LITERATURE CITED

1. T. N. Borisova, A. V. Varlamov, N. D. Sergeeva, A. T. Soldatenkov. O. V. Zvolinskii, A. A. Astakhov, and N. S. Prostakov, Khim. Geterotsikl. Soedin., No. 7, 973 (1987).
2. L. N. Yakhontov, Usp. Khim., No. 5, 840 (1980).
3. H. Budzikiewicz, C. Djerassi, and D. Williams, The Interpretation of the Mass Spectra of Organic Compounds [Russian translation], Mir, Moscow (1966), p. 128.
4. P. B. Terent'ev, Mass Spectrometry in Organic Chemistry [in Russian], Vyssh. Shkola, Moscow (1979), p. 76.
5. A. I. Ermakov and Yu. N. Sheinker, Khim. Geterotsikl. Soedin., No. 2, 221 (1981).
6. R. Johnston, Handbook of Mass Spectrometry for Organic Chemists [Russian translation], Mir, Moscow (1975).

QUANTUM-CHEMICAL INVESTIGATION OF THE DIELS—ALDER REACTION IN CONDENSED ISOINDOLES WITH A NODAL NITROGEN ATOM

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On the basis of calculated data on the electron structures of condensed isoindoles with a nodel nitrogen atom it is hypothesized that these compounds may act as dienes in the Diels—Alder reaction. Conclusions regarding the relative activities and the peculiarities of cycloaddition in the investigated structures were drawn from the static reactivity indexes obtained within the Pariser—Parr—Pople approximation.

Computational methods, together with kinetic studies, are currently the chief sources of information regarding the reactivities of dienes and dienophiles in the Diels—Alder reaction and its stereochemistry and mechanism. Data obtained in recent years [1-5] show that the Woodward—Hoffmann theory [6], which is acknowledged by organic chemists, is not absolute. More thorough and elegant experimental investigations have demonstrated the possibility of the realization of "forbidden" (from the point of view of the theory of orbital symmetry) processes [7], as well as a two-step mechanism of the Diels—Alder reaction, in contrast to the classical one-step synchronous process [1, 3, 5, 8].

Chiefly butadiene, polyenes, benzene, polyacenes, and cyclopentadiene have been included among the dienes that have been investigated by quantum-chemical methods. However, calculations of heterocyclic dienes began to be realized only recently [9, 10]. In particular, several explanations were proposed in [11, 12].

In the course of a systematic study of the chemistry of isoindole and its condensed derivatives we calculated the electron structures of isoindole [13] and a number of azino- [14] and azoloindoles [15]. It was established that the bond orders, π charges, (σ + π) charges, and valence activities of the bonds and fragments [16] in the isoindole part of the condensed systems change little, and, consequently, it is logical to assume that, with respect to chemical properties, they all* will resemble isoindole; in particular, they should undergo the Diels—Alder reaction that is characteristic for the latter. The aim of the present research was to evaluate the relative activities of a number of condensed isoindoles I-XVII in this reaction by means of calculated data.

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*The numbering of the atoms differs from that generally used for a more concise exposition of the material in this paper.

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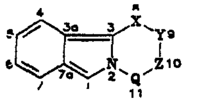
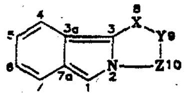


I–IX



X–XVII

I X=Y=Z=Q=CH; II X=N, Y=Z=Q=CH; III X=Z=Q=CH, Y=N; IV X=Y=Q=CH, Z=N; V X=Y=Z=CH, Q=N; VI X=N—Me, Y=Z=CH, Q=C=O; VII X=N—Me, Y=C=O, Z=Q=CH; VIII X=N—Me, Y+Z= o-phenylene Q=C=O; IX X=N—Me, Y=C=O, Z+Q=o-phenyleneX X=N—Me, Y=Z=CH; XI X=Y=CH, Z=N—Me; XII X=N—Me, Y+Z=o-phenylene XIII X=N—Me, Y=CH, Z=N; XIV X=NMe, Y=N, Z=CH; XV X=N, Y=CH, Z=NMe; XVI X=NMe, Y=Z=N; XVII X=Y=N, Z=N—Me

