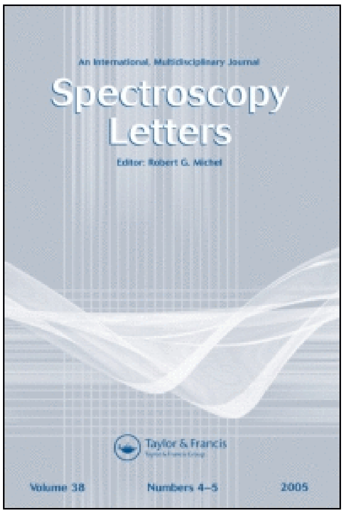

Spectroscopy Letters
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713597299

Dynamic and Electro-Optical Parameters of Aminogroups in Fluorinated Aromatic Amines with Intermolecular Hydrogen Bonding into 1:1 Complexes

V. E. Borisenko[a]; G. G. Furin[b]; S. A. Korobeynikova[a]
[a] Physical Department, Tyumen State University, Tyumen, Russia [b] (Siberian Department), Institute of Organic Chemistry, Russian Academy of Sciences, Novosibirsk, Russia

To cite this Article Borisenko, V. E. , Furin, G. G. and Korobeynikova, S. A.(1995) 'Dynamic and Electro-Optical Parameters of Aminogroups in Fluorinated Aromatic Amines with Intermolecular Hydrogen Bonding into 1:1 Complexes', Spectroscopy Letters, 28: 5, 715 — 733

To link to this Article: DOI: 10.1080/00387019508009914

URL: http://dx.doi.org/10.1080/00387019508009914

SPECTROSCOPY LETTERS, 28(5), 715-733 (1995)

DYNAMIC AND ELECTRO-OPTICAL PARAMETERS OF AMINOGROUPS IN FLUORINATED AROMATIC AMINES WITH INTERMOLECULAR HYDROGEN BONDING INTO 1:1 COMPLEXES

Key words: infrared spectroscopy, hydrogen bonding, halogen-substituted anilines, dynamic and electro-optical aminogroup parameters, equilibrium constants

V.E.Borisenko[*], *G.G.Furin*[**], *S.A.Korobeynikova*[*]

[*] Physical Department, Tyumen State University, Tyumen 625000, Russia

[**] Institute of Organic Chemistry, Russian Academy of Sciences (Siberian Department), Novosibirsk 630090, Russia

ABSTRACT

Infrared spectra of free molecules of 4-methoxytetrofluoroaniline, pentafluoroaniline and 4-aminotetrofluoropyridine and of those ones H-bonded into 1:1 complexes with various proton acceptors have been studied in the region of aminogroup stretching vibrations in CCl_4 medium. Spectral characteristics of absorption bands of monomers and complexes have been determined.

Vibrational and electro-optical problems for free and H-bonded molecules were solved. Valent angles $\gamma(HNH)$, dynamic constants K(NH) and electro-optical parameters $\partial\mu/\partial q$ (derivatives with respect to bond length) and $\partial\mu/\partial q'$ (derivative with respect to adjacent bond) of free and bonded molecules have been calculated.

Correlations between spectral, geometrical, dynamic and electro-optical properties of aminogroups of free molecules and those of bonded ones have been established.

The nature of relationship of $\partial\mu_1/\partial q_1$ (for active in H-bonding group) and $(K_1(NH))^{1/2}$ parameters for weak proton donors is determined predominantly by proton acceptors features. For strong donors it depends mainly on proton donors properties. In intermediate cases correlation between electro-optical and dynamic characteristics of bonded NH-groups is controlled by proton donors and acceptors alike.

INTRODUCTION

Substituents in arene ring of aniline influence sufficiently on spectral features of absorption bands of aminogroups in free molecules in the infrared spectral region.

Proton donating ability of aminogroup in H-bonded intermolecular complexes, valent angle $\gamma(HNH)$, dynamic and electro-optical parameters of aminogroup depend on a type, a position and a number of substituents in arene ring [1-3].

For rather weak proton donors, namely, aniline, mono- and 2,6-di-(CH_3,F,Cl,Br)-substituted anilines bonded into 1:1 complexes with various proton acceptors [1] some regular trends, such as variations in electro-optical parameters $\partial\mu_1/\partial q_1$ (the derivative of dipole moment with respect to bond length) and also in dynamic constant $K_1(NH)$ of bonded NH-group for each proton acceptors have been revealed.

Observed changes in integral intensity of absorption bands of aminogroup stretching vibrations when passing from free molecules to 1:1 bonded ones are caused by polarization of free electron pair of proton acceptor and to a smaller extent by aminogroup polarization under the attraction of the proton acceptor.

As a number of substituents in arene ring and their electronegativity increase [2], so does the proton donating ability of aminogroup in 1:1 H-bonded complexes. Aminogroup polarization caused by proton acceptor becomes more pronounces and plays an essential role in observed spectral changes of aminogroup absorption bands in passing from free molecules to bonded ones.

