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CRYSTAL AND MOLECULAR STRUCTURE OF 5-ETHYL-5,10-DIHYDRIDO-10,10-DIPHENYLPHENAZASILINE

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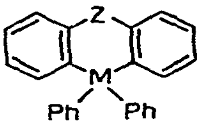
Summary

The structure of 5-ethyl-5,10-dihydro-10,10-diphenylphenazasiline has been determined from three-dimensional X-ray data collected by counter methods. The compound crystallizes in the monoclinic space group $P2_1/b$ with a 10.782(5), b 22.642(9), c 8.830(4) Å and γ 74° 41'(2). The observed and calculated densities ($Z = 4$) are 1.22 and 1.21 g cm^{-3}, respectively. Anisotropic (Si, N, C)-isotropic block-diagonal least squares refinement gave a conventional R factor of 3.9% for 1871 reflections with $I > 2\sigma(I)$. The central six-membered ring of the tricyclic system adopts a folded boat conformation; the dihedral angle between the benzo-group planes is 157.3°. The C—Si—C angle in the heterocycle is 101.1(1)°; the mean Si—C bond length is 1.850(2) Å (in the cycle) and 1.862(2) Å (with Ph group). The nitrogen atom is displaced 0.05 Å from the plane of the adjacent carbon atoms; the sum of the angles about N is 359.7°.

Introduction

The test reported in ref. 1 of a number of compounds of the phenazasiline type as high-temperature antioxidants for silicon rubbers and oils has shown a composition on the basis of phenyl-α-naphthilamine and 5-ethyl-5,10-dihydro-10,10-diphenylphenazasiline (I) to be most effective for oils. It is also known that the compounds of the phenaza-, phenoxa- and phenthia-silines, -germiles and -stanniles types (I—IX) possess a biological activity depending on the nature of both heteroatoms and the molecular geometry. In particular the pharmacological properties of organosilicon compounds with phenazasiline base



	I	II	III	IV	V	VI	VII	VIII	IX
Z	NC_2H_5	O	S	NC_2H_5	O	S	NC_2H_5	O	S
M	Si	Si	Si	Ge	Ge	Ge	Sn	Sn	Sn

have been investigated [2]. As a consequence of the above mentioned properties, there is a considerable degree of interest in the structure of these compounds, as a result of which some important features of their structures have been determined. So, the study of NMR, UV and IR spectra of the compounds I—IX enabled them to be considered as representatives of new types of aromatic systems in which *p*-electrons of nitrogen, oxygen and sulfur and vacant orbitals of the Si, Ge and Sn atoms are included in a general conjugated system [3]. In order to check this assumption for the solid state we have made an X-ray analysis of crystals of I, the tricyclic system for which there is, from spectral data [3], the largest degree of conjugation.

We also expected this study to permit evaluation of how much the electron-accepting bromine substituents in 2,8-dibromo-5-ethyl-5,10-dihydro-10,10-diphenylphenazasiline [4], X, present in the aromatic rings of the tricyclic sys-

