vibrations the binding electrons may not influence the reliability factor to the same extent. But, whenever the reliability factor is used as a criterion for the determination of parameters and the intensities have been measured at low temperatures, the asymmetry of the carbon atom will play a role, and formulas corresponding to equation (1) should be used. It should also be taken into account that, if the elementary cell is very large, the intensities of low orders may be appreciably influenced by the binding electrons and even forbidden reflexes may appear.

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Crystal data for some naphthalene derivatives.

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(*Received* 19 *November* 1959)

The interesting results obtained from the analyses of the crystal structures of several derivatives of anthracene have prompted investigations of the structures of some naphthalene derivatives. It is hoped to carry out complete analyses of several crystals and to compare the bond lengths in the naphthalene skeletons with those in the parent molecule. In the meantime the crystal data are outlined here.

Crystal data

1-Naphthoic acid, $C_{11}H_8O_2$.

Monoclinic, $a=31{\cdot}12$, $b=3{\cdot}87$, $c=6{\cdot}92$ Å, $\beta=92{\cdot}2°$.
Volume of the unit cell $=U=832{\cdot}8$ Å^3,
D_m (measured density) $=1{\cdot}380$ g.cm.$^{-3}$,
$Z=4$, D_x (calculated density) $=1{\cdot}373$ g.cm.$^{-3}$.
Space group $P2_1/a$–C_{2h}^5.

2-Naphthoic acid, $C_{11}H_8O_2$.

Monoclinic, $a=30{\cdot}59$, $b=5{\cdot}00$, $c=5{\cdot}63$ Å, $\beta=92{\cdot}6°$.
$U=858{\cdot}8$ Å^3, $D_m=1{\cdot}320$ g.cm.$^{-3}$, $Z=4$, $D_x=1{\cdot}332$ g.cm.$^{-3}$.
Space group $P2_1/n$–C_{2h}^5.

1,2-Dichloronaphthalene, $C_{10}H_6Cl_2$.

Monoclinic, $a=15{\cdot}11$, $b=3{\cdot}92$, $c=14{\cdot}86$ Å, $\beta=96{\cdot}0°$.
$U=875{\cdot}4$ Å^3, $D_m=1{\cdot}494$ g.cm.$^{-3}$, $Z=4$, $D_x=1{\cdot}495$ g.cm.$^{-3}$.
Space group $P2_1/n$–C_{2h}^5.

1,4-Dibromonaphthalene, $C_{10}H_6Br_2$.

Monoclinic, $a=27{\cdot}45$, $b=16{\cdot}62$, $c=4{\cdot}09$ Å, $\beta=91{\cdot}9°$.
$U=1864{\cdot}9$ Å^3, $D_m>2{\cdot}00$ g.cm.$^{-3}$, $Z=8$, $D_x=2{\cdot}037$ g.cm.$^{-3}$.
Space group $P2_1/a$–C_{2h}^5.

1,5-Dinitronaphthalene, $C_{10}H_6N_2O_4$.

Monoclinic, $a=7{\cdot}76$, $b=16{\cdot}32$, $c=3{\cdot}70$ Å, $\beta=101{\cdot}8°$.
$U=458{\cdot}7$ Å^3, $D_m=1{\cdot}578$ g.cm.$^{-3}$, $Z=2$, $D_x=1{\cdot}579$ g.cm.$^{-3}$.
Space group $P2_1/a$–C_{2h}^5.

Crystal data for 1-naphthoic acid have been reported previously (McCrone, 1953), the axial lengths agreeing well with those of the present investigation, but the crystal system being reported as orthorhombic. The $h0l$ Weissenberg films of all the crystals of 1-naphthoic acid examined in the present analysis do indeed exhibit orthorhombic symmetry at first sight, but closer examination of both the positions and intensities of the reflexions leaves no doubt that the crystals are monoclinic, but twinned on (100).

The structure analysis of 1,5-dinitronaphthalene has been completed (Trotter, 1960), and has shown that the molecule is not completely planar as previously reported (Sevastyanov, Zhdanov & Umansky, 1948). Details of the other structures will be reported in later communications.

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