# Synthesis and X-ray structure of N-phenyl phenylglyoxamide

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Received December 17, 1997

The title compound  $(C_{14}H_{11}NO_2)$  is monoclinic with a = 13.579(2), b = 5.297(1), c = 16.455(2) Å,  $\beta = 98.11(2)^\circ$ , Z = 4, and space group  $P2_1/n$ . The significant structural features lie in the two carbonyl groups of the glyoxamide which are oriented antiperiplanar to each other  $[-163.6(3)^\circ]$ . The central bond C(1)-C(2) is 1.545(4) A. The observed conformation is stabilized by intramolecular hydrogen bonds.

KEY WORDS: N-phenyl phenylglyoxamide; phenylglyoxanilide; synthesis; x-ray structure.

## Introduction

We have recently reported that the electrochemical reaction of terminal alkynes with diaryl disulfides in organic solvents represents a simple and efficient method to synthesize  $\alpha$ -oxo-thioesters.<sup>1,2</sup> We would like to mention that studies on the chemistry of this class of compounds are almost unknown. However, our preliminary experiments showed that  $\alpha$ -oxo-thioesters react in ethanol with o-phenylenediamines under reflux vielding 2-quinoxalone.<sup>3</sup> In a continuation of our study of the chemistry of  $\alpha$ -oxo-thioesters we have next investigated the reaction of  $\alpha$ -oxo-thioesters with aliphatic and aromatic monoamines. In the present paper the preparation of the title compound by reaction of phenyl phenylthioglyoxylate 1 with aniline is reported. In the literature only a few reports on the preparation of **3** have been published.<sup>4-8</sup>

The aim of this study was to examine and to characterize the molecular dimensions of the glyoxa-

mide group, particulary for comparison with the glyoxylate and thioglyoxylate groups (Scheme 1).

# Experimental

#### Synthesis of phenyl phenylglyoxamide

A mixture of 3 mmole (0.73 g) of 1 and 3 mmole (0.3g) of aniline in 6 ml of methanol was heated under reflux for 2 h and then evaporated under reduced pressure to dryness. The crude product was purified by column chromatography on silica gel 40 (70-230 mesh) using a mixture of dichloromethane and cyclohexane (1/1, v/v) as eluant. The eluate ( $R_f$  value ca. 0.6) was concentrated and the residue was crystallized from petroleum ether  $(40-60^{\circ}C)$  - cyclohexane to give 0.5 g (74%) of **3** with m.p.  $64-65^{\circ}$ C (lit.<sup>4</sup> m.p. 63-64°C). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 7.17-7.72 (m,8H,Ar-H), δ 8.40-8.44 (m,2H,Ar-H), δ 8.96 (broad singlet, 1H,NH); MS EI (70 eV) m/z (relative intensity): 225(21.1, M<sup>+</sup>), 120(7.9, M-C<sub>6</sub>H<sub>5</sub>CO), 105 (100,  $M-C_6H_5NHCO$ ). The melting point was determined on a Buchi 510 capillary apparatus. The <sup>1</sup>H NMR spectrum was recorded on a Bruker 300 MSL instrument at 300 MHz. The mass spectrum was obtained on a LKB GC MS 2091 spectrometer at 70 eV.

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#### Crystal structure of phenyl phenylglyoxamide

The crystals of 3 were grown from petroleum ether (40-60°C)-cyclohexane mixture. The data collection was performed on an Enraf-Nonius CAD4 fourcircle X-ray diffractometer with graphite monochromated CuK $\alpha$  radiation; the  $\omega$ -2 $\theta$  scan mode was applied. The corrections for Lorenz and polarization effects but not for absorption were applied. The structure was solved by direct methods (SHELXS-86<sup>9</sup>) and refined using SHELXL-93.<sup>10</sup> All hydrogen atoms were located in the calculated "ideal" positions but the N-H atom was located from difference Fourier map. In subsequent refinements positional and isotropic thermal parameters of H-atoms were refined. The crystal data and details of refinement are summarized in Table 1. Thermal ellipsoids in Fig. 1 are drawn with the **ORTEPII** program.<sup>11</sup>

## **Results and discussion**

Final atomic coordinates and equivalent isotropic displacement parameters are given in Table 2. Bond distances and bond angles are given in Table 3. Figure 1 shows a perspective view of the molecule together with the labelling scheme. The main feature of the conformation of the title compound lies in the two carbonyl groups which are oriented antiperiplanar one to another. The torsion angle O(1)-C(1)-C(2)-O(2) describes the conformation about the central C(1)-C(2) bond and is equal to  $-163.6(3)^{\circ}$  which is a typical value for this class of compounds [e.g.,  $170.2^{\circ}$  for p-methyl-phenyl glyoxylacid-m-trifluoro-anilide<sup>12</sup> and 162.4° for 2'-(N-isopropyloxamoyl)-acetanilide<sup>13</sup>].

