

MSG No. 105.211  $P4_2mc$  [ Type I, tetragonal ]

Table 1: Wyckoff site: **2a**, site symmetry: **2mm**.

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

Table 2: Wyckoff site: **2b**, site symmetry: **2mm**.

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

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

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

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

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

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

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

Table 6: Wyckoff site: **8f**, site symmetry: **1**

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