MSG No. 114.282 $P_I\bar{4}2_1c$ [Type IV, tetragonal]

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

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

Table 2: Wyckoff site: `2b`, site symmetry: `-42'm'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `22'2'.`

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 9

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

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

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