

801. *Electronic Atom and Bond Populations in Unsaturated Molecules.*

By V. W. MASLEN and C. A. COULSON.

The general theory of conjugated systems with π electrons has been extended to include explicit account of overlap integrals commonly neglected. This links it with Mulliken's theory of electronic atom and bond populations. Contour integral and other expressions are obtained for the atom and bond polarizabilities analogous to those first introduced by Coulson and Longuet-Higgins. A series of general theorems concerning these polarizabilities is established. Some numerical calculations show that predictions of chemical and physical behaviour are not greatly affected by this new development.

IN a series of five papers^{1a-1e} Coulson and Longuet-Higgins have applied the simple molecular-orbital (MO) theory, without overlap, to the π -electronic structure of conjugated systems. In these papers, a π -electron density q_r is associated with atom r and a bond order p_{rs} with bond rs . These two quantities, together with a set of polarizabilities, can describe many properties of conjugated systems. The great advantage of the treatment is that, despite its simplicity, it often yields excellent agreement with experiment.

We now try to retain the simplicity and generality of the original treatment, but to

¹ Coulson and Longuet-Higgins, *Proc. Roy. Soc.*, (a) 1947, *A*, **191**, 39, (b) 1947, *A*, **192**, 16, (c) 1948, *A*, **193**, 447, (d) *ibid.*, p. 456, (e) 1948, *A*, **195**, 188.

remove the assumption of zero overlap between adjacent π orbitals. When these overlap integrals are included our previous definitions of charge and bond order require modification. So far as the charge distribution is concerned, Wheland² showed that there is a simple way of re-allocating the total charge among the various atoms. This analysis was extended and generalised by Chirgwin and Coulson,³ who obtained certain general theorems analogous to those in refs. 1*a* and *b*, and by Löwdin,⁴ who gave an alternative definition of charge and bond order (but this omits any question of bond charges). Recent accurate X-ray analysis of molecular crystals has shown that there is a small tendency for charge to concentrate along the bond "lines." It is convenient therefore to introduce bond charges as well as atom charges. In the valence-bond scheme it used to be customary to speak of "charges de liaison." In the molecular-orbital scheme—with which alone we shall be concerned—Mulliken⁵ and McWeeny^{6,7} defined a bond charge in terms of the coefficients of adjacent π orbitals and the corresponding overlap integral. Since the existence of this bond charge is directly dependent on the overlap integral, Mulliken suggested the use of the phrase "overlap population." The overlap population and the atomic population together account for all the electrons considered.

Since there is evidence from X-ray scattering that these atom and bond charges possess rather more physical meaning than the extended atom charges in the theories of Chirgwin, Coulson, and Löwdin (these are identical with Mulliken's "gross atomic populations"), it is interesting to see how far the general theory of Coulson and Longuet-Higgins can be applied to them. We now show that relations similar to those of the earlier work can be obtained, both by means of certain new contour integrals and also in terms of the LCAO coefficients in the occupied molecular orbitals. Thus not only atom and bond charges, but also a series of polarizabilities, can be defined and related. We have also illustrated these relations by some detailed numerical calculations.

When overlap integrals S_{rs} are included, the algebra becomes rather difficult, and it is not always easy to see what the calculations show, so it is often convenient to adopt Wheland's approximation,² that the ratio S_{rs}/β_{rs} for a given link between atoms *r* and *s* has a value (*k*) independent of the length of the link and dependent only on the two atoms at the ends of the link. This constant ratio of resonance integral and overlap integral cannot be rigorously correct, but Mulliken⁸ has shown that it cannot be far wrong at ordinary distances and its use greatly simplifies calculations. For notation, see ref. 1*a*; some familiarity with the work in refs. 1*b*, 1*c* is assumed.

