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Bond-Length Variations in Aromatic Systems

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Carbon–carbon bond-length measurements have been made, by the method of X-ray crystal analysis, on pyrene, $C_{16}H_{10}$, 1:2:5:6-dibenzanthracene, $C_{22}H_{14}$, coronene, $C_{24}H_{12}$, and 1:12 benzperylene, $C_{22}H_{12}$. In all these cases definite evidence has been obtained that the bond lengths vary to a small extent in different parts of the molecules. The variation in many cases is not much greater than the possible experimental error, and so it would not be reasonable at this stage to base any very detailed calculations on these findings. In each case the result of the measurements has been compared with that obtained by taking a linear sum of all the Kekulé structures and deriving the bond lengths by means of the empirical Pauling-Brockway curve. It is found that this simple treatment gives a surprisingly good qualitative account of the results, especially for coronene and pyrene. The high symmetry of these molecules may simplify the problem, otherwise it is difficult to understand how a treatment which takes no account of the very numerous first and second excited structures can give even this measure of agreement.

The chemical properties of these hydrocarbons are discussed in relation to the bond-length data, but no very precise correlation can be made. Application of the Fries rule, which states that structures with benzenoid rings are more important than structures with quininoid rings, tends to improve the agreements in the case of pyrene.

Introduction

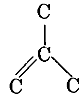
Many methods are now available for the precise measurement of bond lengths in molecules. Calculations based on spectroscopic data certainly yield the most accurate results for simple types, but diffraction methods have a much greater range of application. Both gas diffraction and crystal diffraction have been widely employed in recent years, and a large amount of data has been accumulated. For the more complex types of structure now being investigated crystal diffraction methods are perhaps the most suitable, because even when the structure is governed by a large number of independent parameters these can be refined and accurately determined by successive applications of the well-known Fourier series methods.

Early in the history of X-ray analysis it was recognized that the diamond crystal represents the prototype carbon skeleton for aliphatic compounds, while the planar hexagonal networks of graphite similarly represent the carbon rings of aromatic molecules. With the determination of reliable values for single, double and triple carbon–carbon bond lengths (Table 1) it became clear that the links in aromatic molecules are of a length intermediate between the pure single and pure double bond, although somewhat closer to the latter. Further, the carefully determined values for benzene, naphthalene, anthracene, and graphite show a small but progressive increase in bond length as the number of carbon rings is increased. These variations are not much above the limit of experimental error, but they appear to be confirmed by a number of investigations.

Table 1. *Carbon–carbon bond lengths*

	A.
Single bond (diamond, *n*-hydrocarbons)	1·54
Graphite	1·42
Anthracene	1·41
Naphthalene	1·41
Benzene	1·39
Double bond (ethylene)	1·33–1·34
Triple bond (acetylene)	1·20

These facts have been fully discussed by Pauling (1939), who shows that they receive a simple interpretation in terms of the stable valency bond structures which apply to these molecules. Thus, in benzene, from the contributions of the two Kekulé structures we infer a 'double-bond character' of 50 %; in naphthalene and anthracene linear summations of the corresponding structures (three for naphthalene and four for anthracene—see Table 2) lead to average double-bond characters of about 45 %; while in graphite the superposition of an indefinitely large number of structures of the type



gives a double-bond character of 33 %. When these values are plotted against the bond distances, they are found to lie on or near to a smooth curve connecting the pure single bond (zero double-bond character) to the pure double bond (100 % double-bond character) (Pauling & Brockway, 1937), and this curve can be given a reasonable interpretation in terms of the potential function for a resonating bond (Pauling, 1939). This empirical curve is very useful in assessing bond character (as above defined) from experimental measurements of distance. It is reproduced in Fig. 1.

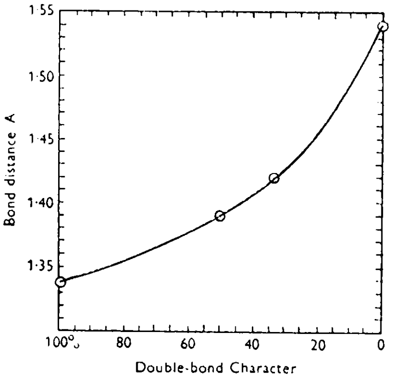


Fig. 1. Bond distance as a function of bond character. (After Pauling and Brockway.)

The bond-length measurements given above are average values. In benzene there is no reason to expect the individual bonds within the molecule to differ from the average of 1·39 A., nor in graphite from the average of 1·42 A. In naphthalene, anthracene, and the higher condensed ring hydrocarbons, however, the situation is different. By summing the relevant Kekulé structures we obtain different values for the double-bond character in different parts of the molecule. Chemical evidence also points very clearly to a difference in reactivity at different centres in these molecules, but the precise relationship between reactivity and bond character is very much a matter for discussion. It may, however, be possible to detect certain differences in bond length, and the present paper is concerned with an experimental investigation of this problem for several of the larger condensed-ring aromatic hydrocarbons.

