MSG No. 111.256 $P_c\bar{4}2m$ [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	$\left[0, 0, \frac{1}{2}\right]$	`[9,10,11,12,13,14,15,16]`

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[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: `222.`

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

Table 6: Wyckoff site: `4f`, site symmetry: `22'2'.`

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

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

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

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

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

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

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

Table 10: Wyckoff site: `8j`, site symmetry: `.2'.`

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

Table 11: Wyckoff site: `8k`, site symmetry: `.2'.`

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

Table 12: Wyckoff site: `8l`, site symmetry: `.2.`

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

Table 13: Wyckoff site: `8m`, site symmetry: `2..`

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

continued ...

Table 13

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

Table 14: Wyckoff site: 8n, 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	$\left[x, x, z+\frac{1}{2}\right]$	[9,16]
6	$\left[x, -x, \frac{1}{2}-z\right]$	[10,13]
7	$\left[-x, x, \frac{1}{2}-z\right]$	[11,14]
8	$\left[-x, -x, z+\frac{1}{2}\right]$	[12,15]

Table 15: Wyckoff site: 16o, 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	$\left[x, y, z+\frac{1}{2}\right]$	[9]
10	$\left[x, -y, \frac{1}{2}-z\right]$	[10]
11	$\left[-x, y, \frac{1}{2}-z\right]$	[11]
12	$\left[-x, -y, z+\frac{1}{2}\right]$	[12]
13	$\left[y, -x, \frac{1}{2}-z\right]$	[13]
14	$\left[-y, x, \frac{1}{2}-z\right]$	[14]
15	$\left[-y, -x, z+\frac{1}{2}\right]$	[15]
16	$\left[y, x, z+\frac{1}{2}\right]$	[16]