MSG No. 132.456 P_c4_2/mcm [Type IV, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4'/mm'm

No.	position	mapping
1	$[0, 0, 0]$	[1,6,7,8,9,14,15,16,18,19,20,21,26,27,28,29]
2	$\left[0, 0, \frac{1}{2}\right]$	[2,3,4,5,10,11,12,13,17,22,23,24,25,30,31,32]

Table 2: Wyckoff site: 2b, site symmetry: 4'/m'm'm

No.	position	mapping
1	$\left[0, 0, \frac{1}{4}\right]$	[1,4,5,6,10,11,15,16,18,19,23,24,25,28,29,30]
2	$\left[0, 0, \frac{3}{4}\right]$	[2,3,7,8,9,12,13,14,17,20,21,22,26,27,31,32]

Table 3: Wyckoff site: 2c, site symmetry: 4'/mm'm

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[1,6,7,8,9,14,15,16,18,19,20,21,26,27,28,29]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[2,3,4,5,10,11,12,13,17,22,23,24,25,30,31,32]

Table 4: Wyckoff site: 2d, site symmetry: 4'/m'm'm

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[1,4,5,6,10,11,15,16,18,19,23,24,25,28,29,30]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[2,3,7,8,9,12,13,14,17,20,21,22,26,27,31,32]

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

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[1,4,5,6,25,28,29,30]
2	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[2,3,7,8,26,27,31,32]
3	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[9,12,13,14,17,20,21,22]
4	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[10,11,15,16,18,19,23,24]

Table 6: Wyckoff site: `4f`, site symmetry: `mm'm'.`

No.	position	mapping
1	$\left[0,\ \frac{1}{2},\ 0\right]$	`[1,6,9,14,20,21,28,29]`
2	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[2,3,10,11,23,24,31,32]`
3	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[4,5,12,13,17,22,25,30]`
4	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[7,8,15,16,18,19,26,27]`

Table 7: Wyckoff site: `4g`, site symmetry: `4'm'm`

No.	position	mapping
1	$[0,\ 0,\ z]$	`[1,6,15,16,18,19,28,29]`
2	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[2,3,12,13,17,22,31,32]`
3	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	`[4,5,10,11,23,24,25,30]`
4	$[0,\ 0,\ -z]$	`[7,8,9,14,20,21,26,27]`

Table 8: Wyckoff site: `4h`, site symmetry: `4'm'm`

No.	position	mapping
1	$\left[\frac{1}{2},\ \frac{1}{2},\ z\right]$	`[1,6,15,16,18,19,28,29]`
2	$\left[\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[2,3,12,13,17,22,31,32]`
3	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[4,5,10,11,23,24,25,30]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ -z\right]$	`[7,8,9,14,20,21,26,27]`

Table 9: Wyckoff site: `8i`, site symmetry: `2m'm'.`

No.	position	mapping
1	$\left[0,\ \frac{1}{2},\ z\right]$	`[1,6,28,29]`
2	$\left[\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[2,3,31,32]`
3	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[4,5,25,30]`
4	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[7,8,26,27]`
5	$\left[0,\ \frac{1}{2},\ -z\right]$	`[9,14,20,21]`
6	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	`[10,11,23,24]`
7	$\left[0,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[12,13,17,22]`
8	$\left[\frac{1}{2},\ 0,\ z\right]$	`[15,16,18,19]`

Table 10: Wyckoff site: `8j`, site symmetry: `m.2m`

No.	position	mapping
1	$[x,\ x,\ 0]$	`[1,7,14,16]`
2	$[-x,\ x,\ \frac{1}{2}]$	`[2,5,11,12]`
3	$[x,\ -x,\ \frac{1}{2}]$	`[3,4,10,13]`
4	$[-x,\ -x,\ 0]$	`[6,8,9,15]`
5	$[x,\ x,\ \frac{1}{2}]$	`[17,23,30,32]`
6	$[-x,\ x,\ 0]$	`[18,21,27,28]`
7	$[x,\ -x,\ 0]$	`[19,20,26,29]`
8	$[-x,\ -x,\ \frac{1}{2}]$	`[22,24,25,31]`

