

SG No. 64 D_{2h}^{18} $Cmce$ [orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site: **8f**, site symmetry: **m** .

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

Table 7: Wyckoff site: **16g**, site symmetry: **1**

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