

MSG No. 59.405 $Pmmn$ [Type I, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: $mm2$

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

Table 2: Wyckoff site: 2b, site symmetry: $mm2$

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

Table 3: Wyckoff site: 4c, site symmetry: -1

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

Table 4: Wyckoff site: 4d, site symmetry: -1

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

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

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

Table 6: Wyckoff site: $4f$, site symmetry: $\bar{4}2m$.

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

Table 7: Wyckoff site: $8g$, site symmetry: 1

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