MSG No. 135.492 P_c4_2/mbc [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `4'/m..`

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `m'.m'm'`

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

Table 4: Wyckoff site: `4d`, site symmetry: `m.m'm'`

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

Table 5: Wyckoff site: `8e`, site symmetry: `4'..`

No.	position	mapping
1	$[0,\ 0,\ z]$	`[1,6,18,19]`
2	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[2,3,17,22]`

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 2.m'm'

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

Table 7: Wyckoff site: 8g, site symmetry: m.2'm'

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

Table 8: Wyckoff site: 8h, site symmetry: m'.2m'

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ \frac{1}{4}\right]$	[1,7,30,32]
2	$\left[\frac{1}{2}-x,\ x,\ \frac{3}{4}\right]$	[2,5,27,28]
3	$\left[x+\frac{1}{2},\ -x,\ \frac{3}{4}\right]$	[3,4,26,29]
4	$\left[-x,\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	[6,8,25,31]
5	$\left[-x,\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	[9,15,22,24]

continued ...

Table 8

No.	position	mapping
6	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{4}\right]$	[10,13,19,20]
7	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{4}\right]$	[11,12,18,21]
8	$\left[x,\ x+\frac{1}{2},\ \frac{3}{4}\right]$	[14,16,17,23]

Table 9: Wyckoff site: 16i, 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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	[4,13]
5	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0\right]$	[5,12]
6	$[-x,\ -y,\ 0]$	[6,9]
7	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[7,16]
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[20,29]
13	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[21,28]
14	$\left[-x,\ -y,\ \frac{1}{2}\right]$	[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 10: Wyckoff site: 16j, 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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[4,29]
5	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[5,28]
6	$\left[-x,\ -y,\ \frac{1}{4}\right]$	[6,25]
7	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{4}\right]$	[7,32]
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	[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	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[12,21]
13	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[13,20]
14	$\left[x,\ y,\ \frac{3}{4}\right]$	[14,17]
15	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	[15,24]

continued ...

Table 10

No.	position	mapping
16	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{3}{4}\right]$	[16,23]

Table 11: Wyckoff site: 16k, site symmetry: ..m'

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

Table 12: Wyckoff site: 32l, 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	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[4]
5	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	[5]
6	$[-x,\, -y,\, z]$	[6]
7	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[7]
8	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[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	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$	[12]
13	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	[13]
14	$[x,\, y,\, -z]$	[14]
15	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[15]
16	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[16]
17	$\left[x,\, y,\, z+\frac{1}{2}\right]$	[17]

continued ...

Table 12

No.	position	mapping
18	$[-y,\, x,\, z]$	[18]
19	$[y,\, -x,\, z]$	[19]
20	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[20]
21	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[21]
22	$\left[-x,\, -y,\, z+\frac{1}{2}\right]$	[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	$\left[-x,\, -y,\, \frac{1}{2}-z\right]$	[25]
26	$[y,\, -x,\, -z]$	[26]
27	$[-y,\, x,\, -z]$	[27]
28	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[28]
29	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[29]
30	$\left[x,\, y,\, \frac{1}{2}-z\right]$	[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]