The Nature of the Chemical Bond. VII. The Calculation of Resonance Energy in Conjugated Systems

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Additional information on J. Chem. Phys.

The Nature of the Chemical Bond. VII. The Calculation of Resonance Energy in Conjugated Systems

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The quantum-mechanical treatment previously applied to benzene, naphthalene, and the hydrocarbon free radicals is used in the calculation of extra resonance energy of conjugation in systems of double bonds, the dihydro-naphthalenes and dihydroanthracenes, phenylethylene, stilbene, isostilbene, triphenylethylene, tetraphenylethyl-ene, biphenyl, *o*, *m*, and *p*-diphenylbenzene, and 1,3,5-triphenylbenzene. The calculated values, which are in approximate agreement with empirical values from thermo-chemical data, are used in the discussion of chemical properties and in the formulation of rules regarding conjugation in overlapping systems.

$\mathbf{W}$ITH the aid of the recently developed method[1] of calculating matrix elements for various electronic structures of molecules, based on Slater's treatment,[2] we have carried out a quantum-mechanical discussion of a number of conjugated systems involving double bonds and aromatic nuclei. This discussion, which is presented in the following pages, is closely similar to that previously given benzene and anthracene and the hydrocarbon free radicals,[3] and has similarly led to an illuminating qualitative and semi-quantitative explanation of the properties of the systems.

ADDITION PRODUCTS OF NAPHTHALENE

The measurements of heats of combustion made by Roth and Auwers[4] show that liquid

1,2-dihydronaphthalene, in which the benzene ring is conjugated with a double bond, is 4.9 kcal. more stable than liquid 1,4-dihydronaphthalene, in which this conjugation does not occur. It is probable that these isomers differ by about 0.1 kcal. in heat of vaporization, the boiling points being 206.5 and 212.0°C, respectively, leading to a difference in energy of the gaseous molecules of 5.0 kcal. This information permits us to discuss the effect of change in carbon-carbon distance on the exchange integral between adjacent atoms. A canonical set of fourteen independent structures for 1,2-dihydronaphthalene (in all of which single bonds between adjacent atoms are left unchanged) is shown in Fig. 1. Of these the two unexcited structures 1 and 2 will contribute most to the normal state of the molecule, so that the carbon-carbon distance for the 3-4 bond and for the six bonds of the unbroken benzene ring will be the double-bond distance of 1.38A, and the corresponding exchange integral will be that previously[3] designated by the symbol α, and found to have a value of about -1.5 v.e. The carbon-carbon distance connecting the 3-4 bond with the benzene ring

[*] Contribution No. 370.

[1] Linus Pauling, J. Chem. Phys. **1**, 280 (1933). The same calculations could be made by the use of the method of Eyring and Kimball, J. Chem. Phys. **1**, 239 (1933).

[2] J. C. Slater, Phys. Rev. **38**, 1109 (1931).

[3] Linus Pauling and G. W. Wheland, J. Chem. Phys. **1**, 362 (1933).

[4] W. A. Roth and K. v. Auwers, Liebig's Ann. **407**, 145 (1915).

will be somewhat larger, lying somewhere between 1.38 and 1.54A, inasmuch as the structures which make this bond a double bond are first-excited structures, and hence play a subordinate rôle in the normal state of the molecule. The corresponding exchange integral, which we may designate as β, will thus have a somewhat different value from α (presumably smaller in absolute value). The remaining three carbon-carbon distances will have the single-bond value 1.54A, for neither the unexcited nor the first-excited structures make them double bonds. The corresponding exchange integral β' will hence differ from α by an amount somewhat larger than for β.

