MSG No. 89.91 $P4'2'2$ [Type III, tetragonal]

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

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

Table 2: Wyckoff site: `1b`, site symmetry: `4'2'2`

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: `4'2'2`

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: `4'2'2`

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: `22'2'.`

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

Table 6: Wyckoff site: `2f`, site symmetry: `22'2'.`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 16

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