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HETEROORGANIC DERIVATIVES OF FURAN.

69.* ANALYSIS OF ELECTRON STRUCTURES OF 2-FURYLTRIETHOXYSILANE AND 1'-(2-FURYL)-SILATRANE BY THE MO LCAO CNDO/2 METHOD

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The electron structures (charges on the atoms, additive populations of the atomic orbitals, and multiplicities of the chemical bonds) of 2-furyltriethoxysilane, 1'-(2-furyl)silatrane, and the starting triethanolamine were analyzed by the MO LCAO CNDO/2 method taking into account the d orbitals. The localized molecular orbitals and the hybrid atomic orbitals that form them were constructed by the Polak projection method.

We have previously investigated the electron structures of furan (I) and trimethyl(2-furyl)silane (II) [4]. In the present research we calculated the electron-density matrixes for 2-furyltriethoxysilane (III), 2-furylsilatrane (IV), and the starting triethanolamine (V).

The description of the electron structures of the indicated compounds was accomplished using characteristics such as the charges on the atoms, the additive populations of the atomic orbitals (AO), and the multiplicities of the chemical bonds — the Wiberg indexes. The structures of the individual bonds in the molecules were investigated by construction of the

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*see [1-3] for Communications 66-68.

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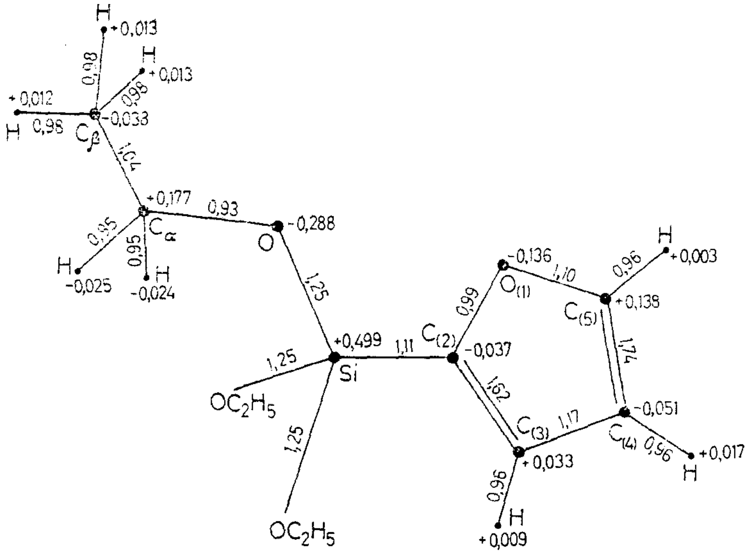

Fig. 1. Molecular diagram of 2-furyltriethoxysilane (III).

TABLE 1. Populations of the AO of the Atoms of the Furyl Fragment in I-IV and the Silicon Atom in II-IV*

Compound	AO	Atom					
		$C_{(2)}$	$C_{(3)}$	$C_{(4)}$	$C_{(5)}$	$O_{(1)}$	Si
I	*s*	1,033	1,006	1,006	1,033	1,602	—
	p	0,955	1,012	1,012	0,955	1,516	—
II	*s*	1,077	1,016	0,999	1,024	1,622	0,864
	p	0,982	0,988	1,017	0,949	1,507	0,589
	d	—	—	—	—	—	0,243
III	*s*	1,072	1,017	0,999	1,024	1,620	0,741
	p	0,988	0,983	1,018	0,946	1,505	0.448
	d	—	—	—	—	—	0.283
IV	*s*	1,071	1,016	1,001	1,024	1,608	0,700
	p	0,982	0,987	1,022	0,949	1,513	0,458
	d	—	—	—	—	—	0,295

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*The populations of the p and d orbitals are the arithmetic means for all possible values of quantum number m_1.

localized molecular orbitals (MO) and the hybrid orbitals that form them. The geometrical parameters of the molecules were taken from [5, 6].

