20.1–13 COLOUR SYMMETRY AND SCALLING IN PHASE TRANSITION AND CRITICAL PHENOMENA THEORY. By V.A.Koptsik, Moscow University, Moscow, USSR

It is shown that the method of generalized representations of the classical space and point groups, and the method of coloured P- and Q-groups in their magnetic interpretation are the equivalent languages for the symmetry description of magnetic structures arising through the phase transitions in crystals. The colour symmetry methods may be effectivelly used in the theory of critical phenomena because the scaling transformations of the appropriate Hamiltonians are nothing but a special realization of the US⇒EUC, BZ⇒RBZ transformations in the colour symmetry groups. The principal idea of colour scaling consists in the abstract symmetry conservation law for isolated physical systems. The commensurate (or incommensurate) modulated structure of a crystal arising through the phase transitions may be described in terms of colour space groups isomorphic (or homorphic) to the initial space groups: $\Phi = TG = T^*\{t_i\}G = T^*G^{(t)} \leftrightarrow T^*G^{(t,w)} = T^{(w)}G^{(w)} = \Phi^{(w)} \subset P^{\Phi}s\Phi$. We use there the non-standard factorization of the space group Φ connected with the enlarged unit cell EUC and go to the isomorphic positional colour space group $\Phi^{(w)} \leftrightarrow \Phi$ which is the subgroup of the wreath products of the groups P and Φ which correspond to the selected model of imperfect crystal. The action of the generalized symmetry operators $\langle p_i^{g_i} \ldots p_i^{g_n} | g_i \rangle \in G^{(t,w)} \leftrightarrow G^{(t)}$ on the field order parameter $\eta(\vec{r})$ depends on the point coordinates $\vec{r}_i = g_i\vec{r}_i$, $g_i \in G^{(t,w)}$. Averaging $\eta(\vec{r})$ throughout the group $G^{(t,w)}$ in the volume of EUC one obtains the uniform distribution of $\eta = \langle\eta(\vec{r})\rangle$. To the scaling transformations US⇒EUS there correspond the transformations from initial microscopic to some block Hamiltonian. If this result coinsides with that of the renormalization group approach and with the experimental data one may take the test model of $T^*G^{(t,w)} = \Phi^{(w)}$ group for the representative subgroup of the generalized microscopic symmetry of modulated phase of a crystal in the class of the equivalent symmetry groups. It follows from abstract symmetry conservation law that $\Phi_\rho^{(w)}$ is isomorphic to the group Φ_{ρ^*} and that Φ_ρ is the common subgroup of Φ_ρ and $\Phi_\rho^{(w)}$ in accordance with the experiment and theory of Landau.

20.2–1 APPLICATION OF EXPLICIT-ORIGIN SPACE GROUP NOTATION. By S.R. Hall, Crystallography Centre, University of Western Australia, Nedlands 6009, Australia.

The explicit-origin space group notation of Hall (Acta Cryst. (1981) A37, 517) has a number of advantages over the commonly-used short and full Hermann-Mauguin symbols for computer-based symmetry operations. Foremost, the new symbols are very simply translated into both site and reflection symmetry information. It has other important advantages as well. There is a clear relationship between space group symmetries related by an inversion centre (e.g. $P22_{ab}$ and $-P22_{ab}$ instead of $P2_12_12$ and Pbam) or by point groups (e.g. $-P2_a2_a$ and $-P2_a2_n$ instead of Pmma and Pbcn); the facility for all possible axial settings with symbols which exhibit the same features; and a difference in notation when an inversion centre is not placed at the origin (e.g. $-P4_a2_b$ and $P42\,{-1}_{ab}$ are the centrosymmetric and non-centrosymmetric forms of P4/nbm).

