MSG No. 140.543 $I4/m'cm$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `42'2'`

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,11,23,29]`
2	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[2,10,22,30]`

continued ...

Table 5

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

Table 6: Wyckoff site: `8f`, site symmetry: `4..`

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

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

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

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

No.	position	mapping
1	$\left[x, x + \frac{1}{2}, 0\right]$	`[1,16,24,27]`
2	$\left[\frac{1}{2} - x, x, 0\right]$	`[2,15,21,26]`
3	$\left[x + \frac{1}{2}, -x, 0\right]$	`[3,14,22,25]`
4	$\left[-x, \frac{1}{2} - x, 0\right]$	`[4,13,23,28]`
5	$\left[-x, x + \frac{1}{2}, \frac{1}{2}\right]$	`[5,10,18,31]`

continued ...

Table 8

No.	position	mapping
6	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[6,9,19,30]
7	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}\right]$	[7,12,20,29]
8	$\left[x+\frac{1}{2},\ x,\ \frac{1}{2}\right]$	[8,11,17,32]

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

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

Table 10: Wyckoff site: 16j, site symmetry: .2'.

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

continued ...

Table 10

No.	position	mapping
16	$\left[\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{4}\right]$	`[24,31]`

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

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

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

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

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