

STRUCTURE OF ORGANIC  
COMPOUNDS

X-ray Mapping in Heterocyclic Design: VI. X-ray Diffraction  
Study of 3-(Isonicotinoyl)-2-Oxooxazolo[3,2-*a*]pyridine  
and the Product of Its Hydrolysis

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Received January 29, 2001

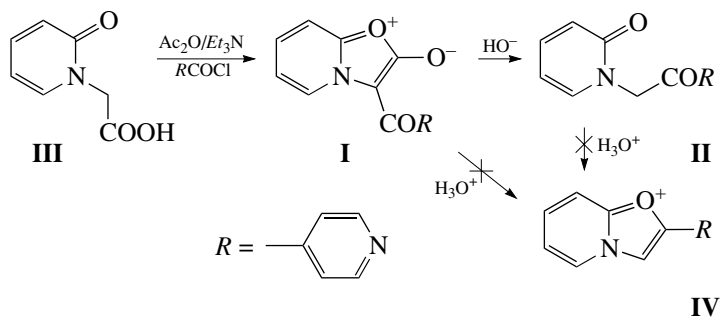
**Abstract**—The structure of 3-(isonicotinoyl)-2-oxooxazolo[3,2-*a*]pyridine,  $C_{13}H_8N_2O_3$ , (**I**) is determined by X-ray powder diffraction analysis. Crystals **I** are orthorhombic,  $a = 16.610(2)$  Å,  $b = 3.853(1)$  Å,  $c = 16.431(2)$  Å,  $Z = 4$ , and space group  $Pna2_1$ . The structure is solved by the grid search procedure and refined by the Reitveld method ( $R_p = 0.086$ ,  $R_{wp} = 0.115$ ,  $R_e = 0.030$ , and  $\chi^2 = 11.138$ ). The structure of the product of hydrolysis of compound **I**,  $C_{12}H_{10}N_2O_2$ , (**II**) is determined by the single-crystal X-ray diffraction technique. Crystals **II** are orthorhombic,  $a = 8.755(4)$  Å,  $b = 10.526(17)$  Å,  $c = 23.088(6)$  Å,  $Z = 8$ , and space group  $Pc2_1b$ . The structure is solved by the direct method and refined by the full-matrix least-squares procedure to  $R = 0.0464$ . A fragment of two fused heterocycles in **I** is planar. The dihedral angle between the plane of the pyridine ring in the isonicotinoyl fragment and the plane of the bicyclic system is  $51.2(2)^\circ$ . Both exocyclic CO groups that are adjacent to the five-membered fragment contain double bonds. The structures of two crystallographically independent molecules **II** are almost identical to each other, and the isonicotinoyl fragment is nearly perpendicular to the plane of the pyridone fragment [ $84.3(1)^\circ$  and  $87.0(1)^\circ$ ]. © 2002 MAIK "Nauka/Interperiodica".

INTRODUCTION

This paper continues a series of our structural investigations of the heterocyclic compounds that are able to enter readily into various chemical rearrangements and reactions of ring transformations [1–12]. In the present work, we concentrated on the structures of 3-(isonicotinoyl)-2-oxooxazolo[3,2-*a*]pyridine,  $C_{13}H_8N_2O_3$  (**I**), which belongs to the class of mesoionic heterocyclic compounds, and the product of its hydrolysis,

$C_{12}H_{10}N_2O_2$  (**II**). Data on the structures of these molecules are unavailable in the Cambridge Structural Database [13].

Our interest in the structure and properties of the molecules belonging to mesoionic compounds, such as **I**, is due to, first, the unusual (ilide) structural type of their heterocycles [9] and, second, the possibility of ready opening of the oxazolone ring and its transformation into the oxazolium ring [14] according to the **I–IV** conversion:



A number of representatives of the mesoionic heterocycles with the general formula  $C_{13}H_8N_2O_3$  (**I**) and aliphatic or aromatic  $R$  residues have been described in the literature. We prepared the first representative of

this series with a heterocyclic residue  $R$  ( $\gamma$ -pyridyl). Compound **I** was obtained from pyridonacetic acid **III** according to the procedure analogous to that used in [14] ( $R = Ar$ ) with isonicotinoyl chloride as an acylating

**Table 1.** Atomic coordinates ( $\times 10^4$ ) and isotropic thermal parameters  $B_{\text{iso}}$  ( $\text{\AA}^2$ ) for structure **I**

