

MSG No. 115.285 $P\bar{4}'m'2$ [Type III, tetragonal]

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

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

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

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: $-4'm'2$

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: $-4'm'2$

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: $2\mathbf{g}$, site symmetry: $2\mathbf{m}'\mathbf{m}'$.

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: $4\mathbf{h}$, site symmetry: $\dots 2$

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

Table 9: Wyckoff site: $4\mathbf{i}$, site symmetry: $\dots 2$

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

Table 10: Wyckoff site: $4\mathbf{j}$, site symmetry: $\dots \mathbf{m}'$.

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: $4\mathbf{k}$, site symmetry: $\dots \mathbf{m}'$.

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]