

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]