In paper [3] the comparative investigation of the influence of halogen- and nitro-substituents in substituted anilines on geometrical, dynamic and electro-optical characteristics of aminogroups in 1:1 H-bonded complexes has been pursued. The interrelation of $\partial\mu_1/\partial q_1$ parameters and $K_1(NH)^{1/2}$ value for complexes of *p*-nitroanilines derivatives with various proton acceptors turned out to be linear. The influence of nitrogroup on a type of variation of $\partial\mu_1/\partial q_1$ and $K_1(NH)$ parameters for bonded *NH*-group proved to be the determining factor. The effects of halogen substituents and individual peculiarities of proton acceptors are, in this instance, of secondary importance.

For all substituted anilines general linear dependence of spectral moment $M_c^{(1)}$ of absorption band $\nu_c(NH)$ for 1:1 bonded complexes on $(K_1(NH))^{1/2}$ value has been established.

Our interest is in studying dynamic and electro-optical characteristics of bonded *NH*-groups in 1:1 complexes of substituted anilines. Here comparable influence of arene ring substituents of various nature and proton accepting molecules on redistribution of electron density in the region of aminogroup localization is expected to be observed.

EXPERIMENT AND CALCULATIONS

Infrared spectra of free and H-bonded (1:1) molecules of 4-methoxytetrafluoroaniline, pentafluoroaniline, 4-aminotetrafluoropyridine with acetonitrile, tetrahydrofurane (THF), dimethylformamide (DMF), dimethylsulphoxide (DMSO) and hexamethylphosphoramide (HMPA) were studied in spectral region 3000-3600 cm^{-1} in CCl_4 media. The concentrations of proton donating molecules in CCl_4 vary in the range 0.010-0.015 M and those of accepting ones fall within the range 0.05 to 0.5 M thus allowing to generate predominantly H-bonded (1:1) complexes in solutions [4].

Infrared spectra were registered by "Specord-75 IR" spectrophotometer (Karl Zeiss Jena). The technique of spectral determinations of absorption bands of aminogroup stretching vibrations in monomeric molecules and in H-bonded (1:1) complexes has been described in [1-3]. The instrumental error of maximums positions determination for bands $\nu^s(NH_2)$ and $\nu^{as}(NH_2)$ of free molecules is about 2 cm^{-1}, and that of integral intensities is within 5% accuracy.

Spectral moments $M_c^{(1)}$ of $\nu_c(NH)$ bands and values of vibration frequencies in maximums of bands $\nu_f(NH)$ for complexes were determined accurate to ±3 cm^{-1}, integral intensities were measured good to ±10%.

Spectral characteristics of absorption bands of monomers and H-bonded (1:1) complexes and equilibrium constants K_{25^oC} (dm^3M^{-1}) monomer-complex are listed in Tables 1,2.

Vibrational and electro-optical problems for free and bonded molecules were solved within the framework of R-NH_2 model. When calculating 1:1 bonded complexes dynamic and electro-optical nonequivalency of aminogroup NH-bonds were taken into account. The evaluation of electro-optical parameters of NH bonds in 1:1

TABLE I

The spectral, geometrical, dynamic and electro-optical characteristics of aminogroup of anilines substituted in CCl_4

Proton donor	$\nu^s(NH_2)$			$\nu^{as}(NH_2)$			B^s/B^{as}	γ(HNH)	K(NH)	$\partial\mu/\partial q$	$\partial\mu/\partial q'$
	ν^s (cm^{-1})	$\Delta\nu^s_{1/2}$ (cm^{-1})	B^s (10^{-3} dm^3 M^{-1} cm^{-2})	ν^{as} (cm^{-1})	$\Delta\nu^{as}_{1/2}$ (cm^{-1})	B^{as} (10^{-3} dm^3 M^{-1} cm^{-2})		(°)	(10^{-6} cm^{-2})	(DA^{-1})	(DA^{-1})
4-OCH_3-tetra-fluoraniline	3405	19	6.91	3496	27.5	5.41	1.28	107.5	11.108	1.57	0.35
pentafluoraniline	3406	17	8.18	3499	24	6.92	1.18	108	11.121	1.74	0.37
4-NH_2-tetra-fluoropyridine	3423	21.5	13.2	3523	25	8.74	1.51	109.75	11.253	2.13	0.61
2,3,5,6 - tetra-fluoraniline [2]	3410	17.5	8.21	3506	24	5.92	1.39	108.75	11.158	1.70	0.43

TABLE 2

The spectral characteristics of absorption bands of stretching vibrations of substituted anilines aminogroup in 1:1 H-bonded complexes with different proton acceptors in CCl_4

