The average values of the bond lengths and bond angles formed by the carbon atoms in sp^2 and sp^3 hybridization correspond to the standard values [10].

The following intermolecular contacts are the most strained in the crystal structure: $Br_6...Br_7$ 3.775 Å ($Br_7:x, y = 1, z$), $Br_6...Br_1$ 3.700 Å ($Br_1: 1 = x, 2 = y, 1 = z$), $Br_1...$ Br_7 3.756 Å ($Br_7: 1 = x, 3 = y, 1 = z$), $Br_5...Br_5$ 3.516 Å ($Br_5: 1 = x, 1 = y, -z$).

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REACTION OF 1,1-DIFLUOROALKYL ISOCYANATES WITH N-TRIMETHYL-

SILYL-N'-PHENYLCARBODIIMIDE

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 α -Chloroalkyl isocyanates R¹R²C(Cl)N=C=O react with N-monosilylated carbodiimides Me₃SiN=C=NR³ to give α -isocyanatoalkycarboiidimes, α -isocyanatoalkylcyanamides, or acylcyanamides, depending on the nature of substituents R¹, R², and R³ [1]. It was observed that the reaction of 1,1-difluoroalkyl isocyanates Ia, b with N-trimethylsilyl-N'-phenylcarbodiimide (in a ratio of 1:2) with subsequent hydrolysis gives amidines IIa, b in high yields (see [2]).

 $\begin{array}{cccc} \operatorname{RCF}_{2} N = C = 0 & \frac{1}{2} & \frac{2\operatorname{Me}_{3}\operatorname{SiN} = C = \operatorname{NPh}}{2} & \begin{array}{c} O \\ \operatorname{RCF}_{2} N = C = 0 & \frac{1}{2} & \frac{2\operatorname{Me}_{3}\operatorname{SiN} = C = \operatorname{NPh}}{2} & \operatorname{RC}_{-} \operatorname{NH}_{-} & C & -\operatorname{NHPh}_{-} \\ & & & & & \\ & & & & & \\ & & & & & \\ I & a, b & & \\ & & & & & \\ I & a, b & & \\ & & & & & \\ I & a, b & & \\ & & & & \\ I, & & \\ I,$

The structure of IIb was proved rigorously by x-ray diffraction analysis. The overall form of the IIb molecule with numbering of the atoms and the bond lengths is shown in Fig. 1. A peculiarity of the structure is the presence of intramolecular hydrogen bonds of the N-H...N type [N(2)...N(5) 2.67 Å, HN(2)...N(5) 1.89 Å, N(2)-HN(2) 0.93 Å; the angle at the HN(2) atom is 140°]. The N(2) and N(3) atoms have a planar-trigonal configuration of the bonds as a consequence of p-m interaction of their unshared electron pairs with the adjacent m systems. As a result, the N(2)-C(1)-N(3)-C(4)-N(5)-HN(2) ring is planar with a deviation

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Atom	x	y	z .	B _{eq}
0	1314(1)	439(1)	591(1)	5,3(1)
N(2)	2504(1)	2196(1)	-153(1)	4,7(1)
N(3)	312(1)	1794(1)		4,5(1)
N(5)	1000(1)	3758(1)	-1709(1)	4,6(1)
C(1)	1420(2)	1415(1)	-6(1)	4,3(1)
C(4)	105(2)	2882(1)		4,0(1)
C(6)	3793(2)	2011(1)	446(1)	4,4(1)
C(7)	4097(2)	997(2)	1261(1)	5,5(1)
C(8)	5385(2)	917(2)	1802(1)	6,3(1)
C(9)	6370(2)	1833(2)	1533(1)	6,4(1)
C(10)	6074(2)	2836(2)	718(1)	6,1(1)
C(11)	4802(2)	2929(2)	166(1)	5,2(1)
C(12)	-1260(2)	2945(1)	-2159(1)	4,1(1)
C(13)	-2670(2)	4270(2)	-2299(1)	5.1(1)
C(14)	-3967(2)	4306(2)	-2822(1)	6,3(1)
C(15)	-3826(2)	3026(2)		6.6(1)
C(16)	-2433(2)	1717(2)		6,2(1)
C(17)		1666(1)	-2549(1)	5,2(1)
C(18)	948(2)	4802(1)	-2545(1)	4,2(1)
C(19)	1436(2)	4383(1)		5,1(1)
C(20)	1502(2)	5420(2)		6,4(1)
C(21)	1082(2)	6882(2)	-4152(1)	6,8(1)
C(22)	598(2)	7304(2)	-3181(2)	6,7(1)
C(23)	551(2)	6274(2)	2379(1)	5,3(1)
C(101)*	3250(2)	127(3)	5163(2)	8,8(1)
C(201)	5502(3)	1137(2)	4483(2)	9,1(1)
C(301)	3738(3)	1257(2)	4645(2)	8,7(1)
	1	3	1	

