

SG No. 71 D_{2h}^{25} $Immm$ [orthorhombic]

* plus set: $+ [0, 0, 0], \quad + [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

Table 1: Wyckoff site: 2a, site symmetry: mmm

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

Table 2: Wyckoff site: 2b, site symmetry: mmm

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

Table 3: Wyckoff site: 2c, site symmetry: mmm

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

Table 4: Wyckoff site: 2d, site symmetry: mmm

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

Table 5: Wyckoff site: 4e, site symmetry: $2mm$

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

Table 6: Wyckoff site: 4f, site symmetry: $2mm$

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

Table 7: Wyckoff site: $4g$, site symmetry: $m2m$

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

Table 8: Wyckoff site: $4h$, site symmetry: $m2m$

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

Table 9: Wyckoff site: $4i$, site symmetry: $mm2$

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

Table 10: Wyckoff site: $4j$, site symmetry: $mm2$

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

Table 11: Wyckoff site: $8k$, site symmetry: -1

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

Table 12: Wyckoff site: $8l$, site symmetry: $m..$

No.	position	mapping
1	$[0, y, z]$	$[1, 8]$
2	$[0, -y, z]$	$[2, 7]$

continued ...

Table 12

No.	position	mapping
3	$[0, y, -z]$	$[3, 6]$
4	$[0, -y, -z]$	$[4, 5]$

Table 13: Wyckoff site: $8\mathbf{m}$, site symmetry: $\bar{3}m$.

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

Table 14: Wyckoff site: $8\mathbf{n}$, site symmetry: $\bar{3}m$

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

Table 15: Wyckoff site: $16\mathbf{o}$, site symmetry: $\bar{3}m$

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