

SG No. 60  $D_{2h}^{14}$   $Pbcn$  [ 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]	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[2, -6]
3	[-X, Y, -Z]	$[0, 0, \frac{1}{2}]$	[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]	$[0, \frac{1}{2}, 0]$	[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]	$[\frac{1}{2}, 0, 0]$	[4, -8]

\* Wyckoff site: 4c, site symmetry: .2.

Table 3: Wyckoff bond: 4a@4c

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

Table 4: Wyckoff bond: 4b@4c

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

Table 5: Wyckoff bond: **8c@4c**

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

\* Wyckoff site: **8d**, site symmetry: **1**

Table 6: Wyckoff bond: **8a@8d**

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