MSG No. 99.164 $P4mm1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 1a, site symmetry: 4mm1'

No.	position	mapping
1	$[0, 0, z]$	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]

Table 2: Wyckoff site: 1b, site symmetry: 4mm1'

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]

Table 3: Wyckoff site: 2c, site symmetry: 2mm.1'

No.	position	mapping
1	$\left[\frac{1}{2}, 0, z\right]$	[1,4,5,6,9,12,13,14]
2	$\left[0, \frac{1}{2}, z\right]$	[2,3,7,8,10,11,15,16]

Table 4: Wyckoff site: 4d, site symmetry: ..m1'

No.	position	mapping
1	$[x, x, z]$	[1,8,9,16]
2	$[-x, x, z]$	[2,5,10,13]
3	$[x, -x, z]$	[3,6,11,14]
4	$[-x, -x, z]$	[4,7,12,15]

Table 5: Wyckoff site: 4e, site symmetry: .m.1'

No.	position	mapping
1	$[x, 0, z]$	[1,6,9,14]
2	$[0, x, z]$	[2,8,10,16]
3	$[0, -x, z]$	[3,7,11,15]
4	$[-x, 0, z]$	[4,5,12,13]

Table 6: Wyckoff site: `4f`, site symmetry: `.m.1'`

No.	position	mapping
1	$\left[x, \frac{1}{2}, z\right]$	`[1,6,9,14]`
2	$\left[\frac{1}{2}, x, z\right]$	`[2,8,10,16]`
3	$\left[\frac{1}{2}, -x, z\right]$	`[3,7,11,15]`
4	$\left[-x, \frac{1}{2}, z\right]$	`[4,5,12,13]`

Table 7: Wyckoff site: `8g`, site symmetry: `11'`

No.	position	mapping
1	$[x, y, z]$	`[1,9]`
2	$[-y, x, z]$	`[2,10]`
3	$[y, -x, z]$	`[3,11]`
4	$[-x, -y, z]$	`[4,12]`
5	$[-x, y, z]$	`[5,13]`
6	$[x, -y, z]$	`[6,14]`
7	$[-y, -x, z]$	`[7,15]`
8	$[y, x, z]$	`[8,16]`