TABLE 1

FINAL POSITIONAL ($\times 10^4$) AND ANISOTROPIC THERMAL ($\times 10^4$) PARAMETERS FOR THE NON-HYDROGEN ATOMS

Atom	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Si	1867(1)	4079(0)	4140(1)	70	16	124	20	−2	−9
N	1556(2)	3009(1)	1866(2)	92	25	169	18	26	−39
C(1)	373(2)	3653(1)	3184(3)	72	16	142	12	6	6
C(2)	−802(2)	3793(1)	3405(3)	100	23	199	33	−12	4
C(3)	−1923(2)	3488(1)	2672(3)	89	30	242	23	−18	31
C(4)	−1866(2)	3014(1)	1713(3)	82	31	221	−6	−64	24
C(5)	−740(2)	2854(1)	1478(3)	111	22	165	−11	−2	−2
C(6)	412(2)	3175(1)	2185(3)	82	17	140	1	−5	0
C(7)	2844(2)	3521(1)	4024(3)	70	18	142	21	19	−3
C(8)	2586(2)	3075(1)	2884(3)	83	18	163	22	59	12
C(9)	3397(3)	2687(1)	2740(4)	123	20	254	40	75	−12
C(10)	4451(3)	2749(1)	3680(4)	139	30	322	73	108	38
C(11)	4708(2)	3183(1)	4805(4)	100	37	256	60	18	39
C(12)	3898(2)	3559(1)	4970(3)	97	27	190	37	−12	5
C(13)	1549(2)	4272(1)	6124(3)	116	26	141	59	−15	−2
C(14)	601(3)	3874(1)	6999(3)	149	45	155	95	58	33
C(15)	414(4)	4014(2)	8495(4)	220	76	177	168	141	66
C(16)	1128(5)	4544(2)	9139(4)	373	81	153	269	−52	−22
C(17)	2043(5)	4935(2)	8315(4)	384	51	210	177	−239	−96
C(18)	2254(3)	4810(1)	6820(3)	199	31	174	64	−81	−39
C(19)	2690(2)	4796(1)	3115(3)	84	18	150	16	−30	−16
C(20)	3881(2)	4876(1)	2428(3)	92	22	220	10	32	0
C(21)	4466(3)	5417(1)	1661(4)	110	27	267	2	36	7
C(22)	3870(3)	5875(1)	1570(4)	149	21	269	−1	−6	20
C(23)	2687(3)	5812(1)	2227(4)	131	20	318	29	−36	1
C(24)	2109(2)	5275(1)	3000(3)	107	19	232	20	24	15
C(25)	1733(3)	2811(1)	299(3)	123	28	184	7	52	−50
C(26)	2890(3)	3239(1)	−464(3)	126	38	192	20	73	−15

Estimated standard deviations are in parentheses. Anisotropic thermal parameters are in the form $\exp[-b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)]$.

tem decrease its planarity. The problem under consideration is of principal importance as it is known that optimum properties are exhibited by the compounds of which the molecules are the most planar in the ground state.

Experimental

Using the procedure previously described [5] we have obtained compound I. It crystallises in the form of colourless transparent crystals. Crystal data are: $C_{26}H_{23}NSi$, mol. wt. 377.66; m.p. 121—122°C, monoclinic, $P2_1/b$, a 10.782(5), b 22.642(9), c 8.830(4) Å, γ 74°41′(2), V 2079,0 Å^3, D_m 1.22 g cm^{-3}, $Z = 4$, $D_x = 1.21$ g cm^{-3}, for Cu-K_α, $\mu = 10.4$ cm^{-1}. Unit cell dimensions are defined more precisely by means of a diffractometer DRON-1 with a monocrystal attachment. Intensities of 1871 independent nonzero ($I > 2\sigma(I)$) reflections for the $hk0$—$hk9$ layers are measured within the angle range of $4.1° \leqslant \theta \leqslant 56.3°$ for a crystal of size 0.8 × 0.25 × 0.1 mm on a DAR-UM semiautomatic diffractometer by the technique of recording every layer with Cu-K_α radiation (graphite monochromator). No absorption correction was made. The structure was solved by direct methods with RENTGEN-75 programm [6]. We used 277 reflections with E values greater than 1.36 to determine signs. The positions of all the 28 nonhydrogen atoms are revealed from E and F maps and those of hydrogen atoms from a difference-Fourier map. The structure was refined by an anisotropic (atoms Si, N, C)-isotropic (H atoms) block-diagonal least squares

