sence of a small amount of titanium and silicon in addition to iron. Chemical analysis showed that the sample was composed of 84·44% Fe_2O_3, 5·78% SiO_2 and 10% H_2O.

Identical X-ray diffraction patterns were obtained from powders of a sample of limonite from Nepal and another from Alabama, U.S.A. This clearly shows that natural limonites are crystalline although incapable of forming single crystals of apprecible size. Further studies are being undertaken.

We thank Prof. K. Banerjee, Sircar Professor of Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta, for his inspiring guidance and Prof. N. N. Chatterjee, Head of the Department of Geology, Calcutta University for the samples of limonite.

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A refinement of the crystal and molecular structures of naphthalene and anthracene.

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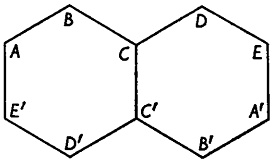
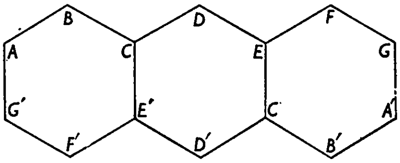
Very complete redeterminations of the crystal and molecular structures of naphthalene (Abrahams, Robertson & White, 1949 *a*, *b*) and of anthracene (Mathieson, Robertson & Sinclair, 1950; Sinclair, Robertson & Mathieson, 1950) have been described recently. In these investigations the carbon co-ordinates were determined from triple Fourier series of observed structure factors evaluated at points throughout the unit cell. No attempt was made to correct the results for the effects of finite series, which were expected to be small; though in the three-dimensional analysis of the hydrocarbon dibenzyl (Jeffrey, 1947) the effects were shown to produce bond-length errors as large as 0.037 Å (Cruickshank, 1949). A detailed estimate of the accuracy of the results is also desirable for the comparison of the experimental bond lengths with quantum-mechanical calculations of Coulson, Daudel & Robertson (1951).





We have now made finite-series corrections to the naphthalene and anthracene bond lengths by Booth's (1945, 1946 *a*) back-correction method. Differential syntheses (Booth, 1946 *b*) were computed with the observed and calculated structure factors given by Robertson and his co-workers, all six second differentials being computed for each atom. From these syntheses new atomic positions were found, from which the bond lengths given in Tables 1 and 2 were derived. The results of Robertson *et al.* are given for comparison. The finite-series corrections average 0.0058 Å per co-ordinate for each molecule, about half that for dibenzyl. The estimated standard deviations (e.s.d.) of the bond lengths are also shown in Tables 1 and 2, and were calculated by Cruickshank's (1949) method using $|F_o - F_c|$ as an estimate of $\sigma(F)$. The chemically equivalent but crystallographically non-equivalent bonds all agree within the e.s.d.'s, and so weighted mean estimates of the chemically independent bonds may be derived. These are given in Tables 3 and 4, together with their e.s.d.'s (allowance has been made for the negative correlation of the lengths of *BC* and *CD* in naphthalene through the common atom *C*, and similarly for *CD* and *DE* in anthracene).

Table 1. *Bond lengths in naphthalene*

Bond	Present refinement	E.s.d.	Robertson *et al.*
AB	1·369 Å	0·010 Å	1·363 Å
BC	1·426	0·007	1·421
CD	1·424	0·009	1·420
DE	1·362	0·008	1·354
AE'	1·404	0·009	1·395
CC'	1·393	0·010	1·395

Table 2. *Bond lengths in anthracene*

Bond	Present refinement	E.s.d.	Robertson *et al.*
AB	1·365 Å	0·009 Å	1·361 Å
BC	1·428	0·007	1·426
CD	1·393	0·007	1·387
DE	1·398	0·006	1·395
EF	1·418	0·008	1·412
FG	1·375	0·007	1·366
AG'	1·408	0·010	1·390
CE'	1·436	0·007	1·440

Tables 3 and 4 also give the theoretical bond lengths according to the molecular orbital calculations of Coulson

Table 3. *Chemically independent bond lengths in naphthalene*

Bond	Experimental	E.s.d.	Theoretical
AB	1·365 Å	0·006 Å	1·384 Å
BC	1·425	0·005	1·416
AE′	1·404	0·009	1·406
CC′	1·393	0·010	1·424

Table 4. *Chemically independent bond lengths in anthracene*

Bond	Experimental	E.s.d.	Theoretical
AB	1·371 Å	0·006 Å	1·382 Å
BC	1·424	0·005	1·420
CD	1·396	0·004	1·406
AG′	1·408	0·010	1·410
CE′	1·436	0·007	1·430

et al. For anthracene the agreement between the experimental and theoretical results is now as close as can be expected from the experimental errors and the admitted imperfections of the theory. For naphthalene the agreement is less good,.the bond *AB* and the central bond *CC′* showing significant differences between theory and experiment.

We have also computed the carbon peak heights in the observed and calculated syntheses. These are given in Tables 5 and 6. Since models with identical atoms were used for each molecule, the variation in the calculated peak heights shows that a substantial part of the variation in the observed heights, previously commented on by Robertson *et al.*, is due to the effect of finite series.

Table 5. *Peak heights in naphthalene*

Atom	Observed synthesis	Calculated synthesis
A	6·86 e.Å^{-3}	6·90 e.Å^{-3}
B	7·33	7·02
C	8·28	7·41
D	7·43	7·06
E	7·05	6·98

Table 6. *Peak heights in anthracene*

Atom	Observed synthesis	Calculated synthesis
A	7·56 e.Å^{-3}	7·94 e.Å^{-3}
B	8·28	8·51
C	9·76	9·10
D	9·27	8·78
E	9·66	8·93
F	8·59	8·47
G	7·61	8·17

The differential syntheses needed in this work were computed in duplicate by Hollerith methods and on the electronic digital computer of the Computing Machine Laboratory of Manchester University. Very close agreement, within 0·02% on the densities, was obtained between the two sets of results. These are the first crystallographic calculations to be made on the Manchester computer. Apart from programming time and about 8 hr. for punching the data tapes, only about 2 hr. 20 min. were needed on the computer itself for the observed and calculated syntheses of the two molecules.

Further work is in progress and a full account will be published later.

Our thanks are due to Prof. E. G. Cox for his encouragement and interest and for the Hollerith computing facilities available in this laboratory; to Dr Mary B. Hesse who joined us in programming the differential syntheses on the Manchester electronic computer; and to Mr R. A. Brooker and other in the Manchester Computing Machine Laboratory for their assistance and for the use of the machine.

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Mechanical twinning of indium.

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It is generally believed (Craig & Clark, 1952) that metals having the face-centred cubic structure cannot deform by twinning, either as a result of impact or of a continuously applied stress.

Recent experiments have shown that indium, which has a face-centred tetragonal structure with $c/a = 1{\cdot}078$, is subject to twinning as a mode of deformation. The twin plane is (011), $(0\bar{1}\bar{1})$, (101) or $(\bar{1}0\bar{1})$, but not (110) or $(\bar{1}\bar{1}0)$; none of these planes can act as twinning planes in the cubic structure, because there would be no difference between the twinned and the original structure.

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