Table 11: Wyckoff site: `8k`, site symmetry: `m'.2'm`

No.	position	mapping
1	$[x,\ x,\ \frac{1}{4}]$	`[1,16,23,30]`
2	$[-x,\ x,\ \frac{3}{4}]$	`[2,12,21,27]`
3	$[x,\ -x,\ \frac{3}{4}]$	`[3,13,20,26]`
4	$[x,\ -x,\ \frac{1}{4}]$	`[4,10,19,29]`
5	$[-x,\ x,\ \frac{1}{4}]$	`[5,11,18,28]`
6	$[-x,\ -x,\ \frac{1}{4}]$	`[6,15,24,25]`
7	$[x,\ x,\ \frac{3}{4}]$	`[7,14,17,32]`
8	$[-x,\ -x,\ \frac{3}{4}]$	`[8,9,22,31]`

Table 12: Wyckoff site: `8l`, site symmetry: `m2'm'.`

No.	position	mapping
1	$[x,\ 0,\ 0]$	`[1,14,20,29]`
2	$[0,\ x,\ \frac{1}{2}]$	`[2,11,23,32]`
3	$[0,\ -x,\ \frac{1}{2}]$	`[3,10,24,31]`
4	$[x,\ 0,\ \frac{1}{2}]$	`[4,13,17,30]`
5	$[-x,\ 0,\ \frac{1}{2}]$	`[5,12,22,25]`
6	$[-x,\ 0,\ 0]$	`[6,9,21,28]`
7	$[0,\ x,\ 0]$	`[7,16,18,27]`
8	$[0,\ -x,\ 0]$	`[8,15,19,26]`

Table 13: Wyckoff site: `8m`, site symmetry: `m'2m'.`

No.	position	mapping
1	$[x,\ 0,\ \frac{1}{4}]$	`[1,4,29,30]`
2	$[0,\ x,\ \frac{3}{4}]$	`[2,7,27,32]`
3	$[0,\ -x,\ \frac{3}{4}]$	`[3,8,26,31]`

continued ...

Table 13

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

Table 14: Wyckoff site: `8n`, site symmetry: `m2'm'`.

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ 0\right]$	`[1,14,20,29]`
2	$\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$	`[2,11,23,32]`
3	$\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[3,10,24,31]`
4	$\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[4,13,17,30]`
5	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[5,12,22,25]`
6	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[6,9,21,28]`
7	$\left[\frac{1}{2},\ x,\ 0\right]$	`[7,16,18,27]`
8	$\left[\frac{1}{2},\ -x,\ 0\right]$	`[8,15,19,26]`

Table 15: Wyckoff site: `8o`, site symmetry: `m'2m'`.

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ \frac{1}{4}\right]$	`[1,4,29,30]`
2	$\left[\frac{1}{2},\ x,\ \frac{3}{4}\right]$	`[2,7,27,32]`
3	$\left[\frac{1}{2},\ -x,\ \frac{3}{4}\right]$	`[3,8,26,31]`
4	$\left[-x,\ \frac{1}{2},\ \frac{1}{4}\right]$	`[5,6,25,28]`
5	$\left[-x,\ \frac{1}{2},\ \frac{3}{4}\right]$	`[9,12,21,22]`
6	$\left[\frac{1}{2},\ -x,\ \frac{1}{4}\right]$	`[10,15,19,24]`
7	$\left[\frac{1}{2},\ x,\ \frac{1}{4}\right]$	`[11,16,18,23]`
8	$\left[x,\ \frac{1}{2},\ \frac{3}{4}\right]$	`[13,14,17,20]`

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

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,14]`
2	$\left[-y,\ x,\ \frac{1}{2}\right]$	`[2,11]`
3	$\left[y,\ -x,\ \frac{1}{2}\right]$	`[3,10]`
4	$\left[x,\ -y,\ \frac{1}{2}\right]$	`[4,13]`
5	$\left[-x,\ y,\ \frac{1}{2}\right]$	`[5,12]`
6	$[-x,\ -y,\ 0]$	`[6,9]`

continued ...