Since this work was completed, similar calculations have been published by Bassett and Brown.^{9,10} There are certain significant differences, usually leading to quite distinct formulæ. Thus whereas we have dealt with the bond charge defined below in (4), Bassett and Brown omitted the overlap integral in their definition and so, although they refer to it as a bond-charge density, they have really been dealing with bond orders and not bond charges. For example, the sum of their atom and bond charges is not equal to the number of π electrons, and has no simple physical meaning. There are corresponding related differences which arise when the fundamental Wheland assumption ($\beta/S = \text{constant}$) is introduced in a polarizability calculation. The bond charge should change both because the bond order changes and also because the degree of overlap changes. We therefore believe that our analysis has more physical significance than theirs, though certain of the results are the same in the two theories.

² Wheland, *J. Amer. Chem. Soc.*, 1942, **64**, 900.

³ Chirgwin and Coulson, *Proc. Roy. Soc.*, 1950, *A*, **201**, 196.

⁴ Löwdin, *J. Chem. Phys.*, 1950, **18**, 365.

⁵ Mulliken, *ibid.*, 1955, **23**, 1833, 1841, and refs. therein.

⁶ McWeeny, *ibid.*, 1951, **19**, 1614.

⁷ *Idem*, *ibid.*, 1952, **20**, 920.

⁸ Mulliken, *J. Chim. phys.*, 1949, **46**, 675.

⁹ Bassett and Brown, *Austral. J. Chem.*, 1956, **9**, 305.

¹⁰ *Idem*, *ibid.*, p. 315.

It follows that E is a function of α_r , β_{rs} , and S_{rs} . By differentiation

$$\delta E_j = \sum_r \frac{\partial E_j}{\partial \alpha_r} \delta \alpha_r + \sum_{r < s} \sum_s \frac{\partial E_j}{\partial \beta_{rs}} \delta \beta_{rs} + \sum_{r < s} \sum_s \frac{\partial E_j}{\partial S_{rs}} \delta S_{rs} \dots \dots \dots (6)$$

From (5) and (6) we obtain

$$\left(\frac{\partial E_j}{\partial \alpha_r} \right)_{\Delta=0} = \frac{c_{rj}^2}{\sum_r c_{rj}^2 + 2 \sum_{r < s} \sum_s c_{rj} c_{sj} S_{rs}} \dots \dots \dots (7)$$

and

$$S_{rs} \left(\frac{\partial E_j}{\partial \beta_{rs}} \right)_{\Delta=0} = \frac{2 S_{rs} c_{rj} c_{sj}}{\sum_r c_{rj}^2 + 2 \sum_{r < s} \sum_s c_{rj} c_{sj} S_{rs}} \dots \dots \dots (8)$$

Summation of (7) and (8) over occupied levels then yields

$$q_r = 2 \sum_{j=1}^m \left(\frac{\partial E_j}{\partial \alpha_r} \right)_{\Delta=0} = \left(\frac{\partial \mathcal{E}}{\partial \alpha_r} \right)_{\Delta=0}$$

$$q_{rs} = 2 S_{rs} \sum_{j=1}^m \left(\frac{\partial E_j}{\partial \beta_{rs}} \right)_{\Delta=0} = S_{rs} \left(\frac{\partial \mathcal{E}}{\partial \beta_{rs}} \right)_{\Delta=0}$$

where $\mathcal{E} = 2 \sum_{j=1}^m E_j$

Proceeding similarly to ref. 1a, we obtain

$$q_r = -2 \sum_{j=1}^m \frac{\Delta_{r,r}(E_j)}{\Delta'(E_j)} = -\frac{1}{\pi i} \oint_{\mathcal{C}} \frac{\Delta_{r,r}(E) \alpha E}{\Delta(E)} \dots \dots \dots (9)$$

$$q_{rs} = -4 S_{rs} (-)^{r+s} \sum_{j=1}^m \frac{\Delta_{r,s}(E_j)}{\Delta'(E_j)} = -\frac{4 S_{rs}}{2\pi i} (-)^{r+s} \oint_{\mathcal{C}} \frac{\Delta_{r,s}(E) dE}{\Delta(E)} \dots \dots (10)$$

