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Regioselectivity in the Reactions of *N*-(Polychloroethylidene)-sulfonamides with 1*H*-Pyrrole and 1-Methyl-1*H*-pyrrole

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Abstract—*N*-(2,2,2-Trichloroethylidene)arenesulfonamides react with 1*H*-pyrrole and 1-methyl-1*H*-pyrrole to give the corresponding *N*-[2,2,2-trichloro-1-(1*H*-pyrrol-2-yl)ethyl]arenesulfonamides. The reaction of *N*-(2,2,2-trichloroethylidene)trifluoromethanesulfonamide with pyrrole leads to a mixture of 2-mono- and 2,5-disubstituted pyrroles, whereas in the reaction with 1-methyl-1*H*-pyrrole only the 2-substituted compound is formed. *N*-(2,2-Dichloro-2-phenylethylidene)-4-methylbenzenesulfonamide reacts with 1*H*-pyrrole to form *N*-[2,2-dichloro-2-phenyl-1-(1*H*-pyrrol-2-yl)ethyl]-4-methylbenzenesulfonamide, and its reaction with 1-methyl-1*H*-pyrrole gives a mixture of 2- and 3-monosubstituted derivatives. The results of quantum-chemical calculations of the initial reactants and products indicate that the process is orbital-controlled. A good agreement is observed between the experimental data and theoretical conclusions concerning the dependence of the reaction regioselectivity on the nature of substituents in the electrophile molecule.

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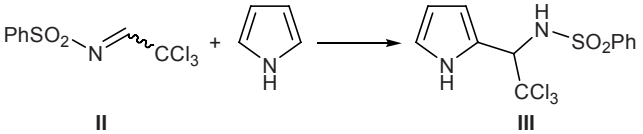
Reactions of *N*-(polychloroethylidene)arenesulfonamides with pyrroles open convenient synthetic approaches to important compounds whose molecules include a pyrrole fragment and aminosulfonyl and polyhaloalkyl groups [1, 2] that are responsible for their biological activity and possibility for further chemical modifications. In continuation of our systematic studies on the reactivity of azomethine systems activated by strong electron-withdrawing substituents toward hetarenes [1], in the present work we examined amidoalkylation of pyrroles with Schiff bases derived from trifluoromethane- and arenesulfonamides, on the one hand, and trichloroacetaldehyde and dichloro(phenyl)acetaldehyde, on the other.

It is known that electrophilic reagents react with pyrroles at both α- and β-positions of the pyrrole ring. For example, the reaction of 1-methyl-1*H*-pyrrole with ethyl (4-tolylsulfonylimino)acetate in the presence of $CuPF_6$ gives a mixture of 2- and 3-[ethoxycarbonyl(*p*-tolylsulfonylamino)methyl]-substituted 1-methylpyrroles with an overall yield of 89% [3]. Analogous reaction with 2-acetyl-1*H*-pyrrole results in the formation of the corresponding 4-substituted derivative.

It was shown previously that 4-chloro-*N*-(2,2,2-trichloroethylidene)benzenesulfonamide regioselectively reacts with pyrrole and 1-substituted pyrroles in the absence of a catalyst or in the presence of boron trifluoride–ether complex, yielding up to 60% of the corresponding 2-monosubstituted derivatives, 4-chloro-*N*-[2,2,2-trichloro-1-(1-R-1*H*-pyrrol-2-yl)ethyl]benzenesulfonamides [2]. In the recent publication [4] we reported on unusual reaction of highly electrophilic *N*-(2,2,2-trichloroethylidene)trifluoromethanesulfonamide (**I**) with pyrrole, which gave either 2-mono- or 2,5-disubstituted pyrrole in up to 80% yield, depending on the conditions.

