

Quantum-chemical Treatment of Cyclization and Recyclization Reactions: XXVI.* Effects of Substituents in the Thermal Rearrangement of Methylene-cyclopropane

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Abstract—Basing on the coupled perturbation Hartree-Fock theory an effect of substituents on the thermal rearrangement of methylenecyclopropane derivatives was considered. The effect is described in the second order of the theory. The activation energy depends both on the first and second power of the parameter characterizing the substituent, and introduction of several groups as a rule cannot be described in the framework of an additive scheme and requires accounting for the interactions between the substituents. The results of computation are in good agreement with the results of kinetic measurements.

Effects of substituents on the rates of chemical reactions proceeding through ionic transition state are described as a rule by various sets of σ -constants [2]. The rates of radical reaction due to the polar effects also frequently correlate with Hammett's σ constants or Brown's σ^+ [3]. At the same time quite a number of reaction series is known where the polar factors play negligible role, and the transition state has pure radical (biradical) character. In this case it is hardly possible to expect good agreement with the mentioned constants of the substituents. Therefore various σ^- -scales were advanced for estimation of the ability of various functional groups to stabilize free radicals. These scales were mostly based on kinetic measurements. For instance, the σ^- of Jackson [4] is founded on the rate of thermal decomposition of dibenzyl-mercury derivatives, the σ_F^- of Fisher [5] utilizes the bromination rate of *para*-substituted 3-cyanotoluenes. Among the non-kinetic methods for estimating the stabilizing substituents effect approaches should be mentioned using evaluation of hyperfine coupling constants in the ESP spectra [6], pK_a -values, and redox potentials [7]. However the transition from σ^- -constants obtained in one reaction series to those calculated in another one "involves the difficulty in complete separation of the polar and radical effects" [6] that apparently ensure respectively stabilization of ionic and radical intermediates; also should be taken into consideration the influence of the substituents on the stability of the initial compound. Therefore all these σ^- -scales are in poor accord with each other and have limited practical application. Besides in the

presence of two or more substituents their effect on the reaction rate commonly does not agree with the additivity rule, and this is not accounted for within the framework of these models. The formerly developed scheme accounting for the substitution effect on physicochemical characteristics of molecules based on the bound version of the perturbation theory (see, e.g., [8]) involves the unique parametrization of the substituents $\Delta\alpha_{R_j}$. The $\Delta\alpha_{R_j}$ values, initially selected using the NMR spectra, are constant for each substituent and independent of the position of substitution, of the substituted substrate and of the characteristic under consideration. Therefore the values can be equally applicable both to radicals and common molecules. Therefore the goal of this study is illustration of the fact that this approach provides a quantitative description of rate constants of recyclization in the alternant systems (by an example of methylenecyclopropane recyclization) not only for mono- but also for disubstitution, and that it excludes the necessity to use various sets of specially chosen radical constants of substituents.

The variation of energy in the system at substitution within accuracy to the terms of the first and second order of the perturbation theory is described as follows:

$$\Delta E^0 = \sum_i q_i^0 \Delta\alpha_{R_i} + \frac{1}{2} \sum_i \pi_{ii}^0 (\Delta\alpha_{R_i})^2 + \sum_{i>k} \pi_{ik} \Delta\alpha_{R_i} \Delta\alpha_{R_k}, \quad (1)$$

where q_i^0 is the π -electron charge of the i -th atom, π_{ik} are mutual atom-atom polarizabilities, and summation is performed over all substituents R . Applying this expression to a noninteracting molecule and a

* For communication XXV see [1].

transition state we get for the variation of activation energy of reaction effected by substitution

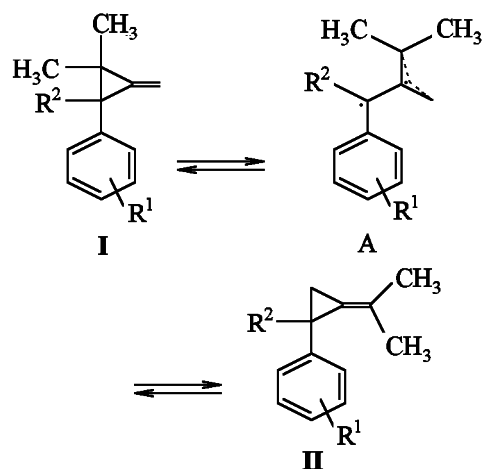
$$\Delta\delta E^0 = \sum (q_i^0 - q^{\ddagger})\Delta\alpha_{R_i} + \frac{1}{2}\sum_i (\pi_{ii}^0 - \pi_{ii}^{\ddagger})(\Delta\alpha_{R_i})^2 + \sum_{i>k} (\pi_{ik}^0 - \pi_{ik}^{\ddagger})\Delta\alpha_{R_i}\Delta\alpha_{R_k} + 2\sum_i \pi_{i,lm}\Delta\alpha_{R_i}\Delta\beta_{lm}, \quad (2)$$

where the last term is introduced to take into account the change in the order of the forming remote l - m bond in the unimolecular electrocyclic reactions ($\Delta\beta$ is the change in the resonance integral corresponding to a dis- or conrotatory motion of bonds).

