MSG No. 191.242 P_c6/mmm [Type IV, hexagonal]

Table 1: Wyckoff site: `2a`, site symmetry: `6/mmm`

No.	position	mapping
1	$[0,\ 0,\ 0]$	`[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]`
2	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]`

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

No.	position	mapping
1	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[1,2,3,4,5,6,19,20,21,22,23,24,31,32,33,34,35,36,37,38,39,40,41,42]`
2	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[7,8,9,10,11,12,13,14,15,16,17,18,25,26,27,28,29,30,43,44,45,46,47,48]`

Table 3: Wyckoff site: `4c`, site symmetry: `-6m2`

No.	position	mapping
1	$\left[\frac{1}{3},\ \frac{2}{3},\ 0\right]$	`[1,3,5,10,11,12,14,16,18,19,20,21]`
2	$\left[\frac{2}{3},\ \frac{1}{3},\ 0\right]$	`[2,4,6,7,8,9,13,15,17,22,23,24]`
3	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}\right]$	`[25,27,29,34,35,36,38,40,42,43,44,45]`
4	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{2}\right]$	`[26,28,30,31,32,33,37,39,41,46,47,48]`

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

No.	position	mapping
1	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{4}\right]$	`[1,3,5,19,20,21,34,35,36,38,40,42]`
2	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{4}\right]$	`[2,4,6,22,23,24,31,32,33,37,39,41]`
3	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	`[7,8,9,13,15,17,26,28,30,46,47,48]`
4	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{3}{4}\right]$	`[10,11,12,14,16,18,25,27,29,43,44,45]`

Table 5: Wyckoff site: `4e`, site symmetry: `6mm`

No.	position	mapping
1	$[0,\ 0,\ z]$	`[1,2,3,4,5,6,19,20,21,22,23,24]`
2	$[0,\ 0,\ -z]$	`[7,8,9,10,11,12,13,14,15,16,17,18]`
3	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[25,26,27,28,29,30,43,44,45,46,47,48]`
4	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	`[31,32,33,34,35,36,37,38,39,40,41,42]`

Table 6: Wyckoff site: `6f`, site symmetry: `mmm`

No.	position	mapping
1	$\left[\frac{1}{2}, 0, 0\right]$	`[1,4,7,11,13,16,19,23]`
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[2,5,9,10,14,17,21,22]`
3	$\left[0, \frac{1}{2}, 0\right]$	`[3,6,8,12,15,18,20,24]`
4	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[25,28,31,35,37,40,43,47]`
5	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[26,29,33,34,38,41,45,46]`
6	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[27,30,32,36,39,42,44,48]`

Table 7: Wyckoff site: `6g`, site symmetry: `m'mm`

No.	position	mapping
1	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[1,4,19,23,31,35,37,40]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	`[2,5,21,22,33,34,38,41]`
3	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[3,6,20,24,32,36,39,42]`
4	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[7,11,13,16,25,28,43,47]`
5	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	`[8,12,15,18,27,30,44,48]`
6	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	`[9,10,14,17,26,29,45,46]`

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

No.	position	mapping
1	$\left[\frac{1}{3}, \frac{2}{3}, z\right]$	`[1,3,5,19,20,21]`
2	$\left[\frac{2}{3}, \frac{1}{3}, z\right]$	`[2,4,6,22,23,24]`
3	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	`[7,8,9,13,15,17]`
4	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[10,11,12,14,16,18]`
5	$\left[\frac{1}{3}, \frac{2}{3}, z+\frac{1}{2}\right]$	`[25,27,29,43,44,45]`
6	$\left[\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2}\right]$	`[26,28,30,46,47,48]`
7	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}-z\right]$	`[31,32,33,37,39,41]`
8	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}-z\right]$	`[34,35,36,38,40,42]`

Table 9: Wyckoff site: `12i`, site symmetry: `2mm`

No.	position	mapping
1	$\left[\frac{1}{2}, 0, z\right]$	`[1,4,19,23]`
2	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[2,5,21,22]`
3	$\left[0, \frac{1}{2}, z\right]$	`[3,6,20,24]`
4	$\left[\frac{1}{2}, 0, -z\right]$	`[7,11,13,16]`
5	$\left[0, \frac{1}{2}, -z\right]$	`[8,12,15,18]`
6	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[9,10,14,17]`
7	$\left[\frac{1}{2}, 0, z+\frac{1}{2}\right]$	`[25,28,43,47]`

continued ...

