

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]