We shall also compare the results obtained with those predicted by summing the Kekulé structures for these molecules, and making use of the Pauling-Brockway empirical curve. While it is of interest to study the measure of agreement obtained by this comparison, it is not to be expected that the Kekulé structures alone make a dominant contribution to the normal state of these larger molecules. The much more numerous first and second excited structures no doubt outweigh the non-excited Kekulé structures, and indeed it has recently been shown that in systems containing more than twelve carbon atoms the non-excited Kekulé forms may hardly be relevant at all (Coulson, private communication; Daudel & Pullman, 1946). In view of this the general pattern of the agreements obtained is rather surprising. It is found that in the large and highly symmetrical molecules of coronene and pyrene there is a distinct qualitative resemblance between the measurements and the predictions based on the Kekulé forms, although this agreement seems to break down to some extent in the case of 1:2:5:6-dibenzanthracene.

Our choice of structures for this investigation has been dictated by considerations of expediency in making the measurements. We should obviously begin with a further refinement of the naphthalene and anthracene results, but although there are indications of bond-length variations in these molecules, their orientation in the crystal is such that the two-dimensional Fourier projections already obtained (Robertson, 1933 *a*, *b*) are not capable of much additional refinement. Further progress should clearly be made by completing full three-dimensional surveys for these crystals, and although this work has been started it is not yet complete. In the meantime we have chosen certain more complex molecules where the orientation in the crystal produces two-dimensional electron density projections which show a high degree of resolution, either for all the atoms or at least for a considerable number of them.

The question of accuracy and limits of error is, of course, all important in this work, but it is not an easy one to answer. We have examined the matter in some detail by making up artificial structures of known bond lengths to simulate the projections obtained from the real hydrocarbons (Robertson & White, 1947 *a*). Various random and systematic errors have been introduced into the calculated structure factors and the effects of these errors on the Fourier projections have been studied. The general conclusion is that maximum errors of about 0·03 A. and probable errors of about 0·015 A. in bond-length determinations may be expected in the most careful work. When it is possible to average a number of distinct measurements for a group of chemically identical bonds in any one structure, then considerably better results can be expected.

This work has been confined to two-dimensional methods, and generally there is obtained for each structure only one really useful projection, which can be refined by successive applications of the Fourier series method. The procedure is then to assume that the molecule has a strictly planar form and deduce its orientation in the crystal. The most probable centres for all the atoms are then decided and the bond lengths are worked out with due allowance for the orientation. If there should be any substantial departure from the planar form in these molecules, our results will be in error. This contingency is not a very likely one, and in any case the assumption of a planar form is tested rather rigorously by the agreements obtained between calculated and observed structure factors in other zones of X-ray reflexions.

It should be emphasized that the results given below are provisional and they may require to be modified if it becomes feasible to complete full three-dimensional surveys for these structures. However, the first requirement for any such more detailed survey is an approximation carried out with as much accuracy as possible by two-dimensional methods. The present results should fulfil this condition, and so the effort expended in deriving them may be useful later on.

Pyrene, $C_{16}H_{10}$

This is a four-molecule crystal belonging to the space group C_{2h}^5–$P2_1/a$. No molecular symmetry element is utilized in building up the crystal structure, although, within the limits of our measurements, two mutually perpendicular axes of symmetry appear to exist in the molecule, in conformity with the accepted chemical structure. The principal evidence regarding bond lengths is derived from the final Fourier projection (Robertson & White, 1947*b*) made along the *b* axis (Fig. 2). In this map nine out of the sixteen carbon atoms are separately resolved, and the positions of their centres can be estimated with some certainty. The other atoms are obscured by the overlap of adjacent molecules lying at different depths in the crystal unit cell, and the positions of these remaining seven atoms are therefore somewhat uncertain. What evidence there is confirms the expected molecular symmetry about the two mutually perpendicular axes, *L* and *M*. Assuming this symmetry to be exact, and allowing for the orientation (the molecular plane is inclined at about 40° to the projection plane), it is then possible to derive all the interatomic distances. These are shown in Fig. 3.

