

# 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]