

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]