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{iso}}$	Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{iso}}$
C(1)	1991(5)	5229(18)	-405	3.55	C(14)	439(4)	1779(21)	-1279(7)	5.70
C(2)	1456(5)	3740(18)	186(6)	3.55	N(1)	1947(4)	3072(16)	863(4)	3.55
C(3)	1744(5)	1900(21)	1618(6)	3.55	O(1)	2741(3)	5340(11)	-24(4)	3.55
C(4)	2349(5)	1259(22)	2183(5)	3.55	O(2)	1945(3)	6360(12)	-1082(4)	6.25
C(5)	3134(5)	2245(22)	1986(6)	3.55	O(3)	270(3)	1934(13)	833(4)	3.06
C(6)	3324(5)	3616(21)	1249(6)	3.55	H(3)	1222(27)	1036(159)	1758(36)	4.0
C(7)	2721(5)	4139(18)	699(6)	3.55	H(4)	2236(36)	335(135)	2691(31)	4.0
C(8)	612(4)	3033(22)	184(6)	3.55	H(5)	2540(31)	1951(175)	2378(30)	4.0
C(9)	191(5)	3327(22)	-533(6)	5.70	H(6)	3854(28)	4289(129)	1126(33)	4.0
C(10)	-576(6)	5040(21)	-491(6)	5.70	H(10)	-730(23)	5917(115)	10(35)	4.0
C(11)	-1022(4)	5424(27)	-1178(7)	5.70	H(11)	-1527(26)	6437(128)	-1144(35)	4.0
N(12)	-767(4)	3916(19)	-1938(5)	5.70	H(13)	157(31)	1329(145)	-2462(33)	4.0
C(13)	-10(6)	2390(28)	-1975(7)	5.70	H(14)	935(25)	666(138)	-1324(35)	4.0

agent. The yield of compound **I** was 47%, even though the reaction was accompanied by a substantial resinification. Heating of compound **I** with an aqueous solution of sodium carbonate resulted in the hydrolytic cleavage of the oxazolone ring and the formation of pyridone **II**. Note that it is impossible to prepare pyridone **II** by another procedure. For example, it would be difficult to follow the standard strategy for preparation of these compounds by the reaction of pyridone-2 with the corresponding bromoketone, because the suitable bromoketone, 4-bromoacetylpyridine, contains both the heteroatom of the pyridine ring and the alkylating fragment, and, therefore, it is capable of self-quaternization.

The transformation of  $\alpha$ -amino acids into  $\alpha$ -amino ketones under the effect of acid halides is usually called the Dakin–West reaction. The step-by-step transformation of pyridonacetic acid **III** (formally, an  $\alpha$ -amino acid) into pyridone **II** (formally, an  $\alpha$ -amino ketone) through the stage of formation of the stable mesoionic heterocycle **I**, which we have accomplished, should also be considered as a Dakin–West reaction.

Our attempts to carry out acid cyclodehydration of pyridone **II** into bicyclic cation **IV** were unsuccessful. Under standard conditions, which provide for an oxazolium ring closure with the other 1-phenacylpyridones (successive treatment with sulfuric and perchloric acids), pyridone **II** formed the stable perchlorate. In the latter compound, the nitrogen heteroatom of the isonicotinoyl fragment, apparently, served as a center of protonation. A similar perchlorate of pyridone **II** was also isolated in an attempt to perform recyclization of mesoionic oxazolopyridine **I** in the acid medium by analogy with the transformation revealed earlier for the case of  $R = Ar$  [14]. Thus, we have at least in part drawn the boundaries of applicability of the recyclization of mesoionic oxazolopyridines into cationoid systems.

Earlier, we characterized systems of types **I** and **II** with  $Ar = C_6H_5$  [3, 9] and *para*- $NO_2-C_6H_4$  [8, 11] by the X-ray powder and single-crystal diffraction techniques. The present study of one more complementary pair of molecules supplements the data on the structures of mesoionic systems and the products of their hydrolysis and provides one more example of the X-ray mapping of chemical reactions [5–7, 11, 12].

