MSG No. 130.434 P_I4/ncc [Type IV, tetragonal]

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

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

Table 2: Wyckoff site: `4b`, site symmetry: `-42'm'`

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[1,9,23,31]`
2	$\left[0, \frac{1}{2}, 0\right]$	`[2,10,21,29]`

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$\left[x, x + \frac{1}{2}, \frac{3}{4}\right]$	[1,7,30,32]
2	$\left[-x, x, \frac{3}{4}\right]$	[2,5,27,28]
3	$\left[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}\right]$	[3,4,26,29]
4	$\left[\frac{1}{2} - x, -x, \frac{3}{4}\right]$	[6,8,25,31]
5	$\left[-x, \frac{1}{2} - x, \frac{1}{4}\right]$	[9,15,22,24]

continued ...

Table 8

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

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

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

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

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

continued ...

Table 10

No.	position	mapping
16	$\left[\frac{1}{4}, x, \frac{1}{2}\right]$	[16,27]

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

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

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

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