MSG No. 200.15 $Pm\bar{3}1'$ [Type II, cubic]

Table 1: Wyckoff site: 1a, site symmetry: m-3.1'

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,
		25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]

Table 2: Wyckoff site: 1b, site symmetry: m-3.1'

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,
		25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]

Table 3: Wyckoff site: 3c, site symmetry: mmm..1'

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[1,2,3,4,13,14,15,16,25,26,27,28,37,38,39,40]
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[5,8,10,12,17,20,22,24,29,32,34,36,41,44,46,48]
3	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[6,7,9,11,18,19,21,23,30,31,33,35,42,43,45,47]

Table 4: Wyckoff site: 3d, site symmetry: mmm..1'

No.	position	mapping
1	$\left[\frac{1}{2}, 0, 0\right]$	[1,2,3,4,13,14,15,16,25,26,27,28,37,38,39,40]
2	$\left[0, \frac{1}{2}, 0\right]$	[5,8,10,12,17,20,22,24,29,32,34,36,41,44,46,48]
3	$\left[0, 0, \frac{1}{2}\right]$	[6,7,9,11,18,19,21,23,30,31,33,35,42,43,45,47]

Table 5: Wyckoff site: 6e, site symmetry: 2mm..1'

No.	position	mapping
1	$[x, 0, 0]$	[1,2,15,16,25,26,39,40]
2	$[-x, 0, 0]$	[3,4,13,14,27,28,37,38]
3	$[0, x, 0]$	[5,12,20,22,29,36,44,46]
4	$[0, 0, x]$	[6,9,19,23,30,33,43,47]
5	$[0, 0, -x]$	[7,11,18,21,31,35,42,45]
6	$[0, -x, 0]$	[8,10,17,24,32,34,41,48]

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

No.	position	mapping
1	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[1,2,15,16,25,26,39,40]`
2	$\left[-x,\ 0,\ \frac{1}{2}\right]$	`[3,4,13,14,27,28,37,38]`
3	$\left[\frac{1}{2},\ x,\ 0\right]$	`[5,12,20,22,29,36,44,46]`
4	$\left[0,\ \frac{1}{2},\ x\right]$	`[6,9,19,23,30,33,43,47]`
5	$\left[0,\ \frac{1}{2},\ -x\right]$	`[7,11,18,21,31,35,42,45]`
6	$\left[\frac{1}{2},\ -x,\ 0\right]$	`[8,10,17,24,32,34,41,48]`

Table 7: Wyckoff site: `6g`, site symmetry: `2mm..1'`

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ 0\right]$	`[1,2,15,16,25,26,39,40]`
2	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[3,4,13,14,27,28,37,38]`
3	$\left[0,\ x,\ \frac{1}{2}\right]$	`[5,12,20,22,29,36,44,46]`
4	$\left[\frac{1}{2},\ 0,\ x\right]$	`[6,9,19,23,30,33,43,47]`
5	$\left[\frac{1}{2},\ 0,\ -x\right]$	`[7,11,18,21,31,35,42,45]`
6	$\left[0,\ -x,\ \frac{1}{2}\right]$	`[8,10,17,24,32,34,41,48]`

Table 8: Wyckoff site: `6h`, site symmetry: `2mm..1'`

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[1,2,15,16,25,26,39,40]`
2	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[3,4,13,14,27,28,37,38]`
3	$\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$	`[5,12,20,22,29,36,44,46]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ x\right]$	`[6,9,19,23,30,33,43,47]`
5	$\left[\frac{1}{2},\ \frac{1}{2},\ -x\right]$	`[7,11,18,21,31,35,42,45]`
6	$\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[8,10,17,24,32,34,41,48]`