and
$$\mathcal{E} = \frac{1}{\pi i} \oint_{\mathcal{C}} E \frac{\Delta'(E)}{\Delta(E)} dE = \frac{1}{\pi i} \oint_{\mathcal{C}} \left(E \frac{\Delta'(E)}{\Delta(E)} - n \right) dE \dots \dots \dots (11)$$

where the contour \mathcal{C} is the infinite semicircular contour shown in Fig. 1 and the energy zero is so adjusted that

$$E_1 < E_2 < \dots < E_m < 0 < E_{m+1} < \dots < E_n$$

This is usually satisfied by taking as energy zero the energy of an electron around a carbon atom. With alternant hydrocarbons this is always possible. To reduce these expressions further, we need to examine the limiting forms of their integrands for large E . The expansion of the secular determinant is

$$\Delta = (-)^n \{ A E^n - B E^{n-1} + \dots \}$$

where

$$A = S, B = \sum_r \sum_s (-)^{r+s} \beta_{rs} S_{r,s}$$

and S is the determinant of the overlap matrix.

$S_{r,s}$ is the determinant obtained from S by striking out the r -th row and s -th column. It follows that for large $|E|$

$$\frac{\Delta_{r,r}}{\Delta} \longrightarrow -\frac{S_{r,r}}{S} \cdot \frac{1}{E}$$

so that the part of the integral in (9) which arises from the infinite semicircle is simply $S_{r,r}/S$. Thus

$$q_r = \frac{S_{r,r}}{S} - \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\Delta_{r,r}(iy)}{\Delta(iy)} \cdot dy \dots \dots \dots (12)$$

Similarly

$$q_{rs} = 2 S_{rs}(-)^{r+s} \left\{ \frac{S_{r,s}}{S} - \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\Delta_{r,s}(iy)}{\Delta(iy)} \cdot dy \right\} \quad \dots \quad (13)$$

and

$$\mathcal{E} = B + \frac{1}{\pi} \int_{-\infty}^{\infty} \left(iy \frac{\Delta'(iy)}{\Delta(iy)} - n \right) dy \quad \dots \quad (14)$$

If we put $S_{rs} = 0$ for all $r \neq s$, the expressions (12) and (14) reduce to (38) and (41) of ref. 1a, whereas (13) reduces to zero, as expected.

FIG. 1. Integral contour in E - and z -space.

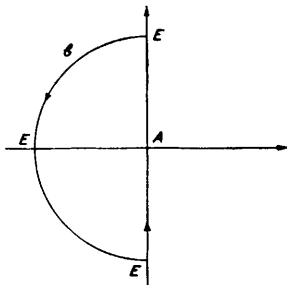
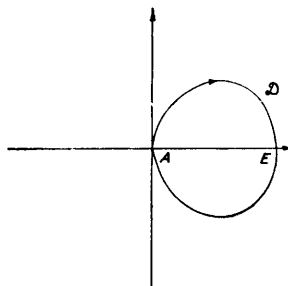


FIG. 2. Integral contour in x -space.



THE WHELAND ASSUMPTION

Our equations (12)—(14) become simpler if we adopt the Wheland assumption that all β_{rs} are proportional to S_{rs} , and all $\alpha_r = \alpha$. Such an assumption is particularly suitable to the case of polycyclic hydrocarbons and polyene chains. Now

$$\beta_{rs} - ES_{rs} = \beta_{rs} (1 - kE)$$

where $k = S_{rs}/\beta_{rs} = a$ constant = S/β , where S and β are standard integrals as, for example, in benzene. Thus

$$\Delta = \det|\beta_{rs} - ES_{rs}| = (1 - kE)^n D(x) \quad \dots \quad (15)$$

where

$$x = (E - \alpha)/(1 - kE) \quad \dots \quad (16)$$

and

$$D(x) = \begin{vmatrix} -x & \beta_{12} & \beta_{13} & \dots & \beta_{1n} \\ \beta_{21} & -x & \beta_{23} & \dots & \\ \beta_{n1} & \dots & & & -x \end{vmatrix} \quad \dots \quad (17)$$

