

SG No. 61 D_{2h}^{15} $Pbca$ [orthorhombic]

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

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

Table 1: Wyckoff bond: **4a@4a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[4, -8]$

* Wyckoff site: **4b**, site symmetry: -1

Table 2: Wyckoff bond: **4a@4b**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, \frac{1}{2}]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, 0]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, 0]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[4, -8]$

* Wyckoff site: **8c**, site symmetry: 1

Table 3: Wyckoff bond: **8a@8c**

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