

SG No. 48 D_{2h}^2 $Pnnn$ [orthorhombic]

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

Table 1: Wyckoff site: 2a, site symmetry: 222

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: 222

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: -1

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

Table 6: Wyckoff site: 4f, site symmetry: -1

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

Table 7: Wyckoff site: 4g, site symmetry: 2..

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

Table 8: Wyckoff site: 4h, site symmetry: 2..

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

Table 9: Wyckoff site: 4i, site symmetry: .2.

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

Table 10: Wyckoff site: 4j, site symmetry: .2.

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

Table 11: Wyckoff site: **4k**, site symmetry: $\dots 2$

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

Table 12: Wyckoff site: **4l**, site symmetry: $\dots 2$

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

Table 13: Wyckoff site: **8m**, site symmetry: **1**

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