MSG No. 125.374 P_I4/nbm [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `422`

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0, 0, 0]$	`[1,7,9,15]`
2	$\left[\frac{1}{2}, 0, 0\right]$	`[2,5,10,13]`

continued ...

Table 5

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

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

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

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

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

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	$\left[-x,\ x,\ \frac{3}{4}\right]$	`[2,12,21,27]`
3	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	`[3,13,20,26]`
4	$\left[x,\ -x,\ \frac{1}{4}\right]$	`[4,10,19,29]`
5	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{4}\right]$	`[5,11,18,28]`

continued ...

Table 8

No.	position	mapping
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: 16i, site symmetry: ..2

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

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

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

continued ...

Table 10

No.	position	mapping
16	$\left[x,\ \frac{3}{4},\ \frac{1}{2}\right]$	[29,30]

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	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[4,29]
5	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{4}\right]$	[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	$\left[y+\frac{1}{2},\ -x,\ \frac{1}{4}\right]$	[10,19]
11	$\left[-y,\ x+\frac{1}{2},\ \frac{1}{4}\right]$	[11,18]
12	$\left[-x,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[12,21]
13	$\left[x+\frac{1}{2},\ -y,\ \frac{3}{4}\right]$	[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 12: Wyckoff site: 16l, site symmetry: ..m

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ z\right]$	[1,16]
2	$\left[-x,\ x,\ z\right]$	[2,12]
3	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ z\right]$	[3,13]
4	$\left[x,\ -x,\ -z\right]$	[4,10]
5	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ -z\right]$	[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	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[18,28]
11	$\left[x,\ -x,\ z+\frac{1}{2}\right]$	[19,29]
12	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[20,26]
13	$\left[-x,\ x,\ \frac{1}{2}-z\right]$	[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 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	$\left[x,\, \frac{1}{2}-y,\, -z\right]$	[4]
5	$\left[\frac{1}{2}-x,\, y,\, -z\right]$	[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	$\left[y+\frac{1}{2},\, -x,\, -z\right]$	[10]
11	$\left[-y,\, x+\frac{1}{2},\, -z\right]$	[11]
12	$\left[-x,\, y+\frac{1}{2},\, z\right]$	[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	$[-y,\, -x,\, z]$	[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	$\left[-y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[18]
19	$\left[y+\frac{1}{2},\, -x,\, z+\frac{1}{2}\right]$	[19]
20	$\left[x+\frac{1}{2},\, -y,\, \frac{1}{2}-z\right]$	[20]
21	$\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[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]
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	$\left[\frac{1}{2}-x,\, y,\, z+\frac{1}{2}\right]$	[28]
29	$\left[x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[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]