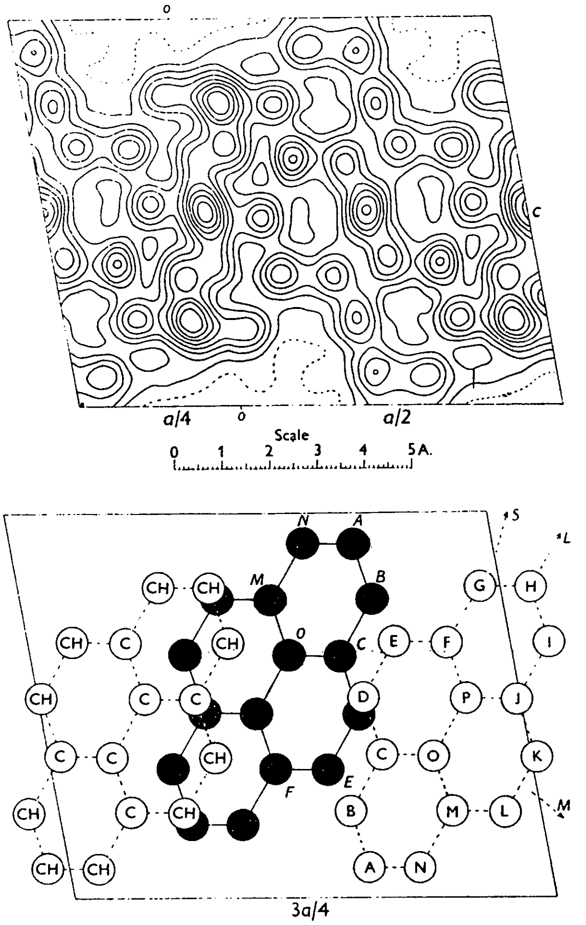


Fig. 2. Electron density map of the pyrene crystal structure.

The bond-length variations are seen to be considerable. Even if errors should be as great as 0·03 or 0·04 A. the conclusion that the bonds do vary in length to some extent is fairly definite. The general pattern of the variations is also an interesting one, with an alternation of long and short bonds around the rings. As far as we can estimate the hexagon angles remain near to 120° in all cases.

With regard to the interpretation of these results in terms of the Kekulé structures, there are six different ways of drawing the bonds for a fixed position of the carbon skeleton (Table 2). We may compute the double-bond character of each link by summing these structures, and the result is given by the percentage figures shown in Fig. 5. Translated into distances by means of the Pauling-Brockway empirical curve, we obtain the values shown in Fig. 4.

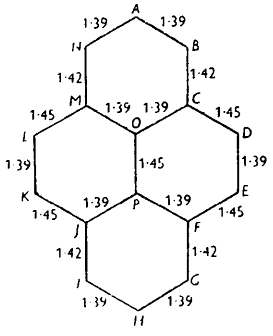


Fig. 3. Pyrene: distances measured.

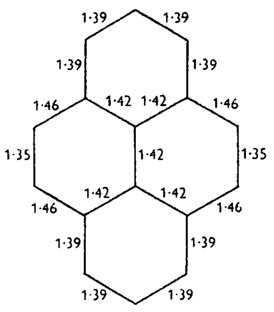


Fig. 4. Pyrene: distances calculated.

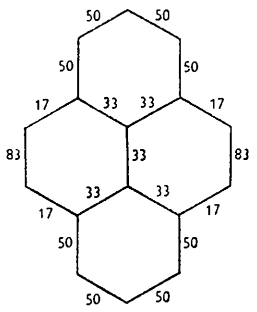
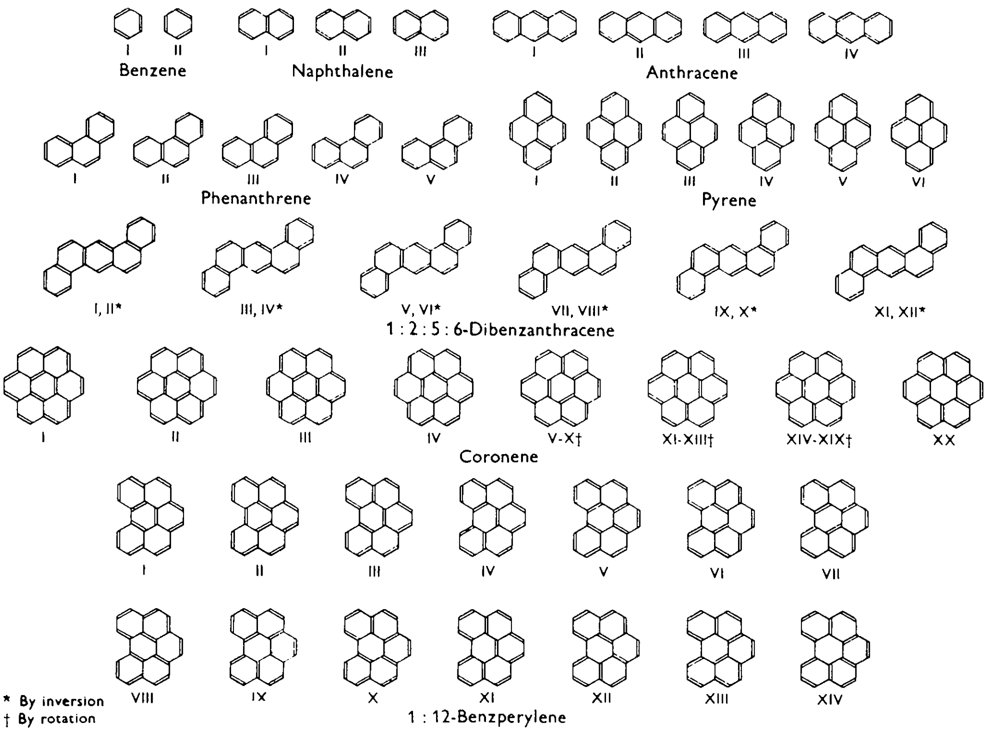


Fig. 5. Pyrene: percentage double-bond character.

