MSG No. 129.421 P_C4/nmm [Type IV, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: 4'/m'mm'

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

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

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

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

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

Table 6: Wyckoff site: `4f`, site symmetry: `m'.mm'`

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

Table 7: Wyckoff site: `4g`, site symmetry: `4mm`

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

Table 8: Wyckoff site: `4h`, site symmetry: `4'mm'`

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

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

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

Table 10: Wyckoff site: 8j, site symmetry: m'm2'.

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

Table 11: Wyckoff site: 8k, site symmetry: m'm2'.

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

Table 12: Wyckoff site: 8l, site symmetry: m'.2'm

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

Table 13: Wyckoff site: 8m, site symmetry: m'.2'm

No.	position	mapping
1	$\left[x, x, \frac{1}{2}\right]$	[1,16,23,30]
2	$\left[\frac{1}{2} - x, x, \frac{1}{2}\right]$	[2,12,21,27]
3	$\left[x, \frac{1}{2} - x, \frac{1}{2}\right]$	[3,13,20,26]

continued ...

Table 13

No.	position	mapping
4	$\left[x + \frac{1}{2}, -x, \frac{1}{2}\right]$	[4,10,19,29]
5	$\left[-x, x + \frac{1}{2}, \frac{1}{2}\right]$	[5,11,18,28]
6	$\left[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}\right]$	[6,15,24,25]
7	$\left[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}\right]$	[7,14,17,32]
8	$\left[-x, -x, \frac{1}{2}\right]$	[8,9,22,31]

Table 14: Wyckoff site: 8n, site symmetry: m'.2m'

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

Table 15: Wyckoff site: 8o, site symmetry: m'.2m'

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

Table 16: Wyckoff site: 16p, site symmetry: m'..

No.	position	mapping
1	$[x, y, 0]$	[1,30]
2	$\left[\frac{1}{2} - y, x, 0\right]$	[2,27]
3	$\left[y, \frac{1}{2} - x, 0\right]$	[3,26]
4	$\left[x + \frac{1}{2}, -y, 0\right]$	[4,29]
5	$\left[-x, y + \frac{1}{2}, 0\right]$	[5,28]
6	$\left[\frac{1}{2} - x, \frac{1}{2} - y, 0\right]$	[6,25]

continued ...

Table 16

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

Table 17: Wyckoff site: 16q, site symmetry: m'..

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

Table 18: Wyckoff site: 16r, site symmetry: .m.

No.	position	mapping
1	$\left[\frac{3}{4},\, y,\, z\right]$	[1,12]
2	$\left[\frac{1}{2}-y,\, \frac{3}{4},\, z\right]$	[2,15]
3	$\left[y,\, \frac{3}{4},\, z\right]$	[3,16]
4	$\left[\frac{1}{4},\, -y,\, -z\right]$	[4,9]
5	$\left[\frac{1}{4},\, y+\frac{1}{2},\, -z\right]$	[5,14]
6	$\left[\frac{3}{4},\, \frac{1}{2}-y,\, z\right]$	[6,13]
7	$\left[y+\frac{1}{2},\, \frac{1}{4},\, -z\right]$	[7,10]
8	$\left[-y,\, \frac{1}{4},\, -z\right]$	[8,11]

continued ...

Table 18

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

Table 19: Wyckoff site: `16s`, site symmetry: `..m`

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

Table 20: Wyckoff site: `16t`, site symmetry: `..m'`

No.	position	mapping
1	$\left[x, x + \frac{1}{2}, z\right]$	[1,32]
2	$[-x, x, z]$	[2,28]
3	$\left[x + \frac{1}{2}, \frac{1}{2} - x, z\right]$	[3,29]
4	$\left[x + \frac{1}{2}, \frac{1}{2} - x, -z\right]$	[4,26]
5	$[-x, x, -z]$	[5,27]
6	$\left[\frac{1}{2} - x, -x, z\right]$	[6,31]
7	$\left[x, x + \frac{1}{2}, -z\right]$	[7,30]
8	$\left[\frac{1}{2} - x, -x, -z\right]$	[8,25]
9	$\left[-x, \frac{1}{2} - x, -z\right]$	[9,24]
10	$[x, -x, -z]$	[10,20]

continued ...

Table 20

No.	position	mapping
11	$\left[\frac{1}{2} - x,\ x + \frac{1}{2},\ -z\right]$	[11,21]
12	$\left[\frac{1}{2} - x,\ x + \frac{1}{2},\ z\right]$	[12,18]
13	$[x,\ -x,\ z]$	[13,19]
14	$\left[x + \frac{1}{2},\ x,\ -z\right]$	[14,23]
15	$\left[-x,\ \frac{1}{2} - x,\ z\right]$	[15,22]
16	$\left[x + \frac{1}{2},\ x,\ z\right]$	[16,17]

Table 21: Wyckoff site: 32u, site symmetry: 1

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