

SG No. 103 C_{4v}^5 $P4cc$ [tetragonal]

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

* Wyckoff site: 2a, site symmetry: 4..

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 4b@2a

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

Table 3: Wyckoff bond: 8c@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]	[3]
4	[Y, -X, Z]	[0, 0, z]	[4]
5	[X, -Y, Z]	[0, 0, $z + \frac{1}{2}$]	[5]
6	[-X, Y, Z]	[0, 0, $z + \frac{1}{2}$]	[6]
7	[-Y, -X, Z]	[0, 0, $z + \frac{1}{2}$]	[7]
8	[Y, X, Z]	[0, 0, $z + \frac{1}{2}$]	[8]

* Wyckoff site: 2b, site symmetry: 4..

Table 4: Wyckoff bond: 2a@2b

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

Table 5: Wyckoff bond: 4b@2b

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

Table 6: Wyckoff bond: 8c@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]	$[\frac{1}{2}, \frac{1}{2}, z]$	[3]
4	[Y, -X, Z]	$[\frac{1}{2}, \frac{1}{2}, z]$	[4]
5	[X, -Y, Z]	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	[-X, Y, Z]	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	[-Y, -X, Z]	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[7]
8	[Y, X, Z]	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[8]

* Wyckoff site: 4c, site symmetry: 2..

Table 7: Wyckoff bond: 4a@4c

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

Table 8: Wyckoff bond: 4b@4c

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

Table 9: Wyckoff bond: 8c@4c

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	$[-Y, X, Z]$	$[\frac{1}{2}, 0, z]$	[3]
4	$[Y, -X, Z]$	$[\frac{1}{2}, 0, z]$	[4]
5	$[X, -Y, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[-X, Y, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	$[-Y, -X, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[7]
8	$[Y, X, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[8]

* Wyckoff site: 8d, site symmetry: 1

Table 10: Wyckoff bond: 8a@8d

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