Proton donor ($M \cdot dm^{-3}$)		Proton acceptor ($M \cdot dm^{-3}$)	$\nu^f(NH)$ (cm^{-1})	B^f ($10^{-3}\ dm^3\ M^{-1}\ cm^{-2}$)	$M_c^{(1)}$ (cm^{-1})	$2(M_c^{(2)})^{1/2}$ (cm^{-1})	B^c ($10^{-3}\ dm^3\ M^{-1}\ cm^{-2}$)	$K_{25°C}$ ($dm^3\ M^{-1}$)
4-OCH_3-tetrafluoraniline (0.015)	1.	CH_3CN (0.5)	3493	5.56	3374	40.2 *	12.3	2.61
	2.	THF (0.3)	3491	5.17	3346	54.4 *	19.5	1.43
	3.	DMF (0.25)	3490	9.33	3291	129.0	48.7	2.85
	4.	DMSO (0.25)	3486	11.4	3273	139.6	58.6	5.28
	5.	HMPA (0.05)	3483	8.8	3227	147.5	89.0	8.73
pentafluoraniline (0.015)	6.	CH_3CN (0.5)	3496	11.4	3371	66.7 *	26.1	2.11
	7.	THF (0.3)	3498	10.2	3334	86.8 *	37.8	2.03
	8.	DMF (0.25)	3498	6.24	3286	141.7	62.2	4.30
	9.	DMSO (0.25)	3497	6.38	3257	151.4	60.6	8.15
	10.	HMPA (0.05)	3497	6.18	3210	154.8	66.2	24.1
4-NH_2-tetrafluoropyridine (0.01)	11.	CH_3CN (0.5)	3502	13.5	3340	117.9	43.8	2.76
	12.	THF (0.3)	3491	11.2	3269	159.2	72.2	3.15
	13.	DMF (0.25)	3491	8.80	3254	176.2	79.9	16.7
	14.	DMSO (0.25)	3487	8.61	3225	179.5	77.2	41.0
	15.	HMPA (0.05)	3486	8.51	3151	185.9	82.6	180.7

* - without taking into account $2\gamma(HNH)$ band

complexes was carried out assuming that some of them retain their values in passing from free molecules to bonded ones.

Calculated data on values of valent angles $\gamma(HNH)$, dynamic constants K(NH) and electro-optical parameters $\partial\mu/\partial q$ and $\partial\mu/\partial q'$ (the derivative of dipole moment with respect to adjacent bond) for aminogroups of free molecules of substituted anilines in CCl_4 are presented in Table 1. Dynamic characteristics of NH bonds and different variants of calculation of aminogroup electro-optical parameters in 1:1 complexes are listed in Table 3.

Parameters of bonded NH group in complexes are indicated by index 1 and of nonbonded one - by index 2. Parameters of free molecules have no any indexes.

RESULTS AND DISCUSSION

Spectral manifestations of H-bond in the region of aminogroup stretching vibrations of 4-methoxitetrafluoroaniline, pentafluoroaniline and 4-aminotetrafluoropyridine in 1:1 complexes with various proton acceptors are shown at Figures 1-3. Spectral displays of complexation are qualitatively typical for the majority of substituted anilines [1-3]. In the region between $\nu^{s}(NH_2)$ and $\nu^{as}(NH_2)$ bands of free molecules (close to $\nu^{as}(NH_2)$ band) bands $\nu_f(NH)$ are observed, the main contribution to which is made by free NH-group of 1:1 complexes. In the region below absorption band $\nu^{s}(NH_2)$ of monomers at 3400-3000 cm^{-1} the band $\nu_c(NH)$ of complexes is observed. The structure of the last band is caused by Fermi resonance of vibrations $\nu_c(NH)$ with overtone of deformational vibration $\gamma(HNH)$ (for free molecules of studied anilines $2\gamma(HNH)$= 3192±3 cm^{-1}, $B^{2\gamma}$= $(0.33\pm0.03)\cdot 10^{3}$ dm^{3}M^{-1}cm^{-2}) and with more weak secondary vibrations of aromatic ring.

In 2,3,5,6-tetrafluoroaniline [2] the increase of frequencies, the growth of integral intensities and the reduction in halfwidths

TABLE 3

The dinamic and electro-optical parameters of substituted anilines aminogroup in 1:1 H-bonded complexes with different proton acceptors in CCl_4

Proton donor	Proton acceptor	K_2 (NH) (10^{-6} cm^{-2})	K_1 (NH) (10^{-6} cm^{-2})	Variant 1		Variant 2		Variant 3	
				$\partial\mu_1/\partial q_1$ (DA^{-1})	$\partial\mu_1/\partial q_2$ (DA^{-1})	$\partial\mu_1/\partial q_1$ (DA^{-1})	$\partial\mu_2/\partial q_2$ (DA^{-1})	$\partial\mu_1/\partial q_1$ (DA^{-1})	$\partial\mu_i/\partial q_j$ (DA^{-1})
4-OCH_3-tetra-fluoraniline	CH_3CN	11.245	10.758	2.15	0.63	2.30	1.34	2.18	0.51
	THF	11.256	10.547	2.66	0.93	2.86	1.22	2.73	0.67
	DMF	11.294	10.173	---	---	4.43	1.61	4.44	0.31
	DMSO	11.273	10.059	---	---	4.84	1.52	4.83	0.11
	HMPA	11.265	9.768	---	---	---	---	5.90	0.14
pentafluoraniline	CH_3CN	11.267	10.733	3.40	0.39	3.41	1.72	3.40	0.39
	THF	11.325	10.461	3.95	0.46	3.97	1.67	3.96	0.44
	DMF	11.348	10.141	---	---	4.98	1.17	4.98	0.75
	DMSO	11.348	9.956	---	---	4.90	1.29	4.90	0.95
	HMPA	11.359	9.661	---	---	---	---	---	---
4-NH_2-tetra-fluoropyridine	CH_3CN	11.330	10.516	4.29	0.67	4.31	2.08	4.29	0.65
	THF	11.295	10.042	5.48	1.00	5.42	1.86	5.40	0.93
	DMF	11.300	9.946	---	---	5.67	1.61	---	---
	DMSO	11.282	9.765	---	---	5.66	1.50	---	---
	HMPA	11.290	9.307	---	---	---	---	---	---

