

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

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

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

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: . . 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]