Acta Cryst. (1959). **12**, 173

On the nomenclature of the 80 plane groups in three dimensions.

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‘International’ symbols for the 80 plane groups in three dimensions have already been proposed (K. Dornberger-Schiff, 1956) and used (K. Dornberger-Schiff, 1957 and in preparation). They have the following advantages:

(*a*) They are self-explanatory to anybody familiar with the international symbols for space groups.

(*b*) They show clearly where the data referring to number of position, point symmetry and coordinates of equivalent positions, and formulae for structure factors and electron-density may be found in Vol. I of the *International Tables for X-ray Crystallography* (1952).

Now similar symbols have been proposed by Holser (1958). They differ from those proposed earlier in two ways:

1) The direction of missing periodicity is not marked explicitly, but the first position is always taken as such.
2) Small letters are used to denote the character of the net.

These two points are of disadvantage for the following reasons:

ad 1) The direction of missing periodicity should be clearly marked as distinct from the other directions, so that it can be recognized as such without further explanation. Round brackets around the letter and/or figure referring to the non-periodic direction have therefore been proposed.

ad 2) A capital letter is preferable to a small letter, to indicate that the symmetry group refers to a three-dimensional object.

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The crystal structures of some mesitylene and durene derivatives. I. Crystal data.

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The infra-red and Raman frequencies, dipole moments, ultra-violet spectra and other physical properties of the nitro and acetyl derivatives of mesitylene and durene suggest that the steric effects of the methyl groups prevent the attainment of completely coplanar configurations, and reduce the resonance interaction between the aromatic π-electrons and the substituent nitro and acetyl groups. These deviations from coplanarity have not been directly measured however.

Similar steric effects and resonance inhibition are observed also in 9-substituted and 9:10-disubstituted anthracenes, where the environments of the substituent groups are very similar to those in mesitylene and durene derivatives. Resonance in 9-nitroanthracene for example would be at a maximum when the nitro group is coplanar with the anthracene nucleus, but this configuration involves distances which are much less than the usual van der Waals separations between the oxygen atoms and neighbouring carbon and hydrogen atoms. Detailed analyses by X-ray diffraction methods of the crystal and molecular structures of 9-nitroanthracene and 9:10-dinitroanthracene (Trotter, 1958, 1959*a*) have shown that the strain due to this ‘overcrowding’ is relieved by rotation of the nitro groups about the C–N bonds, so that the groups are tilted markedly out of the planes of the aromatic rings. The resultant decreases in resonance interaction have been correlated with the variations in the characteristic vibration frequencies of the nitro groups (Trotter, 1959*b*), and further detailed examination of the bond lengths, especially the C–N distances, suggests that the resonance between nitro group and anthracene nucleus is almost completely inhibited in 9-nitroanthracene, where the nitro group is tilted 85° from the coplanar position, but that in the 9:10-dinitro derivative, where the tilts are 64°, there is a small but measurable interaction (Trotter, 1959*b*).

These investigations have now been extended to the nitro derivatives of mesitylene and durene to obtain further accurate measurements of the deviations from coplanarity in this type of molecule. Crystals of nitromesitylene and dinitrodurene were available for the X-ray investigations, and the crystal data are outlined below.

Crystal data

Nitromesitylene, $C_9H_{11}O_2N$

Molecular weight = 165·2; melting point = 44 °C.
Orthorhombic, $a = 15{\cdot}14$, $b = 8{\cdot}41$, $c = 7{\cdot}26$ Å.
Volume of the unit cell = $U = 923{\cdot}8$ Å^3,
D_m (measured density) = 1·176 g.cm.$^{-3}$,
$Z = 4$, D_x (calculated density) = 1·180 g.cm.$^{-3}$.
Space group $Pna2_1$–C_{2v}^9 or $Pnam$–D_{2h}^{16}.

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Dinitrodurene, $C_{10}H_{12}O_4N_2$

M.W. = 224·2; m.p. = 207 °C.
Monoclinic, $a = 9{\cdot}02$, $b = 15{\cdot}43$, $c = 16{\cdot}99$ Å, $\beta = 110°\ 15'$.
$U = 2216{\cdot}4$ Å^3, $D_m = 1{\cdot}330$ g.cm.$^{-3}$,
$Z = 8$, $D_x = 1{\cdot}335$ g.cm.$^{-3}$.
Space group $Cc\text{–}C_s^4$ or $C2/c\text{–}C_{2h}^6$.

