

Michael J. Goldcamp,
Jeanette A. Krause Bauer and
Michael J. Baldwin*

Department of Chemistry, University of Cincinnati,
Cincinnati, OH 45221-0172, USA

Correspondence e-mail: jeanette.krause@uc.edu

Key indicators

Single-crystal X-ray study

$T = 150$ K

Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å

R factor = 0.038

wR factor = 0.104

Data-to-parameter ratio = 11.2

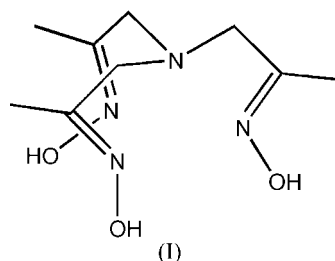
For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Tris(1-propan-2-onyl oxime)amine

The title compound, Ox_3H_3 or $\text{C}_9\text{H}_{18}\text{N}_4\text{O}_3$, adopts an open extended structure which does not restrict solvent accessibility or metallation reactivity. An intermolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond is observed.

Comment

Compounds with several different functional groups are of interest as chelating ligands for transition metals. For the past couple of years, our research effort has focused on the reactivity of Ni, Cu and Zn complexes (Goldcamp, Robison, Krause Bauer & Baldwin, 2002; Goldcamp, Robison, Squires *et al.*, 2002) of ligands sporting the tripodal geometry and incorporating oximate and mixed oxime/amide functionality (Goldcamp, Krause Bauer & Baldwin, 2000; Goldcamp, Rosa *et al.*, 2000). Tris(1-propan-2-onyl oxime)amine, (I), otherwise known as tris(2-hydroxyiminopropyl)amine, Ox_3H_3 , is such a ligand.



The molecular structure of (I) is similar to that observed for [N-(1-propan-2-onyl oxime)]bis[N-2-(N' , N'' -trimethylacetyl)aminoethyl]amine (Goldcamp, Rosa *et al.*, 2000) in that both have an open extended geometry rather than a folded geometry, as exhibited by tris[2-(benzoylamino)ethyl]amine (Goldcamp, Krause Bauer & Baldwin, 2000). Viewing (I) along its threefold axis, one observes a rather shallow symmetrical cavity with a depth of 1.8 Å (distance from N1 to the centroid of the methyl C atoms) and a width of 4.1 Å (distance between methyl C atoms). The opposite side of the molecule is open, making it accessible for reactivity with metals. Upon metallation, the three donor arms clamp down on the metal, forming a tripod motif, as observed in $\text{Ni}(\text{Ox}_3\text{H}_3)\text{Cl}_2$ (Goldcamp, Robison, Squires *et al.*, 2002) and $[\text{Ni}(\text{Ox}_3\text{H}_3)(\text{NO}_3)(\text{H}_2\text{O})]\text{NO}_3\cdot\text{H}_2\text{O}$ (Goldcamp, Robison, Krause Bauer & Baldwin, 2002). An intermolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond is observed (Table 1).

Experimental

The synthesis of (I) has been reported previously (Mattaipoulos, 1898; Oglloblin & Potekhin, 1965).

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Crystal data

$C_9H_{18}N_4O_3$
 $M_r = 230.27$
 Cubic, $I\bar{4}3d$
 $a = 17.1677(9) \text{ \AA}$
 $V = 5059.8(5) \text{ \AA}^3$
 $Z = 16$
 $D_x = 1.209 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation

Cell parameters from 4620 reflections
 $\theta = 2.9\text{--}28.2^\circ$
 $\mu = 0.09 \text{ mm}^{-1}$
 $T = 150(2) \text{ K}$
 Wedge, colorless
 $0.38 \times 0.20 \times 0.18 \text{ mm}$

Data collection

Bruker SMART 1K Platform CCD diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.966$, $T_{\max} = 0.984$
 15 298 measured reflections

573 independent reflections
 518 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.064$
 $\theta_{\text{max}} = 28.2^\circ$
 $h = -22 \rightarrow 19$
 $k = -22 \rightarrow 16$
 $l = -21 \rightarrow 22$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.104$
 $S = 1.07$
 573 reflections
 51 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 1.25P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1\cdots N2^i$	0.87	1.92	2.782 (3)	169

Symmetry codes: (i) $\frac{3}{4} - z, \frac{3}{4} - y, \frac{3}{4} + x$.

The hydroxyl H atom was located directly from a difference map and held fixed at that location ($O-H = 0.87 \text{ \AA}$). The remaining H atoms were either located directly or calculated, based on geometric criteria, and treated with a riding model ($C-H = 0.98$ and 0.99 \AA for CH_3 and CH_2 , respectively). H-atom isotropic displacement parameters were defined as aU_{eq} of the adjacent atom, where $a = 1.2$ for CH_2 and 1.5 for all others. Since this is a light-atom structure collected with data collected with Mo $K\alpha$ radiation, the Friedel pairs were merged.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve

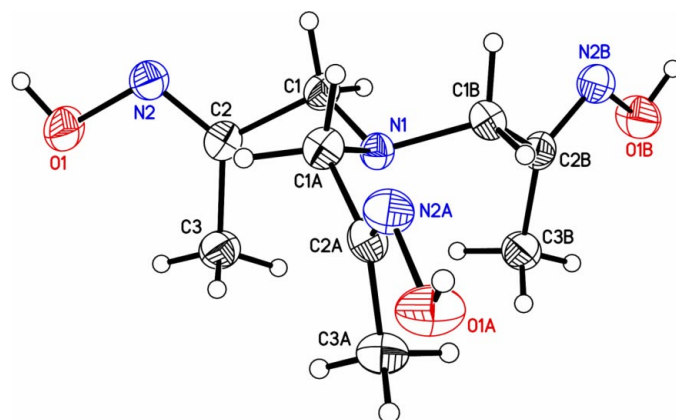


Figure 1

The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering scheme.

structure: SHELXTL (Bruker, 1998); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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