

SG No. 220  $T_d^6$   $I\bar{4}3d$  [ cubic ]

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

\* Wyckoff site: 12a, site symmetry:  $-4..$

Table 1: Wyckoff bond: 12a@12a

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{3}{8}, 0, \frac{1}{4}]$	$[1, 4, -18, -19]$
2	$[-X, 0, 0]$	$[\frac{1}{8}, 0, \frac{3}{4}]$	$[2, 3, -17, -20]$
3	$[0, X, 0]$	$[\frac{1}{4}, \frac{3}{8}, 0]$	$[5, 8, -14, -15]$
4	$[0, -X, 0]$	$[\frac{3}{4}, \frac{1}{8}, 0]$	$[6, 7, -13, -16]$
5	$[0, 0, X]$	$[0, \frac{1}{4}, \frac{3}{8}]$	$[9, 12, -22, -23]$
6	$[0, 0, -X]$	$[0, \frac{3}{4}, \frac{1}{8}]$	$[10, 11, -21, -24]$

Table 2: Wyckoff bond: 24b@12a

No.	vector	center	mapping
1	$[0, X, Y]$	$[\frac{3}{8}, 0, \frac{1}{4}]$	$[1, -4]$
2	$[0, -X, Y]$	$[\frac{1}{8}, 0, \frac{3}{4}]$	$[2, -3]$
3	$[Y, 0, X]$	$[\frac{1}{4}, \frac{3}{8}, 0]$	$[5, -8]$
4	$[Y, 0, -X]$	$[\frac{3}{4}, \frac{1}{8}, 0]$	$[6, -7]$
5	$[X, Y, 0]$	$[0, \frac{1}{4}, \frac{3}{8}]$	$[9, -12]$
6	$[-X, Y, 0]$	$[0, \frac{3}{4}, \frac{1}{8}]$	$[10, -11]$
7	$[X, 0, Y]$	$[\frac{3}{4}, \frac{1}{8}, 0]$	$[13, -16]$
8	$[-X, 0, Y]$	$[\frac{1}{4}, \frac{3}{8}, 0]$	$[14, -15]$
9	$[0, Y, X]$	$[\frac{1}{8}, 0, \frac{3}{4}]$	$[17, -20]$
10	$[0, Y, -X]$	$[\frac{3}{8}, 0, \frac{1}{4}]$	$[18, -19]$
11	$[Y, X, 0]$	$[0, \frac{3}{4}, \frac{1}{8}]$	$[21, -24]$
12	$[Y, -X, 0]$	$[0, \frac{1}{4}, \frac{3}{8}]$	$[22, -23]$

Table 3: Wyckoff bond: 48c@12a

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

*continued ...*

Table 3

No.	vector	center	mapping
12	$[-Y, -Z, X]$	$[0, \frac{1}{4}, \frac{3}{8}]$	[12]
13	$[Y, X, Z]$	$[\frac{3}{4}, \frac{1}{8}, 0]$	[13]
14	$[-Y, -X, Z]$	$[\frac{1}{4}, \frac{3}{8}, 0]$	[14]
15	$[Y, -X, -Z]$	$[\frac{1}{4}, \frac{3}{8}, 0]$	[15]
16	$[-Y, X, -Z]$	$[\frac{3}{4}, \frac{1}{8}, 0]$	[16]
17	$[X, Z, Y]$	$[\frac{1}{8}, 0, \frac{3}{4}]$	[17]
18	$[-X, Z, -Y]$	$[\frac{3}{8}, 0, \frac{1}{4}]$	[18]
19	$[-X, -Z, Y]$	$[\frac{3}{8}, 0, \frac{1}{4}]$	[19]
20	$[X, -Z, -Y]$	$[\frac{1}{8}, 0, \frac{3}{4}]$	[20]
21	$[Z, Y, X]$	$[0, \frac{3}{4}, \frac{1}{8}]$	[21]
22	$[Z, -Y, -X]$	$[0, \frac{1}{4}, \frac{3}{8}]$	[22]
23	$[-Z, Y, -X]$	$[0, \frac{1}{4}, \frac{3}{8}]$	[23]
24	$[-Z, -Y, X]$	$[0, \frac{3}{4}, \frac{1}{8}]$	[24]

