

MSG No. 119.320 $I_c\bar{4}m2$ [Type IV, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: $-4m2$

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

Table 2: Wyckoff site: 4b, site symmetry: $-4m2$

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

Table 3: Wyckoff site: 4c, site symmetry: $-4'm2'$

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

Table 4: Wyckoff site: 4d, site symmetry: $-4'm2'$

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

Table 5: Wyckoff site: 8e, site symmetry: 2.22

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 3, 26, 28]$
2	$[\frac{3}{4}, \frac{3}{4}, 0]$	$[2, 4, 25, 27]$

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	[1, 2, 7, 8]
2	$[\frac{1}{2}, 0, -z]$	[3, 4, 5, 6]
3	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[9, 10, 15, 16]
4	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[11, 12, 13, 14]
5	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[17, 18, 23, 24]

continued ...

Table 8

No.	position	mapping
6	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[19, 20, 21, 22]
7	$[\frac{1}{2}, 0, z]$	[25, 26, 31, 32]
8	$[0, \frac{1}{2}, -z]$	[27, 28, 29, 30]

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

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

Table 10: Wyckoff site: 16j, site symmetry: $\dots 2$

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

continued ...

Table 10

No.	position	mapping
16	$[x, \frac{1}{2} - x, \frac{3}{4}]$	[24, 29]

Table 11: Wyckoff site: 16k, site symmetry: $\dots 2'$

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

Table 12: Wyckoff site: 16l, site symmetry: $\dots 2'$

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

Table 13: Wyckoff site: 16m, site symmetry: $2' . .$

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

Table 14: Wyckoff site: 16n, site symmetry: $.m.$

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

Table 15: Wyckoff site: 32o, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]

continued ...

Table 15

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