MSG No. 140.548 $I4'/m'cm'$ [Type III, tetragonal]

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

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: -42'm'

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1,3,29,31]
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[2,4,30,32]

continued ...

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Table 5

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

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

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

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

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

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

No.	position	mapping
1	$\left[x, x + \frac{1}{2}, 0\right]$	[1,14,19,32]
2	$\left[-x, \frac{1}{2} - x, 0\right]$	[2,13,20,31]
3	$\left[x + \frac{1}{2}, x, \frac{1}{2}\right]$	[3,16,17,30]
4	$\left[\frac{1}{2} - x, -x, \frac{1}{2}\right]$	[4,15,18,29]
5	$\left[x + \frac{1}{2}, -x, 0\right]$	[5,10,24,27]

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2} - x,\, x,\, 0\right]$	[6,9,23,28]
7	$\left[-x,\, x + \frac{1}{2},\, \frac{1}{2}\right]$	[7,12,22,25]
8	$\left[x,\, \frac{1}{2} - x,\, \frac{1}{2}\right]$	[8,11,21,26]

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

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

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

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

continued ...

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Table 10

No.	position	mapping
16	$\left[x+\frac{1}{2},\,\frac{1}{2},\,\frac{1}{4}\right]$	[24,30]

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

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

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

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

Table 13: Wyckoff site: 32m, site symmetry: 1

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