structure factors and the transformed one are identical, i.e. $F(\underline{h})=F'(\underline{h})$. For the same reason, all transformations corresponding to a given coset of G in $N_E(G)$ result in the same set of indices and related structure factors. In the present context it is sufficient, therefore, to treat one representative symmetry operation from each coset. Two cases shall be discussed separately:

(a) The coset can be represented by a pure translation $(\underline{I},\underline{p})$, $\underline{I}$ being the identity matrix: Then all indices remain unchanged ($\underline{h}'=\underline{h}\underline{I}=\underline{h}$) and only the phases change ($\varphi'(\underline{h})=\varphi(\underline{h})-2\pi\underline{h}\underline{p}$). The number n_t of such cosets equals the index between the translation subgroups of G and of $N_E(G)$. The permissible origin translations (C.Giacovazzo, Acta Cryst. (1974) A30, 390) playing a fundamental part in direct methods may be derived directly as those translations of $N_E(G)$ not belonging to G itself.

(b) The coset cannot be represented by a pure translation: Then each corresponding unit cell transformation causes a mapping of the reciprocal lattice with the property, that the two structure factors with the same indices $F(\underline{h})$ and $F'(\underline{h})$ (referring to the original basis and the transformed basis, respectively) are not related by space-group symmetry, i.e. $|F(\underline{h})|\neq|F'(\underline{h})|$. For this, G and $N_E(G)$ have to belong to different crystal classes. If n is the index of G in $N_E(G)$ and n_t is the index between the corresponding two translation subgroups, then n/n_t is the number of symmetrically inequivalent indexing schemes in reciprocal lattice. In the special case of a non-centrosymmetrical crystal structure without anomalous scatterers Friedel's law holds and, therefore, the number of inequivalent indexing schemes is reduced by a factor of 2 (exception: space groups from enantiomorphic pairs). In such a case different indexing schemes occur only if G and $N_E(G)$ belong to different Laue groups.

20.2–3 INVARIANT SUBGROUPS OF SPACE GROUPS.

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Invariant (normal) subgroups play a central role in group theory, for example in the structure of groups, in representation theory, and in group-subgroup relations. We continue our study of the subgroups of space groups (Acta Cryst. A 36, 1980, 845-850) by investigating the properties of invariant subgroups of space groups, in any dimension. Necessary and sufficient conditions for a subgroup H of a space group G to be invariant are established: its translation subgroup T_H must be invariant in G, and the image (factor group) H/T_H must be invariant in G/T_H. These conditions are restated in a form which leads to a computational algorithm (tables of invariant subgroups are being prepared by P. Engel). The structures of the images G/H are also discussed and partially characterized.

20.2–4 GEOMETRIC PROPERTIES OF WYCKOFF SETS IN SPACE GROUPS.

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A collection of symmetry equivalent points in a space group is called Wyckoff positions. Most space groups have positions with point-group symmetry higher than the trivial, and those with the highest site symmetry are particularlly interesting. For convenience, let those with the highest site symmetry be called "very special Wyckoff positions". In some space groups, there are several very special Wyckoff positions that may be permuted by automorphisms of space groups (Koch & Fisher, 1975,Acta Cryst. A31, 88), and they form a "Wyckoff set", so named by Wondratschek (International Tables for Crystallography, 1983, Vol. A, Dordrecht/Boston, Reidel). Thus the Wyckoff sets with the highest site symmetry may also be called "very special Wyckoff sets".

The Dirichlet domains of the very special Wyckoff sets of 3-dimensional space groups are polyhedra, which may be used as geometric units; although their introduction was for the classification and description of cubic crystal structures (Chieh, 1979, Acta Cryst., A35, 946). When the concept of geometric unit was employed to classify tetragonal, hexagonal and rhombohedral space groups (Chieh, 1983, Acta Cryst., A39, 415), the author has realized the need for a theoretical basis, i.e. the rigorous criterion for geometric units. The use of Dirichlet domains of very special Wyckoff sets seems to be the most appropriate.

As an example, the geometric units for the 17 2-dimensional space groups are given in the Figure. There are four categories reflecting the number of geometric units per crystallographic cell. Although some may two types due to the presence (or the lack) of symmetry in the crystal system. A similar scheme for 3-dimensional space groups will be presented.

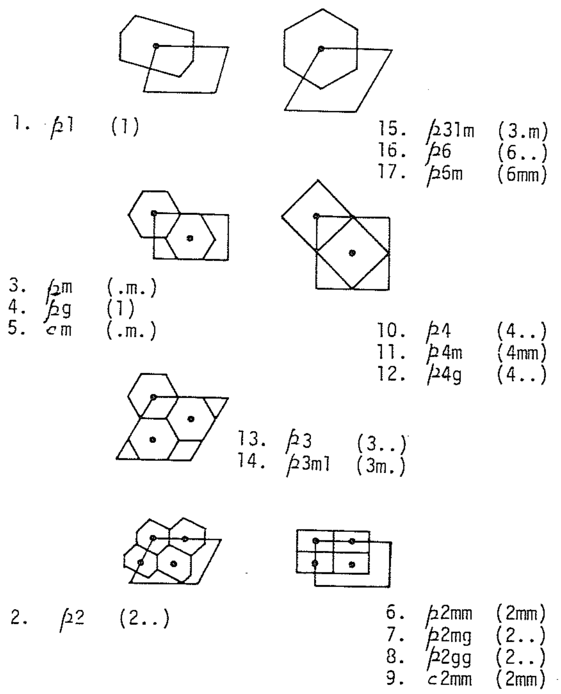

Figure. Geometric units of the 17 2-dimensional space groups. Site symmetry at the centre of these units are given in the bracket.