MSG No. 113.267 $P\bar{4}2_1m$ [Type I, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `-4..`

No.	position	mapping
1	$[0, 0, 0]$	`[1,4,5,6]`
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[2,3,7,8]`

Table 2: Wyckoff site: `2b`, site symmetry: `-4..`

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	`[1,4,5,6]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[2,3,7,8]`

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

No.	position	mapping
1	$\left[0, \frac{1}{2}, z\right]$	`[1,4,7,8]`
2	$\left[\frac{1}{2}, 0, -z\right]$	`[2,3,5,6]`

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

No.	position	mapping
1	$[0, 0, z]$	`[1,4]`
2	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[2,3]`
3	$[0, 0, -z]$	`[5,6]`
4	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[7,8]`

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

No.	position	mapping
1	$\left[x, x + \frac{1}{2}, z\right]$	`[1,8]`
2	$\left[x + \frac{1}{2}, -x, -z\right]$	`[2,5]`
3	$\left[\frac{1}{2} - x, x, -z\right]$	`[3,6]`
4	$\left[-x, \frac{1}{2} - x, z\right]$	`[4,7]`

Table 6: Wyckoff site: 8f, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[2]
3	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$	[3]
4	$[-x,\ -y,\ z]$	[4]
5	$[y,\ -x,\ -z]$	[5]
6	$[-y,\ x,\ -z]$	[6]
7	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z\right]$	[7]
8	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z\right]$	[8]

1	$[x,\ y,\ z]$	[1]
2	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[2]
3	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$	[3]