

MSG No. 175.142 P_6/m [Type IV, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: $6/m..$

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: $6/m'..$

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

Table 3: Wyckoff site: 4c, site symmetry: $-6..$

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

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

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

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

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

Table 6: Wyckoff site: **6f**, site symmetry: $2/m'..$

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

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

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

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	$[\frac{2}{3}, \frac{1}{3}, -z]$	$[7, 9, 11]$
4	$[\frac{1}{3}, \frac{2}{3}, -z]$	$[8, 10, 12]$
5	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	$[13, 15, 17]$
6	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	$[14, 16, 18]$
7	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	$[19, 21, 23]$
8	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	$[20, 22, 24]$

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	$[\frac{1}{2}, 0, -z]$	$[7, 10]$
5	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[8, 11]$
6	$[0, \frac{1}{2}, -z]$	$[9, 12]$
7	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[13, 16]$

continued ...

Table 9

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

Table 10: Wyckoff site: 12j, site symmetry: $m..$

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

Table 11: Wyckoff site: 12k, site symmetry: $m'..$

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

Table 12: Wyckoff site: 241, 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	$[-x, -y, -z]$	[7]
8	$[-x + y, -x, -z]$	[8]
9	$[y, -x + y, -z]$	[9]
10	$[x, y, -z]$	[10]
11	$[x - y, x, -z]$	[11]
12	$[-y, x - y, -z]$	[12]
13	$[x, y, z + \frac{1}{2}]$	[13]
14	$[x - y, x, z + \frac{1}{2}]$	[14]
15	$[-y, x - y, z + \frac{1}{2}]$	[15]
16	$[-x, -y, z + \frac{1}{2}]$	[16]
17	$[-x + y, -x, z + \frac{1}{2}]$	[17]
18	$[y, -x + y, z + \frac{1}{2}]$	[18]
19	$[-x, -y, \frac{1}{2} - z]$	[19]
20	$[-x + y, -x, \frac{1}{2} - z]$	[20]
21	$[y, -x + y, \frac{1}{2} - z]$	[21]
22	$[x, y, \frac{1}{2} - z]$	[22]
23	$[x - y, x, \frac{1}{2} - z]$	[23]
24	$[-y, x - y, \frac{1}{2} - z]$	[24]