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X-RAY STRUCTURAL INVESTIGATION OF TRICYCLIC 2,3-TETRA- AND 2,3-PENTAMETHYLENE-3,4-DIHYDROQUINAZOL-4-ONES AND THEIR DERIVATIVES

B. Tashkhodzhaev, K. K. Turgunov, A. L. D'yakonov,
G. A. Belova, and Kh. Shakhidoyatov

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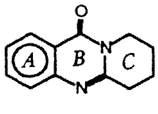
The fine structures of the alkaloid 2,3-tetramethylene-3,4-dihydroquinazol-4-one and its synthetic analogs 2,3-pentamethylene-3,4-dihydro- and -1,2,3,4-tetrahydroquinazol-4-ones and the complex of 2,3-pentamethylene-3,4-dihydroquinazol-4-one with succininide in a ratio of 2:1 have been studied by the x-ray structural method. By an analysis of the lengths of the valence bonds, including those given in the literature, the degree of delocalization of the π-electron system of the N1=C2 double bond and the role of the C=O bond in the overall conjugation have been evaluated.

The alkaloid 2,3-tetramethylene-3,4-dihydroquinazol-4-one (6,7,8,9-tetrahydropyrido[2.1-*b*]quinazol-11-one) and homologs of it isolated previously from various plants and possessing diverse physiological activities are attracting the attention of researchers by their chemical properties, as well [1, 2]. These compounds differ from one another in their chemical behaviors, and the directions of their reaction with electrophilic reagents depend substantially on the size of their ring *C* [2].

In our opinion, this property is determined by the fine structure of the −N=C−N−C=O fragment of ring *B*. In these compounds, thanks to $p-\pi$ conjugation, the π-electronic system of double bonds (N1=C2, C4=O) and of the benzene ring creates a kind of pseudoaromatic system sensitive to very small changes in the overall molecular structure: a change in the length of the polymethylene chain in ring *C*, the presence of various substituents in rings *A* and *C*, and the presence or absence of an N1=C2 double bond. With the aim of studying the fine structure of the alkaloid 2,3-tetramethylene-3,4-dihydroquinazol-4-one (**1**) and its synthetic analogs 2,3-pentamethylene-3,4-dihydroquinazol-4-one (**2**) and 2,3-pentamethylene-1,2,3,4-tetrahydroquinazol-4-one (**3**) and the complex of 2,3-pentamethylene-3,4-dihydroquinazol-4-one with succininide in a ratio of 2:1 (**4**), we have performed an x-ray structural analysis (XSA).



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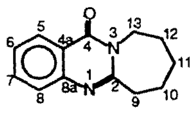

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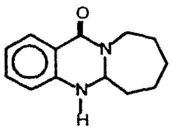

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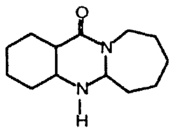

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On the whole, the quinazolone moiety of the compounds under investigation forms a simplified bicyclic system, and the conformational differences are shown mainly in relation to ring *C*. In compound (**1**) the six-membered ring *C* assumes the half-chair conformation, and in the (**2**), (**3**), and (**4**) molecules the seven-membered ring *C* has the chair conformation. In the molecule of (**3**) there is no double bond at N1−C2, and ring *B* therefore has a sofa conformation with a deviation of the C2 atom from the plane of the other atoms by 0.55 Å.

The geometric parameters of the (**1**)-(**3**) molecules that are necessary for analyzing the fine geometry of the $C_{ar}-N1-C2-N3-C4-C_{ar}$ section are given in Table 1.

Institute of the Chemistry of Plant Substances, Academy of Sciences of the Republic of Uzbekistan, Tashkent, fax (3712) 89 14 75. Translated from Khimiya Prirodnykh Soedinenii, No. 3, pp. 410-420, May-June, 1995. Original article submitted June 20, 1994.

