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o-Benzoquinone dioxime

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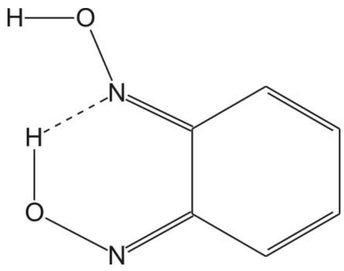
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.082; data-to-parameter ratio = 4.7.

The title compound, $C_6H_6N_2O_2$, 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 C=N—OH. One oxime group is involved in the formation of a strong intramolecular O—H$\cdots$N hydrogen bond, while another links molecules into zigzag chains along the c axis *via* intermolecular O—H$\cdots$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

$C_6H_6N_2O_2$
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^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 K
0.24 × 0.12 × 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 $I > 2\sigma(I)$
$R_{\rm int}$ = 0.055
$\theta_{\max}$ = 23.3°
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
$\Delta\rho_{\max}$ = 0.19 e Å^{-3}
$\Delta\rho_{\min}$ = −0.13 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$\cdots$N2$^{\rm i}$	0.85 (7)	1.92 (7)	2.745 (4)	162 (6)
O2—H2$\cdots$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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Mégnamisi-Bélombé, M. & Endres, H. (1985). *Acta Cryst.* C**41**, 513–515.
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supplementary materials

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o-Benzoquinone dioxime

G. Gervasio, **D. Marabello** and **F. Bertolotti**

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).

Experimental

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

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 $U_{iso}(H) = 1.2U_{eq}(C)$. 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.

Figures

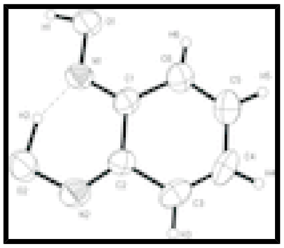

Fig. 1. The molecular structure of trhe title compound showing the atomic numbering and 50% of probability displacements ellipsoids.

o-Benzoquinone dioxime

Crystal data

$C_6H_6N_2O_2$

$M_r = 138.13$

Orthorhombic, $Pca2_1$

$a = 15.009 (5)$ Å

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

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 500 reflections

$\theta = 2.7–23.3°$

$b = 3.8181$ (13) Å

$c = 10.694$ (3) Å

$V = 612.8$ (4) Å^3

$Z = 4$

$F(000) = 288$

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

$T = 293$ K

Prism, orange

0.24 × 0.12 × 0.04 mm

Data collection

Siemens–Bruker APEX diffractometer

Radiation source: fine-focus sealed tube

graphite

φ scans

Absorption correction: multi-scan (Blessing, 1995)

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

2330 measured reflections

468 independent reflections

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

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

$\theta_{\text{max}} = 23.3°$, $\theta_{\text{min}} = 2.7°$

$h = -16 \rightarrow 16$

$k = -4 \rightarrow 3$

$l = -11 \rightarrow 11$

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 methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.19$ e Å^{-3}

$\Delta\rho_{\text{min}} = -0.13$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{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 (Å^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, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2^{i}	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 codes: (i) $-x+1, -y+1, z-1/2$.

Fig. 1