

SG No. 57 D_{2h}^{11} $Pbcm$ [orthorhombic]

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

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

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

Table 2: Wyckoff site: 4b, site symmetry: -1

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

Table 3: Wyckoff site: 4c, site symmetry: 2..

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

Table 4: Wyckoff site: 4d, site symmetry: ..m

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

Table 5: Wyckoff site: 8e, site symmetry: 1

No.	position	mapping
1	[x , y , z]	[1]

continued ...

Table 5

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