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## Structure Reports

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## o-Benzoquinone dioxime

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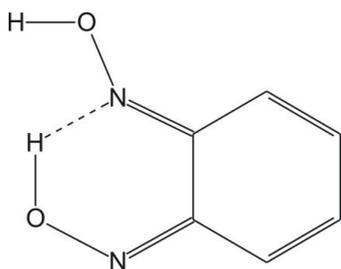
Received 14 September 2010; accepted 4 October 2010

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.034;  $wR$  factor = 0.082; data-to-parameter ratio = 4.7.

The title compound,  $\text{C}_6\text{H}_6\text{N}_2\text{O}_2$ , was obtained as a product of an *in vitro* study of the metabolism of benzofuroxan. The molecule exhibits a *amphi* configuration of the oxime groups  $\text{C}=\text{N}-\text{OH}$ . One oxime group is involved in the formation of a strong intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond, while another links molecules into zigzag chains along the  $c$  axis via intermolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds.

## Related literature

For details of the synthesis, see: Grosa *et al.* (2004). For a related structure, see: Mégnamisi-Bélombé & Endres (1985).



## Experimental

## Crystal data

 $\text{C}_6\text{H}_6\text{N}_2\text{O}_2$   
 $M_r = 138.13$ 

 Orthorhombic,  $Pca2_1$   
 $a = 15.009$  (5) Å

 $b = 3.8181$  (13) Å  
 $c = 10.694$  (3) Å  
 $V = 612.8$  (4) Å<sup>3</sup>  
 $Z = 4$ 

 Mo  $K\alpha$  radiation  
 $\mu = 0.12$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.24 \times 0.12 \times 0.04$  mm

## Data collection

 Siemens-Bruker APEX  
 diffractometer  
 Absorption correction: multi-scan  
 (Blessing, 1995)  
 $T_{\min} = 0.856$ ,  $T_{\max} = 1.000$   
 2330 measured reflections

 468 independent reflections  
 418 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.055$   
 $\theta_{\text{max}} = 23.3^\circ$   
 11 standard reflections every 60 min  
 intensity decay: none

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.082$   
 $S = 1.01$   
 468 reflections  
 99 parameters  
 1 restraint

 H atoms treated by a mixture of  
 independent and constrained  
 refinement  
 $\Delta\rho_{\text{max}} = 0.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.13$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\cdots\text{N2}^i$	0.85 (7)	1.92 (7)	2.745 (4)	162 (6)
$\text{O2}-\text{H2}\cdots\text{N1}$	1.06 (8)	1.57 (8)	2.532 (4)	147 (6)

Symmetry code: (i)  $-x + 1, -y + 1, z - \frac{1}{2}$ .

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

We thank Professor A. Gasco for supplying crystals of the title compound.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2766).

## References

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 Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.  
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 Mégnamisi-Bélombé, M. & Endres, H. (1985). *Acta Cryst.* **C41**, 513–515.  
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## supporting information

*Acta Cryst.* (2010). E66, o2764 [https://doi.org/10.1107/S1600536810039619]

### ***o*-Benzoquinone dioxime**

**Giuliana Gervasio, Domenica Marabello and Federica Bertolotti**

#### **S1. Comment**

The title compound, *o*-benzoquinone dioxime, has been obtained according to Grosa *et al.* (2004). In the C1—C6 ring the C3-C4 and C5-C6 bond distances correspond to formal double bonds (1.336 (5) Å *av.*). Also the C1-N1 and C2-N2 distances agree with a double bond character (1.304 (5) Å *av.*). Noteworthy is the presence of a strong intramolecular hydrogen bond O2-H2...N2 that probably stabilize the *syn* form of the dioxime. A further intermolecular hydrogen bond O1-H1...N2 forms chains of molecules. *O*-benzoquinone dioxime is known as an excellent ligand which forms bis-chelated transition metal complexes especially with the dipositive metal ions of the Ni triad (cf. Mégnamisi-Bélombé & Endres, 1985).

#### **S2. Experimental**

The *o*-benzoquinone dioxime has been obtained according to Grosa *et al.* (2004)

#### **S3. Refinement**

A very small and poorly diffracting crystal has been used; it was not possible to obtain a better crystal because it is a product of a metabolism. C-bound H atoms were placed in geometrically idealized positions (C—H = 0.93 Å), and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . Two O-bound H atoms were located on a difference map and refined isotropically. A restraint has been imposed on the planarity of the hexagonal ring. In the absence of any significant anomalous scatterers in the molecule, 368 Friedel pairs were merged before the final refinement.

