Molecular Crystal Global Phase Diagrams: II. Reference Lattices

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

Table 8: Order Parameters

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

Sphere Packings:

ZNOXAC01
Parent: 227 Oh-7, Fd-3m, F4_1/d-32/m, origin choice 2
Subgroup: 227 Oh-7, Fd-3m, F4_1/d-32/m, origin choice 2
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 0 0

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

GM1+ is the primary OP.

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

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

GM2- is the primary OP.

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

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

GM2- is the primary OP.

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

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

K4 is the primary OP.

DILWIE01 & ZEYHIU

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

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

A2 is the primary OP.

TCYMET

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

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

Coupled OP.

ZIZHIZ

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

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

Coupled OP.

MTRETC10

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

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

LD3 is the primary OP.

FUZLUH & VAFWAA

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

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

GM3+ is the primary OP.

ZZZKNW01

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

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

GM5- is the primary OP.

KUJSIR

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

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

W3 is the primary OP.

YEMRIR

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

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

Coupled OP.

ADAMAN08 & GERHOA

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

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

Coupled OP.

KANGUB01

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

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

GM3+ is the primary OP.

(methane III)

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

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

Coupled OP.

YIMWEW

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

Irrep	k params	Dir	Subgroup	Size
GM1+		(a)	229 Im-3m	1
GM3+		(a,-1.732a)	139 I4/mmm	1
GM5+		(0,0,a)	69 Fmmm	1

DT5	5/6	(a,-a,a,a,0,0,0,0,0,0,0,0)	64	Cmca	6
DT1	1/3	(a,0,0,0,0,0)	139	I4/mmm	3
DT3	1/3	(0,a,0,0,0,0)	69	Fmmm	3
H4+		(a,-a,0)	64	Cmca	2
H5+		(a,a,0)	64	Cmca	2
N1-		(0,0,a,0,0,0)	68	Ccca	2
N4-		(0,0,a,0,0,0)	63	Cmcm	2
D2	1/6	(0,0,a,0,0,0,0,0,0,0,0,0)	68	Ccca	6
D3	1/6	(0,0,0,0,0,0,0,0,0,a,0,0)	63	Cmcm	6

Coupled OP.

RASDOE & TFMETH02

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

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

GM3+ is the primary OP.

REKYUB

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

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

L3- is the primary OP.

MECKOU

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

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

L3- is the primary OP.

MECKUA

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

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

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

Coupled OP.

TOHSUE

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

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

Coupled OP.

CARBTC07 & CTBROM

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

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

C2 is the primary OP.

MEZDIE01 & MEZDOK01

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

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

Coupled OP.

OHABEE

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

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

Coupled OP.

Dimer Packings:

FOJBUB & VADRAU

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

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

X5+ is the primary OP.

LUFYEQ

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

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

GM3+ is the primary OP.

CARBTC

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

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

F2+ is the primary OP.

Mixed

KOXKOX, RUQMEV, & SENLAY

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

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

GM2- is the primary OP.

Richard B. McClurg, April, 2008