There are considerable deviations between the measured and calculated values, especially in the centre of the molecule where the measurements indicate one very long bond (1·45 A.) while the predicted values are constant and of the graphite order (1·42 A.). In the upper and lower ring the predicted values are again more constant than the measurements indicate. In spite of these deviations there is a general qualitative resemblance which appears to be more than fortuitous, and the average values over the whole molecule are in excellent agreement, the measured average being 1·412 A. and the predicted, 1·408 A. Further, more detailed theoretical calculations of bond orders and bond lengths by the method of molecular orbitals (Coulson, private communication) also lead to some very encouraging agreements with our measurements.

The chemistry of pyrene (Vollmann, Becker, Corell, Streeck & Langbein, 1937) shows the atoms *G* and *B* or *G* and *N* (Fig. 3) to be the most reactive centres. These positions are always attacked when two substituents are introduced into the molecule, mixtures of 3:8- and 3:10-compounds being formed. It is certainly rather difficult to make any definite correlation between these facts and the bond-length measurements. It would appear that those parts of the molecule of more normal aromatic character (the upper and lower rings where the bond lengths are rather similar to those in benzene itself) are more readily attacked than those other parts where the bonds show more extreme variations in length. In this latter region the reactivity may be transferred, as in a conjugated system. However, a very interesting observation has recently been made by Cook & Schoental (private communication), who show that the reaction between osmium tetroxide and pyrene gives a complex which is hydrolysed to 1:2-dihydroxy-1:2-dihydropyrene. In this case the reactive positions are therefore *D* and *E* of Fig. 3 situated between the long and short bonds.

Table 2. *Stable valence-bond structures.*



* By inversion
† By rotation

In general, the relation between reactivity and bond length is not likely to be a very direct one, especially as the state of the molecule during reaction will be different from that observed in the crystal.

1:2:5:6-dibenzanthracene, $C_{22}H_{14}$

Two different crystalline modifications of this compound are known, a two-molecule monoclinic form of low symmetry (Iball & Robertson, 1933), space group $C_2^2\text{-}P2_1$, and a four-molecule orthorhombic form, space group $D_{2h}^{15}\text{-}Pcab$ (Krishnan & Banerjee, 1935; Iball, 1936). We have now been able to complete the X-ray analysis of both these crystalline modifications (Robertson & White, 1947*c*, in the Press), and a comparison of the results obtained in the two cases is of great interest in helping us to decide whether the bond-length variations observed in this work are really genuine. It is to be expected that the internal bond lengths will be invariant with respect to the particular crystal modification adopted, as the different crystal modifications merely represent very minor differences of packing of the molecules in the unit cell. The energy difference between the two forms is very small, and corresponds to very slight adjustments and rearrangements in the equilibrium of the van der Waals forces around the molecules.

In the analysis of the orthorhombic modification the work is somewhat simplified by the fact that each molecule displays an exact centre of symmetry in the crystal structure. With regard to the determination of atomic positions, the situation is somewhat similar to that in the pyrene structure, no clear picture of the whole molecule being obtained. The most useful two-dimensional Fourier projection is shown in Fig. 6 which gives separate resolution of nine out of the eleven crystallographically independent atoms. The molecular planes are inclined at only about 31° to the projection plane (*bc*), but again the picture is obscured by the overlapping effects of neighbouring molecules situated at different depths in the unit cell.