The mutual *trans* orientation of the two carbonyl groups is stabilized by four intramolecular hydrogen bonds. The O(1) atom is involved in two almost symmetrical C-H...O hydrogen bonds to the two phenyl substituents to complete the 6-membered rings. The O(2) atom forms one hydrogen bond of the N(1)-H(1)...O(2) type and one of the C(4)-H(4)...O(2) type both to complete 5-membered rings. Such attractive intramolecular interactions create

 
 Table 1. Crystal data and summary of intensity data collection and structure refinement

Compound Color	C <sub>14</sub> H <sub>11</sub> NO <sub>2</sub> Pale-yellow
Formula weight	225.25
Space group	P2 <sub>1</sub> /n
Temp., °C	20
Cell constants (25 reflections,	
$8 < \theta < 25^{\circ}$ )	
a, Å	13.579(2)
b, Å	5.297(1)
<i>c</i> , Å	16.455(2)
β, deg	98.11(2)
Cell volume, Å <sup>3</sup>	1171.7(6)
Formula units/unit cell	4
$D_{\text{calc}}$ , g cm <sup>-3</sup>	1.277
$\mu_{calc}, cm^{-1}$	6.99
Diffractometer/scan	Enraf-Nonius CAD4/ω-2θ
Radiation, graphite monochromator	$CUK\alpha \ (\lambda = 1.54178)$
Max. crystal dimensions, mm	$0.28 \times 0.35 \times 0.42$
Scan width	$0.90 + 0.35 \tan \theta$
Standard reflections	3
Decay of standards	<2%
Reflections measured	2500
2θ range, deg	$3.96 < \theta < 76.92$
Range of h, k, l	-17 0, -6 0, -20 20
Reflections observed $[F_{o} > 4\sigma(F_{o})]$	1955
Independent reflections	2401 [ $R_{int} = 0.0201$ ]
Computer programs	SHELXL-93 <sup>10</sup>
Structure solution	SHELXS-86 <sup>9</sup>
Refinement method	Full-matrix least-squares on $F^2$
No. of parameters varied	199
Weights	$[\sigma^2 (F_0^2) + (0.058P)^2]^{-1} \text{ where} P = (F_0^2 + 2F_c^2)/3$
GOF	1.037
Final R indices $[l > 2\sigma l]$	$R_1 = 0.053, wR_2 = 0.117$
R indices (all data)	$R_1 = 0.120, wR_2 = 0.185$
Largest feature final diff. map	0.161 and $-0.106 e^- Å^{-3}$

a barrier to rotation about the central C(1)-C(2) bond and stabilize the antiperiplanar conformation of the title compound. The details of the geometry of the hydrogen bonds are presented in Table 4. Besides the formation of intramolecular hydrogen bonds the oxygen atom O(2) and the N(1)-H(1) group are involved in intermolecular hydrogen bonds to two adjacent molecules of 3 and form a one-dimensional chain of heli-

**Table 2.** Atomic coordinates (× 10<sup>4</sup>) and equivalent isotropic displacement parameters ( $\mathring{A}^2 \times 10^3$ ) for  $3^a$ 