\* Wyckoff site: 12b, site symmetry:  $-4..$

Table 4: Wyckoff bond: 12a@12b

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{7}{8}, 0, \frac{1}{4}]$	[1, 4, -18, -19]
2	$[-X, 0, 0]$	$[\frac{5}{8}, 0, \frac{3}{4}]$	[2, 3, -17, -20]
3	$[0, X, 0]$	$[\frac{1}{4}, \frac{7}{8}, 0]$	[5, 8, -14, -15]
4	$[0, -X, 0]$	$[\frac{3}{4}, \frac{5}{8}, 0]$	[6, 7, -13, -16]
5	$[0, 0, X]$	$[0, \frac{1}{4}, \frac{7}{8}]$	[9, 12, -22, -23]
6	$[0, 0, -X]$	$[0, \frac{3}{4}, \frac{5}{8}]$	[10, 11, -21, -24]

Table 5: Wyckoff bond: 24b@12b

No.	vector	center	mapping
1	$[0, X, Y]$	$[\frac{7}{8}, 0, \frac{1}{4}]$	[1, -4]
2	$[0, -X, Y]$	$[\frac{5}{8}, 0, \frac{3}{4}]$	[2, -3]
3	$[Y, 0, X]$	$[\frac{1}{4}, \frac{7}{8}, 0]$	[5, -8]
4	$[Y, 0, -X]$	$[\frac{3}{4}, \frac{5}{8}, 0]$	[6, -7]
5	$[X, Y, 0]$	$[0, \frac{1}{4}, \frac{7}{8}]$	[9, -12]
6	$[-X, Y, 0]$	$[0, \frac{3}{4}, \frac{5}{8}]$	[10, -11]
7	$[X, 0, Y]$	$[\frac{3}{4}, \frac{5}{8}, 0]$	[13, -16]
8	$[-X, 0, Y]$	$[\frac{1}{4}, \frac{7}{8}, 0]$	[14, -15]
9	$[0, Y, X]$	$[\frac{5}{8}, 0, \frac{3}{4}]$	[17, -20]
10	$[0, Y, -X]$	$[\frac{7}{8}, 0, \frac{1}{4}]$	[18, -19]
11	$[Y, X, 0]$	$[0, \frac{3}{4}, \frac{5}{8}]$	[21, -24]
12	$[Y, -X, 0]$	$[0, \frac{1}{4}, \frac{7}{8}]$	[22, -23]

Table 6: Wyckoff bond: 48c@12b

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{7}{8}, 0, \frac{1}{4}]$	[1]
2	$[-X, -Y, Z]$	$[\frac{5}{8}, 0, \frac{3}{4}]$	[2]
3	$[-X, Y, -Z]$	$[\frac{5}{8}, 0, \frac{3}{4}]$	[3]
4	$[X, -Y, -Z]$	$[\frac{7}{8}, 0, \frac{1}{4}]$	[4]
5	$[Z, X, Y]$	$[\frac{1}{4}, \frac{7}{8}, 0]$	[5]
6	$[Z, -X, -Y]$	$[\frac{3}{4}, \frac{5}{8}, 0]$	[6]
7	$[-Z, -X, Y]$	$[\frac{3}{4}, \frac{5}{8}, 0]$	[7]
8	$[-Z, X, -Y]$	$[\frac{1}{4}, \frac{7}{8}, 0]$	[8]
9	$[Y, Z, X]$	$[0, \frac{1}{4}, \frac{7}{8}]$	[9]
10	$[-Y, Z, -X]$	$[0, \frac{3}{4}, \frac{5}{8}]$	[10]
11	$[Y, -Z, -X]$	$[0, \frac{3}{4}, \frac{5}{8}]$	[11]
12	$[-Y, -Z, X]$	$[0, \frac{1}{4}, \frac{7}{8}]$	[12]
13	$[Y, X, Z]$	$[\frac{3}{4}, \frac{5}{8}, 0]$	[13]
14	$[-Y, -X, Z]$	$[\frac{1}{4}, \frac{7}{8}, 0]$	[14]
15	$[Y, -X, -Z]$	$[\frac{1}{4}, \frac{7}{8}, 0]$	[15]
16	$[-Y, X, -Z]$	$[\frac{3}{4}, \frac{5}{8}, 0]$	[16]
17	$[X, Z, Y]$	$[\frac{5}{8}, 0, \frac{3}{4}]$	[17]
18	$[-X, Z, -Y]$	$[\frac{7}{8}, 0, \frac{1}{4}]$	[18]
19	$[-X, -Z, Y]$	$[\frac{7}{8}, 0, \frac{1}{4}]$	[19]
20	$[X, -Z, -Y]$	$[\frac{5}{8}, 0, \frac{3}{4}]$	[20]
21	$[Z, Y, X]$	$[0, \frac{3}{4}, \frac{5}{8}]$	[21]
22	$[Z, -Y, -X]$	$[0, \frac{1}{4}, \frac{7}{8}]$	[22]
23	$[-Z, Y, -X]$	$[0, \frac{1}{4}, \frac{7}{8}]$	[23]
24	$[-Z, -Y, X]$	$[0, \frac{3}{4}, \frac{5}{8}]$	[24]

