Acta Cryst. (1958). **11**, 564

The crystal structures of some anthracene derivatives. I. Crystal data.

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(*Received* 16 *May* 1958)

In investigating photoconduction effects in anthracene and some of its derivatives, more detailed information can be obtained if polarized light is used, and the magnitudes of the photocurrents are examined in various directions in the crystals. Knowledge of the orientation of the unit cell axes with respect to the external crystal form, and of the molecules in the unit cell, is required, and since this information can be obtained generally only by complete structure analyses, the structures of some anthracene derivatives are being fully investigated by X-ray diffraction methods.

Some anthracene derivatives with substituents in the 9 and 10 positions have photocurrents which are 10^2 to 10^3 times as great as those in anthracene itself, although since all of these substances are insulators, the currents are always extremely small (of the order of 10^{-7}–10^{-11} amps.). The present series of X-ray investigations has been confined to these derivatives. Full details of the analyses will be given in subsequent communications, but the crystal data are outlined here.

Crystal data

9:10-Dibromoanthracene, $C_{14}H_8Br_2$.

Triclinic, $a = 4{\cdot}06$, $b = 8{\cdot}88$, $c = 16{\cdot}15$ Å,
$\alpha = 98° 50'$, $\beta = 97° 05'$, $\gamma = 100° 21'$.

$U = 559{\cdot}3$ Å^3, D_m (measured density) $= 1{\cdot}981$ g.cm.$^{-3}$,
$Z = 2$, D_x (observed density) $= 1{\cdot}983$ g.cm.$^{-3}$.
Space group $P\bar{1}$–C_i.

9:10-Dichloroanthracene, $C_{14}H_8Cl_2$.

Monoclinic, $a = 7{\cdot}04$, $b = 17{\cdot}93$, $c = 8{\cdot}63$ Å,
$\beta = 102° 56'$.

$U = 1062{\cdot}3$ Å^3, $D_m = 1{\cdot}525$ g.cm.$^{-3}$,
$Z = 4$, $D_x = 1{\cdot}535$ g.cm.$^{-3}$.
Space group $P2_1/a$–C^5_{2h}.

9:10-Dinitroanthracene, $C_{14}H_8N_2O_4$.

Triclinic, $a = 3{\cdot}95$, $b = 8{\cdot}68$, $c = 8{\cdot}76$ Å,
$\alpha = 106° 46'$, $\beta = 98° 59'$, $\gamma = 98° 01'$.

$U = 278{\cdot}6$ Å^3, $D_m = 1{\cdot}591$ g.cm.$^{-3}$,
$Z = 1$, $D_x = 1{\cdot}589$ g.cm.$^{-3}$.
Space group $P\bar{1}$–C_i.

9-Nitroanthracene, $C_{14}H_9NO_2$.

Monoclinic, $a = 7{\cdot}49$, $b = 13{\cdot}77$, $c = 11{\cdot}44$ Å,
$\beta = 115° 11'$.

$U = 1068{\cdot}5$ Å^3, $D_m = 1{\cdot}375$ g.cm.$^{-3}$,
$Z = 4$, $D_x = 1{\cdot}379$ g.cm.$^{-3}$.
Space group $P2_1/a$–C^5_{2h}.

Structure analyses of all of these crystals are in progress; since the dibromo and dichloro derivatives are not isomorphous, they are being investigated independently.

In order to study photoconduction in these crystals the atomic positions need be determined only approximately, but since relatively little more labour is required to refine the approximate structures, full structure analyses are being carried out, and reasonably accurate atomic parameters and molecular dimensions obtained. It will also be of interest to compare the dimensions of these molecules with those of the parent compound, and to examine any effects of the substituents on the bond lengths in the anthracene nucleus.

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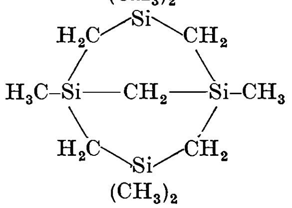
Kristallgitter zyklischer Silicium-Kohlenwasserstoffe.

Von M. Renninger und W. Renninger, *Kristallographisches Institut der Universität, Marburg-Lahn, Gutenbergstrasse* 18, *Deutschland*

(*Eingegangen am* 28. *April* 1958)

Bei Untersuchungen über die thermische Zersetzung von Tetramethyl- und Tetraäthyl-Silan fanden G. Fritz & B. Raabe (1956) unter verschiedenen teils dampfförmigen und flüssigen, teils wachsartigen und festen Zersetzungsprodukten auch ein sehr schön in langen Nadeln kristallisierendes von der Bruttoformel $Si_4C_{11}H_{28}$. Chemische und sterische Indizien führten die Autoren auf die nachstehende Strukturformel, deren Richtigkeit wenn auch nicht völlige Sicherheit, so doch grosse Wahrscheinlichkeit für sich hat:



Das Verlangen nach Klärung der Molekülstruktur liess