

MSG No. 84.55 $P4'_2/m'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: $4\mathbf{g}$, site symmetry: $2..$

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

Table 8: Wyckoff site: $4\mathbf{h}$, site symmetry: $2..$

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

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

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

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

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

Table 11: Wyckoff site: $8\mathbf{k}$, site symmetry: 1

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

continued ...

Table 11

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