MSG No. 176.148 P_c6_3/m [Type IV, hexagonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, 0, z\right]$	[1,16]
2	$\left[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}\right]$	[2,17]
3	$\left[0, \frac{1}{2}, z\right]$	[3,18]
4	$\left[\frac{1}{2}, 0, z + \frac{1}{2}\right]$	[4,13]
5	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[5,14]
6	$\left[0, \frac{1}{2}, z + \frac{1}{2}\right]$	[6,15]
7	$\left[\frac{1}{2}, 0, -z\right]$	[7,22]

continued ...

Table 9

No.	position	mapping
8	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z\right]$	[8,23]
9	$\left[0, \frac{1}{2}, -z\right]$	[9,24]
10	$\left[\frac{1}{2}, 0, \frac{1}{2} - z\right]$	[10,19]
11	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	[11,20]
12	$\left[0, \frac{1}{2}, \frac{1}{2} - z\right]$	[12,21]

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

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

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

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

Table 12: Wyckoff site: 241, site symmetry: 1

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