If we assume that structures 1 and 2 have the same coefficients in the wave function for the normal state, and similarly 3, 4, 5; 6, 7, 8; 9, 10, 11; and 12, 13, 14, we obtain the following secular equation, in which x represents the quantity $(Q-W')/\alpha$, and b the ratio β/α. The energy $W_{1,2}$ of the molecule is equal to $W'-3/2\beta$, the latter term being omitted in the secular equation for convenience.
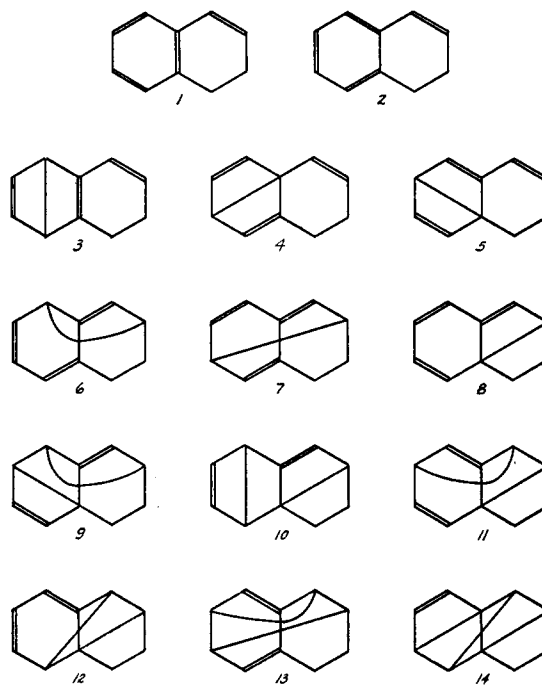

FIG. 1. Complete set of canonical structures for 1,2-dihydro-naphthalene.

$$\begin{vmatrix} 5x/2+17/2-5b/4 & 3x+12-3b/2 & 7x/4+25/4+7b/4 & 7x/4+25/4-b/8 & x+4+b \\ 3x+12-3b/2 & 9x/2+27/2-9b/4 & 9x/4+33/4+9b/4 & 9x/4+33/4 & 3x/2+9/2+3b/2 \\ 7x/4+25/4+7b/4 & 9x/4+33/4+9b/4 & 11x/2+7/4+11b/2 & 5x/2+53/8+5b/2 & 5x/2+7/4+5b/2 \\ 7x/4+25/4-b/8 & 9x/4+33/4 & 5x/2+53/8+5b/2 & 11x/2+5/2-11b/4 & 11x/8+4+11b/8 \\ x+4+b & 3x/2+9/2+3b/2 & 5x/2+7/4+5b/2 & 11x/8+4+11b/8 & 5x/2-11/4+5b/2 \end{vmatrix} = 0.$$

Because of the small contribution of the second and third-excited states, we may neglect them, which reduces the equation to a cubic, of the form

$$b^2(198z-63)+b(234z^2+132z-390)$$
$$+(68z^3+44z^2-884z-582)=0, \quad (1)$$

in which $z=-x-b$.

If as an approximation we assume $b=1(\beta=\beta'=\alpha)$, we find as the pertinent root of this equation $z=2.3062$, corresponding to $W_{1,2}=Q+1.8062\alpha$. A similar treatment applied to 1,4-dihydrobenzene (which involves no interaction between the benzene ring and the double bond) leads to $W_{1,4}=Q+3.6055\alpha-2\beta'$, or, in this case, $Q+1.6055\alpha$. (In this paper as in the previous one

