

1. SPACE GROUPS AND THEIR SUBGROUPS

conjugate in  $\mathcal{P}$ . Therefore, by Proposition 1.4.6.1.3, the number of these groups is either 1 or 3:

**Corollary 1.4.6.2.2.** Let  $\mathcal{R}$  be a three-dimensional space group.

If the order of the point group of  $\mathcal{R}$  is not divisible by 3 then  $\mathcal{R}$  has no  $t$ -subgroups of index 3.

If 3 is a factor of the order of the point group of  $\mathcal{R}$ , then  $\mathcal{R}$  has either one  $t$ -subgroup of index 3 (which is then normal in  $\mathcal{R}$ ) or three conjugate  $t$ -subgroups of index 3.  $\square$

1.4.7. Qualitative results

1.4.7.1. General theory

In this section, we want to comment on the very subtle question of deciding whether two space groups  $\mathcal{R}_1$  and  $\mathcal{R}_2$  are isomorphic.

This problem can be treated in several stages:

Let  $\mathcal{R}_1$  and  $\mathcal{R}_2$  be space groups. Since the translation subgroups  $\mathcal{T}(\mathcal{R}_i)$  are characteristic subgroups of  $\mathcal{R}_i$  (the maximal Abelian normal subgroup of finite index), each isomorphism  $\varphi: \mathcal{R}_1 \rightarrow \mathcal{R}_2$  induces isomorphisms of the corresponding translation subgroups

$$\varphi' : \mathcal{T}(\mathcal{R}_1) \rightarrow \mathcal{T}(\mathcal{R}_2)$$

(by restriction) as well as of the point groups

$$\bar{\varphi} : \mathcal{P}_1 := \mathcal{R}_1/\mathcal{T}(\mathcal{R}_1) \rightarrow \mathcal{R}_2/\mathcal{T}(\mathcal{R}_2) =: \mathcal{P}_2.$$

It is convenient to view  $\mathcal{T}(\mathcal{R}_i)$  as a lattice on which the point group  $\mathcal{P}_i$  acts as group of linear mappings (cf. the start of Section 1.4.4). Then the isomorphism  $\varphi'$  is an isomorphism of  $\mathcal{P}_1$ -sets, where  $\mathcal{P}_1$  acts on  $\mathcal{T}(\mathcal{R}_1)$  via conjugation and on  $\mathcal{T}(\mathcal{R}_2)$  via

$$g\mathcal{T}(\mathcal{R}_1) \cdot t := \varphi(g)t\varphi(g)^{-1} \text{ for all } g\mathcal{T}(\mathcal{R}_1) \in \mathcal{P}_1, t \in \mathcal{T}(\mathcal{R}_2).$$

Since  $\varphi(\mathcal{T}(\mathcal{R}_1)) = \mathcal{T}(\mathcal{R}_2)$  and  $\mathcal{T}(\mathcal{R}_2)$  centralizes itself, this action is well defined, i.e. independent of the choice of the coset representative  $g$ .

The following theorem will show that the isomorphism of sufficiently large factor groups of  $\mathcal{R}_1$  and  $\mathcal{R}_2$  implies a ‘near’ isomorphism of the space groups themselves. To give a precise formulation we need one further definition.

**Definition 1.4.7.1.1.** For  $d \in \mathbb{N}$  define

$$O_d := \left\{ \frac{a}{b} \mid a, b \in \mathbb{Z}, b \neq 0, \gcd(b, d) = 1 \right\} \leq \mathbb{Q},$$

which is the set of all rational numbers for which the denominator is prime to  $d$ . For the space group  $\mathcal{R} \leq \mathcal{E}_n$  let  $\mathcal{R} \leq \mathcal{R}_{(d)} \leq \mathcal{E}_n$  be the group  $\mathcal{R}_{(d)} := \langle \mathcal{T}(\mathcal{R})_{(d)}, \mathcal{R} \rangle$ , where

$$\mathcal{T}(\mathcal{R})_{(d)} = \{at \mid a \in O_{(d)}, t \in \mathcal{T}(\mathcal{R})\} \leq \mathcal{T}_n,$$

i.e. one allows denominators that are prime to  $d$  in the translation subgroup.  $\square$