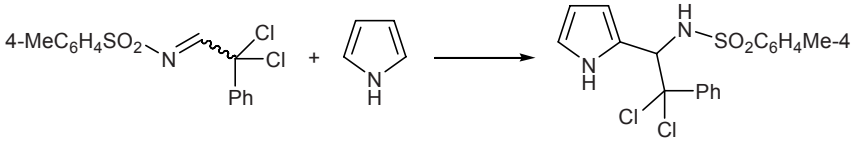
We failed to obtain disubstituted product in the reaction of pyrrole with *N*-(2,2,2-trichloroethylidene)-benzenesulfonamide (**II**) even using 2 equiv of the latter, i.e., under the conditions ensuring formation of

Scheme 1.



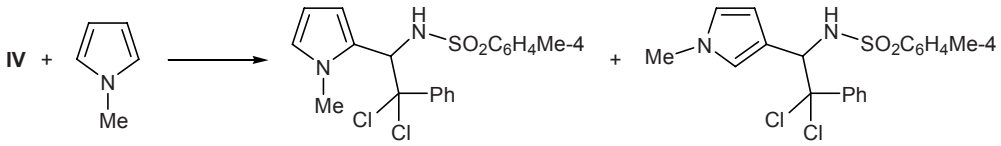
II **III**

Scheme 2.



IV **V**

Scheme 3.



VI **VII**

2,5-disubstituted pyrrole from compound **I** [4]. Instead, 2-substituted pyrrole **III** was isolated in 74% yield (Scheme 1).

N-(2,2-Dichloro-2-phenylethylidene)-4-methylbenzenesulfonamide (**IV**) is less reactive than compounds **I** and **II** toward pyrrole and 1-methyl-1*H*-pyrrole [2, 4]; this follows from the fact that its reactions are less exothermic. No disubstituted pyrroles were formed in the reaction with compound **IV**. The reaction of **IV** with pyrrole gave 82% of 2-substituted derivative **V** (Scheme 2), as in the reactions of pyrrole with *N*-(2,2,2-trichloroethylidene)benzenesulfonamide (**II**) and 4-chloro-*N*-(2,2,2-trichloroethylidene)benzenesulfonamide [2]. However, compound **IV** reacted with 1-methyl-1*H*-pyrrole to produce a mixture of isomeric 2- and 3-substituted 1-methyl-1*H*-pyrroles **VI** and **VII** at a ratio of 4:1 (overall yield 81%; Scheme 3).

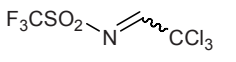
The formation of a mixture of isomers **VI** and **VII** was proved by ^{1}H and ^{13}C NMR spectroscopy. The ^{1}H and ^{13}C NMR spectra of the product mixture obtained from compound **IV** and 1-methyl-1*H*-pyrrole contained two sets of signals from aromatic protons and carbon nuclei and those present in the 1-methylpyrrole fragment. Furthermore, the NHCH moiety gave rise to two doublets of doublets in the ^{1}H NMR spectrum, which is typical of *N*-polychloroethyl sulfonamides [2, 4]. The presence of 2- and 3-substituted pyrrole ring in molecules **VI** and **VII**, respectively, was unambiguously proved by two-dimensional NMR techniques. The assignment was made using ^{1}H–^{13}C correlation (HMBC) optimized for $^nJ_{CH}$ = 10 Hz (coupling through 2–3 chemical bonds).

In the HMBC spectrum of **VI** we observed cross peaks for protons in the 1-methyl group, on the one hand, and C^2 and C^5, on the other. The CH proton showed two cross peaks due to coupling with C^2 and C^3, respectively (coupling through 2 and 3 bonds). The COSY spectrum of **VI** revealed correlation between 3-H and 4-H in the pyrrole ring, as well as between 4-H and 5-H. These findings confirm the structure of **VI** as 2-substituted pyrrole. In the HMBC spectrum of **VII**, the 3-CH proton showed three cross peaks with C^3, C^2, and C^4, while protons in the methyl group displayed correlations with C^2 and C^5. The COSY spectrum of **VII** contained only one cross peak for protons in the pyrrole ring, which corresponded to coupling between 4-H and 5-H. The other signals in the ^{1}H and ^{13}C NMR spectra of isomers **VI** and **VII** were assigned using HSQC ^{1}H–^{13}C correlation technique.

