

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]