The recent addition of an origin shift parameter to the notation provides for site compatability with all previous (and future) space group settings. This, and the above features, make the explicit-origin symbols ideal for computer data-base and archival purposes. For this reason they have been adopted by the XTAL Program System (Hall et al., Acta Cryst. (1980) A36, 979) and the Standard Crystallographic File Structure (Brown, Acta Cryst. (1983) A39, 216). The origin shift update, the symbol translation algorithm and some applications will be described.

20.2–2 THE IMPLICATION OF EUCLIDEAN NORMALIZERS OF SPACE GROUPS ON INDICES AND PHASES OF STRUCTURE FACTORS. By E. Koch, Institute for Mineralogy, University of Marburg, Lahnberge, D-3550 Marburg, FRG.

The Euclidean normalizer $N_E(G)$ of a space group G forms the appropriate tool to derive all equivalent descriptions of a crystal structure or its enantiomorph from a given one. For this, two different methods may be used:

(1) The space group (the location of its symmetry elements) and the unit cell (basis vectors and origin) are kept fixed in space, whereas the coordinates of all atoms are transformed by the symmetry operations of $N_E(G)$ (W. Fischer & E. Koch, Acta Cryst. (1983) A39,907). By this means the crystal structure or its enantiomorph is embedded into the unit cell in n different ways, each referring to one of the n cosets of G in $N_E(G)$ and each giving rise to another coordinate description.

(2) The crystal structure itself and therewith its symmetry elements (the space group) are kept fixed in space, whereas the original chosen unit cell is transformed (rotated, inverted, translated) by the symmetry operations of $N_E(G)$. This procedure results in the same n coordinate descriptions as method (1),but the transition to the enantiomorph is replaced by the change of the handedness of the basis system.

For studying the implication of Euclidean normalizers in reciprocal space the second approach is more adequate: Each change of coordinate system in direct space, described by a matrix-vector pair $(\underline{P},\underline{p})$, causes a basis transformation in reciprocal space and, as a consequence, a change of indices for all reflections from $\underline{h}$ to $\underline{h}' = \underline{h}\underline{P}$ and of structure-factor phases from $\varphi(\underline{h})$ to $\varphi'(\underline{h}') = \varphi(\underline{h}) - 2\pi\underline{h}\underline{p}$ (for symbolism cf. H. Arnold in: International Tables for Crystallography, Vol. A (1983) D. Reidel). If $(\underline{P},\underline{p})$ corresponds to a symmetry operation of G itself, the original set of indices and related

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.

By M. Senechal, Professor of Mathematics, Smith College, Northampton, MA 01063

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.

By Chung Chieh, Guelph-Waterloo Centre for Graduate Work in Chemistry, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

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.

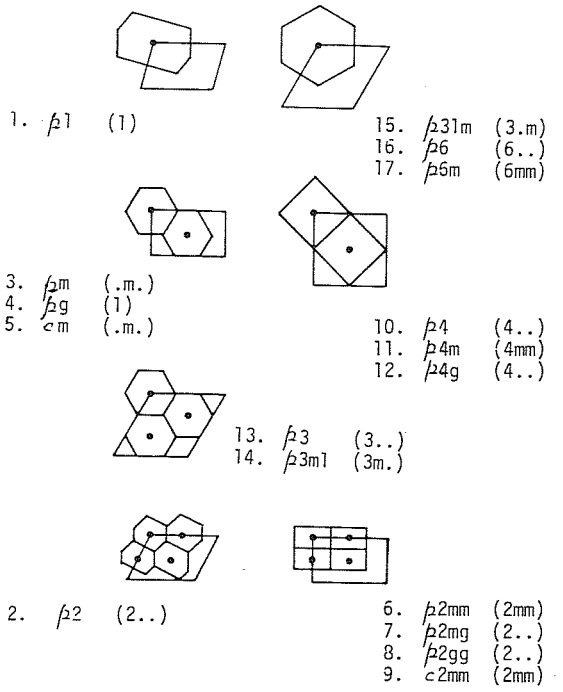

Figure. Geometric units of the 17 2-dimensional space groups. Site symmetry at the centre of these units are given in the bracket.