TABLE 2

FINAL HYDROGEN-ATOM POSITIONAL PARAMETERS (× 10^3) AND THERMAL PARAMETERS

Atom	x	y	z	B
H(1)	—81(2)	415(1)	409(3)	3.1
H(2)	—300(2)	359(1)	278(2)	1.6
H(3)	—263(3)	279(1)	117(3)	4.1
H(4)	—74(2)	252(1)	79(3)	2.1
H(5)	319(3)	237(1)	191(3)	4.9
H(6)	497(3)	245(1)	351(3)	3.9
H(7)	554(2)	320(1)	545(3)	3.4
H(8)	405(3)	386(1)	583(3)	5.8
H(9)	14(4)	342(2)	636(4)	8.4
H(10)	—24(3)	375(2)	901(4)	5.8
H(11)	87(5)	465(2)	1021(6)	11.9
H(12)	258(4)	534(2)	865(5)	9.7
H(13)	293(2)	508(1)	623(3)	3.4
H(14)	443(3)	455(1)	242(3)	4.0
H(15)	532(3)	544(1)	114(4)	5.9
H(16)	423(3)	625(2)	99(4)	8.6
H(17)	228(3)	614(1)	220(4)	6.1
H(18)	117(2)	522(1)	348(3)	2.1
H(19)	91(3)	280(1)	—33(3)	4.7
H(20)	187(3)	239(1)	40(3)	4.4
H(21)	371(3)	323(1)	8(3)	4.9
H(22)	297(3)	316(1)	—158(4)	5.6
H(23)	270(3)	365(1)	—51(4)	7.2

Isotropic temperature parameters (Å^2) are given in the form exp $[-B(\sin\theta/\lambda)^2]$. Estimated standard deviations are in parentheses.

procedure using Cruickshank's weight scheme. The final discrepancy value was $R = 0.039$. At this stage the maximum shifts in the defined parameters of the nonhydrogen atoms were less than a half their estimated standard deviations. The coordinates and thermal parameters of these atoms are given in Tables 1 and 2.

Results and discussion

The molecule conformation is shown in Fig. 1 as drawn by the ELLIDS programme. The bond lengths and valence angles are listed in Table 3. Table 4 gives the main data of the molecule geometry.

The tricyclic framework of the molecule is not planar. The molecule is bent along the $Si\cdots N$ line, the dihedral angle between $C(1)\cdots C(6)$ and $C(7)\cdots C(12)$ planar benzo groups is equal to 157.3°. The heterocycle exhibits the boat conformation. The Si and N atoms are displaced out of the averaged plane V drawn through the remaining atoms of the central cycle by 0.40 and 0.26 Å. The Si C(1)C(7) and N C(6)C(8) planes are bent relative to the bottom of the boat