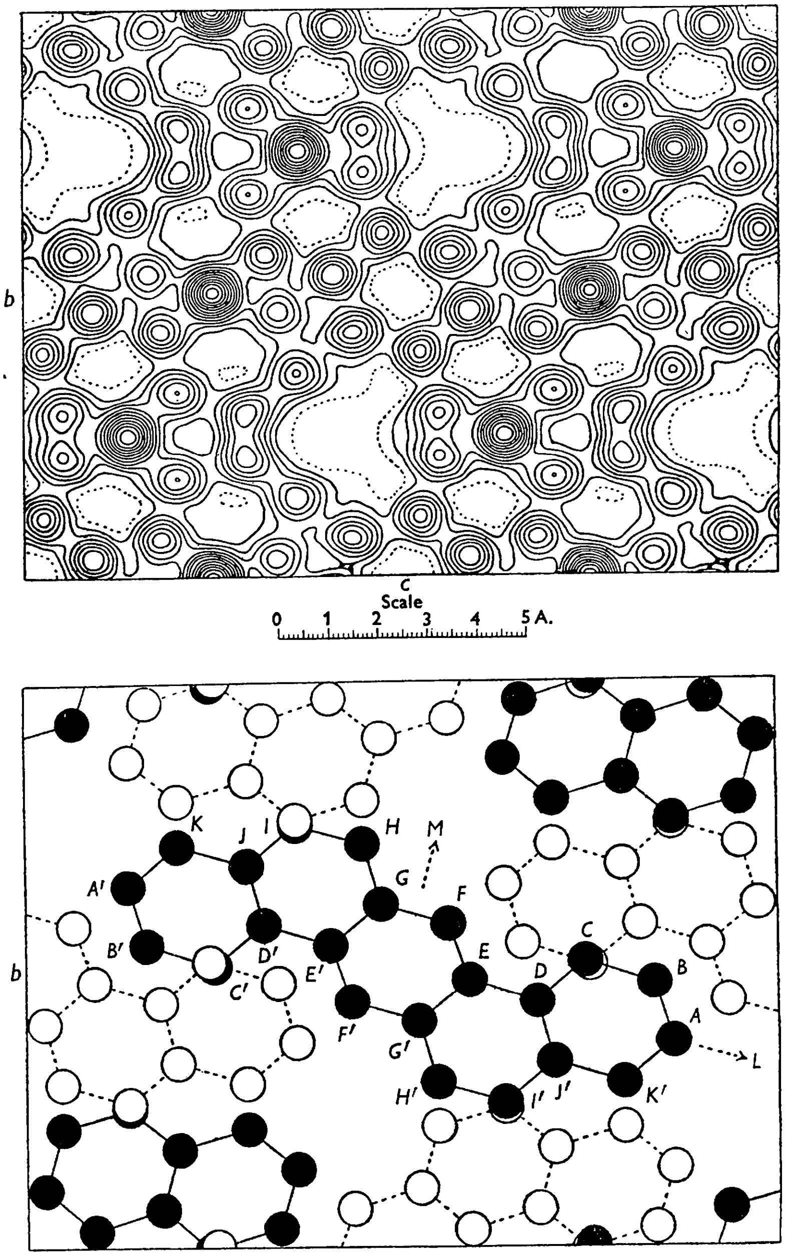


Fig. 6. Electron density map of the orthorhombic 1:2:5:6-dibenzanthracene crystal structure.

When allowance is made for the orientation of the molecule (assumed to be planar) the bond lengths may be determined as before and the results are given in Fig. 7. The atoms of the central ring are clearly defined and fairly definite measurements of distance can be made in this region, and here errors in bond length should not exceed 0·02 A. In the other parts of the molecule direct measurements can be made only for some of the bonds, and the picture is therefore incomplete. The position of the atom marked K is very uncertain, and bond lengths adjacent to it (KA and KJ) are doubtful.

In the monoclinic modification the contour map has a rather similar appearance, but no centre of symmetry is required by the crystal structure. The twenty-two carbon atoms are all crystallographically independent, and eighteen of them can be separately resolved. The results show that to a high degree of approximation the molecules contain an inherent centre of symmetry, although this is not used in building up the crystal structure. If we assume this centre of symmetry to be exact, then distances can be worked out for all the bond lengths in the molecule. The results of this calculation are shown in Fig. 8.

The results obtained from these two independent crystal structures give some confirmation of the more outstanding bond-length variations. The distortion of the central ring with the long *EG* bonds appears to be definite. On the whole, the central ring of the orthorhombic structure is probably more accurate, but in the rest of the molecule the monoclinic structure is likely to give the more reliable values.

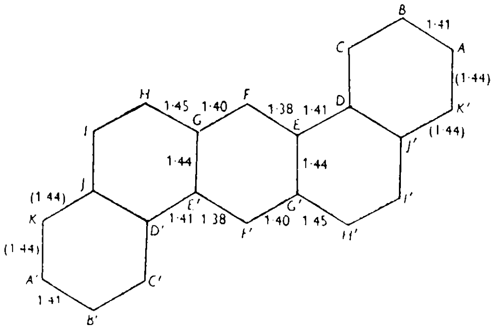


Fig. 7. Dibenzanthracene (orthorhombic form): distances measured.

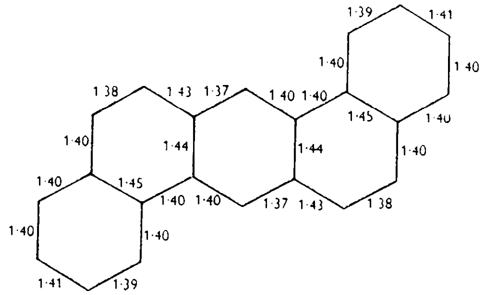


Fig. 8. Dibenzanthracene (monoclinic form): distances measured.

For this molecule twelve different Kekulé structures can be drawn, keeping the carbon skeleton in a fixed position. The double-bond character of the various links may then be assessed by a simple summation, and the results are given in Fig. 10 as percentage values. The corresponding bond lengths derived from the Pauling-Brockway curve are given in Fig. 9.

