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Spatial and Electronic Structure of 2-(2-Furyl)- and 2-(2-Thienyl)pyrroles According to ^{1}H and ^{13}C NMR Data

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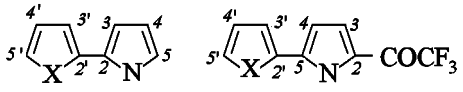
Abstract—In 2-(2-furyl)- and 2-(2-thienyl)pyrroles the heterocycles are in efficient π,π-conjugation. The presumably possible for this compounds intramolecular hydrogen bond N–H···O or N–H···S is lacking. The $COCF_3$ group in position 2 of the pyrrole ring is syn-oriented with respect to pyrrole fragment, and the orientation is fixed by an intramolecular hydrogen bond N–H···O. However no bifurcating hydrogen bonds arise in the molecules containing $COCF_3$ group.

The analysis of ^{1}H and ^{13}C NMR spectra of a number of 2(pyridyl)pyrrole and their trifluoroacetylated derivatives allowed revealing some specific features of their structure. It was demonstrated that an efficient π,π-conjugation existed between the heterocycles; in the 2-(2-pyridyl)pyrrole a weak intramolecular hydrogen bond N–H···N stabilized the conformation with syn-position of the heterocycles; in compounds with a $COCF_3$ group in the *2* position of the pyrrole ring an intermolecular hydrogen bond N–H···O formed which fixed the *syn*(O,N)-orientation of this fragment [1].

In extension of these investigations we continued the systematic studies of pyrrole derivatives structures by NMR method [2–10] and report here on the registration and analysis of ^{1}H and ^{13}C NMR spectra of 2-(2-furyl)- and 2-(2-thienyl)pyrroles (**I, II**), and their trifluoroacetyl derivatives **III, IV**.



I, II **III, IV**

X = O (**I, III**); S (**II, IV**).

The ^{1}H and ^{13}C NMR data for pyrroles **I–IV** are presented in Tables 1, 2, the coupling constants ^{13}C-^{1}H and those with fluorine nuclei are listed in Table 3. The assignment of some signals in the ^{1}H and ^{13}C NMR spectra of the compounds under study posed difficult problems. In the ^{1}H spectrum of 2-(2-furyl)pyrrole (**I**) the signals were assigned unambiguously. With the use of HSQC method [11] were attributed signals of C^3, C^4, C^5 and $C^{3'}$, $C^{4'}$, $C^{5'}$. The assignment of the ^{1}H signals of the thienyl ring in the spectrum of compound **II** was not unambiguous. A large coupling constant ^{13}C–1H permits identification of $C^{5'}$ (Table 3), and the HSQC experiment indicated those of $H^{3'}$, $H^{4'}$, $H^{5'}$. The positions of signals from $H^{3'}$ and $H^{4'}$ were refined by analysis of 1M projections of the 2M HSQC spectrum [12] at 120.97 and 127.71 ppm on the scale F_1 (^{13}C). The signals of C^3, C^4 and C^5 were assigned by HSQC procedure.

The application of the HSQC experiment was sufficient for assignment of carbon signals in the ^{13}C NMR spectrum of 2-trifluoroacetyl-5-(2-furyl)pyrrole (**III**). The $C^{5'}$ signal in the spectrum of thienylpyrrole **IV** was assigned basing on the value of direct ^{1}H–^{13}C coupling constant as was done with the spectrum of compound **II** (Table 3). The signals of C^5, C^4, $C^{3'}$, $C^{4'}$ were identified by HSQC procedure. The assignment of signals from carbon atoms C^2, C^5 and $C^{2'}$ required performing HMBC experiment [13]. For the signal of C^2 a coupling through three bonds with H^4 was observed, and similar interaction for signals of carbon atoms C^5 and $C^{2'}$ with H^3, $H^{3'}$ and H^3, $H^{4'}$ respectively was revealed.

