MSG No. 125.372 P_c4/nbm [Type IV, tetragonal]

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

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	`[1,2,3,4,5,6,7,8]`
2	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	`[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: `42'2'`

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

Table 3: Wyckoff site: `4c`, 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	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	`[17,20,21,22,26,27,31,32]`
4	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	`[18,19,23,24,25,28,29,30]`

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

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

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	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[17,23,25,31]`
6	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[18,21,26,29]`
7	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[19,20,27,28]`
8	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[22,24,30,32]`

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

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

Table 7: Wyckoff site: `8g`, site symmetry: `4..`

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ z\right]$	`[1,2,3,6]`
2	$\left[\frac{1}{4},\ \frac{1}{4},\ -z\right]$	`[4,5,7,8]`
3	$\left[\frac{3}{4},\ \frac{3}{4},\ -z\right]$	`[9,10,11,14]`
4	$\left[\frac{3}{4},\ \frac{3}{4},\ z\right]$	`[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 8: Wyckoff site: `8h`, 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	$\left[\frac{3}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[17,22,31,32]`

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[18,19,28,29]
7	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[20,21,26,27]
8	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[23,24,25,30]

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	$\left[x,\ x,\ \frac{1}{2}\right]$	[17,23]
10	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{2}\right]$	[18,21]
11	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[19,20]
12	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[22,24]
13	$\left[-x,\ -x,\ \frac{1}{2}\right]$	[25,31]
14	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	[26,29]
15	$\left[-x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[27,28]
16	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[30,32]

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

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

continued ...

Table 10

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

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

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

Table 12: Wyckoff site: 16l, site symmetry: .2'.

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

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

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

Table 14: Wyckoff site: 32n, 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	$\left[x,\ y,\ z+\frac{1}{2}\right]$	[17]
18	$\left[\frac{1}{2}-y,\ x,\ z+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	[21]
22	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[22]
23	$\left[y,\ x,\ \frac{1}{2}-z\right]$	[23]

continued ...

Table 14

No.	position	mapping
24	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[24]
25	$\left[-x,\ -y,\ \frac{1}{2}-z\right]$	[25]
26	$\left[y+\frac{1}{2},\ -x,\ \frac{1}{2}-z\right]$	[26]
27	$\left[-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[27]
28	$\left[-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[28]
29	$\left[x+\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[29]
30	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[30]
31	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	[31]
32	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[32]