$D(x)$ is the secular determinant that would be obtained by putting all overlap integrals equal to zero. As Wheland¹¹ has shown, the relation (16) is equivalent to

$$E - \alpha = M\gamma/(1 + MS) \quad \dots \quad (18)$$

where $\gamma = \beta - S\alpha$ and $M = x/\beta$. We shall shortly use the latter relation. Its physical advantage is that it introduces the "revised" resonance integral γ instead of the earlier one β . γ is invariant for a change in zero of energy, but β is not.¹² In these terms

$$q_r = - \frac{1}{\pi i} \oint_{\mathcal{C}} (1 - kE)^{-1} \frac{D_{r,r}(x)}{D(x)} dE$$

with a similar equation for q_{rs} .

¹¹ Wheland, *J. Amer. Chem. Soc.*, 1941, **63**, 2025.

¹² Mulliken and Rieke, *ibid.*, p. 1770.

If we now put $z = E - \alpha$ this becomes

$$q_r = -\frac{1}{\pi i} \oint \frac{\beta}{(\gamma - Sz)} \cdot \frac{D_{r,r}(x)}{D(x)} \cdot dz$$

We next alter the variable of integration from z to x . The relation between these two co-ordinates is that

$$x = \frac{\beta z}{\gamma - Sz}; \quad z = \frac{\gamma x}{\beta + Sx} \quad (19)$$

The contour \mathcal{C} of Fig. 1 transforms into the contour \mathcal{D} of Fig. 2, but since β and γ are negative, and S and M are positive for the occupied levels, and $S < \frac{1}{2}$ in all cases of conventional π -electron chemistry, all the poles in the integrand lie either between E and A or on the negative real axis of x . We may therefore deform the contour so that it becomes the imaginary axis and the infinite semicircle to the right of it. The contribution to the integral from the semicircle is zero, and so

$$q_r = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\beta}{\beta + iSy} \cdot \frac{D_{r,r}(iy)}{D(iy)} \cdot dy \quad (20)$$

In exactly the same way

$$q_{rs} = -\frac{2(-)^{r+s} S_{rs}}{\pi} \int_{-\infty}^{\infty} \frac{\beta}{\beta + iSy} \cdot \frac{D_{r,s}(iy)}{D(iy)} \cdot dy \quad . . . (21)$$

$$\mathcal{E} = 2m\alpha + \frac{\gamma}{\pi} \int_{-\infty}^{\infty} \left\{ \frac{iy}{\beta + iSy} \cdot \frac{D'(iy)}{D(iy)} - \frac{n}{\beta + iSy} \right\} \cdot dy \quad . . (22)$$

Equations (20) and (21) have not been given before, but (22) has been obtained in a rather different way by de Heer.¹³ This completes our derivation of the formulæ for atom charge, bond charge, and total π energy.

ATOM AND BOND POLARIZABILITIES

The definitions of these quantities follow as closely as possible those of ref. 1a. They are

$$\pi_{r,s} = \frac{\partial q_r}{\partial \alpha_s}; \quad \pi_{rs,t} = \frac{\partial q_{rs}}{\partial \alpha_t}; \quad \pi_{t,rs} = \frac{\partial q_t}{\partial \beta_{rs}}; \quad \pi_{rs,tu} = \frac{\partial q_{rs}}{\partial \beta_{tu}} \quad . . (23)$$

General expressions for these quantities can be written down at once by partial differentiation of (12) and (13). But we shall find it convenient to discuss two particular cases: (a) We imagine the overlap integrals to be kept constant in the course of the differentiations (23); (b) we use the Wheland assumption, from which it follows that $\delta S_{rs} = (S_{rs}/\beta_{rs})\delta\beta_{rs} = \hbar\delta\beta_{rs}$. In making the differentiations, we must now use equations analogous to (6), allowing for this variation of S_{rs} .