\* Wyckoff site: 16c, site symmetry: .3.

Table 7: Wyckoff bond: 16a@16c

No.	vector	center	mapping
1	$[X, X, X]$	$[x, x, x]$	[1,5,9]
2	$[-X, -X, X]$	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	[2,7,12]
3	$[-X, X, -X]$	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	[3,8,10]
4	$[X, -X, -X]$	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	[4,6,11]
5	$[X, X, X]$	$[x + \frac{1}{4}, x + \frac{1}{4}, x + \frac{1}{4}]$	[13,17,21]
6	$[-X, -X, X]$	$[\frac{1}{4} - x, \frac{3}{4} - x, x + \frac{3}{4}]$	[14,19,24]
7	$[X, -X, -X]$	$[x + \frac{3}{4}, \frac{1}{4} - x, \frac{3}{4} - x]$	[15,20,22]
8	$[-X, X, -X]$	$[\frac{3}{4} - x, x + \frac{3}{4}, \frac{1}{4} - x]$	[16,18,23]

Table 8: Wyckoff bond: 48b@16c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, x]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	[2]
3	$[-X, Y, -Z]$	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	[3]
4	$[X, -Y, -Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	[4]
5	$[Z, X, Y]$	$[x, x, x]$	[5]
6	$[Z, -X, -Y]$	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	[6]
7	$[-Z, -X, Y]$	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	[7]
8	$[-Z, X, -Y]$	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	[8]
9	$[Y, Z, X]$	$[x, x, x]$	[9]
10	$[-Y, Z, -X]$	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	[10]
11	$[Y, -Z, -X]$	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	[11]
12	$[-Y, -Z, X]$	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	[12]
13	$[Y, X, Z]$	$[x + \frac{1}{4}, x + \frac{1}{4}, x + \frac{1}{4}]$	[13]
14	$[-Y, -X, Z]$	$[\frac{1}{4} - x, \frac{3}{4} - x, x + \frac{3}{4}]$	[14]
15	$[Y, -X, -Z]$	$[x + \frac{3}{4}, \frac{1}{4} - x, \frac{3}{4} - x]$	[15]
16	$[-Y, X, -Z]$	$[\frac{3}{4} - x, x + \frac{3}{4}, \frac{1}{4} - x]$	[16]
17	$[X, Z, Y]$	$[x + \frac{1}{4}, x + \frac{1}{4}, x + \frac{1}{4}]$	[17]
18	$[-X, Z, -Y]$	$[\frac{3}{4} - x, x + \frac{3}{4}, \frac{1}{4} - x]$	[18]
19	$[-X, -Z, Y]$	$[\frac{1}{4} - x, \frac{3}{4} - x, x + \frac{3}{4}]$	[19]
20	$[X, -Z, -Y]$	$[x + \frac{3}{4}, \frac{1}{4} - x, \frac{3}{4} - x]$	[20]
21	$[Z, Y, X]$	$[x + \frac{1}{4}, x + \frac{1}{4}, x + \frac{1}{4}]$	[21]
22	$[Z, -Y, -X]$	$[x + \frac{3}{4}, \frac{1}{4} - x, \frac{3}{4} - x]$	[22]
23	$[-Z, Y, -X]$	$[\frac{3}{4} - x, x + \frac{3}{4}, \frac{1}{4} - x]$	[23]
24	$[-Z, -Y, X]$	$[\frac{1}{4} - x, \frac{3}{4} - x, x + \frac{3}{4}]$	[24]

\* Wyckoff site: 24d, site symmetry: 2..