interactions involving the single bonds between adjacent atoms are neglected, on the reasonable assumption that they are effectively the same for all the structures considered.) Hence the 1,2 compound is calculated to be more stable than the 1,4 compound by -0.2007α or, for $\alpha=-1.5$ v.e., 0.301 v.e. This is in rough agreement with the experimental value 5.0 kcal. or 0.22 v.e. given above. The comparison indicates that β and β' differ from α by a few percent. If we assume, as is reasonable because of the relative interatomic distances, that β lies midway between β' and α, and that a safe lower limit for the extra stability of the 1,2 compound is 4.6 kcal. or -0.14α, we write as a second equation connecting b and z
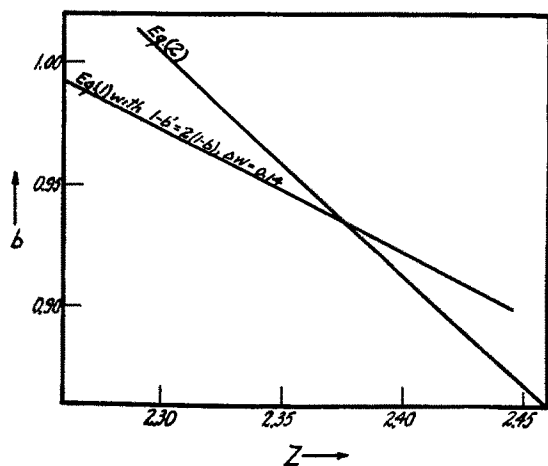
$$z=4.2455-2b. \quad (2)$$

FIG. 2.

The simultaneous solution of Eqs. (1) and (2) is shown in Fig. 2, in which the two curves represent the two relations between the variables. Their intersection corresponds to $\beta = 0.935\alpha$ and $\beta' = 0.87\alpha$, which are thus minimum values for these exchange integrals.

It is probable that the errors introduced by the neglect of all except unexcited and first-excited structures and by equating β and β' to α cancel each other to a considerable extent, especially for more complicated molecules than the dihydro-

naphthalenes. These approximations are made throughout the rest of this paper.

Calculated resonance energies for $1,2-C_{10}H_{10}$, $1,4-C_{10}H_{10}$, $1,5-C_{10}H_{10}$, and $9,10-C_{10}H_{10}$, the last two involving a chain of four and two chains of two conjugated double bonds (discussed in a following section), are given in Table I. No data are available regarding the two least stable dihydronaphthalenes.

TABLE I. Calculated resonance energies for dihydronaphthalenes.

	W	$W - W_{1,2}$	$W - W_{1,2}$
$1,2-C_{10}H_{10}$	$Q+1.8062\alpha$	0	0
$1,4-C_{10}H_{10}$	$Q+1.6055\alpha$	-0.2007α	0.301 v.e.
$1,5-C_{10}H_{10}$	$Q+1.225\alpha$	-0.581α	0.872
$9,10-C_{10}H_{10}$	$Q+0.964\alpha$	-0.842α	1.263

ADDITION PRODUCTS OF ANTHRACENE

The secular equation for 1,2-dihydroanthracene resulting from the consideration of (I) the symmetrical unexcited structure, (II) the two unsymmetrical unexcited structures, (III) the sixteen first-excited structures not involving conjugation of the double bond and the naphthalene nucleus, and (IV) the six first-excited structures involving this conjugation, is

$$\begin{vmatrix} x+5/2 & x/2+7/2 & 35x/8+361/16 & 19x/16+7 \\ x/2+7/2 & 17x/8+103/16 & 19x/2+47 & 35x/16+403/32 \\ 35x/8+361/16 & 19x/2+47 & 557x/8+4627/16 & 427x/32+2599/32 \\ 19x/16+7 & 35x/16+403/32 & 427x/32+2599/32 & 119x/8+595/16 \end{vmatrix} = 0.$$

