

SG No. 74 D_{2h}^{28} *Imma* [orthorhombic]

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

Table 1: Wyckoff site: 4a, site symmetry: 2/m..

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

Table 2: Wyckoff site: 4b, site symmetry: 2/m..

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

Table 3: Wyckoff site: 4c, site symmetry: .2/m.

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: mm2

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff site: 16j, site symmetry: 1

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

continued ...

Table 10

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