A molecular diagram of 2-furyltriethoxysilane is presented in Fig. 1. In trimethyl(2-furyl)silane (II) the charge on the silicon atom is +0.153 au [4]. Replacement of the methyl groups in II by ethoxy groups leads to an increase in the charge on the silicon atom to +0.499; one observes a decrease in the s and p AO of silicon and a significant increase in the populations of its d orbitals (Table 1). This redistribution of the populations of the AO of silicon was not noted in previously studied 2-furylsilanes and arises only when oxygen atoms are attached to the silicon atom. A shift of the electron cloud from silicon to oxygen along the line of the σ bond occurs by virtue of the high electronegativity of the oxygen atom. This leads to a decrease in the populations of the s and p orbitals of the silicon atom and to an increase in its positive charge. Delocalization of the electrons of the unshared electron pairs of the oxygen atom may be one of the reasons that leads to an increase in the populations of the d orbitals of the silicon atom. The Wiberg index of the siloxane bond in 2-furyltriethoxysilane is 1.25, which indicates a shift of the electron cloud to the internuclear region. An increase in the positive charge on the silicon atom has only a slight effect on the character of the electron-density distribution in the ring. As compared with methyl(2-furyl)silanes [4], the charges on the $C_{(4)}$ and $C_{(5)}$ atoms of the furyl fragment remain virtually unchanged, whereas a small increase in the negative charge on the $C_{(2)}$ atom occurs due to an increase in the populations of its p orbitals. A certain decrease in the elec-

TABLE 2. Populations (n) and Structures of the Hybrid AO that Form the Localized MO of the Bonds of the Furyl Fragment and the Si—C(Furyl) Bond in I-IV

Compound	Hybrid AO (HAO)	$h_1(C_{(2)})$	$h_1(C_{(3)})$	$\mu_1(C_{(2)}-C_{(3)})$ n	$h_2(C_{(2)})$	$h_2(C_{(3)})$
I	n_{HAO}	1,02	0,97	1,99	0,96	0,96
	s contribution	0,47	0,33		0	0
	p contribution	0,55	0,64		0,96	0,96
II	n_{HAO}	0,96	1,00	1,96	0,95	0,86
	s contribution	0,36	0,30		0	0
	p contribution	0,60	0,70		0,95	0,86
III	n_{HAO}	0,97	0,99	1,96	0,98	0,84
	s contribution	0,37	0,29		0	0
	p contribution	0,60	0,70		0,98	0,84
IV	n_{HAO}	0,95	1,01	1,96	0,95	0,88
	s contribution	0,35	0,39		0	0
	p contribution	0,60	0,62		0,95	0,88

Compound	HAO	$h_2(C_{(4)})$	$h_2(C_{(5)})$	$\mu_2(C_{(4)}-C_{(5)})$ n	$h_1(C_{(5)})$	$h_1(O_{(1)})$
I	n_{HAO}	0,96	0,96	1,92	0,78	1,20
	s contribution	0	0		0,22	0,24
	p contribution	0,96	0,96		0,56	0,96
II	n_{HAO}	0,98	0,91	1,89	0,84	1,14
	s contribution	0	0		0,29	0,20
	p contribution	0,98	0,91		0,55	0,94
III	n_{HAO}	0,98	0,91	1,89	0,84	1,14
	s contribution	0	0		0,29	0,21
	p contribution	0,98	0,91		0,55	0,93
IV	n_{HAO}	0,99	0,91	1,90	0,83	1,16
	s contribution	0	0		0,26	0,24
	p contribution	0,99	0,91		0,57	0,92

Compound.	HAO	$h_2(C_{(2)})$	$h_2(O_{(1)})$	$\mu_2(C_{(2)}-O_{(1)})$ n	$h(C_{(2)})$
I	n_{HAO}	0,34	1,59	1,93	
	s contribution	0	0		
	p contribution	0,34	1,59		
II	n_{HAO}	0,26	1,64	1,90	1,25
	s contribution	0	0		0,59
	p contribution	0,26	1,64		0,66
	d contribution	—	—		—
III	n_{HAO}	0,27	1,63	1,90	1,22
	s contribution	0	0		0,57
	p contribution	0,27	1,63		0.65
	d contribution	—	—		—
IV	n_{HAO}	0,27	1,63	1,90	1,24
	s contribution	0	0		0,59
	p contribution	0,27	1,63		0,65
	d contribution	—	—		—

TABLE 2 (Continued)