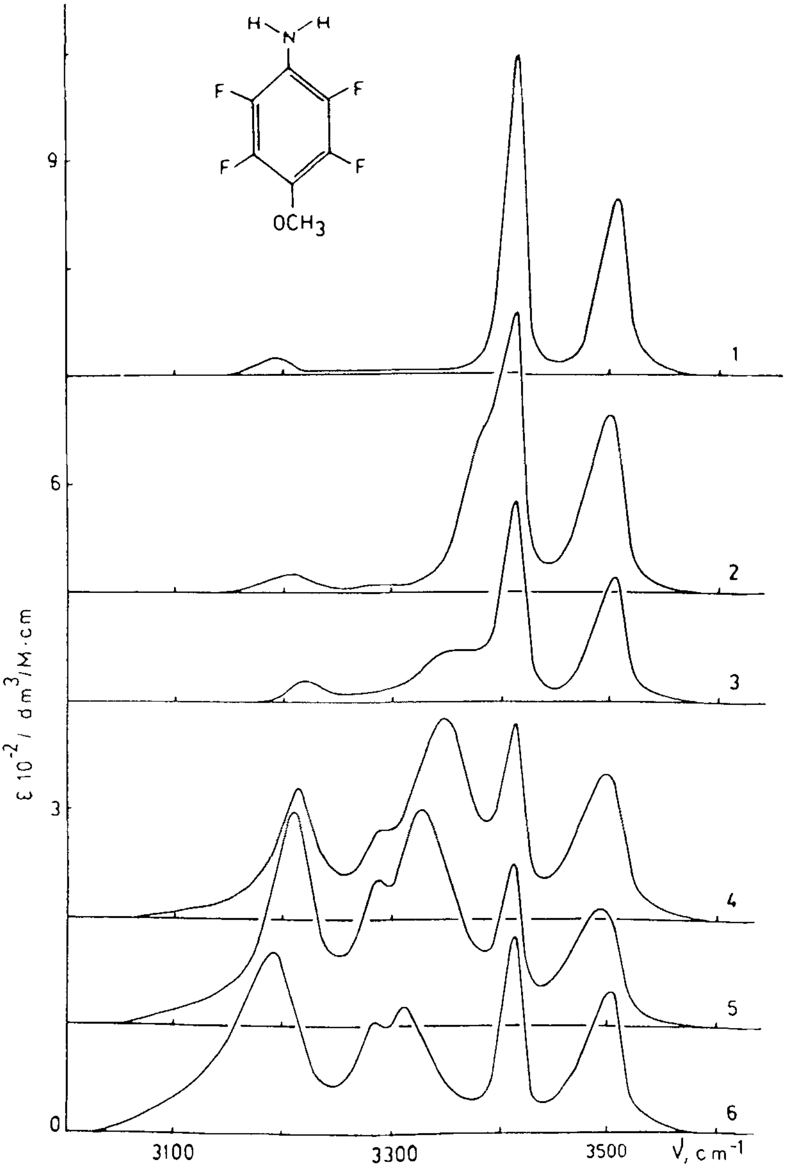

Fig.1. Spectral display of hydrogen bonding in (1:1) complexes of 4-methoxytetrafluoroaniline in the region of aminogroup stretching vibrations in different solvents:
(1) - CCl_4,(2) - CCl_4+ CH_3CN, (3) - CCl_4+ THF, (4) - CCl_4+ DMF,
(5) - CCl_4 + DMSO, (6) - CCl_4 + HMPA.

