

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

* Wyckoff site: **2a**, site symmetry: **23**.

 Table 1: Wyckoff bond: **6a@2a**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, 0]$	$[1, -2, -3, 4]$
2	$[0, X, 0]$	$[0, 0, 0]$	$[5, -6, -7, 8]$
3	$[0, 0, X]$	$[0, 0, 0]$	$[9, -10, -11, 12]$

 Table 2: Wyckoff bond: **8b@2a**

No.	vector	center	mapping
1	$[X, X, X]$	$[0, 0, 0]$	$[1, 5, 9]$
2	$[-X, -X, X]$	$[0, 0, 0]$	$[2, 7, 12]$
3	$[-X, X, -X]$	$[0, 0, 0]$	$[3, 8, 10]$
4	$[X, -X, -X]$	$[0, 0, 0]$	$[4, 6, 11]$

 Table 3: Wyckoff bond: **12c@2a**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, 0]$	$[1, -2]$
2	$[-X, Y, 0]$	$[0, 0, 0]$	$[3, -4]$
3	$[0, X, Y]$	$[0, 0, 0]$	$[5, -6]$
4	$[0, -X, Y]$	$[0, 0, 0]$	$[7, -8]$
5	$[Y, 0, X]$	$[0, 0, 0]$	$[9, -10]$
6	$[Y, 0, -X]$	$[0, 0, 0]$	$[11, -12]$

 Table 4: Wyckoff bond: **24d@2a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[0, 0, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[0, 0, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[0, 0, 0]$	$[4]$
5	$[Z, X, Y]$	$[0, 0, 0]$	$[5]$
6	$[Z, -X, -Y]$	$[0, 0, 0]$	$[6]$
7	$[-Z, -X, Y]$	$[0, 0, 0]$	$[7]$
8	$[-Z, X, -Y]$	$[0, 0, 0]$	$[8]$
9	$[Y, Z, X]$	$[0, 0, 0]$	$[9]$
10	$[-Y, Z, -X]$	$[0, 0, 0]$	$[10]$

continued ...

Table 4

No.	vector	center	mapping
11	$[Y, -Z, -X]$	$[0, 0, 0]$	$[11]$
12	$[-Y, -Z, X]$	$[0, 0, 0]$	$[12]$

* Wyckoff site: 6b, site symmetry: 222..

Table 5: Wyckoff bond: 6a@6b

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, -3, 4]$
2	$[0, X, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -6, -7, 8]$
3	$[0, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -10, -11, 12]$

Table 6: Wyckoff bond: 6b@6b

No.	vector	center	mapping
1	$[0, 0, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, -3, -4]$
2	$[X, 0, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, 6, -7, -8]$
3	$[0, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, 10, -11, -12]$

Table 7: Wyckoff bond: 6c@6b

No.	vector	center	mapping
1	$[0, X, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, 3, -4]$
2	$[0, 0, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -6, 7, -8]$
3	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -10, 11, -12]$

Table 8: Wyckoff bond: 12d@6b

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2]$
2	$[-X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -4]$
3	$[0, X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -6]$
4	$[0, -X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[7, -8]$
5	$[Y, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -10]$
6	$[Y, 0, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[11, -12]$

Table 9: Wyckoff bond: 12e@6b

No.	vector	center	mapping
1	$[Y, 0, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -3]$
2	$[-Y, 0, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, -4]$
3	$[X, Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -7]$
4	$[X, -Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[6, -8]$
5	$[0, X, Y]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -11]$
6	$[0, X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[10, -12]$

Table 10: Wyckoff bond: 12f@6b

No.	vector	center	mapping
1	$[0, X, Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -4]$
2	$[0, -X, Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, -3]$
3	$[Y, 0, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -8]$
4	$[Y, 0, -X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[6, -7]$
5	$[X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -12]$
6	$[-X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[10, -11]$

Table 11: Wyckoff bond: 24g@6b

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1]$
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3]$
4	$[X, -Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[4]$
5	$[Z, X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5]$
6	$[Z, -X, -Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[6]$
7	$[-Z, -X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[7]$
8	$[-Z, X, -Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[8]$
9	$[Y, Z, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9]$
10	$[-Y, Z, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[10]$
11	$[Y, -Z, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[11]$
12	$[-Y, -Z, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[12]$

* Wyckoff site: 8c, site symmetry: .3.

Table 12: Wyckoff bond: 8a@8c

No.	vector	center	mapping
1	$[X, X, X]$	$[x, x, x]$	$[1, 5, 9]$

continued ...

Table 12

No.	vector	center	mapping
2	$[-X, -X, X]$	$[-x, -x, x]$	[2,7,12]
3	$[-X, X, -X]$	$[-x, x, -x]$	[3,8,10]
4	$[X, -X, -X]$	$[x, -x, -x]$	[4,6,11]

Table 13: Wyckoff bond: 24b@8c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, x]$	[1]
2	$[-X, -Y, Z]$	$[-x, -x, x]$	[2]
3	$[-X, Y, -Z]$	$[-x, x, -x]$	[3]
4	$[X, -Y, -Z]$	$[x, -x, -x]$	[4]
5	$[Z, X, Y]$	$[x, x, x]$	[5]
6	$[Z, -X, -Y]$	$[x, -x, -x]$	[6]
7	$[-Z, -X, Y]$	$[-x, -x, x]$	[7]
8	$[-Z, X, -Y]$	$[-x, x, -x]$	[8]
9	$[Y, Z, X]$	$[x, x, x]$	[9]
10	$[-Y, Z, -X]$	$[-x, x, -x]$	[10]
11	$[Y, -Z, -X]$	$[x, -x, -x]$	[11]
12	$[-Y, -Z, X]$	$[-x, -x, x]$	[12]

* Wyckoff site: 12d, site symmetry: 2..

