

SG No. 68 D_{2h}^{22} $Ccce$ [orthorhombic]

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

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: -1

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

Table 4: Wyckoff site: 8d, site symmetry: -1

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

Table 5: Wyckoff site: 8e, site symmetry: 2..

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

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

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

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

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

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

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

Table 9: Wyckoff site: **16i**, site symmetry: 1

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