

MSG No. 187.214  $P_c\bar{6}m2$  [ Type IV, hexagonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $-6m2$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$
2	$[0, 0, \frac{1}{2}]$	$[13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 2: Wyckoff site: 2b, site symmetry:  $-6'm2'$

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 2, 3, 10, 11, 12, 16, 17, 18, 19, 20, 21]$
2	$[0, 0, \frac{3}{4}]$	$[4, 5, 6, 7, 8, 9, 13, 14, 15, 22, 23, 24]$

Table 3: Wyckoff site: 2c, site symmetry:  $-6m2$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$
2	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 4: Wyckoff site: 2d, site symmetry:  $-6'm2'$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[1, 2, 3, 10, 11, 12, 16, 17, 18, 19, 20, 21]$
2	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[4, 5, 6, 7, 8, 9, 13, 14, 15, 22, 23, 24]$

Table 5: Wyckoff site: 2e, site symmetry:  $-6m2$

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 6: Wyckoff site: 2f, site symmetry:  $-6'm2'$

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[1, 2, 3, 10, 11, 12, 16, 17, 18, 19, 20, 21]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[4, 5, 6, 7, 8, 9, 13, 14, 15, 22, 23, 24]$

Table 7: Wyckoff site: 4g, site symmetry: 3m.

No.	position	mapping
1	[0, 0, z]	[1, 2, 3, 10, 11, 12]
2	[0, 0, -z]	[4, 5, 6, 7, 8, 9]
3	[0, 0, $z + \frac{1}{2}$ ]	[13, 14, 15, 22, 23, 24]
4	[0, 0, $\frac{1}{2} - z$ ]	[16, 17, 18, 19, 20, 21]

Table 8: Wyckoff site: 4h, site symmetry: 3m.

No.	position	mapping
1	[ $\frac{1}{3}, \frac{2}{3}, z$ ]	[1, 2, 3, 10, 11, 12]
2	[ $\frac{1}{3}, \frac{2}{3}, -z$ ]	[4, 5, 6, 7, 8, 9]
3	[ $\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}$ ]	[13, 14, 15, 22, 23, 24]
4	[ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z$ ]	[16, 17, 18, 19, 20, 21]

Table 9: Wyckoff site: 4i, site symmetry: 3m.

No.	position	mapping
1	[ $\frac{2}{3}, \frac{1}{3}, z$ ]	[1, 2, 3, 10, 11, 12]
2	[ $\frac{2}{3}, \frac{1}{3}, -z$ ]	[4, 5, 6, 7, 8, 9]
3	[ $\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$ ]	[13, 14, 15, 22, 23, 24]
4	[ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z$ ]	[16, 17, 18, 19, 20, 21]

Table 10: Wyckoff site: 6j, site symmetry: mm2

No.	position	mapping
1	[x, -x, 0]	[1, 6, 8, 11]
2	[x, 2x, 0]	[2, 4, 9, 12]
3	[-2x, -x, 0]	[3, 5, 7, 10]
4	[x, -x, $\frac{1}{2}$ ]	[13, 18, 20, 23]
5	[x, 2x, $\frac{1}{2}$ ]	[14, 16, 21, 24]
6	[-2x, -x, $\frac{1}{2}$ ]	[15, 17, 19, 22]

Table 11: Wyckoff site: 6k, site symmetry: m'm2'

No.	position	mapping
1	[x, -x, $\frac{1}{4}$ ]	[1, 11, 18, 20]
2	[x, 2x, $\frac{1}{4}$ ]	[2, 12, 16, 21]

*continued ...*

Table 11

No.	position	mapping
3	$[-2x, -x, \frac{1}{4}]$	[3,10,17,19]
4	$[x, 2x, \frac{3}{4}]$	[4,9,14,24]
5	$[-2x, -x, \frac{3}{4}]$	[5,7,15,22]
6	$[x, -x, \frac{3}{4}]$	[6,8,13,23]