In the central ring the agreements are good, as the measurements do not show much deviation from the benzene value of 1·39 A. With regard to the other parts of the molecule, little can be said with certainty except that there is no obvious correspondence between the calculated and observed values. It may be inferred that excited structures, which have been completely neglected in the above treatment, make the more important contribution to the normal state of this molecule.

With regard to chemical properties, it is well known that the 9 and 10 positions (*F* and *F′* in Fig. 7) are the most reactive. The 9:10-quinone is formed as principal product by oxidation with chromic acid, together with some 3:4-quinone (positions *H* and *I* in Fig. 7) as a minor product. Again, it is difficult to make any correlation between these facts and the bond-length measurements. There is, indeed, some similarity to the rather anomalous situation which we encountered in the case of pyrene, namely, that the parts of the molecule most susceptible to attack are those where the bond lengths do not appear to differ much from the benzene values.

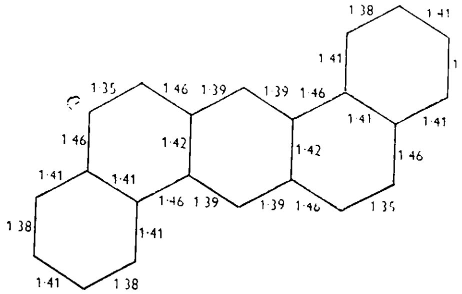


Fig. 9. Dibenzanthracene: distances calculated.

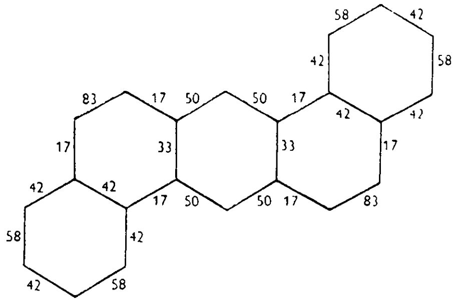


Fig. 10. Dibenzanthracene: percentage double-bond character.

Coronene, $C_{24}H_{12}$

This hydrocarbon forms small but beautifully shaped monoclinic crystals belonging to the space group C_{2h}^5-$P2_1/a$. As there are only two molecules in the unit cell, each molecule must possess an exact centre of symmetry. The structure proves to be a very favourable one for study by two-dimensional Fourier series methods (Robertson & White, 1945) and the projection along the short *b* crystal axis gives a map showing excellent resolution for all the carbon atoms (Fig. 11). The great plane of the molecule is inclined at 44° to this projection plane, and there is no overlap by neighbouring molecules to obscure the picture, as was the case in our previous examples. The diagram shown in Fig. 11 was obtained after the initial structure determination had been refined by several successive applications of the Fourier series method.

Assuming a strictly planar model and allowing for the orientation in the usual way, the bond lengths within the molecule can be determined with some accuracy. The errors in placing individual atoms should not be greater than about 0·02 A. and are probably less. Insignificant deviations were found in the lengths of the bonds of the central ring and in the 'spokes', and the average value of 1·43 A. is probably correct to within 0·01 A. Similarly, the bond lengths in the outer ring are found to group themselves very closely around the two average values of 1·385 and 1·415 A. arranged as shown in Fig. 12.

