985
0	0.9181114	0.0164553
0	0	0.4795676

71 CANFOM
a= 18.4086
b= 16.9106 b/a= 0.918625
c= 8.8343 c/a= 0.4799007
alpha= 88.064 alpha= 88.064
beta= 90.834 beta= 90.834
gamma= 88.084 gamma= 88.084

a	b	c	
1	0.918625	0.4799007	
88.064	90.834	88.084	
alpha	beta	gamma	

Transformation to Planar Coordinates

0.006985	-0.030726	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	0.030726	-0.006985	-0.248254
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

-3.90214E-08	-1.29356E-05	1
0.0164553	0.918111404	0
0.479567629	0	0

a	b	c
0.479849859	0.918111404	1
90.00080726	90.00000466	88.03479
alpha	beta	gamma

		|G|	Z	|G|/Z
Daughter	2iii	2	8	0.25
Plane	2_1	2	4	0.5
		2	2	
		(size)	(index)	

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

i: 1 nearest neighbor
3 neighbors within 8% of nearest
next neighbor 26% farther than nearest
i: 1 nearest neighbor
3 neighbors within 8% of nearest
next neighbor 29% farther than ne
i: 1 nearest neighbor
3 neighbors within 7% of nearest
next neighbor 33% farther than nearest
i: 1 nearest neighbor
3 neighbors within 9% of nearest
next neighbor 32% farther than ne

Center of Mass Coordinates

i	1			
x,y,z	0.1987578	0.0060756	0.5133267	1
1-x,1-y,1-z	0.8012422	0.9939244	0.4866733	1

x= 0.1987578
y= 0.0060756
z= 0.5133267

i	1			
x,y,z	0.2997033	0.5063144	0.9700989	1
1-x,1-y,1-z	0.7002967	0.4936856	0.0299011	1

planar

plane normal:

1	0	0

plane origin:

0.25	0	0.25

Transformation to orthogonal axes:

0.006985		
-0.030726		

rotation angle:

0 degrees

1/4,0,-z 0.263326667 0.006075556 -0.052895 1
0.236673333 0.993924444 0.580129 1

3/4,1/2,z 0.720098889 0.506314444 0.060231 1
-0.220098889 0.493685556 0.467003 1

z= 0.056562756
error= 0.013326667 0.006075556 0.003668

Z'= 4

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	

R. B. McClurg, July, 2008