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TABLE 1. Bond Lengths *r* (Å) and Valence Angles ω (degrees) in Structures (1), (2), and (3)

Bond	r_1	r_2	r_3	Angle	ω_1	ω_2	ω_3
O–C4	1.224(4)	1.216(8)	1.242(3)	C2–N1–C8a	118.1(3)	118.0(6)	117.7(2)
N1–C8a	1.388(4)	1.409(9)	1.370(3)	N3–C2–N1	123.3(3)	124.1(6)	108.5(2)
N1–C2	1.295(4)	1.296(9)	1.448(4)	C9–C2–N1	117.7(3)	118.3(7)	109.2(2)
C2–C9	1.497(5)	1.498(12)	1.515(3)	C9–C2–N3	119.0(3)	117.6(7)	11.8(2)
N3–C4	1.390(4)	1.416(10)	1.359(3)	C2–N3–C4	122.2(3)	121.6(6)	120.2(2)
N3–C2	1.389(4)	1.389(8)	1.474(3)	C2–N3–C12	122.0(3)		
N3–C12	1.485(5)			C4–N3–C12	115.6(3)		
N3–C13		1.475(10)	1.459(4)	C2–N3–C13		121.9(6)	119.3(2)
C4a–C4	1.452(5)	1.455(9)	1.463(4)	C4–N3–C13		116.4(6)	119.4(2)
C5–C4a	1.400(5)	1.392(11)	1.399(4)	N3–C4–O1	120.2(3)	120.7(7)	121.4(3)
C5–C6	1.367(6)	1.382(11)	1.375(6)	C4a–C4–N3	115.1(3)	114.6(6)	117.3(2)
C6–C7	1.391(6)	1.384(13)	1.378(5)	C4a–C4–O1	124.7(3)	124.8(7)	121.2(2)
C7–C8	1.370(6)	11.373(11)	1.371(4)	C4–C4a–C5	121.2(3)	119.8(6)	121.0(2)
C8–C8a	1.406(5)	1.377(10)	1.401(5)	C4–C4a–C8a	118.7(3)	119.7(6)	119.2(2)
C8a–C4a	1.395(5)	1.396(10)	1.402(3)	C8a–C4a–C5	120.1(3)	120.5(7)	119.4(3)
C9–C10	1.498(7)	1.531(12)	1.517(5)	C4a–C5–C6	120.2(4)	118.7(7)	120.8(3)
C10–C11	1.498(7)	1.533(10)	1.528(6)	C7–C6–C5	119.9(4)	120.5(8)	119.5(3)
C11–C12	1.483(7)	1.536(12)	1.519(4)	C8–C7–C6	120.9	120.5(7)	121.1(4)
C12–C13		1.507(13)	1.509(5)	C8a–C8–C7	120.0(4)	120.0(7)	120.5(3)
				C8–C8a–N1	118.5(3)	118.4(5)	11.7(2)
				C4a–C8a–C8	118.9(3)	119.7(7)	118.7(2)
				C4a–C8a–N1	122.9(6)	121.9(5)	118.5(3)
				C10–C9–C2	114.7(3)	114.3(8)	115.4(2)
				C11–C10–C9	109.4(4)	113.2(7)	113.6(3)
				C12–C11–C10	111.5(4)	112.2(6)	115.0(3)
				N3–C12–C22	114.7(4)		
				C13–C12–C11		114.8(8)	114.7(3)
				C12–C13–N3		113.8(7)	112.9(3)

In the (3) molecule the lengths of the ordinary N1–C2 and N3–C2 bonds (1.448 and 1.474 Å, respectively) are close to those observed in the (5) molecule, the structure of which has been established by XSA for the two diasteroisomeric forms [3]. A slight shortening of the N1–C8a (1.370 Å) and N3–C4 (1.359 Å) bonds and lengthening of the C4═O bond (1.242 Å) shows conjugation of the π-electronic system of the aromatic ring and the double bond of the carbonyl group (C4═O) with the unshared pairs of electrons of the N1 and N3 atoms, respectively. The shortening of the N3–C4 bond, as compared with the N1–C8a bond in (3) and with that observed in known quinazol-4-ones containing an alicylic, rather than an aromatic, ring *A* (for example, in compound (5) the length of the N3–C4 bond is 1.385 Å [3]) is possibly connected with the presence of additional conjugation of the unshared pair of N3 with the π-electrons of the benzene ring through the C4 atom. Moreover, *p*-π conjugation forces the N3 atom to assume the planar N_{sp2} hybridized form, which is reflected in the sum of the valence angles at this heteroatom, 358.9°. The geometric parameters of the other sections of the (3) molecule do not undergo appreciable distortions and are close to the corresponding standard values [4].

