MSG No. 194.272 P_c6_3/mmc [Type IV, hexagonal]

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

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

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

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

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

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

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

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

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

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

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

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

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	$\left[\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2}\right]$	`[2,4,6,22,23,24]`
3	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	`[7,8,9,13,15,17]`
4	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}-z\right]$	`[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	$\left[\frac{2}{3}, \frac{1}{3}, z\right]$	`[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	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[34,35,36,38,40,42]`

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

No.	position	mapping
1	$\left[\frac{1}{2}, 0, z\right]$	`[1,19,28,47]`
2	$\left[\frac{1}{2}, \frac{1}{2}, z+\frac{1}{2}\right]$	`[2,22,29,45]`
3	$\left[0, \frac{1}{2}, z\right]$	`[3,20,30,48]`
4	$\left[\frac{1}{2}, 0, z+\frac{1}{2}\right]$	`[4,23,25,43]`
5	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[5,21,26,46]`
6	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	`[6,24,27,44]`
7	$\left[\frac{1}{2}, 0, -z\right]$	`[7,13,35,40]`

continued ...

Table 9

No.	position	mapping
8	$\left[0,\ \frac{1}{2},\ -z\right]$	[8,15,36,42]
9	$\left[\frac{1}{2},\ \frac{1}{2},\ -z\right]$	[9,17,34,38]
10	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[10,14,33,41]
11	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	[11,16,31,37]
12	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[12,18,32,39]

Table 10: Wyckoff site: 12j, site symmetry: m2'm'

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x,\, 0,\, z]$	`[1,47]`
2	$\left[x,\, x,\, z+\frac{1}{2}\right]$	`[2,45]`
3	$[0,\, x,\, z]$	`[3,48]`
4	$\left[-x,\, 0,\, z+\frac{1}{2}\right]$	`[4,43]`
5	$[-x,\, -x,\, z]$	`[5,46]`
6	$\left[0,\, -x,\, z+\frac{1}{2}\right]$	`[6,44]`
7	$[x,\, 0,\, -z]$	`[7,40]`
8	$[0,\, x,\, -z]$	`[8,42]`
9	$[-x,\, -x,\, -z]$	`[9,38]`

continued ...

Table 14

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

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

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

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

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

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

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,40]`
2	$\left[x-y,\ x,\ \frac{1}{2}\right]$	`[2,41]`
3	$[-y,\ x-y,\ 0]$	`[3,42]`
4	$\left[-x,\ -y,\ \frac{1}{2}\right]$	`[4,37]`
5	$[-x+y,\ -x,\ 0]$	`[5,38]`
6	$\left[y,\ -x+y,\ \frac{1}{2}\right]$	`[6,39]`
7	$[x-y,\ -y,\ 0]$	`[7,47]`
8	$[y,\ x,\ 0]$	`[8,48]`
9	$[-x,\ -x+y,\ 0]$	`[9,46]`
10	$\left[x,\ x-y,\ \frac{1}{2}\right]$	`[10,45]`
11	$\left[-x+y,\ y,\ \frac{1}{2}\right]$	`[11,43]`
12	$\left[-y,\ -x,\ \frac{1}{2}\right]$	`[12,44]`
13	$[-x,\ -y,\ 0]$	`[13,28]`
14	$\left[-x+y,\ -x,\ \frac{1}{2}\right]$	`[14,29]`
15	$[y,\ -x+y,\ 0]$	`[15,30]`

continued ...

Table 17

No.	position	mapping
16	$\left[x,\, y,\, \frac{1}{2}\right]$	[16,25]
17	$[x-y,\, x,\, 0]$	[17,26]
18	$\left[-y,\, x-y,\, \frac{1}{2}\right]$	[18,27]
19	$[-x+y,\, y,\, 0]$	[19,35]
20	$[-y,\, -x,\, 0]$	[20,36]
21	$[x,\, x-y,\, 0]$	[21,34]
22	$\left[-x,\, -x+y,\, \frac{1}{2}\right]$	[22,33]
23	$\left[x-y,\, -y,\, \frac{1}{2}\right]$	[23,31]
24	$\left[y,\, x,\, \frac{1}{2}\right]$	[24,32]

Table 18: Wyckoff site: 48r, 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	$[x-y,\, -y,\, -z]$	[7]
8	$[y,\, x,\, -z]$	[8]
9	$[-x,\, -x+y,\, -z]$	[9]
10	$\left[x,\, x-y,\, \frac{1}{2}-z\right]$	[10]
11	$\left[-x+y,\, y,\, \frac{1}{2}-z\right]$	[11]
12	$\left[-y,\, -x,\, \frac{1}{2}-z\right]$	[12]
13	$[-x,\, -y,\, -z]$	[13]
14	$\left[-x+y,\, -x,\, \frac{1}{2}-z\right]$	[14]
15	$[y,\, -x+y,\, -z]$	[15]
16	$\left[x,\, y,\, \frac{1}{2}-z\right]$	[16]
17	$[x-y,\, x,\, -z]$	[17]
18	$\left[-y,\, x-y,\, \frac{1}{2}-z\right]$	[18]
19	$[-x+y,\, y,\, z]$	[19]
20	$[-y,\, -x,\, z]$	[20]
21	$[x,\, x-y,\, z]$	[21]
22	$\left[-x,\, -x+y,\, z+\frac{1}{2}\right]$	[22]
23	$\left[x-y,\, -y,\, z+\frac{1}{2}\right]$	[23]
24	$\left[y,\, x,\, z+\frac{1}{2}\right]$	[24]
25	$\left[x,\, y,\, z+\frac{1}{2}\right]$	[25]
26	$[x-y,\, x,\, z]$	[26]
27	$\left[-y,\, x-y,\, z+\frac{1}{2}\right]$	[27]
28	$[-x,\, -y,\, z]$	[28]
29	$\left[-x+y,\, -x,\, z+\frac{1}{2}\right]$	[29]
30	$[y,\, -x+y,\, z]$	[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	$[x,\, x-y,\, -z]$	[34]
35	$[-x+y,\, y,\, -z]$	[35]
36	$[-y,\, -x,\, -z]$	[36]
37	$\left[-x,\, -y,\, \frac{1}{2}-z\right]$	[37]
38	$[-x+y,\, -x,\, -z]$	[38]
39	$\left[y,\, -x+y,\, \frac{1}{2}-z\right]$	[39]
40	$[x,\, y,\, -z]$	[40]
41	$\left[x-y,\, x,\, \frac{1}{2}-z\right]$	[41]
42	$[-y,\, x-y,\, -z]$	[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	$[-x,\, -x+y,\, z]$	[46]
47	$[x-y,\, -y,\, z]$	[47]
48	$[y,\, x,\, z]$	[48]