MSG No. 120.326 $I_c\bar{4}c2$ [Type IV, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: -4'm'2

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: -4m'2'

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

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

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

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

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[1,11,20,26]
2	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[2,12,19,25]

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[1,2,23,24]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z\right]$	[3,4,21,22]
3	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	[5,6,19,20]
4	$\left[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}\right]$	[7,8,17,18]
5	$\left[0, 0, z + \frac{1}{2}\right]$	[9,10,31,32]

continued ...

Table 8

No.	position	mapping
6	$[0, 0, -z]$	[11,12,29,30]
7	$\left[0, 0, \frac{1}{2} - z\right]$	[13,14,27,28]
8	$[0, 0, z]$	[15,16,25,26]

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

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

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

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

continued ...

Table 10

No.	position	mapping
16	$\left[\frac{1}{2}-x,\, x+\frac{1}{2},\, \frac{3}{4}\right]$	[30,31]

Table 11: Wyckoff site: `16k`, site symmetry: `..2'`

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

Table 12: Wyckoff site: `16l`, site symmetry: `..2'`

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

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

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

Table 14: Wyckoff site: `16n`, site symmetry: .m'.

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

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	$[y, x, \frac{1}{2} - z]$	[3]
4	$[-y, -x, \frac{1}{2} - z]$	[4]
5	$[y, -x, -z]$	[5]
6	$[-y, x, -z]$	[6]
7	$[-x, y, z + \frac{1}{2}]$	[7]
8	$[x, -y, z + \frac{1}{2}]$	[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	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[11]
12	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[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	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[15]
16	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[16]
17	$[x, y, z + \frac{1}{2}]$	[17]
18	$[-x, -y, z + \frac{1}{2}]$	[18]
19	$[y, x, -z]$	[19]
20	$[-y, -x, -z]$	[20]
21	$[y, -x, \frac{1}{2} - z]$	[21]
22	$[-y, x, \frac{1}{2} - z]$	[22]
23	$[-x, y, z]$	[23]
24	$[x, -y, z]$	[24]
25	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[25]
26	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[26]
27	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[27]
28	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[28]
29	$[y + \frac{1}{2}, \frac{1}{2} - x, -z]$	[29]
30	$[\frac{1}{2} - y, x + \frac{1}{2}, -z]$	[30]
31	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[31]
32	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[32]