Thus the substituent effects in reactions proceeding through carbocations (carbanions) formation, and also through systems with considerable separation of charges, can be sufficiently accurately described in the first order perturbation theory with respect to $\Delta\alpha_{R_j}$ [the first term in formula (2)]. However for alternant molecules and radicals the variation of reaction rates under the influence of the chemical substitution should be described not in the first, but in the second order perturbation theory since due to level pairing theorem all the residual charges on the atoms of these compounds would be equal to zero. One among the conformations of the above is the familiar fact that electrophilic and nucleophilic attack on the benzoid hydrocarbons occurs at the same positions (see, e.g., [9]), and also relatively small effect of substitution on the rate of alternant radicals formation (see, e.g., [10]). It should be stressed that the second and third terms of expression (2) are quantities of the same order of magnitude, therefore *a priori* neither of them can be neglected.

To illustrate the approach we consider the thermal rearrangements of substituted methylenecyclopropanes. The choice of this type reactions is not casual and is caused by the following reasons. Firstly, the biradical species arising in the course of reaction are nearer to the transition state than the initial compounds, and therefore the application of the index approach directly to the biradicals is theoretically more justified. Secondly, the rearrangements of such kind are used as tests of pure free-radical substituent effects [11] (in contrast to polar effects). Within the framework of the applied approach it means application of the second order perturbation theory with respect to $\Delta\alpha_{R_j}$ and $\Delta\beta_{ik}$. Finally, a large amount of published data exists on methylenecyclopropane rearrangement dependence on the type, position, and number of substituents. Therefore the comparison of theoretical and experimental results may be more complete than with the radical series.

Scheme 1.



One of the most thoroughly studied in this respect reactions [12–14] is the rearrangement of 3,3-dimethyl-2-phenylmethylenecyclopropane (**I**) into 2-phenylisopropylidenecyclopropane (**II**). Therewith according to equation (2) the change in the rate of this reaction due to the chemical substitution originates from nonzero contributions both of the first (3rd and 4th terms) and second (2nd term) powers of $\Delta\alpha_{R_j}$.

It is possible therefore regarding equation (2) as a correlation avoid the calculation of π_{ii} , π_{ik} , $\pi_{i,lm}$ and describe the experimental rate values of the reaction [12] basing on their correlation with $\Delta\alpha_{R_j}$ and $\Delta\alpha_{R_j}^2$. Actually, for the *para*-substituents a sufficiently reliable description of the rearrangement rate was obtained:

$$\log k = -(3.41 \pm 0.02) + (0.049 \pm 0.010)\Delta\alpha + (0.115 \pm 0.006)\Delta\alpha^2, \\ n \ 11, \ R \ 0.990, \ S \ 0.043. \quad (3)$$

Similar results were obtained also for *meta*-substituents:

$$\log k = -(3.455 \pm 0.009) - (0.039 \pm 0.006)\Delta\alpha - (0.023 \pm 0.005)\Delta\alpha^2, \\ n \ 9, \ R \ 0.946, \ S \ 0.018. \quad (4)$$

The regression factors at $\Delta\alpha_{R_j}^2$ in these equations in keeping with expression (2) should be proportional to the difference of the atomic polarizabilities of the initial molecule and the triplet biradical A. The values calculated for the *meta*- and *para*-positions $\pi_{ii}^0 - \pi_{ii}^{\ddagger}$ (-0.0015 and 0.0033 eV^{-1}) provide overall correct dependence of the reaction rates on substitution posi-

tion. In the first case the rate constant decreases, and in the second case increases as compared to the reaction rate constant for the unsubstituted molecule. However the combining of correlations (3) and (4) is hampered since the term proportional to the first power of $\Delta\alpha_{R_j}$ is governed by a sum of two factors: interaction of functional groups, and effect caused by the change in the order of the remote bond due to substitution. The relative contribution from these factors cannot be precisely evaluated because of uncertainty of the change in the value of the resonance integral $\Delta\beta$.