$\mu_2(C_{(2)}-C_{(3)})$ n	$h(C_{(3)})$	$h(C_{(4)})$	$\mu(C_{(3)}-C_{(4)})$ n	$h_1(C_{(4)})$	$h_1(C_{(5)})$	$\mu_1(C_{(4)}-C_{(5)})$ n
1,92	0,99	0,99	1,98	0,97	1,02	1,99
	0,34	0,34		0,33	0,47	
	0,65	0,65		0,64	0,55	
1,81	1,00	0,96	1,96	1,01	0,98	1,99
	0,39	0,25		0,41	0,41	
	0,61	0,71		0,60	0,57	
1,82	1,01	0,95	1,96	1,00	0,99	1,99
	0,40	0,25		0,40	0,41	
	0,61	0,70		0,60	0,58	
1,83	0,97	0,99	1,96	0,99	1,00	1,99
	0,31	0,31		0,35	0,43	
	0,66	0,68		0,64	0,57	

$\mu_1(C_{(5)}-O_{(1)})$ n	$h_2(C_{(5)})$	$h_2(O_{(1)})$	$\mu_2(C_{(5)}-O_{(1)})$ n	$h_1(C_{(2)})$	$h_1(O_{(1)})$	$\mu_1(C_{(2)}-O_{(1)})$ n
1,98	0,34	1,59	1,93	0,78	1,20	1,98
	0	0		0,22	0,24	
	0,34	1,59		0,56	0,96	
1,98	0,31	1,63	1,94	0,73	1,22	1,95
	0	0		0,17	0,26	
	0,31	1,63		0,56	0,96	
1,98	0,30	1,64	1,94	0,74	1,21	1,95
	0	0		0,18	0,25	
	0,30	1,64		0,56	0,96	
1,99	0,32	1,62	1,94	0,74	1,21	1,95
	0	0		0,17	0,26	
	0,32	1,62		0,57	0,95	

$h(Si)$	$\mu(C_{(2)}-Si)$ n
0,73	1,98
0,23	
0,37	
0,13	
0,77	1,99
0,34	
0,31	
0,12	
0,74	1,98
0,29	
0,31	
0,14	

tron density on the $C_{(3)}$ and $O_{(1)}$ atoms is also noted. The multiplicities of the ring bonds in trimethyl(2-furyl)silane and 2-furyltriethoxysilane are the same.

The results of construction of the localized MO for the bonds of the furyl fragment in I-IV are presented in Table 2. Two MO are localized for the $C_{(2)}-C_{(3)}$ bond in the furan molecule: $\mu_1[C_{(2)}-C_{(3)}]$ and $\mu_2[C_{(2)}-C_{(3)}]$ with filling numbers $n(\mu_1) = 1.99$ au and $n(\mu_2) = 1.92$ au. The hybrid AO of the $C_{(2)}$ and $C_{(3)}$ atoms that form the μ_1 orbital are directed virtually toward one another. The $h_1[C_{(2)}]$ hybrid AO is an sp orbital, the $h_1[C_{(3)}]$ orbital is an sp^2 orbital, and the $\mu_1[C_{(2)}-C_{(3)}]$ orbital describes an ordinary σ bond. The hybrid AO that form the localized $\mu_2[C_{(2)}-C_{(3)}]$ MO are pure 2p orbitals that are oriented perpendicularly to the plane of the ring, i.e., the μ_2 orbital describes a π bond. The filling number of this two-center MO is considerably smaller than two, which attests to delocalization of the π electrons along the ring bonds. To find the optimal localized MO one must evidently increase the number of its centers. In trimethyl(2-furyl)silane and 2-furyltriethoxysilane one observes a decrease in the $n(\mu_1)$ filling number to 1.96 au and the $n(\mu_2)$ filling number to 1.82 au. The μ_2 orbital in these cases can be regarded as the principal component of a certain multicenter localized MO.