## EXPERIMENTAL

The X-ray diffraction experiment for **I** was performed in an evacuated Enraf–Nonius Guinier–Johansson FR552 camera ( $\lambda CuK_{\alpha 1}$ , quartz monochromator). The intensities and angle parameters of the X-ray spectrum were measured using an LS18 densitometer in  $0.01^\circ$  steps. The unit cell parameters were determined according to the ITO indexing program [15] in the  $2\theta$  angle range  $4^\circ$ – $86^\circ$  and the index ranges  $0 \leq h \leq 13$ ;  $0 \leq k \leq 3$ ,  $0 \leq l \leq 13$ . The space group was determined from the systematic absences of reflections. Crystals **I** are orthorhombic,  $a = 16.610(2)$  Å,  $b = 3.853(1)$  Å,  $c = 16.431(2)$  Å,  $V = 1051.6(3)$  Å<sup>3</sup>,  $d_{\text{calcd}} = 1.436$  g/cm<sup>3</sup>,  $\mu(\lambda Cu) = 8.89$  cm<sup>-1</sup>,  $Z = 4$ , and space group  $Pna2_1$ .

Structure **I** was solved by the grid search procedure [16] using the given molecular fragments. The full-profile refinement of the structure was performed by the Reitveld method with the MRIA program [17]. The pseudo-Voigt function was used as a profile shape function, and the background was approximated by the Chebyshev polynomials of the fifth order. The parameters of the texture in the [010] direction were refined within the March–Dollase model [18]. The final refinement parameters are as follows:  $R_p = 0.086$ ,  $R_{wp} = 0.115$ ,  $R_e = 0.030$ , and  $\chi^2 = 11.138$ , where  $R_p = \sum |I_o - I_c| / \sum I_o$ ,  $R_{wp} = \sum w|I_o - I_c| / \sum wI_o$ ,  $R_e = \sum \sigma I_o / \sum I_o$ ;  $I_o$  is

**Table 2.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic thermal parameters  $U_{\text{eq}}$  ( $\text{\AA}^2 \times 10^3$ ) for structure **II**

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{eq}}$	Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{eq}}$
N(1A)	2515(2)	8000(2)	8031(1)	48(1)	C(9B)	3677(2)	10598(2)	1727(1)	49(1)
C(2A)	1987(3)	6861(2)	8234(1)	73(1)	C(10B)	4385(2)	9734(2)	1367(1)	53(1)
O(2A)	1588(2)	6042(2)	7876(1)	99(1)	C(11B)	4500(3)	10009(3)	792(1)	75(1)
C(3A)	1910(3)	6746(2)	8837(1)	87(1)	N(12B)	4008(2)	11056(2)	534(1)	86(1)
C(4A)	2353(3)	7668(3)	9192(1)	83(1)	C(13B)	3352(4)	11873(3)	892(1)	104(1)
C(5A)	2886(2)	8805(2)	8969(1)	66(1)	C(14B)	3157(3)	11706(2)	1472(1)	94(1)
C(6A)	2941(2)	8969(2)	8400(1)	59(1)	H(3A)	1452(16)	6081(17)	8983(6)	43(5)
C(7A)	2556(2)	8171(2)	7410(1)	52(1)	H(4A)	2360(20)	7600(20)	9573(9)	118(9)
C(8A)	1018(2)	8316(2)	7142(1)	44(1)	H(5A)	3320(20)	9570(20)	9262(8)	99(8)
O(8A)	-94(1)	8508(1)	7440(1)	64(1)	H(6A)	3310(30)	9750(20)	8165(9)	125(9)
C(9A)	860(2)	8207(2)	6511(1)	46(1)	H(7A1)	3105(17)	8840(20)	7319(7)	62(6)
C(10A)	-426(2)	8675(2)	6240(1)	72(1)	H(7A2)	3070(20)	7520(20)	7223(7)	81(7)
C(11A)	-541(3)	8557(3)	5654(1)	91(1)	H(10A)	-1249(19)	8970(20)	6485(7)	72(6)
N(12A)	483(2)	8031(2)	5308(1)	81(1)	H(11A)	-1415(19)	8860(10)	5453(7)	70(6)
C(13A)	1714(3)	7602(2)	5576(1)	67(1)	H(13A)	2474(18)	7325(18)	5314(7)	73(7)
C(14A)	1946(2)	7643(2)	6159(1)	58(1)	H(14A)	2790(20)	7330(20)	6319(8)	86(7)
N(1B)	2442(2)	10839(1)	3307(1)	46(1)	H(3B)	4471(17)	11115(19)	4465(7)	67(6)
C(2B)	3687(2)	11161(2)	3631(1)	47(1)	H(4B)	2344(15)	10235(15)	4846(6)	35(4)
O(2B)	4809(2)	11629(2)	3383(1)	62(1)	H(5B)	328(18)	9553(17)	4283(7)	55(6)
C(3B)	3611(2)	10883(2)	4226(1)	57(1)	H(6B)	365(18)	10010(18)	3314(7)	54(5)
C(4B)	2377(3)	10337(2)	4458(1)	62(1)	H(7B1)	1432(13)	11137(14)	2540(6)	23(4)
C(5B)	1169(3)	9984(2)	4110(1)	71(1)	H(7B2)	2890(20)	12030(20)	2672(8)	98(7)
C(6B)	1220(2)	10253(2)	3552(1)	63(1)	H(10B)	4680(20)	8880(30)	1554(8)	112(8)
C(7B)	2454(2)	11184(2)	2700(1)	52(1)	H(11B)	5040(20)	9540(20)	550(8)	82(7)
C(8B)	3423(2)	10284(2)	2346(1)	47(1)	H(13B)	2820(30)	12440(30)	706(12)	151(11)
O(8B)	3962(1)	9335(1)	2551(1)	59(1)	H(14B)	2690(20)	12230(20)	1716(8)	80(7)

