

MSG No. 25.62 $P_a mm2$ [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: **2c**, site symmetry: **m'm2'**

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

Table 4: Wyckoff site: **2d**, site symmetry: **m'm2'**

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

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

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

Table 6: Wyckoff site: 4f, site symmetry: .m.

No.	position	mapping
1	$[x, \frac{1}{2}, z]$	[1,4]
2	$[-x, \frac{1}{2}, z]$	[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 7: Wyckoff site: 4g, site symmetry: m..

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

Table 8: Wyckoff site: 4h, site symmetry: m'..

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

Table 9: Wyckoff site: 8i, 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	$[x + \frac{1}{2}, y, z]$	[5]
6	$[\frac{1}{2} - x, -y, z]$	[6]
7	$[\frac{1}{2} - x, y, z]$	[7]
8	$[x + \frac{1}{2}, -y, z]$	[8]