	x	у	-	U <sub>eq</sub>
N(1)	9236(2)	-1442(4)	2548(1)	69(1)
C(1)	9404(2)	199(5)	1951(2)	69(1)
<b>O</b> (1)	10176(1)	405(4)	1650(1)	98(1)
C(2)	8496(2)	1912(5)	1681(2)	65(1)
O(2)	7850(1)	1992(3)	2135(1)	80(1)
C(3)	8423(2)	3423(5)	921(2)	63(1)
C(4)	7778(2)	5503(5)	848(2)	73(1)
C(5)	7670(3)	6939(7)	138(2)	89(1)
C(6)	8184(3)	6355(9)	- 502(2)	98(1)
C(7)	8806(3)	4300(9)	- 437(2)	98(1)
C(8)	8935(2)	2829(7)	269(2)	81(1)
C(9)	9893(2)	-3266(5)	2960(2)	74(1)
C(10)	9534(3)	-4672(7)	3563(2)	100(1)
C(11)	10122(4)	-6541(9)	3981(3)	129(2)
C(12)	11054(4)	-7001(9)	3810(4)	131(2)
C(13)	11414(4)	-5613(10)	3211(3)	123(2)
C(14)	10840(3)	-3723(8)	2778(2)	98(1)

<sup>*a*</sup>  $U_{eq}$  is defined as one third of the trace of the orthogonalized  $U_{u}$  tensor.

cally arranged molecules along a  $2_1$  crystallographic axis (Fig. 2). A number of short intermolecular C-H...O contacts additionally stabilize the structure (see Table 4).

The conformation about the central bond of the glyoxamide group is very similar to that observed for the p-tolyl phenylthioglyoxylate<sup>14</sup> but differs from that

Table 3. Selected bond lengths (Å), angles (°) and torsion angles (°) for 3

$\mathbf{N}(1) = \mathbf{C}(1)$	1 354(3)
N(1) = C(1)	1.334(3)
N(1) = C(9)	1.421(3)
C(1) = O(1)	1.226(3)
C(1) - C(2)	1.545(4)
C(2) - O(2)	1.230(3)
C(2) - C(3)	1.477(3)
C(1) - N(1) - C(9)	128.6 (2)
O(1) - C(1) - N(1)	126.3 (3)
O(1) - C(1) - C(2)	121.7 (3)
N(1)-C(1)-C(2)	112.1 (2)
O(2) - C(2) - C(3)	121.9 (2)
O(2) - C(2) - C(1)	117.0 (2)
C(3) - C(2) - C(1)	121.1 (2)
C(9) = N(1) = C(1) = O(1)	0.2 (5)
C(9) - N(1) - C(1) - C(2)	-178.7 (2)
O(1) - C(1) - C(2) - O(2)	-163.6 (3)
N(1)-C(1)-C(2)-O(2)	15.4 (3)
O(1)-C(1)-C(2)-C(3)	15.1 (4)
N(1)-C(1)-C(2)-C(3)	-166.0 (2)

observed for the glyoxylate<sup>15-17</sup> and 1,2-diketo systems.<sup>18</sup> In the structure of phenylthioglyoxylate the two carbonyl groups are oriented antiperiplanar one to another with torsion angle equal to  $-168.2^{\circ}$ .<sup>14</sup> Such a conformation is a consequence of the existence of the nonbonded intramolecular interaction S-O of the 1.4 type between the acceptor sulfur and the donor oxygen atoms. It was found that ethyl phenylglyoxylate exists in a conformation where the two carbonyl groups have been rotated by 75° from cis-coplanarity.<sup>15</sup> In the case of the (-)menthyl p-bromophenylglyoxylate the two C=O groups are twisted about the central bond by 104°.<sup>17</sup> X-ray studies of benzil show a twist of 68.8° for the corresponding torsion angle.<sup>18</sup> Because of the twist about the central bond between the carbonyl groups  $p_z$ - $p_z$  overlap does not exist and, as a consequence, there is no  $\pi$  bond formation and thus conjugation plays a minor role in these compounds.

It is worth pointing out that the central C(1)-C(2)bond [1.545(4) Å] in the glyoxamide group of the title compound is significantly longer than the value accepted for a  $C(sp^2) - C(sp^2)$  single bond which was found to range between 1.47 and 1.52 Å.<sup>19</sup> The C(1)-C(2) distance is as long as the typical  $C(sp^3)-C(sp^3)$  distance. A similar phenomenon has been observed for the p-methyl-phenyl glyoxylacidm-trifluoro-anilide (1.546 Å)<sup>12</sup> and 2'-(N-isopropyloxamoyl)-acetanilide (1.530 Å).<sup>13</sup> It should be mentioned here that these observations are not restricted only to glyoxamides. Lengthening of the corresponding C-Cdistances was also found in the thioglyoxylate group,14 various glyoxalates<sup>15-17</sup> and 1,2-diketo systems,<sup>18</sup> In Table 5 geometrical details for some of the above mentioned compounds are collected. It appears that the length of the C(1)-C(2) bond correlates with the corresponding torsion angle O(1)-C(1)-C(2)-O(2).

