MSG No. 126.385 P_C4/nnc [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `4'22'`

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `422`

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[1,9,22,30]`
2	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[2,10,19,27]`

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 2.22

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

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

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

Table 8: Wyckoff site: 8h, site symmetry: 4..

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{3}{4}, z\right]$	[1,2,3,6]
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z\right]$	[4,5,7,8]
3	$\left[\frac{1}{4}, \frac{1}{4}, -z\right]$	[9,10,11,14]
4	$\left[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}\right]$	[12,13,15,16]
5	$\left[\frac{1}{4}, \frac{1}{4}, z\right]$	[17,18,19,22]

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}-z\right]$	[20,21,23,24]
7	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	[25,26,27,30]
8	$\left[\frac{3}{4}, \frac{3}{4}, z+\frac{1}{2}\right]$	[28,29,31,32]

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

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

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

No.	position	mapping
1	$\left[\frac{3}{4}, y, \frac{3}{4}\right]$	[1,5]
2	$\left[\frac{1}{2}-y, \frac{3}{4}, \frac{3}{4}\right]$	[2,8]
3	$\left[y, \frac{3}{4}, \frac{3}{4}\right]$	[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	$\left[y+\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[10,16]
7	$\left[-y, \frac{1}{4}, \frac{1}{4}\right]$	[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	$\left[-y, \frac{1}{4}, \frac{3}{4}\right]$	[18,24]
11	$\left[y+\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[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	$\left[y, \frac{3}{4}, \frac{1}{4}\right]$	[26,32]
15	$\left[\frac{1}{2}-y, \frac{3}{4}, \frac{1}{4}\right]$	[27,31]

continued ...

Table 10

No.	position	mapping
16	$\left[\frac{3}{4}, y, \frac{1}{4}\right]$	[28,30]

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

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

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

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

Table 13: Wyckoff site: 16m, 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	$\left[x,\, \frac{1}{2}-y,\, 0\right]$	[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	$[y,\, x,\, 0]$	[7,32]
8	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, 0\right]$	[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	$\left[-x,\, y+\frac{1}{2},\, 0\right]$	[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	$[-y,\, -x,\, 0]$	[15,24]
16	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, 0\right]$	[16,23]

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	$\left[x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[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	$\left[y,\, x,\, \frac{1}{2}-z\right]$	[7]
8	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[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	$\left[-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[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	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[15]
16	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[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	$\left[x+\frac{1}{2},\, -y,\, \frac{1}{2}-z\right]$	[20]
21	$\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[21]
22	$[-x,\, -y,\, z]$	[22]
23	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[23]

continued ...

Table 14

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