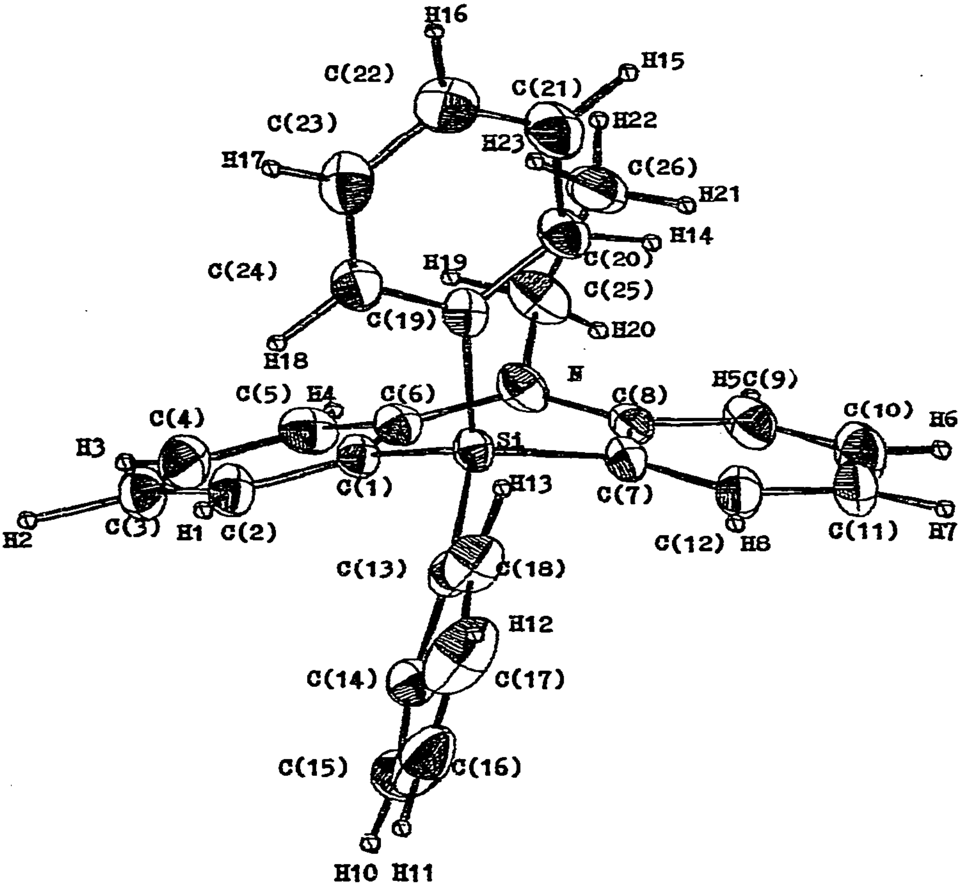


Fig. 1. The molecular structure of 5-ethyl-5,10-dihydro-10,10-diphenylphenazasiline and the numbering scheme of the atoms. The thermal ellipsoids are at 30% probability.

TABLE 3

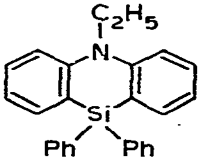
BOND LENGTHS (Å) AND ANGLES (°) WITH THEIR ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

Si—C(1)	1.849(2)	C(13)—C(14)	1.402(3)
Si—C(7)	1.850(2)	C(13)—C(18)	1.397(3)
Si—C(13)	1.859(2)	C(14)—C(15)	1.385(4)
Si—C(19)	1.865(2)	C(14)—H(9)	1.16(4)
N—C(6)	1.409(3)	C(15)—C(16)	1.367(5)
N—C(8)	1.406(3)	C(15)—H(10)	0.92(3)
N—C(25)	1.482(3)	C(16)—C(17)	1.351(5)
C(1)—C(2)	1.399(3)	C(16)—H(11)	1.03(5)
C(1)—C(6)	1.405(3)	C(17)—C(18)	1.382(4)
C(2)—C(3)	1.384(3)	C(17)—H(12)	1.00(4)
C(2)—H(1)	1.02(2)	C(18)—H(13)	0.97(2)
C(3)—C(4)	1.380(4)	C(19)—C(20)	1.387(3)
C(3)—H(2)	1.25(2)	C(19)—C(24)	1.392(3)
C(4)—C(5)	1.371(4)	C(20)—C(21)	1.396(3)
C(4)—H(3)	0.97(3)	C(20)—H(14)	1.05(3)
C(5)—C(6)	1.408(3)	C(21)—C(22)	1.359(4)
C(5)—H(4)	0.98(2)	C(21)—H(15)	1.02(3)
C(7)—C(8)	1.400(3)	C(22)—C(23)	1.375(4)
C(7)—C(12)	1.395(3)	C(22)—H(16)	0.98(3)
C(8)—C(9)	1.400(3)	C(23)—C(24)	1.391(3)
C(9)—C(10)	1.385(4)	C(23)—H(17)	0.97(4)
C(9)—H(5)	1.01(3)	C(24)—H(18)	1.07(2)
C(10)—C(11)	1.373(4)	C(25)—C(26)	1.519(3)
C(10)—H(6)	1.01(3)	C(25)—H(19)	1.04(3)
C(11)—C(12)	1.378(4)	C(25)—H(20)	1.00(3)
C(11)—H(7)	1.05(3)	C(26)—H(21)	1.01(3)
C(12)—H(8)	1.00(3)	C(26)—H(22)	1.01(3)
		C(26)—H(23)	1.01(3)
C(1)—Si—C(7)	101.1(1)	C(8)—C(7)—C(12)	118.6(2)
C(1)—Si—C(13)	111.3(1)	N—C(8)—C(7)	122.5(2)
C(1)—Si—C(19)	112.4(1)	N—C(8)—C(9)	118.8(2)
C(7)—Si—C(13)	112.8(1)	C(7)—C(8)—C(9)	118.7(2)
C(7)—Si—C(19)	110.0(1)	C(8)—C(9)—C(10)	120.9(3)
C(13)—Si—C(19)	109.1(1)	C(8)—C(9)—H(5)	117(2)
C(6)—N—C(8)	124.5(2)	C(10)—C(9)—H(5)	122(2)
C(6)—N—C(25)	117.3(2)	C(9)—C(10)—C(11)	120.8(3)
C(8)—N—C(25)	117.9(2)	C(9)—C(10)—H(6)	116(2)
Si—C(1)—C(2)	122.3(2)	C(11)—C(10)—H(6)	124(2)
Si—C(1)—C(6)	119.3(2)	C(10)—C(11)—C(12)	118.5(3)
C(2)—C(1)—C(6)	118.4(2)	C(10)—C(11)—H(7)	116(2)
C(1)—C(2)—C(3)	123.1(3)	C(12)—C(11)—H(7)	126(2)
C(1)—C(2)—H(1)	118(2)	C(7)—C(12)—C(11)	122.5(2)
C(3)—C(2)—H(1)	119(2)	C(7)—C(12)—H(8)	119(2)
C(2)—C(3)—C(4)	117.5(3)	C(11)—C(12)—H(8)	118(2)
C(2)—C(3)—H(2)	127(1)	Si—C(13)—C(14)	121.1(2)
C(4)—C(3)—H(2)	116(2)	Si—C(13)—C(18)	121.9(2)
C(3)—C(4)—C(5)	121.5(2)	C(14)—C(13)—C(18)	117.1(2)
C(3)—C(4)—H(3)	120(2)	C(13)—C(14)—C(15)	120.2(3)
C(5)—C(4)—H(3)	118(2)	C(13)—C(14)—H(9)	112(2)
C(4)—C(5)—C(6)	121.2(2)	C(15)—C(14)—H(9)	127(2)
C(4)—C(5)—H(4)	119(2)	C(14)—C(15)—C(16)	121.0(3)
C(6)—C(5)—H(4)	120(2)	C(14)—C(15)—H(10)	117(2)
N—C(6)—C(1)	122.5(2)	C(16)—C(15)—H(10)	122(2)
N—C(6)—C(5)	119.2(2)	C(15)—C(16)—C(17)	119.7(3)
C(1)—C(6)—C(5)	118.3(2)	C(15)—C(16)—H(11)	117(2)
Si—C(7)—C(8)	119.5(2)	C(17)—C(16)—H(11)	123(2)
Si—C(7)—C(12)	121.8(2)	C(16)—C(17)—C(18)	120.8(3)
		C(16)—C(17)—H(12)	126(3)
		C(18)—C(17)—H(12)	113(3)