Case (a): δS put equal to zero.—From (9), by analogy with eqn. (57) of ref. 1a:

$$\pi_{r,s} = \frac{1}{\pi i} \oint \left(\frac{\Delta_{r,s}}{\Delta} \right)^2 \cdot dE$$

By successive transformations, first to z and then to x :

$$\pi_{r,s} = \frac{1}{\pi} \cdot \frac{\beta}{\gamma} \int_{-\infty}^{\infty} \left\{ \frac{D_{r,s}(iy)}{D(iy)} \right\}^2 dy = \frac{\beta}{\gamma} (\pi_{r,s})_0 \quad (24)$$

¹³ de Heer, *Phil. Mag.*, 1950, **41**, 370.

Similarly:

$$\pi_{rs,t} = 2 S_{rs} \beta / \gamma (\pi_{rs,t})_0 \quad . \quad . \quad . \quad . \quad . \quad . \quad (25)$$

$$\pi_{t,rs} = \beta / \gamma (\pi_{t,rs})_0 \quad . \quad . \quad . \quad . \quad . \quad . \quad (26)$$

$$\pi_{rs,tu} = 2 S_{rs} \beta / \gamma (\pi_{rs,tu})_0 \quad . \quad . \quad . \quad . \quad . \quad . \quad (27)$$

where the suffix zero denotes that the polarizabilities are calculated with complete neglect of all overlap integrals.

Case (b): $\delta\beta$ proportional to δS .—The polarizabilities $\pi_{r,s}$ and $\pi_{rs,t}$ defined in this case are independent of any variations of β_{rs} , and are therefore still given by (24) and (25). A discussion similar to that in ref. 1a shows that the other two polarizabilities are given by

$$\pi_{t,rs} = \frac{2(-)^{r+s}}{\pi} \int_{-\infty}^{\infty} \frac{\beta}{\beta + iSy} \cdot \frac{D_{r,t} D_{s,t}}{D^2} \cdot dy \quad . \quad . \quad . \quad (28)$$

$$\pi_{rs,tu} = \frac{q_{tu}}{\beta_{tu}} \delta_{rs}^{tu} + \frac{2(-)^{r+s+t+u}}{\pi} S_{rs} \int_{-\infty}^{\infty} \frac{\beta}{\beta + iSy} \cdot \frac{D_{r,u} D_{s,t} + D_{r,t} D_{s,u}}{D^2} \cdot dy \quad (29)$$

In (28) and (29) the function, $D_{r,s}$, etc., are all functions of the variable iy , and δ_{rs}^{tu} is the Kronecker "delta function." It is possible^{1a} to derive alternative expressions for these polarizabilities in terms of the fundamental coefficients c_{rj} in the various molecular orbitals. The expressions in case (a) follow at once from eqns. (64)—(67), of ref. 1a. But instead of (28) and (29) we have

$$\pi_{t,rs} = 4 \sum_{j=1}^m \left\{ \sum_{k=1}^n \frac{c_{tj} c_{tk} (c_{rj} c_{sk} + c_{sj} c_{rk})}{N_j^2 (\epsilon_j - \epsilon_k)} - \frac{S}{\beta} \frac{c_{rj} c_{sj} c_{tj}^2}{N_j^4} \right\} \quad . \quad . \quad (28a)$$

$$\pi_{rs,tu} = \frac{q_{tu}}{\beta_{tu}} \delta_{rs}^{tu} + 4 S_{rs} \sum_{j=1}^m \left\{ \sum_{k=1}^n \frac{(c_{tj} c_{uk} + c_{uj} c_{tk})(c_{rj} c_{sk} + c_{sj} c_{rk})}{N_j^2 (\epsilon_j - \epsilon_k)} - \frac{2S}{\beta} \cdot \frac{c_{rj} c_{sj} c_{tj} c_{uj}}{N_j^4} \right\} \quad (29a)$$

SOME GENERAL THEOREMS

Several theorems proved earlier^{1a,b} can be modified to apply to our new atom and bond charges. The results are given below without proof for a few important cases.

