MSG No. 98.162 I_c4_122 [Type IV, tetragonal]

Table 1: Wyckoff site: 8a, site symmetry: 2.22

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

Table 2: Wyckoff site: 8b, site symmetry: 2.22

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

Table 3: Wyckoff site: 8c, site symmetry: 2.2'2'

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

Table 4: Wyckoff site: `8d`, site symmetry: `2.22`

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

Table 5: Wyckoff site: `8e`, site symmetry: `2'22'`.

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

Table 6: Wyckoff site: `8f`, site symmetry: `2'22'`.

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

Table 7: Wyckoff site: `16g`, site symmetry: `2'..`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, z\right]$	[1,30]
2	$\left[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{4}\right]$	[2,27]
3	$\left[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{4}\right]$	[3,26]

continued ...

Table 7

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

Table 8: Wyckoff site: `16h`, site symmetry: `2'..`

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, 0, z\right]$	[1,6]
2	$\left[0, 0, z + \frac{1}{4}\right]$	[2,3]
3	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4} - z\right]$	[4,5]
4	$\left[0, \frac{1}{2}, -z\right]$	[7,8]
5	$\left[0, \frac{1}{2}, z + \frac{1}{2}\right]$	[9,14]

continued ...

Table 9

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

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

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

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

No.	position	mapping
1	$\left[x, \frac{1}{2} - x, \frac{1}{4}\right]$	[1,16]
2	$\left[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}\right]$	[2,12]
3	$\left[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}\right]$	[3,13]
4	$[x, x, 0]$	[4,10]
5	$[-x, -x, 0]$	[5,11]
6	$\left[-x, x + \frac{1}{2}, \frac{1}{4}\right]$	[6,15]
7	$\left[\frac{1}{2} - x, x, \frac{3}{4}\right]$	[7,14]

continued ...

Table 11

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

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

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

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

No.	position	mapping
1	$\left[x, \frac{1}{2}-x, 0\right]$	[1,32]
2	$\left[x+\frac{1}{2}, x+\frac{1}{2}, \frac{1}{4}\right]$	[2,28]
3	$\left[\frac{1}{2}-x, \frac{1}{2}-x, \frac{1}{4}\right]$	[3,29]
4	$\left[x, x, \frac{1}{4}\right]$	[4,26]
5	$\left[-x, -x, \frac{1}{4}\right]$	[5,27]
6	$\left[-x, x+\frac{1}{2}, 0\right]$	[6,31]
7	$\left[\frac{1}{2}-x, x, 0\right]$	[7,30]
8	$\left[x+\frac{1}{2}, -x, 0\right]$	[8,25]
9	$\left[x+\frac{1}{2}, -x, \frac{1}{2}\right]$	[9,24]

continued ...

Table 13

No.	position	mapping
10	$\left[x, x, \frac{3}{4}\right]$	[10,20]
11	$\left[-x, -x, \frac{3}{4}\right]$	[11,21]
12	$\left[x+\frac{1}{2}, x+\frac{1}{2}, \frac{3}{4}\right]$	[12,18]
13	$\left[\frac{1}{2}-x, \frac{1}{2}-x, \frac{3}{4}\right]$	[13,19]
14	$\left[\frac{1}{2}-x, x, \frac{1}{2}\right]$	[14,23]
15	$\left[-x, x+\frac{1}{2}, \frac{1}{2}\right]$	[15,22]
16	$\left[x, \frac{1}{2}-x, \frac{1}{2}\right]$	[16,17]

Table 14: Wyckoff site: `16n`, site symmetry: `.2.`.

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

Table 15: Wyckoff site: `16o`, site symmetry: `.2'`.

No.	position	mapping
1	$\left[x, \frac{1}{4}, \frac{3}{8}\right]$	[1,20]
2	$\left[\frac{3}{4}, x+\frac{1}{2}, \frac{5}{8}\right]$	[2,31]
3	$\left[\frac{1}{4}, \frac{1}{2}-x, \frac{5}{8}\right]$	[3,32]
4	$\left[x, \frac{1}{4}, \frac{7}{8}\right]$	[4,17]
5	$\left[-x, \frac{3}{4}, \frac{7}{8}\right]$	[5,22]
6	$\left[-x, \frac{3}{4}, \frac{3}{8}\right]$	[6,21]
7	$\left[\frac{1}{4}, x, \frac{5}{8}\right]$	[7,26]
8	$\left[\frac{3}{4}, -x, \frac{5}{8}\right]$	[8,27]
9	$\left[x+\frac{1}{2}, \frac{3}{4}, \frac{7}{8}\right]$	[9,28]
10	$\left[\frac{1}{4}, x, \frac{1}{8}\right]$	[10,23]
11	$\left[\frac{3}{4}, -x, \frac{1}{8}\right]$	[11,24]

Table 15

No.	position	mapping
12	$\left[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{8}\right]$	[12,25]
13	$\left[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{8}\right]$	[13,30]
14	$\left[\frac{1}{2} - x, \frac{1}{4}, \frac{7}{8}\right]$	[14,29]
15	$\left[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{8}\right]$	[15,18]
16	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{8}\right]$	[16,19]

Table 16: Wyckoff site: 32p, site symmetry: 1

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