

SG No. 196 $T^2 F23$ [cubic]

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

* Wyckoff site: **4a**, site symmetry: **23**.

Table 1: Wyckoff bond: **12a@4a**

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: **16b@4a**

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: **24c@4a**

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: **48d@4a**

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: 4b, site symmetry: 23.

Table 5: Wyckoff bond: 12a@4b

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

Table 6: Wyckoff bond: 16b@4b

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

Table 7: Wyckoff bond: 24c@4b

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

Table 8: Wyckoff bond: 48d@4b

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

continued ...

Table 8

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

* Wyckoff site: 4c, site symmetry: 23.

Table 9: Wyckoff bond: 12a@4c

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

Table 10: Wyckoff bond: 16b@4c

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

Table 11: Wyckoff bond: 24c@4c

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

Table 12: Wyckoff bond: 48d@4c

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

* Wyckoff site: 4d, site symmetry: 23.

Table 13: Wyckoff bond: 12a@4d

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

Table 14: Wyckoff bond: 16b@4d

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

Table 15: Wyckoff bond: 24c@4d

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

Table 16: Wyckoff bond: 48d@4d

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

* Wyckoff site: 16e, site symmetry: $\cdot 3$.

Table 17: Wyckoff bond: 16a@16e

No.	vector	center	mapping
1	$[X, X, X]$	$[x, x, x]$	[1,5,9]
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 18: Wyckoff bond: 48b@16e

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: 24f, site symmetry: $2..$

Table 19: Wyckoff bond: 24a@24f

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 20: Wyckoff bond: 24b@24f

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	$[0, 0, X]$	$[0, 0, x]$	$[9, 12]$
6	$[0, 0, -X]$	$[0, 0, -x]$	$[10, 11]$

Table 21: Wyckoff bond: 48c@24f

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: 24g, site symmetry: 2..

Table 22: Wyckoff bond: 24a@24g

No.	vector	center	mapping
1	$[0, X, Y]$	$[x, \frac{1}{4}, \frac{1}{4}]$	$[1, -4]$

continued ...

Table 22

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

Table 23: Wyckoff bond: 24b@24g

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

Table 24: Wyckoff bond: 48c@24g

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

* Wyckoff site: 48h, site symmetry: 1

Table 25: Wyckoff bond: 48a@48h

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]

continued ...

Table 25

No.	vector	center	mapping
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]