There are presently two groups of approaches to the quantum-chemical description of the Diels–Alder reaction: the construction of potential surfaces of the reactions [7, 17, 18] by means of nonempirical and semiempirical methods of calculation and the use of static reactivity indexes from semiempirical calculations [19-21]. The first pathway is modern and extremely promising. However, the construction of potential surfaces is a very complex procedure, particularly if the reactions of dienes and dienophiles other than the simplest are examined, and the potential surfaces of the Diels–Alder reaction for complex compounds such as isoindole therefore have not yet been calculated. In addition, there are data that indicate that calculations of this sort do not always lead to unequivocal results [22, 23]. We therefore selected the second approach, especially since the use of static indexes in series of similarly constructed compounds (this is obvious for our structures) has been justified [24, 25].

In the complete analysis of static reactivity indexes one should take into account the fact that cycloaddition may occur both synchronously [18, 23, 26] and nonsynchronously [2, 26]. In the latter case either a concerted mechanism [18] or a two-step mechanism with the intermediate formation of a zwitterion or a diradical [1, 27] is possible. However, it follows from the literature that, regardless of the mechanism, many peculiarities of the diene synthesis are determined by the donor-acceptor properties of the reagents and by the difference in the stabilization of the reagents and the reaction products, which is associated with the localization energy [22, 28-31]. From our point of view, the symmetry of the starting molecules should also be added to these two important features. Thus in the Diels–Alder reaction of N-methylisoindole (a symmetrical diene) [32] and 1-ethylthio-2-phenylisoindole (an unsymmetrical diene) [3] with N-substituted maleinimides, exclusively supra-supra-cycloaddition adducts (endo and exo) are formed in the first case, whereas in the second case the formation of supra-antara-cycloaddition adducts is possible, which constitutes evidence for a nonsynchronous mechanism.

Considering the material set forth above, for convenience in analysis of the static reactivity indexes of dienes we propose to separate the cycloaddition process into three arbitrary stages: I) mutual orientation of the reacting molecules (indexes used: the π charges and the boundary electron densities at the ends of the diene fragments, and other indexes); II) donor-acceptor interaction, which leads either to a donor-acceptor complex or to the formation of an intermediate particle* [the energy of the highest occupied molecular orbital (HOMO)]; III) formation of an adduct, which is accompanied by cleavage of the overall π system and liberation of individual π fragments (the localization energy).

Compounds I-V contain formally three cis-diene fragments, while VI-XVI contain two. Proceeding from the π charges (q_π) at the ends of the diene fragments, as well as the boundary electron densities (f_π) in these positions, calculated within the Pariser–Parr–Pople (PPP) approximation (Table 1), it may be concluded that the initial attach of the dienophile in all of the compounds will be realized at the pyrrole ring, just as one observes in the case of isoindole. In addition, in the case of addition to the pyrrole diene fragment a new π bond that is involved in the aromatic sextet of the benzene ring, which is energically favorable, is formed. On the other hand, alternative cycloaddition in the 4,7 or 8,11 positions (the latter for I-V) should lead to the less energically favorable π systems of pyrroloazines or isoindole, respectively, in conjunction with extremely reactive isolated double bonds.

It follows from the data in Table 1 that the π charges, as well as the boundary electron densities in the 1 and 3 positions, differ from one another to a greater or lesser extent (for different structures). On the one hand, this means that a nonsynchronous mechanism of

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*Completion of the reaction with the formation of a Michael adduct is possible at this stage.

