MSG No. 132.448 $P4_2/mcm1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: m.mm1'

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

Table 2: Wyckoff site: 2b, site symmetry: -42m1'

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

Table 3: Wyckoff site: 2c, site symmetry: m.mm1'

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

Table 4: Wyckoff site: 2d, site symmetry: -42m1'

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

Table 5: Wyckoff site: 4e, site symmetry: 222.1'

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

Table 6: Wyckoff site: `4f`, site symmetry: `2/m..1'`

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

Table 7: Wyckoff site: `4g`, site symmetry: `2.mm1'`

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

Table 8: Wyckoff site: `4h`, site symmetry: `2.mm1'`

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

Table 9: Wyckoff site: `4i`, site symmetry: `m.2m1'`

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

Table 10: Wyckoff site: `4j`, site symmetry: `m.2m1'`

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

Table 11: Wyckoff site: `8k`, site symmetry: `2..1'`

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

Table 12: Wyckoff site: `8l`, site symmetry: `.2.1'`

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

Table 13: Wyckoff site: `8m`, site symmetry: `.2.1'`

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

Table 14: Wyckoff site: `8n`, site symmetry: `m..1'`

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,14,17,30]`
2	$\left[-y,\ x,\ \frac{1}{2}\right]$	`[2,11,18,27]`
3	$\left[y,\ -x,\ \frac{1}{2}\right]$	`[3,10,19,26]`

continued ...

Table 14

No.	position	mapping
4	$\left[x, -y, \frac{1}{2}\right]$	[4,13,20,29]
5	$\left[-x, y, \frac{1}{2}\right]$	[5,12,21,28]
6	$[-x, -y, 0]$	[6,9,22,25]
7	$[y, x, 0]$	[7,16,23,32]
8	$[-y, -x, 0]$	[8,15,24,31]

Table 15: Wyckoff site: 8o, site symmetry: ..m1'

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

Table 16: Wyckoff site: 16p, site symmetry: 11'

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