

MSG No. 140.541 *I4/mcm* [Type I, tetragonal]

Table 1: Wyckoff site: **4a**, site symmetry: 422

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

Table 2: Wyckoff site: **4b**, site symmetry: -42m

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

Table 3: Wyckoff site: **4c**, site symmetry: 4/m..

No.	position	mapping
1	$[0, 0, 0]$	[1,2,3,6,9,10,11,14]
2	$[0, 0, \frac{1}{2}]$	[4,5,7,8,12,13,15,16]
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[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 4: Wyckoff site: **4d**, site symmetry: 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	$[0, \frac{1}{2}, \frac{1}{2}]$	[4,5,12,13,18,19,26,27]
4	$[\frac{1}{2}, 0, \frac{1}{2}]$	[7,8,15,16,17,22,25,30]

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1,7,25,31]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[2,5,26,29]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 4..

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

Table 7: Wyckoff site: 8g, site symmetry: 2.mm

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	[1,6,31,32]
2	$[\frac{1}{2}, 0, z]$	[2,3,28,29]
3	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[4,5,26,27]
4	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[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	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[12,13,18,19]
8	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[15,16,17,22]

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

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	$[-x, x + \frac{1}{2}, \frac{1}{2}]$	[5,12,18,27]

continued ...

Table 8

No.	position	mapping
6	$[-x, \frac{1}{2} - x, 0]$	[6,9,24,31]
7	$[x + \frac{1}{2}, x, \frac{1}{2}]$	[7,16,17,30]
8	$[\frac{1}{2} - x, -x, \frac{1}{2}]$	[8,15,22,25]

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

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

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

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

continued ...

Table 10

No.	position	mapping
16	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[29,30]

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

No.	position	mapping
1	$[x, y, 0]$	[1,14]
2	$[-y, x, 0]$	[2,11]
3	$[y, -x, 0]$	[3,10]
4	$[x, -y, \frac{1}{2}]$	[4,13]
5	$[-x, y, \frac{1}{2}]$	[5,12]
6	$[-x, -y, 0]$	[6,9]
7	$[y, x, \frac{1}{2}]$	[7,16]
8	$[-y, -x, \frac{1}{2}]$	[8,15]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[17,30]
10	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}]$	[18,27]
11	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2}]$	[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 12: Wyckoff site: 16l, 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	$[-x, x + \frac{1}{2}, \frac{1}{2} - z]$	[5,27]
6	$[-x, \frac{1}{2} - x, z]$	[6,31]
7	$[x + \frac{1}{2}, x, \frac{1}{2} - z]$	[7,30]
8	$[\frac{1}{2} - x, -x, \frac{1}{2} - z]$	[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	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[12,18]
13	$[x, \frac{1}{2} - x, z + \frac{1}{2}]$	[13,19]
14	$[x, x + \frac{1}{2}, -z]$	[14,23]
15	$[\frac{1}{2} - x, -x, z + \frac{1}{2}]$	[15,22]
16	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	[16,17]

Table 13: Wyckoff site: 32m, site symmetry: 1

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