One has the following:

**Theorem 1.4.7.1.2.** Let  $\mathcal{R}_1$  and  $\mathcal{R}_2$  be two space groups with point groups of order  $d_i := |\mathcal{R}_i/\mathcal{T}(\mathcal{R}_i)|$ . Let  $\mathbf{N}(\mathcal{R}_i)$  denote the set of normal subgroups of  $\mathcal{R}_i$  having finite index in  $\mathcal{R}_i$ . Then the following three conditions are equivalent:

- (i) There are normal subgroups  $\mathcal{S}_i \trianglelefteq \mathcal{R}_i$  with  $\mathcal{R}_1/\mathcal{S}_1 \cong \mathcal{R}_2/\mathcal{S}_2$  and with  $\mathcal{S}_i \subseteq d_i^2\mathcal{T}(\mathcal{R}_i)$  if  $d_i \neq 2$  and  $\mathcal{S}_i \subseteq 16\mathcal{T}(\mathcal{R}_i)$  if  $d_i = 2$  ( $i = 1, 2$ ).
- (ii)  $(\mathcal{R}_1)_{(d_1)} \cong (\mathcal{R}_2)_{(d_2)}$ .
- (iii) There is a bijection  $\mu: \mathbf{N}(\mathcal{R}_1) \rightarrow \mathbf{N}(\mathcal{R}_2)$  such that  $\mathcal{R}_1/\mathcal{N} \cong \mathcal{R}_2/\mu(\mathcal{N})$  for all  $\mathcal{N} \in \mathbf{N}(\mathcal{R}_1)$ .  $\square$

For a proof of this theorem, see Finken *et al.* (1980).

*Remark.* If  $\mathcal{R}_i$  are three- or four-dimensional space groups, the isomorphism in (ii) already implies the isomorphism of  $\mathcal{R}_1$  and  $\mathcal{R}_2$ , but there are counterexamples for dimension 5.

1.4.7.2. Three-dimensional space groups

**Corollary 1.4.7.2.1.** Let  $\mathcal{R}$  be a three-dimensional space group with translation subgroup  $\mathcal{T}$  and  $p$  be a prime not dividing the order of the point group  $\mathcal{R}/\mathcal{T}$ . Let  $\mathcal{U}$  be a subgroup of  $\mathcal{R}$  of index  $p^\alpha$  for some  $\alpha \in \mathbb{Z}_{>0}$ . Then

- (a)  $\mathcal{U}$  is a  $k$ -subgroup.
- (b)  $\mathcal{U}$  is isomorphic to  $\mathcal{R}$ .  $\square$

*Proof.*

(a)  $\mathcal{U} \leq \mathcal{UT} \leq \mathcal{R}$  implies that  $[\mathcal{R} : \mathcal{UT}]$  divides  $[\mathcal{R} : \mathcal{U}] = p^\alpha$ . Since  $\mathcal{T} \leq \mathcal{UT} \leq \mathcal{R}$ , one obtains  $[\mathcal{R} : \mathcal{UT}]$  as a factor of  $[\mathcal{R} : \mathcal{T}]$ . But  $p$  is not a factor of  $[\mathcal{R} : \mathcal{T}]$ , hence  $[\mathcal{R} : \mathcal{UT}] = 1$  and  $\mathcal{R} = \mathcal{UT}$ . According to the remark following Definition 1.4.4.2.2,  $\mathcal{U}$  is a  $k$ -subgroup.