(1) q_r must be positive. (2) For alternant hydrocarbons, where we assume (i) equality of all α_r , (ii) equality of all β_{rs} for neighbour atoms, and neglect of all other β_{rs} , and (iii) β_{rs} proportional to S_{rs} ,

$$q_r + \frac{1}{2} \sum_{s \neq r} q_{rs} = 1.$$

$$(3) \text{ In all cases } q_r + \frac{1}{2} \sum_{s \neq r} q_{sr} \leq 2$$

$$(4) q_{rs}^2 \leq 4 S_{rs}^2 q_r q_s$$

(5) $\pi_{r,r}$ and $\pi_{rs,rs}$ are both negative, whether we consider case (a) or case (b) of p. 4046.

$$(6) \mathcal{E} = \sum_r q_r \alpha_r + \sum_{r < s} \sum q_{rs} (\beta_{rs} / S_{rs}).$$

In particular, for alternant hydrocarbons, as in theorem (2):

$$\mathcal{E} = \text{constant} + k^{-1} \sum_{r < s} \sum q_{rs}$$

showing that the bond charge q_{rs} may be used as an indication of the contribution of the

bond r s to the total π -electron energy. We are indebted to Dr. J. A. R. Coope for pointing this out to us (see also Mulliken⁵).

$$(7) \sum_r q_r + \sum_{r < s} q_{rs} = 2m$$

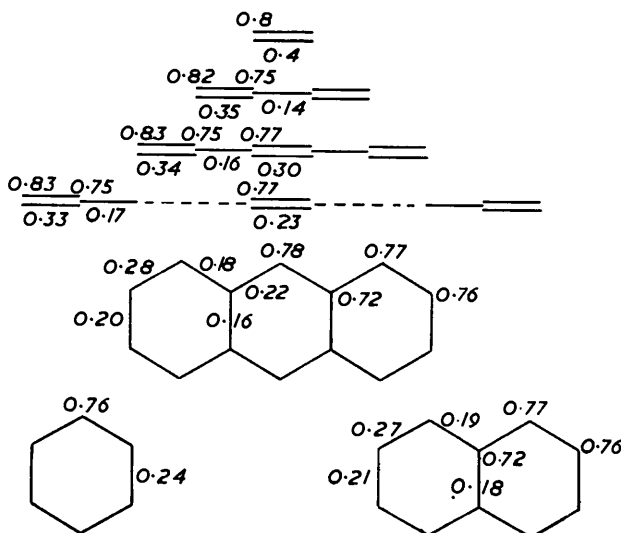
$$(8) \sum_r \pi_{r,t} + \sum_{r < s} \pi_{rs,t} = 0 \text{ for both cases (a) and (b)}$$

$$(9) \sum_r \pi_{r,tu} + \sum_{r < s} \pi_{rs,tu} = 0 \text{ for both cases (a) and (b)}.$$

NUMERICAL CALCULATIONS

We have made some calculations for alternant hydrocarbons [with the approximations cited in Theorem (2)] but, in agreement with the energy calculations of de Heer¹³ and others (cf. refs. in de Heer's paper), we find that the agreement with experiment is generally

FIG. 3. *Atom and bond charge densities for several polyacenes and linear polyenes* ($S = 1/4$).



unchanged when overlap is included. There is practically no change in the correlation of free valence with localization energy, or of bond charge (as compared with bond order) with bond length.

