

Table 3. Comparison of the crystal data of the *p*-polyphenyls

	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β (°)	<i>Z</i>	Space group	DC
Biphenyl	8.04	5.51	9.39	94.5	2	<i>P</i> 2 ₁ / <i>a</i>	4.20
<i>p</i> -Terphenyl	8.08	5.60	13.59	91.9	2	<i>P</i> 2 ₁ / <i>a</i>	4.22
<i>p</i> -Quadriphenyl	8.05	5.55	17.81	95.8	2	<i>P</i> 2 ₁ / <i>a</i>	4.18
<i>p</i> -Quinquephenyl	8.04	5.485	21.99	92.0	2	<i>P</i> 2 ₁ / <i>a</i>	4.24
<i>p</i> -Hexaphenyl	8.09	5.60	26.23	91.8	2	<i>P</i> 2 ₁ / <i>a</i>	

quaphenyl was available of which no good single crystals could be isolated, no single-crystal work was carried out. But with the above considerations about the homologous isomorphism of the *p*-polyphenyls and the result for the *p*-hexaphenyl, the available powder pattern could easily be indexed. After this a refinement was carried out, computing $\sin^2 \theta$ values to find the best agreement between observed and calculated $\sin^2 \theta$ values. The final agreement obtained for the most important reflexions is given in Table 2.

A final comparison between the linear polyphenyls so far investigated is presented in Table 3.

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The existence of a chromium-molybdenum A15 structure. By F. J. A. DEN BROEDER and W. G. BURGERS, *Laboratory for Physical Chemistry of the Solid State, Technological University, Delft, The Netherlands*

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In the course of an investigation of Cr–Mo alloys under way in this laboratory an A15 or β -W structure (*Strukturbericht*, 1937) was found, which is probably a chromium-molybdenum suboxide. The Cr–Mo alloy was made by argon-arc melting of a mixture of chromium blocks and molybdenum wire. An X-ray diffraction pattern with Cr $K\alpha$ radiation of the button showed only the presence of the b.c.c. primary solid solution with a lattice constant of $a_\alpha = 2.94$ Å (corresponding to ~ 18 at. % Mo). The alloy was then homogenized by heating in an evacuated (pressure about 0.1 mmHg) sealed silica tube for 65 hr at 1230°C and slowly cooled. The X-ray pattern (Fig. 1) showed, in addition to the b.c.c. reflexions of the solid solution, strong extra lines, which could be indexed on a cubic cell with lattice constant $a_\beta = 4.65$ Å. The ratio between the lattice constants of both phases ($a_\beta/a_\alpha = 1.58$) is, within the accuracy attained, practically the same as the ratio between β -W ($a = 5.036$ Å) and b.c.c. W ($a_\alpha = 3.158$ Å), which is $a_\beta/a_\alpha = 1.59$. The indices of the reflexions of the new phase

correspond to those of β -W, whereas the relative intensities are approximately the same (Burgers & van Liempt, 1931).

According to Hägg & Schönberg (1954) β -W is not a tungsten modification, but a metallic oxide with the probable ideal formula W_3O . They assumed that the 6 W atoms and the 2 O atoms are distributed at random over the 8 (*a*) and (*c*) positions of the A15 cell. Schönberg (1954a) also prepared a chromium oxide with the β -W structure, having the probable formula Cr_3O and with a lattice constant of $a_\beta = 4.544$ Å. From intensity calculations of the X-ray pattern the conclusion was drawn that this structure was ordered with 6 Cr atoms situated on the 6(*c*) sites and 2 O atoms on the 2(*a*) sites of the A15 cell. Also for the Cr structure the ratio of the lattice constants a_β/a_α appears to be 1.58. Therefore we suggest that the phase found is a Cr, Mo oxide with the formula $(Cr, Mo)_3O$, having an A15 crystal structure. Of the weak 110 and 220 reflexions which must be present in the case of an ordered structure, only a very weak 110 reflexion was detectable. Thus it could not be decided if this structure was ordered. The possibility that the relative amounts of Cr and Mo can vary in the $(Cr, Mo)_3O$ phase is indicated by a diffraction pattern from a Cr, Mo alloy (~ 46 at. % Mo) that was heated under the same conditions as above. Besides the b.c.c. reflexions of the solid solution (lattice constant $a_\alpha = 3.02$ Å) also the 222, 320, 321 and 400 reflexions, which are strong for the β -W structure, were present. The lattice constant of the assumed A15 cell was $a_\beta = 4.77$ Å, and also in this case the ratio $a_\beta/a_\alpha = 1.58$, as for W_3O with respect to W, and Cr_3O with respect to Cr.

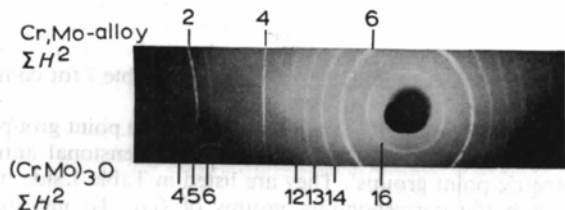


Fig. 1. Straumanis pattern, with Cr $K\alpha$ radiation, of Mo–Cr alloy and $(Mo, Cr)_3O$ phase. Camera diameter 57.3 mm.

