MSG No. 89.87   *P*422   [Type I, tetragonal]

Table 1: Wyckoff site: 1a, site symmetry: 422

No.	position	mapping
1	$[0, 0, 0]$	[1,2,3,4,5,6,7,8]

Table 2: Wyckoff site: 1b, site symmetry: 422

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

Table 3: Wyckoff site: 1c, site symmetry: 422

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

Table 4: Wyckoff site: 1d, site symmetry: 422

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

Table 5: Wyckoff site: 2e, site symmetry: 222.

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

Table 6: Wyckoff site: 2f, site symmetry: 222.

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

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

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

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

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

Table 9: Wyckoff site: `4i`, site symmetry: `2..`

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

Table 10: Wyckoff site: `4j`, site symmetry: `..2`

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

Table 11: Wyckoff site: `4k`, site symmetry: `..2`

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

Table 12: Wyckoff site: `4l`, site symmetry: `.2.`

No.	position	mapping
1	$[x, 0, 0]$	[1,4]
2	$[0, x, 0]$	[2,7]
3	$[0, -x, 0]$	[3,8]
4	$[-x, 0, 0]$	[5,6]

Table 13: Wyckoff site: `4m`, site symmetry: `.2.`

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

Table 14: Wyckoff site: `4n`, site symmetry: `.2.`

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	[1,4]
2	$\left[0, x, \frac{1}{2}\right]$	[2,7]
3	$\left[0, -x, \frac{1}{2}\right]$	[3,8]
4	$\left[-x, 0, \frac{1}{2}\right]$	[5,6]

Table 15: Wyckoff site: `4o`, site symmetry: `.2.`

No.	position	mapping
1	$\left[x, \frac{1}{2}, 0\right]$	[1,4]
2	$\left[\frac{1}{2}, x, 0\right]$	[2,7]
3	$\left[\frac{1}{2}, -x, 0\right]$	[3,8]
4	$\left[-x, \frac{1}{2}, 0\right]$	[5,6]

Table 16: Wyckoff site: `8p`, site symmetry: `1`

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x, z]$	[2]
3	$[y, -x, z]$	[3]
4	$[x, -y, -z]$	[4]

continued ...

3

Table 16

No.	position	mapping
5	$[-x,\ y,\ -z]$	[5]
6	$[-x,\ -y,\ z]$	[6]
7	$[y,\ x,\ -z]$	[7]
8	$[-y,\ -x,\ -z]$	[8]