

SG No. 97 D_4^9 $I422$ [tetragonal]

* plus set: $+ [0, 0, 0]$, $+ [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

* Wyckoff site: **2a**, site symmetry: **422**

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, 0]$	$[1, 2, 3, 4, -5, -6, -7, -8]$

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

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

Table 3: Wyckoff bond: **4c@2a**

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

Table 4: Wyckoff bond: **8d@2a**

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

Table 5: Wyckoff bond: **8e@2a**

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

Table 6: Wyckoff bond: 8f@2a

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

Table 7: Wyckoff bond: 16g@2a

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

* Wyckoff site: 2b, site symmetry: 422

Table 8: Wyckoff bond: 2a@2b

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

Table 9: Wyckoff bond: 4b@2b

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

Table 10: Wyckoff bond: 4c@2b

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

Table 11: Wyckoff bond: **8d@2b**

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

Table 12: Wyckoff bond: **8e@2b**

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

Table 13: Wyckoff bond: **8f@2b**

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

Table 14: Wyckoff bond: **16g@2b**

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

* Wyckoff site: **4c**, site symmetry: **222**.

Table 15: Wyckoff bond: 4a@4c

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

Table 16: Wyckoff bond: 4b@4c

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

Table 17: Wyckoff bond: 4c@4c

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

Table 18: Wyckoff bond: 8d@4c

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

Table 19: Wyckoff bond: 8e@4c

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

Table 20: Wyckoff bond: 8f@4c

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

Table 21: Wyckoff bond: 16g@4c

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

* Wyckoff site: 4d, site symmetry: 2.22

Table 22: Wyckoff bond: 4a@4d

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

Table 23: Wyckoff bond: 4b@4d

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

Table 24: Wyckoff bond: 4c@4d

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

Table 25: Wyckoff bond: **8d@4d**

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

Table 26: Wyckoff bond: **8e@4d**

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

Table 27: Wyckoff bond: **8f@4d**

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

Table 28: Wyckoff bond: **16g@4d**

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

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

Table 29: Wyckoff bond: **4a@4e**

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

Table 30: Wyckoff bond: **8b@4e**

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

Table 31: Wyckoff bond: **16c@4e**

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	$[-X, Y, -Z]$	$[0, 0, -z]$	$[5]$
6	$[X, -Y, -Z]$	$[0, 0, -z]$	$[6]$
7	$[Y, X, -Z]$	$[0, 0, -z]$	$[7]$
8	$[-Y, -X, -Z]$	$[0, 0, -z]$	$[8]$

* Wyckoff site: **8f**, site symmetry: $2..$

Table 32: Wyckoff bond: **8a@8f**

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	$[-X, Y, 0]$	$[0, \frac{1}{2}, -z]$	$[5, -6]$
4	$[Y, X, 0]$	$[\frac{1}{2}, 0, -z]$	$[7, -8]$

Table 33: Wyckoff bond: **8b@8f**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, \frac{1}{2}, z]$	$[1, 2]$

continued ...

Table 33

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

Table 34: Wyckoff bond: 16c08f

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	$[-X, Y, -Z]$	$[0, \frac{1}{2}, -z]$	[5]
6	$[X, -Y, -Z]$	$[0, \frac{1}{2}, -z]$	[6]
7	$[Y, X, -Z]$	$[\frac{1}{2}, 0, -z]$	[7]
8	$[-Y, -X, -Z]$	$[\frac{1}{2}, 0, -z]$	[8]

* Wyckoff site: 8g, site symmetry: . . 2

Table 35: Wyckoff bond: 8a08g

No.	vector	center	mapping
1	$[X, -X, Z]$	$[x, x, 0]$	[1,-7]
2	$[-X, X, Z]$	$[-x, -x, 0]$	[2,-8]
3	$[X, X, Z]$	$[-x, x, 0]$	[3,-5]
4	$[-X, -X, Z]$	$[x, -x, 0]$	[4,-6]

Table 36: Wyckoff bond: 8b08g

No.	vector	center	mapping
1	$[X, X, 0]$	$[x, x, 0]$	[1,7]
2	$[-X, -X, 0]$	$[-x, -x, 0]$	[2,8]
3	$[-X, X, 0]$	$[-x, x, 0]$	[3,5]
4	$[X, -X, 0]$	$[x, -x, 0]$	[4,6]

Table 37: Wyckoff bond: $16c@8g$

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

* Wyckoff site: $8h$, site symmetry: $.2$.

Table 38: Wyckoff bond: $8a@8h$

No.	vector	center	mapping
1	$[0, X, Z]$	$[x, 0, 0]$	[1,-6]
2	$[0, -X, Z]$	$[-x, 0, 0]$	[2,-5]
3	$[-X, 0, Z]$	$[0, x, 0]$	[3,-7]
4	$[X, 0, Z]$	$[0, -x, 0]$	[4,-8]

Table 39: Wyckoff bond: $8b@8h$

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	[1,6]
2	$[-X, 0, 0]$	$[-x, 0, 0]$	[2,5]
3	$[0, X, 0]$	$[0, x, 0]$	[3,7]
4	$[0, -X, 0]$	$[0, -x, 0]$	[4,8]

Table 40: Wyckoff bond: $16c@8h$

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

* Wyckoff site: 8i, site symmetry: .2.

Table 41: Wyckoff bond: 8a@8i

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

Table 42: Wyckoff bond: 8b@8i

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

Table 43: Wyckoff bond: 16c@8i

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

* Wyckoff site: 8j, site symmetry: .2

Table 44: Wyckoff bond: 8a@8j

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

Table 45: Wyckoff bond: **8b@8j**

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

Table 46: Wyckoff bond: **16c@8j**

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

* Wyckoff site: **16k**, site symmetry: **1**

Table 47: Wyckoff bond: **16a@16k**

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	$[-X, Y, -Z]$	$[-x, y, -z]$	[5]
6	$[X, -Y, -Z]$	$[x, -y, -z]$	[6]
7	$[Y, X, -Z]$	$[y, x, -z]$	[7]
8	$[-Y, -X, -Z]$	$[-y, -x, -z]$	[8]