

MSG No. 83.46 $P4/m'$ [Type III, tetragonal]

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

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

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

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

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

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: $4/m' \dots$

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: $2/m' \dots$

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

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

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

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

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

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

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

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

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

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

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

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

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

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