Acta Cryst. (1960). **13**, 277

The unit cells and space groups of the *cis*- and *trans*-isomers of dimethyl-9:10-dihydroanthracene-9:10-dicarboxylate.

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(*Received* 19 *October* 1959)

The structure of 9:10-dihydroanthracene (Ferrier & Iball, 1954) and 9:10-dihydro-1:2:5:6-dibenz-anthracene (Iball & Young, 1958) have already been determined. It was shown that in the former compound the molecule is not planar but is folded about the line joining the 9 and 10 carbon atoms whereas in the latter compound there is no such folding and the molecule is virtually planar. It is of interest to examine other derivatives of dihydroanthracene to find out what effect various groups, substituted for two of the hydrogen atoms, will have on the shape. Beckett & Mulley (1955*a*, *b*) and Herbstein (1959) have discussed the theoretical stereo-chemical factors which determine the shape of this group of compounds. The two compounds under investigation (Fig. 1) were prepared by Dr A. H. Beckett and his colleagues at The Chelsea College of Science and Technology, London and we are very grateful to him for providing excellent crystals of both isomers.

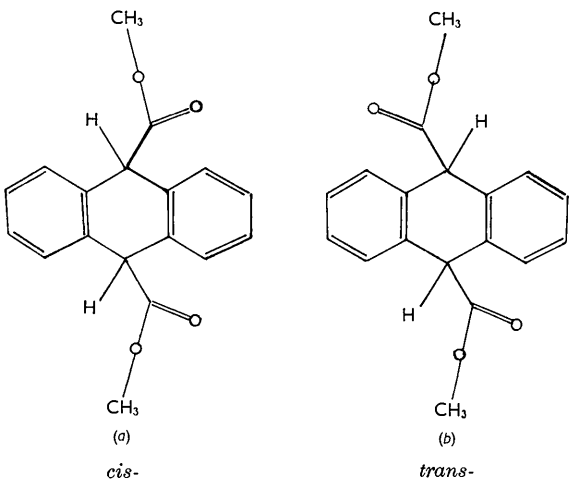

Fig. 1. Dimethyl-9:10-dihydroanthracene-9:10-dicarboxylates ($C_{18}H_{16}O_4$)

Dimethyl-*cis*-9:10-dihydroanthracene-9:10-dicarboxylate

The crystals are colourless, equidimensional triclinic prisms. The unit-cell dimensions are:

$$a = 8{\cdot}38,\ b = 13{\cdot}20,\ c = 7{\cdot}55\ \text{Å};$$
$$\alpha = 99°\ 40',\ \beta = 116°\ 37',\ \gamma = 87°\ 50'.$$

$d_o = 1{\cdot}338$ g.cm.$^{-3}$; $d_c = 1{\cdot}338$ g.cm.$^{-3}$.
2 mol. ($C_{18}H_{16}O_4$) per unit cell. Probable space group $P\bar{1}$.

Application of the statistical test to the structure factors for the *hk*0, *h*0*l* and 0*kl* zones indicates quite clearly that the unit cell possesses a centre of symmetry.

Dimethyl-*trans*-9:10-dihydroanthracene-9:10-dicarboxylate

Crystals of this compound are colourless monoclinic prisms. The unit-cell dimensions are:

$$a = 7{\cdot}81,\ b = 11{\cdot}15,\ c = 9{\cdot}23\ \text{Å};\ \beta = 111°\ 33'.$$

$d_o = 1{\cdot}320$ g.cm.$^{-3}$; $d_c = 1{\cdot}317$ g.cm.$^{-3}$.
2 mol. ($C_{18}H_{16}O_4$) per unit cell. Space group $P2_1/a$.

(Systematic absences were *h*0*l* when *h* is odd and 0*k*0 when *k* is odd.)

Although it is not possible at this stage to say anything about the shape of the *cis*-isomer, one can be quite definite about some features of the *trans*-isomer.

The space group $P2_1/a$ with only 2 molecules per unit cell requires that the molecules possess a centre of symmetry. This rules out at once any configuration involving the folded shape of 9:10-dihydroanthracene. In fact one can say that the three rings must be virtually planar as it appears to be impossible to construct any other model which would be reasonable and would possess a centre of symmetry. This result, in so far as the molecular structure in the solid is concerned, does not support the theoretical structure put forward by Beckett & Mulley (1955) as with a centro-symmetrical molecule the central ring cannot have the 'shallow boat' shape which is the basis of their discussion.

The structures of both isomers are being studied further. Structure factors for the three main zones have been measured and three-dimensional data are being collected.

We are indebted to the British Empire Cancer Campaign and to the Royal Society for grants in support of this investigation.

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