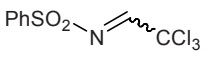
We succeeded in isolating isomer **VI** as individual substance by fractional crystallization, and special experiments proved that 2-substituted pyrrole **VI** is not converted into 3-substituted isomer **VII** even on prolonged heating in boiling carbon tetrachloride.

To interpret our experimental results we performed quantum-chemical calculations of the electrophiles, i.e., *N*-(polychloroethylidene) sulfonamides **I**, **II**, and **VIII**, isomeric 2- and 3-monosubstituted products **III**, **IX**, **X**, and **XI**–**XIII**, and isomeric disubstitution products **XIV**–**XVI**. Insofar as compounds **XIV**–**XVI** possess two asymmetric carbon atoms, calculations were performed for each diastereoisomer couple. The calculations were performed in terms of the density functional theory (DFT) using B3LYP/6-311G(*d*,*p*) basis set with full geometry optimization with the aid of Gaussian 03 software [5].

It is well known that the α-position in the pyrrole is more reactive than the β-position, though the difference in their reactivities is minimal as compared to other five-membered heterocycles, thiophene and furan [6]. Reduction in the reactivity of *N*-sulfonyl imines in the series **I** > **II** > **VIII** is well consistent with increase

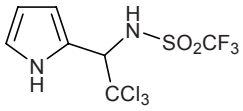


I

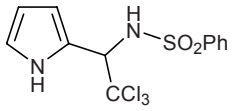


II

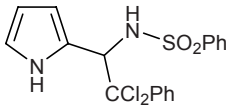
VIII



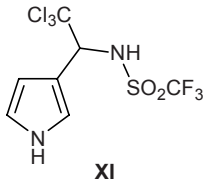
IX



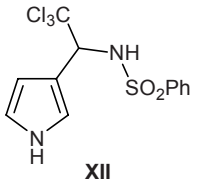
III



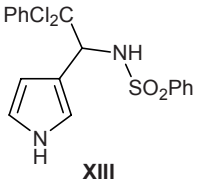
X



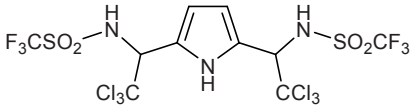
XI



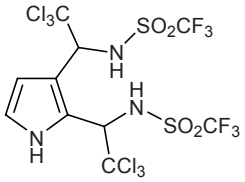
XII



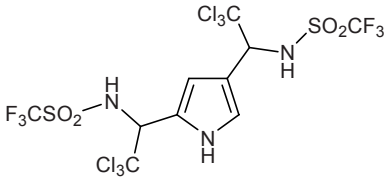
XIII



XIV



XV



XVI

in the energy of the lowest unoccupied molecular orbital in the same series: –0.117, –0.100, and –0.085 eV, respectively, but there is no correlation with the charge on the C=N carbon atom (0.131, 0.103, and 0.138, respectively). These findings suggest that the reactions of imines **I**, **II**, and **VIII** as electrophiles are orbital-controlled.

The β-carbon atom in the pyrrole molecule possesses larger electron density, while the contribution of the α-carbon atom to the highest occupied molecular orbital is much greater than that of the β-carbon atom. Therefore, orbital-controlled reactions with electrophiles **I**, **II**, and **VIII** should occur at the α-position, which is observed experimentally. The structure of isomeric α- and β-substituted products is shown in Fig. 1. The total energies of α-substituted compounds **III**, **IX**, and **X** are lower than those of isomeric β-substitution products **XI**–**XIII**, which also favors formation of the former. However, it should be noted that the energy difference ΔE between 2- and 3-substituted isomers strongly depends on the initial imine. The ΔE values for trichloroacetaldehyde imine derivatives **IX**/**XI** and **III**/**XII** are 7.2 and 13.6 kcal/mol, respectively, whereas the energy difference between isomeric 2- and 3-[2,2-dichloro-2-phenyl-1-(phenylsulfonylamino)ethyl]pyrroles **X** and **XIII** is as small as 0.6 kcal/mol.

