

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

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

Table 1: Wyckoff site: 2a, site symmetry:  $\text{mmm}$

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

Table 2: Wyckoff site: 2b, site symmetry:  $\text{mmm}$

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:  $\text{mmm}$

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:  $\text{mmm}$

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:  $2\text{mm}$

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:  $2\text{mm}$

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:  $\text{m}2\text{m}$ 

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:  $\text{m}2\text{m}$ 

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:  $\text{mm}2$ 

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:  $\text{mm}2$ 

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:  $\text{m..}$ 

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: 8m, site symmetry: .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: 8n, site symmetry: ...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: 16o, site symmetry: 1

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]