Table 16

No.	position	mapping
7	$[y,\ x,\ 0]$	`[7,16]`
8	$[-y,\ -x,\ 0]$	`[8,15]`
9	$\left[x,\ y,\ \frac{1}{2}\right]$	`[17,30]`
10	$[-y,\ x,\ 0]$	`[18,27]`
11	$[y,\ -x,\ 0]$	`[19,26]`
12	$[x,\ -y,\ 0]$	`[20,29]`
13	$[-x,\ y,\ 0]$	`[21,28]`
14	$\left[-x,\ -y,\ \frac{1}{2}\right]$	`[22,25]`
15	$\left[y,\ x,\ \frac{1}{2}\right]$	`[23,32]`
16	$\left[-y,\ -x,\ \frac{1}{2}\right]$	`[24,31]`

Table 17: Wyckoff site: `16q`, site symmetry: `m'..`

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{4}\right]$	`[1,30]`
2	$\left[-y,\ x,\ \frac{3}{4}\right]$	`[2,27]`
3	$\left[y,\ -x,\ \frac{3}{4}\right]$	`[3,26]`
4	$\left[x,\ -y,\ \frac{1}{4}\right]$	`[4,29]`
5	$\left[-x,\ y,\ \frac{1}{4}\right]$	`[5,28]`
6	$\left[-x,\ -y,\ \frac{1}{4}\right]$	`[6,25]`
7	$\left[y,\ x,\ \frac{3}{4}\right]$	`[7,32]`
8	$\left[-y,\ -x,\ \frac{3}{4}\right]$	`[8,31]`
9	$\left[-x,\ -y,\ \frac{3}{4}\right]$	`[9,22]`
10	$\left[y,\ -x,\ \frac{1}{4}\right]$	`[10,19]`
11	$\left[-y,\ x,\ \frac{1}{4}\right]$	`[11,18]`
12	$\left[-x,\ y,\ \frac{3}{4}\right]$	`[12,21]`
13	$\left[x,\ -y,\ \frac{3}{4}\right]$	`[13,20]`
14	$\left[x,\ y,\ \frac{3}{4}\right]$	`[14,17]`
15	$\left[-y,\ -x,\ \frac{1}{4}\right]$	`[15,24]`
16	$\left[y,\ x,\ \frac{1}{4}\right]$	`[16,23]`

Table 18: Wyckoff site: `16r`, site symmetry: `..m`

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,16]`
2	$\left[-x,\ x,\ z+\frac{1}{2}\right]$	`[2,12]`
3	$\left[x,\ -x,\ z+\frac{1}{2}\right]$	`[3,13]`
4	$\left[x,\ -x,\ \frac{1}{2}-z\right]$	`[4,10]`
5	$\left[-x,\ x,\ \frac{1}{2}-z\right]$	`[5,11]`
6	$[-x,\ -x,\ z]$	`[6,15]`
7	$[x,\ x,\ -z]$	`[7,14]`
8	$[-x,\ -x,\ -z]$	`[8,9]`

continued ...

Table 18

No.	position	mapping
9	$\left[x,\, x,\, z+\frac{1}{2}\right]$	[17,32]
10	$[-x,\, x,\, z]$	[18,28]
11	$[x,\, -x,\, z]$	[19,29]
12	$[x,\, -x,\, -z]$	[20,26]
13	$[-x,\, x,\, -z]$	[21,27]
14	$\left[-x,\, -x,\, z+\frac{1}{2}\right]$	[22,31]
15	$\left[x,\, x,\, \frac{1}{2}-z\right]$	[23,30]
16	$\left[-x,\, -x,\, \frac{1}{2}-z\right]$	[24,25]

Table 19: Wyckoff site: 16s, site symmetry: .m'.

No.	position	mapping
1	$[x,\, 0,\, z]$	[1,29]
2	$\left[0,\, x,\, z+\frac{1}{2}\right]$	[2,32]
3	$\left[0,\, -x,\, z+\frac{1}{2}\right]$	[3,31]
4	$\left[x,\, 0,\, \frac{1}{2}-z\right]$	[4,30]
5	$\left[-x,\, 0,\, \frac{1}{2}-z\right]$	[5,25]
6	$[-x,\, 0,\, z]$	[6,28]
7	$[0,\, x,\, -z]$	[7,27]
8	$[0,\, -x,\, -z]$	[8,26]
9	$[-x,\, 0,\, -z]$	[9,21]
10	$\left[0,\, -x,\, \frac{1}{2}-z\right]$	[10,24]
11	$\left[0,\, x,\, \frac{1}{2}-z\right]$	[11,23]
12	$\left[-x,\, 0,\, z+\frac{1}{2}\right]$	[12,22]
13	$\left[x,\, 0,\, z+\frac{1}{2}\right]$	[13,17]
14	$[x,\, 0,\, -z]$	[14,20]
15	$[0,\, -x,\, z]$	[15,19]
16	$[0,\, x,\, z]$	[16,18]

