

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

Table 1: Wyckoff site: **2a**, site symmetry: $.2/\text{m.1}'$

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: $.2/\text{m.1}'$

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: $.2/\text{m.1}'$

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: $.2/\text{m.1}'$

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: $\text{mm}21'$

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: $\text{mm}21'$

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]