

SG No. 49 D_{2h}^3 $Pccm$ [orthorhombic]

* plus set: $+ [0, 0, 0]$

Table 1: Wyckoff site: 2a, site symmetry: $\dots 2/m$

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

Table 2: Wyckoff site: 2b, site symmetry: $\dots 2/m$

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

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

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

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

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

Table 5: Wyckoff site: 2e, 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 6: Wyckoff site: 2f, 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 7: Wyckoff site: 2g, site symmetry: 222

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

Table 8: Wyckoff site: 2h, site symmetry: 222

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 9: Wyckoff site: 4i, 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 10: Wyckoff site: 4j, site symmetry: 2..

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

Table 11: Wyckoff site: $4k$, 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 12: Wyckoff site: $4l$, site symmetry: $.2$.

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

Table 13: Wyckoff site: $4m$, site symmetry: $.2$

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

Table 14: Wyckoff site: $4n$, 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	$[\frac{1}{2}, \frac{1}{2}, -z]$	[5,6]
4	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[7,8]

Table 15: Wyckoff site: $4o$, site symmetry: $.2$

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

Table 16: Wyckoff site: $4p$, site symmetry: $\dots 2$

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

Table 17: Wyckoff site: $4q$, site symmetry: $\dots m$

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

Table 18: Wyckoff site: $8r$, site symmetry: 1

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