Spectroscopic study of the most important combinations of atomic groups in complex molecules of organic compounds

3.* Nitroaromatic compounds

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The IR spectra of several compounds containing the nitro group were studied. Based on these and previous data, the state of the nitro group depending on the structure of the fragments bound to the nitrophenyl group was discussed. The redistribution of the electron density at vibrations of the nitro group and the substituent atoms was considered. The effects of the π-bond system, bridging atoms separating the nitrophenyl group from the substituents, and heavy atoms adjacent to the bridging atom were characterized. The data obtained facilitates the orientation in the selection of molecular structures satisfying the specified requirements of practical applications.

Key words: nitroaromatic compounds, IR band intensity, conjugation, donor-acceptor interaction, effect of heavy atom.

Manifestations of the mutual effect of atomic groups in many types of complex organic molecules have been described in many publications, including spectroscopic data. Spectroscopic methods make it possible to easily determine some parameters with high accuracy, for example, frequencies of atomic vibrations. The accuracy accessible for estimation of the rigidity or order of chemical bonds is sufficiently high only for very simple molecules. The differences experimentally observed in frequencies of 1—10 cm^{-1} usually do not give reliable information on details in the structure of complex molecules compared. A combination of several methods allows one to supplement and control conclusions, but the difficulties that appear are due to the fact that interrelations between different parameters of the effect of atomic groups are insufficiently studied, and many of the correlations established can be applied only to a restricted series of compounds similar in structure. Under these conditions, extension of information on the interactions of active centers in polyatomic molecules remains urgent.

The totality of manifestations of conjugation and deviations from additivity of complex molecules includes the specific character of the distribution (redistribution) of the electron density between fragments of different types, which affects the values of dipole moments and intensities of IR absorption bands. This redistribution can be considered as one aspect of donor-acceptor interaction and is described by the predominant contribution of the vacant orbital of the electron-acceptor group to the delocalized highest occupied molecular orbital (HOMO). The donor-acceptor interaction affects the intensity of IR absorption bands, static atomic polarizability, and electron density evolutions in the transition state of the chemical reaction, *etc.*

In this work, based on the study of the spectra of nitroaromatic compounds, we determined the main tendencies of substituents and the structure of intermediate units to affect the nitro group, which is an active π-acceptor in these compounds.

The fragments adjacent to the *p*-nitrophenyl group are known to affect noticeably the frequencies of the symmetrical (ω_s) and antisymmetrical (ω_{as}) stretching vibrations of the nitro group,[1—4] although in most cases, they almost do not contribute to the corresponding normal coordinates Q_s and Q_{as}.* Therefore, even minor differences in frequencies (2—5 cm^{-1}) in the spectra of similar compounds are worthy of attention and, in some cases, can be used for approximate estimation of the character of the N—O bond.

Intramolecular interactions of active centers can be characterized more comprehensively if data on the intensities of bands in the IR and Raman spectra are used along with the frequencies. The intensity of the IR band of the antisymmetrical vibration of the nitro groups (A_{as}) is related to the average electron density distribution

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* For Part 2, see Ref. 1.

*The exception is, in particular, *p*-dinitrobenzene. In dinitro compounds with a very weak bond between the nitro groups, the latter can be considered as two independent vibrational subsystems.

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between the molecular fragments, the polarity of the N—O bonds, and some local effects, and the intensity of the IR band of the symmetrical vibration (A_s) is additionally related to the electron density migration between the nitro group and other fragments of the molecule during atomic vibrations ("dynamic effects"), *i.e.*, to the dependence of charges on the atoms on the Q_s coordinate.