The pertinent root of this is $x = -4.599$, corresponding to the energy $W_{1,2} = Q - x\alpha - 3\alpha/2 = Q + 3.099\alpha$, of which $Q + 2.976\alpha$ results from resonance within the naphthalene nucleus (calculated by neglecting all structures other than the three unexcited and the sixteen naphthalene first-excited structures), and the difference, 0.123α, is the energy of conjugation of the naphthalene nucleus and the double bond. The total energy of 1,4-dihydroanthracene, in which this conjugation does not occur, is $W_{1,4} = Q + 2.976\alpha$, and that of 9,10-dihydroanthracene, involving two unconjugated benzene rings, is $W_{9,10} = Q + 3.190\alpha$ (Table II). Table II could be easily extended to include
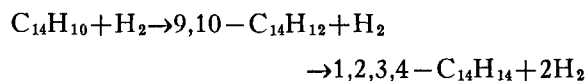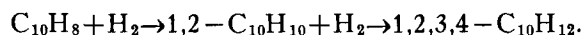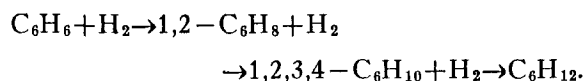
additional less stable and as yet unprepared dihydroanthracenes and higher addition products. No thermal data are available for comparison with the calculated energy values of Table II.

TABLE II. Calculated resonance energies for dihydroanthracenes.

	W	$W - W_{9,10}$	$W - W_{9,10}$
$9,10-C_{14}H_{12}$	$Q+3.190\alpha$	0	0
$1,2-C_{14}H_{12}$	$Q+3.099\alpha$	-0.091α	0.137 v.e.
$1,4-C_{14}H_{12}$	$Q+2.976\alpha$	-0.214α	0.321 v.e.

The resonance energies are essentially independent of the nature of the atoms attached to the nucleus; hydrogen is mentioned for convenience.

It is, however, reasonable to assume that, in the case of closely similar reactions, that reaction leading to the most stable product will occur most easily. This hypothesis leads to a complete explanation of the observed courses of hydrogenation of benzene, naphthalene, and anthracene, which are represented by the following schemes, showing only the reactions for which data are available.[5]

$$C_6H_6+H_2 \rightarrow 1,2-C_6H_8+H_2$$
$$\rightarrow 1,2,3,4-C_6H_{10}+H_2 \rightarrow C_6H_{12}.$$

$$C_{10}H_8+H_2 \rightarrow 1,2-C_{10}H_{10}+H_2 \rightarrow 1,2,3,4-C_{10}H_{12}.$$

$$C_{14}H_{10}+H_2 \rightarrow 9,10-C_{14}H_{12}+H_2$$
$$\rightarrow 1,2,3,4-C_{14}H_{14}+2H_2$$

$$\rightarrow 1,2,3,4,5,6,7,8-C_{14}H_{18}+3H_2 \rightarrow C_{14}H_{24}.$$

With this hypothesis, the calculated stability of the 9,10 addition compound of anthracene provides an explanation of the ease of attack of the 9,10 positions for addition. A similar calculation for phenanthrene shows that for this molecule too the 9,10 positions should be most reactive.

CONJUGATED DOUBLE-BOND SYSTEMS

In Table III are given calculated values of the resonance energy for straight conjugated chains containing two, three, and four double bonds and a branched chain with three double bonds (the list could be easily extended). In each case the secular equation was solved as a quadratic, all first-excited structures being given the same

TABLE III. *Resonance energies in systems of double bonds.*

System	Number of first-excited structures	Resonance energy
= — =	1	$-0.232\alpha = 0.348$ v.e.
= — = — =	3	$-0.482\alpha = 0.723$ v.e.
= — = — = — =	6	$-0.725\alpha = 1.09$ v.e.
(branched)	2	$-0.438\alpha = 0.657$ v.e.

[5] W. Hückel, *Theoretische Grundlagen der organischen Chemie*, 1, p. 359, Akad. Verlag. M. B. H., Leipzig, 1931.

coefficient. No reliable thermochemical data are available for comparison with these values. It may be mentioned that our hypothesis provides no information regarding addition in various positions (1,2 *vs.* 1,4 in dienes), which must instead be discussed on the basis of detailed mechanisms.

PHENYLETHYLENE, STILBENE, ETC.