Table 9: Wyckoff site: `8i`, site symmetry: `.3.1'`

No.	position	mapping
1	$[x,\ x,\ x]$	`[1,5,6,25,29,30]`
2	$[x,\ -x,\ -x]$	`[2,10,11,26,34,35]`
3	$[-x,\ x,\ -x]$	`[3,7,12,27,31,36]`
4	$[-x,\ -x,\ x]$	`[4,8,9,28,32,33]`
5	$[-x,\ -x,\ -x]$	`[13,17,18,37,41,42]`
6	$[-x,\ x,\ x]$	`[14,22,23,38,46,47]`
7	$[x,\ -x,\ x]$	`[15,19,24,39,43,48]`
8	$[x,\ x,\ -x]$	`[16,20,21,40,44,45]`

Table 10: Wyckoff site: `12j`, site symmetry: `m..1'`

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,14,25,38]`
2	$[0,\ -y,\ -z]$	`[2,13,26,37]`
3	$[0,\ y,\ -z]$	`[3,16,27,40]`
4	$[0,\ -y,\ z]$	`[4,15,28,39]`
5	$[z,\ 0,\ y]$	`[5,24,29,48]`
6	$[y,\ z,\ 0]$	`[6,21,30,45]`
7	$[-y,\ z,\ 0]$	`[7,23,31,47]`
8	$[-z,\ 0,\ y]$	`[8,22,32,46]`
9	$[-y,\ -z,\ 0]$	`[9,18,33,42]`
10	$[z,\ 0,\ -y]$	`[10,20,34,44]`
11	$[y,\ -z,\ 0]$	`[11,19,35,43]`
12	$[-z,\ 0,\ -y]$	`[12,17,36,41]`

Table 11: Wyckoff site: `12k`, site symmetry: `m..1'`

No.	position	mapping
1	$\left[\frac{1}{2},\ y,\ z\right]$	`[1,14,25,38]`
2	$\left[\frac{1}{2},\ -y,\ -z\right]$	`[2,13,26,37]`
3	$\left[\frac{1}{2},\ y,\ -z\right]$	`[3,16,27,40]`
4	$\left[\frac{1}{2},\ -y,\ z\right]$	`[4,15,28,39]`
5	$\left[z,\ \frac{1}{2},\ y\right]$	`[5,24,29,48]`
6	$\left[y,\ z,\ \frac{1}{2}\right]$	`[6,21,30,45]`
7	$\left[-y,\ z,\ \frac{1}{2}\right]$	`[7,23,31,47]`
8	$\left[-z,\ \frac{1}{2},\ y\right]$	`[8,22,32,46]`
9	$\left[-y,\ -z,\ \frac{1}{2}\right]$	`[9,18,33,42]`
10	$\left[z,\ \frac{1}{2},\ -y\right]$	`[10,20,34,44]`
11	$\left[y,\ -z,\ \frac{1}{2}\right]$	`[11,19,35,43]`
12	$\left[-z,\ \frac{1}{2},\ -y\right]$	`[12,17,36,41]`

Table 12: Wyckoff site: `24l`, site symmetry: `11'`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1,25]`
2	$[x,\ -y,\ -z]$	`[2,26]`
3	$[-x,\ y,\ -z]$	`[3,27]`
4	$[-x,\ -y,\ z]$	`[4,28]`
5	$[z,\ x,\ y]$	`[5,29]`
6	$[y,\ z,\ x]$	`[6,30]`
7	$[-y,\ z,\ -x]$	`[7,31]`
8	$[-z,\ -x,\ y]$	`[8,32]`
9	$[-y,\ -z,\ x]$	`[9,33]`

continued ...

Table 12

No.	position	mapping
10	$[z, -x, -y]$	[10,34]
11	$[y, -z, -x]$	[11,35]
12	$[-z, x, -y]$	[12,36]
13	$[-x, -y, -z]$	[13,37]
14	$[-x, y, z]$	[14,38]
15	$[x, -y, z]$	[15,39]
16	$[x, y, -z]$	[16,40]
17	$[-z, -x, -y]$	[17,41]
18	$[-y, -z, -x]$	[18,42]
19	$[y, -z, x]$	[19,43]
20	$[z, x, -y]$	[20,44]
21	$[y, z, -x]$	[21,45]
22	$[-z, x, y]$	[22,46]
23	$[-y, z, x]$	[23,47]
24	$[z, -x, y]$	[24,48]