MSG No. 118.314 $P_I\bar{4}n2$ [Type IV, tetragonal]

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

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'm'2`

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: `2c`, site symmetry: `-4m'2'`

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 9

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

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

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