The high reactivity of imine **I** ensures facile formation of disubstituted product **XIV**. In order to rationalize the regioselectivity in the reaction of **I** with pyrrole we analyzed the structure of frontier molecular orbitals in **IX** which acts as nucleophile in the reaction with **I**. The maximal contribution to the highest occupied molecular orbital of **IX** is that of the C^5 atom (31.4% against 8.3% of C^3 and 11.2% of C^4). Taking into account that the process is orbital-controlled, 2,5-disubstituted product should be formed, as is observed experimentally.

The ^{1}H NMR spectrum of 2,5-bis[2,2,2-trichloro-1-(trifluoromethylsulfonylamino)ethyl]pyrrole (**XIV**) contained a singlet from the CCl_3CH proton (δ 5.25 ppm), a doublet from 3-H and 4-H (δ 6.47 ppm, $^4J_{NH,CH}$ = 2.3 Hz), a broadened singlet from the pyrrole NH proton (δ 11.07 ppm) and a singlet from the SO_2NH proton (δ 11.62 ppm); in addition, singlets at δ 5.22 ppm (CCl_3CH) and 11.73 ppm (SO_2NH) were present due to the minor diastereoisomer. In the ^{13}C NMR spectrum, signals at δ_C 66.65 (CH), 100.74 (CCl_3), 109.38 (C^3, C^4), 119.07 (CF_3, J_{CF} = 322.5 Hz), and 124.05 ppm (C^2, C^5) were assigned to the major diastereoisomer, while the minor one displayed signals at δ_C 100.68 and 109.23 ppm due to the CCl_3 carbon atom and C^3/C^4, respectively. The diastereoisomer ratio was ~6:1. On the basis of the NMR data it was impossible to determine whether racemic mixture of optically active diastereoisomers (*RR* + *SS*) or *meso* form (*RS*) of **XIV** prevails. Therefore, we compared their energies calculated at the B3LYP/6-311G(*d*,*p*) level. The *meso* form (*RS*) in the gas phase is slightly

