

SG No. 84 C_{4h}^2 $P4_2/m$ [tetragonal]

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

Table 1: Wyckoff site: 2a, site symmetry: $2/\mathfrak{m}..$

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: $2/\mathfrak{m}..$

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: $2/\mathfrak{m}..$

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

Table 4: Wyckoff site: 2d, site symmetry: $2/\mathfrak{m}..$

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

Table 5: Wyckoff site: 2e, site symmetry: $-4..$

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

Table 6: Wyckoff site: 2f, site symmetry: $-4..$

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

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

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

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

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

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

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

Table 10: Wyckoff site: 4j, site symmetry: $m..$

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

Table 11: Wyckoff site: $8k$, site symmetry: 1

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