

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]	[\mathbf{\frac{1}{2}}, 0, z]	[3,-4]
3	[-X, Y, 0]	[0, $\frac{1}{2}$, -z]	[5,-6]
4	[Y, X, 0]	[\mathbf{\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: 16c@8f

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: 8a@8g

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: 8b@8g

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]