MSG No. 112.266 $P_I\bar{4}2c$ [Type IV, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: -4'2m'

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: 222.

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: 2.m'm'

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

Table 6: Wyckoff site: **8f**, site symmetry: `.2.`

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

Table 7: Wyckoff site: **8g**, site symmetry: `.2.`

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

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

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

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

No.	position	mapping
1	$\left[x, x+\frac{1}{2}, z\right]$	[1,16]
2	$\left[x, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[2,13]
3	$\left[-x, x+\frac{1}{2}, \frac{1}{2}-z\right]$	[3,14]

continued ...

Table 9

No.	position	mapping
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	$\left[\frac{1}{2}-x,\ -x,\ z+\frac{1}{2}\right]$	[7,12]
8	$\left[x+\frac{1}{2},\ x,\ z+\frac{1}{2}\right]$	[8,9]

Table 10: Wyckoff site: 16j, site symmetry: 1

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