the observed intensity, and  $I_c$  is the calculated intensity. The atomic coordinates and isotropic thermal parameters are listed in Table 1.

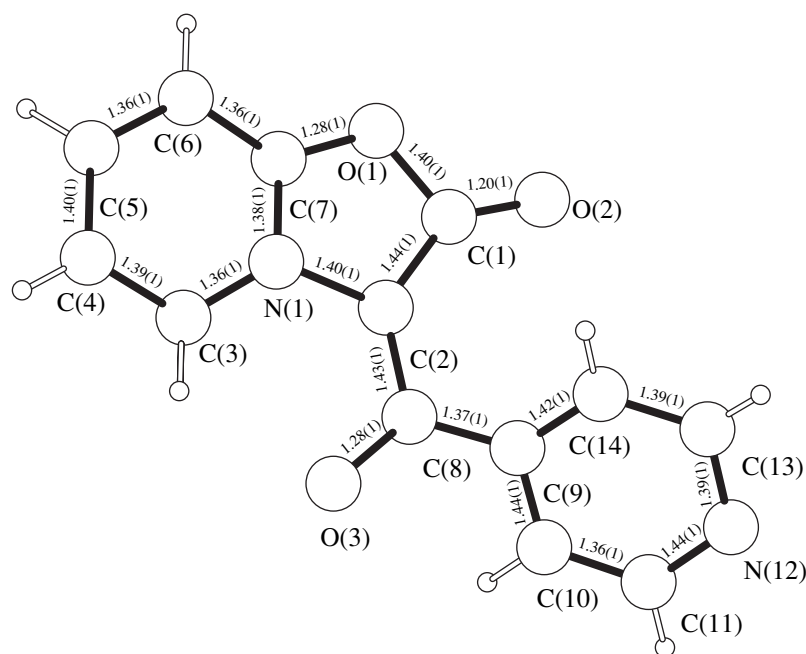
The unit cell parameters of **II** were determined and refined using 25 reflections in the  $\theta$  range  $14^\circ$ – $16^\circ$  on a CAD4 automated diffractometer [19] ( $\lambda\text{MoK}\alpha$ , graphite monochromator). Crystals **II** are orthorhombic,  $a = 8.755(4)$   $\text{\AA}$ ,  $b = 10.526(17)$   $\text{\AA}$ ,  $c = 23.088(6)$   $\text{\AA}$ ,  $V = 2128(4)$   $\text{\AA}^3$ ,  $d_{\text{calcd}} = 1.337$   $\text{g/cm}^3$ ,  $\mu(\lambda\text{Mo}) = 0.093$   $\text{mm}^{-1}$ ,  $Z = 8$ , space group  $Pc2_1b$ . A set of 1266 reflections with  $I \geq 2\sigma(I)$  was collected by the  $\omega$ -scan technique in the range  $\theta \leq 21.96^\circ$  on the same diffractometer. The preliminary processing of the diffraction data set was performed with the WinGX98 program [20]. The structure was solved by the direct method and refined by the least-squares procedure in the anisotropic approximation using the SHELX97 program package [21]. The hydrogen atoms were located from the electron-density difference synthesis and refined in the isotropic approximation. The final discrepancy factors are  $R_1 = 0.0461$  and  $wR_2 = 0.0868$ . The residual electron density lies

between  $\Delta\rho_{\text{max}} = 0.139$  and  $\Delta\rho_{\text{min}} = -0.116$   $\text{e/\AA}^3$ . The atomic coordinates and equivalent thermal parameters are listed in Table 2.

