

MSG No. 25.61 $P_{\bar{c}}mm2$ [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: $mm2$

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

Table 4: Wyckoff site: 2d, site symmetry: $mm2$

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

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

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

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

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

Table 7: Wyckoff site: **4g**, site symmetry: $m\bar{2}$.

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

Table 8: Wyckoff site: **4h**, site symmetry: $m\bar{2}$.

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

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	$[x, y, z + \frac{1}{2}]$	[5]
6	$[-x, -y, z + \frac{1}{2}]$	[6]
7	$[-x, y, z + \frac{1}{2}]$	[7]
8	$[x, -y, z + \frac{1}{2}]$	[8]