MSG No. 125.373 P_C4/nbm [Type IV, tetragonal]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, 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	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[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	$\left[0, 0, \frac{1}{2}\right]$	[6,8,14,16,17,23,25,31]

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[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	$[0, 0, 0]$	`[6,8,14,16,17,23,25,31]`

Table 7: Wyckoff site: `4g`, site symmetry: `4'm'm`

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

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

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

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	$\left[0, \frac{1}{2}, z\right]$	`[2,13,19,28]`
3	$\left[\frac{1}{2}, 0, z\right]$	`[3,12,18,29]`
4	$\left[\frac{1}{2}, 0, -z\right]$	`[4,11,21,26]`
5	$\left[0, \frac{1}{2}, -z\right]$	`[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'm'2.`

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

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

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

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	$[-x,\ x,\ 0]$	`[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	$\left[\frac{1}{2}-x,\ -x,\ 0\right]$	`[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'.2'm`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[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 13

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	$\left[\frac{1}{2}-x,\, -x,\, \frac{1}{2}\right]$	`[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 14: Wyckoff site: `8n`, site symmetry: `m'.2m'`

No.	position	mapping
1	$[x,\, x,\, 0]$	`[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	$\left[\frac{1}{2}-x,\, \frac{1}{2}-x,\, 0\right]$	`[6,8,25,31]`
5	$[-x,\, -x,\, 0]$	`[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	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, 0\right]$	`[14,16,17,23]`

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

No.	position	mapping
1	$\left[x,\, x,\, \frac{1}{2}\right]$	`[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	$\left[\frac{1}{2}-x,\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	`[6,8,25,31]`
5	$\left[-x,\, -x,\, \frac{1}{2}\right]$	`[9,15,22,24]`
6	$\left[x+\frac{1}{2},\, -x,\, \frac{1}{2}\right]$	`[10,13,19,20]`
7	$\left[-x,\, x+\frac{1}{2},\, \frac{1}{2}\right]$	`[11,12,18,21]`
8	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}\right]$	`[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	$\left[\frac{1}{2}-x,\, y,\, 0\right]$	`[5,28]`
6	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, 0\right]$	`[6,25]`

continued ...

Table 16

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

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

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

continued ...

Table 18

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

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

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

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

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

continued ...

Table 20

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