

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: .m.

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]