

MSG No. 136.504 P_c4_2/mnm [Type IV, tetragonal]

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: $m.mm$

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

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

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1,6,18,19]
2	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[2,3,17,22]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 2.m̄m

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

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

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

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

No.	position	mapping
1	$[x, x, \frac{1}{4}]$	[1,16,23,30]
2	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}]$	[2,12,21,27]
3	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[3,13,20,26]
4	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$	[4,10,19,29]
5	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}]$	[5,11,18,28]

continued ...

Table 8

No.	position	mapping
6	$[-x, -x, \frac{1}{4}]$	[6,15,24,25]
7	$[x, x, \frac{3}{4}]$	[7,14,17,32]
8	$[-x, -x, \frac{3}{4}]$	[8,9,22,31]

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

No.	position	mapping
1	$[x, y, 0]$	[1,14]
2	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}]$	[2,11]
3	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[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	$[y, x, 0]$	[7,16]
8	$[-y, -x, 0]$	[8,15]
9	$[x, y, \frac{1}{2}]$	[17,30]
10	$[\frac{1}{2} - y, x + \frac{1}{2}, 0]$	[18,27]
11	$[y + \frac{1}{2}, \frac{1}{2} - x, 0]$	[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	$[y, x, \frac{1}{2}]$	[23,32]
16	$[-y, -x, \frac{1}{2}]$	[24,31]

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

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	[1,30]
2	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{3}{4}]$	[2,27]
3	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[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	$[y, x, \frac{3}{4}]$	[7,32]
8	$[-y, -x, \frac{3}{4}]$	[8,31]
9	$[-x, -y, \frac{3}{4}]$	[9,22]
10	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$	[10,19]
11	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{4}]$	[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	$[-y, -x, \frac{1}{4}]$	[15,24]

continued ...

Table 10

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

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

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

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

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

continued ...

Table 12

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