MSG No. 123.340 $P4/mmm1'$ [Type II, tetragonal]

Table 1: Wyckoff site: `1a`, site symmetry: `4/mmm1'`

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

Table 2: Wyckoff site: `1b`, site symmetry: `4/mmm1'`

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

Table 3: Wyckoff site: `1c`, site symmetry: `4/mmm1'`

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

Table 4: Wyckoff site: `1d`, site symmetry: `4/mmm1'`

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

Table 5: Wyckoff site: `2e`, site symmetry: `mmm.1'`

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

Table 6: Wyckoff site: `2f`, site symmetry: `mmm.1'`

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

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

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

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

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

Table 9: Wyckoff site: 4i, site symmetry: 2mm.1'

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

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

No.	position	mapping
1	$[x,\ x,\ 0]$	[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	$[-x,\ -x,\ 0]$	[6,8,9,15,22,24,25,31]

Table 11: Wyckoff site: 4k, site symmetry: m.2m1'

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

Table 12: Wyckoff site: 4l, site symmetry: m2m.1'

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

Table 13: Wyckoff site: 4m, site symmetry: m2m.1'

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

Table 14: Wyckoff site: 4n, site symmetry: m2m.1'

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

Table 15: Wyckoff site: 4o, site symmetry: m2m.1'

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

Table 16: Wyckoff site: 8p, site symmetry: m..1'

No.	position	mapping
1	$[x,\ y,\ 0]$	[1,14,17,30]
2	$[-y,\ x,\ 0]$	[2,11,18,27]
3	$[y,\ -x,\ 0]$	[3,10,19,26]
4	$[x,\ -y,\ 0]$	[4,13,20,29]

continued ...

Table 16

No.	position	mapping
5	$[-x,\ y,\ 0]$	`[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 17: Wyckoff site: `8q`, site symmetry: `m..1'`

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{2}\right]$	`[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]`
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	$\left[-x,\ -y,\ \frac{1}{2}\right]$	`[6,9,22,25]`
7	$\left[y,\ x,\ \frac{1}{2}\right]$	`[7,16,23,32]`
8	$\left[-y,\ -x,\ \frac{1}{2}\right]$	`[8,15,24,31]`

Table 18: Wyckoff site: `8r`, site symmetry: `..m1'`

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,16,17,32]`
2	$[-x,\ x,\ z]$	`[2,12,18,28]`
3	$[x,\ -x,\ z]$	`[3,13,19,29]`
4	$[x,\ -x,\ -z]$	`[4,10,20,26]`
5	$[-x,\ x,\ -z]$	`[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 19: Wyckoff site: `8s`, site symmetry: `.m.1'`

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

continued ...

Table 19

No.	position	mapping
8	$[0, -x, -z]$	`[8,10,24,26]`

Table 20: Wyckoff site: `8t`, site symmetry: `.m.1'`

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

Table 21: Wyckoff site: `16u`, site symmetry: `11'`

No.	position	mapping
1	$[x, y, z]$	`[1,17]`
2	$[-y, x, z]$	`[2,18]`
3	$[y, -x, z]$	`[3,19]`
4	$[x, -y, -z]$	`[4,20]`
5	$[-x, y, -z]$	`[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	$[y, -x, -z]$	`[10,26]`
11	$[-y, x, -z]$	`[11,27]`
12	$[-x, y, z]$	`[12,28]`
13	$[x, -y, z]$	`[13,29]`
14	$[x, y, -z]$	`[14,30]`
15	$[-y, -x, z]$	`[15,31]`
16	$[y, x, z]$	`[16,32]`