MSG No. 99.163 *P4mm*   [Type I, tetragonal]

Table 1: Wyckoff site: 1a, site symmetry: 4mm

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

Table 2: Wyckoff site: 1b, site symmetry: 4mm

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

Table 3: Wyckoff site: 2c, site symmetry: 2mm.

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

Table 4: Wyckoff site: 4d, site symmetry: ..m

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

Table 5: Wyckoff site: 4e, site symmetry: .m.

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

Table 6: Wyckoff site: `4f`, site symmetry: `.m.`

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

Table 7: Wyckoff site: `8g`, 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]
5	$[-x, y, z]$	[5]
6	$[x, -y, z]$	[6]
7	$[-y, -x, z]$	[7]
8	$[y, x, z]$	[8]