Table 9

No.	position	mapping
8	$\left[\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[26,29,45,46]
9	$\left[0,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[27,30,44,48]
10	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	[31,35,37,40]
11	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[32,36,39,42]
12	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[33,34,38,41]

Table 10: Wyckoff site: 12j, site symmetry: m2m

No.	position	mapping
1	$[x,\ 0,\ 0]$	[1,7,16,23]
2	$[x,\ x,\ 0]$	[2,10,17,21]
3	$[0,\ x,\ 0]$	[3,8,18,24]
4	$[-x,\ 0,\ 0]$	[4,11,13,19]
5	$[-x,\ -x,\ 0]$	[5,9,14,22]
6	$[0,\ -x,\ 0]$	[6,12,15,20]
7	$\left[x,\ 0,\ \frac{1}{2}\right]$	[25,31,40,47]
8	$\left[x,\ x,\ \frac{1}{2}\right]$	[26,34,41,45]
9	$\left[0,\ x,\ \frac{1}{2}\right]$	[27,32,42,48]
10	$\left[-x,\ 0,\ \frac{1}{2}\right]$	[28,35,37,43]
11	$\left[-x,\ -x,\ \frac{1}{2}\right]$	[29,33,38,46]
12	$\left[0,\ -x,\ \frac{1}{2}\right]$	[30,36,39,44]

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

No.	position	mapping
1	$\left[x,\ 0,\ \frac{1}{4}\right]$	[1,23,31,40]
2	$\left[x,\ x,\ \frac{1}{4}\right]$	[2,21,34,41]
3	$\left[0,\ x,\ \frac{1}{4}\right]$	[3,24,32,42]
4	$\left[-x,\ 0,\ \frac{1}{4}\right]$	[4,19,35,37]
5	$\left[-x,\ -x,\ \frac{1}{4}\right]$	[5,22,33,38]
6	$\left[0,\ -x,\ \frac{1}{4}\right]$	[6,20,36,39]
7	$\left[x,\ 0,\ \frac{3}{4}\right]$	[7,16,25,47]
8	$\left[0,\ x,\ \frac{3}{4}\right]$	[8,18,27,48]
9	$\left[-x,\ -x,\ \frac{3}{4}\right]$	[9,14,29,46]
10	$\left[x,\ x,\ \frac{3}{4}\right]$	[10,17,26,45]
11	$\left[-x,\ 0,\ \frac{3}{4}\right]$	[11,13,28,43]
12	$\left[0,\ -x,\ \frac{3}{4}\right]$	[12,15,30,44]

Table 12: Wyckoff site: `12l`, site symmetry: `mm2`

No.	position	mapping
1	$[x,\ 2x,\ 0]$	`[1,11,16,19]`
2	$[-x,\ x,\ 0]$	`[2,9,17,22]`
3	$[-2x,\ -x,\ 0]$	`[3,12,18,20]`
4	$[-x,\ -2x,\ 0]$	`[4,7,13,23]`
5	$[x,\ -x,\ 0]$	`[5,10,14,21]`
6	$[2x,\ x,\ 0]$	`[6,8,15,24]`
7	$\left[x,\ 2x,\ \frac{1}{2}\right]$	`[25,35,40,43]`
8	$\left[-x,\ x,\ \frac{1}{2}\right]$	`[26,33,41,46]`
9	$\left[-2x,\ -x,\ \frac{1}{2}\right]$	`[27,36,42,44]`
10	$\left[-x,\ -2x,\ \frac{1}{2}\right]$	`[28,31,37,47]`
11	$\left[x,\ -x,\ \frac{1}{2}\right]$	`[29,34,38,45]`
12	$\left[2x,\ x,\ \frac{1}{2}\right]$	`[30,32,39,48]`