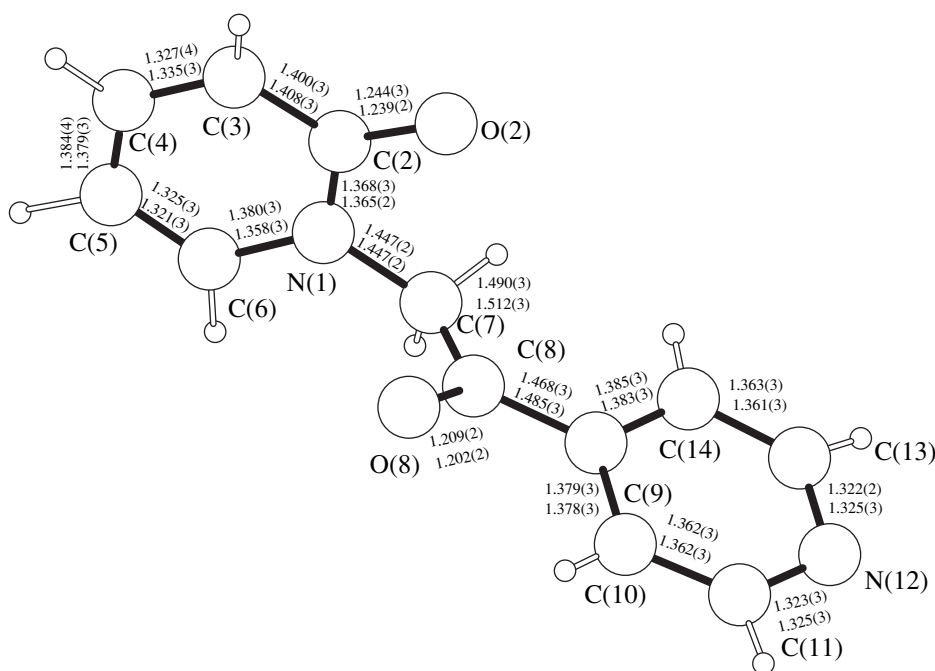
The spatial arrangements of atoms in molecules **I** and **II** with atomic numberings are shown in Figs. 1 and 2, respectively. The figures were drawn using the PLUTON96 graphical program package [22].

## RESULTS AND DISCUSSION

The angle between the planes of oxazolo[3,2-*a*]pyridine bicycle and the six-membered pyridine ring in molecule **I** is equal to  $51.2(2)^\circ$ . The C(1)–C(2) bond (1.44  $\text{\AA}$ ) appeared to be significantly longer than the expected double bond, whereas the exocyclic C(1)–O(2) bond is 1.20  $\text{\AA}$ . It follows from these bond lengths that the geometry of the C(2)–C(1)=O(2) fragment is similar to that of the exocyclic C(2)–C(8)=O(3) keto group. The parameters of the O(2)=C(1)–C(2)–C(8)=O(3) structural fragment correspond to a combination of two ordinary carbonyl groups linked through



**Fig. 1.** Structure of molecule **I** with the atomic numbering and interatomic distances (A).



**Fig. 2.** Structure of molecule **II** with the atomic numbering and interatomic distances (A; the upper value refers to molecule A, and the lower value refers to molecule B).

the C(2) atom. This can be explained by the localization of the negative charge at the C(2) atom of the mesoionic molecule. The positive charge is delocalized in the N(1)–C(7)–O(1) chain and does not touch the pyridine fragment of the mesoionic bicycle. We revealed a similar but more pronounced delocalization of the positive

charge in the molecule of the chemical analogue of **I**, which was described earlier in [9].