It seems to be the most probable that both carbonyl groups C(1)=O(1) and C(2)=O(2) possess the same electron configuration on the C atoms and, consequently, an excess of charge of the same character which causes a Coulomb repulsion between the two C atoms thus leading to C(1)-C(2) bond lengthening.<sup>20</sup>

On the other hand shortening of the C(2)-C(3)and N(1)-C(9) bond distances which are equal to 1.477(3) Å and 1.421(3) Å, respectively, (compared to the corresponding single bonds) can be explained by the conjugation of the bonds of the adjacent phenyl ring and have been observed in a number of analogous structures of the aromatic amides.<sup>21–23</sup>

The C(1)-N(1) distance of 1.354(3) Å seems to be relatively longer. This value is similar to that found



Fig. 1. View of the title compound with the labeling scheme.

**Table 4.** Hydrogen-bond parameters (Å,°) and short C-H…O contacts with their esd's (in parentheses)<sup>a</sup>

	D-H	D····A	HA	D-H····A
$N(1) = H(1) \cdots O(2)$	1.02(3)	2,637(3)	2.17(3)	106(2)
$C(8) - H(8) \cdots O(1)$	0.98(3)	2.928(4)	2.25(3)	125(2)
$C(14) - H(14) \cdots O(1)$	0.99(4)	2.927(5)	2.24(3)	125(3)
$C(4) - H(4) \cdots O(2)$	1.03(3)	2.810(3)	2.49(3)	97(2)
$N(1) - H(1) - O(2)^{i}$	1.02(3)	3.060(3)	2.14(3)	150(2)
C(10) - H(10) - O(2)'	1.03(4)	3.996(4)	2.56(3)	138(3)
$C(4) = H(4) \cdots O(2)^{n}$	1.03(4)	3.627(4)	2.67(3)	155(2)
$C(7) - H(7) \cdots O(1)^{m}$	1.02(3)	3.589(5)	2.73(3)	142(2)

<sup>a</sup> Symmetry related positions: (i) 3/2 - x, -1/2 + y, 1/2 - z; (ii) 3/2 - x, 1/2 + y, 1/2 - z; (iii) 2 - x, -y, -z.



Fig. 2. View of the chain of helically arranged molecules in the crystal packing of 3. Broken lines shown intermolecular N(1)-H(1) O(2) hydrogen bonds.

in p-methyl-phenyl glyoxylacid-m-trifluoro-anilide  $(1.348 \text{ Å})^{12}$  but larger than the one in primary (1.326 Å) and secondary (1.341 Å) amides.<sup>24</sup> This suggests that the Coulomb repulsion between C(1) and C(2) gives rise to an additional lengthening of the adjacent C(1)-N(1) bonds and also C(2)-C(3) bond since the conjugation of the C(1)-C(2) single bond is no longer posible.

The observed carbonyl C=O distances 1.230(3)Å for C(2)=O(2) and 1.226(3) Å for C(1)=O(1) are slightly longer than those found for p-tolyl phenylthioglyoxylate,<sup>14</sup> glyoxylate<sup>17</sup> and benzil<sup>18</sup> (see Table 5). The above is consistent with the concept that N-H O=C bond formation is associated with an enhanced delocalization of  $\pi$ -electrons of the amidic group and implies elongation of the C=O distances.<sup>25</sup> In fact, the C=O distances of 1.229(9) Å in the tertiary amides (where the formation of a hydrogen bond is impossible) are only a little shorter than those of 1.238(9) Å found for secondary and primary amides where the hydrogen bonds are always formed.<sup>24</sup> The small elongation of the C=O bond distance observed for the reported structure may be a consequence of a weaker  $\pi$ -electron delocalization and longer intermolecular hydrogen bond. This is also influenced by the concomitant presence of the intramolecular N(1) - H(1) - O(2) hydrogen bond which results in weakening of both inter- and intramolecular N-H O hydrogen bonds.

