

SG No. 77 C_4^3 $P4_2$ [tetragonal]

* 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	[-Y, X, 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	[-Y, X, Z]	[0, 0, $z + \frac{1}{2}$]	[3]
4	[Y, -X, 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]	[\frac{1}{2}, \frac{1}{2}, z]	[1, -2]
2	[-Y, X, 0]	[\frac{1}{2}, \frac{1}{2}, $z + \frac{1}{2}$]	[3, -4]

Table 5: Wyckoff bond: 2b@2b

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 6: Wyckoff bond: 4c@2b

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	$[-Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[3]
4	$[Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[4]

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

Table 7: Wyckoff bond: 2a@2c

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

Table 8: Wyckoff bond: 2b@2c

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

* Wyckoff site: 4d, site symmetry: 1

Table 10: Wyckoff bond: 4a@4d

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