One two-center localized $\mu[C_{(3)}-C_{(4)}]$ MO with filling number $n(\mu) = 1.98$ au is isolated for the $C_{(3)}-C_{(4)}$ bond of the furan molecule. The attachment of substituents to the ring $C_{(2)}$ atom (II-IV) does not lead to substantial changes in the population of this MO, introducing only asymmetry into the structure of the boundary $h[C_{(3)}]$ and $h[C_{(4)}]$ AO. As compared with I, in the II-IV molecule for the $h[C_{(3)}]$ orbital one notes an increase in the s contribution and a decrease in the p contribution, whereas for the $h[C_{(4)}]$ orbital, on the other hand, the fraction of the 2p orbitals increases, and the contribution of the 2s orbitals decreases. The multiplicity of the $C_{(3)}-C_{(4)}$ bond is 1.17, which exceeds the multiplicity of single C–C bonds and confirms the fact of delocalization of the π electrons of the ring double bonds.

The localized $\mu_1[C_{(4)}-C_{(5)}]$ and $\mu_2[C_{(4)}-C_{(5)}]$ MO are similar in structure to the already examined $\mu_1[C_{(2)}-C_{(3)}]$ and $\mu_2[C_{(2)}-C_{(3)}]$ orbitals and less sensitive to replacement of the substituents attached to the $C_{(2)}$ atom because of remoteness from it.

A study of the structures of the $C_{(5)}-O_{(1)}$ and $C_{(2)}-O_{(1)}$ bonds of furan was made by diagonalization of the corresponding blocks of the electron-density matrix. It is known that the oxygen atom has two unshared electron pairs. Calculation shows that only one unshared electron pair is completely localized on the $O_{(1)}$ atom with a population of 1.99 au; the second such pair has a population of 1.74 au. If it is assumed that the second pair participates in some way in the formation of a chemical bond, then, for example, for the furan $C_{(5)}-O_{(1)}$ bond two MO are localized, viz., $\mu_1[C_{(5)}-O_{(1)}]$ and $\mu_2[C_{(5)}-O_{(1)}]$, where $\mu_1[C_{(5)}-O_{(1)}] = 0.627h_1[C_{(5)}] + 0.799h_1[O_{(1)}]$ and $\mu_2[C_{(5)}-O_{(1)}] = 0.422h_2[C_{(5)}] + 0.906h_2[O_{(1)}]$, i.e., in addition to the $\mu_1[C_{(5)}-O_{(1)}]$ orbital, which describes a σ bond, there is an additional localized MO, which describes the interaction of the electrons of the unshared electron pair of oxygen and the π electrons of the double bond. An increase in the Wiberg index of the $C_{(5)}-O_{(1)}$ bond in the furan molecule to 1.09 is a consequence of this additional interaction. In II and III the multiplicity of the $C_{(2)}-O_{(1)}$ bond adjacent to the $C_{(2)}$ atom decreases to 0.99-1.00 by virtue of a shift of the electron cloud from the internuclear region to the $C_{(2)}$ atom, whereas the multiplicity of the $C_{(5)}-O_{(1)}$ bond remains virtually unchanged.

Let us examine the structures of the bonds of the ethoxysilyl fragment and the $C_{(2)}-Si$ bond in III (Tables 2 and 3). Calculation shows that one unshared electron pair with filling number 1.91 au is isolated on the oxygen atom of the ethoxy group which indicates its delocalization; the second unshared electron pair is populated to an even lesser extent (1.77 au). Two localized MO, viz., $\mu_1 = 0.493h_1(Si) + 0.870h_1(O)$, with filling number 1.99 au, and $\mu_2 = 0.327h_2(Si) + 0.945h_2(O)$, with filling number 1.97 au, are realized for the Si–O bond. The first localized MO describes a σ bond, while the second is due to the participation of the π electrons of the unshared electron pair of oxygen in the formation of the bond. The contribution of the d orbitals of the silicon atom to the hybrid $h_2(Si)$ AO is 0.14 au (67%). The isolated additional localized $\mu_2(Si-O)$ MO and the structures of the hybrid $h_2(Si)$ and $h_2(O)$ can be interpreted within the framework of the concept of $d_\pi-p_\pi$ interaction.

The multiplicity of the $C_\alpha-O$ bond is 0.93; this is evidently due to shifting of the electron cloud toward the oxygen atom. The C_α atom has a positive charge of +0.177. The multiplicity of the $C_\alpha-C_\beta$ bond is close to unity, and the hybrid AO that form the MO of the $C_\alpha-C_\beta$ bond are, respectively, sp^2 and sp^3 orbitals.

