

SG No. 102 C_{4v}^4 $P4_2nm$ [tetragonal]

* plus set: $+ [0, 0, 0]$

* Wyckoff site: **2a**, site symmetry: **2.mm**

Table 1: Wyckoff bond: **2a@2a**

No.	vector	center	mapping
1	$[X, X, 0]$	$[0, 0, z]$	$[1, -2, -7, 8]$
2	$[-X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3, -4, -5, 6]$

Table 2: Wyckoff bond: **2b@2a**

No.	vector	center	mapping
1	$[X, -X, 0]$	$[0, 0, z]$	$[1, -2, 7, -8]$
2	$[X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3, -4, 5, -6]$

Table 3: Wyckoff bond: **2c@2a**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	$[1, 2, 7, 8]$
2	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3, 4, 5, 6]$

Table 4: Wyckoff bond: **4d@2a**

No.	vector	center	mapping
1	$[X, X, Z]$	$[0, 0, z]$	$[1, 8]$
2	$[-X, -X, Z]$	$[0, 0, z]$	$[2, 7]$
3	$[-X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3, 6]$
4	$[X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[4, 5]$

Table 5: Wyckoff bond: **4e@2a**

No.	vector	center	mapping
1	$[X, -X, Z]$	$[0, 0, z]$	$[1, 7]$
2	$[-X, X, Z]$	$[0, 0, z]$	$[2, 8]$
3	$[X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3, 5]$
4	$[-X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[4, 6]$

Table 6: Wyckoff bond: **4f@2a**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	$[1, -2]$
2	$[-Y, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3, -4]$
3	$[X, -Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[5, -6]$
4	$[-Y, -X, 0]$	$[0, 0, z]$	$[7, -8]$

Table 7: Wyckoff bond: **8g@2a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, z]$	$[1]$
2	$[-X, -Y, Z]$	$[0, 0, z]$	$[2]$
3	$[-Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3]$
4	$[Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[4]$
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	$[-Y, -X, Z]$	$[0, 0, z]$	$[7]$
8	$[Y, X, Z]$	$[0, 0, z]$	$[8]$

* Wyckoff site: **4b**, site symmetry: $2..$

Table 8: Wyckoff bond: **4a@4b**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, z]$	$[1, -2]$
2	$[-Y, X, 0]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[3, -4]$
3	$[X, -Y, 0]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[5, -6]$
4	$[-Y, -X, 0]$	$[\frac{1}{2}, 0, z]$	$[7, -8]$

Table 9: Wyckoff bond: **4b@4b**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, \frac{1}{2}, z]$	$[1, 2]$
2	$[0, 0, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[3, 4]$
3	$[0, 0, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[5, 6]$
4	$[0, 0, Z]$	$[\frac{1}{2}, 0, z]$	$[7, 8]$

Table 10: 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	$[-Y, X, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[3]
4	$[Y, -X, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[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	$[-Y, -X, Z]$	$[\frac{1}{2}, 0, z]$	[7]
8	$[Y, X, Z]$	$[\frac{1}{2}, 0, z]$	[8]

* Wyckoff site: **4c**, site symmetry: $\bar{3}m$

Table 11: Wyckoff bond: **4a@4c**

No.	vector	center	mapping
1	$[X, X, Z]$	$[x, x, z]$	[1,8]
2	$[-X, -X, Z]$	$[-x, -x, z]$	[2,7]
3	$[-X, X, Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]$	[3,6]
4	$[X, -X, Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[4,5]

Table 12: Wyckoff bond: **4b@4c**

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, x, z]$	[1,-8]
2	$[-X, X, 0]$	$[-x, -x, z]$	[2,-7]
3	$[X, X, 0]$	$[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]$	[3,-6]
4	$[-X, -X, 0]$	$[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[4,-5]

Table 13: Wyckoff bond: **8c@4c**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, z]$	[1]
2	$[-X, -Y, Z]$	$[-x, -x, z]$	[2]
3	$[-Y, X, Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]$	[3]
4	$[Y, -X, Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[4]
5	$[X, -Y, Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[5]
6	$[-X, Y, Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	$[-Y, -X, Z]$	$[-x, -x, z]$	[7]
8	$[Y, X, Z]$	$[x, x, z]$	[8]

* Wyckoff site: **8d**, site symmetry: **1**

Table 14: 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	$[-Y, X, Z]$	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[3]
4	$[Y, -X, Z]$	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[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	$[-Y, -X, Z]$	$[-y, -x, z]$	[7]
8	$[Y, X, Z]$	$[y, x, z]$	[8]