The character of π,π-interaction between the heterocycles in compounds **I, II** is revealed by the changes in the chemical shifts of carbon signals with respect to those in the "isolated" parts of these molecules (pyrrole, furan, and thiophene) (Table 1). The $C^{3'}$ and $C^{5'}$ nuclei in the furan ring of compound **I** suffer additional shielding that results in upfield shift of these signals compared to the corresponding signals

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Table 1. ^{13}C NMR spectra of substituted pyrroles **I**–**IV**[a]

Compd. no.	Chemical shifts, δ, ppm									
	C^2	C^3	C^4	C^5	$C^{2'}$	$C^{3'}$	$C^{4'}$	$C^{5'}$	C(O)	CF_3
I	124.12	105.39 (–2.8)[b]	109.84 (+1.6)[b]	118.20 (+0.4)[b]	148.39	102.30 (–7.3)[c]	111.53 (+1.9)[c]	140.41 (–2.2)[c]	–	–
II	126.72	106.81 (–1.4)[b]	110.11 (+1.9)[b]	118.59 (+0.8)[b]	136.32	120.97 (–6.2)[d]	127.71 (+0.5)[d]	122.75 (–2.6)[d]	–	–
III	125.86	123.63 (+13.8)[e]	109.50 (+4.1)[e]	134.43	145.49	109.25 (+7.0)[e]	112.32 (+0.8)[e]	143.65 (+3.2)[e]	169.31	117.34
IV	126.11	123.88 (+13.8)[f]	110.95 (+4.1)[f]	137.93	132.71	125.92 (+5.0)[f]	128.54 (+0.8)[f]	127.15 (+4.4)[f]	169.36	117.34

[a] δ, ppm: 117.76 ($C^{2,5}$), 108.23 ($C^{3,4}$), pyrrole; 142.6 ($C^{2,5}$), 109.6 ($C^{3,4}$), furan; 125.4 ($C^{2,5}$), 127.2 ($C^{3,4}$), thiophene [30].
[b] Shift of the signal position with respect to the corresponding singlet in the pyrrole spectrum δ_p, $\Delta\delta = \delta - \delta_p$.
[c] Shift of the signal position with respect to the corresponding signal in the furan spectrum δ_f, $\Delta\delta = \delta - \delta_f$.
[d] Shift of the signal position with respect to the corresponding signal in the thiophene spectrum δ_t, $\Delta\delta = \delta - \delta_t$.
[e] Shift of the signal position with respect to the corresponding signal in the spectrum of pyrrole I δ_I, $\Delta\delta = \delta - \delta_I$.
[f] Shift of the signal position with respect to the corresponding signal in the spectrum of pyrrole I δ_{II}, $\Delta\delta = \delta - \delta_{II}$.

Table 2. ^1H and IR spectra of substituted pyrroles **I**–**IV**

Compd. no.	^1H NMR spectrum, δ, ppm							IR spectrum, ν(NH), cm^{-1}
	H^3	H^4	H^5	$H^{3'}$	$H^{4'}$	$H^{5'}$	NH	
I	6.43	6.25	6.79	6.33	6.41	7.33	8.49	3482
II	6.39	6.24	6.79	7.00	6.99	7.13	8.27	3482
III	7.28	6.62	–	6.93	6.54	7.52	9.88	3437
IV	7.27	6.61	–	7.48	7.15	7.42	9.86	3436

Table 3. Coupling constants ^{13}C–^1H, ^{19}F–^1H and ^{19}F–^{13}C in pyrroles **I**–**IV**, Hz

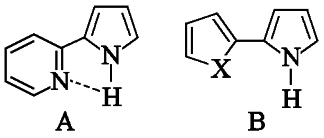
Compd. no.	$^1J(C^3H^3)$	$^1J(C^4H^4)$	$^1J(C^5H^5)$	$^1J(C^{3'}H^{3'})$	$^1J(C^{4'}H^{4'})$	$^1J(C^{5'}H^{5'})$	$^1J_{CF}$	$^2J_{CF}$	$^4J(C^3F)$	$^5J(C^3F)$
I	171.6	171.1	186.7	174.7	175.0	203.8	–	–	–	–
II	171.0	171.3	186.1	166.5	168.0	187.2	–	–	–	–
III	172.9	178.9	–	176.5	176.5	205.1	288.6	36.3	3.6	1.8
IV	175.1	177.1	–	167.9	168.9	188.3	288.3	36.4	3.5	1.9