The secular equation for phenylethylene, in which a phenyl group is conjugated with a double bond, is the same as for 1,2-dihydronaphthalene, and leads to the same value for the resonance energy.
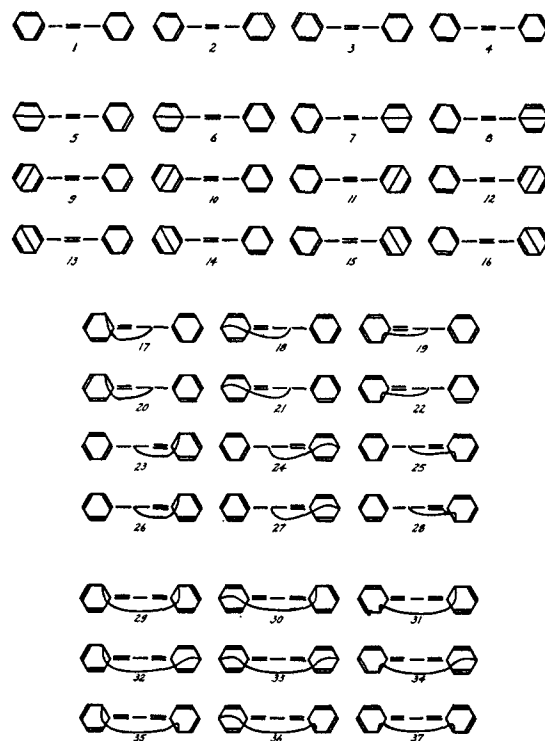

FIG. 3. Unexcited and first-excited canonical structures of sym.-diphenylethylene.

For stilbene, sym.-diphenylethylene, we consider the thirty-seven structures shown in Fig. 3, grouping together the four unexcited structures, the twelve first-excited structures not involving conjugation, the twelve in which there is conjugation of the double bond and a phenyl group, and the nine in which there is conjugation of the two phenyl groups by way of the double bond. This leads to the biquadratic secular equation

$$\begin{vmatrix} 25x/4+30 & 15x+81 & 35x/4+453/8 & 49x/16+399/16 \\ 15x+81 & 81x/2+207 & 87x/4+1185/8 & 63x/8+519/8 \\ 35x/4+453/8 & 87x/4+1185/8 & 269x/8+1107/8 & 77x/4+753/8 \\ 49x/16+399/16 & 63x/8+519/8 & 77x/4+753/8 & 121x/4+759/8 \end{vmatrix} = 0,$$

which on solution as a biquadratic leads to $W=Q+5.5889\alpha$. The energy the molecule would have without resonance, found by equating the upper left-hand quadratic part of the secular determinant to zero, is $W'=Q+5.1898\alpha$, corresponding to an extra resonance energy of conjugation of 0.3891α.

The secular equation for isostilbene, in which there is no conjugation of the two phenyl groups with each other, is just the cubic equation obtained from the stilbene determinant by omitting the fourth row and column.

The secular equation for triphenylethylene, corresponding to 8, 36, 36, and 36 structures of the four kinds described for stilbene, is

$$\begin{vmatrix} 125x/8+1675/16 & 225x/4+3285/8 & 525x/16+4395/16 & 245x/16+4921/32 \\ 225x/4+3285/8 & 1755x/8+25,569/16 & 1935x/16+17,019/16 & 231x/4+2379/4 \\ 525x/16+4395/16 & 1935x/16+17,019/16 & 2385x/16+31,653/32 & 3423x/32+12,465/16 \\ 245x/16+4921/32 & 231x/4+2379/4 & 3423x/32+12,465/16 & 2959x/16+3985/4 \end{vmatrix} = 0.$$

That for tetraphenylethylene, with 16, 96, 196, and 144 structures, respectively, of these four kinds, is

$$\begin{vmatrix} 625x/16+5375/16 & 375x/2+1725 & 875x/8+17,975/16 & 1225x/16+7315/8 \\ 375x/2+1725 & 3825x/4+35,685/4 & 4275x/8+91,815/16 & 3045x/8+18,699/4 \\ 875x/8+17,975/16 & 4275x/8+91,815/16 & 9175x/16+41,245/8 & 12,845x/32+273,911/64 \\ 1225x/16+7315/8 & 3045x/8+18,699/4 & 12,845x/32+273,911/64 & 74,761x/64+557,465/64 \end{vmatrix} = 0.$$

The energy values obtained on solution of these equations are given in Table IV.