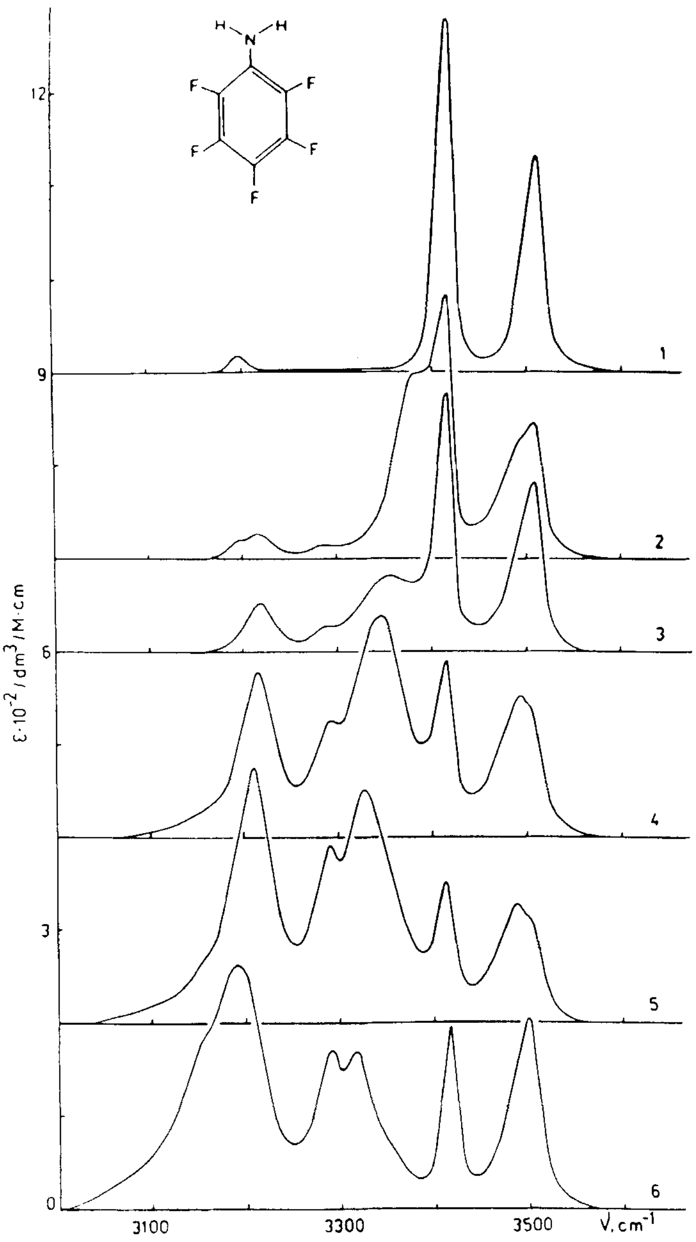

Fig.2. Spectral display of hydrogen bonding in (1:1) complexes of pentafluoroaniline in different solvents:

(1) - CCl_4, (2) - CCl_4+ CH_3CN, (3) - CCl_4+ THF, (4) - CCl_4+ DMF, (5) - CCl_4 + DMSO, (6) - CCl_4 + HMPA.

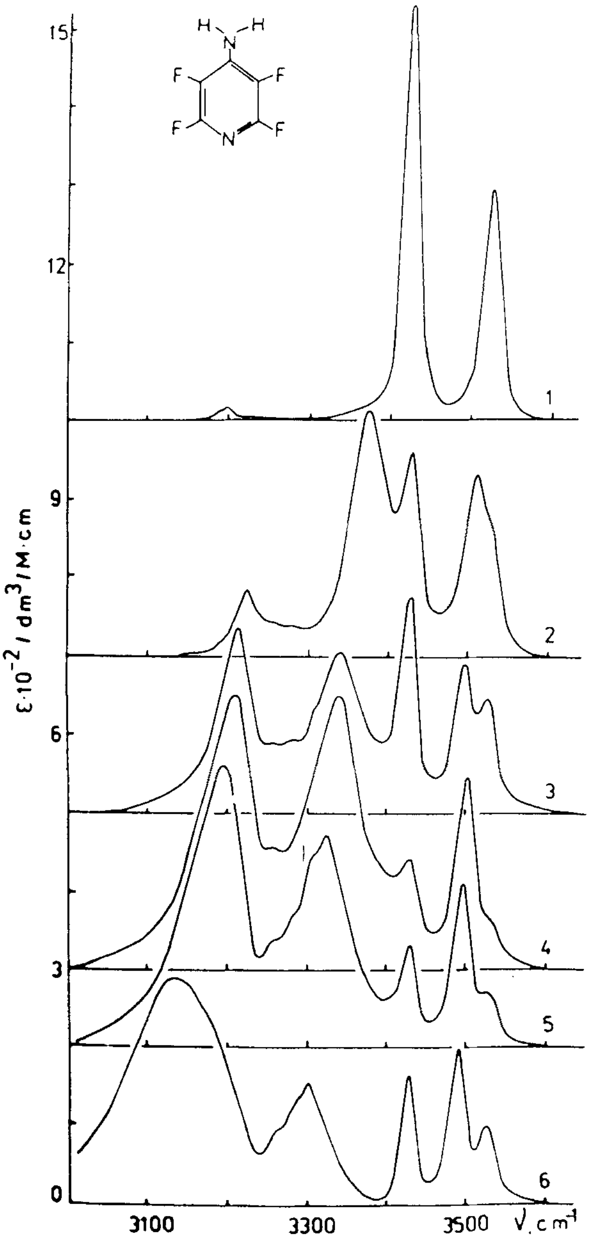

Fig.3. Spectral display of hydrogen bonding in (1:1) complexes of 4-aminotetrafluoropyridine in different solvents:
(1) - CCl_4, (2) - CCl_4+ CH_3CN, (3) - CCl_4+ THF, (4) - CCl_4+ DMF, (5) - CCl_4 + DMSO, (6) - CCl_4 + HMPA.

of aminogroup stretching vibrations in comparison with similar values for aniline [1] has been observed.

When CH_3O-radical with summary inductive effect described by negative Taft constant ($\sigma_p^o(CH_3O)=-0.12$ [5]) is introduced into *p*-position of arene ring of tetrafluoroaniline, some decrease in frequencies and integral intensities along with growth of absorption bands halfwidths of aminogroup stretching vibrations is reached.

The change-over from 2,3,5,6-tetrafluoroaniline to pentafluoroaniline has no virtual influence on halfwidths of both bands and on integral intensity of band $\nu^s(NH_2)$ of free molecules but followed by growth of integral intensity of band $\nu^{as}(NH_2)$ and by diminution of frequencies of aminogroup stretching vibrations.

