

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]