MSG No. 111.257 $P_C\bar{4}2m$ [Type IV, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `-42m`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `.2.`

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

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

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

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

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