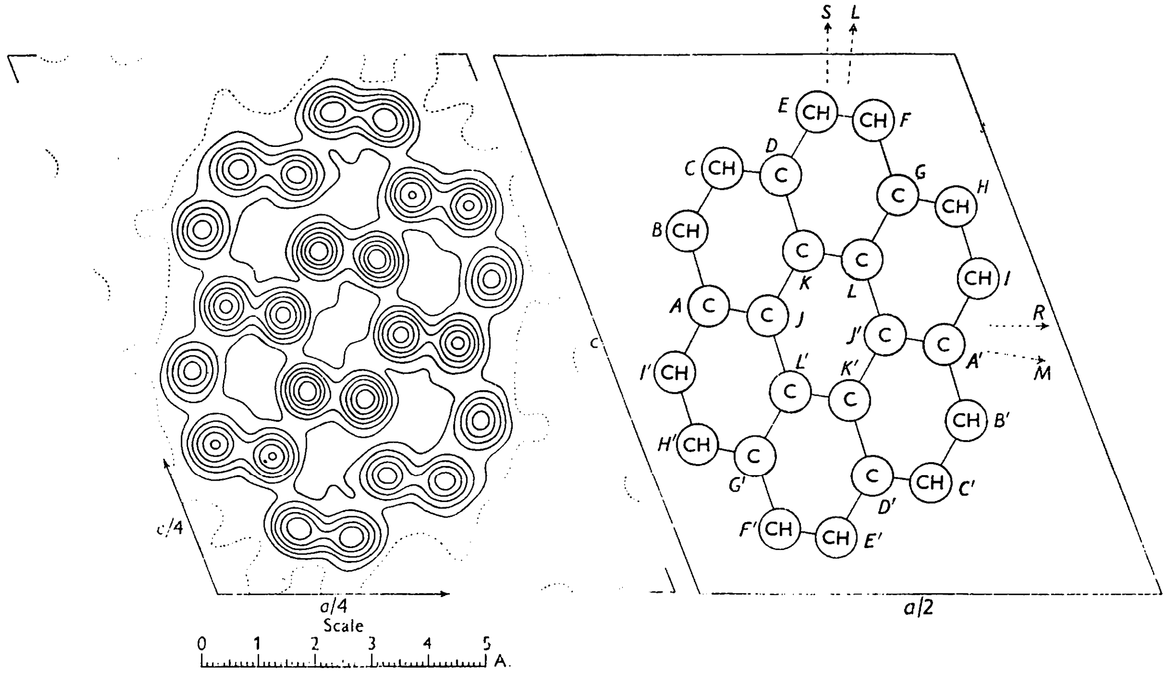


Fig. 11. Electron density map for coronene.

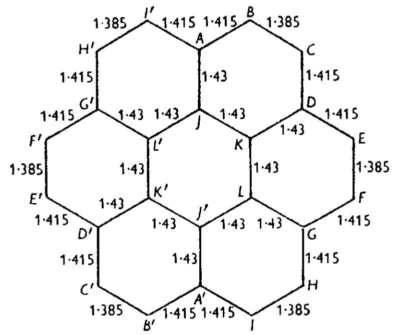


Fig. 12. Coronene: distances measured.

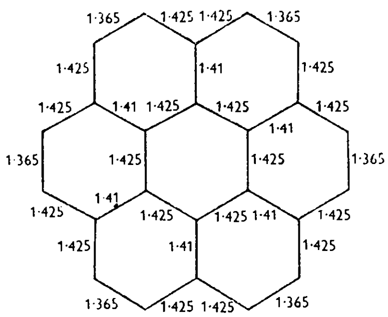


Fig. 13. Coronene: distances calculated.

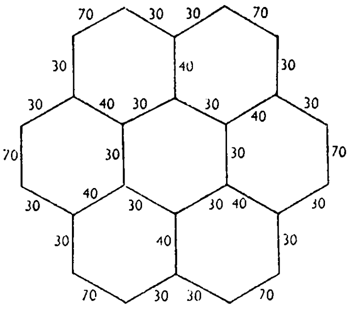


Fig. 14. Coronene: percentage double-bond character.

The distribution of the bond-length variations revealed by these measurements is an interesting one. In all the central parts of the molecule, where the structure is clearly similar to graphite, the bond lengths are found to exceed slightly the graphite value of 1·42 A., while on the outer edge the values alternate between those of benzene (1·39 A.) and a slightly higher figure.

The relevant Kekulé structures in this case number twenty in all, and the double-bond characters of the various links derived from these structures are shown as percentages in Fig. 14. When these are translated into distances we obtain the values shown in Fig. 13.

The general pattern of the agreements obtained between the measured and calculated values is surprisingly good. The chief discrepancy lies in an inversion of the values obtained for the 'spokes' and the longer set of bonds on the outer rim of the molecule. The predicted alternation of values in the outer bonds is also more extreme than the measurements indicate.

Reference should also be made to the more satisfactory and detailed calculations of Coulson (1944) for the coronene structure by the method of molecular orbitals. The general conclusions derived from his study of the problem are in very good agreement with our observations.

With regard to the chemistry of this hydrocarbon, the initial reactions are obviously confined to the outer ring. On hydrogenation a dihydro-derivative is first formed, with addition of hydrogen at *B* and *C* (Fig. 12). Further treatment yields a tetrahydro-compound, the addition being at *B*, *C*, *H* and *I*, and finally the hexahydro-compound with the extra hydrogen atoms at *B*, *C*, *H*, *I*, *E′* and *F′* can be formed (Clar & Frommherz, private communication). The addition is therefore at the positions of the shorter bonds, but the dimensions alone do not provide any reason for the particular sequence of positions occupied.

1:12-benzperylene, $C_{22}H_{12}$

The coronene results receive very interesting confirmation from the analysis of benzperylene, a molecule which differs by only two carbon atoms from that of the coronene skeleton. The crystal structure of benzperylene is of the complex four molecule type, space group C^5_{2h}–$P2_1/a$, without any internal molecular symmetry. However, the parameters of the twenty-two carbon atoms have now been determined with considerable accuracy by White (in the Press). The structure is somewhat similar to that of pyrene, but the molecular planes are inclined at a steeper angle to the main projection plane. In addition, some of the atoms are obscured by overlapping effects of adjacent molecules, and only the eleven out of the twenty-two crystallographically independent atoms can be resolved even on the most favourable two-dimensional Fourier projection of the structure. As a result, there is no direct information concerning some of the most interesting bond lengths.

The final results of the measurements are shown in Fig. 15, from which it can be seen that the main pattern of the variations corresponds rather closely to that of the coronene structure. The central bonds are all distinctly longer than the benzene value, and on the outside edge there is a distinct alternation of long and short bonds.

