MSG No. 51.298 P_amma [Type IV, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: mmm'

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: mmm'

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

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

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

Table 5: Wyckoff site: 2e, site symmetry: mmm'

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

Table 6: Wyckoff site: 2f, site symmetry: m'mm'

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

Table 7: Wyckoff site: 2g, site symmetry: mmm'

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

Table 8: Wyckoff site: 2h, site symmetry: m'mm'

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

Table 9: Wyckoff site: 4i, site symmetry: 2'mm'

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

Table 10: Wyckoff site: 4j, site symmetry: 2'mm'

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

Table 11: Wyckoff site: 4k, site symmetry: 2'mm'

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

Table 12: Wyckoff site: 4l, site symmetry: 2'mm'

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

Table 13: Wyckoff site: 4m, site symmetry: m2'm'

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

Table 14: Wyckoff site: 4n, site symmetry: m2'm'

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

Table 15: Wyckoff site: 4o, site symmetry: m'2m'

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

Table 16: Wyckoff site: 4p, site symmetry: m'2m'

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

Table 17: Wyckoff site: `4q`, site symmetry: `mm2`

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

Table 18: Wyckoff site: `4r`, site symmetry: `mm2`

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

Table 19: Wyckoff site: `4s`, site symmetry: `m'm2'`

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

Table 20: Wyckoff site: `4t`, site symmetry: `m'm2'`

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

Table 21: Wyckoff site: `8u`, site symmetry: `m..`

No.	position	mapping
1	$\left[\frac{3}{4}, y, z\right]$	`[1,6]`
2	$\left[\frac{1}{4}, -y, -z\right]$	`[2,5]`
3	$\left[\frac{1}{4}, y, -z\right]$	`[3,8]`
4	$\left[\frac{3}{4}, -y, z\right]$	`[4,7]`

continued ...

Table 21

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

Table 22: Wyckoff site: 8v, site symmetry: m'..

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

Table 23: Wyckoff site: 8w, site symmetry: .m.

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

Table 24: Wyckoff site: 8x, site symmetry: .m.

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

continued ...

Table 24

No.	position	mapping
8	$\left[-x,\, \frac{1}{2},\, z\right]$	[12,14]

Table 25: Wyckoff site: 8y, site symmetry: ..m'

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

Table 26: Wyckoff site: 8z, 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	$\left[-x,\, y,\, \frac{1}{2}\right]$	[3,14]
4	$\left[\frac{1}{2}-x,\, -y,\, \frac{1}{2}\right]$	[4,13]
5	$\left[-x,\, -y,\, \frac{1}{2}\right]$	[5,12]
6	$\left[\frac{1}{2}-x,\, y,\, \frac{1}{2}\right]$	[6,11]
7	$\left[x,\, -y,\, \frac{1}{2}\right]$	[7,10]
8	$\left[x+\frac{1}{2},\, y,\, \frac{1}{2}\right]$	[8,9]

Table 27: Wyckoff site: 16A, site symmetry: 1

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

continued ...

Table 27

No.	position	mapping
11	$\left[\frac{1}{2} - x,\, y,\, -z\right]$	[11]
12	$[-x,\, -y,\, z]$	[12]
13	$\left[\frac{1}{2} - x,\, -y,\, -z\right]$	[13]
14	$[-x,\, y,\, z]$	[14]
15	$\left[x + \frac{1}{2},\, -y,\, z\right]$	[15]
16	$[x,\, y,\, -z]$	[16]