PG No. 31 T_d $\bar{4}3m$ [cubic]

* Wyckoff site: `4a`, site symmetry: `.3m`

Table 1: Wyckoff bond: `4a@4a`

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

Table 2: Wyckoff bond: `12b@4a`

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

Table 3: Wyckoff bond: `12c@4a`

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

Table 4: Wyckoff bond: `24d@4a`

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]
13	$[Y, X, Z]$	$[x, x, x]$	[13]
14	$[-Y, -X, Z]$	$[-x, -x, x]$	[14]
15	$[Y, -X, -Z]$	$[x, -x, -x]$	[15]
16	$[-Y, X, -Z]$	$[-x, x, -x]$	[16]
17	$[X, Z, Y]$	$[x, x, x]$	[17]
18	$[-X, Z, -Y]$	$[-x, x, -x]$	[18]
19	$[-X, -Z, Y]$	$[-x, -x, x]$	[19]
20	$[X, -Z, -Y]$	$[x, -x, -x]$	[20]
21	$[Z, Y, X]$	$[x, x, x]$	[21]
22	$[Z, -Y, -X]$	$[x, -x, -x]$	[22]
23	$[-Z, Y, -X]$	$[-x, x, -x]$	[23]
24	$[-Z, -Y, X]$	$[-x, -x, x]$	[24]

* Wyckoff site: `6b`, site symmetry: `2.mm`

Table 5: Wyckoff bond: `6a@6b`

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

Table 6: Wyckoff bond: `6b@6b`

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	[1,4,17,20]
2	$[-X, 0, 0]$	$[-x, 0, 0]$	[2,3,18,19]

continued ...

Table 6

No.	vector	center	mapping
3	$[0, X, 0]$	$[0, x, 0]$	[5,8,13,16]
4	$[0, -X, 0]$	$[0, -x, 0]$	[6,7,14,15]
5	$[0, 0, X]$	$[0, 0, x]$	[9,12,21,24]
6	$[0, 0, -X]$	$[0, 0, -x]$	[10,11,22,23]

Table 7: Wyckoff bond: `12c@6b`

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

Table 8: Wyckoff bond: `12d@6b`

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]
7	$[X, 0, Y]$	$[0, x, 0]$	[13,-16]
8	$[-X, 0, Y]$	$[0, -x, 0]$	[14,-15]
9	$[0, Y, X]$	$[x, 0, 0]$	[17,-20]
10	$[0, Y, -X]$	$[-x, 0, 0]$	[18,-19]
11	$[Y, X, 0]$	$[0, 0, x]$	[21,-24]
12	$[Y, -X, 0]$	$[0, 0, -x]$	[22,-23]

Table 9: Wyckoff bond: `24e@6b`

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]
13	$[Y, X, Z]$	$[0, x, 0]$	[13]
14	$[-Y, -X, Z]$	$[0, -x, 0]$	[14]
15	$[Y, -X, -Z]$	$[0, -x, 0]$	[15]
16	$[-Y, X, -Z]$	$[0, x, 0]$	[16]
17	$[X, Z, Y]$	$[x, 0, 0]$	[17]
18	$[-X, Z, -Y]$	$[-x, 0, 0]$	[18]
19	$[-X, -Z, Y]$	$[-x, 0, 0]$	[19]
20	$[X, -Z, -Y]$	$[x, 0, 0]$	[20]
21	$[Z, Y, X]$	$[0, 0, x]$	[21]
22	$[Z, -Y, -X]$	$[0, 0, -x]$	[22]
23	$[-Z, Y, -X]$	$[0, 0, -x]$	[23]
24	$[-Z, -Y, X]$	$[0, 0, x]$	[24]

* Wyckoff site: `12c`, site symmetry: `..m`

Table 10: Wyckoff bond: `12a@12c`

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

Table 11: Wyckoff bond: `12b@12c`

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

Table 12: Wyckoff bond: `24c@12c`

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

* Wyckoff site: `24d`, site symmetry: `1`

Table 13: Wyckoff bond: `24a@24d`

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]
13	$[Y, X, Z]$	$[y, x, z]$	[13]
14	$[-Y, -X, Z]$	$[-y, -x, z]$	[14]
15	$[Y, -X, -Z]$	$[y, -x, -z]$	[15]
16	$[-Y, X, -Z]$	$[-y, x, -z]$	[16]
17	$[X, Z, Y]$	$[x, z, y]$	[17]
18	$[-X, Z, -Y]$	$[-x, z, -y]$	[18]
19	$[-X, -Z, Y]$	$[-x, -z, y]$	[19]
20	$[X, -Z, -Y]$	$[x, -z, -y]$	[20]
21	$[Z, Y, X]$	$[z, y, x]$	[21]
22	$[Z, -Y, -X]$	$[z, -y, -x]$	[22]
23	$[-Z, Y, -X]$	$[-z, y, -x]$	[23]
24	$[-Z, -Y, X]$	$[-z, -y, x]$	[24]