

MSG No. 112.261 $P\bar{4}'2'c$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 2e, site symmetry: $-4'$.

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

Table 6: Wyckoff site: 2f, site symmetry: $-4'$.

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 13: Wyckoff site: 4m, site symmetry: 2 . .

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

Table 14: Wyckoff site: 8n, site symmetry: 1

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