

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: ...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: ...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: . . 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: . . 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]