

MSG No. 84.54 $P4_2/m'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 11: Wyckoff site: $8k$, site symmetry: 1

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

continued ...

Table 11

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