TABLE 3. Populations (n) and Structures of the Hybrid AO that Form the Localized MO of the Si—O—C_α—C_β Bond in 2-Furyltriethoxysilane (III), the Si—O—C_α—C_β—N Bond in 1-(2-Furyl)-silatrane (IV), and the —O—C_α—C_β—N Bond in Triethanolamine (V)

HAO	n_{HAO}	s contribution	p contribution	d contribution
	III			
h_1(Si)	0,48	0,15	0,21	0,12
h_1(O)	1,51	0,61	0,90	—
μ_1(Si—O), n		1,99		
h_2(Si)	0,21	0	0,07	0,14
h_2(O)	1,76	0	1,76	—
μ_2(Si—O), n		1,97		
$h(C_\alpha)$	0,83	0,21	0,62	—
h(O)	1,09	0,13	0,96	—
$\mu(C_\alpha$—O), n		1,92		
$h(C_\alpha)$	1,00	0,32	0,68	—
$h(C_\beta)$	1,00	0,25	0,75	—
$\mu(C_\alpha—C_\beta)$, n		2,0		
	IV			
h(Si)	0,24	0,05	0,11	0,08
h(N)	1,72	0,35	1,37	—
μ(Si—N), n		1,96		
h_1(O)	1.52	0.58	0,94	—
h_1(Si)	0,47	0,14	0,21	0,12
μ_1(O—Si), n		1,99		
h_2(O)	1,76	0	1,76	—
h_2(Si)	0,21	0	0,07	0,14
μ_2(O—Si), n		1,97		
$h(C_\alpha)$	0,96	0,33	0,63	—
$h(C_\beta)$	1,03	0,24	0,79	—
$\mu(C_\alpha—C_\beta)$, n		1,99		
$h(C_\alpha)$	0,86	0,17	0,69	—
h(O)	1,07	0,12	0,95	—
$\mu(C_\alpha$—O), n		1,93		
$h(C_\beta)$	0,84	0,19	0,65	—
h(N)	1,12	0,24	0,88	—
$\mu(C_\beta$—N), n		1,96		
	V			
$h(C_\alpha)$	1,00	0,36	0,64	—
$h(C_\beta)$	0,99	0.23	0,76	—
$\mu(C_\alpha—C_\beta)$, n		1,99		
$h(C_\alpha)$	0,85	0,17	0,68	—
h(O)	1,14	0,22	0,92	—
$\mu(C_\alpha$—O), n		1,99		
$h(C_\beta)$	0,92	0,21	0,71	—
h(N)	1,05	0,27	0,78	—
$\mu(C_\beta$—N), n		1,97		

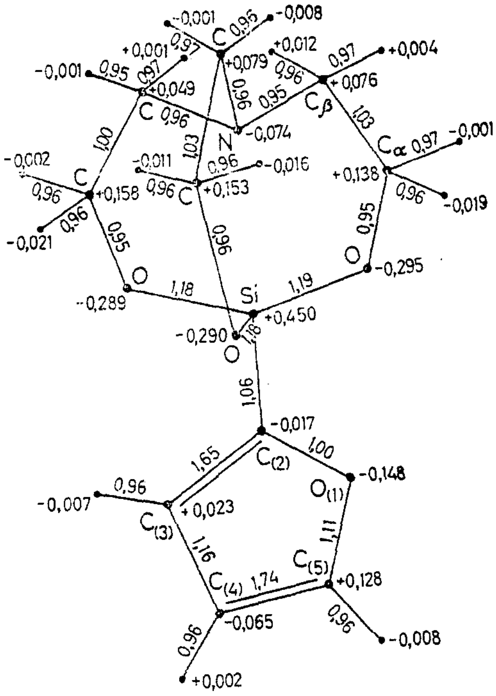

Fig. 2. Molecular diagram of 1'-(2-furyl)-silatrane (IV).

Replacement of the methyl groups by ethoxy groups causes virtually no change in the multiplicity and structure of the $C_{(2)}$—Si bond (Table 2). The certain amount of decrease in the p contribution to the hybrid h(Si) AO is associated with the fact that the 3p electrons of silicon migrate toward the oxygen atoms of the ethoxy groups.

