MSG No. 123.349 P_C4/mmm [Type IV, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `4/mmm`

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

Table 2: Wyckoff site: `2b`, site symmetry: `4/mmm`

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

Table 3: Wyckoff site: `2c`, site symmetry: `4'/mmm'`

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

Table 4: Wyckoff site: `2d`, site symmetry: `4'/mmm'`

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

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

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

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

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

Table 7: Wyckoff site: `4g`, site symmetry: `4mm`

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

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

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

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

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

Table 10: Wyckoff site: `8j`, site symmetry: `mm2.`

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

Table 11: Wyckoff site: `8k`, site symmetry: `mm2.`

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

Table 12: Wyckoff site: `8l`, site symmetry: `m.2m`

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

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

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

continued ...

Table 13

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

Table 14: Wyckoff site: `8n`, site symmetry: `m.2'm'`

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

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

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

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	$[x,\, -y,\, 0]$	`[4,13]`
5	$[-x,\, y,\, 0]$	`[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	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ 0\right]$	[17,30]
10	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ 0\right]$	[18,27]
11	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ 0\right]$	[19,26]
12	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	[20,29]
13	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0\right]$	[21,28]
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ 0\right]$	[22,25]
15	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$	[23,32]
16	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ 0\right]$	[24,31]

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

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

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

No.	position	mapping
1	$[0,\ y,\ z]$	[1,12]
2	$[-y,\ 0,\ z]$	[2,15]
3	$[y,\ 0,\ z]$	[3,16]
4	$[0,\ -y,\ -z]$	[4,9]
5	$[0,\ y,\ -z]$	[5,14]
6	$[0,\ -y,\ z]$	[6,13]
7	$[y,\ 0,\ -z]$	[7,10]
8	$[-y,\ 0,\ -z]$	[8,11]

continued ...

Table 18

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

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

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

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

No.	position	mapping
1	$\left[x, x+\frac{1}{2}, z\right]$	[1,32]
2	$\left[\frac{1}{2}-x, x, z\right]$	[2,28]
3	$\left[x+\frac{1}{2}, -x, z\right]$	[3,29]
4	$\left[x, \frac{1}{2}-x, -z\right]$	[4,26]
5	$\left[-x, x+\frac{1}{2}, -z\right]$	[5,27]
6	$\left[-x, \frac{1}{2}-x, z\right]$	[6,31]
7	$\left[x+\frac{1}{2}, x, -z\right]$	[7,30]
8	$\left[\frac{1}{2}-x, -x, -z\right]$	[8,25]
9	$\left[-x, \frac{1}{2}-x, -z\right]$	[9,24]
10	$\left[x+\frac{1}{2}, -x, -z\right]$	[10,20]

continued ...

Table 20

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

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	$[x,\, -y,\, -z]$	[4]
5	$[-x,\, y,\, -z]$	[5]
6	$[-x,\, -y,\, z]$	[6]
7	$[y,\, x,\, -z]$	[7]
8	$[-y,\, -x,\, -z]$	[8]
9	$[-x,\, -y,\, -z]$	[9]
10	$[y,\, -x,\, -z]$	[10]
11	$[-y,\, x,\, -z]$	[11]
12	$[-x,\, y,\, z]$	[12]
13	$[x,\, -y,\, z]$	[13]
14	$[x,\, y,\, -z]$	[14]
15	$[-y,\, -x,\, z]$	[15]
16	$[y,\, x,\, z]$	[16]
17	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z\right]$	[17]
18	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, z\right]$	[18]
19	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, z\right]$	[19]
20	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[20]
21	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	[21]
22	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z\right]$	[22]
23	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, -z\right]$	[23]
24	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, -z\right]$	[24]
25	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, -z\right]$	[25]
26	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, -z\right]$	[26]
27	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, -z\right]$	[27]
28	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$	[28]
29	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	[29]
30	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[30]
31	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, z\right]$	[31]
32	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z\right]$	[32]