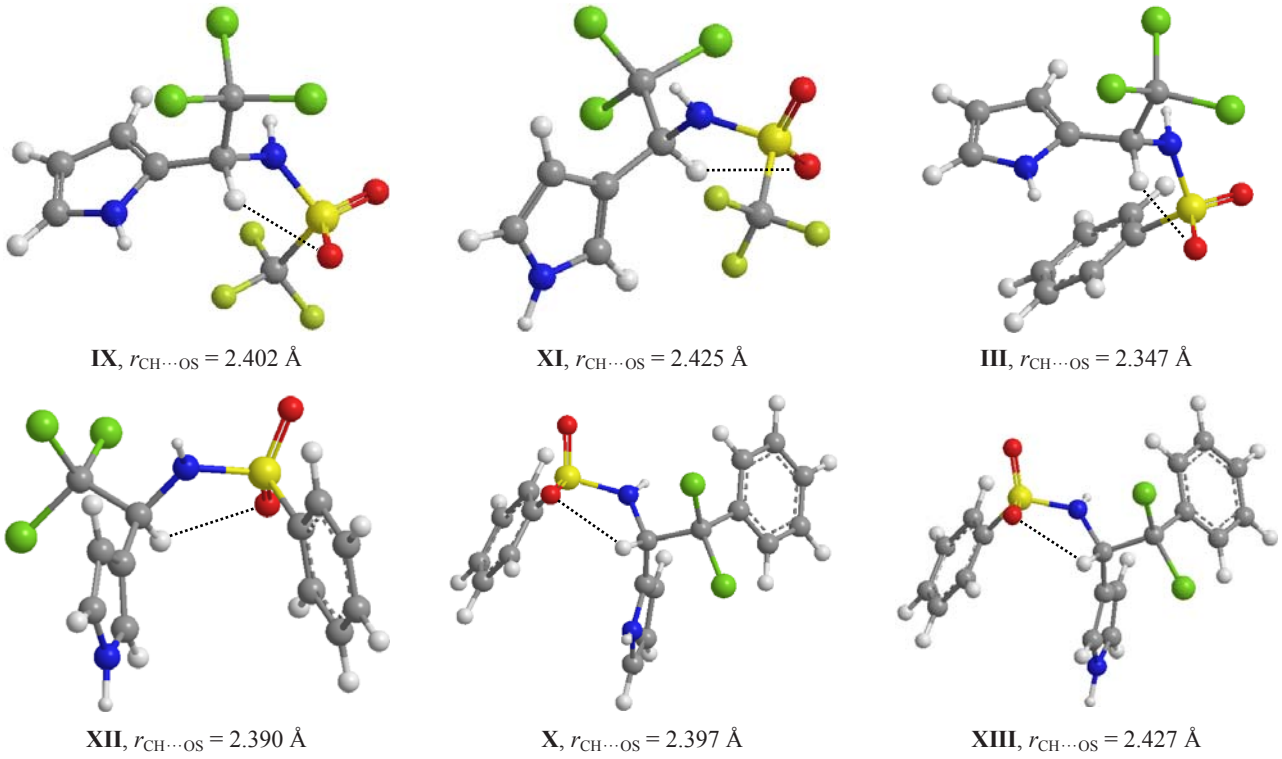


Fig. 1. Molecular structures of 2- and 3-substituted pyrroles **III** and **X**–**XIII** according to B3LYP/6-311G(*d*,*p*) calculations. Intramolecular hydrogen bonds are shown with dashed lines.

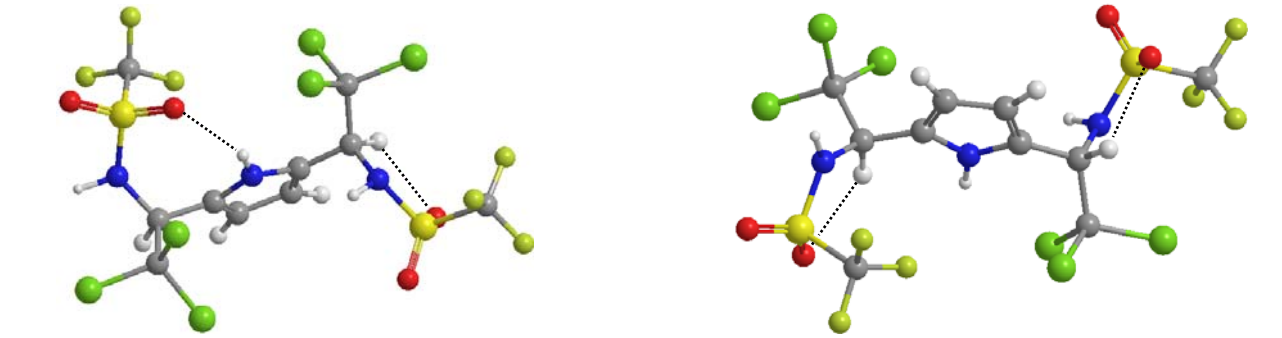


Fig. 2. Molecular structures of (2*S*,5*S*)- and (2*R*,5*S*)-diastereoisomers of 2,5-bis[2,2,2-trichloro-1-(trifluoromethylsulfonylamino)-ethyl]pyrrole (**XIV**) according to B3LYP/6-311G(*d*,*p*) calculations. Intramolecular hydrogen bonds are shown with dashed lines.