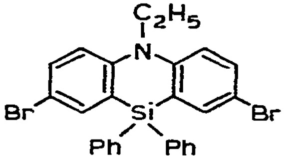
TABLE 3 (continued)

		C(22)—C(23)—H(17)	121(2)
C(13)—C(18)—C(17)	121.2(3)	C(24)—C(23)—H(17)	120(2)
C(13)—C(18)—H(13)	118(2)	C(19)—C(24)—C(23)	121.9(3)
C(17)—C(18)—H(13)	121(2)	C(19)—C(24)—H(18)	119(2)
Si—C(19)—C(20)	122.5(2)	C(23)—C(24)—H(18)	119(2)
Si—C(19)—C(24)	120.3(2)	N—C(25) C(26)	111.8(2)
C(20)—C(19)—C(24)	117.2(2)	N—C(25)—H(19)	109(2)
C(19)—C(20)—C(21)	121.0(3)	N—C(25)—H(20)	106(2)
		C(26)—C(25)—H(19)	109(1)
C(19)—C(20)—H(14)	126(2)	C(26)—C(25)—H(20)	110(2)
C(21)—C(20)—H(14)	113(2)	H(19)—C(25)—H(20)	112(2)
C(20)—C(21)—C(22)	120.2(3)	C(25)—C(26)—H(21)	110(2)
C(20)—C(21)—H(15)	117(2)	C(25)—C(26)—H(22)	115(2)
C(22)—C(21)—H(15)	123(2)	C(25)—C(23)—H(23)	106(2)
C(21)—C(22)—C(23)	120.6(3)	H(21)—C(26)—H(22)	109(2)
C(21)—C(22)—H(16)	122(2)	H(21)—C(26)—H(23)	116(2)
C(23)—C(22)—H(16)	117(2)	H(22)—C(26)—H(23)	100(3)
C(22)—C(23)—C(24)	119.1(3)		