in furan spectrum by 7.3 and 2.2 ppm respectively, whereas the $C^{4'}$ nucleus is deshielded and its signal is shifted downfield by 1.9 ppm (Table 1). In the pyrrole ring of molecule **I** only C^3 nucleus is shielded stronger than in pyrrole (Δδ –2.8 ppm), and nuclei C^4 and C^5 are deshielded (Δδ 1.6 and 0.4 ppm respectively). Thus the heterocycles of molecule **I** are effectively conjugated, and this is possible only at coplanar or nearly coplanar position.

Since the shielding of $C^{3'}$ carbon is 2.6 times stronger than that of C^3 nucleus, and carbon $C^{5'}$ is shielded in contrast to C^5 it may be concluded that the pyrrole ring in compound **I** shows stronger π-donor ability than the furan ring. Similar shifts

of ^{13}C signals are observed in the spectrum of 2-(2-thienyl)pyrrole (**II**) (Table 1) evidencing effective π,π-conjugation of heterocycles also in this compound. The $C^{3'}$ nucleus in compound **II** is 4.4 times more shielded than C^3 carbon. The $C^{5'}$ nucleus is considerably shielded($\Delta\delta$ −2.6 ppm), whereas C^5 is deshielded ($\Delta\delta$ 0.8 ppm). Therefore we may assume that the pyrrole ring in the molecule in question plays role of a donor with respect to the thiophene ring. In the trifluoroacetylpyrroles **III, IV** the electronic effect of the $COCF_3$ group produced strong shifts of the carbon signals from pyrrole, furan, and thiophene rings as compared with the ^{13}C NMR spectra of compounds **I, II** (Table 1). It especially concerns the signal from C^3 atom that in the spectra of compounds **III, IV** under the influence of electron-withdrawing effect of the $COCF_3$ group is displaced downfield nearly by 14 ppm with respect to the signal in the spectra of **I, II** analogs (Table 1). The transfer of electronic effect of the $COCF_3$ group to furan or thiophene ring through the pyrrole one is quite pronounced as seen from the downfield shift of the signals corresponding to atoms $C^{3'}$, $C^{4'}$ and $C^{5'}$ ($\Delta\delta$ 7.0, 0.8, and 3.2 respectively for compound **III**; 5.0, 0.8, and 4.4 respectively for compound **IV**) (Table 1).

Similar pattern of π,π-interaction between heterocycles and of transfer of $COCF_3$ group effect was revealed in a series of 2-(pyridyl)pyrroles [1] thus indicating the analogy in their electronic structure to that of compounds **I**–**IV**. Therefore it was reasonable to expect a likeness of these molecules in the other structural aspects. For instance, ^1H NMR and IR spectral data testify to the presence in the 2-(2-pyrrolyl)pyridine of an intramolecular hydrogen bond N–H···N that stabilizes the *syn*-position of the heterocycles (structure A).



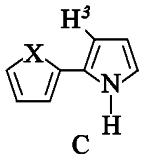
A **B**

X = O, S.

Analogous hydrogen bonds N–H···O and N–H···S might be expected to exist in 2-(2-furyl)pyrrole (**I**) and 2-(2-thienyl)pyrrole (**II**) respectively (structure B). However these bonds would have produced a downfield shift of the NH proton in the ^1H NMR spectra of pyrroles **I, II**; but it is not the case (the corresponding signals appear at 8.49 and 8.27 ppm respectively). These values are close to the chemical shifts of NH proton in the spectra of 2-phenyl-, 2-(3-pyridyl)-, and 2-(4-pyridyl)pyrroles where the intramolecular hydrogen bond is lacking. The chemical shifts of the NH proton in the spectra of these compounds lie in the 8.4–8.7 ppm range [1] whereas the hydrogen bond in 2-(2-pyrrolyl)pyridine effects a downfield shift of NH proton resonance to 9.6 ppm [1].