more favorable (by 1.6 kcal/mol), but its dipole moment (1.82 D) is lower than the dipole moment of the (*RR*)-diastereoisomer or identical (*SS*)-diastereoisomer (2.88 D). This means that the relative stability may depend on the solvent nature. SCRF (self-consistent reaction field) calculations of the structures optimized by the B3LYP/6-311G(*d*,*p*) method showed that the ΔE value in methylene chloride (i.e., in the same solvent as in experimental studies) is 2.5 kcal/mol in favor of the *meso* form (like in the gas phase). Taking into account the above data we presumed that the (*RS*)-diastereoisomer is the major component, and racemic mixture of optically active (*RR*)- and (*SS*)-diastereoisomers is the minor component.

According to the calculations, intramolecular hydrogen bonds are formed in both diastereoisomers. The *meso*-form (*RS*) is characterized by CH···OS hydrogen bonds in both side chains, while in the (*SS*)-diastereoisomer analogous CH···OS hydrogen bond is formed in one side chain, and the other side chain is involved in NH···OS hydrogen bond with participation of the pyrrole NH proton (Fig. 2).

One of the most interesting results of the reactions of *N*-(polychloroethylidene) sulfonamides with pyrroles is the formation of [2,2-dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-2-phenylethyl]-4-methylbenzenesulfonamide (**VI**) as the major product and *N*-[2,2-dichloro-1-(1-methyl-1*H*-pyrrol-3-yl)-2-phenylethyl]-4-methylbenzenesulfonamide (**VII**) as the minor product from *N*-[2,2-dichloro-2-phenylethylidene]-4-methylbenzenesulfonamide (**IV**) and 1-methyl-1*H*-pyrrole (Scheme 3). β-Substituted product is formed only in the reaction with the least reactive electrophile among the examined ones. This result is consistent with the theoretical data. The difference in the energies of α- and β-substituted isomers **X** and **XIII** is very small, 0.6 kcal/mol against 7.2 and 13.6 kcal/mol for isomer couples **IX**/**XI** and **III**/**XII**, respectively. This means that the probabilities for formation of isomers **X** and **XIII** are almost similar from the viewpoint of thermodynamics. In addition, the lowest unoccupied molecular orbital of imine **IV** as electrophile (as well as the LUMO of imine **VIII**) has a higher energy than those of **I** and **II** (E_{LUMO} = –0.117, –0.100, –0.085, and –0.083 eV for compounds **I**, **II**, **VIII**, and **IV**, respectively), while the positive charge on the C=N carbon atom is maximal (0.131, 0.103, 0.138, and 0.137 a.u. for **I**, **II**, **VIII**, and **IV**, respectively). Increase of the gap between the HOMO of pyrrole and LUMO of electrophile should lead to reduction in the contribution of orbital control and increase in the contribution of charge control and hence to increased probability of β-substitution, in keeping with the experimental data.

Thus our experimental data and the results of quantum-chemical calculations indicate that reactions of *N*-sulfonylpolychloroacetaldehyde imines with pyrroles are orbital-controlled and that they give mainly the corresponding α-substituted pyrrole derivatives, though least reactive electrophiles could give rise to isomeric β-substituted products.

EXPERIMENTAL

The IR spectra were recorded in KBr on a Bruker IFS-25 spectrometer. The ^{1}H and ^{13}C NMR spectra were measured from solutions in DMSO-d_6 on Bruker DPX-400 and Bruker Avance-400 spectrometers at 400.13 MHz for ^{1}H and 100.62 MHz for ^{13}C using tetramethylsilane as reference. Initial compounds **I** [7], **II** [2], **IV** [8], **IX**, and **XIV** [4] were synthesized according to known procedures.

