MSG No. 136.500 $P4'_2/m'n'm$ [Type III, tetragonal]

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

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `2/m'..`

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

Table 4: Wyckoff site: `4d`, site symmetry: `-4..`

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

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

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

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

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

Table 7: Wyckoff site: `4g`, site symmetry: `m'.m2'`

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

Table 8: Wyckoff site: `8h`, site symmetry: `2..`

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

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

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

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

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

Table 11: Wyckoff site: `16k`, site symmetry: `1`

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