The results obtained by calculations of rate constants in keeping with correlation equations (3, 4) are compared with the experimental data in Table 1, where are also given the $\Delta\alpha_{R_j}$ values (in -3.8972 eV units) for the functional groups under consideration. Note that the $\Delta\alpha_{R_j}$ values are linearly related to the Taft's inductive constants σ^* (see [8]), except that the halogens fall out of this series. A similar pattern is observed with the *meta*-substituents. However if increase the values of their parameters by 1.4 as was done before [15], these points fall on the common straight line.

As was pointed out in [16], the relative rates of the rearrangement in question did not correlate with any standard set of substituents constants (σ , σ^+ , σ^-). It is obvious from equation (2) that the rate constants should have been correlated not only with the proper substituent constants but also with the squares of the latter.

In going to discussion of the rearrangements occurring with disubstituted derivatives of 2-phenyl-3,3-dimethylmethylenecyclopropane (**I**) it should be noted that the additive model of substituent effect on the rate of chemical reactions is justified only in the first order perturbation theory. Therefore the introduction into an alternant system of several substituents may cause deviation from additivity as is actually observed experimentally [13, 14]. The value of this deviation as follows from expression (2) (the term proportional to $\Delta\alpha_{R_i}\Delta\alpha_{R_k}$) can be calculated basing on mutual atom-atom polarizabilities. For instance, the calculation demonstrated that the interaction between functional groups in the *meta*-positions of compound **I** is relatively weak ($\pi_{35}^0 - \pi_{35}^\# = -0.0006$ eV $^{-1}$). As a result the effects of two substituents in this case should follow the additivity rule. Actually, the values of logarithms of rate constants for 3,5-dimethyl and 3,5-dichloro derivatives of compound **I** calculated according to the additive scheme agree well with the

experimental data [12] given in parentheses: -3.54 (-3.54); and -3.42 (-3.37).

At the same time for the substituents located in 2 position of the three-membered ring and in *para*-position of the six-membered ring the $\pi_{n2}^\#$ value amounts to 0.0075 eV $^{-1}$, and in the framework of the approach under consideration it means that either synergistic or antisnergistic effect is observed respectively when both substituents are donors (acceptors) or one is donor and another acceptor. This conclusion is in total agreement with the experiment [13, 14] where has been demonstrated that in the presence of one donor and another acceptor substituent the reaction is accelerated, and with two acceptor substituents it is retarded.

In order to find in expression (2) the term corresponding to the interaction of the functional groups it is necessary to have the reaction rate constants both for disubstituted (k_{ik}) and the corresponding monosubstituted (k_i and k_k) and unsubstituted (k_0) compounds, and all the data should be measured under the same conditions. Then it is easy to show that

$$\log(k_{ik}k_0/k_i k_k) = A(\pi_{ik}^0 - \pi_{ik}^{\#})\Delta\alpha_{R_i}\Delta\alpha_{R_k}. \quad (5)$$

To illustrate this relation let us consider the rearrangements of 3,3-dimethyl-2-phenylmethylenecyclopropane (**I**) in isoctane at a fixed substituent in the 2 position ($R^2 = \text{COOEt}$ on Scheme 1) and a

Table 1. Effect of substitution on the rate of thermal rearrangement in derivatives of 2-phenyl-3,3-dimethylmethylenecyclopropane

Substituent	$\Delta\alpha_{R_j}$	-log <i>k</i> <i>para</i> -substituted		-log <i>k</i> <i>meta</i> -substituted	
		calcd.	exp. data	calcd.	exp. data
NMe ₂	-3.00	2.52	2.55	3.55	-
SMe	-1.89	3.09	3.02	3.46	3.48
OMe	-1.6	3.19	3.21	3.45	3.47
<i>t</i> -Bu	-1.2	3.30	3.32	3.44	-
Me	-0.9	3.36	3.33	3.44	3.42
H	0	3.41	3.45	3.46	3.45
Br	0.55	3.35	3.31	3.48	-
CF ₃	0.68	3.32	3.37	3.49	3.51
Cl	0.74	3.31	3.32	3.50	3.48
F	0.92	3.27	3.53	3.51	3.50
CN	1.61	3.03	2.99	3.58	3.57
NO ₂	1.99	2.86	2.87	3.55	3.56

variable substituent in the para-position R^1 . As seen, the obtained correlation (6) well supports this relation

$$\log(k_{n_2}k_0/k_n k_2) = -(0.230 \pm 0.021)\Delta\alpha_{R_n}\Delta\alpha_{R_2},$$

$$n \ 4, \ r \ 0.986, \ S \ 0.041. \quad (6)$$

The calculation in keeping with this equation of the relative rate of rearrangement for $R^1 = \text{H, OMe, Me, CO}_2\text{Et}$ respectively gives 1 (1); 3.92 (4.35); 2.00 (1.89); 1.49 (1.63). The figures in parentheses are the experimental data from [13].