CONJUGATED BENZENE RINGS

For biphenyl we consider four unexcited structures, twelve first-excited structures not involving conjugation, and nine involving conjugation, as shown in Fig. 4. These lead to the secular equation

$$\begin{vmatrix} 25x/4+215/8 & 15x+147/2 & 49x/8+301/8 \\ 15x+147/2 & 81x/2+747/4 & 63x/4+393/4 \\ 49x/8+301/8 & 63x/4+393/4 & 121x/4+319/4 \end{vmatrix} = 0,$$

whose solution is given in Table V.

For ortho, meta, and para diphenylbenzene we consider eight unexcited structures of the type indicated by the letter A in Fig. 5, thirty-six first-excited structures of type B, and thirty-six of type C, in which there is conjugation with the central ring. This includes all first-excited structures for m-diphenylbenzene. For ortho and para diphenylbenzene, however, there are in addition nine first-excited structures of type D, in which the two end rings are conjugated together. The secular equation for the ortho compound is

$$
\begin{vmatrix}
125x/8+775/8 & 225x/4+765/2 & 245x/8+3941/16 & 245x/64+1169/32 \\
225x/4+765/2 & 1755x/8+11,907/8 & 231x/2+1917/2 & 231x/16+4527/32 \\
245x/8+3941/16 & 231x/2+1917/2 & 5771x/32+7813/8 & 539x/16+3367/16 \\
245x/64+1169/32 & 231x/16+4527/32 & 539x/16+3367/16 & 121x/4+110
\end{vmatrix} = 0.
$$

The secular equation for the meta compound is obtained from this by omitting the fourth row and column. That for the para compound is:

$$
\begin{vmatrix}
125x/8+775/8 & 225x/4+765/2 & 245x/8+3941/16 & 49x/16+497/16 \\
225x/4+765/2 & 1755x/8+11,907/8 & 231x/2+1917/2 & 399x/32+981/8 \\
245x/8+3941/16 & 231x/2+1917/2 & 2959x/16+16,151/16 & 77x/2+1891/8 \\
49x/16+497/16 & 399x/32+981/8 & 77x/2+1891/8 & 121x/4+110
\end{vmatrix} = 0.
$$

For 1,3,5-triphenylbenzene, with 16 unexcited, 96 unconjugated first-excited, and 108 conjugated first-excited structures, the secular equation is

$$
\begin{vmatrix}
625x/16+10,125/32 & 375x/2+6525/4 & 3675x/32+9135/8 \\
375x/2+6525/4 & 3825x/4+67,545/8 & 9135x/16+23,481/4 \\
3675x/32+9135/8 & 9135x/16+23,481/4 & 50,265x/64+799,227/128
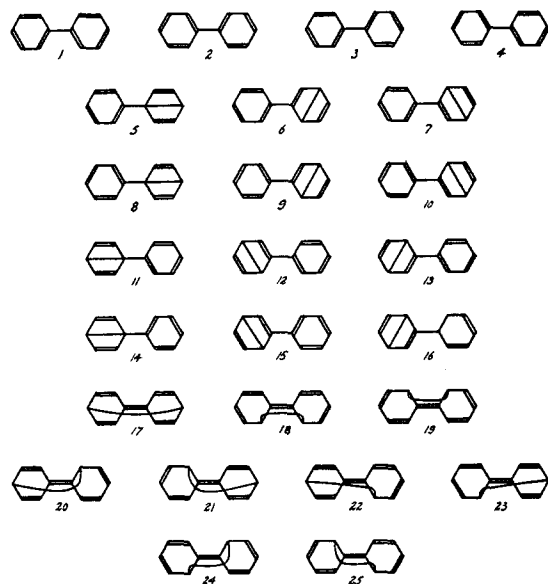\end{vmatrix} = 0.
$$

