ucts that absorb in a valley adjacent to λ_{max} are formed. As can be seen from Table 1, the rate of this reaction increases with the increase in [SDS], which is characteristic of micellar catalysis. It can be noted that in freshly prepared solutions R_{pv} does not depend on [SDS] and is close to the corresponding value in water. However, one cannot be sure that in these solutions the equilibrium distribution of the solubilized molecules is established.

The dependence of both λ_{max} and R_{pv} on [CTAB] is observed in CTAB solutions, namely, when the surfactant concentration decreases (that is, as the filling of the micelles with the solubilizate increases), the absorption band shifts to short waves and λ_{max} is considerably higher than in water. When [CTAB] decreases, R_{pv} decreases from a value close to R_{pv} in ethanol (when [CTAB] = $1.1 \cdot 10^{-2}$ mol L^{-1}) to a value somewhat smaller than that in a 2-propanol—water mixture (see Table 1). Thus, the average polarity of the microenvironment in CTAB solutions increases as the concentration of dihydroquinolines in the micelles increases. It is worth noting, that in the solubilization of **1** and **2** in CTAB micelles the R_{pv} values are close to those in aqueous solutions of alcohols, and λ_{max} are close to the corresponding values in water-free organic solvents.

These results can be interpreted by assuming that the solubilized molecules have two preferential locations: inside the micelle and on the micelle-water interface. The observed R_{pv} and λ_{max} are averaged over these two positions. In this case, the filling of the CTAB micelles starts from the core. Unlike dihydroquinolines, benzene and its homologs at low concentrations are located on the interface of the CTAB micelles and penetrate inside the micelles as their concentrations increase. In SDS, the filling of micelles begins from the core.[2,3]

Thus, the results obtained demonstrate not only the effect of the nature of surfactant on the location of dihydroquinoline molecules in micelles, but confirm the known fact that different solubilized species may have different locations and orientations in micelles.

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Rearrangement of *O*-perfluoroisobutenylacetone oxime. The structure of 2,2-bis(trifluoromethyl)-5-methyl-Δ^4-pyrrolin-3-one

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Dehydrofluorination of *O*-(β-hydroperfluoroisobutyl)acetone oxime affords 2,2-bis(trifluoromethyl)-5-methyl-Δ^4-pyrrolin-3-one; the molecular structure of the latter was unambiguously established by X-ray diffraction method.

Key words: *O*-perfluoroisobutenylacetone oxime, rearrangement; 2,2-bis(trifluoromethyl)-5-methyl-Δ^4-pyrrolin-3-one, the X-ray crystal structure.

Previously,[1] after dehydrofluorination of *O*-(β-hydroperfluoroisobutyl)acetone oxime (**1**), a crystalline compound (m.p. 139—140 °C) was isolated, to which the structure of 3,3-bis(trifluoromethyl)-5-methyl-Δ^4-pyrrolin-2-one (**2**) was assigned. It is the author's opinion that unstable *O*-perfluoroisobutenylacetone oxime (**3**)

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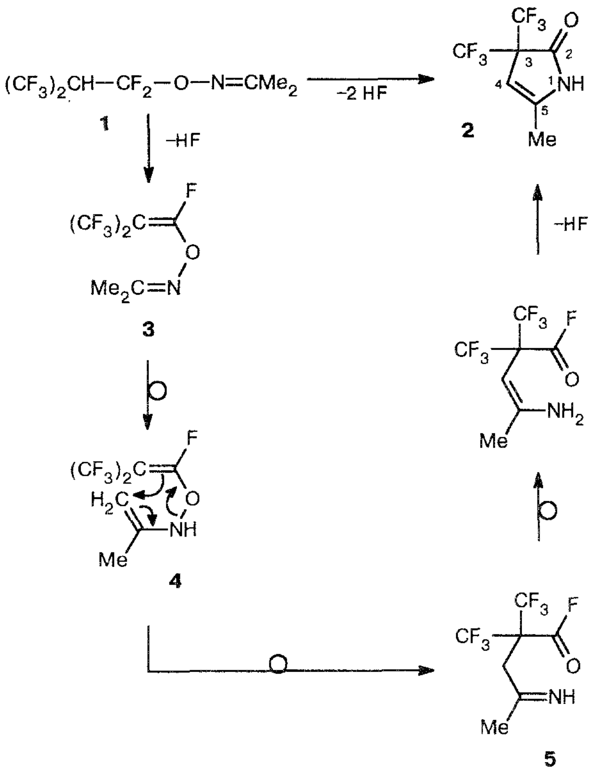
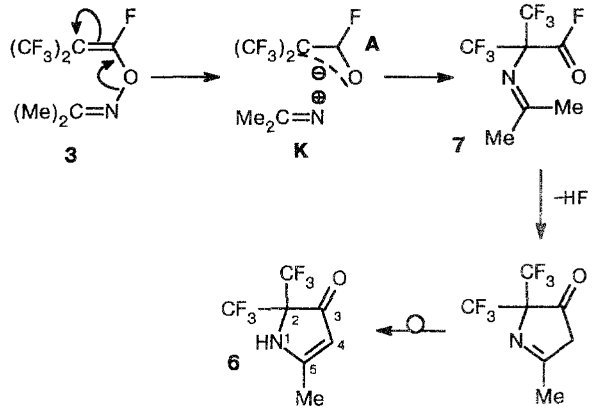
Scheme 1