The presence of an N1═C2 double bond is characteristic for compounds (1) and (2), unlike (3). In the (1) and (2) molecules the π-electronic system of this bond is conjugated with the unshared pair of electrons of the N3 atom. This conjugation appears as an appreciable lengthening of the N1═C2* double bond (1.295 Å) and a considerable shortening of the N3–C2 ordinary bond (1.389 Å) in comparison with the generally known figures for N═C (1.255 Å) and N–C (1.470 Å) bonds [5]. The interaction of the π-system of the N1═C2 bond with the unshared pair of electrons of the N3 atom leads to a weakening of the competitive tendencies of N1–C8a and N3–C4 for conjugation, which is expressed in a lengthening of the N1–C8a and N3–C4 bonds (1.399 and 1.403 Å, respectively) in comparison with those observed in (3) (1.370 and 1.359 Å, respectively). Weakening of the alternative *p*–π conjugation of N3 and the carbonyl group leads to a shortening of the C4═O bond (1.220 Å), which approximates the length of a pure double bond, 1.210 Å [3].

Thus, interaction of the *p*-π type in the quinazol-4-ones leads to a local redistribution of the π-electronic system. In compounds (1) and (2) the order of the π-bond in N1═C2 decreases to 0.70, and in C2–N3 it increases to 0.27, according to Bayer [5].

A comparative analysis of the valence angles of ring *B* in (1) and (2) shows that a lengthening of the polymethylene chain of ring *C* by one methylene unit does not lead to change in the strain in ring *B*: the valence angles of correponding atoms of ring *B* in (1) and (2) are identical within the limits of experimental error.

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*Here and below, the averaged lengths of the bonds and valence angles for structures (1) and (2) are to be understood.

TABLE 2. Bond Lengths (Å) and Valence Angles (ω) in Structure (4)