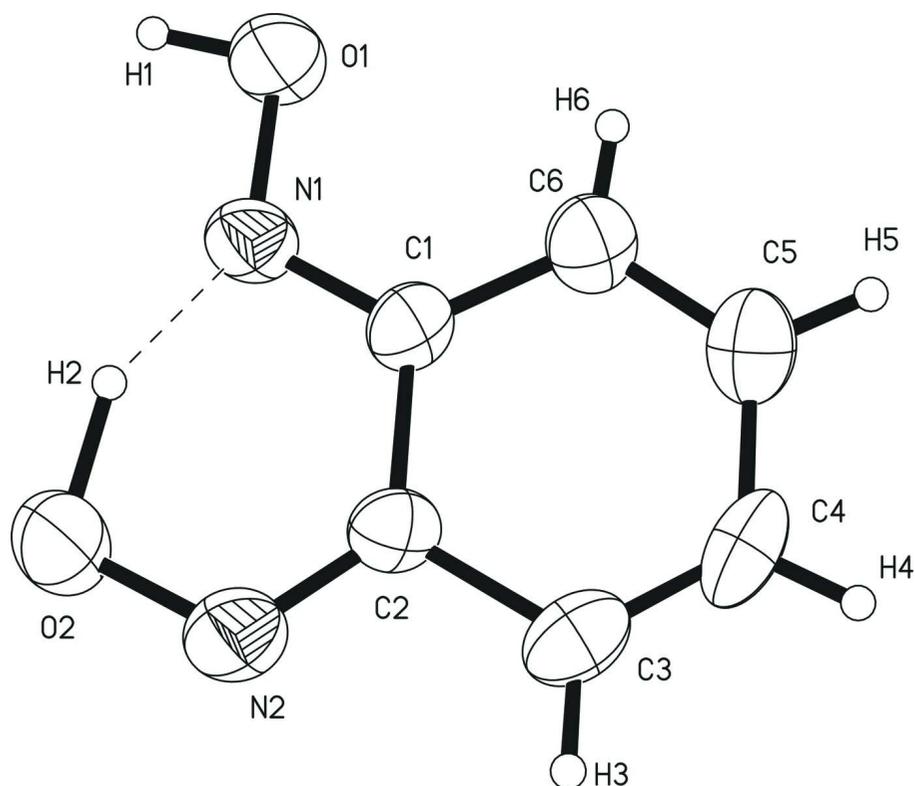


Figure 1

The molecular structure of the title compound showing the atomic numbering and 50% of probability displacements ellipsoids.

### *o*-Benzoquinone dioxime

#### Crystal data

$C_6H_6N_2O_2$

$M_r = 138.13$

Orthorhombic,  $Pca2_1$

$a = 15.009 (5) \text{ \AA}$

$b = 3.8181 (13) \text{ \AA}$

$c = 10.694 (3) \text{ \AA}$

$V = 612.8 (4) \text{ \AA}^3$

$Z = 4$

$F(000) = 288$

$D_x = 1.497 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 500 reflections

$\theta = 2.7\text{--}23.3^\circ$

$\mu = 0.12 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Prism, orange

$0.24 \times 0.12 \times 0.04 \text{ mm}$

#### Data collection

Siemens–Bruker APEX  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  scans

Absorption correction: multi-scan  
(Blessing, 1995)

$T_{\min} = 0.856$ ,  $T_{\max} = 1.000$

2330 measured reflections

468 independent reflections

418 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.055$

$\theta_{\max} = 23.3^\circ$ ,  $\theta_{\min} = 2.7^\circ$

$h = -16 \rightarrow 16$

$k = -4 \rightarrow 3$

$l = -11 \rightarrow 11$

11 standard reflections every 60 min

intensity decay: none

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.034$  $wR(F^2) = 0.082$  $S = 1.01$ 