The values of the stretching vibrations frequency of N–H bonds in the IR spectra of compounds **I, II** do not suffer any shift to lower frequencies expected at hydrogen bonds formation [14]; thus the IR spectra also indicate the lack of hydrogen bonds in **I, II** molecules. The ν(N–H) values in the spectra of compounds **I, II** is nearly identic to those in the IR spectra of 2-phenyl-, 2-(3-pyridyl)-, and 2-(4-pyridyl)-pyrroles {ν(N–H) 3484, 3478, and 3482 cm^{-1} respectively [1]}. The hydrogen bond formation in the 2-(2-pyrrolyl)pyridine results in decrease in ν(NH) to 3460 cm^{-1} [1].

Thus the ^1H NMR and IR spectra show the lack of an internal hydrogen bond in furyl- and thienylpyrroles **I, II**. This may be caused by nonplanar structure of molecules **I, II**. However the existence of significantly populated conformations with strong deviation of heterorings from coplanarity disagrees with the data of *ab initio* quantum-chemical calculations [15] and is improbable in view of effective π,π-conjugation of the heterocycles. Another reason of the nonexistence of hydrogen bond in compounds **I, II** may consist in considerably populated conformation with the anti-position of the heterocycles (structure C); the latter assumption is consistent with the *ab initio* quantum-chemical calculations [15].



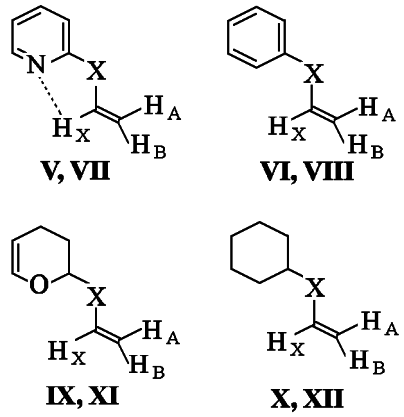
C

X = O, S.

Under such occasion at X = NH should be observed a strong downfield shift of proton signal from H^3 and increase in the coupling constant $^1J(C^3H^3)$ due to specific intramolecular interaction with H^3 atom [16, 17]. In furyl- and thienylpyrroles **I, II** the signal of H^3 proton is displaced downfield compared to the signal of H^3 proton only by 0.15–0.20 ppm (caused by the anisotropic influence of the furan or thiophene ring [18]) (Table 2). The coupling constants $^1J(C^3H^3)$ in the spectra of compounds **I, II** also hardly differ from the coupling constants $^1J(C^4H^4)$ (Table 3).

This means that in any of B or C conformation of furyl- and thienylpyrroles **I, II** the doubly coordinated O and S atoms do not form hydrogen bonds and do not participate in specific intramolecular interactions unlike atom N. It was remarked previously that at the replacement of a nitrogen by some other heteroatoms (among then doubly coordinated chalcogenes) specific intramolecular interactions of the C–H···heteroatom type became inefficient [19, 20].This fact is due to unlike energy state of the unshared pairs in different heteroatom [21].

This statement can be illustrated by comparison of ^{1}H chemical shifts of some model compounds. The signal of H_X proton in the ^{1}H NMR spectra of 2-vinyloxypyridine (**V**) and 2-vinylsulfanylpyridine (**VII**) is shifted downfield by 0.98 and 0.59 ppm as compared to analogous signals of phenyl vinyl ether (**VI**) and vinyl phenyl sulfide (**VIII**) respectively (Table 4) due to an intramolecular hydrogen bond C–H···N [16, 17].



X = O (**V, VI, IX, X**), S (**VII, VIII, XI, XII**).

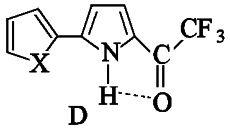
Table 4. ^{1}H NMR spectral data of vinyl ethers **V, VII, IX, XI** and sulfides **VI, VIII, X, XII**

Compd. no.	Chemical shifts, δ, ppm			
	H_A	H_B	H_X	$\Delta\delta^a$
V	4.49	4.87	7.55	0.38
VI	4.35	4.69	6.77	0.34
VII	5.49	5.56	7.11	0.07
VIII	5.33	5.31	6.52	–0.02
IX	4.13	4.48	6.46	0.35
X	3.96	4.26	6.31	0.30
XI	5.29	5.36	6.52	0.07
XII	5.19	5.19	6.38	0.00

[a] $\Delta\delta = \delta_A - \delta_B$.