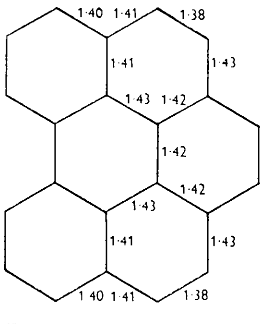


Fig. 15. Benzperylene: distances measured.

For this molecule, a total of fourteen stable valence-bond structures can be drawn. The double-bond characters of the various links, computed by summing these structures, are shown in Fig. 17, and the theoretical distances derived from these figures are given in Fig. 16. Again, a very fair measure of agreement is found between these calculations and the observations, although it is a pity that some of the more extreme values predicted for the 'open' side of the molecule cannot be checked by measurement.

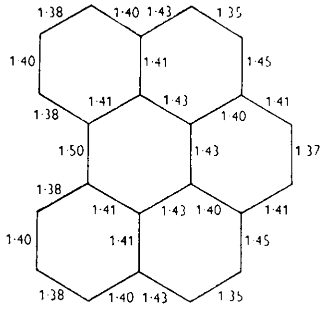


Fig. 16. Benzperylene: distances calculated.

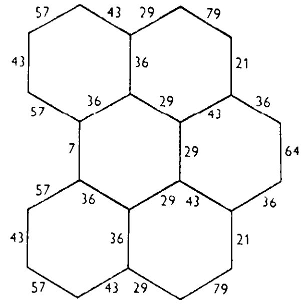


Fig. 17. Benzperylene: percentage double-bond character.

Conclusions

In the examples discussed above definite evidence has been obtained that the carbon–carbon bond lengths vary to a small extent in different parts of the molecules. The variation in many cases is not much greater than the possible experimental error, and so it would not be reasonable at this stage to base any very detailed calculations on these findings. In each case we have compared the result of our measurements with that obtained by taking a linear sum of all the Kekulé structures and deriving the bond lengths by means of the empirical Pauling-Brockway curve. It is found that this simple treatment gives a surprisingly good qualitative account of the results, especially for coronene and pyrene. The high symmetry of these molecules may simplify the problem, otherwise it is difficult to understand how a treatment which takes no account of the very numerous first and second excited structures can give even this measure of agreement.

The chemical properties of these hydrocarbons can sometimes be expressed by stating a preference for one or a certain group of the Kekulé structures. This does not imply bond fixation, but rather that some of the structures are more probable than others. Perhaps the most useful generalization in this connexion is that expressed by the Fries rule, which states that structures with benzenoid rings are more important than structures with quininoid rings. It is of interest to test the application of this rule to some of the structures and its effect on the bond-length predictions.

In the case of pyrene, two of the six structures each have three benzenoid rings, two have two benzenoid rings, and two have only one. If the contributions of these structures to the normal state are weighted in proportion to their benzenoid character, the most important effect is to increase the length of the central bond in Fig. 4 to 1·46 A., in good agreement with the observations. The four inner bonds adjacent to it become 1·40 A. instead of 1·42 A., while the other four long bonds on the outer edge become 1·50 A. instead of 1·46 A. The general effect is thus to make some qualitative improvement in the predicted bond lengths.

When the dibenzanthracene structures are treated in the same way the effect is disappointing. The predicted bond lengths in the central ring become equalized at the benzene value of 1·39 A., while in other parts of the molecule the values obtained are more extreme than those shown in Fig. 9 and not in any better agreement with the observations.

Of the twenty coronene structures, one contains five benzenoid rings, eight contain four benzenoid rings, six contain three benzenoid rings, three contain two benzenoid rings and two contain only one benzenoid ring. Weighting the contributions of the structures according to these benzenoid characters has little effect on the dimensions given in Fig. 13. Rather more extreme values are obtained for the bond-length variations, but the general picture is the same. In particular it may be noted that no combination of the Kekulé structures is capable of differentiating the longer bonds of the outer ring from the bonds of the inner ring.

The general impression based on our very limited data is that application of the Fries rule tends to improve the agreements slightly, and this finding is in accordance with chemical experience as well as theoretical expectation.

Figs. 2, 6 and 11 are reproduced by kind permission from the *Journal of the Chemical Society*.

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Indexing Method of Powder Photographs of Long-Spacing Compounds

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A method suitable for indexing X-ray powder photographs of compounds which give long-spacing reflexions is described. The method reduces the problem to that of a two-dimensional lattice. As an example, the unit cell of potassium caproate is deduced from its powder pattern by means of two graphical variants of the method. Limitations of the method are discussed.

Introduction

Crystal structure study of many long-chain substances, such as certain forms of soaps, fats and fatty acids, is considerably hampered by the difficulty of growing single crystals large enough for a complete X-ray diffraction analysis. However, a considerable amount of information can be obtained from powder photographs and from other properties of the long-chain compounds, provided the 'long spacings' can be measured. This is due to certain characteristic peculiarities of their crystals, which reduce the three-dimensional problem of the determination of their crystal lattice to a simpler