It should be noted that the terminology used does not create special difficulties outside the scope of the semiclassical theory, and for the introduction of matrix elements of the dipole moment of the transition (μ_{om}) formed of vibrational wave functions of an atomic oscillator (U_v). The relation to the normal Q coordinate is mapped in the integrand on each Q value, which, strictly speaking, should not be accepted as the determining location of atoms. For simplicity, let us consider a diatomic molecule as a unidimensional harmonic oscillator with charges on the atoms $+z(Q)$ and $-z(Q)$ and write the modulus of the matrix element of the transition dipole moment in the form $|\mu_{01}| = |<u_0|z(Q)|u_1>|$. Neglecting secondary contributions, this expression can be rewritten in the form of the binomial $z(Q) \cdot Q_{01} + (\partial z(Q)/\partial Q) \cdot r_0 \cdot Q_{01}$, where r_0 is the equilibrium internuclear distance; Q is the coordinate counted from the r_0 value; and Q_{01} is the matrix element of this coordinate (zero amplitude). The use of the $z(Q)$ function does not restrict the choice of approaches to the description of the interrelations of Q and time, but it is the same, of course, as the standard[*] formulation of the adiabatic Born—Oppenheimer approximation. The second term of the expression presented above reflects the contribution of the electron density migration during oscillation of Q.

In terms of these concepts, we can note that migration of the electron density during atomic vibrations can result in the appearance of some nondiagonal force coefficients relating nonadjacent active centers of the molecules and in noticeable delocalization of the vibrations (which, in principle, is possible even when the intermediate unit is motionless!). The concept of "migration" is an acceptable conventionality, which does not contradict standard methods of quantum chemistry using the adiabatic approximation. It is noteworthy that the time dependence of the coordinate operator $\dot{Q}(t)$ corresponding to Heisenberg's concept is similar to the $Q(t)$ dependence of the classic oscillator; however, this does not give any additional arguments for the consideration of the problem of acceptability of the classic model.[*] The analysis of evolutions of packets of the wave functions u_v of the atomic oscillator (at least for standard experimental conditions) does not lead to concepts about the adequate and full-value model of harmonic vibrations of atoms and parameters characterizing the electron density distribution. Therefore, the migration should be considered not as an immutable fact, but as one of the compact variants of representation of the problem of the IR band intensity, which is convenient for qualitative description under conditions when the damping constant for the electron subsystem is sufficiently high.

As for the interpretation of data on the IR band intensity using "electrooptical parameters" of chemical bonds, these parameters have no physical sense and give no new information.[6] The same concerns the concepts about "transitions between resonance structures" upon atomic vibrations (see, *e.g.*, Ref. 7).

The results of spectral studies of the nitro compounds are presented in Table 1.

As can be seen from the experimental data, the structure of the system of conjugated bonds has different effects on different conjugation indicators. For example, in molecules of the X—П—NO_2 type (where П is the system of π-bonds), only the most active π-donors among the X groups affect noticeably A_{as} and, probably, the polarity of the N—O bonds. The data on the dipole moments of the molecules (see, *e.g.*, their comparison in Ref. 10) do not contradict this assertion. Unlike A_{as}, the A_s values depend more explicitly on the structure of adjacent and nonadjacent molecular fragments. The A_s value of nitrobenzene is almost threefold greater than those of nitroalkanes; it is still higher for compounds with a longer chain of π-bonds, and the deviation of the π-bond system from the complanar character, as should be expected, results in a decrease in A_s (*cf.* data in Table 1 for the nonplanar system of *p*-nitrodiphenyl and for 2-nitrofluorene).

Although the dependences of the effect of substituents X on the structure of intermediate units are different for the A_s and ω_s values, there are some common features. This is valid to a somewhat lesser extent for the Raman line intensity of the nitro group (I_s), which varies in the series of the compounds studied within considerably wider limits.[4,9] It should be noted than the elongation of the chain of the carbon—carbon π-bonds adjacent to the nitrophenyl group affects strongly the UV absorption spectrum and the I_s value, but has a slight effect on A_s and A_{as} (as well as on ω_s and ω_{as}), which depend to a greater extent on the donor-acceptor interaction.