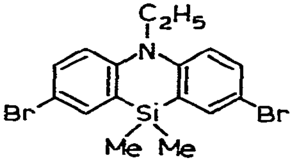
(plane V) at angles of 159.8° and 156.2°. The bond configuration of the Si atom is tetrahedral, with a certain degree of distortion. This is shown by the endocyclic Si—C(1) (1.849(2) Å) and Si—C(7) (1.850(2) Å) bonds and the angle C(1)—Si—C(7) (101.1(1)°) being noticeably less than the appropriate exocyclic Si—C(13) (1.859(2) Å) and Si—C(19) (1.865(2) Å) bonds and the angles C—Si—C (111.1(1)° (average)). The bond configuration of the N atom is close to planar: the deviation of N from the plane of C(6), C(8) and C(25) atoms bound with it is 0.05 Å and the sum of N valence angles equals 359.7°. The endocyclic N—C bonds are identical (1.409(3) and 1.406(3) Å), differing from the exocyclic N—C(25) (1.482(3) Å) bond by a value corresponding to the difference of covalence radii of C atom in sp^2 and sp^3 hybridization states. In the C(1)···C(6) and C(7)···C(12) benzene cycles the peripheral C(2)—C(3)—C(4)—C(6) and C(9)—C(10)—C(11)—C(12) bonds are on the average shortened by approximately 0.02 Å in comparison with C(2)—C(1)—C(6)—C(5) and C(9)—C(8)—C(7)—C(12) which are adjacent to the heterocycle.



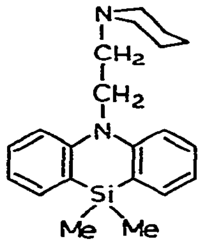
(I)



(X)



(XI)



(XII)

The study carried out enables us to make a comparison of the structure parameters of the tricyclic ring system of four related derivatives of phenazasiline, the most important of them being given in Table 5. The comparison of the molecular bend angles, the deviations of Si and N atoms from the plane drawn through the remaining atoms of the heterocycle, the sum of the valence angles of N atoms and the height of N-pyramids point out the conformation of molecule I to be closest to planar. From previously reported data [9] the intro-

(Continued on p. 276)

TABLE 4

LEAST-SQUARES PLANES OF THE MOLECULE, DISPLACEMENTS(d) OF ATOMS FROM THE PLANES AND DIHEDRAL ANGLES

Plane	Equation $Ax + By + Cz = D$				d (Å)							
	A	B	C	D								
I	0.462	13.854	−6.729	2.936	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	Si*	N*
					0.00	0.01	−0.01	0.00	0.01	−0.01	−0.02	−0.05
					H(1)*	H(2)*	H(3)*	H(4)*				
					−0.02	−0.03	−0.02	0.01				
II	4.468	11.775	−5.600	3.158	C(7)	C(8)	C(9)	C(10)	C(11)	C(12)	Si*	N*
					−0.01	0.00	0.01	−0.01	0.00	0.01	−0.16	−0.04
					H(5)*	H(6)*	H(7)*	H(8)*				
					0.01	0.02	−0.04	0.07				
III	−8.950	15.308	−2.600	3.568	C(13)	C(14)	C(15)	C(16)	C(17)	C(18)		
					0.01	−0.01	0.00	0.00	0.00	−0.01		
					H(9)*	H(10)*	H(11)*	H(12)*	H(13)*	Si*		
					0.11	−0.05	−0.12	−0.06	0.03	0.07		
IV	3.849	6.498	7.473	6.479	C(19)	C(20)	C(21)	C(22)	C(23)	C(24)		
					0.00	0.00	0.00	0.00	0.00	0.00		
					H(14)*	H(15)*	H(16)*	H(17)*	H(18)*	Si*		
					0.01	0.05	0.05	−0.04	0.04	0.02		
V	2.685	13.419	−6.065	3.059	C(1)	C(6)	C(7)	C(8)	Si*	N*	C(25)*	
					0.01	−0.01	0.01	−0.01	−0.40	−0.26	−1.00	
VI	3.000	6.863	−7.749	0.151	Si	C(1)	C(7)					
VII	1.883	18.997	−3.149	5.421	N	C(6)	C(8)					
VIII	1.728	19.633	−2.577	5.742	C(6)	C(8)	C(25)	N*				
								0.05				