TABLE 1. Reactivity Indexes of Condensed Isoindoles in the Ground State

Compound	π charges at the ends of the diene (q_π)					Boundary electron densities (f_π) in positions						E_{HOMO}, kJ/mole		E_{loc}, kJ/mole
	position		sum in positions											
	1	3	1,3	4,7	8,11	1	3	4	7	8	11	PPP	CNDO/2	
I	−0,23	−0,16	−0,39	−0,02	−0,09	0,27	0,12	0,09	0,14	0,03	0,10	−825	−853	2883
II	−0,24	−0,10	−0,34	−0,01	−0,27	0,27	0,14	0,12	0,15	0,01	0,06	−830	−873	2855
III	−0,19	−0,17	−0,36	−0,01	+0,01	0,24	0,10	0,10	0,14	0,01	0,13	−854	−854	
IV	−0,23	−0,14	−0,37	−0,01	+0,07	0,27	0,10	0,08	0,13	0,03	0,11	−833	−818	
V	−0,21	−0,16	−0,37	−0,02	−0,17	0,26	0,13	0,10	0,14	0,01	0,08	−840	−862	
VI	−0,18	−0,19	−0,37	−0,02		0,25	0,17	0,11	0,13			−837	−821	2799
VII	−0,22	−0,18	−0,40	+0,00		0,25	0,18	0,13	0,14			−851	−841	2811
VIII	−0,20	−0,17	−0,37	−0,01		0,25	0,17	0,10	0,12			−820	−806	
IX	−0,21	−0,18	−0,39	−0,02		0,25	0,19	0,13	0,14			−836	−824	2814
X	−0,26	−0,19	−0,45	−0,02		0,29	0,14	0,10	0,14			−812	−802	2854
XI	−0,26	−0,18	−0,44	−0,02		0,28	0,12	0,08	0,13			−810	−804	
XII	−0,25	−0,18	−0,43	−0,02		0,28	0,15	0,10	0,13			−801	−801	2839
XIII	−0,24	−0,20	−0,44	−0,02		0,29	0,17	0,12	0,15			−820	−812	
XIV	−0,26	−0,19	−0,45	−0,02		0,30	0,13	0,10	0,14			−818	−780	2855
XV	−0,27	−0,12	−0,39	−0,02		0,28	0,14	0,11	0,15			−815	−812	
XVI	−0,25	−0,20	−0,45	−0,02		0,29	0,15	0,12	0,15			−828	−831	2861
XVII	−0,25	−0,13	−0,38	−0,02		0,27	0,16	0,11	0,15			−832	−835	

the Diels–Alder reaction is possible for compounds that have a substantial difference in charges on the ends of the pyrrole butadiene fragment (for example, the II, XV, XVII, etc. molecules). However, a synchronous mechanism is more likely for isoindolopyrimidones VI and VII and isoindoloquinazolones VIII and IX. The latter conclusion is also confirmed by the small differences in the boundary electron densities in the 1 and 3 positions of these compounds (Table 1). However, this option does not always prove to be unequivocal. An example of this is structure II, where a synchronous mechanism is predicted judging from the Δq_π values, whereas a nonsynchronous mechanism is also extremely likely from the Δf_π value.

On the other hand, a difference in the π charges of the 1 and 3 positions can be interpreted as a measure of the probability of Michael addition in the α-position of the pyrrole ring. With respect to this characteristic, structures II, VI-IX, and XII should be considered to be the least inclined to form Michael adducts; in general, this is in agreement with the small corresponding Δf_π values in these compounds (Table 1).

Considering the material set forth above, let us analyze the activity of condensed isoindoles stage by stage. From our point of view, under the assumption of a synchronous mechanism it is logical to evaluate the activity of the compounds with respect to the smaller of the two q_π values at the ends of the diene fragments (since a certain limiting value of the charge, below which cycloaddition does not occur, possibly exists), whereas under the assumption of a nonsynchronous mechanism it is logical to evaluate the activity of the compounds on the basis of the sum of the π charges in the same positions (the probability of initial attach is determined by the greater of the two q_π values, while the probability of subsequent cycloaddition is determined by the q_π value in the 2 position). One can then construct orders of the activities of the various isoindoles in the Diels–Adler reaction for synchronous (1) and nonsynchronous (2) mechanisms:

$$\begin{gathered}\text{XIII, XVI}>\text{VI, X, XIV}>\text{VII, IX, XI, XII}>\text{III, VIII}>\text{I,}\\ \text{V}>\text{IV}>\text{XVII}>\text{XV}>\text{II}\end{gathered} \tag{1}$$

$$\begin{gathered}\text{X, XIV, XVI}>\text{XI, XIII}>\text{XII}>\text{VII}>\text{I, IX, XV}>\text{XVII}>\text{IV,}\\ \text{V, VI, VIII}>\text{III}>\text{II}\end{gathered} \tag{2}$$