Table 9: Wyckoff bond: 24a@24d

No.	vector	center	mapping
1	$[0, X, Y]$	$[x, 0, \frac{1}{4}]$	[1, -4]
2	$[0, -X, Y]$	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[2, -3]
3	$[Y, 0, X]$	$[\frac{1}{4}, x, 0]$	[5, -8]
4	$[Y, 0, -X]$	$[\frac{3}{4}, \frac{1}{2} - x, 0]$	[6, -7]
5	$[X, Y, 0]$	$[0, \frac{1}{4}, x]$	[9, -12]
6	$[-X, Y, 0]$	$[0, \frac{3}{4}, \frac{1}{2} - x]$	[10, -11]
7	$[X, 0, Y]$	$[\frac{1}{4}, x + \frac{1}{4}, \frac{1}{2}]$	[13, -16]
8	$[-X, 0, Y]$	$[\frac{1}{4}, \frac{3}{4} - x, 0]$	[14, -15]
9	$[0, Y, X]$	$[x + \frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[17, -20]
10	$[0, Y, -X]$	$[\frac{3}{4} - x, 0, \frac{1}{4}]$	[18, -19]
11	$[Y, X, 0]$	$[\frac{1}{2}, \frac{1}{4}, x + \frac{1}{4}]$	[21, -24]
12	$[Y, -X, 0]$	$[0, \frac{1}{4}, \frac{3}{4} - x]$	[22, -23]

Table 10: Wyckoff bond: 24b@24d

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, \frac{1}{4}]$	[1,4]
2	$[-X, 0, 0]$	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[2,3]
3	$[0, X, 0]$	$[\frac{1}{4}, x, 0]$	[5,8]
4	$[0, -X, 0]$	$[\frac{3}{4}, \frac{1}{2} - x, 0]$	[6,7]
5	$[0, 0, X]$	$[0, \frac{1}{4}, x]$	[9,12]
6	$[0, 0, -X]$	$[0, \frac{3}{4}, \frac{1}{2} - x]$	[10,11]
7	$[0, X, 0]$	$[\frac{1}{4}, x + \frac{1}{4}, \frac{1}{2}]$	[13,16]
8	$[0, -X, 0]$	$[\frac{1}{4}, \frac{3}{4} - x, 0]$	[14,15]
9	$[X, 0, 0]$	$[x + \frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[17,20]
10	$[-X, 0, 0]$	$[\frac{3}{4} - x, 0, \frac{1}{4}]$	[18,19]
11	$[0, 0, X]$	$[\frac{1}{2}, \frac{1}{4}, x + \frac{1}{4}]$	[21,24]
12	$[0, 0, -X]$	$[0, \frac{1}{4}, \frac{3}{4} - x]$	[22,23]