Earlier, we investigated the structures of *N*-substituted pyridones-2, in which the phenacyl [3] and *para*-nitrophenacyl groups are located at the nitrogen atom [8]. The structure of **II** agrees closely with the molecu-

**Table 3.** Parameters of the interatomic contacts\* in structure **I**

<i>D</i> – <i>H</i>	<i>d</i> ( <i>D</i> – <i>H</i> ), Å	<i>d</i> ( <i>D</i> ⋯ <i>A</i> ), Å	<i>d</i> ( <i>H</i> ⋯ <i>A</i> ), Å	ω( <i>D</i> – <i>H</i> ⋯ <i>A</i> ), deg	<i>A</i> [symmetry code]
C(3)–H(3)	0.96(5)	2.77(1)	2.22(5)	115(3)	O(3) [ <i>x</i> , <i>y</i> , <i>z</i> ]
C(10)–H(10)	0.93(6)	2.85(1)	2.64(5)	94(3)	O(3) [ <i>x</i> , <i>y</i> , <i>z</i> ]
C(14)–H(14)	0.93(5)	3.08(1)	2.79(5)	99(3)	O(2) [ <i>x</i> , <i>y</i> , <i>z</i> ]
C(4)–H(4)	0.93(5)	3.08(1)	2.46(5)	124(4)	O(2) [1/2 – <i>x</i> , <i>y</i> – 1/2, 1/2 + <i>z</i> ]
C(5)–H(5)	0.94(5)	3.20(1)	2.67(5)	116(4)	O(2) [1/2 – <i>x</i> , <i>y</i> – 1/2, 1/2 + <i>z</i> ]
C(14)–H(14)	0.93(5)	3.27(1)	2.39(5)	158(4)	O(2) [ <i>x</i> , <i>y</i> – 1, <i>z</i> ]

\* *D* is a donor, *A* is an acceptor, and *H* is a hydrogen atom.

**Table 4.** Parameters of the interatomic contacts\* in structure **II**

<i>D</i> – <i>H</i>	<i>d</i> ( <i>D</i> – <i>H</i> ), Å	<i>d</i> ( <i>D</i> ⋯ <i>A</i> ), Å	<i>d</i> ( <i>H</i> ⋯ <i>A</i> ), Å	ω( <i>D</i> – <i>H</i> ⋯ <i>A</i> ), deg	<i>A</i> (symmetry code)
C(7 <i>A</i> )–H(7 <i>A</i> 2)	0.93(2)	2.626(4)	2.52(2)	86(1)	O(2 <i>A</i> ) [ <i>x</i> , <i>y</i> , <i>z</i> ]
C(10 <i>A</i> )–H(10 <i>A</i> )	0.97(2)	2.791(3)	2.48(2)	99(1)	O(8 <i>A</i> ) [ <i>x</i> , <i>y</i> , <i>z</i> ]
C(5 <i>B</i> )–H(5 <i>B</i> )	0.95(2)	3.498(4)	2.86(2)	125(1)	N(12 <i>A</i> ) [ <i>x</i> , <i>y</i> , <i>z</i> ]
C(7 <i>B</i> )–H(7 <i>B</i> 2)	0.97(2)	2.638(3)	2.39(2)	94(1)	O(2 <i>B</i> ) [ <i>x</i> , <i>y</i> , <i>z</i> ]
C(10 <i>B</i> )–H(10 <i>B</i> )	1.03(2)	2.790(3)	2.44(2)	99(1)	O(8 <i>B</i> ) [ <i>x</i> , <i>y</i> , <i>z</i> ]
C(3 <i>B</i> )–H(3 <i>B</i> )	0.97(2)	3.674(3)	2.81(2)	150(1)	N(12 <i>B</i> ) [1 – <i>x</i> , <i>y</i> , <i>z</i> + 1/2]
C(7 <i>A</i> )–H(7 <i>A</i> 1)	0.88(2)	3.302(3)	2.68(2)	130(1)	O(8 <i>B</i> ) [1 – <i>x</i> , <i>y</i> , <i>z</i> + 1/2]
C(6 <i>A</i> )–H(6 <i>A</i> )	1.04(3)	3.424(5)	2.62(3)	134(2)	O(2 <i>B</i> ) [1 – <i>x</i> , <i>y</i> , <i>z</i> + 1/2]
C(6 <i>A</i> )–H(6 <i>A</i> )	1.04(3)	3.378(3)	2.81(2)	114(1)	O(8 <i>B</i> ) [1 – <i>x</i> , <i>y</i> , <i>z</i> + 1/2]
C(7 <i>A</i> )–H(7 <i>A</i> 1)	0.88(2)	3.207(5)	2.71(2)	117(2)	O(2 <i>A</i> ) [ <i>x</i> , <i>y</i> + 1/2, 3/2 + <i>z</i> ]
C(7 <i>A</i> )–H(7 <i>A</i> 2)	0.93(2)	3.363(3)	2.51(2)	153(2)	O(2 <i>B</i> ) [1 – <i>x</i> , <i>y</i> – 1/2, 1 – <i>z</i> ]
C(14 <i>A</i> )–H(14 <i>A</i> )	0.89(2)	3.213(3)	2.33(2)	171(2)	O(2 <i>B</i> ) [1 – <i>x</i> , <i>y</i> – 1/2, 1 – <i>z</i> ]
C(13 <i>A</i> )–H(13 <i>A</i> )	0.95(2)	3.640(3)	2.72(2)	163(1)	N(12 <i>B</i> ) [ <i>x</i> , <i>y</i> – 1/2, 1/2 – <i>z</i> ]
C(10 <i>B</i> )–H(10 <i>B</i> )	1.03(2)	3.340(6)	2.38(3)	155(2)	O(2 <i>B</i> ) [ <i>x</i> , <i>y</i> – 1/2, 1/2 – <i>z</i> ]
C(6 <i>B</i> )–H(6 <i>B</i> )	0.96(2)	3.307(3)	2.57(2)	133(1)	O(8 <i>A</i> ) [– <i>x</i> , <i>y</i> , <i>z</i> – 1/2]
C(7 <i>B</i> )–H(7 <i>B</i> 2)	0.97(2)	3.218(4)	2.91(2)	100(1)	O(8 <i>A</i> ) [– <i>x</i> , <i>y</i> + 1/2, 1 – <i>z</i> ]
C(7 <i>B</i> )–H(7 <i>B</i> 1)	0.97(1)	3.218(4)	2.76(2)	110(1)	O(8 <i>A</i> ) [– <i>x</i> , <i>y</i> + 1/2, 1 – <i>z</i> ]
C(7 <i>B</i> )–H(7 <i>B</i> 1)	0.97(1)	3.783(3)	2.82(1)	177(1)	O(2 <i>A</i> ) [– <i>x</i> , <i>y</i> + 1/2, 1 – <i>z</i> ]
C(7 <i>B</i> )–H(7 <i>B</i> 2)	0.97(2)	3.617(5)	2.66(2)	172(2)	O(8 <i>B</i> ) [ <i>x</i> , <i>y</i> + 1/2, 1/2 – <i>z</i> ]