It is apparent that in some cases the hypothetical mechanism of cycloaddition does not have a substantial effect on the relative activity. Thus, for example, XVI, XIV, and XII occupy initial positions in both orders, while II is found at the end. At the same time, it is much more favorable for VI to react via a synchronous mechanism rather than via a nonsynchronous mechanism, whereas the opposite is true for XV.

Such orders of activities of dienes under the assumption of two alternative mechanisms can also be composed on the basis of the boundary electron densities. With respect to the lower value of two f_π values for a synchronous mechanism

$$\begin{gathered}\text{IX}>\text{VII}>\text{VI, VIII, XIII}>\text{XVII}>\text{XII, XVI}>\text{II, X, XV}>\text{V,}\\ \text{XIV}>\text{I, XI}>\text{III, IV}\end{gathered} \tag{3}$$

and with respect to their sum for a nonsynchronous mechanism

$$\begin{gathered}\text{XIII}>\text{IX, XVI}>\text{VII, X, XII, XVII}>\text{VI, VIII, XV}>\text{II}>\text{XI}>\text{I,}\\ \text{V}>\text{IV}>\text{III}\end{gathered} \tag{4}$$

The position of pyrimido[2,1-a]isoindole (II) changed somewhat as compared with the first two orders; the remaining azinoisoindoles I and III-V remain the least active. As in the preceding predictions, VI-IX should be the most reactive in synchronous cycloaddition. Azoloisoindoles that contain an N-methyl fragment in the 8 position (see the structural formulas) are more active than their positional isomers. However, on the whole, despite individual differences, the general tendency of the location of the systems in orders (1)-(4) is clear and corresponds to the electron-acceptor character of the fragment annelated along side *a* of the azoindole ring [33].

Let us then assume that the same dienophile was selected for all of the investigated compounds. The energy of the highest occupied molecular orbital of the diene (E_{HOMO}) will then be the reactivity index in the second arbitrary stage. Two orders of the relative activities of the condensed isoindoles can be composed from the E_{HOMO} values calculated by the Pariser–Parr–Pople (PPP) (5) and CNDO/2 (6) methods (Table 1):

$$\begin{gathered}\text{XII}>\text{XI}>\text{X}>\text{XV}>\text{XIV}>\text{VIII}>\text{XIII}>\text{I}>\text{XVI}>\\ >\text{II}>\text{XVII}>\text{IV}>\text{VI}>\text{IX}>\text{V}>\text{VII}>\text{III}\end{gathered} \tag{5}$$

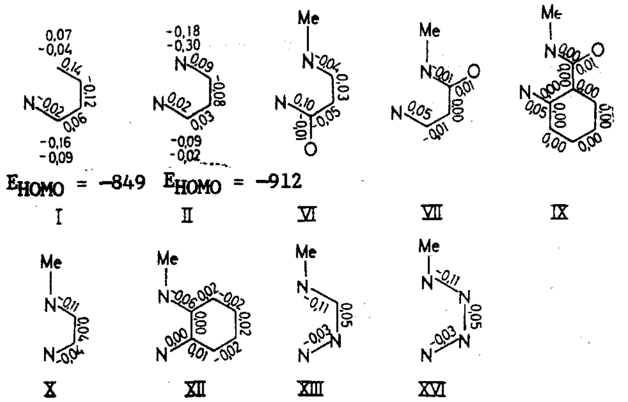

Fig. 1. Change in the bond orders on passing from the starting molecule of condensed isoindole (the number is indicated under the structure) to the localized fragment. The π charges at the ends of the diene fragments that contain atoms 8-11 in the starting molecule (top number) and in the localized part (bottom number) and the energies of the highest occupied molecular orbitals (HOMO) of the fragments in kilojoules per mole are also presented for I and II.

