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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) = $1{\cdot}176$ g.cm.$^{-3}$,
$Z = 4$, D_x (calculated density) = $1{\cdot}180$ g.cm.$^{-3}$.
Space group $Pna2_1$–C_{2v}^9 or $Pnam$–D_{2h}^{16}.

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