The fact that these ratios are constant means that, if these structures are oxides, M_3O , apparently only the crystal atomic diameter of the metal atoms determines the lattice constants of the $A15$ structures mentioned. In the light of the foregoing it is remarkable that pure Mo_3O , according to Schönberg (1954*b*), does not crystallize in the $A15$ structure.

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The nomenclature of crystallographic symmetry groups. By J. BOHM and K. DORNBERGER-SCHIFF, *Deutsche Akademie der Wissenschaften zu Berlin, II. Physikalisch-Technisches Institut and Institut für Strukturforschung, Berlin-Adlershof, Germany.*

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Additional to the well known crystallographic space groups and point groups there exist further kinds of symmetry group, such as groups in other than three dimensions, groups of antisymmetry, black-white symmetry, cryptosymmetry, colour symmetry, multiple symmetry and so on.

Different nomenclatures and symbols for the individual groups belonging to some of these kinds of symmetry group were proposed by various authors. But the fact that in each case these symmetry groups have geometrical representations may be used to obtain a survey and classification (Holser, 1961; Bohm, 1963), and geometrical symbols may be given to all symmetry groups. Such 'International Symbols' for the 230 space groups and the 32 point groups are familiar to crystallographers; corresponding symbols for the 80 'antisymmetric plane groups' or the 'plane space groups' have been proposed by Dornberger-Schiff (1956, 1959, 1964) and in a somewhat modified manner by Holser (1958). Geometrical symbols avoid the use of special antisymmetric or other special symmetry elements. They have the great advantage that all data given for the three-dimensional space groups in *International Tables for X-ray Crystallography* (1952) (coordinates of general and special positions, structure factor formulae *etc.*) may be used as they stand or after a simple transformation.

In this paper proposals will be made for a nomenclature of some further kinds of symmetry group. Various names of these different kinds are quoted; in this paper a symbol $G_{rst\dots}$ is used, as proposed by one of us (Bohm, 1963). In such a symbol the indices $rst\dots$ give the dimensions of the sub-spaces which remain invariant under the operations of the particular symmetry groups and lie one inside the other. (This proposal is a generalization of a proposal by Niggli 1959); details are given in Bohm (1963), where, however, no mention is made of the fact that some of the listed kinds of symmetry group are identical.)

In the following, geometrical symbols of the groups of G_{31} , $G_{310} = G_{320}$, G_{321} , G_{3210} , G_{21} and G_{210} are described and listed. Together with the earlier proposals (Dornberger-Schiff, 1956) they furnish a complete set of geometrical symbols for all kinds of symmetry group up to three dimensions.

1. The groups of G_{31} ; the groups of G_{310}

('Linear space groups', 'three-dimensional line groups', 'Balkengruppen', 'one-dimensional colour groups', 'one-dimensional cryptosymmetric groups', and the corresponding point groups.)

The number of the groups of G_{31} is, strictly speaking unlimited. But if only subgroups of the three-dimensional space groups are admitted, there are 75 different groups. The proposed symbols of the groups are listed in Table 1. The symbols begin with the lattice-symbol P , because the lattice of groups with a single periodicity is necessarily primitive; a capital letter is used because the objects are three-dimensional (*cf.* § 3, where p is used in G_{21} for two-dimensional objects). The symbols of the symmetry elements retain their well known meaning: 1, $\bar{1}$, m , c , 2, 2_1 , 3, $\bar{3}$, 3_1 , 3_2 , \dots *etc.* The sequence of symbols is exactly as in space group notation; for certain cases a 1 (monad axis) is added (corresponding *e.g.* to space group $P31m$). For the symmetry elements there are three positions in the symbol; the two positions corresponding to the directions of missing periodicity are put into a pair of brackets (see Table 1).

There are possibilities to write abbreviated symbols, which are not listed. Table 1 contains some further information: Those groups which permit enantiomorphy are marked by +. There exist pairs of 'enantiomorphous groups' among the G_{31} groups (as among the ordinary space groups). They contain an enantiomorphous screw axis and are not to be confused with those groups which permit enantiomorphy (*cf.* Bohm & Kleber, 1958/59). The enantiomorphous pairs are marked in Table 1 by a curly bracket before their numbers. Amongst the 75 G_{31} groups there are 8 pairs of enantiomorphous groups. Symbols of the G_{31} groups according to Alexander (1929) are given in Table 1 for comparison.

The point groups G_{310} are identical with the point groups G_{320} of a 'two-sided plane' or the 'two-dimensional antisymmetric point groups'. They are listed in Table 1 side by side with the corresponding groups of G_{31} . To indicate which dimensions are transformed separately from the others the symbols of two positions are enclosed in one pair