Table 11: Wyckoff bond: 48c@24d

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, \frac{1}{4}]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[2]
3	$[-X, Y, -Z]$	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[3]
4	$[X, -Y, -Z]$	$[x, 0, \frac{1}{4}]$	[4]
5	$[Z, X, Y]$	$[\frac{1}{4}, x, 0]$	[5]
6	$[Z, -X, -Y]$	$[\frac{3}{4}, \frac{1}{2} - x, 0]$	[6]
7	$[-Z, -X, Y]$	$[\frac{3}{4}, \frac{1}{2} - x, 0]$	[7]
8	$[-Z, X, -Y]$	$[\frac{1}{4}, x, 0]$	[8]
9	$[Y, Z, X]$	$[0, \frac{1}{4}, x]$	[9]
10	$[-Y, Z, -X]$	$[0, \frac{3}{4}, \frac{1}{2} - x]$	[10]
11	$[Y, -Z, -X]$	$[0, \frac{3}{4}, \frac{1}{2} - x]$	[11]
12	$[-Y, -Z, X]$	$[0, \frac{1}{4}, x]$	[12]
13	$[Y, X, Z]$	$[\frac{1}{4}, x + \frac{1}{4}, \frac{1}{2}]$	[13]
14	$[-Y, -X, Z]$	$[\frac{1}{4}, \frac{3}{4} - x, 0]$	[14]
15	$[Y, -X, -Z]$	$[\frac{1}{4}, \frac{3}{4} - x, 0]$	[15]
16	$[-Y, X, -Z]$	$[\frac{1}{4}, x + \frac{1}{4}, \frac{1}{2}]$	[16]
17	$[X, Z, Y]$	$[x + \frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[17]
18	$[-X, Z, -Y]$	$[\frac{3}{4} - x, 0, \frac{1}{4}]$	[18]
19	$[-X, -Z, Y]$	$[\frac{3}{4} - x, 0, \frac{1}{4}]$	[19]
20	$[X, -Z, -Y]$	$[x + \frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[20]
21	$[Z, Y, X]$	$[\frac{1}{2}, \frac{1}{4}, x + \frac{1}{4}]$	[21]
22	$[Z, -Y, -X]$	$[0, \frac{1}{4}, \frac{3}{4} - x]$	[22]
23	$[-Z, Y, -X]$	$[0, \frac{1}{4}, \frac{3}{4} - x]$	[23]
24	$[-Z, -Y, X]$	$[\frac{1}{2}, \frac{1}{4}, x + \frac{1}{4}]$	[24]

\* Wyckoff site: 48e, site symmetry: 1

Table 12: Wyckoff bond: 48a@48e

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[2]
3	$[-X, Y, -Z]$	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[3]
4	$[X, -Y, -Z]$	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[4]
5	$[Z, X, Y]$	$[z, x, y]$	[5]
6	$[Z, -X, -Y]$	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[6]
7	$[-Z, -X, Y]$	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[7]
8	$[-Z, X, -Y]$	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[8]
9	$[Y, Z, X]$	$[y, z, x]$	[9]
10	$[-Y, Z, -X]$	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[10]
11	$[Y, -Z, -X]$	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[11]
12	$[-Y, -Z, X]$	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[12]
13	$[Y, X, Z]$	$[y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}]$	[13]
14	$[-Y, -X, Z]$	$[\frac{1}{4} - y, \frac{3}{4} - x, z + \frac{3}{4}]$	[14]
15	$[Y, -X, -Z]$	$[y + \frac{3}{4}, \frac{1}{4} - x, \frac{3}{4} - z]$	[15]
16	$[-Y, X, -Z]$	$[\frac{3}{4} - y, x + \frac{3}{4}, \frac{1}{4} - z]$	[16]
17	$[X, Z, Y]$	$[x + \frac{1}{4}, z + \frac{1}{4}, y + \frac{1}{4}]$	[17]
18	$[-X, Z, -Y]$	$[\frac{3}{4} - x, z + \frac{3}{4}, \frac{1}{4} - y]$	[18]
19	$[-X, -Z, Y]$	$[\frac{1}{4} - x, \frac{3}{4} - z, y + \frac{3}{4}]$	[19]
20	$[X, -Z, -Y]$	$[x + \frac{3}{4}, \frac{1}{4} - z, \frac{3}{4} - y]$	[20]
21	$[Z, Y, X]$	$[z + \frac{1}{4}, y + \frac{1}{4}, x + \frac{1}{4}]$	[21]
22	$[Z, -Y, -X]$	$[z + \frac{3}{4}, \frac{1}{4} - y, \frac{3}{4} - x]$	[22]
23	$[-Z, Y, -X]$	$[\frac{3}{4} - z, y + \frac{3}{4}, \frac{1}{4} - x]$	[23]
24	$[-Z, -Y, X]$	$[\frac{1}{4} - z, \frac{3}{4} - y, x + \frac{3}{4}]$	[24]