Bond	r_a	r_b	r_c	r_d	Angle	ω_a	ω_b	ω_c	ω_d
O–C4	1.21(1)	1.25(1)	1.23(2)	1.19(2)	C2–N1–C8a	114.4(9)	120.2(8)	97.1(9)	117.5(9)
N1–C8a	1.41(1)	1.42(1)	1.54(2)	1.45(2)	N1–C2–N3	127.2(1.2)	121.9(1.0)	136.6(1.2)	124.1(1.1)
N1–C2	1.31(2)	1.26(2)	1.43(2)	1.30(2)	N1–C2–C9	118.6(1.0)	116.3(9)	113.2(9)	116.0(1.1)
C2–C9	1.52(2)	1.49(2)	1.56(2)	1.44(2)	N3–C2–C9	114.2(1.1)	121.4(1.1)	110.1(1.2)	119.7(1.2)
N3–C2	1.40(1)	1.37(1)	1.34(2)	1.40(2)	C2–N3–C4	117.9(9)	125.2(1.1)	124.1(1.2)	116.5(1.0)
N3–C4	1.45(2)	1.35(2)	1.44(2)	1.41(2)	C2–N3–C13	122.5(1.0)	118.6(1.0)	125.1(1.1)	123.4(1.0)
N3–C13	1.51(2)	1.43(2)	1.59(2)	1.42(2)	C4–N3–C13	118.9(9)	116.2(0.9)	110.8(1.0)	120.1(1.0)
C4–C4a	1.45(2)	1.45(2)	1.48(2)	1.37(2)	N3–C4–C4a	115.4(9)	113.9(9)	108.9(1.0)	121.8(1.0)
C4a–C5	1.40(2)	1.41(2)	1.40(2)	1.41(2)	O–C4–N3	117.9(1.2)	123.4(1.2)	124.9(1.3)	112.5(1.4)
C4a–C8a	1.35(1)	1.41(2)	1.40(2)	1.36(2)	O–C4–C4a	126.2(1.2)	122.5(1.1)	126.2(1.2)	125.7(1.4)
C5–C6	1.37(2)	1.38(2)	1.38(2)	1.37(2)	C4–C4a–C5	120.0(1.1)	119.8(1.1)	120.4(1.1)	118.3(1.1)
C6–C7	1.38(2)	1.39(2)	1.39(2)	1.39(2)	C8a–C4a–C4	118.9(1.1)	121.7(1.0)	119.2(1.1)	121.5(1.1)
C7–C8	1.39(2)	1.37(2)	1.38(2)	1.38(2)	C8a–C4a–C5	121.2(1.2)	118.5(1.2)	120.4(1.3)	120.1(1.2)
C8–C8a	1.37(2)	1.45(2)	1.39(2)	1.42(2)	C4a–C5–C6	117.8(1.2)	11.3(1.0)	122.4(1.2)	116.8(1.2)
C9–C10	1.52(2)	1.56(2)	1.56(2)	1.54(2)	C5–C6–C7	124.6(1.1)	115.7(1.3)	118.2(1.4)	121.3(1.4)
C10–C11	1.51(2)	1.52(2)	1.49(2)	1.55(2)	C6–C7–C8	113.4(1.2)	128.1(1.3)	118.3(1.4)	124.2(1.6)
C11–C12	1.55(2)	1.49(2)	1.52(2)	1.52(2)	C7–C8–C8a	125.4(1.1)	113.7(1.0)	125.4(1.3)	112.5(1.3)
C12–C13	1.50(2)	1.55(2)	1.54(2)	1.53(2)	C8–C8a–N1	117.5(9)	119.5(9)	112.5(1.0)	113.5(1.0)
					C4a–C8a–C8	117.7(1.1)	121.5(1.0)	115.1(1.1)	125.0(1.3)
					N1–C8a–C4a	124.8(1.1)	118.9(1.1)	132.4(1.2)	121.0(1.1)
					C2–C9–Ч10	112.8(1.0)	112.0(1.0)	109.0(1.1)	115.9(1.3)
					C9–C10–C11	114.2(1.0)	116.2(1.0)	110.8(1.2)	114.3(1.1)
					C10–C11–C12	111.4(1.1)	118.6(1.2)	117.9(1.2)	111.2(1.3)
					C11–C12–C13	113.0(1.1)	114.1(1.1)	109.0(1.3)	120.8(1.2)
					N3–C13–C12	110.8(1.1)	115.6(1.0)	112.9(1.1)	112.2(1.1)
		The succinimide molecules							
O1–C1	1.23(2)	1.15(2)			N–C4–C1	111.6(9)	118.2(1.1)		
O2–C4	1.27(2)	1.19(2)			C1–N–O2	123.4(1.0)	129.4(1.3)		
N6–C1	1.37(2)	1.39(2)			C1–C2–O2	125.8(1.1)	127.5(1.3)		
N6–C4	1.35(2)	1.36(2)			C1–C2–N	110.5(1.1)	102.9(1.2)		
C1–C2	1.47(2)	1.57(2)			C2–C3–C1	101.7(1.0)	108.2(1.1)		
C2–C3	1.59(2)	1.45(2)			C3–C4–C2	104.7(1.1)	105.3(1.1)		
					C4–N–O1	125.9(1.0)	126.1(1.1)		
					C4–C3–O1	122.8(1.2)	128.5(1.2)		
					C4–C3–N	111.3(1.1)	105.4(1.1)		

TABLE 3. Main Crystallographic Parameters of Compounds (**1-4**).

Compound	Cell parameters						Space group	d_{calc}, g/cm^3	Number of reflections	Divergence factor
	Å			degrees						
	a	*b*	*c*	α	β	γ				
1	5.076	7.583	26.083	90.00	90.00	90.00	$P2_12_12_1$	1.33	827	0.046
2	12.865	8.857	9.719	90.00	90.00	90.0	$Pca2_1$	1.29	813	0.058
3	10.128	8.751	13.596	90.00	110.71	90.00	$P2_1$	1.27	1105	0.047
4	7.961	10.273	16.797	98.01	95.99	101.55	P_1	1.19	2661	0.066

TABLE 4. Coordinates (× 10^4) of the Nonhydrogen Atoms in Structures (**1**), (**2**), and (**3**)

