

MSG No. 115.287 $P\bar{4}m'2'$ [Type III, tetragonal]

Table 1: Wyckoff site: 1a, site symmetry: $-4m'2'$

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

Table 2: Wyckoff site: 1b, site symmetry: $-4m'2'$

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

Table 3: Wyckoff site: 1c, site symmetry: $-4m'2'$

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

Table 4: Wyckoff site: 1d, site symmetry: $-4m'2'$

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

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

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

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

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

Table 7: Wyckoff site: 2g, site symmetry: 2m'm'.

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

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

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

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

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

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

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

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

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