The aforesaid can be clarified in the simplest form using the molecular orbital (MO) methods. The dependence of the energy of the frontier MO (energy gap) on the given normal coordinate Q is substantial for the intensity of lines in Raman and IR spectra. This dependence can be explained by some mixing of these MO when $Q \neq 0$. However, the difference in the predominant localization along the atomic chain of the occupied and vacant MO is substantial for the IR line intensity,

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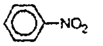
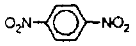
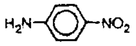
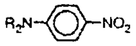
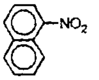
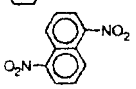
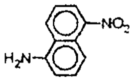
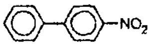
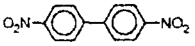
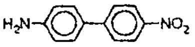
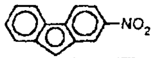
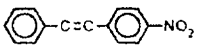
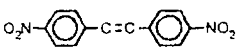
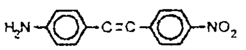
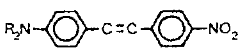
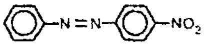
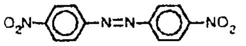
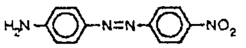
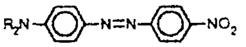
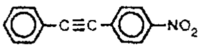
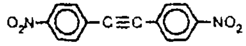
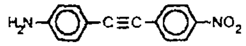
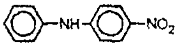
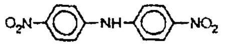
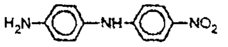
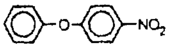
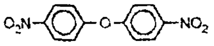
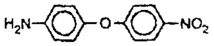
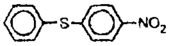
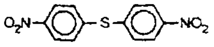
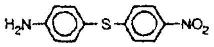
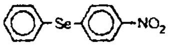
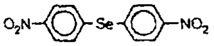
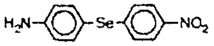
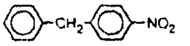
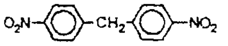
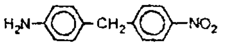
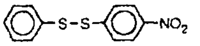
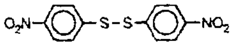
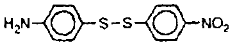
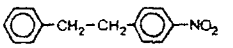
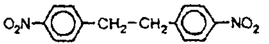
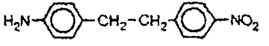
[*] Retaining conditions of the nonrelativistic approximation, the full wave function of molecules with weakly interacting subsystems can be also presented in the form $\Psi_e = \varphi_{e(v)} \cdot U_{(e)v}$, where φ is the electron wave function; *e* and *v* are the quantum numbers of the electron and nuclear subsystems; no parametric dependence of φ on Q was introduced.

[**] For other, more general aspects of the classic theory and metaphysical approaches, see review (Ref. 5).

Table 1. Parameters of lines of the nitro group in the IR and Raman spectra and of the long-wave absorption band in the UV spectra

Compound	$\Delta\omega_s$	$\Delta\omega_{as}$	A_s	A_{as}	I_s	$\Delta\lambda_1$
	cm^{-1}					/nm
	0 (1348)	0 (1533)	1.9	2.5	700	0 (252)
	3	7	2	2.3	—	3
	−18*	−22	8.5	3.4	20000	68
	−25	−31*	12	3.5	250000	102
	−4*	−6	[2.6]	[2.6]	1600	58
	−2	0	[2.2]	[2.7]	—	[60]
	−8	—	—	—	—	[100]
	−2	−9	3	2.6	5500	42
	−2	−11	2.6	—	—	43
	−7	−15	6.7	3.8	—	95
	−6	−7	3.5	2.4	—	72
	−5	—	—	—	—	73
	−13	−13	7.5	—	—	118
	−6	−10	3.7	2.7	22000	82
	−5	−11	3.5	—	—	82
	−8	−12	8	[5.6]	[500000]	135
	−9	−12	11	[6.5]	5000000	161
	−3	−6	3.5	3.3	—	73
	—	—	—	—	—	[80]
	[−7]	−7	—	—	—	155
	−8	−5	7.8	5.3	—	191
	−4	−11	—	—	—	68
	−3	−9	[2]	—	—	68
	−6	−13	4	—	—	[110]
	−25*	−27	[11]	[5]	—	101
	−17*	−19	[11]	5.8	150000	108
	−26*	[−25]	[12]	5.9	—	108
	−6	−9	3.9	—	4000	41
	−2	−8	2.8	—	2500	39
	−6	[−9]	4.0	—	—	41
	[−8]	[−13]	—	—	[20000]	78
	−5	−10	3.2	—	—	78
	−10	−18	3.7	—	—	78
	[−6]	—	—	—	[30000]	[82]
	−4	−13	2.6	—	—	83
	−6	−18	2.6	—	—	88
	[−2]	[−8]	2.7	—	[1500]	13
	−2	−8	2.6	3.1	—	13
	−3	[−8]	3.2	3.2	—	15
	−7	−11	3.8	—	—	58
	−7	−8	3.4	—	5000	53
	[−8]	—	—	—	—	[58]
	[−2]	[−10]	[2.5]	—	[1500]	[13]
	−1	−9	3.0	—	—	12
	−2	−10	2.8	—	—	13