***N*-[2,2,2-Trichloro-1-(1*H*-pyrrol-2-yl)ethyl]benzenesulfonamide (III).** Pyrrole, 0.67 g (0.01 mol), was added dropwise under stirring to a mixture of 5.72 g (0.02 mol) of compound **II** and 50 ml of anhydrous carbon tetrachloride, cooled to –15°C. After 30 min, the cooling bath was removed, and the mixture was stirred for 5 h at room temperature and was kept for 12 h in the cold. The precipitate was filtered off and washed with 50 ml of 10% aqueous ammonia. Yield 2.62 g (74%), mp 178–182°C. IR spectrum, ν, cm^{-1}: 3420, 3230 (NH); 1320, 1160 (SO_2). ^{1}H NMR spectrum, δ, ppm: 5.25 d (1H, NCH, ^3J = 9.0 Hz), 5.78 m (1H, 4-H), 6.17 m (1H, 3-H), 6.53 m (1H, 5-H), 7.32 m (1H, *p*-H) 7.44 m (2H, *m*-H), 7.60 m (2H, *o*-H), 8.86 d (1H, NH, ^3J = 9.0 Hz), 10.69 s (1H, 1-H). ^{13}C NMR spectrum, δ_C, ppm: 66.26 (NCH), 102.26 (CCl_3), 107.57 (C^4), 108.68 (C^3), 117.73 (C^5), 123.92 (C^2), 126.16 (C^o), 128.51 (C^m), 132.07 (C^p), 140.69 (C^i). Found, %: C 41.03; H 3.26; Cl 30.66; N 7.52; S 9.22. $C_{12}H_{11}Cl_3N_2O_2S$. Calculated, %: C 40.76; H 3.14; Cl 30.07; N 7.92; S 9.07.

***N*-[2,2-Dichloro-2-phenyl-1-(1*H*-pyrrol-2-yl)-ethyl]-4-methylbenzenesulfonamide (V).** A mixture of 1.71 g (5 mmol) of compound **IV**, 0.47 g (7 mmol) of pyrrole, and 15 ml of anhydrous carbon tetrachloride was stirred for 45 min. The precipitate was filtered off, washed with 50 ml of 10% aqueous ammonia, dried, and recrystallized from chloroform. Yield 1.67 g (82%), mp 182–184°C. IR spectrum, ν, cm^{-1}: 3400, 3210 (NH); 1305, 1140 (SO_2). ^{1}H NMR spectrum, δ, ppm: 2.26 s (3H, CH_3), 5.25 d (1H, NCH, ^3J = 10.0 Hz), 5.67 m (1H, 4-H), 5.77 m (1H, 3-H), 6.38 m (1H, 5-H), 7.07 d (2H, *m*-H in C_6H_4), 7.33 d (2H, *o*-H in C_6H_4), 7.35 m (2H, *m*-H in C_6H_5), 7.39 m (1H, *p*-H in C_6H_5), 7.55 m (2H, *o*-H in C_6H_5), 8.22 d (1H, NH, ^3J = 10.0 Hz), 10.19 s (1H, 1-H). ^{13}C NMR spectrum, δ_C, ppm: 21.57 (CH_3), 65.03 (NCH), 94.80 (CCl_2), 108.24 (C^4), 110.31 (C^3), 118.33 (C^5), 124.65 (C^2), 127.15 (C^o in C_6H_4), 127.28 (C^o in C_6H_5), 128.25 (C^m in C_6H_5), 129.46 (C^m in C_6H_4), 129.61 (C^p in C_6H_5), 137.00 (C^i in C_6H_4), 139.56 (C^i in C_6H_5), 143.48 (C^p in C_6H_4). Found, %: C 56.02; H 4.36; Cl 16.99; N 6.32; S 7.22. $C_{20}H_{20}Cl_2N_2O_2S$. Calculated, %: C 55.75; H 4.43; Cl 17.32; N 6.84; S 7.83.