Table 13: Wyckoff site: `12m`, site symmetry: `m'm2'`

No.	position	mapping
1	$\left[x,\ 2x,\ \frac{1}{4}\right]$	`[1,19,35,40]`
2	$\left[-x,\ x,\ \frac{1}{4}\right]$	`[2,22,33,41]`
3	$\left[-2x,\ -x,\ \frac{1}{4}\right]$	`[3,20,36,42]`
4	$\left[-x,\ -2x,\ \frac{1}{4}\right]$	`[4,23,31,37]`
5	$\left[x,\ -x,\ \frac{1}{4}\right]$	`[5,21,34,38]`
6	$\left[2x,\ x,\ \frac{1}{4}\right]$	`[6,24,32,39]`
7	$\left[-x,\ -2x,\ \frac{3}{4}\right]$	`[7,13,28,47]`
8	$\left[2x,\ x,\ \frac{3}{4}\right]$	`[8,15,30,48]`
9	$\left[-x,\ x,\ \frac{3}{4}\right]$	`[9,17,26,46]`
10	$\left[x,\ -x,\ \frac{3}{4}\right]$	`[10,14,29,45]`
11	$\left[x,\ 2x,\ \frac{3}{4}\right]$	`[11,16,25,43]`
12	$\left[-2x,\ -x,\ \frac{3}{4}\right]$	`[12,18,27,44]`

Table 14: Wyckoff site: `24n`, site symmetry: `..m`

No.	position	mapping
1	$[x,\ 0,\ z]$	`[1,23]`
2	$[x,\ x,\ z]$	`[2,21]`
3	$[0,\ x,\ z]$	`[3,24]`
4	$[-x,\ 0,\ z]$	`[4,19]`
5	$[-x,\ -x,\ z]$	`[5,22]`
6	$[0,\ -x,\ z]$	`[6,20]`
7	$[x,\ 0,\ -z]$	`[7,16]`
8	$[0,\ x,\ -z]$	`[8,18]`
9	$[-x,\ -x,\ -z]$	`[9,14]`

continued ...

Table 14

No.	position	mapping
10	$[x,\ x,\ -z]$	[10,17]
11	$[-x,\ 0,\ -z]$	[11,13]
12	$[0,\ -x,\ -z]$	[12,15]
13	$\left[x,\ 0,\ z+\frac{1}{2}\right]$	[25,47]
14	$\left[x,\ x,\ z+\frac{1}{2}\right]$	[26,45]
15	$\left[0,\ x,\ z+\frac{1}{2}\right]$	[27,48]
16	$\left[-x,\ 0,\ z+\frac{1}{2}\right]$	[28,43]
17	$\left[-x,\ -x,\ z+\frac{1}{2}\right]$	[29,46]
18	$\left[0,\ -x,\ z+\frac{1}{2}\right]$	[30,44]
19	$\left[x,\ 0,\ \frac{1}{2}-z\right]$	[31,40]
20	$\left[0,\ x,\ \frac{1}{2}-z\right]$	[32,42]
21	$\left[-x,\ -x,\ \frac{1}{2}-z\right]$	[33,38]
22	$\left[x,\ x,\ \frac{1}{2}-z\right]$	[34,41]
23	$\left[-x,\ 0,\ \frac{1}{2}-z\right]$	[35,37]
24	$\left[0,\ -x,\ \frac{1}{2}-z\right]$	[36,39]

Table 15: Wyckoff site: 24o, site symmetry: .m.

No.	position	mapping
1	$[x,\ 2x,\ z]$	[1,19]
2	$[-x,\ x,\ z]$	[2,22]
3	$[-2x,\ -x,\ z]$	[3,20]
4	$[-x,\ -2x,\ z]$	[4,23]
5	$[x,\ -x,\ z]$	[5,21]
6	$[2x,\ x,\ z]$	[6,24]
7	$[-x,\ -2x,\ -z]$	[7,13]
8	$[2x,\ x,\ -z]$	[8,15]
9	$[-x,\ x,\ -z]$	[9,17]
10	$[x,\ -x,\ -z]$	[10,14]
11	$[x,\ 2x,\ -z]$	[11,16]
12	$[-2x,\ -x,\ -z]$	[12,18]
13	$\left[x,\ 2x,\ z+\frac{1}{2}\right]$	[25,43]
14	$\left[-x,\ x,\ z+\frac{1}{2}\right]$	[26,46]
15	$\left[-2x,\ -x,\ z+\frac{1}{2}\right]$	[27,44]
16	$\left[-x,\ -2x,\ z+\frac{1}{2}\right]$	[28,47]
17	$\left[x,\ -x,\ z+\frac{1}{2}\right]$	[29,45]
18	$\left[2x,\ x,\ z+\frac{1}{2}\right]$	[30,48]
19	$\left[-x,\ -2x,\ \frac{1}{2}-z\right]$	[31,37]
20	$\left[2x,\ x,\ \frac{1}{2}-z\right]$	[32,39]
21	$\left[-x,\ x,\ \frac{1}{2}-z\right]$	[33,41]
22	$\left[x,\ -x,\ \frac{1}{2}-z\right]$	[34,38]
23	$\left[x,\ 2x,\ \frac{1}{2}-z\right]$	[35,40]
24	$\left[-2x,\ -x,\ \frac{1}{2}-z\right]$	[36,42]