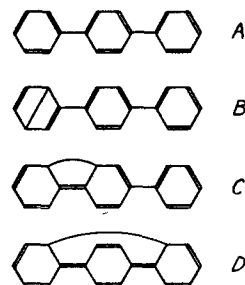FIG. 4. Unexcited and first-excited structures of biphenyl.

FIG. 5.

TABLE IV. *Calculated resonance energies for phenyl-substituted ethylenes.*

Molecule	W	W'	$W'-W$	
Phenylethylene	$Q+ 3.3062\alpha$	$Q+3.1055\alpha$	-0.2007α	$=0.301$ v.e.
Sym. diphenyl-ethylene	$Q+ 5.589\alpha$	$Q+5.190\alpha$	-0.389α	$=0.584$ v.e.
Unsym. diphenyl-ethylene	$Q+ 5.545\alpha$	$Q+5.190\alpha$	-0.355α	$=0.533$ v.e.
Triphenylethylene	$Q+ 7.804\alpha$	$Q+7.285\alpha$	-0.519α	$=0.779$ v.e.
Tetraphenyl-ethylene	$Q+10.080\alpha$	$Q+9.362\alpha$	-0.719α	$=1.08$ v.e.

The energy values found on solution of these equations and of the non-conjugated parts of them, together with their differences, the energy of conjugation, are given in Table V.

TABLE V. *Calculated resonance energies for conjugated benzene rings.*

Molecule	W	W'	$W'-W$
Biphenyl	$Q+4.867\alpha$	$Q+4.690\alpha$	$-0.177\alpha=0.266$ v.e.
m-Diphenylbenzene	$Q+7.086\alpha$	$Q+6.785\alpha$	$-0.301\alpha=0.452$ v.e.
p-Diphenylbenzene	$Q+7.094\alpha$	$Q+6.785\alpha$	$-0.309\alpha=0.464$ v.e.
o-Diphenylbenzene	$Q+7.103\alpha$	$Q+6.785\alpha$	$-0.318\alpha=0.477$ v.e.
1,3,5-Triphenylbenzene	$Q+9.273\alpha$	$Q+8.862\alpha$	$-0.411\alpha=0.617$ v.e.

COMPARISON WITH EXPERIMENT

The meager existant results of experiments on heats of combustion, given in the previous paper of this series,[6] are in rough agreement with the theoretical calculations, the discrepancies in most cases lying within the experimental error. The calculated energy of conjugation of a benzene ring and a double bond, 0.30 v.e., is in excellent agreement with the extra resonance energy 0.29 v.e. for phenylethylene. For stilbene and isostilbene[7] the empirical values 0.67 and 0.45 v.e. agree less well with the calculated values 0.58 and 0.53 v.e., respectively. For biphenyl the agreement is good, 0.35 v.e. empirical, 0.27 v.e. calculated; for 1,3,5-triphenylbenzene the difference of 0.5 v.e. between the empirical value 1.1 v.e. and the calculated value 0.62 v.e., while large, may be due to error in the reported heat of combustion or in part in the estimated heat of sublimation.

CONCLUSIONS REGARDING CONJUGATION

The calculations provide us with sufficient information to permit the formulation with considerable confidence of a set of rules regarding conjugation.

A phenyl group is 20 or 30 percent less effective in conjugation than a double bond, and a naphthyl group is less effective than a phenyl group. Thus the resonance energy of biphenyl is only 77 percent of that for two conjugated

double bonds, and the ratios of energy of conjugation of a double bond with another double bond, a phenyl group, and a naphthyl group are 1 : 0.86 : 0.53.

