MSG No. 127.395 $P4/m'b'm'$ [Type III, tetragonal]

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

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

Table 2: Wyckoff site: `2b`, site symmetry: `4/m'..`

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `4..`

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff site: `8j`, site symmetry: `m'..`

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

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

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

Table 12: Wyckoff site: `16l`, site symmetry: `1`

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