MSG No. 139.531 $I4/mmm$ [Type I, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `4/mmm`

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

Table 2: Wyckoff site: `2b`, site symmetry: `4/mmm`

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

Table 3: Wyckoff site: `4c`, site symmetry: `mmm.`

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

Table 4: Wyckoff site: `4d`, site symmetry: `-4m2`

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

Table 5: Wyckoff site: `4e`, site symmetry: `4mm`

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

Table 6: Wyckoff site: `8f`, site symmetry: `..2/m`

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `m2m.`

No.	position	mapping
1	$[x, 0, 0]$	`[1,4,13,14]`
2	$[0, x, 0]$	`[2,7,11,16]`
3	$[0, -x, 0]$	`[3,8,10,15]`

continued ...

Table 9

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

Table 10: Wyckoff site: `8j`, site symmetry: `m2m.`

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

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

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

Table 12: Wyckoff site: `16l`, 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	$[x,\ -y,\ 0]$	`[4,13]`
5	$[-x,\ y,\ 0]$	`[5,12]`
6	$[-x,\ -y,\ 0]$	`[6,9]`
7	$[y,\ x,\ 0]$	`[7,16]`
8	$[-y,\ -x,\ 0]$	`[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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[20,29]`
13	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[21,28]`
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[22,25]`
15	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[23,32]`
16	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[24,31]`

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

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

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

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,12]`

continued ...

Table 14

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

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

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

continued ...

Table 15

No.	position	mapping
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	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[28]
29	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[29]
30	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[31]
32	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[32]