Reaction of *N*-(2,2-dichloro-2-phenylethylidene)-4-methylbenzenesulfonamide (IV) with 1-methyl-1*H*-pyrrole. A mixture of 1.71 g (5 mmol) of compound **IV**, 0.57 g (7 mmol) of 1-methyl-1*H*-pyrrole, and 15 ml of anhydrous carbon tetrachloride was heated for 5 h under reflux with stirring. The mixture was then kept in the cold, and the precipitate was filtered off, washed with 50 ml of 10% aqueous ammonia, and dried. According to the NMR data, the product was a mixture of *N*-[2,2-dichloro-1-(1-methyl-1*H*-pyr-

rol-2-yl)-2-phenylethyl]-4-methylbenzenesulfonamide (**VI**) and *N*-[2,2-dichloro-1-(1-methyl-1*H*-pyrrol-3-yl)-2-phenylethyl]-4-methylbenzenesulfonamide (**VII**) at a ratio of 4:1. Overall yield 1.72 g (81%). Isomer **VI** was isolated as individual substance by fractional crystallization of the isomer mixture from carbon tetrachloride, yield 0.49 g.

Compound **VI**. mp 140–142°C. IR spectrum, ν, cm^{-1}: 3230 (NH); 1320, 1150 (SO_2). ^1H NMR spectrum, δ, ppm: 2.26 s (3H, C**H**$_3C_6H_4$), 2.78 s (3H, 1-CH_3), 4.90 d (1H, NCH, ^3J = 9.7 Hz), 5.72 m (1H, 4-H), 6.23 m (1H, 3-H), 6.24 m (1H, 5-H), 7.08 d (2H, *m*-H in C_6H_4), 7.34 d (2H, *m*-H in C_6H_5), 7.35 m (3H, *o*-H in C_6H_4, *p*-H in C_6H_5), 7.48 m (2H, *o*-H in C_6H_5), 8.58 d (1H, NH, ^3J = 9.7 Hz). ^{13}C NMR spectrum, δ_C, ppm: 20.86 (**C**$H_3C_6H_4$), 32.67 (1-CH_3), 61.88 (NCH), 95.69 (CCl_2), 106.54 (C^4), 109.67 (C^3), 121.65 (C^5), 126.08 (C^2), 126.12 (C^o in C_6H_4), 127.50 (C^o in C_6H_5), 127.82 (C^m in C_6H_5), 128.77 (C^m in C_6H_4), 129.31 (C^p in C_6H_5), 137.81 (C^i in C_6H_5), 139.30 (C^i in C_6H_4), 141.99 (C^p in C_6H_4). Found, %: C 56.53; H 4.36; Cl 16.66; N 6.32; S 7.22. $C_{20}H_{20}Cl_2N_2O_2S$. Calculated, %: C 56.74; H 4.76; Cl 16.75; N 6.62; S 7.57.

Compound **VII**. ^1H NMR spectrum, δ, ppm: 2.28 s (3H, C**H**$_3C_6H_4$), 3.26 s (3H, 1-CH_3), 5.05 d (1H, NCH, ^3J = 9.7 Hz), 5.52 m (1H, 4-H), 6.10 m (1H, 2-H), 6.21 m (1H, 5-H), 7.12 d (2H, *m*-H in C_6H_4), 7.32 m (2H, *m*-H in C_6H_5), 7.37 m (1H, *p*-H in C_6H_5), 7.42 d (2H, *o*-H in C_6H_4), 7.50 m (2H, *o*-H in C_6H_5), 8.25 d (1H, NH, ^3J = 9.7 Hz). ^{13}C NMR spectrum, δ_C, ppm: 20.87 (**C**$H_3C_6H_4$), 35.29 (1-CH_3), 64.73 (NCH), 96.36 (CCl_2), 108.36 (C^4), 117.15 (C^3), 120.45 (C^5), 121.99 (C^2), 126.01 (C^o in C_6H_5), 126.48 (C^o in C_6H_4), 127.23 (C^m in C_6H_5), 128.51 (C^m in C_6H_4), 128.96 (C^p in C_6H_5), 138.57 (C^i in C_6H_5), 140.45 (C^i in C_6H_4), 141.74 (C^p in C_6H_4).

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