Table 16: Wyckoff site: 24p, site symmetry: m..

No.	position	mapping
1	$[x,\ y,\ 0]$	[1,16]
2	$[x-y,\ x,\ 0]$	[2,17]
3	$[-y,\ x-y,\ 0]$	[3,18]
4	$[-x,\ -y,\ 0]$	[4,13]
5	$[-x+y,\ -x,\ 0]$	[5,14]
6	$[y,\ -x+y,\ 0]$	[6,15]
7	$[x-y,\ -y,\ 0]$	[7,23]
8	$[y,\ x,\ 0]$	[8,24]
9	$[-x,\ -x+y,\ 0]$	[9,22]
10	$[x,\ x-y,\ 0]$	[10,21]
11	$[-x+y,\ y,\ 0]$	[11,19]
12	$[-y,\ -x,\ 0]$	[12,20]
13	$\left[x,\ y,\ \frac{1}{2}\right]$	[25,40]
14	$\left[x-y,\ x,\ \frac{1}{2}\right]$	[26,41]
15	$\left[-y,\ x-y,\ \frac{1}{2}\right]$	[27,42]
16	$\left[-x,\ -y,\ \frac{1}{2}\right]$	[28,37]
17	$\left[-x+y,\ -x,\ \frac{1}{2}\right]$	[29,38]
18	$\left[y,\ -x+y,\ \frac{1}{2}\right]$	[30,39]
19	$\left[x-y,\ -y,\ \frac{1}{2}\right]$	[31,47]
20	$\left[y,\ x,\ \frac{1}{2}\right]$	[32,48]
21	$\left[-x,\ -x+y,\ \frac{1}{2}\right]$	[33,46]
22	$\left[x,\ x-y,\ \frac{1}{2}\right]$	[34,45]
23	$\left[-x+y,\ y,\ \frac{1}{2}\right]$	[35,43]
24	$\left[-y,\ -x,\ \frac{1}{2}\right]$	[36,44]

Table 17: Wyckoff site: 24q, site symmetry: m'..

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{4}\right]$	[1,40]
2	$\left[x-y,\ x,\ \frac{1}{4}\right]$	[2,41]
3	$\left[-y,\ x-y,\ \frac{1}{4}\right]$	[3,42]
4	$\left[-x,\ -y,\ \frac{1}{4}\right]$	[4,37]
5	$\left[-x+y,\ -x,\ \frac{1}{4}\right]$	[5,38]
6	$\left[y,\ -x+y,\ \frac{1}{4}\right]$	[6,39]
7	$\left[x-y,\ -y,\ \frac{3}{4}\right]$	[7,47]
8	$\left[y,\ x,\ \frac{3}{4}\right]$	[8,48]
9	$\left[-x,\ -x+y,\ \frac{3}{4}\right]$	[9,46]
10	$\left[x,\ x-y,\ \frac{3}{4}\right]$	[10,45]
11	$\left[-x+y,\ y,\ \frac{3}{4}\right]$	[11,43]
12	$\left[-y,\ -x,\ \frac{3}{4}\right]$	[12,44]
13	$\left[-x,\ -y,\ \frac{3}{4}\right]$	[13,28]
14	$\left[-x+y,\ -x,\ \frac{3}{4}\right]$	[14,29]
15	$\left[y,\ -x+y,\ \frac{3}{4}\right]$	[15,30]

continued ...