468 reflections

99 parameters

1 restraint

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sitesH atoms treated by a mixture of independent  
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0605P)^2]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -0.13 \text{ e } \text{\AA}^{-3}$ *Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6109 (3)	0.3317 (8)	0.4796 (3)	0.0377 (8)
C2	0.5481 (2)	0.2457 (9)	0.5795 (3)	0.0377 (8)
C3	0.5843 (3)	0.0751 (9)	0.6896 (3)	0.0479 (10)
H3A	0.5461	0.0119	0.7543	0.057*
C4	0.6706 (3)	0.0072 (9)	0.6998 (3)	0.0520 (12)
H4A	0.6919	-0.1043	0.7711	0.062*
C5	0.7312 (3)	0.1027 (10)	0.6031 (3)	0.0532 (10)
H5A	0.7916	0.0552	0.6128	0.064*
C6	0.7028 (3)	0.2599 (9)	0.4981 (3)	0.0461 (9)
H6A	0.7437	0.3225	0.4368	0.055*
N1	0.5761 (2)	0.4735 (7)	0.3794 (3)	0.0426 (8)
N2	0.4629 (2)	0.3068 (8)	0.5828 (3)	0.0489 (8)
O1	0.6388 (2)	0.5573 (8)	0.2905 (2)	0.0561 (8)
H1	0.603 (4)	0.638 (17)	0.236 (6)	0.11 (2)*
O2	0.4235 (2)	0.4598 (7)	0.4801 (2)	0.0584 (9)
H2	0.477 (5)	0.541 (17)	0.422 (6)	0.13 (2)*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.045 (2)	0.0412 (18)	0.0267 (15)	-0.0013 (15)	-0.0039 (15)	-0.0047 (13)
C2	0.043 (2)	0.0426 (19)	0.0278 (15)	-0.0044 (16)	0.0022 (16)	-0.0053 (14)
C3	0.067 (3)	0.046 (2)	0.0306 (17)	-0.0030 (17)	0.0005 (18)	-0.0007 (18)
C4	0.072 (3)	0.050 (2)	0.035 (2)	0.004 (2)	-0.018 (2)	0.0031 (14)

C5	0.054 (3)	0.055 (2)	0.050 (2)	0.0067 (19)	-0.012 (2)	-0.0059 (17)
C6	0.047 (2)	0.053 (2)	0.0382 (18)	0.0039 (18)	-0.0018 (17)	-0.0051 (17)
N1	0.041 (2)	0.0576 (19)	0.0294 (14)	-0.0035 (13)	0.0044 (16)	-0.0011 (12)
N2	0.051 (2)	0.0646 (18)	0.0306 (14)	0.0003 (17)	0.0034 (15)	-0.0015 (16)
O1	0.0470 (18)	0.091 (2)	0.0303 (12)	-0.0017 (14)	0.0032 (14)	0.0104 (13)
O2	0.046 (2)	0.090 (2)	0.0393 (14)	0.0042 (14)	-0.0021 (14)	0.0018 (13)

*Geometric parameters (Å, °)*

C1—N1	1.309 (5)	C4—H4A	0.9300
C1—C6	1.420 (5)	C5—C6	1.342 (5)
C1—C2	1.462 (5)	C5—H5A	0.9300
C2—N2	1.299 (4)	C6—H6A	0.9300
C2—C3	1.450 (5)	N1—O1	1.375 (4)
C3—C4	1.326 (6)	N2—O2	1.377 (4)
C3—H3A	0.9300	O1—H1	0.85 (7)
C4—C5	1.425 (6)	O2—H2	1.06 (8)
N1—C1—C6	125.5 (3)	C5—C4—H4A	119.5
N1—C1—C2	115.8 (3)	C6—C5—C4	121.2 (4)
C6—C1—C2	118.7 (3)	C6—C5—H5A	119.4
N2—C2—C3	115.3 (3)	C4—C5—H5A	119.4
N2—C2—C1	127.8 (3)	C5—C6—C1	120.8 (4)
C3—C2—C1	116.9 (3)	C5—C6—H6A	119.6
C4—C3—C2	121.4 (4)	C1—C6—H6A	119.6
C4—C3—H3A	119.3	C1—N1—O1	112.9 (3)
C2—C3—H3A	119.3	C2—N2—O2	118.5 (3)
C3—C4—C5	120.9 (3)	N1—O1—H1	97 (4)
C3—C4—H4A	119.5	N2—O2—H2	105 (4)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1...N2 <sup>i</sup>	0.85 (7)	1.92 (7)	2.745 (4)	162 (6)
O2—H2...N1	1.06 (8)	1.57 (8)	2.532 (4)	147 (6)

Symmetry code: (i)  $-x+1, -y+1, z-1/2$ .