MSG No. 87.80 I_c4/m [Type IV, tetragonal]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `8e`, site symmetry: `2'/m..`

No.	position	mapping
1	$\left[\frac{3}{4},\ \frac{1}{4},\ 0\right]$	`[1,8,28,29]`
2	$\left[\frac{3}{4},\ \frac{3}{4},\ 0\right]$	`[2,7,27,30]`

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: 8g, site symmetry: 4..

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

Table 8: Wyckoff site: 8h, site symmetry: 4'..

No.	position	mapping
1	$\left[0, \frac{1}{2}, z\right]$	[1,4,26,27]
2	$\left[\frac{1}{2}, 0, z\right]$	[2,3,25,28]
3	$\left[0, \frac{1}{2}, -z\right]$	[5,8,30,31]
4	$\left[\frac{1}{2}, 0, -z\right]$	[6,7,29,32]
5	$\left[\frac{1}{2}, 0, z+\frac{1}{2}\right]$	[9,12,18,19]

continued ...

Table 8

No.	position	mapping
6	$\left[0,\, \frac{1}{2},\, z+\frac{1}{2}\right]$	`[10,11,17,20]`
7	$\left[\frac{1}{2},\, 0,\, \frac{1}{2}-z\right]$	`[13,16,22,23]`
8	$\left[0,\, \frac{1}{2},\, \frac{1}{2}-z\right]$	`[14,15,21,24]`

Table 9: Wyckoff site: `16i`, site symmetry: `2'..`

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

Table 10: Wyckoff site: `16j`, site symmetry: `m..`

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

continued ...

Table 10

No.	position	mapping
16	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ 0\right]$	[28,29]

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

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

Table 12: Wyckoff site: 32l, 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	$[y,\ -x,\ -z]$	[6]
7	$[-y,\ x,\ -z]$	[7]
8	$[x,\ y,\ -z]$	[8]
9	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[9]
10	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[10]
11	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[11]
12	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[12]
13	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[13]
14	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[14]
15	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[15]
16	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[16]
17	$\left[x,\ y,\ z+\frac{1}{2}\right]$	[17]

continued ...

Table 12

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