Table 17

No.	position	mapping
16	$\left[x,\, y,\, \frac{3}{4}\right]$	[16,25]
17	$\left[x-y,\, x,\, \frac{3}{4}\right]$	[17,26]
18	$\left[-y,\, x-y,\, \frac{3}{4}\right]$	[18,27]
19	$\left[-x+y,\, y,\, \frac{1}{4}\right]$	[19,35]
20	$\left[-y,\, -x,\, \frac{1}{4}\right]$	[20,36]
21	$\left[x,\, x-y,\, \frac{1}{4}\right]$	[21,34]
22	$\left[-x,\, -x+y,\, \frac{1}{4}\right]$	[22,33]
23	$\left[x-y,\, -y,\, \frac{1}{4}\right]$	[23,31]
24	$\left[y,\, x,\, \frac{1}{4}\right]$	[24,32]

Table 18: Wyckoff site: 48r, 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	$[x-y,\, -y,\, -z]$	[7]
8	$[y,\, x,\, -z]$	[8]
9	$[-x,\, -x+y,\, -z]$	[9]
10	$[x,\, x-y,\, -z]$	[10]
11	$[-x+y,\, y,\, -z]$	[11]
12	$[-y,\, -x,\, -z]$	[12]
13	$[-x,\, -y,\, -z]$	[13]
14	$[-x+y,\, -x,\, -z]$	[14]
15	$[y,\, -x+y,\, -z]$	[15]
16	$[x,\, y,\, -z]$	[16]
17	$[x-y,\, x,\, -z]$	[17]
18	$[-y,\, x-y,\, -z]$	[18]
19	$[-x+y,\, y,\, z]$	[19]
20	$[-y,\, -x,\, z]$	[20]
21	$[x,\, x-y,\, z]$	[21]
22	$[-x,\, -x+y,\, z]$	[22]
23	$[x-y,\, -y,\, z]$	[23]
24	$[y,\, x,\, z]$	[24]
25	$\left[x,\, y,\, z+\frac{1}{2}\right]$	[25]
26	$\left[x-y,\, x,\, z+\frac{1}{2}\right]$	[26]
27	$\left[-y,\, x-y,\, z+\frac{1}{2}\right]$	[27]
28	$\left[-x,\, -y,\, z+\frac{1}{2}\right]$	[28]
29	$\left[-x+y,\, -x,\, z+\frac{1}{2}\right]$	[29]
30	$\left[y,\, -x+y,\, z+\frac{1}{2}\right]$	[30]
31	$\left[x-y,\, -y,\, \frac{1}{2}-z\right]$	[31]

continued ...

Table 18

No.	position	mapping
32	$\left[y,\, x,\, \frac{1}{2}-z\right]$	[32]
33	$\left[-x,\, -x+y,\, \frac{1}{2}-z\right]$	[33]
34	$\left[x,\, x-y,\, \frac{1}{2}-z\right]$	[34]
35	$\left[-x+y,\, y,\, \frac{1}{2}-z\right]$	[35]
36	$\left[-y,\, -x,\, \frac{1}{2}-z\right]$	[36]
37	$\left[-x,\, -y,\, \frac{1}{2}-z\right]$	[37]
38	$\left[-x+y,\, -x,\, \frac{1}{2}-z\right]$	[38]
39	$\left[y,\, -x+y,\, \frac{1}{2}-z\right]$	[39]
40	$\left[x,\, y,\, \frac{1}{2}-z\right]$	[40]
41	$\left[x-y,\, x,\, \frac{1}{2}-z\right]$	[41]
42	$\left[-y,\, x-y,\, \frac{1}{2}-z\right]$	[42]
43	$\left[-x+y,\, y,\, z+\frac{1}{2}\right]$	[43]
44	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[44]
45	$\left[x,\, x-y,\, z+\frac{1}{2}\right]$	[45]
46	$\left[-x,\, -x+y,\, z+\frac{1}{2}\right]$	[46]
47	$\left[x-y,\, -y,\, z+\frac{1}{2}\right]$	[47]
48	$\left[y,\, x,\, z+\frac{1}{2}\right]$	[48]