

13. ISOMORPHIC SUBGROUPS OF SPACE GROUPS

Table 13.2.2.1. Three-dimensional derivative lattices of indices 2 to 7 (cont.)

Index 7	1(7a, b, c); 2(a, 7b, c); 3(a, b, 7c); 4(7a, b + a, c); 5(7a, b, c + b); 6(a, 7b, c + b); 7(7a, b - a, c); 8(7a, b, c - a); 9(a, 7b, c - b); 10(7a, b + 2a, c); 11(7a, b, c - 3a); 12(a, 7b, c + 2b); 13(7a, b - 3a, c); 14(7a, b, c + 2a); 15(a, 7b, c - 3b); 16(7a, b - 2a, c); 17(7a, b, c + 3a); 18(a, 7b, c - 2b); 19(7a, b + 3a, c); 20(7a, b, c - 2a); 21(a, 7b, c + 3b); 22(7a, b + a, c + a); 23(7a, b + a, c - a); 24(7a, b - a, c + a); 25(7a, b - a, c - a); 26(7a, b + a, c + 2a); 27(7a, b + a, c - 2a); 28(7a, b + 2a, c + a); 29(7a, b - 2a, c + a); 30(7a, b + 3a, c - 3a); 31(7a, b - 3a, c + 3a); 32(7a, b + a, c + 3a); 33(7a, b + a, c - 3a); 34(7a, b + 3a, c + a); 35(7a, b - 3a, c + a); 36(7a, b + 2a, c - 2a); 37(7a, b - 2a, c + 2a); 38(7a, b + 2a, c + 2a); 39(7a, b - 3a, c - a); 40(7a, b - a, c - 3a); 41(7a, b - 2a, c - 2a); 42(7a, b + 3a, c - a); 43(7a, b - a, c + 3a); 44(7a, b + 2a, c + 3a); 45(7a, b + 3a, c + 2a); 46(7a, b - 2a, c - 3a); 47(7a, b - 3a, c + 2a); 48(7a, b + 2a, c - 3a); 49(7a, b - 3a, c - 2a); 50(7a, b - 2a, c + 3a); 51(7a, b + 3a, c - 2a); 52(7a, b + 3a, c + 3a); 53(7a, b - 2a, c - a); 54(7a, b - a, c - 2a); 55(7a, b - 3a, c - 3a); 56(7a, b + 2a, c - a); 57(7a, b - a, c + 2a)
---------	---

Example

One can derive easily the 7 derivative lattices of index 2.

$$1(2a, b, c); 2(a, 2b, c); 3(a, b, 2c); 4(2a, b + a, c);$$

$$5(2a, b, c + a); 6(a, 2b, c + b); 7(2a, b + a, c + a).$$

Another primitive cell of a given derivative lattice is obtained if one of the following three elementary transformations is performed on the vectors of a primitive cell of this derivative lattice:

- (i) the sign of a vector is changed;
  - (ii) two vectors are interchanged;
  - (iii) to a vector is added  $q$  times another vector ( $q$  integer).
- (i) and (ii) are left-handed transformations, (iii) is right-handed.

Example

The primitive cell  $a'', b'', c''$  ( $a'' = -2b - a, b'' = 9a - 2c - 2b, c'' = c - a + 3b$ ) belongs to the derivative lattice of index 10 given by the primitive cell  $a', b', c'$  ( $a' = 5a, b' = 2b + a, c' = c - 2a + b$ ) because these two cells are related by the following

Table 13.2.3.1. Two-dimensional derivative lattices of indices 2 to 7

The entry for each derivative lattice starts with a running number which is followed, between parentheses, by the appropriate basis-vector relations.

Index 2	1(2a, b); 2(a, 2b); 3(2a, b + a)
Index 3	1(3a, b); 2(a, 3b); 3(3a, b + a); 4(3a, b - a)
Index 4	1(4a, b); 2(a, 4b); 3(4a, b + a); 4(4a, b - a); 5(4a, b + 2a); 6(2a, 2b + a); 7(2a, 2b)
Index 5	1(5a, b); 2(a, 5b); 3(5a, b + a); 4(5a, b - a); 5(5a, b + 2a); 6(5a, b - 2a)
Index 6	1(6a, b); 2(a, 6b); 3(6a, b + a); 4(6a, b - a); 5(6a, b + 2a); 6(3a, 2b + a); 7(6a, b - 2a); 8(3a, 2b - a); 9(6a, b + 3a); 10(2a, 3b + a); 11(3a, 2b); 12(2a, 3b)
Index 7	1(7a, b); 2(a, 7b); 3(7a, b + a); 4(7a, b - a); 5(7a, b + 2a); 6(7a, b - 3a); 7(7a, b - 2a); 8(7a, b + 3a)

sequence of elementary transformations:

$$(-2b - a, 9a - 2c - 2b, c - a + 3b) \xrightarrow{(iii)}$$

$$(-2b - a, 9a - 2c - 2b, c - 2a + b) \xrightarrow{(iii)}$$

$$(-2b - a, 5a, c - 2a + b) \xrightarrow{(i)} (2b + a, 5a, c - 2a + b)$$

$$\xrightarrow{(ii)} (5a, 2b + a, c - 2a + b);$$

( $a'', b'', c''$ ) and ( $a', b', c'$ ) have the same handedness.

13.2.3. Two-dimensional derivative lattices

All previous considerations are valid also for two-dimensional lattices and their derivative lattices (Table 13.2.3.1). The relevant formula for any index is

$$a' = p_1 a, \quad b' = p_2 b + q a$$

[a direction is kept]

( $p_1, p_2$  positive integers, not necessarily prime;

index =  $p_1 p_2 > 1$ ;  $q$  any integer;  $-p_1/2 < q \leq p_1/2$ ).

A similar formula is obtained by interchange of  $a$  and  $b$ .

References

13.1

Bertaut, E. F. (1956). *Structure de FeS stoechiométrique*. *Bull. Soc. Fr. Minéral. Cristallogr.* **79**, 276–292.

Bertaut, E. F. & Billiet, Y. (1979). *On equivalent subgroups and supergroups of the space groups*. *Acta Cryst.* **A35**, 733–745.

Billiet, Y. (1973). *Les sous-groupes isosymboliques des groupes spatiaux*. *Bull. Soc. Fr. Minéral. Cristallogr.* **96**, 327–334.

Billiet, Y. (1978). *Some remarks on the 'family tree' of Bärnighausen*. *Acta Cryst.* **A34**, 1023–1025.

Billiet, Y. (1979). *Le groupe P1 et ses sous-groupes. I. Outillage*

*mathématique: automorphisme et factorisation matricielle*. *Acta Cryst.* **A35**, 485–496.

Billiet, Y. & Rolley Le Coz, M. (1980). *Le groupe P1 et ses sous-groupes. II. Tables de sous-groupes*. *Acta Cryst.* **A36**, 242–248.

13.2

Billiet, Y. & Rolley Le Coz, M. (1980). *Le groupe P1 et ses sous-groupes. II. Tables de sous-groupes*. *Acta Cryst.* **A36**, 242–248.