$$\mathrm{XIV}>\mathrm{XII}>\mathrm{X}>\mathrm{XI}>\mathrm{VIII}>\mathrm{XIII},\ \mathrm{XV}>\mathrm{IV}>\mathrm{VI}> >\mathrm{IX}>\mathrm{XVI}>\mathrm{XVII}>\mathrm{VII}>\mathrm{I}>\mathrm{III}>\mathrm{V}>\mathrm{II} \tag{6}$$

If one does not regard a shift within the limits of two to three positions as being a fundamental change, orders (5) and (6) are extremely similar to one another. It should be noted that some compounds that were determined to be included among the most active with respect to the first type of indexes (q_π and f_π) also turn out to be active in the second stage (for example, X and XIV). Similar symbatic character is also characteristic for the low-activity structures (for example, III and V). Judging from the E_{HOMO} values, the relative reactivities of XIII and XV are somewhat decreased as compared with the preceding orders, while the relative reactivities of XI, XII, and XV are somewhat increased.

In the third arbitrary stage the overall π system of the condensed isoindoles is cleaved, and isolated π fragments are formed: the benzene ring of the isoindole part and the residue annelated along the *a* side of isoindole. The difference between the sums of the energies of these two π fragments and the energy of the starting diene determines the localization energy (E_{loc}),* from which for some of the investigated compounds (Table 1) one can compose the following order of activities:

$$\mathrm{VI}>\mathrm{VII}>\mathrm{IX}>\mathrm{XII}>\mathrm{X}>\mathrm{XIV}>\mathrm{II}>\mathrm{XVI}>\mathrm{I} \tag{7}$$

Isoindolopyrimidones VI and VII and isoindoloquinazolone IX, for which, in addition to the benzene ring of the isoindole part (as in all of the investigated structures), fragments that have low valence activity are formed during the Diels–Alder reaction, have the lowest localization energies [14]. Cleavage of the π system of these compounds and isolation of the fragments as a result of cycloaddition therefore make a smaller contribution to the activation barrier. A similar situation arises when one compares the localization energies of imidazoisoindole X and isoindolobenzimidazole XII. The E_{loc} value of the latter is lower because of the fact that isolation of the benzene ring is more favorable than isolation of a double bond.

The change in localization in the molecule during cycloaddition can be traced from the differences in the multiplicities of the bonds in isolated fragments 8-11 and in the corresponding starting condensed isoindole (Fig. 1). It is apparent that localization of the π bonds increases appreciably in I and II, whereas the change in the bond orders is small in structures VI, VII, and IX. This fact is in agreement with the preceding activity orders.

Thus an analysis of various static indexes that are determining factors in one of three arbitrary stages of the Diels–Alder reaction makes it possible to hope to establish the relative reactivities of the condensed isoindoles under consideration. The conclusions are most accurate if the corresponding indexes vary symbatically.

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*One should not confuse this characteristic with the known energy of para localization [34].

TABLE 2. π Charges at the Ends of the Diene Fragments in the Triplet Excited State Obtained by the Pariser—Parr—Pople (PPP) Method

Compound	π charges in positions					Compound	π charges in positions			
	1	3	4	7	8 (11)		1	3	4	7
I	−0,12	−0.13	0,03	0,04	−0,00	IX	−0,05	−0,09	0,06	0,08
					(−0,20)	X	−0,11	−0,23	−0,04	0,02
II	−0,09	−0,08	0,05	0,06	−0,28	XII	−0,10	−0,19	−0,02	0,02
					(−0,17)	XIII	−0,09	−0,19	−0,01	0,04
VI	−0,05	−0,14	0,04	0,08		XVI	−0,06	−0,17	0,01	0,06
VII	−0,07	−0,12	0,06	0,08						

For the investigation of the Diels—Alder reaction in condensed isoindoles it is extremely useful to know not only their relative activities but also the activities as compared with dienes that are already known. The lowest of the π charges in the 1 and 3 positions of almost all of the investigated compounds (Table 1) is close to the q_π value in the α position of isoindole (−0.18 [13]). Consequently, under the assumption of a synchronous cycloaddition mechanism all of these compounds have comparable reactivities. Only structures II, IV, XV, and XVII constitute an exception. However, in the case of nonsynchronous cycloaddition, all of them, judging from the sum of the π charges, will have activities that are close to the activity of isoindole.