Scheme 2



undergoes prototropic rearrangement to the enamine **4** followed by Claisen isomerization, and then the iminofluoric anhydride **5** undergoes cyclization to pyrrolinone **2** (Scheme 1).

The conversion of the unsaturated ether of oxime **3** to iminofluoric anhydride **5** under mild conditions is attributable to the known fact that Claisen rearrangement occurs readily in the presence of electron-acceptor substituents on the vinyl group.[2]

However, by X-ray diffraction analysis of the obtained crystalline compound, we showed that this compound is actually 2,2-bis(trifluoromethyl)-5-methyl-Δ^4-pyrrolin-3-one (**6**) rather than compound **2**.

Apparently, the instability of *O*-perfluoroisobutenylacetone oxime **3** results from the lability of the N—O bond, because anion **A** is a readily leaving group[3,4] (Scheme 2).

After heterocyclic cleavage of the N—O bond, the cationoid particle **K** migrates (without any structural changes) from the O atom to the C atom of the mesomeric anion **A**. Stabilization of this tight ionic pair occurs *via* formation of a C—N bond.

Evidently, fluoroanhydride, which was determined by ^{19}F NMR spectroscopy (see Ref. 1), has the structure of **7** rather than **5**. The subsequent cyclization of the intermediate **7** yields the final product, pyrrolinone **6**.

Based on the X-ray diffraction data, pyrrolinone **6** has a planar structure; the root-mean square deviation of the atoms from the plane of the cycle is 0.008 Å. The bond lengths and bond angles in the molecule are close to the expected values.[5] In particular, the distribution of the bond lengths in the transoid O=C(1)—C(3)=C(4) fragment is indicative of the possibility for conjugation in the given atomic chain. Among the characteristic features of the molecular geometry of **6**, the lengthening of the C(1)—C(2) bond to 1.57(1) Å, which can be caused by the steric requirements, *i.e.*, by the presence of two bulky CF_3 groups at the C(2) atom should be mentioned. In crystals, molecules of **6** are linked in chains *via* intermolecular hydrogen bonds of the N—H...O type (N—H, 0.73 Å; H...O, 2.04 Å; the N—H...O angle, 158°; the N...O distance, 2.725(9) Å). Apparently, it is the formation of this H-bond that causes the enlargement of the exocyclic O—C(1)—C(3) bond angle at the carbonyl C atom to 134.2(7)°.

Table 1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic temperature factors ($U \times 10^3$/Å^2) for non-hydrogen atoms in structure **6**

Atom	*x*	*y*	*z*	*U*
F(1)	5008(2)	1957(2)	1048	55(2)
F(2)	4903(2)	799(2)	1262(5)	57(2)
F(3)	5952(2)	1754(2)	512(5)	66(2)
F(4)	5783(2)	2146(2)	−1418(5)	64(2)
F(5)	4620(2)	1506(2)	−2123(5)	55(2)
F(6)	4846(2)	2371(2)	−937(5)	52(2)
O	5458(2)	493(2)	−1089(5)	48(2)
N	3857(3)	763(3)	−265(5)	34(3)
C(1)	4798(4)	407(3)	−865(7)	32(3)
C(2)	4723(3)	1130(3)	−445(7)	31(3)
C(3)	4012(4)	−238(3)	−906(7)	40(3)
C(4)	3491(3)	−5(3)	−539(7)	27(3)
C(5)	2606(4)	−506(4)	−427(7)	44(4)
C(6)	5147(4)	1409(4)	601(8)	46(4)
C(7)	4987(4)	1784(4)	−1223(8)	43(4)