Note. $\Delta\omega_s$ and $\Delta\omega_{as}$ are the shifts of the frequencies of stretching vibrations of the nitro group compared to the frequencies of nonsubstituted nitrobenzene; A_s and A_{as} are the integral intensities of the IR bands of these vibrations; I_s are the relative molar integral intensities of the Raman lines with frequency ω_s (the intensity of the line at 313 cm^{-1} in the spectrum of CCl_4 was assumed to be 100);[4,8,9] and $\Delta\lambda_1$ is the shift of the long-wave intense UV absorption band ($\pi\rightarrow\pi^*$ or $n,\pi\rightarrow\pi^*$) compared to the spectrum of nitrobenzene according to the published data for solutions in heptane. The ω and λ_1 values for nonsubstituted nitrobenzene are given in parentheses; the results of tentative estimations for benzene solutions by the published data related to solutions in polar solvents and estimations based on analogies are presented in brackets. For dinitro compounds, the A_s, A_{as}, and I_s values were recalculated per nitro group by division by 2, and $\Delta\omega_s$ is the arithmetic mean of values determined in the IR and Raman spectra (the latter differed by no more than 12 cm^{-1}); for dinitrobenzene, $\Delta\omega_{as}$ is the arithmetic mean, but for all other dinitro compounds, the ω_{as} frequencies were detected only in the IR spectra. When the line of the nitro group is split (up to 10—40 cm^{-1}), the total intensity of the two components and the intermediate value of the frequency (marked with asterisk) are given. All data on IR and Raman spectra concern solutions in benzene. Designations: R is the methyl group, Ф and hexahedron indicate the *para*-phenylene fragment.

while the Raman spectra are determined by the difference between their contributions to the corresponding equilibrium interatomic distances (which are affected by the arrangement of the nodal points of the wave functions) and, of course, "resonance denominators" (see Ref. 9) depending on the frequency of exciting light. Of course, "mixing" of orbitals is only a convenient method for description of changes in the structure of the electronic shell of a molecule and the corresponding modification of linear combinations of AO.

In the series of compounds $X—\Pi—NO_2$, the studied indicators of conjugation with the nitro group somewhat weaken under the effect of the electron-accepting X groups (which can be considered as the result of competition between two acceptors) and are enhanced dramatically when π-electron-donating substituents, for example, amino group, are introduced. The activity of the X substituent depends to a great extent on nonadjacent atoms composing the X group (for example, the Z atom in the $Z—M—\Pi—NO_2$ system) rather than on the atom directly linked to the $\Pi—NO_2$ fragment. The electron-donating ability of the HCO—NH group in $CO—NH—\Pi—NO_2$ is considerably lower than that of the NH_2 group, and the effect of the F atoms in the F—NH and F_2N groups should be more considerable; the metal Z atom (σ-donor) adjacent to nitrogen, by contrast, greatly increases the π-electron-donating activity of the Z—NH substituent. The electron-donating ability of the amino group changes strongly when the molecule is electron-excited, increases on going from the gas phase to solutions (especially for some forms of solvation), increases sharply when the proton is eliminated, and decreases to zero due to protonation. It is very important that the electron-donating ability of the amino group depends strongly on the conformation (on the rotation angle around the $H_2N—C$ bond) and on the type of electron-accepting ability of the adjacent group-partner; these facts emphasize the conventional character of separation (classification) of atomic groups to electron-donating and electron-accepting groups and restrict quantitative estimations of their electronegativity.