As may be inferred from previous reasoning, some increase of frequencies of aminogroup stretching vibrations in pentafluoroaniline molecule ($\sigma_p^o(F)=0.17$ [5]), would be expected in comparison with data observed for 2,3,5,6-tetrafluoroaniline. However, the effect of fluorine atoms in *p*-position of arene ring on aminogroup frequencies $\nu^s(NH_2)$ and $\nu^{as}(NH_2)$ in free molecules is analogous to that of electropositive radical CH_3O. This effect emerges also in *p*-fluoroaniline [1], where stretching vibrations frequencies, force constants K(*NH*) and valent angle $\gamma(HNH)$ are lower than in case of aniline, whereas for *o*- and *m*- fluoroanilines inverse regularity is observed.

The introduction of heteroatom into tetrafluoroaniline arene ring is accompanied by frequencies increase, growth of halfwidths and integral intensities of absorption bands of aminogroup stretching vibrations, Table 1.

Spectral variations of aminogroup absorption bands of *p*-substituted tetrafluoroanilines as compared with model substance, 2,3,5,6-tetrafluoroaniline, are caused by changes of geometrical, dynamic and electro-optical parameters of aminogroup, Table 1, which appear to be highly sensitive to a position, a number and a type of substituents in arene ring.

Frequencies deferential $\Delta\nu=\nu^{as}(NH_2)-\nu^{s}(NH_2)$ for free molecules of *p*-substituted tetrafluoroanilines is linearly dependent on valent angle $\gamma(HNH)$ value and follows general regularity for all substituted anilines with equivalent *NH*-bonds [1-3]:

$$\Delta\nu=4.00\ \gamma(HNH)\ -339.0;\ r=\ 1.000 \qquad (1)$$

As spectral characteristics of complex band $\nu_c(NH)$ of 1:1 complexes, Table 2, first spectral moment $M_c^{(1)}$ and "effective" band halfwidth connected with second central moment by correlation [6]:

$$(\Delta\nu_{1/2})_{eff}=\ 2(M_c^{(2)})^{1/2} \qquad (2)$$

are presented.

Data of Table 2 show integral intensities B^c,low frequency shift $M_c^{(1)}$ of bands $\nu_c(NH)$ of compounds under study and equilibrium constants K_{25^oC} to increase when proton donating ability of molecules rises in the next row: CH_3CN, THF, DMF, DMSO, HMPA. Relative shift of band $\nu_f(NH)$ into low frequency field in this row is no more than 10-15 cm^{-1}.

Equilibrium constants for H-bonded complexes of similar type can serve as a measure of proton donating ability of donor molecules, Table 2. In most cases their values increase in the row: 4-methoxytetrafluoroanilins, pentafluoroaniline, 4-aminotetrafluoropyridine. Proton donating ability of 2,3,5,6-tetrafluoroaniline [2] is comparable to that of pentafluoroaniline.

The position of spectral moment $M_c^{(1)}$ of band $\nu_c(NH)$ is observed to be linear dependent on $(K(NH))^{1/2}$ value for all *p*-substituted tetrafluoroanilines, Fig. 4, this dependence being approximated by linear regression equation:

$$M_{c}^{(1)} = 0.965\ (K_{1}(NH))^{1/2} + 221{,}2;\ r = 0.999 \qquad (3)$$

Analogous relationship has been found previously for a number of other substituted anilines [1,3].

Dynamic nonequivalency of aminogroup *NH*-bonds in 1:1 complexes, Table 3, comprises 10-15%. As this takes place, a character of dynamic constant $K_2(NH)$ change with increase in H-bond strength is different depending on nature of proton donors. Definite regularity is observed for H-bonded complexes of 4-methoxytetrafluoroaniline (maximum $K_2(NH)$ value for complex with DMF) and pentafluoroaniline (monotone increase of $K_2(NH)$ value when H-bond is strengthened). Regularities of $K_2(NH)$ change for complexes of 4-aminotetrafluoropyridine with various proton acceptors are more complex.

An assumption that electro-optical parameters of nonbonded *NH*-group are conserved when passing from free molecules to 1:1 complexes was adopted to carry out calculations (variant 1, $\partial\mu_2/\partial q_2 = \partial\mu/\partial q =$ const, $\partial\mu_2/\partial q_1 = \partial\mu/\partial q' =$ const). In this approximation it's turned out to be possible to calculate electro-optical parameters $\partial\mu_1/\partial q_1$ and $\partial\mu_1/\partial q_2$ of bonded *NH*-group only for the least firm complexes with CH_3CN and THF, for which aminogroup polarization by proton acceptors action is relatively small. For complexes including DMF, DMSO and HMPA this assumption was proved to be unacceptable because of in compatibility of conclusion equations [7].

