Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

An instance of tandem hydrogen bonding: the geometry of indan-1,2-dione 2-oxime in the solid state

Jens Hartung,[a]* Kristina Špehar,[a] Ingrid Svoboda[b] and Hartmut Fuess[b]

[a]Fachbereich Chemie, Organische Chemie, Technische Universität Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern, Germany, and [b]Strukturforschung, FB11 Material- und Geowissenschaften, Technische Universität Darmstadt, Petersenstraße 23, D-64287 Darmstadt, Germany

Correspondence e-mail: hartung@chemie.uni-kl.de

Key indicators

Single-crystal X-ray study
T = 300 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.107
Data-to-parameter ratio = 11.7

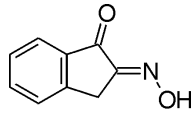
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 1 March 2004
Accepted 31 March 2004
Online 9 April 2004

The title compound, $C_9H_7NO_2$, adopts a planar geometry in the solid state and forms tandem hydrogen-bonded dimers.

Comment

Indan-1,2-dione 2-oxime, (I), crystallizes in the monoclinic space group $P2_1/n$. The unit cell contains four molecules of the title compound, (I), which form pairs of tandem hydrogen-bonded dimers (Table 1, Figs. 1 and 2). Neighbouring pairs of these dimers are orthogonally arranged with respect to each other. The atoms of the oxime group [N1—C2—C1—O2 = 0.8 (3)° and H—O1—N1—C2 = 178 (2)°] are located in a plane of sp^2-hybridized C atoms [*e.g.* C1—C2—C3—C4 = 0.0 (2)° and C1—C5—C4—C3 = 0.3 (2)°]. The distance N1—O1 = 1.400 (2) Å is in agreement with an N—O single bond (Hartung *et al.*, 1996).



(I)

Experimental

Indan-1,2-dione 2-oxime crystallized from a solution of analytically pure *N*-hydroxy-4*H*-indeno[1,2-*d*]thiazole-2(3*H*)-thione (Hartung *et al.*, 2004) in CH_2Cl_2 on standing for 14 d at 293 K. *N*-Hydroxy-4*H*-indeno[1,2-*d*]thiazole-2(3*H*)-thione was prepared from 2-indanone in an extension to a literature procedure (Hartung & Schwarz, 2002).

Crystal data

$C_9H_7NO_2$
M_r = 161.16
Monoclinic, $P2_1/n$
a = 6.169 (2) Å
b = 5.410 (2) Å
c = 22.606 (4) Å
β = 95.97 (2)°
V = 750.4 (4) Å^3
Z = 4
D_x = 1.427 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1212 reflections
θ = 3.4–22.2°
μ = 0.10 mm^{-1}
T = 300 (2) K
Prism, brown
0.40 × 0.16 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur CCD diffractometer
ω scans
Absorption correction: none
4349 measured reflections
1527 independent reflections
1075 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.4°
$h = -7 \rightarrow 6$
$k = -6 \rightarrow 6$
$l = -28 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.107
S = 1.04
1527 reflections
131 parameters
Only coordinates of H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.012 (5)

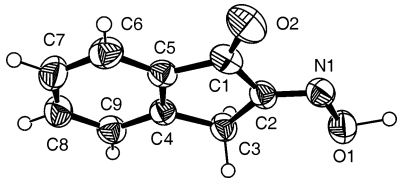


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	1.03 (2)	1.80 (2)	2.770 (2)	155.0 (16)

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

All H atom coordinates were refined, but displacement parameters were constrained to $1.2U_{eq}$ of the parent atoms.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2001); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2001); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997) and *PLATON*2002 (Spek, 2002); software used to prepare material for publication: *SHELXL*97.

This work was supported by the Deutsche Forschungsgemeinschaft (Graduiertenkolleg 690: Elektronendichte – Theorie und Experiment).

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hartung, J., Gottwald, T. & Špehar, K. (2004). In preparation.
Hartung, J., Hiller, M., Schwarz, M., Svoboda, I. & Fuess, H. (1996). *Liebigs Ann. Chem.* pp. 2091–2097.
Hartung, J. & Schwarz, M. (2002). *Org. Synth.* **79**, 228–235.

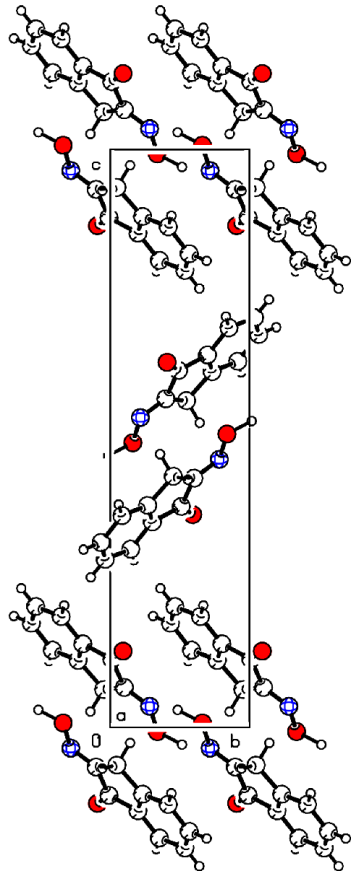


Figure 2
Packing of (I) in the unit cell, viewed along 100.

Oxford Diffraction (2001). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2002) *PLATON*. Version 160902. Utrecht University, The Netherlands.