According to the data in [13], E_{HOMO} = −910 kJ/mole for isoindole, i.e., an energy that is lower than the energies for the investigated structures. Consequently, condensed isoindoles should display greater donor properties than isoindole itself. Calculation of E_{loc} in the case of cycloaddition to the isoindole molecule gives 6087 kJ/mole, which substantially exceeds E_{loc} for each of structures I-XVII. From the set of characteristics one can therefore, on the whole, assume high diene activities of the investigated compounds.

Up to this point we have examined the addition to isoindoles with respect to the pyrrole diene fragment with the formation of a 1:1 adduct of the diene and dienophile. However, an isolated diene fragment in the azine part of the system develops in this adduct for I-V; this means that repeated cycloaddition in the 8,11 positions is possible (see the strucural formulas). The question as to the stage in which a second molecule of the dienophile enters into coordination then is important: when the electron-density distribution is still close to the distribution in the starting molecule (case 1) or after the formation of a 1:1 adduct, when diene fragment 8-11 can be considered to be completely isolated (case 2). Judging from the substantial difference in the q_π and f_π values in the 8 and 11 positions (see Fig. 1 and Table 1), in the first case secondary cycloaddition for all of the azinoisoindoles should proceed via a nonsynchronous mechanism. For structures I and II we also calculated the q_π values in isolated fragments 8-11 (Fig. 1). It is apparent that for both compounds the negative charges in the 8 position increase on passing from the molecule to the fragment, whereas the negative charges in the 11 position decrease. As a result, a certain probability of synchronous cycloaddition develops for pyrido[2,1-a]isoindole (I), but the chances of a nonsynchronous mechanism increase to an even greater extent for pyrimido[2,1-a]isoindole (II). It is interesting that the energies of the HOMO of the same isolated fragments (Fig. 1), which can be equated approximately with the energy of the HOMO of the 1:1 adduct, for I and II lie within the limits that are characteristic for typical dienes. Hence it follows that the secondary addition of a dienophile is extremely likely; the fragment that remains after primary cycloaddition to pyrido[2,1-a]isoindole (I) is a stronger donor than the fragment of pyrimido[2,1-a]isoindole (II).

To describe the photochemical reactions of the investigated compounds it is of interest to examine how the electron-density distribution at the ends of the diene fragments changes in the case of excitation. The results of calculations of the structures of several compounds in the first triplet excited state are presented in Table 2. An analysis of them shows that the most active positions in almost all of the calculated molecules are the ends of the diene fragment of the pyrrole ring. Structure II, for which alternative addition in the 8,11 positions seems more likely, i.e., it seems possible to obtain, via a photochemical pathway, a 1:1 adduct involving the diene fragment of the pyrimidine ring, constitutes an exception.

