

MSG No. 127.398 P_I4/mbm [Type IV, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 42'2'

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

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

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

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	$[\frac{1}{2}, \frac{1}{2}, 0]$	[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	$[0, 0, \frac{1}{2}]$	[20,21,23,24,28,29,31,32]

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1,15,23,25]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[2,13,21,26]

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, 0]$	[1,7,14,16]
2	$[\frac{1}{2} - x, x, 0]$	[2,5,11,12]
3	$[x + \frac{1}{2}, -x, 0]$	[3,4,10,13]
4	$[-x, \frac{1}{2} - x, 0]$	[6,8,9,15]
5	$[x + \frac{1}{2}, x, \frac{1}{2}]$	[17,23,30,32]

continued ...

Table 8

No.	position	mapping
6	$[-x, x + \frac{1}{2}, \frac{1}{2}]$	[18, 21, 27, 28]
7	$[x, \frac{1}{2} - x, \frac{1}{2}]$	[19, 20, 26, 29]
8	$[\frac{1}{2} - x, -x, \frac{1}{2}]$	[22, 24, 25, 31]

Table 9: Wyckoff site: 16i, site symmetry: $\dots 2'$

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

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

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

continued ...

Table 10

No.	position	mapping
16	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[16,27]

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	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	[4,13]
5	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	[5,12]
6	$[-x, -y, 0]$	[6,9]
7	$[y + \frac{1}{2}, x + \frac{1}{2}, 0]$	[7,16]
8	$[\frac{1}{2} - y, \frac{1}{2} - x, 0]$	[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	$[x, -y, \frac{1}{2}]$	[20,29]
13	$[-x, y, \frac{1}{2}]$	[21,28]
14	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2}]$	[22,25]
15	$[y, x, \frac{1}{2}]$	[23,32]
16	$[-y, -x, \frac{1}{2}]$	[24,31]

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

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

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	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[4]
5	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[5]
6	$[-x, -y, z]$	[6]
7	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[7]
8	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[8]
9	$[-x, -y, -z]$	[9]
10	$[y, -x, -z]$	[10]
11	$[-y, x, -z]$	[11]
12	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[12]
13	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[13]
14	$[x, y, -z]$	[14]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[15]
16	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[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	$[x, -y, \frac{1}{2} - z]$	[20]
21	$[-x, y, \frac{1}{2} - z]$	[21]
22	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[22]
23	$[y, x, \frac{1}{2} - z]$	[23]
24	$[-y, -x, \frac{1}{2} - z]$	[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	$[-x, y, z + \frac{1}{2}]$	[28]
29	$[x, -y, z + \frac{1}{2}]$	[29]
30	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[30]
31	$[-y, -x, z + \frac{1}{2}]$	[31]
32	$[y, x, z + \frac{1}{2}]$	[32]