A molecular diagram of 1'-(2-furyl)silatrane is depicted in Fig. 2. As compared with 2-furyltriethoxysilane, a slight decrease in the positive charge of silicon is noted as a consequence of an increase in the populations of its 3p and 3d orbitals. Weakening of the inductive effect on the furyl fragment leads to a decrease in the populations of the 2p orbitals of the ring $C_{(2)}$ atom and to an increase in the electron densities on the $C_{(3)}$ and $O_{(1)}$ atoms. A certain increase in the multiplicities of the $C_{(2)}=C_{(3)}$ and $C_{(2)}-O_{(1)}$ bonds was noted. The localized MO and the hybrid AO that form them, constructed for the bonds of the furyl fragment in III and IV, have similar structures.

Two-center MO $\mu[C_{(2)}-Si] = 0.79h[C_{(2)}] + 0.61h(Si)$, with filling number 1.98 au, is realized for the $C_{(2)}-Si$ bond in 2-furylsilatrane. The structures of this localized MO and the hybrid AO that form it in 2-furylsilatrane and 2-furyltriethoxysilane are virtually identical.

The oxygen atoms of the atrane skeleton have negative charges ranging from −0.289 to −0.295, which differ only slightly from the charge of the oxygen atom in the ethoxy group of III. One unshared pair of electrons with filling number $n = 1.93$ au is isolated on the $O_{(1)}$ atom of the atrane part of 2-furylsilatrane: the second unshared pair is delocalized to an even greater extent, and its filling number is 1.78 au. Localized MO $\mu_1 = 0.49h(Si) + 0.87h(O)$, which describes a σ bond, and orbital $\mu_2 = 0.33h(Si) + 0.94h(O)$, which describes interaction of the π electrons of the unshared pair of the oxygen atom with the 3d orbitals of the silicon atom, are realized for the Si—O bond. The multiplicity of the Si—O bond in 2-furylsilatrane is 1.19, which is somewhat smaller than the multiplicity of the siloxane bond in 2-furyltriethoxysilane.

The C_α atom of the atrane skeleton is characterized by a positive charge of +0.138. The multiplicity of the $C_\alpha-O$ bond is somewhat smaller than unity. A two-center MO with filling number 1.93 au is realized for this bond. The contribution of the 2p orbitals to the hybrid $h(C_\alpha)$ AO is 80%, while the contribution of the 2p orbitals to the h(O) AO is 89%.

The positive charge of the C_β atom is +0.076, and, as compared with the C_α atom, a 0.06 au increase in the population of its 2p orbitals is noted. Two-center MO $\mu(C_\alpha-C_\beta) = 0.7h(C_\alpha)$ $0.72h(C_\beta)$, with filling number 1.99, is isolated for the $C_\alpha-C_\beta$ bond. The hybrid $h(C_\alpha)$ and $h(C_\beta)$ atomic orbitals are, respectively, sp^2 and sp^3 orbitals. The multiplicity of the $C_\alpha-C_\beta$ bond is close to unity.

The nitrogen atom has one unshared electron pair; however, a hybrid AO that describes the unshared electron pair with a population of only 1.73 au, which attests to its substantial delocalization, is isolated in the construction of the localized MO of the $C_\beta-N$ bond in 2-furylsilatrane on the nitrogen atom. Two-center MO $\mu(C_\beta-N) = 0.66h(C_\beta) + 0.75h(N)$, with filling number 1.96, is realized for the $C_\beta-N$ bond. The multiplicity of the $C_\beta-N$ bond is 0.95. The hybrid AO that participate in the formation of the localized MO $\mu(C_\beta-N)$ give the following contribution: $h(C_\beta) = 0.19(s) + 0.65(p)$, and $h(N) = 0.24(s) + 0.88(p)$.

According to the results of x-ray diffraction analysis, the distance between the nitrogen and silicon atoms in 2-furylsilatrane is 2.11 Å [5, 6]. The Wiberg index for the Si ← N coordinate bond in 2-furylsilatrane has a value of 0.4, which somewhat exceeds the multiplicity of this bond in, for example, 1-phenylsilatrane (0.38) [7]. Construction of the two-center MO was accomplished for the Si ← N bond: $\mu(Si-N) = 0.35h(Si) + 0.94h(N)$. The filling number of this MO is 1.96 au. The hybrid AO of silicon and nitrogen have the following form: $h(Si) = 0.05(s) + 0.11(p) + 0.08(d)$ and $h(N) = 0.35(s) + 1.37(p)$, i.e., the hybrid AO that form the MO of the Si ← N bond are not pure 3d and 2p orbitals but have more complex character.

