MSG No. 121.332 $I_c\bar{4}2m$ [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `-42m`

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `-42'm'`

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

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

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

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

No.	position	mapping
1	$[0, 0, z]$	`[1,4,7,8]`
2	$[0, 0, -z]$	`[2,3,5,6]`

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[0,\ y,\ 0]$	`[1,3]`
2	$[0,\ -y,\ 0]$	`[2,4]`
3	$[y,\ 0,\ 0]$	`[5,8]`
4	$[-y,\ 0,\ 0]$	`[6,7]`
5	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[9,11]`

continued ...

Table 8

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

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

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

Table 10: Wyckoff site: 16j, site symmetry: ..m

No.	position	mapping
1	$[x,\ x,\ z]$	[1,8]
2	$[x,\ -x,\ -z]$	[2,5]
3	$[-x,\ x,\ -z]$	[3,6]
4	$[-x,\ -x,\ z]$	[4,7]
5	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[9,16]
6	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[10,13]
7	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[11,14]

continued ...

Table 10

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

Table 11: Wyckoff site: 16k, site symmetry: ..m'

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

Table 12: Wyckoff site: 32l, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$[x,\ -y,\ -z]$	[2]
3	$[-x,\ y,\ -z]$	[3]
4	$[-x,\ -y,\ z]$	[4]
5	$[y,\ -x,\ -z]$	[5]
6	$[-y,\ x,\ -z]$	[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]

continued ...

Table 12

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