

MSG No. 128.408 P_c4/mnc [Type IV, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 4/m..

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

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

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: 4..

No.	position	mapping
1	[0, 0, z]	[1,2,3,6]
2	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[4,5,7,8]

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: 8g, site symmetry: m.2'm'

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, \frac{1}{4}]$	[1,7,30,32]
2	$[\frac{1}{2} - x, x, \frac{1}{4}]$	[2,5,27,28]
3	$[x + \frac{1}{2}, -x, \frac{1}{4}]$	[3,4,26,29]
4	$[-x, \frac{1}{2} - x, \frac{1}{4}]$	[6,8,25,31]
5	$[-x, \frac{1}{2} - x, \frac{3}{4}]$	[9,15,22,24]

continued ...

Table 8

No.	position	mapping
6	$[x + \frac{1}{2}, -x, \frac{3}{4}]$	[10,13,19,20]
7	$[\frac{1}{2} - x, x, \frac{3}{4}]$	[11,12,18,21]
8	$[x, x + \frac{1}{2}, \frac{3}{4}]$	[14,16,17,23]

Table 9: Wyckoff site: 16i, site symmetry: $m\ldots$

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

Table 10: Wyckoff site: 16j, site symmetry: $m'\ldots$

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

continued ...

Table 10

No.	position	mapping
16	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	[16,23]

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

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

Table 12: Wyckoff site: 321, site symmetry: 1

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

continued ...

Table 12

No.	position	mapping
18	$[-y, x, z + \frac{1}{2}]$	[18]
19	$[y, -x, z + \frac{1}{2}]$	[19]
20	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[20]
21	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[21]
22	$[-x, -y, z + \frac{1}{2}]$	[22]
23	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[23]
24	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[24]
25	$[-x, -y, \frac{1}{2} - z]$	[25]
26	$[y, -x, \frac{1}{2} - z]$	[26]
27	$[-y, x, \frac{1}{2} - z]$	[27]
28	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[28]
29	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[29]
30	$[x, y, \frac{1}{2} - z]$	[30]
31	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[31]
32	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[32]