

SG No. 104  $C_{4v}^6$   $P4nc$  [ 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]	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[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]	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[5, -6]
4	[-Y, -X, 0]	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[7, -8]

Table 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]	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[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: 4b, site symmetry: 2..

Table 4: Wyckoff bond: 4a@4b

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

Table 5: Wyckoff bond: **4b@4b**

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

Table 6: Wyckoff bond: **8c@4b**

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

\* Wyckoff site: **8c**, site symmetry: **1**

Table 7: Wyckoff bond: **8a@8c**

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