

SG No. 63 D_{2h}^{17} $Cmcm$ [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, 0, $\frac{1}{2}$]	[2,3,6,7]

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

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

Table 3: Wyckoff site: 4c, site symmetry: m2m

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

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

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

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

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

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

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

Table 7: Wyckoff site: 8g, site symmetry: ..m

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

Table 8: Wyckoff site: 16h, site symmetry: 1

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