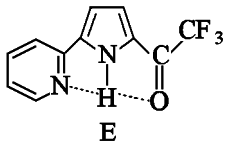
Ethers **IX, X** and sulfides **XI, XII** exist prevailingly in the *s-trans*-conformation as show the differences in the chemical shifts of the β-protons of the vinyl group (parameter $\Delta\delta = \delta_A - \delta_B$) [16, 17, 22] (Table 4). In ether **IX** and sulfide **XI** analogously to 2-vinyloxy and 2-vinylsulfanylpyridines **V, VII** presumably can exist an intramolecular hydrogen bond C–H···O. However the downfield shifts of H_X signals in the ^{1}H NMR spectra of compounds **IX**, **XI** relative to the corresponding signals in the spectra of ether **X** and sulfide **XII** respectively where such interactions are excluded are only 0.13–0.15 ppm (Table 4). Thus in a similar stereochemical situation the interaction C–H···O turned out to be inefficient as compared to that of C–H···N.

In (trifluoroacetyl)pyrroles **III, IV** a remote coupling was observed between ^{19}F and H^3 nuclei through 5 bonds, and ^{19}F and C^3 nuclei through 4 bonds (Table 3). The first interaction occurs through space [23, 24], and the second through an intermediate bond C^3–H^3 [25, 26]. Previously such coupling was observed in the other 5-substituted 2-trifluoroacetylpyrroles [1, 27]. It indicates that the trifluoroacetyl group is located in *syn*-position with respect to pyrrole ring [1] (structure D).



X = O, S.

The proton signal corresponding to NH group in the spectra of (trifluoroacetyl)pyrroles **III, IV** is shifted downfield by 1.4–1.5 ppm as compared to the spectra of the **I, II** analogs lacking the $COCF_3$ group. The absorption band of the N–H bond in the IR spectra of compounds **III, IV** suffers an infrared shift by 45–46 cm^{-1} as compared with the spectra of pyrroles **I, II**. These spectral effects indicate the presence of an intramolecular hydrogen bond N–H···O that is common also for the other compounds of this class [1]. On the other hand, in the ^{1}H NMR spectrum of 2-trifluoroacetyl-5-(2-pyridyl)-pyrrole the NH proton signal is additionally shifted downfield by 0.8 ppm, and the absorption band of the N–H bond in its IR spectrum is displaced to lower frequencies by 15–20 cm^{-1} as compared with the corresponding bands in the spectra of 2-trifluoroacetyl-5-(3-pyridyl)pyrrole and 2-trifluoroacetyl-5-phenylpyrrole [1]. These effects are due to the presence in the first molecule of a bifurcating hydrogen bond (structure E).



E

In 2-trifluoroacetyl-5-(2-furyl)pyrrole (**III**) and 2-(2-thienyl)-5-trifluoroacetylpyrrole (**IV**) the shifts compared to the above compounds are insignificant (Table 2 in [1]) evidencing the lack of bifurcating hydrogen bond in pyrroles **III, IV** [28, 29].

EXPERIMENTAL

^{1}H and ^{13}C NMR spectra were registered on spectrometer Bruker DPX-250 at operating frequencies 250.1 and 62.9 MHz respectively from solutions in $CDCl_3$ using HMDS as internal reference. The concentration of solutions was 5–10 wt% for registering ^{13}C NMR spectra, and 0.1 wt% for ^{1}H NMR spectra. The parameters of pulse sequence in registering of ^{1}H and ^{13}C NMR spectra were described in [1]. The experiments HSQC and HMBC were carried out by standard programs provided with the Bruker DPX spectrometer optimized for coupling constants $^1J_{CH}$ of 160 and 8 Hz respectively. The coupling constants ^{13}C–^{1}H were measured by gated decoupling [31].

Synthesis of compounds under study was described in [32–34].

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