Atom	x	y	z	U_{eq}	x	y	z	U_{eq}	x	y	z	U_{eq}
		Molecule **1**				Molecule **2**				Molecule **3**		
N1	−899(6)	2575(4)	4140(1)	48(1)	4888(4)	2846(6)	5890(6)	45(1)	3428(2)	3078(3)	8904(2)	45(1)
C2	688(7)	2601(4)	3751(1)	44(1)	4228(5)	3886(8)	5545(8)	53(1)	4223(3)	1834(3)	8681(2)	43(1)
N3	987(6)	4055(3)	3433(1)	45(1)	3208(4)	3943(6)	6011(6)	42(1)	4341(2)	2106(2)	7645(1)	42(1)
C4	−437(7)	5601(4)	3504(1)	47(1)	2826(5)	2902(8)	6995(8)	56(1)	3216(3)	2642(3)	6834(2)	41(1)
C4a	−2221(7)	5591(4)	3939(1)	47(1)	3551(5)	1705(8)	7356(8)	55(1)	2023(3)	3242(3)	7084(2)	42(1)
C5	−3809(9)	7051(6)	4050(2)	60(1)	3250(6)	0586(9)	8280(10)	68(2)	785(4)	3722(4)	6289(2)	56(2)
C6	−5528(9)	6996(6)	4454(2)	64(2)	3953(7)	−0538(9)	8609(10)	70(2)	−272(4)	4432(4)	6530(3)	65(2)
C7	−5671(9)	5493(6)	4759(2)	61(2)	4950(7)	−0515(9)	8074(9)	66(2)	−113(4)	4667(4)	7568(2)	63(2)
C8	−4132(8)	4051(6)	4657(1)	55(1)	5285(6)	0596(8)	7170(8)	64(2)	1080(3)	4192(3)	8365(2)	53(2)
C8a	−2382(7)	4074(4)	4239(1)	45(1)	4558(5)	1724(8)	6820(8)	54(1)	2176(3)	3474(3)	8139(2)	43(1)
C9	2289(9)	981(5)	3649(2)	58(2)	4578(7)	5095(9)	4573(11)	63(1)	5646(3)	1717(3)	9559(2)	48(1)
C10	3272(12)	812(6)	3110(2)	65(2)	4643(6)	6671(8)	5214(10)	73(2)	6667(4)	3007(4)	9608(2)	53(2)
C11	4559(11)	2503(6)	2952(2)	68(2)	3600(6)	7508(9)	5217(10)	70(2)	7589(4)	2717(5)	8948(3)	64(2)
C12	2683(10)	4001(6)	2969(2)	55(2)	2775(6)	6693(9)	6085(11)	63(2)	6795(4)	2631(4)	7769(3)	53(2)
C13					2484(6)	5143(9)	5574(10)	57(2)	5570(3)	1529(4)	7439(2)	47(2)
O	−196(6)	6826(3)	3201(1)	70(1)	1953(3)	3031(6)	7459(6)	63(1)	3233(2)	2709(2)	5926(1)	63(1)

TABLE 5. Coordinates (× 10^4) of the Nonhydrogen Atoms in Structure (**4**)

