MSG No. 177.149 $P622$ [Type I, hexagonal]

Table 1: Wyckoff site: `1a`, site symmetry: `622`

No.	position	mapping
1	[0, 0, 0]	`[1,2,3,4,5,6,7,8,9,10,11,12]`

Table 2: Wyckoff site: `1b`, site symmetry: `622`

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

Table 3: Wyckoff site: `2c`, site symmetry: `3.2`

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

Table 4: Wyckoff site: `2d`, site symmetry: `3.2`

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

Table 5: Wyckoff site: `2e`, site symmetry: `6..`

No.	position	mapping
1	$[0, 0, z]$	`[1,2,3,4,5,6]`
2	$[0, 0, -z]$	`[7,8,9,10,11,12]`

Table 6: Wyckoff site: `3f`, site symmetry: `222`

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

Table 7: Wyckoff site: `3g`, site symmetry: `222`

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

Table 8: Wyckoff site: `4h`, site symmetry: `3..`

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

Table 9: Wyckoff site: `6i`, site symmetry: `2..`

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

Table 10: Wyckoff site: `6j`, site symmetry: `.2.`

No.	position	mapping
1	$[x, 0, 0]$	`[1,7]`
2	$[x, x, 0]$	`[2,10]`
3	$[0, x, 0]$	`[3,8]`
4	$[-x, 0, 0]$	`[4,11]`
5	$[-x, -x, 0]$	`[5,9]`
6	$[0, -x, 0]$	`[6,12]`

Table 11: Wyckoff site: `6k`, site symmetry: `.2.`

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	`[1,7]`

continued ...

Table 11

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

Table 12: Wyckoff site: `6l`, site symmetry: `..2`

No.	position	mapping
1	$[x,\, -x,\, 0]$	`[1,12]`
2	$[2x,\, x,\, 0]$	`[2,7]`
3	$[x,\, 2x,\, 0]$	`[3,10]`
4	$[-x,\, x,\, 0]$	`[4,8]`
5	$[-2x,\, -x,\, 0]$	`[5,11]`
6	$[-x,\, -2x,\, 0]$	`[6,9]`

Table 13: Wyckoff site: `6m`, site symmetry: `..2`

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

Table 14: Wyckoff site: `12n`, site symmetry: `1`

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

continued ...

Table 14

No.	position	mapping
11	$[-x+y,\ y,\ -z]$	`[11]`
12	$[-y,\ -x,\ -z]$	`[12]`