

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]