LITERATURE CITED

1. M. J. S. Dewar and A. B. Pierini, J. Am. Chem. Soc., 106, 203 (1984).
2. M. J. S. Dewar, J. Am. Chem. Soc., 106, 209 (1984).
3. V. A. Kovtunenko, T. T. Dobrenko, Z. V. Voitenko, A. K. Tyltin, and F. S. Babichev, Khim. Geterotsikl. Soedin., No. 9, 1200 (1984).
4. N. Epiotis, Structural Theory of Organic Chemistry [Russian translation], Mir, Moscow (1981).
5. M. Blain, S. Odiot, G. J. Martin, and J. P. Gouesnard, Tetrahedron, 36, 2663 (1980).
6. R. B. Woodward and R. Hoffman, Retention of Orbital Symmetry [Russian translation], Mir, Moscow (1971).
7. L. Salem, Electron Structure in Chemical Reactions [Russian translation], Mir, Moscow (1985).
8. M. Blain, S. Odiot, G. J. Martin, J. P. Gouesnard, and O. Chalvet, Tetrahedron, 36, 2775 (1980).
9. P. B. Terent'ev, N. P. Lomakina, M. Islam Rahimi, K. Dager Riad, Ya. B. Zelikhover, and A. N. Kost, Khim. Geterotsikl. Soedin., No. 9, 1255 (1980).
10. P. B. Terent'ev, V. G. Kartsev, A. V. Golepov, I. I. Gloriozov, Yu. A. Gulevich, and A. N. Kost, Khim. Geterotsikl. Soedin., No. 9, 1248 (1980).
11. E. Chacko, J. Bornstein, and D. J. Sardella, J. Am. Chem. Soc., 99, 8248 (1977).
12. M. H. Palmer and S. M. F. Kennedy, J. Chem. Soc., Perkin II, No. 1, 81 (1976).
13. V. A. Kovtunenko, Z. V. Voitenko, V. L. Sheptun, A. K. Tyltin, A. I. Chernega, Yu. T. Struchkov, and F. S. Babichev, Khim. Geterotsikl. Soedin., No. 11, 1497 (1984).
14. V. A. Kovtunenko, Z. V. Voitenko, V. L. Sheptun, L. I. Savranskii, A. K. Tyltin, and F. S. Babichev, Ukr. Khim. Zh., 51, 976 (1985).
15. V. A. Kovtunenko, Z. V. Voitenko, V. L. Sheptun, L. I. Savranskii, A. K. Tyltin, and F. S. Babichev, Khim. Geterotsikl. Soedin., No. 5, 646 (1987).
16. V. I. Baranovskii, V. F. Brattsev, A. I. Panin, and V. M. Tret'yak, Methods for the Calculation of the Electron Structures of Atoms and Molecules [in Russian], Izd. LGU, Leningrad (1976).
17. M. J. S. Dewar, S. Olivella, and H. S. Rzepa, J. Am. Chem. Soc., 100, 5650 (1978).
18. J. Pancir, J. Am. Chem. Soc., 104, 7424 (1982).
19. R. T. Kohl, T. Katto, J. N. Brahan, and I. K. Steille, Macromolecules, 11, 340 (1978).
20. P. V. Alston and R. M. Ottenbrite, J. Org. Chem., 39, 1584 (1974).
21. A. I. Naimushin, V. V. Simonov, and A. F. Anishchenko, Zh. Obshch. Khim., 45, 141 (1975).
22. A. I. Konovalov, Usp. Khim., 52, 1852 (1983).
23. M. V. Basilevskii (Basilevsky), A. G. Shamov, and V. A. Tikhomirov, J. Am. Chem. Soc., 99, 1369 (1977).
24. I. R. Epstein, Trans. Faraday Soc., 63, 2085 (1967).
25. O. Eisenstein and A. Nguen-Trong, Bull. Soc. Chim. France, Nos. 9/10, 2721 (1974).
26. H. Fijimoto, S. Inagaki, and K. Fukui, J. Am. Chem. Soc., 98, 2670 (1976).
27. M. J. S. Dewar, A. S. Griffin, and S. Kirschner, J. Am. Chem. Soc., 96, 6225 (1974).
28. O. Kikuchi, Tetrahedron, 27, 2791 (1971).
29. L. A. Burke, G. Lerou, and M. Sana, Theor. Chim. Acta, 40, 313 (1975).
30. N. N. Vainberg, Master's Dissertation, Kiev State University, Kiev (1981).
31. A. I. Konovalov, in: Structure and Reactivity of Organic Compounds [in Russian], Mir, Moscow (1978).
32. V. A. Kovtunenko, Z. V. Voitenko, A. K. Tyltin, A. V. Turov, and F. S. Babichev, Ukr. Khim. Zh., 49, 1287 (1983).
33. J. Joule and H. Smith, Fundamentals of the Chemistry of Heterocyclic Comopunds [Russian translation], Mir, Moscow (1975).
34. R. D. Brown, J. Chem. Soc., 691 (1950).