

SG No. 86 C_{4h}^4 $P4_2/n$ [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]	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1, 2, -7, -8]
2	[0, 0, Z]	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[3, 4, -5, -6]

Table 2: Wyckoff bond: 4b@2a

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

Table 3: Wyckoff bond: 8c@2a

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

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

Table 4: Wyckoff bond: 2a@2b

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

Table 5: Wyckoff bond: 4b@2b

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

Table 6: Wyckoff bond: 8c@2b

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

* Wyckoff site: 4c, site symmetry: -1

Table 7: Wyckoff bond: 4a@4c

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

* Wyckoff site: 4d, site symmetry: -1

Table 8: Wyckoff bond: 4a@4d

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

* Wyckoff site: 4e, site symmetry: 2..

Table 9: Wyckoff bond: 4a@4e

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

Table 10: Wyckoff bond: 4b@4e

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

Table 11: Wyckoff bond: 8c@4e

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

* Wyckoff site: 4f, site symmetry: 2..

Table 12: Wyckoff bond: 4a@4f

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

Table 13: Wyckoff bond: 4b@4f

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

Table 14: Wyckoff bond: 8c@4f

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

* Wyckoff site: 8g, site symmetry: 1

Table 15: Wyckoff bond: 8a@8g

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