MSG No. 124.360 P_c4/mcc [Type IV, tetragonal]

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

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

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

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

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

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

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

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

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	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[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	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[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	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[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	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[7,8,15,16,18,19,26,27]`

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

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

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

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

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	$\left[\frac{1}{2},\ 0,\ z\right]$	`[2,3,31,32]`
3	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[4,5,25,30]`
4	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	`[7,8,26,27]`
5	$\left[0,\ \frac{1}{2},\ -z\right]$	`[9,14,20,21]`
6	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[10,11,23,24]`
7	$\left[0,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[12,13,17,22]`
8	$\left[\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[15,16,18,19]`

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ 0,\ \frac{1}{4}\right]$	`[1,4,29,30]`
2	$\left[0,\ x,\ \frac{1}{4}\right]$	`[2,7,27,32]`
3	$\left[0,\ -x,\ \frac{1}{4}\right]$	`[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	$\left[0,\ -x,\ \frac{3}{4}\right]$	`[10,15,19,24]`
7	$\left[0,\ x,\ \frac{3}{4}\right]$	`[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	$\left[\frac{1}{2},\ x,\ 0\right]$	`[2,11,23,32]`
3	$\left[\frac{1}{2},\ -x,\ 0\right]$	`[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	$\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$	`[7,16,18,27]`
8	$\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[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	$\left[\frac{1}{2},\ x,\ \frac{1}{4}\right]$	`[2,7,27,32]`
3	$\left[\frac{1}{2},\ -x,\ \frac{1}{4}\right]$	`[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	$\left[\frac{1}{2},\ -x,\ \frac{3}{4}\right]$	`[10,15,19,24]`
7	$\left[\frac{1}{2},\ x,\ \frac{3}{4}\right]$	`[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	$[-y,\ x,\ 0]$	`[2,11]`
3	$[y,\ -x,\ 0]$	`[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	$\left[y,\, x,\, \frac{1}{2}\right]$	[7,16]
8	$\left[-y,\, -x,\, \frac{1}{2}\right]$	[8,15]
9	$\left[x,\, y,\, \frac{1}{2}\right]$	[17,30]
10	$\left[-y,\, x,\, \frac{1}{2}\right]$	[18,27]
11	$\left[y,\, -x,\, \frac{1}{2}\right]$	[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	$[y,\, x,\, 0]$	[23,32]
16	$[-y,\, -x,\, 0]$	[24,31]

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

No.	position	mapping
1	$\left[x,\, y,\, \frac{1}{4}\right]$	[1,30]
2	$\left[-y,\, x,\, \frac{1}{4}\right]$	[2,27]
3	$\left[y,\, -x,\, \frac{1}{4}\right]$	[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	$\left[y,\, x,\, \frac{1}{4}\right]$	[7,32]
8	$\left[-y,\, -x,\, \frac{1}{4}\right]$	[8,31]
9	$\left[-x,\, -y,\, \frac{3}{4}\right]$	[9,22]
10	$\left[y,\, -x,\, \frac{3}{4}\right]$	[10,19]
11	$\left[-y,\, x,\, \frac{3}{4}\right]$	[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	$\left[-y,\, -x,\, \frac{3}{4}\right]$	[15,24]
16	$\left[y,\, x,\, \frac{3}{4}\right]$	[16,23]

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

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

continued ...

Table 18

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

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

No.	position	mapping
1	$[x,\ 0,\ z]$	[1,29]
2	$[0,\ x,\ z]$	[2,32]
3	$[0,\ -x,\ z]$	[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	$\left[0,\ x,\ \frac{1}{2}-z\right]$	[7,27]
8	$\left[0,\ -x,\ \frac{1}{2}-z\right]$	[8,26]
9	$[-x,\ 0,\ -z]$	[9,21]
10	$[0,\ -x,\ -z]$	[10,24]
11	$[0,\ x,\ -z]$	[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	$\left[0,\ -x,\ z+\frac{1}{2}\right]$	[15,19]
16	$\left[0,\ x,\ z+\frac{1}{2}\right]$	[16,18]

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

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ z\right]$	[1,29]
2	$\left[\frac{1}{2},\ x,\ z\right]$	[2,32]
3	$\left[\frac{1}{2},\ -x,\ z\right]$	[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	$\left[\frac{1}{2},\ x,\ \frac{1}{2}-z\right]$	[7,27]
8	$\left[\frac{1}{2},\ -x,\ \frac{1}{2}-z\right]$	[8,26]
9	$\left[-x,\ \frac{1}{2},\ -z\right]$	[9,21]
10	$\left[\frac{1}{2},\ -x,\ -z\right]$	[10,24]

continued ...

Table 20

No.	position	mapping
11	$\left[\frac{1}{2}, x, -z\right]$	[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	$\left[\frac{1}{2}, -x, z+\frac{1}{2}\right]$	[15,19]
16	$\left[\frac{1}{2}, x, z+\frac{1}{2}\right]$	[16,18]

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

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