Table 12: Wyckoff site: 121, site symmetry:  $\mathbf{m}..$ 

No.	position	mapping
1	$[x, y, 0]$	[1,8]
2	$[-y, x - y, 0]$	[2,9]
3	$[-x + y, -x, 0]$	[3,7]
4	$[x, x - y, 0]$	[4,12]
5	$[-x + y, y, 0]$	[5,10]
6	$[-y, -x, 0]$	[6,11]
7	$[x, y, \frac{1}{2}]$	[13,20]
8	$[-y, x - y, \frac{1}{2}]$	[14,21]
9	$[-x + y, -x, \frac{1}{2}]$	[15,19]
10	$[x, x - y, \frac{1}{2}]$	[16,24]
11	$[-x + y, y, \frac{1}{2}]$	[17,22]
12	$[-y, -x, \frac{1}{2}]$	[18,23]

Table 13: Wyckoff site: 12m, site symmetry:  $\mathbf{m}'..$ 

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	[1,20]
2	$[-y, x - y, \frac{1}{4}]$	[2,21]
3	$[-x + y, -x, \frac{1}{4}]$	[3,19]
4	$[x, x - y, \frac{3}{4}]$	[4,24]
5	$[-x + y, y, \frac{3}{4}]$	[5,22]
6	$[-y, -x, \frac{3}{4}]$	[6,23]
7	$[-x + y, -x, \frac{3}{4}]$	[7,15]
8	$[x, y, \frac{3}{4}]$	[8,13]
9	$[-y, x - y, \frac{3}{4}]$	[9,14]
10	$[-x + y, y, \frac{1}{4}]$	[10,17]
11	$[-y, -x, \frac{1}{4}]$	[11,18]
12	$[x, x - y, \frac{1}{4}]$	[12,16]

Table 14: Wyckoff site: 12n, site symmetry: .m.

No.	position	mapping
1	[ $x, -x, z$ ]	[1,11]
2	[ $x, 2x, z$ ]	[2,12]
3	[ $-2x, -x, z$ ]	[3,10]
4	[ $x, 2x, -z$ ]	[4,9]
5	[ $-2x, -x, -z$ ]	[5,7]
6	[ $x, -x, -z$ ]	[6,8]
7	[ $x, -x, z + \frac{1}{2}$ ]	[13,23]
8	[ $x, 2x, z + \frac{1}{2}$ ]	[14,24]
9	[ $-2x, -x, z + \frac{1}{2}$ ]	[15,22]
10	[ $x, 2x, \frac{1}{2} - z$ ]	[16,21]
11	[ $-2x, -x, \frac{1}{2} - z$ ]	[17,19]
12	[ $x, -x, \frac{1}{2} - z$ ]	[18,20]

Table 15: Wyckoff site: 24o, site symmetry: 1

No.	position	mapping
1	[ $x, y, z$ ]	[1]
2	[ $-y, x - y, z$ ]	[2]
3	[ $-x + y, -x, z$ ]	[3]
4	[ $x, x - y, -z$ ]	[4]
5	[ $-x + y, y, -z$ ]	[5]
6	[ $-y, -x, -z$ ]	[6]
7	[ $-x + y, -x, -z$ ]	[7]
8	[ $x, y, -z$ ]	[8]
9	[ $-y, x - y, -z$ ]	[9]
10	[ $-x + y, y, z$ ]	[10]
11	[ $-y, -x, z$ ]	[11]
12	[ $x, x - y, z$ ]	[12]
13	[ $x, y, z + \frac{1}{2}$ ]	[13]
14	[ $-y, x - y, z + \frac{1}{2}$ ]	[14]
15	[ $-x + y, -x, z + \frac{1}{2}$ ]	[15]
16	[ $x, x - y, \frac{1}{2} - z$ ]	[16]
17	[ $-x + y, y, \frac{1}{2} - z$ ]	[17]
18	[ $-y, -x, \frac{1}{2} - z$ ]	[18]
19	[ $-x + y, -x, \frac{1}{2} - z$ ]	[19]
20	[ $x, y, \frac{1}{2} - z$ ]	[20]
21	[ $-y, x - y, \frac{1}{2} - z$ ]	[21]
22	[ $-x + y, y, z + \frac{1}{2}$ ]	[22]
23	[ $-y, -x, z + \frac{1}{2}$ ]	[23]
24	[ $x, x - y, z + \frac{1}{2}$ ]	[24]