

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: 12l, site symmetry: $m\bar{3}m$.

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: $m\bar{3}m$.

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]