Apparently in the above example because of the groups interaction the weight of the linear in $\Delta\alpha_{R_j}$ term in correlations of (3, 4) type is higher than for the *para*-monosubstituted compounds. Therefore somewhat better correlation of the kinetic data with the σ^+ constants of the donor substituents was remarked [13]. Note however that the electron-withdrawing groups fall out of such correlations as before [12, 13].

We like to point out that the relation (5) is observed not only for the data obtained in isoctane as solvent but also for the kinetic measurements carried out in C_6D_6 [14].

$$\log(k_{n_2}k_0/k_n k_2) = -(0.050 \pm 0.021) - (0.126 \pm 0.017)\Delta\alpha_{R_i}\Delta\alpha_{R_k},$$

$$n \ 8, \ r \ 0.951, \ s \ 0.050. \quad (7)$$

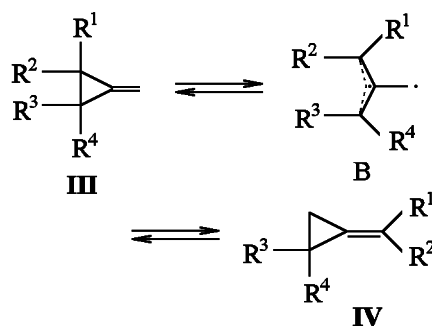
The calculated and experimental (in parentheses) values of the relative reaction rates are here for substituents CF_3 and $R^1 = \text{COOEt}$ 1.80 (1.67); for CF_3 and OMe 2.79 (2.77); for CF_3 and SMe 3.88 (3.32); for CF_3 and NMe_2 16.84 (18.97); for CO_2Et and CF_3 0.81 (0.79); for Me and CF_3 1.20 (1.34); and for CO_2Et and SMe 4.19 (3.83).

The different conditions of reactions carried out with substituted derivatives of methylenecyclopropane proper hampers the comparison of the available rate constants (see book [16] and references therein). In this connection more accurate comparison may be performed on activation energies. Besides the presence of disubstituted derivatives requires taking into account all the terms in expression (3), for instance, with the help of correlation equation of the type

$$\log k = A + B \Delta\alpha_{R_i} + C \Delta\alpha_{R_i} \Delta\alpha_{R_j} + D \Delta\alpha_{R_i}^2, \quad (8)$$

where the regression factors B, C, D in a general case depend on the position of substitution. Since the

Scheme 2.



regression factors in equations (6) and (3) (the term containing $\Delta\alpha^2$) reasonably correspond to the respective polarizabilities before $\Delta\alpha_{R_i}\Delta\alpha_{R_k}$ and $\Delta\alpha^2$ in expression (2), the terms 3 and 4 in the latter would be appropriate to combine.

Thus for the empirical activation energies E_a of the reactions in question (from data of [17]) in full agreement with expression (2) we obtained the following correlation with the parameters of electronic structure and substituents constants ($l-m$ is the index of the bond forming in the course of the reaction)

$$E_a = (173.3 \pm 2.8) - (354 \pm 40) \sum_{i,k>i} \left(\frac{1}{2} \pi_{ii} \Delta\alpha_{R_i}^2 + \pi_{ik} \Delta\alpha_{R_i} \Delta\alpha_{R_k} \right) + (530 \pm 54) \sum_i \pi_{i,lm} \Delta\alpha_{R_i},$$

$$n \ 8, \ r \ 0.989, \ S \ 3.57 \text{ kJ mol}^{-1}. \quad (9)$$

Here were used the following values of mutual polarizabilities for the triplet state of trimethylenemethane $\pi_{2,23} = 0.0257$; $\pi_{2,34} = \pi_{2,3} = -0.0192$; $\pi_{22} = 0.0706 \text{ eV}^{-1}$. It should be once again stressed that the term proportional to $\Delta\alpha_{R_i}\Delta\alpha_{R_k}$ is introduced to take into account the interaction between the functional groups since the calculation according to the additive scheme (that is given in Table 2 in parentheses) furnishes strongly underestimated values of the activation energy.

