MSG No. 58.394 *Pnnm*1′ [Type II, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: ..2/m1'

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

Table 2: Wyckoff site: 2b, site symmetry: ..2/m1'

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

Table 3: Wyckoff site: 2c, site symmetry: ..2/m1'

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

Table 4: Wyckoff site: 2d, site symmetry: ..2/m1'

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

Table 5: Wyckoff site: 4e, site symmetry: ..21'

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

Table 6: Wyckoff site: `4f`, site symmetry: `..21'`

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

Table 7: Wyckoff site: `4g`, site symmetry: `..m1'`

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

Table 8: Wyckoff site: `8h`, site symmetry: `11'`

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