Table 14: Wyckoff bond: 12a@12d

No.	vector	center	mapping
1	$[0, X, Y]$	$[x, 0, 0]$	[1,-4]
2	$[0, -X, Y]$	$[-x, 0, 0]$	[2,-3]
3	$[Y, 0, X]$	$[0, x, 0]$	[5,-8]
4	$[Y, 0, -X]$	$[0, -x, 0]$	[6,-7]
5	$[X, Y, 0]$	$[0, 0, x]$	[9,-12]
6	$[-X, Y, 0]$	$[0, 0, -x]$	[10,-11]

Table 15: Wyckoff bond: 12b@12d

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	[1,4]
2	$[-X, 0, 0]$	$[-x, 0, 0]$	[2,3]
3	$[0, X, 0]$	$[0, x, 0]$	[5,8]
4	$[0, -X, 0]$	$[0, -x, 0]$	[6,7]
5	$[0, 0, X]$	$[0, 0, x]$	[9,12]

continued ...

Table 15

No.	vector	center	mapping
6	$[0, 0, -X]$	$[0, 0, -x]$	$[10, 11]$

Table 16: Wyckoff bond: 24c@12d

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, 0, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[-x, 0, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[x, 0, 0]$	$[4]$
5	$[Z, X, Y]$	$[0, x, 0]$	$[5]$
6	$[Z, -X, -Y]$	$[0, -x, 0]$	$[6]$
7	$[-Z, -X, Y]$	$[0, -x, 0]$	$[7]$
8	$[-Z, X, -Y]$	$[0, x, 0]$	$[8]$
9	$[Y, Z, X]$	$[0, 0, x]$	$[9]$
10	$[-Y, Z, -X]$	$[0, 0, -x]$	$[10]$
11	$[Y, -Z, -X]$	$[0, 0, -x]$	$[11]$
12	$[-Y, -Z, X]$	$[0, 0, x]$	$[12]$

* Wyckoff site: 12e, site symmetry: 2 . .

Table 17: Wyckoff bond: 12a@12e

No.	vector	center	mapping
1	$[0, X, Y]$	$[x, \frac{1}{2}, 0]$	$[1, -4]$
2	$[0, -X, Y]$	$[-x, \frac{1}{2}, 0]$	$[2, -3]$
3	$[Y, 0, X]$	$[0, x, \frac{1}{2}]$	$[5, -8]$
4	$[Y, 0, -X]$	$[0, -x, \frac{1}{2}]$	$[6, -7]$
5	$[X, Y, 0]$	$[\frac{1}{2}, 0, x]$	$[9, -12]$
6	$[-X, Y, 0]$	$[\frac{1}{2}, 0, -x]$	$[10, -11]$

Table 18: Wyckoff bond: 12b@12e

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, \frac{1}{2}, 0]$	$[1, 4]$
2	$[-X, 0, 0]$	$[-x, \frac{1}{2}, 0]$	$[2, 3]$
3	$[0, X, 0]$	$[0, x, \frac{1}{2}]$	$[5, 8]$
4	$[0, -X, 0]$	$[0, -x, \frac{1}{2}]$	$[6, 7]$
5	$[0, 0, X]$	$[\frac{1}{2}, 0, x]$	$[9, 12]$
6	$[0, 0, -X]$	$[\frac{1}{2}, 0, -x]$	$[10, 11]$

Table 19: Wyckoff bond: 24c@12e

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, \frac{1}{2}, 0]$	[1]
2	$[-X, -Y, Z]$	$[-x, \frac{1}{2}, 0]$	[2]
3	$[-X, Y, -Z]$	$[-x, \frac{1}{2}, 0]$	[3]
4	$[X, -Y, -Z]$	$[x, \frac{1}{2}, 0]$	[4]
5	$[Z, X, Y]$	$[0, x, \frac{1}{2}]$	[5]
6	$[Z, -X, -Y]$	$[0, -x, \frac{1}{2}]$	[6]
7	$[-Z, -X, Y]$	$[0, -x, \frac{1}{2}]$	[7]
8	$[-Z, X, -Y]$	$[0, x, \frac{1}{2}]$	[8]
9	$[Y, Z, X]$	$[\frac{1}{2}, 0, x]$	[9]
10	$[-Y, Z, -X]$	$[\frac{1}{2}, 0, -x]$	[10]
11	$[Y, -Z, -X]$	$[\frac{1}{2}, 0, -x]$	[11]
12	$[-Y, -Z, X]$	$[\frac{1}{2}, 0, x]$	[12]

* Wyckoff site: 24f, site symmetry: 1

Table 20: Wyckoff bond: 24a@24f

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-X, -Y, Z]$	$[-x, -y, z]$	[2]
3	$[-X, Y, -Z]$	$[-x, y, -z]$	[3]
4	$[X, -Y, -Z]$	$[x, -y, -z]$	[4]
5	$[Z, X, Y]$	$[z, x, y]$	[5]
6	$[Z, -X, -Y]$	$[z, -x, -y]$	[6]
7	$[-Z, -X, Y]$	$[-z, -x, y]$	[7]
8	$[-Z, X, -Y]$	$[-z, x, -y]$	[8]
9	$[Y, Z, X]$	$[y, z, x]$	[9]
10	$[-Y, Z, -X]$	$[-y, z, -x]$	[10]
11	$[Y, -Z, -X]$	$[y, -z, -x]$	[11]
12	$[-Y, -Z, X]$	$[-y, -z, x]$	[12]