MSG No. 136.506 P_I4_2/mnm [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	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[2,3,4,5,10,11,12,13,17,22,23,24,25,30,31,32]

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

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

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

No.	position	mapping
1	$\left[0, \frac{1}{2}, 0\right]$	[1,6,9,14,20,21,28,29]
2	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[2,3,10,11,23,24,31,32]
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[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 4: Wyckoff site: 4d, site symmetry: -4m'2'

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

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

No.	position	mapping
1	$[0, 0, z]$	[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	$[0, 0, -z]$	[7,8,9,14,20,21,26,27]

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

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `m2'm'.`

No.	position	mapping
1	$[x, 0, 0]$	`[1,14,20,29]`
2	$\left[\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}\right]$	`[2,11,23,32]`
3	$\left[\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}\right]$	`[3,10,24,31]`

continued ...

Table 9

No.	position	mapping
4	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[4,13,17,30]`
5	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[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 10: Wyckoff site: `8j`, site symmetry: `m2'm'`.

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ 0\right]$	`[1,14,20,29]`
2	$\left[0,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[2,11,23,32]`
3	$\left[0,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[3,10,24,31]`
4	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[4,13,17,30]`
5	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}\right]$	`[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 11: Wyckoff site: `16k`, site symmetry: `..2'`

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

Table 12: Wyckoff site: `16l`, site symmetry: `m..`

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,14]`
2	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[2,11]`
3	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[3,10]`
4	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[4,13]`
5	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[5,12]`
6	$[-x,\ -y,\ 0]$	`[6,9]`
7	$[y,\ x,\ 0]$	`[7,16]`
8	$[-y,\ -x,\ 0]$	`[8,15]`
9	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[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	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[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 13: Wyckoff site: `16m`, site symmetry: `..m`

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,16]`
2	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[2,12]`
3	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	`[3,13]`
4	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	`[4,10]`
5	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[5,11]`
6	$[-x,\ -x,\ z]$	`[6,15]`
7	$[x,\ x,\ -z]$	`[7,14]`
8	$[-x,\ -x,\ -z]$	`[8,9]`
9	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[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	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	`[22,31]`
15	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[23,30]`
16	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	`[24,25]`

Table 14: Wyckoff site: `16n`, site symmetry: `.m'.`

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,28]`

continued ...

Table 14

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

Table 15: Wyckoff site: 32o, site symmetry: 1

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

continued ...

Table 15

No.	position	mapping
26	$[y,\, -x,\, -z]$	[26]
27	$[-y,\, x,\, -z]$	[27]
28	$[-x,\, y,\, z]$	[28]
29	$[x,\, -y,\, z]$	[29]
30	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[31]
32	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[32]