Small contribution of $\partial\mu_i/\partial q_j$ parameters (i,j= 1,2; i≠j) to integral intensity of $\nu_c(NH)$ and $\nu_f(NH)$ bands of 1:1 complexes allows to estimate a value and a direction of change of parameter

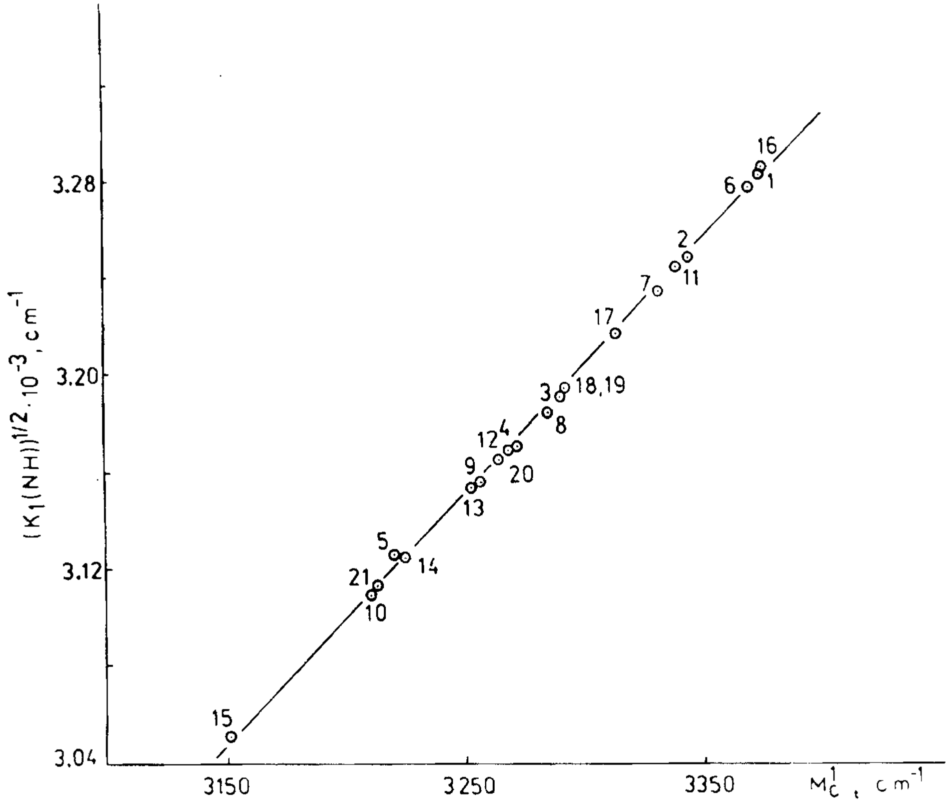

Fig.4. First spectral moment $M_c^{(1)}$ of absorption bands $\nu_c(NH)$ for H-bonded (1:1) complexes of substituted anilines: the dependence on $(K_1(NH))^{1/2}$ value.

(1-5) - 4-methoxytetrafluoroaniline, (6-10) - pentafluoroaniline, (11-15)- 4-aminotetrafluoropyridine, (16-21)-2,3,5,6-tetrafluoroaniline.

$\partial\mu_2/\partial q_2$ of nonbonded *NH*-group (variant 2, $\partial\mu_i/\partial q_j = \partial\mu/\partial q' =$ const). Data of Table 3 demonstrate $\partial\mu_2/\partial q_2$ parameters to be in most cases less than equivalent parameters $\partial\mu/\partial q$ for free molecules in CCl_4, Table 1. For H-bonded complexes of 4-methoxytetrafluoroaniline these variations are moderately great whereas for complexes of pentafluoroaniline and 4-aminotetrafluoropyridine the tendency is observed for parameter $\partial\mu_2/\partial q_2$ to be diminished the strength of H-bond being increased.

Electro-optical parameters of bonded *NH*-group calculated under the assumption that $\partial\mu\ /\partial q = \partial\mu/\partial q =$ const, $\partial\mu/\partial q = \partial\mu\ /\partial q_1$ (variant 3) in comparable cases, Table 3, appear to have values sufficiently close to those calculated by variant 1. The assumption that electro-optical parameters of nonbonded *NH*-group in complexes with HMPA are preserved hasn't proved itself. Most likely this is correlated to marked polarization of aminogroup caused by proton acceptor.

Electro-optical parameters $\partial\mu_2/\partial q_2$ and $\partial\mu_i/\partial q_j$ calculated by variants 1-3 represent only approximate estimates. Parameter $\partial\mu_1/\partial q_1$ is shown to be practically independent on calculation variant. Under our approximations this parameter can be determined most perfectly.

Fig.5 shows the relationship between $\partial\mu_1/\partial q_1$ parameters of studied compounds and $(K_1(NH))^{1/2}$ value for 1:1 complexes. The character of this dependence is individual for each compound.

Thus, the dependence of dynamic and electro-optical parameters of aminogroup in molecules of aniline and its derivatives on individual properties of proton donors and acceptors has been established to be apparent.

For weak proton donors (aniline, mono- and 2,6-di- (CH_3, *F*, *Cl*, *Br*)- substituted anilines [1]) peculiarities of the relationship between $\partial\mu_1/\partial q_1$ and $(K_1(NH))^{1/2}$, Fig.5, are specified

