

SG No. 27 C_{2v}^3 $Pcc2$ [orthorhombic]

* plus set: + [0, 0, 0]

* Wyckoff site: 2a, site symmetry: . . 2

Table 1: Wyckoff bond: 2a@2a

No.	vector	center	mapping
1	[X, Y, 0]	[0, 0, z]	[1, -2]
2	[X, -Y, 0]	[0, 0, z + $\frac{1}{2}$]	[3, -4]

Table 2: Wyckoff bond: 2b@2a

No.	vector	center	mapping
1	[0, 0, Z]	[0, 0, z]	[1, 2]
2	[0, 0, Z]	[0, 0, z + $\frac{1}{2}$]	[3, 4]

Table 3: Wyckoff bond: 4c@2a

No.	vector	center	mapping
1	[X, Y, Z]	[0, 0, z]	[1]
2	[-X, -Y, Z]	[0, 0, z]	[2]
3	[X, -Y, Z]	[0, 0, z + $\frac{1}{2}$]	[3]
4	[-X, Y, Z]	[0, 0, z + $\frac{1}{2}$]	[4]

* Wyckoff site: 2b, site symmetry: . . 2

Table 4: Wyckoff bond: 2a@2b

No.	vector	center	mapping
1	[X, Y, 0]	[0, $\frac{1}{2}$, z]	[1, -2]
2	[X, -Y, 0]	[0, $\frac{1}{2}$, z + $\frac{1}{2}$]	[3, -4]

Table 5: Wyckoff bond: 2b@2b

No.	vector	center	mapping
1	[0, 0, Z]	[0, $\frac{1}{2}$, z]	[1, 2]
2	[0, 0, Z]	[0, $\frac{1}{2}$, z + $\frac{1}{2}$]	[3, 4]

Table 6: Wyckoff bond: 4c@2b

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, z]$	[1]
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, z]$	[2]
3	$[X, -Y, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[3]
4	$[-X, Y, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[4]

* Wyckoff site: 2c, site symmetry: $\dots 2$

Table 7: Wyckoff bond: 2a@2c

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, 0, z]$	[1, -2]
2	$[X, -Y, 0]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[3, -4]

Table 8: Wyckoff bond: 2b@2c

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, 0, z]$	[1, 2]
2	$[0, 0, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[3, 4]

Table 9: Wyckoff bond: 4c@2c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, 0, z]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, z]$	[2]
3	$[X, -Y, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[3]
4	$[-X, Y, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[4]

* Wyckoff site: 2d, site symmetry: $\dots 2$

Table 10: Wyckoff bond: 2a@2d

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[1, -2]
2	$[X, -Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[3, -4]

Table 11: Wyckoff bond: 2b@2d

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[1,2]
2	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[3,4]

Table 12: Wyckoff bond: 4c@2d

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[2]
3	$[X, -Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[3]
4	$[-X, Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[4]

* Wyckoff site: 4e, site symmetry: 1

Table 13: Wyckoff bond: 4a@4e

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