MSG No. 83.45 $P4'/m$ [Type III, tetragonal]

Table 1: Wyckoff site: `1a`, site symmetry: `4'/m..`

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

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

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'/m..`

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'/m..`

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: `2/m..`

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

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

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

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	$\left[0, \frac{1}{2}, -z\right]$	[3,4]
3	$\left[\frac{1}{2}, 0, z\right]$	[5,6]
4	$\left[\frac{1}{2}, 0, -z\right]$	[7,8]

Table 10: Wyckoff site: 4j, site symmetry: m..

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

Table 11: Wyckoff site: 4k, site symmetry: m..

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

Table 12: Wyckoff site: 8l, site symmetry: 1

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

1	$[x,\,y,\,z]$	[1]
2	$[-x,\,-y,\,z]$	[2]
3	$[-x,\,-y,\,-z]$	[3]
6	$[y,\,-x,\,z]$	