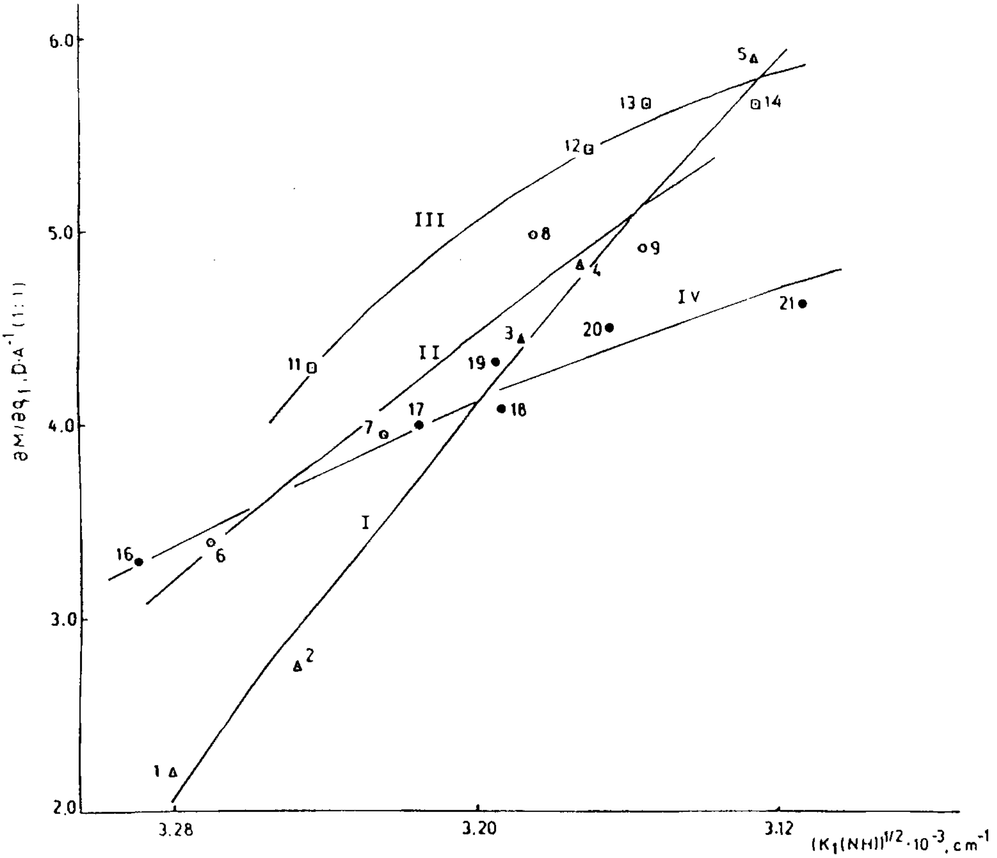

Fig.5. The relationship of $\partial\mu_1/\partial q_1$ and $(K_1(NH))^{1/2}$ parameters of *NH*-group in substituted anilines, taking part in H-bonding into (1:1) complexes.

(1-5) - 4-methoxytetrafluoroaniline, (6-10) - pentafluoroaniline, (11-15)- 4-aminotetrafluoropyridine, (16-21)- 2,3,5,6-tetrafluoroaniline.

by individual features of proton acceptors. Points for different donors are plotted as a function of definite proton acceptors.

For strong proton donors (substituted *p*-nitroanilines) the character of this dependence is dictated by nitro-group in *p*-position of arene ring.

For all derivatives of *p*-nitroanilines the relationship between $\partial\mu_1/\partial q_1$ and $(K_1(NH))^{1/2}$ is described by general equation of linear regression [3].

For medium proton donors, to say, compounds studied in the present work, a type of interrelation between electro-optical parameter $\partial\mu_1/\partial q_1$ and dynamic characteristic of a bond $(K_1(NH))^{1/2}$ in 1:1 complexes is defined by properties of proton donors as well as proton acceptors, effects of substituents in arene ring and of proton acceptors on a type of this dependence being comparable in magnitude.

REFERENCES

1. Borisenko V.E., Greseva E.I., Dukhnova E.V. and Nacheva I.V. Infrared spectra and electro-optical parameters of substituted anilines in H-bonded complexes of 1:1 composition. J.Mol. Struct., 1994; 324: 199-213
2. V.E.Borisenko, I.N.Pospelova, G.G.Furin Infrared spectra and electro-optical parameters of substituted anilines in (1:1) H-bonded complexes (2,3,5,6-tetrafluro-aniline, 4-nitrotetrafluoro aniline). Khimicheskaya fizika, 1993; 12: 957-965
3. V.E.Borisenko, E.I.Tuchkova. Infrared spectra, dynamic and electro-optical parameters of aminogroup of substituted anilines in (1:1) H-bonded complexes. 4-nitroaniline, 2-chloro- and 2,6-dichloro-4-nitroaniline. Spectroscopy Letters, 1994; 27(6):741-762

4. Wolff H., Hagedorn W. Hydrogen bonding and Fermi resonance of of mixed adducts of aniline. The behavior of NH_2 deformation vibrations. J.Phys.Chem., 1980; 84(18): 2335-2337
5. Gordon A.J., Ford R.A. The chemist's Compound. A hand book of practical date techniques and references. New York- London- Sidney- Toronto, 1972
6. Shchepkin D.N. Anharmonic effects in spectra of hydrogen bonded complexes. Depos. VINITI. 1987; 7511- B 87, 86 p.
7. Borisenko V.E., Filarovski A.I. The electro-optical parameters of aniline and its halogene derivatives in hydrogen bonded complexes. J.Mol.Struct., 1989; 196: 353-370

Date Received: January 31, 1995
Date Accepted: March 13, 1995