\* *D* is a donor, *A* is an acceptor, and *H* is a hydrogen atom.

lar structures of these phenacylpyridones. For example, molecules *A* and *B* in structure **II** are almost identical to each other, and the O(2) and C(7) atoms (the pyridone fragment), as well as the C(8) and O(8) atoms (the acyl fragment), lie in the planes of the corresponding heterocycles.

In the pyridone fragment, the partially single and partially double bonds alternate with the formation of the quasi-diene C(3)=C(4)–C(5)=C(6) structural fragment.

The plane of the heterocycle of the acyl fragment is nearly perpendicular to the plane of the pyridone fragment; the dihedral angles are 84.34(8)° and 86.96(8)° for molecules *A* and *B*, respectively. The mutual

arrangement of the six-membered rings in the molecule almost coincides with that in phenacylpyridone [87.55(6)°] [8]. In *para*-nitrophenacylpyridone [3], the corresponding dihedral angle [77.21(1)°] is, on average, 10° smaller than that in molecules *A* and *B*. Hence, we can conclude that the geometry of the molecule does not depend on the type of the acyl radical (phenyl, *para*-nitrophenyl, or  $\gamma$ -pyridyl).

In the crystal structures of compounds **I** and **II**, the systems of interatomic contacts involving hydrogen, nitrogen, and oxygen atoms are formed (Tables 3 and 4). These contacts were calculated with the PARST95 program [23].

## ACKNOWLEDGMENTS

This study was supported by the Netherlands Society of Basic Research (NWO). The synthetic part of this work was supported by the Russian Foundation for Basic Research, project no. 99-03-33076. We are also grateful to this Foundation for the payment of the license for using the Cambridge Structural Database, project no. 99-07-90133.

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*Translated by I. Polyakova*