To give some idea of the magnitude of the atom and bond charges, we give in Fig. 3 their values for linear polyenes and for some polyacenes. (All numerical results in the Figures and Tables were evaluated at $S = \frac{1}{4}$.) It is clear from this Figure that the alternant nature of these molecules is now apparent from both their atom and bond charges; this was not so with the simpler theory where the atom charges were all unity. It is difficult at present, however, to say whether the atom charge or Mulliken's "gross atomic population"⁵ is the better for studies of reactivity. Perhaps, when the experimental data for the susceptibility to attack of the α - and β -positions of naphthalene become more definite, we shall be able to clear up this point.

One difference in the predictions for zero overlap and for inclusion of S occurs in the value of the bond-bond self-polarizability. As implied in eqn. (29), this depends critically upon the relation of δS to $\delta\beta$. In Tables 1 and 2 we give the values of the bond-bond polarizabilities for benzene and naphthalene for the two cases (a) $\delta S = 0$ and (b) $\delta S = k\delta\beta$.

In Tables 3 and 4 we list the atom-bond polarizabilities for case (b). For case (a) these are zero, but in case (b) some of these polarizabilities also are quite large. In Tables 1-4 the units are $1/\gamma$.

TABLE 1. *Mutual bond polarizabilities in benzene.*

(a) $k\beta = S, \delta S = 0$		(b) $k\beta = S, k\delta\beta = \delta S$	
Bond	1-2		1-2
1-2	0.1204		0.2877
2-3	-0.1019		-0.0931
3-4	0.0648		0.0625
4-5	-0.0463		-0.0457

TABLE 2. *Mutual bond polarizabilities in naphthalene.*

Case (a): $k\beta = S, \delta S = 0$								
Case (b): $k\beta = S, k\delta\beta = \delta S$.								
Bond	10-9		9-1		1-2		2-3	
	(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
10-9	0.127	0.231	-0.055	-0.048	0.033	0.032	-0.021	-0.020
9-1	-0.055	-0.048	0.144	0.261	-0.091	-0.083	0.056	0.054
1-2	0.033	0.032	-0.091	-0.083	0.105	0.300	-0.105	-0.095
2-3	-0.021	-0.020	0.056	0.054	-0.105	-0.095	0.148	0.283
3-4	0.033	0.032	-0.037	-0.037	0.062	0.060	-0.105	-0.095
4-10	-0.055	-0.048	0.048	0.046	-0.037	-0.037	0.056	0.054
10-5	-0.055	-0.048	-0.013	-0.013	0.013	0.013	-0.023	-0.022
5-6	0.033	0.032	0.013	0.013	-0.010	-0.010	0.016	0.016
6-7	-0.021	-0.020	-0.023	-0.022	0.016	0.016	-0.016	-0.016
7-8	0.033	0.032	0.030	0.029	-0.016	-0.016	-0.016	0.016
8-9	-0.055	-0.048	-0.073	-0.065	0.030	0.029	-0.023	-0.022

TABLE 3. *Atom bond polarizabilities in benzene.*

Case (b): $k\beta = S, k\delta\beta = \delta S$			
Bond rs	1-2	2-3	3-4
$\pi_{1,rs}$	-0.097	0.015	-0.008

TABLE 4. *Atom bond polarizabilities in naphthalene.*

Case (b): $k\beta = S, k\delta\beta = \delta S$			
Bond	Atom 1	2	9
1-2	-0.109	-0.102	0.011
2-3	0.021	-0.094	-0.006
1-9	-0.089	0.015	-0.074
8-9	0.018	-0.003	-0.074
4-10	-0.005	-0.009	0.007
3-4	-0.012	0.018	-0.004
9-10	0.008	-0.006	-0.067
5-10	0.000	0.005	-0.009
5-6	-0.001	-0.003	-0.004
6-7	0.003	0.000	-0.006
7-8	-0.007	+0.000	0.012

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