Since there are 8 molecules of dinitrodurene in the monoclinic unit cell it seemed likely that the true space-group would be the centrosymmetric one, $C2/c$. Examination of the $hk0$ weighted reciprocal lattice indicated that the benzene rings were perpendicular to the c-axis, with two opposite bonds parallel to b, while the length of the c-axis and the intensity of the 004 reflexion suggested that the molecules were separated by $\frac{1}{4}c$. This orientation of the molecules is such that if the space group is $C2/c$ there should be a large peak in the $0kl$ Patterson projection at $y = 0$, $z = \frac{1}{4}$. The $0kl$ Patterson map has a ridge of density at $z = \frac{1}{4}$, corresponding to vectors between molecules separated by $\frac{1}{4}c$, but there is no maximum at $y = 0$, $z = \frac{1}{4}$, so that the space group is probably not $C2/c$, but Cc with two molecules in the asymmetric unit. This of course makes the analysis much more complex, and in addition the determination of accurate molecular dimensions would probably require a three-dimensional analysis. Since the type of information required can be obtained with much less labour from an analysis of nitromesitylene, which has a much simpler crystal structure, no further detailed investigation of the dinitrodurene structure is being carried out and work is being confined to nitromesitylene.

Preliminary analysis of the mesitylene derivative has shown that the nitro group is tilted out of the aromatic plane by a large amount in this molecule; details of the analysis will be reported in a later communication.

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Trotter, J. (1958). *Acta Cryst.* **11**, 564.
Trotter, J. (1959*a*). *Acta Cryst.* (In the press.)
Trotter, J. (1959*b*). *Canad. J. Chem.* (In the press.)

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 333 Jay Street, Brooklyn 1, N.Y., U.S.A.) or to the Technical Editor (R. W. Asmussen, Chemical Laboratory B of the Technical University of Denmark, Sølvgade 83, Copenhagen K, Denmark)

International Union of Crystallography

The Union has accepted with gratitude the kind invitation of the Academy of Sciences of the U. S. S. R. to hold an intermediate Symposium in Leningrad during the period 21–27 May 1959, on the occasion of the commemoration of the great Russian crystallographer E. S. Federov. The topics of this Symposium will be Crystallographic Analysis and Crystal Chemistry. A Symposium on Electron Diffraction will be held concurrently under the auspices of the Commission on Electron Diffraction of the Union. Although the meetings are primarily intended for specialists in the fields concerned, all crystallographers and electron diffractionists will be welcome in so far as accomodation is available.

The organization of the meetings will be in the hands of the National Committee of Soviet Crystallographers. All correspondence and offers of papers (except of those for the Electron-Diffraction Symposium) should be directed to this Committee, at the address Pyzjewsky per d. 3, Moscow, B-17, U. S. S. R. Papers for the Electron-Diffraction Symposium should be offered to the chairman of the Commission concerned, Professor L. O. Brockway, Chemistry Department, University of Michigan, Mich., U. S. A.

Books Received

The undermentioned works have been received by the Editors. Mention here does not preclude review at a later date

Experimentelle Kristallphysik. By W. A. Wooster. Pp. 133 with 48 figs. Berlin: VEB Deutscher Verlag der Wissenschaften. 1958. Price DM. 14·40.

A Handbook of Lattice Spacings and Structures of Metals and Alloys. By W. B. Pearson. Pp. 1044 with many figs. and tables. London: Pergamon Press. 1958. Price 12½ gns.

Handbuch der Physik. Bd. VII.2. Kristallphysik II. Ed by S. Flügge. Pp. 273 with 190 figs. Berlin: Springer-Verlag. 1958. Price DM. 76.

Tables of Interatomic Distances and Configuration in Molecules and Ions. (Chemical Society Special Publication No 11. Scientific Editor: L. E. Sutton). Pp. 384. London: The Chemical Society. 1958. Price £ 2·2·0, $ 6·00.

Concepts of Classical Optics. By J. Strong. Pp. XXI + 692 with 414 figs. London: Bailey Bros & Swinfen, Ltd. San Francisco: W. H. Freeman and Company. 1958. Price $ 9·50.

Nomogramy pro Kubické mřížky; Grafické řešení Braggovy rovnice. (Charts for Cubic Lattices; Graphical Solution of the Bragg Equation) by Martin Černohorský. Acta Academiae Scientiarum Čechoslovenicae Basis Brunensis Vol. XXX no 4, 1958 pg. 131–159. Published by the Cechoslovak Academy of Science. [Text in Czech, ample summaries in Russian and English]. Price Kčs 5·10