The last term in equation (9) may be applied to estimation of the percentage of various isomers present in the mixture for just from this term originates the difference in the activation energy for compounds with the same substituents. Thus, according to (9) the equilibrium in the reaction shown on Scheme 2 (at relatively low temperature) will be shifted to the left in the case of electron-donor substituents. With the electron-acceptor groups on the contrary will dominate the direct process. For instance, when $R^2 = R^4 = \text{H}$, $R^1 = R^3 = \text{COOMe}$,

Table 2. Activation parameters of methylenecyclopropane rearrangement

Substituent				E_a , kJ mol ⁻¹	
R^1	R^2	R^3	R^4	calculation	experiment
D	D	D	D	173	174
CH ₃	H	H	H	172	169
CH ₃	CH ₃	H	H	171	172
OC ₂ H ₅	H	H	H	158	156
H	H	OC ₂ H ₅	H	119	116
CH ₃	CH ₃	OCH ₃	H	137 (114)	142
OCH ₃	H	CH ₃	CH ₃	132 (109)	131
CH ₃	CH ₃	CH ₃	CH ₃	149 (124)	152

the content of the initial 2,3-bis(methoxymethylene)cyclopropane in the equilibrium mixture amounts only to 6–8% [18]. Note that oxo and aza-substitution also can be described within the framework of the used substituent model (they are treated as electron-acceptor groups). Therefore the last conclusion is to the same extent valid for the allene oxide and *N*-methylmethylenaziridine which readily rearrange into cyclopropanone and *N*-methylcyclopropylimine [16].

It should be mentioned that the stated above rules on dependence of reactions in alternant systems on the character and number of substituents are revealed also in the other physicochemical characteristics.

Actually, because of validity of the theorem on levels pairing the diagonal elements of the orbital-spin polarizability matrix in the alternant radicals are equal to zero, i.e. the variation of spin density effected by chemical substitution should be described not in the first but in the second order perturbation theory with respect to $\Delta\alpha_{R_j}$. Let us show it by an example of the *para*-substituted benzyl radicals. Thus for the most sensitive to substitution constant of hyperfine coupling belonging to the proton of the methylene group we get (for experimental data see [6, 19]):

$$a_{7H} = (16.35 \pm 0.07) - (0.249 \pm 0.041)\Delta\alpha_{R_i}^2, \\ n \ 11, \ r \ 0.896, \ s \ 0.153 \ \text{Gauss}, \quad (10)$$

whereas the correlation with the first power of $\Delta\alpha_{R_j}$ is not detected (the angular factor is insignificant).

$$a_{7H} = (16.05 \pm 0.12) + (0.055 \pm 0.104)\Delta\alpha_{R_i}, \\ n \ 11, \ r \ 0.174, \ s \ 0.340 \ \text{Gauss}. \quad (11)$$

However already in cumyl radical due to interaction of the *para*-substituents with two methyl groups the constants of the hyperfine coupling from the β -protons correlate not only with $\Delta\alpha_{R_j}^2$, but also with $\Delta\alpha_{R_j}$:

$$a_{7H} = (16.25 \pm 0.06) - (0.131 \pm 0.040)\Delta\alpha_{R_i} \\ - (0.220 \pm 0.035)\Delta\alpha_{R_j}^2, \ n \ 11, \ r \ 0.918, \ s \ 0.129 \ \text{Gauss}. \quad (12)$$

Note that in the correlation obtained the regression factors are significant both at $\Delta\alpha_{R_j}$ and $\Delta\alpha_{R_j}^2$. The experimental data utilized in correlations (10–12) are taken from [6, 19].

The observed nonadditive changes in the a_H values at introducing several substituents into allyl radical [20] and the other alternant system [21] also is in agreement with accounting for the influence of the substituents on the ESR spectra in the second order perturbation theory.

Just the observed relation (10) of the constants of hyperfine coupling to $\Delta\alpha_{R_j}^2$ allows the use of the changes in these constants in correlations which cannot be described by the standard σ -Hammett approach. For instance, basing on the difference in the constants of hyperfine coupling of the *para*-substituted and unsubstituted benzyl radicals [6] was constructed a radical scale for substituents σ^- that together with a set of σ constants was used in describing the substituents effects in the reaction shown in Scheme 1. However as was pointed out in [22] the application the constants of hyperfine coupling in themselves as indices of reactivity (and not their changes effected by substitution) or the application of closely related spin densities [23] is not quite proper for the orbital perturbation of the atomic or bond type does not result in dependence of change in the system energy from the spin densities or their corrections.

Thus we demonstrated that a simple approach based on a unique parametrization of the substituents valid for ionic and radical systems allows sufficiently reliable quantitative description of the substitution effect both on kinetics of the thermal rearrangement of methylenecyclopropane and some other physicochemical properties of alternant radicals.

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