

MSG No. 48.259 *Pn'nn* [Type III, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: 22'2'

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

Table 2: Wyckoff site: 2b, site symmetry: 22'2'

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

Table 3: Wyckoff site: 2c, site symmetry: 22'2'

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

Table 4: Wyckoff site: 2d, site symmetry: 22'2'

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

Table 5: Wyckoff site: 4e, site symmetry: -1'

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

Table 6: Wyckoff site: 4f, site symmetry: -1'.

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

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

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

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

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

Table 9: Wyckoff site: 4i, site symmetry: .2'.

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

Table 10: Wyckoff site: 4j, site symmetry: .2'.

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

Table 11: Wyckoff site: 4k, site symmetry: . . 2'

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

Table 12: Wyckoff site: 4l, site symmetry: . . 2'

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

Table 13: Wyckoff site: 8m, site symmetry: 1

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