

MSG No. 192.245 $P6/m'cc$ [Type III, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: 62'2'

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

Table 2: Wyckoff site: 2b, site symmetry: 6/m'..

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

Table 3: Wyckoff site: 4c, site symmetry: 3.2'

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

Table 4: Wyckoff site: 4d, site symmetry: -6'..

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

Table 5: Wyckoff site: 4e, site symmetry: 6..

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

Table 6: Wyckoff site: 6f, site symmetry: 22'2'

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

Table 7: Wyckoff site: 6g, site symmetry: 2/m'..

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

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

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

Table 9: Wyckoff site: 12i, site symmetry: 2..

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1, 4]
2	$[\frac{1}{2}, \frac{1}{2}, z]$	[2, 5]
3	$[0, \frac{1}{2}, z]$	[3, 6]
4	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[7, 11]
5	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[8, 12]
6	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[9, 10]
7	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[13, 17]

continued ...

Table 9

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

Table 10: Wyckoff site: 12j, site symmetry: .2'.

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

Table 11: Wyckoff site: 12k, site symmetry: . .2'

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

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

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

Table 13: Wyckoff site: 24m, site symmetry: 1

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