MSG No. 134.482 P_I4_2/nnm [Type IV, tetragonal]

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: -4'm'2

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

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

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

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

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `m'2m'`.

No.	position	mapping
1	$\left[x, \frac{1}{4}, \frac{3}{4}\right]$	[1,4,29,30]
2	$\left[\frac{1}{4}, x, \frac{1}{4}\right]$	[2,7,27,32]
3	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}\right]$	[3,8,26,31]

continued ...

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: m'2m'.

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

Table 11: Wyckoff site: 16k, site symmetry: ..2

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

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

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

Table 13: Wyckoff site: `16m`, site symmetry: `..m`

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

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

No.	position	mapping
1	$\left[\frac{3}{4}, y, z\right]$	[1,28]

continued ...

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Table 14

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

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

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

continued ...

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Table 15

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

$\left[\frac{1}{2}-x,\ y,\ z\right]$

$\left[x,\ \frac{1}{2} \quad 6 \quad \right]$

$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$

$\left[y,\ x,\ z+\frac{1}{2}\right]$