

SG No. 62 D_{2h}^{16} $Pnma$ [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]	$[0, \frac{1}{2}, 0]$	[3, -7]
4	[X, -Y, -Z]	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[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]	$[0, \frac{1}{2}, \frac{1}{2}]$	[3, -7]
4	[X, -Y, -Z]	$[\frac{1}{2}, \frac{1}{2}, 0]$	[4, -8]

* Wyckoff site: 4c, site symmetry: .m.

Table 3: Wyckoff bond: 4a@4c

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

Table 4: Wyckoff bond: 4b@4c

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

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

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