Dihedral angles (deg):
I,II = 157°20′; I,V = 167°12′; I,VIII = 147°; II,V = 169°54′; II,VIII = 150°06′; III,IV = 111°, III,VIII = 66°27′; IV,VIII = 79°27′; V,VI = 159°48′; V, VII = 156°12′.

Atoms not included in the plane calculation are indicated by asterisks.

TABLE 5

STRUCTURAL PARAMETERS OF THE TRICYCLIC SYSTEM OF PHENAZASILINE DERIVATIVES

Compound	Bend angle [a] (°)	C—Si—C (°)	Si—C (Å)	C—N—C (°)	N—C (Å)	Sum of angles about N (°)	Height of N-pyramid, (Å)	Deviations (Å) of Si and N atoms from the plane of the central cycle.	Ref.
I	157.3	101.1(1)	1.849(2)	124.5(2)	1.406(3)	359.7	0.05	0.40(Si)	this work
			1.850(2)		1.409(3)			0.26(N)	
X	138.8	99.8(1)	1.850(3)	121.3(2)	1.394(4)	357.6	0.13	0.64(Si)	4
			1.864(2)		1.419(3)			0.40(N)	
XI	140.9	98.7(6)	1.84(1)	120(1)	1.42(2)	358.2	0.12 [b]	0.62(Si)	7
			1.87(1)		1.43(2)			0.38(N)	
XII	143								8

[a] Dihedral angle between the benzo-group planes. [b] Calculated from data given in ref. 7.