Table 2. Bond lengths (d) in structure **6**

Bond	d/Å	Bond	d/Å
F(1)—C(6)	1.34(1)	N—C(4)	1.327(7)
F(2)—C(6)	1.33(1)	C(1)—C(2)	1.57(1)
F(3)—C(6)	1.351(1)	C(1)—C(3)	1.397(8)
F(4)—C(7)	1.352(8)	C(2)—C(6)	1.53(1)
F(5)—C(7)	1.33(1)	C(2)—C(7)	1.49(1)
F(6)—C(7)	1.34(1)	C(3)—C(4)	1.37(1)
O—C(1)	1.23(1)	C(4)—C(5)	1.485(7)
N—C(2)	1.466(8)		

Table 3. Bond angles (ω) in structure **6**

Angle	ω/deg	Angle	ω/deg
C(2)—N—C(4)	109.8(6)	C(3)—C(4)—C(5)	127.6(5)
O—C(1)—C(2)	120.6(5)	F(1)—C(6)—F(2)	107.2(7)
O—C(1)—C(3)	134.2(7)	F(1)—C(6)—F(3)	106.3(5)
C(2)—C(1)—C(3)	105.2(7)	F(2)—C(6)—F(3)	107.4(7)
N—C(2)—C(1)	102.3(4)	F(1)—C(6)—C(2)	112.0(7)
N—C(2)—C(6)	107.9(6)	F(2)—C(6)—C(2)	111.5(5)
C(1)—C(2)—C(6)	110.3(7)	F(3)—C(6)—C(2)	112.1(7)
N—C(2)—C(7)	109.9(6)	F(4)—C(7)—F(5)	106.4(7)
C(1)—C(2)—C(7)	112.0(7)	F(4)—C(7)—F(6)	105.8(4)
C(6)—C(2)—C(7)	113.8(5)	F(5)—C(7)—F(6)	106.9(7)
C(1)—C(3)—C(4)	110.0(6)	F(4)—C(7)—C(2)	112.4(7)
N—C(4)—C(3)	112.7(4)	F(5)—C(7)—C(2)	111.3(5)
N—C(4)—C(5)	119.7(6)	F(6)—C(7)—C(2)	113.6(8)

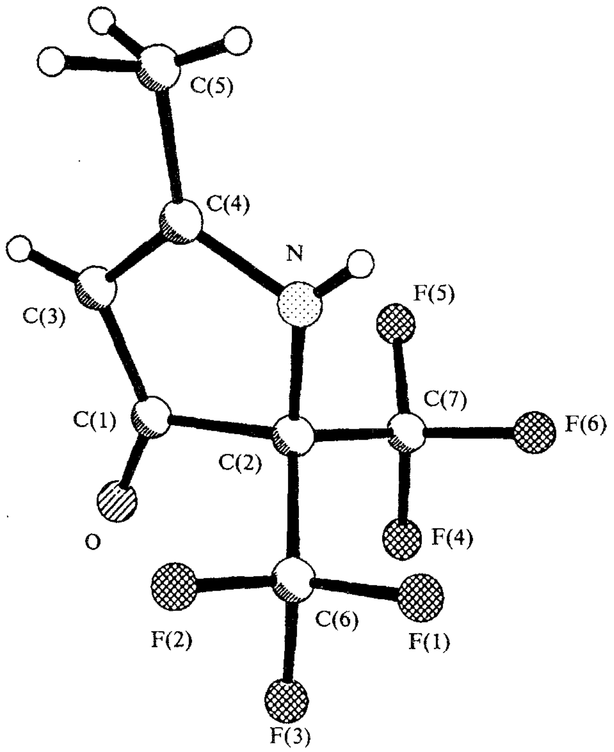


Fig. 1. The molecular structure of pyrrolinone **6**.

Experimental

X-ray diffraction study of a single crystal of **6** was performed on an automated four-circle Siemens P3/PC diffractometer at 148 K (λMo-Kα radiation, graphite monochromator, θ/2θ-scan technique, 2θ ≤ 46°). The crystals of **6** are rhombohedral, at 148 K, $a = b = 19.241(3)$ Å, $c = 12.911(2)$ Å, $V = 4139(2)$ Å^3, $Z = 18$, and the space group is $R3c$.

In subsequent calculations and refinement 773 independent observed reflections with $I \geq 2\sigma(I)$ were used out of a total of 1450 measured ones. The structure was solved by the direct method and refined anisotropically by the full-matrix least-squares procedure. Positions of the H atoms were located from a difference electron density synthesis, and these atoms were refined isotropically. The final refinement converged to $R = 0.046$, $R_w = 0.036$, GOF = 1.39. The fractional atomic coordinates and equivalent isotropic temperature factors for non-hydrogen atoms are given in Table 1. The bond lengths and bond angles are listed in Tables 2 and 3, respectively. The overall view of molecule **6** and the atomic numbering scheme are shown in Fig. 1. All calculations were performed on an IBM-PC/AT personal computer using the SHELXTL PLUS program package.

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