MSG No. 131.438 $P4'_2/mm'c$ [Type III, tetragonal]

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

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

Table 2: Wyckoff site: `2b`, site symmetry: `mm'm'`.

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

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

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

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

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

Table 5: Wyckoff site: `2e`, site symmetry: `-4'm'2`

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

Table 6: Wyckoff site: `2f`, site symmetry: `-4'm'2`

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

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

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

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

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

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

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

Table 10: Wyckoff site: `4j`, site symmetry: `m2'm'`.

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

Table 11: Wyckoff site: `4k`, site symmetry: `m2'm'`.

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

Table 12: Wyckoff site: `4l`, site symmetry: `m2'm'`.

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

Table 13: Wyckoff site: `4m`, site symmetry: `m2'm'`.

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

Table 14: Wyckoff site: `8n`, site symmetry: `..2`

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

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

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

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

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

Table 17: Wyckoff site: 8q, site symmetry: m..

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

Table 18: Wyckoff site: 16r, site symmetry: 1

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