

MSG No. 83.47 $P4'/m'$ [Type III, tetragonal]

Table 1: Wyckoff site: **1a**, site symmetry: $4'/m'$. .

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

Table 2: Wyckoff site: **1b**, site symmetry: $4'/m'$. .

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

Table 3: Wyckoff site: **1c**, site symmetry: $4'/m'$. .

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

Table 4: Wyckoff site: **1d**, site symmetry: $4'/m'$. .

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

Table 5: Wyckoff site: **2e**, site symmetry: $2/m'$. .

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

Table 6: Wyckoff site: **2f**, site symmetry: $2/m'$. .

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

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 5, 6]$
2	$[0, 0, -z]$	$[3, 4, 7, 8]$

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

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

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

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

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

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

Table 11: Wyckoff site: $4k$, site symmetry: m' . .

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

Table 12: Wyckoff site: **81**, site symmetry: **1**

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