If a conjugated system can be resolved into two overlapping parts with a common double bond or benzene ring, and with no conjugation from one part to the other by way of the double bond or benzene ring, the total conjugation energy is 10 or 15 percent less than the sum of the conjugation energies for the two parts. Examples are isostilbene, with conjugation energy 1.77 times that for phenylethylene, metadiphenylbenzene, 1.70 times the biphenyl energy, and branched triene, 1.89 times the diene energy. The conjugation energy of 1,3,5-triphenylbenzene, in which the central benzene ring forms a part of three biphenyl systems, is 23 percent less than three times the biphenyl conjugation energy.

In an overlapping system in which there is conjugation from one part to another by way of a double bond this extra conjugation may counteract the effect of overlapping, so that the total conjugation energy is approximately equal to the sum for the parts. Thus the conjugation energy of stilbene is 1.94 times that for phenylethylene, that for unbranched triene 2.08 times that for diene, and for unbranched tetraene 3.12 times that for diene. A phenyl group is not so effective as a link in a conjugated chain, however; no doubt for the reason that, because of resonance between the two Kekulé structures, the average path between ortho or para positions is three bonds long. In consequence the conjugation energy for p-diphenylbenzene is only three percent greater than for the meta compound, and that for the ortho compound (in which the bridge is more effective) only six percent greater.

Conjugation of phenyl groups and double bonds is of quite appreciable effect in stabilizing molecules, as is, of course, evident from the early recognition of the phenomenon by chemists. The extra resonance energy of tetraphenylethylene, amounting to 1.08 v.e., is more than enough to overcome the unsaturation of the double bond, amounting to 0.74 v.e. (the difference in energy of two carbon-carbon single bonds and a double bond), in consequence of which the properties of the substance differ radically from those of an

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[6] L. Pauling and J. Sherman, J. Chem. Phys. 1, 606 (1933).

[7] The value for this compound, omitted from the previous paper, is calculated from the heat of combustion by the methods described there.

unsaturated compound such as ethylene.[8] Using the bond-energy values given in earlier papers,[9] we calculate for ΔH for the reactions $C_2(C_6H_5)_4 + X_2 \rightarrow C_2(C_6H_5)_4X_2$ the values -0.30 v.e., -0.42 v.e., and $+0.24$ v.e. for $X_2 = H_2$, Cl_2, and Br_2, respectively. Assuming that ΔF and ΔH do not differ greatly, these values suggest that tetraphenylethylene will add hydrogen and chlorine but not bromine.[10] This is in agreement with experiment; tetraphenylethylene has been hydro-

genated catalytically to tetraphenylethane,[11] and has been shown to add chlorine directly,[12] but it does not add bromine, and attempts to prepare tetraphenyldibromethane have led to tetraphenylethylene itself.[13]

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[8] We are indebted to Professor G. E. K. Branch and to Dr. G. W. Wheland for pointing this out to us.

[9] L. Pauling and J. Sherman, J. Chem. Phys. **1**, 606 (1933); L. Pauling, J. Am. Chem. Soc. **54**, 3570 (1932).

[10] The values of ΔH for addition to a non-conjugated double bond are 1.08 v.e. less than these, so that such addition reactions are all exothermic.

[11] W. H. Zartman and H. Adkins, J. Am. Chem. Soc. **54**, 1668 (1932).

[12] H. Finkelstein, Ber. Dtsch. Chem. Ges. **43**, 1533 (1910); J. F. Norris, R. Thomas and B. M. Brown, ibid. **43**, 2940 (1910). See also J. Schmidlin and R. v. Escher, ibid. **43**, 1153 (1910). The resultant dichlortetraphenylethane decomposes easily, mainly with the liberation of HCl and the formation of tetraphenylethylene with Cl substituted in the para position in one of the phenyl groups.

[13] H. Biltz, Ann. d. Chemie **296**, 231 (1897). H. Finkelstein, reference 12.