

MSG No. 51.290 $Pmma1'$ [Type II, orthorhombic]

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

No.	position	mapping
1	$[0, 0, 0]$	$[1, 3, 5, 7, 9, 11, 13, 15]$
2	$[\frac{1}{2}, 0, 0]$	$[2, 4, 6, 8, 10, 12, 14, 16]$

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

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	$[1, 3, 5, 7, 9, 11, 13, 15]$
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, 4, 6, 8, 10, 12, 14, 16]$

Table 3: Wyckoff site: 2c, site symmetry: $.2/m.1'$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 3, 5, 7, 9, 11, 13, 15]$
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, 4, 6, 8, 10, 12, 14, 16]$

Table 4: Wyckoff site: 2d, site symmetry: $.2/m.1'$

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 3, 5, 7, 9, 11, 13, 15]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, 4, 6, 8, 10, 12, 14, 16]$

Table 5: Wyckoff site: 2e, site symmetry: $mm21'$

No.	position	mapping
1	$[\frac{1}{4}, 0, z]$	$[1, 4, 6, 7, 9, 12, 14, 15]$
2	$[\frac{3}{4}, 0, -z]$	$[2, 3, 5, 8, 10, 11, 13, 16]$

Table 6: Wyckoff site: 2f, site symmetry: $mm21'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{2}, z]$	$[1, 4, 6, 7, 9, 12, 14, 15]$
2	$[\frac{3}{4}, \frac{1}{2}, -z]$	$[2, 3, 5, 8, 10, 11, 13, 16]$

Table 7: Wyckoff site: 4g, site symmetry: $.2.1'$

No.	position	mapping
1	$[0, y, 0]$	$[1, 3, 9, 11]$
2	$[\frac{1}{2}, -y, 0]$	$[2, 4, 10, 12]$
3	$[0, -y, 0]$	$[5, 7, 13, 15]$
4	$[\frac{1}{2}, y, 0]$	$[6, 8, 14, 16]$

Table 8: Wyckoff site: 4h, site symmetry: $.2.1'$

No.	position	mapping
1	$[0, y, \frac{1}{2}]$	$[1, 3, 9, 11]$
2	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[2, 4, 10, 12]$
3	$[0, -y, \frac{1}{2}]$	$[5, 7, 13, 15]$
4	$[\frac{1}{2}, y, \frac{1}{2}]$	$[6, 8, 14, 16]$

Table 9: Wyckoff site: 4i, site symmetry: $.m.1'$

No.	position	mapping
1	$[x, 0, z]$	$[1, 7, 9, 15]$
2	$[x + \frac{1}{2}, 0, -z]$	$[2, 8, 10, 16]$
3	$[-x, 0, -z]$	$[3, 5, 11, 13]$
4	$[\frac{1}{2} - x, 0, z]$	$[4, 6, 12, 14]$

Table 10: Wyckoff site: 4j, site symmetry: $.m.1'$

No.	position	mapping
1	$[x, \frac{1}{2}, z]$	$[1, 7, 9, 15]$
2	$[x + \frac{1}{2}, \frac{1}{2}, -z]$	$[2, 8, 10, 16]$
3	$[-x, \frac{1}{2}, -z]$	$[3, 5, 11, 13]$
4	$[\frac{1}{2} - x, \frac{1}{2}, z]$	$[4, 6, 12, 14]$

Table 11: Wyckoff site: 4k, site symmetry: $m..1'$

No.	position	mapping
1	$[\frac{1}{4}, y, z]$	$[1, 6, 9, 14]$
2	$[\frac{3}{4}, -y, -z]$	$[2, 5, 10, 13]$
3	$[\frac{3}{4}, y, -z]$	$[3, 8, 11, 16]$
4	$[\frac{1}{4}, -y, z]$	$[4, 7, 12, 15]$

Table 12: Wyckoff site: 81, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	[1,9]
2	$[x + \frac{1}{2}, -y, -z]$	[2,10]
3	$[-x, y, -z]$	[3,11]
4	$[\frac{1}{2} - x, -y, z]$	[4,12]
5	$[-x, -y, -z]$	[5,13]
6	$[\frac{1}{2} - x, y, z]$	[6,14]
7	$[x, -y, z]$	[7,15]
8	$[x + \frac{1}{2}, y, -z]$	[8,16]