TABLE 1. Coordinates of the Nonhydrogen Atoms (×10⁴) and Their Equivalent Isotropic Temperature Factors B_{ed} (Å²) in IIb

*The coordinates of the atoms of the solvate benzene molecule located at the center of symmetry.

of the atoms from the average plane that does not exceed ± 0.02 Å. In the crystal the molecules are connected into infinite chains by intermolecular hydrogen bonds of the N-H...O type: N(3)...O 2.90 Å, HN(3)...O 2.02 Å, and N(3)-HN(3) 0.90 Å; the angle at the HN(3) atom is ~ 164°C. The remaining geometrical parameters of the molecule have the expected values.

The assignment of the signals in the PMR spectrum of the IIb molecule was made on the basis of x-ray diffraction analysis. (IIb): the signal of the hydrogen atom that participates in the formation of an H-N(2) intermolecular hydrogen bond is shifted to weak field and has a chemical shift of 1.21 ppm, the signal at 8.6 pm can be assigned to an H-N(3) hydrogen bond, while the signals of aromatic hydrogen bonds are located at 6.65-7.28 ppm.

The cell parameters and the intensities of 2368 independent reflections were measured with a CaD-4) automatic four-circle diffractometer (λ MoK_Q, graphite monochromator, ratio of the scanning rates $\theta:\omega = 2:1, 2\theta \leq 56^{\circ}$). The structure was decoded by the method of least squares within the anisotropic approximation with respect to 1912 reflections with $F^2 \geq 3\sigma$. All of the hydrogen atoms were localized in differential syntheses; in the latter stages they were included in refinement within the isotropic approximation. The final divergence factors R = 0.033 and R_w = 0.046. All of the calculations were made with a PDP 11/23 PLUS computer by means of SDP programs [3].

The coordinates of the atoms and their temperature factors are presented in Table 1.

Isocyanate Ia was obtained by the method in [4], while isocyanate Ib was obtained by the method in [5].

<u>N-Phenyl-N'-anilinoformylamidimes IIa, b.</u> A solution of 0.02 mole of carbodiimide in 15 ml of benzene was added with stirring $(20^{\circ}C)$ to a solution of 0.01 mole of isocyanate Ia, b in 5 ml of benzene, after which the mixture was refluxed for 1 h and cooled to 20°C. The



Fig. 1. Overall form of the N-phenyl-N'-anilinoformylbenzamidine IIb molecule.

resulting precipitate was removed by filtration, washed on the filter with water, and crystallized from benzene-ether (3:1).

<u>N-Phenyl-N'-anilinoformyltrichloroacetamidine (IIa).</u> This compound was obtained in 85% yield and had mp 135-136°C. IR spectrum (CH_2Cl_2 , cm⁻¹): 3420, 3060, 1715, 1680, 1560, 1520. Found, %: Cl 29.52; N 11.79. $C_{15}H_{12}Cl_3N_3O$. Calculated, %: Cl 29.82; N 11.78.

<u>N-Phenyl-N'-anilinoformylbenzamidine (IIb).</u> This compound was obtained in 80% yield and had mp 169-170°C [2]. IR spectrum $(CH_2C]_2$, cm⁻¹): 3420, 3040, 1710, 1640, 1600, 1560, 1500. PMR spectrum (CDCl₃, δ , ppm): 12.10 s (1H, NH), 8.58 s (1H, NH), 6.65-7.28 m (15H, 3Ph). Found, %: C 75.76; H 5.31; N 12.63. $C_{20}H_{17}N_3O$. Calculated, %: C 76.17; H 5.43; N 13.32.

The IR spectra were recorded with a UR-20 spectrometer. The PMR spectrum was obtained with a Tesla BS-467 spectrometer (60 MHz) with hexamethyldisiloxane (HMDS) as the internal standard.

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