

MSG No. 51.289 *Pmma* [Type I, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: $.2/m$.

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

Table 2: Wyckoff site: 2b, site symmetry: $.2/m$.

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

Table 3: Wyckoff site: 2c, site symmetry: $.2/m$.

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

Table 4: Wyckoff site: 2d, site symmetry: $.2/m$.

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

Table 5: Wyckoff site: 2e, site symmetry: $mm2$

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

Table 6: Wyckoff site: 2f, site symmetry: $mm2$

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 7: Wyckoff site: $4g$, site symmetry: $.2$.

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

Table 8: Wyckoff site: $4h$, site symmetry: $.2$.

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

Table 9: Wyckoff site: $4i$, site symmetry: $.m$.

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

Table 10: Wyckoff site: $4j$, site symmetry: $.m$.

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

Table 11: Wyckoff site: $4k$, site symmetry: $m..$

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

Table 12: Wyckoff site: 81 , site symmetry: 1

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