It has been mentioned above that the X substituents of the π-donor type have the greatest effect on the IR bands of the nitro group. On the other hand, the nitro group favors[11,12] a considerable increase in the intensity of the bands of the electron-donating NH_2 groups. Variations of the structure of the intermediate units result in parallel changes in the intensity of the bands of the amino and nitro groups. These changes are especially great for the bands with symmetrical modes, which can be attributed to the considerable redistribution (migration) of the electron density between the terminal groups. However, the frequencies of stretching vibrations of the amino group and the rigidity of the N—H bonds do not decrease and, by contrast, even increase under the effect of the nitro group, although the participation of other atomic groups (such as C=O, C≡N, $N=\dot{O}$, C≡CH, C—H, O—H, and the nitro group mentioned above) in the conjugation systems is usually accompanied by a decrease in the vibrational frequencies, rigidity, and order of the bonds. These specific features of the amino group can hardly be explained by changes in the C—N—H bond angles, as has been supposed in several works. Most likely, the N atom is modified when it participates in the conjugation system, and the occupied MO with contributions from the atomic orbitals of nitrogen and hydrogen decreases in the energy scale. This favors an increase in the rigidity of the N—H bonds and an increase in the corresponding ionization potential and frequencies of the electronic $n\rightarrow\pi^*$-transitions related to the amino group.

When the structure of the X group is varied, the limits of changes in the A_s and ω_s values are maximum for $X—NO_2$ molecules, very considerable for $X—\Phi—NO_2$, substantially lower for more complex systems of intermediate π-bonds, and quite insignificant in $X—\Phi—M—\Phi—NO_2$ molecules, where M is the bridging atom with its environment. The effect of the nitro group on the X group weakens in the same sequence. The concepts on weakening of the donor-acceptor interaction of terminal groups are in accordance with the data on the electron density distribution and the effect of the partner-group on the vibrational frequencies, interatomic distances, rigidity and order of the N—O and N—H bonds, ionization potentials, and some parameters of the reactivity. According to the calculations,[13] the transfer of ~0.2 electron charge from the NH_2 group to the nitro group should be observed in nitramine, a smaller (by almost an order of magnitude) charge should be transferred in *p*-nitroaniline (see, *e.g.*, Ref. 8), and a smaller (by almost two orders of magnitude) electron charge should be transferred in nitroaminostilbene. Thus, the excess negative charge on the O atoms of the nitro group should decrease in this series, although A_s is retained almost at the same level, and deviations from additivity in the dipole moments even increase. Such considerable differences in different manifestations of the donor-acceptor interactions are not surprising, because several factors, including an increase in the effective dipole length, play simultaneously an important role.

The optical indicators of conjugation are related to some extent to the parameters of electron excitation levels of a molecule. Under standard experimental conditions, the molar electron polarizability and the intensity of the Raman lines of nitramine do not differ strongly from the data of the additivity scheme. In the case of an intermediate system of π-bonds and an increase in the number of units, deviations from additivity increase along with the bathochromic shift of the UV absorption $n,\pi\rightarrow\pi^*$ band. The correlations between I_s and λ_1 fit in terms of the semiclassic theory; they suggest that the $\pi_1{}^*$ excitation level contributes strongly to I_s and is characterized by an increase in the equilibrium interatomic N—O distances. The correlation becomes more evident for deeply colored compounds, *i.e.*, when the situation is close to the resonance conditions.

In compounds of the X—Φ—M—Φ—NO_2 and X—Φ—M—M—Φ—NO_2 types, including those with methylene bridges, the mutual effect of active centers is still rather noticeable. For example, in aminonitro compounds (X = NH_2) ω_s is somewhat lower, and A_s and $\Delta\lambda_1$ are slightly higher than those of similar dinitro compounds (X = NO_2). Thus, here the properties of the effect of substituents have the same character as those of compound X—Φ—NO_2, but they are considerably less pronounced and, hence, cannot always be reliably interpreted. No properties of the donor-acceptor interaction were obtained in the spectra of compounds similar to R_2N—CH_2—Φ—NO_2, while they are more pronounced for the R_2N—CH_2—NO_2 and R_2N—CH_2—CN molecules than for *p*-nitroaniline; this is indicated by the values of the energy of the electron excitation $n \to \sigma^*, \pi^*$,[14] basicity constants of the amino group, and many other parameters. Based on these facts, the R_2N—CH_2 should be attributed to σ- (but not to π) donors.

