

MSG No. 51.295 $Pmm'a'$ [Type III, orthorhombic]

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

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: $.2'/\mathbf{m}'$.

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: $.2'/\mathbf{m}'$.

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: $.2'/\mathbf{m}'$.

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: $\mathbf{mm}'2'$.

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: $\mathbf{mm}'2'$.

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]	[1,5]
2	[$\frac{1}{2}$, $-y$, 0]	[2,6]
3	[0, $-y$, 0]	[3,7]
4	[$\frac{1}{2}$, y , 0]	[4,8]

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

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

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]	[1,4]
2	[$\frac{3}{4}$, $-y$, $-z$]	[2,3]
3	[$\frac{3}{4}$, y , $-z$]	[5,8]
4	[$\frac{1}{4}$, $-y$, z]	[6,7]

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]