MSG No. 112.260 $P\bar{4}2c1'$ [Type II, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `222.1'`

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

Table 2: Wyckoff site: `2b`, site symmetry: `222.1'`

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

Table 3: Wyckoff site: `2c`, site symmetry: `222.1'`

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

Table 4: Wyckoff site: `2d`, site symmetry: `222.1'`

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

Table 5: Wyckoff site: `2e`, site symmetry: `-4..1'`

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

Table 6: Wyckoff site: `2f`, site symmetry: `-4..1'`

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

Table 7: Wyckoff site: `4g`, site symmetry: `.2.1'`

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

Table 8: Wyckoff site: `4h`, site symmetry: `.2.1'`

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

Table 9: Wyckoff site: `4i`, site symmetry: `.2.1'`

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

Table 10: Wyckoff site: `4j`, site symmetry: `.2.1'`

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

Table 11: Wyckoff site: `4k`, site symmetry: `2..1'`

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

Table 12: Wyckoff site: 4l, site symmetry: 2..1'

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

Table 13: Wyckoff site: 4m, site symmetry: 2..1'

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

Table 14: Wyckoff site: 8n, site symmetry: 11'

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