

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]