The Z—CH_2—Φ—NO_2 structures and similar Z—M—Φ—NO_2 systems, where Z is the heavy atom that constitutes the major fragment of the X group-substituent, are of considerable interest. Let us designate these compounds by the general formula X—M—Φ—NO_2. Several similar compounds with iodine,[2] mercury, and some other p- and d-elements, which have been previously studied in detail,[15–17] are included in Table 2. The effect of substituents on all the parameters is especially strong in the derivatives of Au, Pt, and Sb^V and in the structures with the NH and O bridges. These compounds can be described by the conjugation mechanism[8] and concepts on contributions of the interaction of active centers through the bridging atom and space.[4] The effect of the X substituents on the spectral parameters ω_s and A_a and on the electron density distribution can be related to mixing of orbitals assigned to molecular fragments, participation of vacant orbitals of the electron-accepting zone, and dependences of the energy and structure of delocalized MO on the normal Q_s coordinate. It is significant that the frontier orbitals of the X substituent containing the heavy atom are close in energy, and the contribution of the latter to HOMO can be related qualitatively to the small electronegativity of X. The X group containing the metal atom should be attributed to σ-donors, while the X—M group (unlike H_2N—M) should be assigned to π-donors. The combination of the X—M group with the π-accepting *p*-nitrophenyl group creates conditions for considerable polarization of the system.

Variations of the Z atom (going "from top to bottom" in the Periodic System) favors the formation of substantially delocalized MO, a decrease in the energy gap between frontier orbitals, and electron density redistribution in favor of the nitro group, and increases the influence of relativistic effects on conjugation. On going from right to left in the Periodic System, the interaction increases and, under certain conditions, can result in the formation of the ion structure.

Table 2. Effect of substituents X—M— on lines of the nitro group in the IR and Raman spectra and on the long-wave UV absorption band of compounds X—M—Φ—NO_2

X—M— group	$\Delta\omega_s$ (cm^{-1})	$\Delta\omega_{as}$ (cm^{-1})	A_s	A_{as}	I_s/I_s^{nb}	$\Delta\lambda_1$ /nm
H—	0 (1348)	0 (1533)	1.9	2.5	1	0 (262)
R—	−2	−8	2.5	2.9	2	13
ClHg—	−1	[0]	2.7	—	1	1
ICH_2—	−3	−5	—	—	4	16
$ClHgCH_2$	−5	−13	[4]	—	4.5	30
$IHgCH_2$—	−7	−15	[6]	—	5	40
HO—	−5	−10	3	3	5	39
RO—	−5	−16	4	3.6	6	46
Ph_3PAuO—	−30*	−45	13.8	—	[250]	100
PhHgO—	−30*	−33	[6]	[3]	[30]	75
O^-—	[−60]	—	[18]	—	[1000]	[140]
PhHgNH—	−40	−38	[11]	[3]	[600]	126
HS—	−6	−12	1.9	—	8	56
Ph_3PAuS—	−16	−30	5.5	—	—	127
PhHgS—	−7	−16	3.8	3	[40]	84
Ph_3PbS—	−8	—	3	—	[35]	81
Ph_2SbS—	−6	—	—	—	[40]	80
Ph_4SbS—	−20	—	4.2	—	[800]	132
$Ph(PPh_3)_2PtS$—	−26	—	10	—	—	186
S—	[−50]	—	[14]	—	[1000]	[200]

Note. For designations, see Table 1. All the data (including UV spectra) are given for benzene solutions.

We obtained additional information on the interrelations of active centers, including different manifestations of the donor-acceptor interaction, which confirms the significance of the previous[8,10] general conclusions. The above-mentioned tendencies on the effects of substituents on the properties of nitro compounds and the conclusions can be extended to other compounds similar in structure and containing π-acceptors (ketones, aldehydes, nitriles, and others).

Experimental

IR spectra were recorded on a DS-301 spectrophotometer (JASCO, Japan); all results are for solutions of compounds in benzene. Integral intensities of the IR absorption bands were determined by direct integration. As the measurements showed, for the absorption bands of the nitro group, this method gave almost the same accuracy (±5—10%) as the more labor-consuming extrapolation methods.

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