

MSG No. 25.63 P_Cmm2 [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $. . 2'$

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

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

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

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

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

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

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