MSG No. 134.481 P_C4_2/nnm [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `m'.mm`

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

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

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `-42m`

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

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[17,20,21,22,26,27,31,32]`
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[18,19,23,24,25,28,29,30]`

Table 6: Wyckoff site: `4f`, site symmetry: `-4'2m'`

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

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	$\left[\frac{1}{4}, \frac{3}{4}, z+\frac{1}{2}\right]$	`[2,3,12,13]`
3	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}-z\right]$	`[4,5,10,11]`
4	$\left[\frac{1}{4}, \frac{3}{4}, -z\right]$	`[7,8,9,14]`
5	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	`[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	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	`[23,24,25,30]`

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

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

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

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

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

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

Table 11: Wyckoff site: `8k`, site symmetry: `m'.2m'`

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

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

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ 0\right]$	`[1,16,23,30]`
2	$\left[-x,\ x,\ \frac{1}{2}\right]$	`[2,12,21,27]`
3	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[3,13,20,26]`

continued ...

Table 12

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

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

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

Table 14: Wyckoff site: 16n, site symmetry: .2.

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

Table 15: Wyckoff site: `16o`, site symmetry: `..m`

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

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

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

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

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{2}\right]$	`[1,30]`

continued ...

Table 17

No.	position	mapping
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	$\left[\frac{1}{2}-x,\, y,\, 0\right]$	[5,28]
6	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[6,25]
7	$\left[y,\, x,\, \frac{1}{2}\right]$	[7,32]
8	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	[8,31]
9	$\left[-x,\, -y,\, \frac{1}{2}\right]$	[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	$\left[-x,\, y+\frac{1}{2},\, 0\right]$	[12,21]
13	$\left[x+\frac{1}{2},\, -y,\, 0\right]$	[13,20]
14	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[14,17]
15	$\left[-y,\, -x,\, \frac{1}{2}\right]$	[15,24]
16	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}\right]$	[16,23]

Table 18: Wyckoff site: 32r, 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	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z\right]$	[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	$[-x,\, -y,\, z]$	[22]
23	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, -z\right]$	[23]
24	$[-y,\, -x,\, -z]$	[24]
25	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, -z\right]$	[25]

continued ...

Table 18

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