An interesting point to be noted are the bond angles at the N(1) atom. The large bond angle C(1)-N(1)-C(9) [128.6(2)°] suggests sp<sup>2</sup> hybridization for the nitrogen N(1) atom of the amide. This is further demonstrated by the nearness to 360° of the sums of the bond angles around N(1). We assume that the observed bond angles result from the conjugation between the N(1) atom and phenyl ring. The C(1)-N(1)-C(9) angle is close to a value found for p-methyl-phenyl glyoxylacid-m-trifluoro-anilide

**Table 5.** A comparison of the selected bond distances (Å) and torsion angles (°) for phenyl phenylglyoxamide (X=NH,R=Ph) (present work), p-tolyl phenylthioglyoxylate (X=S, R=PhMe).<sup>14</sup> (-)-menthyl p-bromophenylglyoxylate (X=O, R=(-)-menthyl)<sup>17</sup> and benzil<sup>18</sup>

		Distances			
Compounds	C(2) = C(3)	C(1)-C(2)	C(1)=O(1)	C(2)-O(2)	O(1)-C(1)-C(2)-O(2)
Glyoxamide	1.48	1.55	1.23	1.230	-163.6
Thioglyoxylate	1.47	1.55	1.2	1.22	-168.2
Glyoxylate	1.48	1.53	1.19	1.23	104
Benzil	1.48	1.52	1.210	1.210	68.8

 $(127.6^{\circ})$ .<sup>12</sup> Similar values were observed in the structure of N-aromatic amides where the corresponding angles tend to decrease with the increase in the dihedral angle between the planes of the amide group and the aromatic ring.<sup>26</sup>

The conformation about the N(1)-C(9) as well as about the C(2)-C(3) bonds describe torsion angles C(1)-N(1)-C(9)-C(14) and C(1)-C(2)-C(3)-C(3)-C(3)C(8) which equal -2.8(5) and  $22.8(4)^{\circ}$ , respectively. These torsion angles are adjusted under the influence of the two weak intramolecular interactions C(8)-H(8)-O(1) H(14)-C(14), which stabilize the observed conformation of the two phenyl rings within the molecule. Therefore, both phenyl rings could have avoided steric hindrance due to slight rotation around the N(1)-C(9) and C(2)-C(3) bonds, thus simultaneously improving the coplanarity of the whole molecule  $(\sigma_{av} = 0.283 \text{ Å})$ . The conformation about these bonds differs from that observed for the corresponding bonds in the crystal structure of thioglyoxylate<sup>14</sup> and glyoxylate.<sup>16,17</sup>

The attractive N(H) O interactions imply a dramatic change in the bond angles at C(1) and C(2). The O(2)-C(2)-C(1) and N(1)-C(1)-C(2) bond angles are decreased to 117.0(2) and 112.1(2)°, respectively, while the O(1)-C(1)-N(1) is enlarged to 126.3(3)°. As a result of steric interactions between H(8) and O(1), respectively, H(14) and O(1), the corresponding adjacent outer angles, are enlarged. The angle C(8)-C(3)-C(2) [123.3 (3)°] is clearly larger than the neighbouring angle C(4)-C(3)-C(2) [117.6(2)°]. The situation at the other phenyl group is analogous: i.e., the angle C(14)-C(9)-N(1) [123.8(3)°] is distinctly larger than the adjacent C(10)-C(9)-N(1)[116.6(3)°].

Comparison of the crystal structures of p-tolyl phenylthioglyoxylate and phenyl phenylglyoxamide showed close conformational similarities among these molecules. In both cases the two carbonyl groups are oriented antiperiplanar to each other. These conformations result from either the nonbonded attractive intramolecular interaction of sulfur and oxygen in the case of p-tolyl phenylthioglyoxylate or the intramolecular hydrogen bond  $C=O\cdots H-N$  and short contacts  $C-H\cdots O=C$  in the crystal structure of phenyl phenylglyoxamide. These types of interaction imply the change in the bond distances and correspondingly modifie bond angles.

# Acknowledgments

This study was supported partly by the Silesian School of Medicine and partly by the Centre National de la Recherche Scientifique.

Supplementary material. Crystallographic data (excluding structure factors) for the structure(s) reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1003/5382. Copies of available material can be obtained, free of charge, on application to the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44-(0)1223-336033 or Email: deposit@ccdc.cam.ac.uk).

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