Atom	*x*	*y*	*z*	*U*eq	*x*	*y*	*z*	*U*eq.
		Molecule 4a				Molecule 4b		
O	3366(12)	−1312(9)	−0002(5)	70(5)	5118(13)	2961(9)	4286(6)	73(4)
N1	6514(11)	1008(9)	1970(6)	42(4)	1902(13)	0598(8)	2355(5)	43(3)
C2	5683(17)	1490(7)	1410(7)	52(5)	2713(13)	0107(11)	2880(7)	32(4)
N3	4440(13)	0757(9)	0761(6)	42(4)	3786(12)	0905(11)	3536(6)	46(4)
C4	4178(18)	−0695(13)	0631(8)	56(5)	4086(13)	2261(13)	3695(7)	42(4)
C4a	5124(16)	−1244(11)	1236(7)	43(4)	3187(15)	2853(12)	3089(8)	46(5)
C5	4891(20)	−2643(14)	1170(10)	81(7)	3392(17)	4259(11)	3143(7)	49(5)
C6	5808(16)	−3141(10)	1751(8)	57(5)	2511(17)	4835(15)	2582(8)	72(6)
C7	6970(17)	−2358(11)	2387(9)	66(6)	1439(16)	3939(12)	1948(7)	48(5)
C8	7086(16)	−0981(13)	2412(8)	53(5)	1120(16)	2563(11)	1821(7)	45(5)
C8a	6210(16)	−0409(11)	1856(7)	44(5)	2108(13)	2015(11)	2419(7)	44(4)
C9	5991(14)	3009(12)	1445(7)	45(5)	2290(18)	−1390(12)	2806(7)	53(5)
C10	6989(15)	3486(12)	0777(8)	56(5)	1346(17)	−1868(13)	3521(6)	57(5)
C11	5863(17)	3469(12)	−0008(7)	58(6)	2489(16)	−1759(13)	4322(8)	66(6)
C12	4873(16)	2024(13)	−0382(7)	54(5)	3627(19)	−0427(14)	4691(8)	64(6)
C13	3587(18)	1423(15)	0131(8)	69(6)	4708(14)	0276(11)	4091(8)	49(4)
		Molecule 4c				Molecule 4d		
O	5753(14)	9945(12)	7585(7)	69(5)	1619(17)	1780(12)	6744(9)	121(6)
N1	3925(14)	6336(14)	5859(8)	166(8)	4178(10)	5000(6)	8275(4)	31(3)
C2	3597(15)	7001(10)	6612(8)	46(4)	4723(17)	4574(14)	7602(7)	55(5)
N3	4412(16)	8066(15)	7171(6)	109(6)	3833(12)	3446(9)	7041(5)	46(3)
C4	5984(15)	8977(13)	7079(7)	46(5)	2314(18)	2703(13)	7256(9)	55(6)
C4a	6503(15)	8545(15)	6281(9)	64(5)	1743(15)	3054(10)	7981(7)	43(4)
C5	7942(17)	9328(15)	6036(7)	60(6)	0312(17)	2239(15)	8226(10)	72(7)
C6	8540(21)	8953(17)	5311(8)	78(7)	−0163(18)	2691(15)	8958(10)	78(8)
C7	7728(17)	7732(18)	4836(9)	82(8)	0704(22)	3920(18)	9424(10)	84(8)
C8	5302(17)	6978(16)	5087(9)	71(6)	2092(21)	4763(17)	9207(8)	78(7)
C8a	5597(15)	7340(12)	5789(7)	45(5)	2567(16)	4237(14)	8456(8)	60(5)
C9	1836(14)	6352(13)	6863(9)	55(5)	6405(20)	5269(15)	7481(10)	71(7)
C10	0571(15)	7327(14)	6785(10)	69(6)	7825(17)	4441(14)	7484(7)	63(5)
C11	0607(16)	8187(16)	7578(8)	68(6)	7808(19)	3526(16)	6664(10)	83(7)
C12	2255(20)	9230(17)	7919(8)	94(8)	6071(15)	2537(12)	6406(9)	67(6)
C13	3768(17)	8514(12)	8012(8)	58(5)	4397(18)	3038(17)	6292(8)	79(7)
		Coordinates of the molecules (A and B) of the succinimide of crystallization						
		A				B		
O1	9792(12)	−8854(10)	4008(6)	76(4)	0326(14)	−3194(10)	0974(6)	73(4)
O2	8086(12)	−5143(9)	3264(7)	78(4)	−1405(12)	0512(9)	0308(5)	64(4)
N	8677(12)	−7198(10)	3489(6)	47(4)	−0420(13)	−1193(10)	0798(6)	54(4)
C1	8705(16)	−5866(12)	3726(7)	51(5)	−0381(17)	−2546(13)	0610(10)	64(5)
C2	9661(19)	−5385(13)	4544(7)	65(5)	−1420(22)	−2966(15)	−0270(10)	89(7)
C3	10331(18)	−6678(12)	4736(8)	65(5)	−1982(18)	−1799(12)	−0505(8)	88(5)
C4	9591(16)	−7689(13)	4056(7)	45(4)	−1271(16)	−0632(14)	0239(8)	53(5)

The molecule of 2,3-pentamethylene-3,4-dihydroquinazol-4-one in a complex with succinimide (in the crystal (**4**)) retains the chair conformation of ring *C* observed in the structure of (**2**). However, the experimental material does not permit us to make a fine analysis of the geometry of the molecules in the structure of (**4**). This is connected with the fact that there proved to be six molecules in the independent part of the unit cell of the (**4**) crystal: four molecules of the alkaloid and two molecules of succinimide. Consequently, the errors in the determination of bond lengths and valence angles were fairly high (about 0.030 Å and 1.5°, respectively) (Table 2). However, it may be assumed that the geometry of the quinazol-4-one molecule in the complex (**4**) is identical with that observed in (**2**).

The errors in the determination of the bond lengths and valence angles in (**1**) and (**3**) are of the order of 0.003-0.006 Å and 0.2-0.4°, and in (**2**) somewhat larger (about 0.013 Å and 0.8°, respectively).

