

SG No. 72  $D_{2h}^{26}$  *Ibam* [ orthorhombic ]

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

Table 1: Wyckoff site: 4a, site symmetry: 222

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

Table 2: Wyckoff site: 4b, site symmetry: 222

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

Table 3: Wyckoff site: 4c, site symmetry:  $\cdot\cdot 2/m$

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

Table 4: Wyckoff site: 4d, site symmetry:  $\cdot\cdot 2/m$

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

Table 5: Wyckoff site: 8e, 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	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[3, 7]$
4	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[4, 8]$

Table 6: Wyckoff site: 8f, site symmetry: 2..

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

Table 7: Wyckoff site: 8g, site symmetry: .2.

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: ..2

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

Table 10: Wyckoff site: 8j, site symmetry: ..m

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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