(b) Let  $d_1 := |\mathcal{R}/\mathcal{T}| = |\mathcal{U}/\mathcal{T}(\mathcal{U})|$ . Let  $d := d_1^2$  if  $d_1 \neq 2$  and  $d := 16$  otherwise, and let  $\mathcal{T}' := d\mathcal{T}$ . Since  $\gcd([\mathcal{R} : \mathcal{U}], d) = 1$ , one has  $\mathcal{UT}' = \mathcal{R}$  and  $\mathcal{T}' \cap \mathcal{U} = d\mathcal{T}(\mathcal{U})$ . By the third isomorphism theorem, Theorem 1.4.3.5.2, it follows that

$$\mathcal{R}/\mathcal{T}' = \mathcal{UT}'/\mathcal{T}' \cong \mathcal{U}/\mathcal{T}' \cap \mathcal{U} = \mathcal{U}/d\mathcal{T}(\mathcal{U}).$$

By Theorem 1.4.7.1.2 (i)  $\Rightarrow$  (ii), one has  $\mathcal{R}_{(d_1)} \cong \mathcal{U}_{(d_1)}$ . By the remark above, this already implies that  $\mathcal{R}$  and  $\mathcal{U}$  are isomorphic. **QED**

**Theorem 1.4.7.2.2.** Let  $\mathcal{R}$  be a three-dimensional space group and  $\mathcal{U}$  be a maximal subgroup of  $\mathcal{R}$  of index  $> 4$ . Then

- (a)  $\mathcal{U}$  is a  $k$ -subgroup.
- (b)  $\mathcal{U}$  is isomorphic to  $\mathcal{R}$ .  $\square$

*Proof.* Since  $\mathcal{R}$  is soluble, the index  $[\mathcal{R} : \mathcal{U}] = p^\alpha$  is a prime power (see Theorem 1.4.5.3.1). If  $p$  is not a factor of  $|\mathcal{R}/\mathcal{T}(\mathcal{R})|$ , the statement follows from Corollary 1.4.7.2.1. Hence we only have to consider the cases  $p = 2, \alpha > 2$  and  $p = 3, \alpha > 1$ . Since 9 is not a factor of the order of any crystallographic point group in dimension 3, assertion (a) follows if the index of  $\mathcal{U}$  is divisible by 9. If  $\mathcal{U}$  is a maximal  $t$ -subgroup, then  $\mathcal{R}/\mathcal{U}$  is a primitive  $\mathcal{P}$ -set for the point group  $\mathcal{P}$  of  $\mathcal{R}$ . Since the point groups  $\mathcal{P}$  of dimension 3 have no primitive  $\mathcal{P}$ -sets of order divisible by 8, assertion (a) also follows if the index of  $\mathcal{U}$  is divisible by 8.

For all three-dimensional space groups  $\mathcal{R}$ , the module  $\mathbf{L}(\mathcal{R})/2\mathbf{L}(\mathcal{R})$  [where  $\mathcal{T}(\mathcal{R})$  is identified with the corresponding lattice  $\mathbf{L}(\mathcal{R})$  in  $\tau(\mathbb{E}_3)$  as in Section 1.4.4] is not simple as a module for the point group  $\mathcal{P} = \mathcal{R}/\mathcal{T}(\mathcal{R})$ . [It suffices to check this property for the two maximal point groups  $\mathcal{C}_{yc_2} \times \mathcal{S}ym_4 (= m\bar{3}m)$  and  $\mathcal{C}_{yc_2} \times \mathcal{C}_{yc_2} \times \mathcal{S}ym_3 (= 6/mmm)$ .] This means that  $2\mathbf{L}(\mathcal{R})$  is not a maximal  $\mathcal{R}$ -invariant sublattice of  $\mathbf{L}(\mathcal{R})$ . Since the translation subgroup  $\mathcal{T}(\mathcal{U})$  of a maximal  $k$ -subgroup  $\mathcal{U}$  of index equal to a power of 2 in  $\mathcal{R}$  is a maximal  $\mathcal{R}$ -invariant subgroup of  $\mathcal{T}(\mathcal{R})$  that contains  $2\mathcal{T}(\mathcal{R})$ , one now finds that  $\mathcal{R}$  has no maximal  $k$ -subgroup of index 8.