MSG No. 140.549 $I4/m'c'm'$ [Type III, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 422

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

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

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

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	$\left[0, 0, \frac{1}{2}\right]$	[4,5,7,8,12,13,15,16]
3	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[17,18,19,22,25,26,27,30]
4	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[20,21,23,24,28,29,31,32]

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1,7,25,31]
2	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[2,5,26,29]

continued ...

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Table 5

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

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

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

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

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

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

No.	position	mapping
1	$\left[x, x + \frac{1}{2}, 0\right]$	[1,14,23,32]
2	$\left[\frac{1}{2} - x, x, 0\right]$	[2,11,21,28]
3	$\left[x + \frac{1}{2}, -x, 0\right]$	[3,10,20,29]
4	$\left[x, \frac{1}{2} - x, \frac{1}{2}\right]$	[4,13,19,26]
5	$\left[-x, x + \frac{1}{2}, \frac{1}{2}\right]$	[5,12,18,27]

continued ...

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Table 8

No.	position	mapping
6	$\left[-x,\ \frac{1}{2}-x,\ 0\right]$	[6,9,24,31]
7	$\left[x+\frac{1}{2},\ x,\ \frac{1}{2}\right]$	[7,16,17,30]
8	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}\right]$	[8,15,22,25]

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

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

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

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

Table 10

No.	position	mapping
16	$\left[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[29,30]

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	$\left[x, -y, \frac{1}{2}\right]$	[4,13]
5	$\left[-x, y, \frac{1}{2}\right]$	[5,12]
6	$[-x, -y, 0]$	[6,9]
7	$\left[y, x, \frac{1}{2}\right]$	[7,16]
8	$\left[-y, -x, \frac{1}{2}\right]$	[8,15]
9	$\left[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}\right]$	[17,30]
10	$\left[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}\right]$	[18,27]
11	$\left[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}\right]$	[19,26]
12	$\left[x + \frac{1}{2}, \frac{1}{2} - y, 0\right]$	[20,29]
13	$\left[\frac{1}{2} - x, y + \frac{1}{2}, 0\right]$	[21,28]
14	$\left[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2}\right]$	[22,25]
15	$\left[y + \frac{1}{2}, x + \frac{1}{2}, 0\right]$	[23,32]
16	$\left[\frac{1}{2} - y, \frac{1}{2} - x, 0\right]$	[24,31]

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

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

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	$\left[x,\, -y,\, \frac{1}{2}-z\right]$	[4]
5	$\left[-x,\, y,\, \frac{1}{2}-z\right]$	[5]
6	$[-x,\, -y,\, z]$	[6]
7	$\left[y,\, x,\, \frac{1}{2}-z\right]$	[7]
8	$\left[-y,\, -x,\, \frac{1}{2}-z\right]$	[8]
9	$[-x,\, -y,\, -z]$	[9]
10	$[y,\, -x,\, -z]$	[10]
11	$[-y,\, x,\, -z]$	[11]
12	$\left[-x,\, y,\, z+\frac{1}{2}\right]$	[12]
13	$\left[x,\, -y,\, z+\frac{1}{2}\right]$	[13]
14	$[x,\, y,\, -z]$	[14]
15	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[15]
16	$\left[y,\, x,\, z+\frac{1}{2}\right]$	[16]
17	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[17]
18	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[18]
19	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[19]
20	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[20]
21	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	[21]
22	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[22]
23	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, -z\right]$	[23]
24	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, -z\right]$	[24]
25	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[25]
26	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[26]
27	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[27]
28	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$	[28]
29	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	[29]
30	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, z\right]$	[31]
32	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z\right]$	[32]