MSG No. 50.287 P_Cban [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 9: Wyckoff site: `4i`, site symmetry: `m'2m'`

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

Table 10: Wyckoff site: `4j`, site symmetry: `m'2m'`

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

Table 11: Wyckoff site: `4k`, site symmetry: `m'm'2`

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

Table 12: Wyckoff site: `4l`, site symmetry: `m'm'2`

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

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

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

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

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

Table 15: Wyckoff site: 8o, site symmetry: .m'.

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

Table 16: Wyckoff site: 8p, site symmetry: ..m'

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

Table 17: Wyckoff site: 8q, site symmetry: ..m'

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

Table 18: Wyckoff site: 16r, site symmetry: 1

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

continued ...

Table 18

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