

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