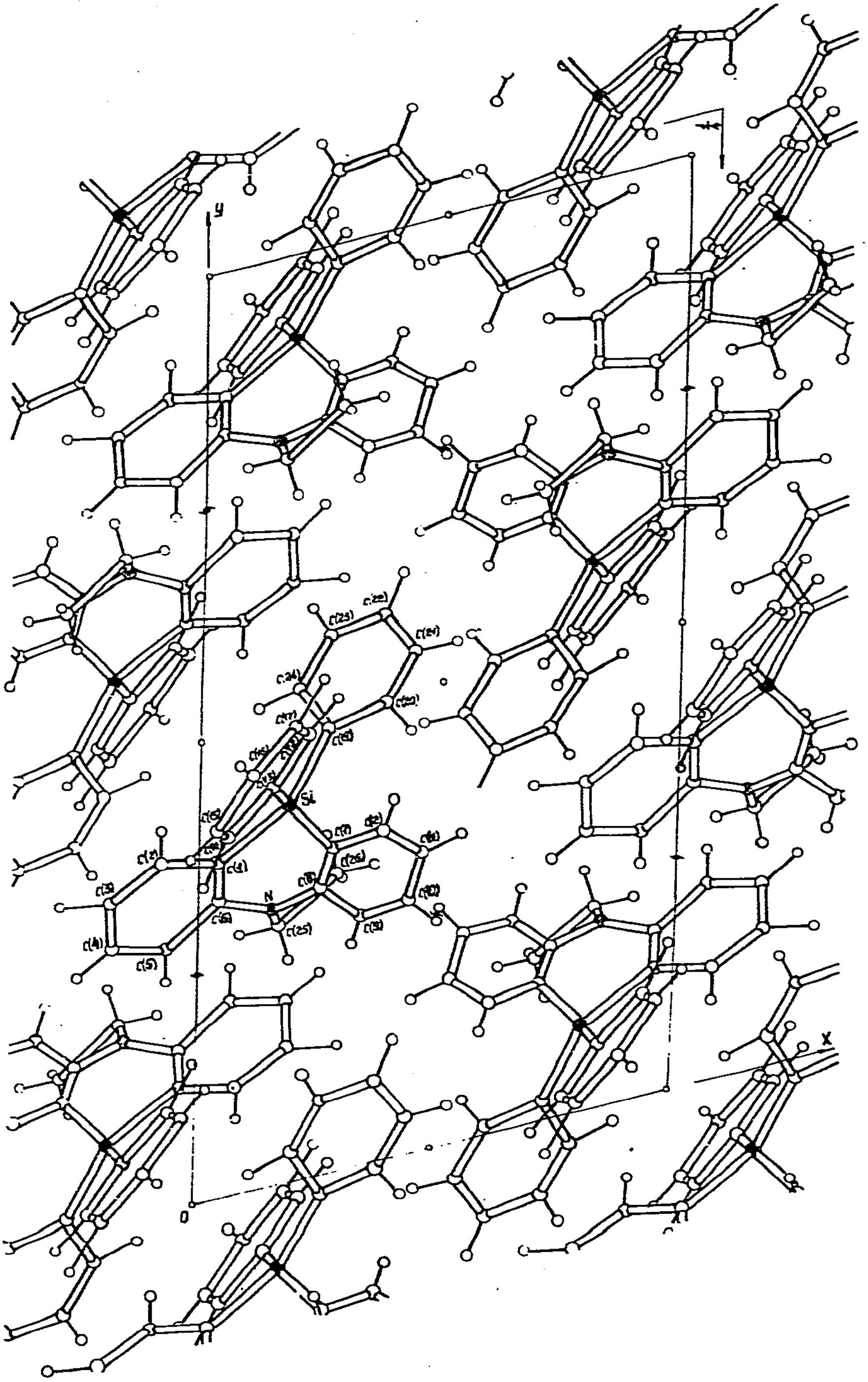


Fig. 2. Projection of the structure along the *c* axis.

duction of typically electron-accepting substituents into the aromatic rings results in the displacement of the charge transfer bands into a high-frequency region of the spectrum. So, the ν (charge transfer) value of compound X amounts to 14800 cm^{-1} and in the compounds of type I it is about 11300 cm^{-1}. Thus substitution of H atoms in the 2-, 8-positions of the benzene cycles of phenazasiline by Br atoms results in an increase of ν (charge transfer) by 3500 cm^{-1}. According to the results of our X-ray structure determination the displacement of the charge transfer band into the high-frequency region is consistent with the decrease of molecule planarity of 18.5°.

The ethyl group occupies an axial position unsymmetrical to the rest of the molecule, being inclined to the benzene C(7)···C(12) cycle compared with X and XI where it is turned to the C(1)···C(6) cycle (in XI it is the corresponding C(6)···C(9)C(14) C(13) ring). This result is indicative of a considerable mobility of the C_2H_5 substituent, which enables different conformers of the ethyl derivatives of phenazasiline to exist. The equatorial C(13)···C(18) and axial C(19)···C(24) phenyl substituents of Si atoms are displaced in such a way that their planes III and IV form a dihedral angle of 111.0° as distinct from 87.3° in X. Their symmetry noticeably differs from the ideal D_{6h} one. This, to a great degree, refers to the endocyclic angles of C(13) and C(19) which are nearly 3° less than the usual value of 120°. A similar decrease of the endocyclic angles in the phenyl substituents is also discovered in structure X (117.4(3)° and 118.5(3)°). These findings, in accordance with the regularities of the structural chemistry of benzene with its substituents [10], testify the phenazasiline tricyclic system to be a strong σ-donor.

The structural features mentioned above, such as molecular conformation close to planar, the trend to shortening endocylic bonds of the Si atom, the practically planar configuration of the N atom and the redistribution of electron density in the benzene rings condensed with the heterocycle, allow us to conclude that molecule I, in its crystalline form, is an aromatic system in which the lone electron pair of the N atom interacts with *d*-orbitals of the Si atom through the π-electron system of the benzene rings.

The molecular arrangement of I in the crystal is shown in Fig. 2. There are no intermolecular contacts less than Van der Waal's distances.

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