Let us examine the electron structure of triethanolamine as a model compound (Fig. 3). The oxygen atom has a negative charge of −0.248. A decrease in the electron density on the oxygen atom of triethanolamine as compared with 1'-(2-furyl)silatrane occurred because of a decrease in the population of its 2p orbitals, and the population of the 2s orbital increased somewhat (Table 4). Two unshared electron pairs with populations $n_1 = 2$ and $n_2 = 1.98$ au were localized on the oxygen atom, while in 2-furylsilatrane both unshared pairs were delocalized.

The charge of the C_α atom is the same in triethanolamine and 1'-(2-furyl)silatrane. The multiplicity of the $C_\alpha-O$ bond increased from 0.95 for the silatrane to 0.99 in triethanolamine. A two-center MO of the following form was constructed for this bond; $\mu(C_\alpha-O) = 0.654h(C_\alpha) + 0.76h(O)$.

A slight increase in the positive charge due to a decrease in the population of the 2p orbitals is noted for the C_β atoms bonded to the nitrogen atom. A two-center MO with filling number 1.99 au is realized for the $C_\alpha-C_\beta$ bond, the contributions of the hybrid $h(C_\alpha)$ and $h(C_\beta)$ AO to the localized MO are identical, and the multiplicity of this σ bond is close to unity.

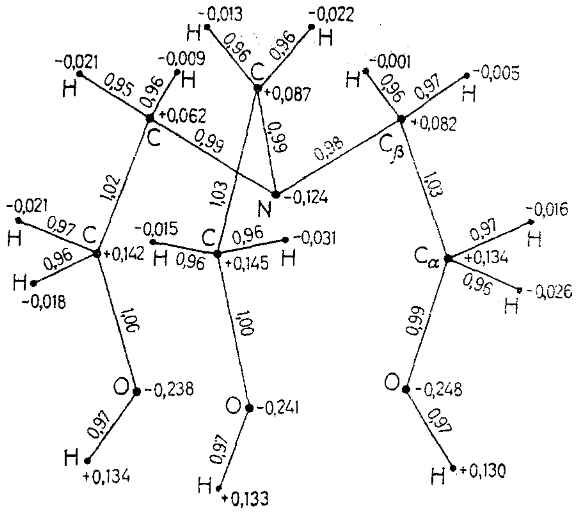

Fig. 3. Molecular diagram of triethanolamine (V).

TABLE 4. Populations of the AO of the Atoms of the Ethoxysilyl Fragment Si—O—C_α—C_β in 2-Furyltriethoxysilane, the Alkoxysilyl Fragment Si—O—C_α—C_β—N in 1'-(2-Furyl)silatrane, and the —O—C_α—C_β—N Fragment in Triethanolamine

Compound	AO	Atom			
		O	C_α	C_β	N
III	*s*	1,571	0,989	1,022	—
	p	1,572	0,945	1,005	—
IV	*s*	1,594	0,974	0,977	1,199
	p	1,567	0,962	0,982	1,292
V	*s*	1,660	0,984	0,976	1,271
	p	1,529	0,961	0,981	1,285

The nitrogen atom in triethanolamine is characterized by a negative charge of −0.124. As compared with the nitrogen atom of 1'-(2-furyl)silatrane, for it one observes a 0.072 au increase in the population of the 2s orbital and a 0.021 au decrease in the population of the 2p orbital.

The unshared electron pair on the nitrogen atom in triethanolamine is localized with a population of 1.954 au, while in the case of 1'-(2-furyl)silatrane the population was only 1.73 au. Construction of the two-center MO was accomplished for the C_β—N bond: $\mu(C_\beta{-}N) = 0.68h(C_\beta) + 0.73h(N)$. The hybrid AO of the C_β and N atoms, which participate in the formation of a σ bond, are sp^3 orbitals. The multiplicity of the C_β—N bond is close to unity.

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