Table 20: Wyckoff site: 16t, site symmetry: .m'.

No.	position	mapping
1	$\left[x,\, \frac{1}{2},\, z\right]$	[1,29]
2	$\left[\frac{1}{2},\, x,\, z+\frac{1}{2}\right]$	[2,32]
3	$\left[\frac{1}{2},\, -x,\, z+\frac{1}{2}\right]$	[3,31]
4	$\left[x,\, \frac{1}{2},\, \frac{1}{2}-z\right]$	[4,30]
5	$\left[-x,\, \frac{1}{2},\, \frac{1}{2}-z\right]$	[5,25]
6	$\left[-x,\, \frac{1}{2},\, z\right]$	[6,28]
7	$\left[\frac{1}{2},\, x,\, -z\right]$	[7,27]
8	$\left[\frac{1}{2},\, -x,\, -z\right]$	[8,26]
9	$\left[-x,\, \frac{1}{2},\, -z\right]$	[9,21]
10	$\left[\frac{1}{2},\, -x,\, \frac{1}{2}-z\right]$	[10,24]

continued ...

Table 20

No.	position	mapping
11	$\left[\frac{1}{2}, x, \frac{1}{2}-z\right]$	[11,23]
12	$\left[-x, \frac{1}{2}, z+\frac{1}{2}\right]$	[12,22]
13	$\left[x, \frac{1}{2}, z+\frac{1}{2}\right]$	[13,17]
14	$\left[x, \frac{1}{2}, -z\right]$	[14,20]
15	$\left[\frac{1}{2}, -x, z\right]$	[15,19]
16	$\left[\frac{1}{2}, x, z\right]$	[16,18]

Table 21: Wyckoff site: 32u, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$\left[-y, x, z+\frac{1}{2}\right]$	[2]
3	$\left[y, -x, z+\frac{1}{2}\right]$	[3]
4	$\left[x, -y, \frac{1}{2}-z\right]$	[4]
5	$\left[-x, y, \frac{1}{2}-z\right]$	[5]
6	$[-x, -y, z]$	[6]
7	$[y, x, -z]$	[7]
8	$[-y, -x, -z]$	[8]
9	$[-x, -y, -z]$	[9]
10	$\left[y, -x, \frac{1}{2}-z\right]$	[10]
11	$\left[-y, x, \frac{1}{2}-z\right]$	[11]
12	$\left[-x, y, z+\frac{1}{2}\right]$	[12]
13	$\left[x, -y, z+\frac{1}{2}\right]$	[13]
14	$[x, y, -z]$	[14]
15	$[-y, -x, z]$	[15]
16	$[y, x, z]$	[16]
17	$\left[x, y, z+\frac{1}{2}\right]$	[17]
18	$[-y, x, z]$	[18]
19	$[y, -x, z]$	[19]
20	$[x, -y, -z]$	[20]
21	$[-x, y, -z]$	[21]
22	$\left[-x, -y, z+\frac{1}{2}\right]$	[22]
23	$\left[y, x, \frac{1}{2}-z\right]$	[23]
24	$\left[-y, -x, \frac{1}{2}-z\right]$	[24]
25	$\left[-x, -y, \frac{1}{2}-z\right]$	[25]
26	$[y, -x, -z]$	[26]
27	$[-y, x, -z]$	[27]
28	$[-x, y, z]$	[28]
29	$[x, -y, z]$	[29]
30	$\left[x, y, \frac{1}{2}-z\right]$	[30]
31	$\left[-y, -x, z+\frac{1}{2}\right]$	[31]
32	$\left[y, x, z+\frac{1}{2}\right]$	[32]