The results of our work and those reported in the literature (Cambridge Crystallogaphic Data Center, 1992 version) on the geometry of ring *B* show that in various derivatives of quinazol-4-one a variation in the size of ring *C* (number of methylene groups in ring *C*, n = 3 [6, 7], n = 4 [8-12], n = 5 [13]) or its opening [14] is not reflected in the lengths of the N1═C2 and N3−C2 valence bonds in ring *B*.

The mean value of literature figures for the lengths of the N1═C2 and N3−C2 valence bonds (1.289 and 1.385 Å, respectively) agree well with our results obtained for compounds (**1**) and (**2**), within the limits of experimental error (3σ).

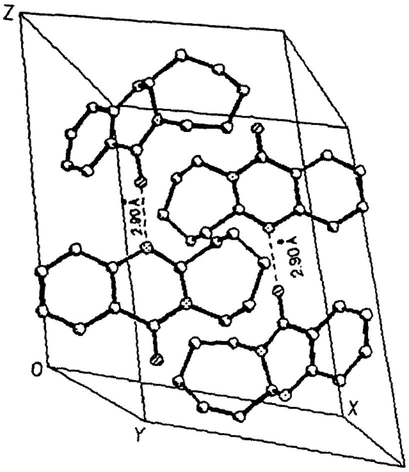

Fig. 1. Packing of the (3) molecules.

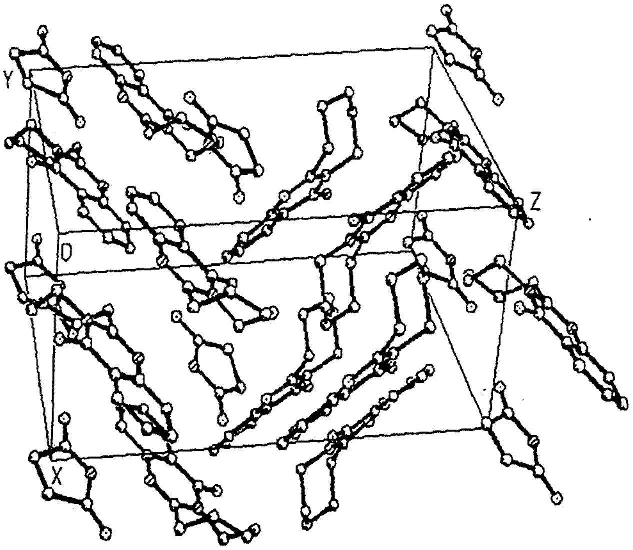

Fig. 2. Packing of the (2) molecules in the crystal of complex (4).

Analysis of the intermolecular contacts in structures (1-4) shows that only in the (3) crystal are there intermolecular hydrogen bonds. A hydrogen bond of the N—H···O═C type exists between molecules linked by 2_1 screw symmetry along the axis of monoclinicity (Fig. 1). In the other crystals the molecules are present at the distances of van der Waals interactions. In the (4) crystal, a succinimide molecule possibly interacts with the π-electronic system of the aromatic ring of 2,3-pentamethylene-3,4-dihydroquinazol-4-one (Fig. 2). This is indicated by the observed approach of the oxygen atoms of succinimide to the hydrogen atoms of the aromatic ring of 2,3-pentamethylene-3,4-dihydroquinazol-4-one.

EXPERIMENTAL

Crystals of compounds (1-4) were first investigated by the photo method. The space groups and the parameters of the unit cells were established from precession x-ray diagrams. These parameters were subsequently refined on a Syntex $P2_1$ diffractometer (USA) using CuK_α radiation. The intensities of the reflections were measured on the same diffractometer. The structure was interpreted by the direct method using the SHELXS program [15] in the automatic regime, apart from (4). For (4) we used the TEXR instruction, which permitted an enhancement of the possibilities of the direct method, since the indeppendent part of the unit cell contained 78 nonhydrogen atoms: four molecules of 2,3-pentamethylene-3,4-dihydroquinazol-4-one and two of succinimide.

The structures were refined by the method of least squares (MLS) in the full-matrix anisotropic approximation by the SHELX-76 program [16]. The coordinates of the hydrogen atoms were determined geometrically and were refined isotropically. The coordinates of the nonhydrogen atoms of structures (**1-4**) taken from the last stage of the MLS are given in Tables 4 and 5. All the computations were performed on a personal computer of the type of an IBM PC AT. Table 3 gives the main crystallographic parameters of the compounds investigated.

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