MSG No. 132.453 $P4_2/mc'm'$ [Type III, tetragonal]

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

No.	position	mapping
1	$[0, 0, 0]$	`[1,4,5,8,11,12,15,16]`
2	$\left[0, 0, \frac{1}{2}\right]$	`[2,3,6,7,9,10,13,14]`

Table 2: Wyckoff site: `2b`, site symmetry: `-42'm'`

No.	position	mapping
1	$\left[0, 0, \frac{1}{4}\right]$	`[1,4,6,7,9,10,15,16]`
2	$\left[0, 0, \frac{3}{4}\right]$	`[2,3,5,8,11,12,13,14]`

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[1,4,5,8,11,12,15,16]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[2,3,6,7,9,10,13,14]`

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	`[1,4,6,7,9,10,15,16]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	`[2,3,5,8,11,12,13,14]`

Table 5: Wyckoff site: `4e`, site symmetry: `22'2'.`

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[1,4,9,10]`
2	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[2,3,11,12]`
3	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	`[5,8,13,14]`
4	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[6,7,15,16]`

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

No.	position	mapping
1	$\left[0,\ \frac{1}{2},\ 0\right]$	`[1,4,5,8]`
2	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[2,3,6,7]`
3	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[9,10,13,14]`
4	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[11,12,15,16]`

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

No.	position	mapping
1	$[0,\ 0,\ z]$	`[1,4,15,16]`
2	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[2,3,13,14]`
3	$[0,\ 0,\ -z]$	`[5,8,11,12]`
4	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	`[6,7,9,10]`

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

No.	position	mapping
1	$\left[\frac{1}{2},\ \frac{1}{2},\ z\right]$	`[1,4,15,16]`
2	$\left[\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[2,3,13,14]`
3	$\left[\frac{1}{2},\ \frac{1}{2},\ -z\right]$	`[5,8,11,12]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[6,7,9,10]`

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

No.	position	mapping
1	$[x,\ x,\ 0]$	`[1,8,11,16]`
2	$\left[-x,\ x,\ \frac{1}{2}\right]$	`[2,7,10,13]`
3	$\left[x,\ -x,\ \frac{1}{2}\right]$	`[3,6,9,14]`
4	$[-x,\ -x,\ 0]$	`[4,5,12,15]`

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

No.	position	mapping
1	$\left[x,\ x,\ \frac{1}{2}\right]$	`[1,8,11,16]`
2	$[-x,\ x,\ 0]$	`[2,7,10,13]`
3	$[x,\ -x,\ 0]$	`[3,6,9,14]`
4	$\left[-x,\ -x,\ \frac{1}{2}\right]$	`[4,5,12,15]`

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

No.	position	mapping
1	$\left[0,\ \frac{1}{2},\ z\right]$	`[1,4]`
2	$\left[\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[2,3]`
3	$\left[0,\ \frac{1}{2},\ -z\right]$	`[5,8]`
4	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	`[6,7]`
5	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[9,10]`
6	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[11,12]`
7	$\left[0,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[13,14]`
8	$\left[\frac{1}{2},\ 0,\ z\right]$	`[15,16]`

Table 12: Wyckoff site: `8l`, site symmetry: `.2'.`

No.	position	mapping
1	$\left[x,\ 0,\ \frac{1}{4}\right]$	`[1,9]`
2	$\left[0,\ x,\ \frac{3}{4}\right]$	`[2,11]`
3	$\left[0,\ -x,\ \frac{3}{4}\right]$	`[3,12]`
4	$\left[-x,\ 0,\ \frac{1}{4}\right]$	`[4,10]`
5	$\left[-x,\ 0,\ \frac{3}{4}\right]$	`[5,13]`
6	$\left[0,\ -x,\ \frac{1}{4}\right]$	`[6,15]`
7	$\left[0,\ x,\ \frac{1}{4}\right]$	`[7,16]`
8	$\left[x,\ 0,\ \frac{3}{4}\right]$	`[8,14]`

Table 13: Wyckoff site: `8m`, site symmetry: `.2'.`

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ \frac{1}{4}\right]$	`[1,9]`
2	$\left[\frac{1}{2},\ x,\ \frac{3}{4}\right]$	`[2,11]`
3	$\left[\frac{1}{2},\ -x,\ \frac{3}{4}\right]$	`[3,12]`
4	$\left[-x,\ \frac{1}{2},\ \frac{1}{4}\right]$	`[4,10]`
5	$\left[-x,\ \frac{1}{2},\ \frac{3}{4}\right]$	`[5,13]`
6	$\left[\frac{1}{2},\ -x,\ \frac{1}{4}\right]$	`[6,15]`
7	$\left[\frac{1}{2},\ x,\ \frac{1}{4}\right]$	`[7,16]`
8	$\left[x,\ \frac{1}{2},\ \frac{3}{4}\right]$	`[8,14]`

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

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

continued ...

Table 14

No.	position	mapping
4	$[-x, -y, 0]$	`[4,5]`
5	$\left[x, -y, \frac{1}{2}\right]$	`[9,14]`
6	$\left[-x, y, \frac{1}{2}\right]$	`[10,13]`
7	$[y, x, 0]$	`[11,16]`
8	$[-y, -x, 0]$	`[12,15]`

Table 15: Wyckoff site: `8o`, site symmetry: `..m'`

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

Table 16: Wyckoff site: `16p`, site symmetry: `1`

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