MSG No. 117.305 $P_C\bar{4}b2$ [Type IV, tetragonal]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `2.22`

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

Table 6: Wyckoff site: `4f`, site symmetry: `2.22`

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ x,\ \frac{1}{2}\right]$	`[1,11]`
2	$\left[-x,\ -x,\ \frac{1}{2}\right]$	`[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	$\left[x,\ -x,\ \frac{1}{2}\right]$	`[5,16]`
6	$\left[-x,\ x,\ \frac{1}{2}\right]$	`[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 11: Wyckoff site: `8k`, site symmetry: `..2`

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

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

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

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

No.	position	mapping
1	$\left[\frac{3}{4},\ \frac{3}{4},\ z\right]$	`[1,10]`
2	$\left[\frac{1}{4},\ \frac{1}{4},\ z\right]$	`[2,9]`
3	$\left[\frac{1}{4},\ \frac{1}{4},\ -z\right]$	`[3,12]`

continued ...

Table 13

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

Table 14: Wyckoff site: 8n, site symmetry: .m'.

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

Table 15: Wyckoff site: 16o, site symmetry: 1

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