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2-(1,3-Dioxolan-2-yl)phenol

Tonia Kretz, Hans-Wolfram Lerner and Michael Bolte*

Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany
Correspondence e-mail: bolte@chemie.uni-frankfurt.de

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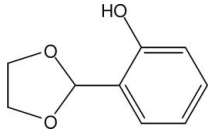
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.093; data-to-parameter ratio = 12.8.

Geometric parameters of the title compound, $C_9H_{10}O_3$, are in the usual ranges. The dioxolane ring adopts an envelope conformation with one of the ring O atoms deviating by 0.477 (4) Å from the plane of the remaining four atoms [C—O—C—C torsion angle = −0.6 (3)°]. The molecules are linked by an O—H···O hydrogen bond, forming zigzag chains running along the *a* axis.

Related literature

For related literature, see: Kretz *et al.* (2007); Lerner *et al.* (2006).



Experimental

Crystal data

$C_9H_{10}O_3$
M_r = 166.17
Orthorhombic, *Pbca*
a = 7.4564 (15) Å
b = 11.172 (2) Å
c = 19.633 (4) Å
V = 1635.5 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 173 (2) K
0.24 × 0.12 × 0.03 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: none
5325 measured reflections
1413 independent reflections
774 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.093
S = 0.86
1413 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O12^{i}	0.84	1.92	2.745 (3)	167

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2361).

References

Kretz, T., Bats, J. W., Lerner, H.-W. & Wagner, M. (2007). *Z. Naturforsch. Teil B*, **62**, 66–74.
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supplementary materials

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2-(1,3-Dioxolan-2-yl)phenol

T. Kretz, H.-W. Lerner and M. Bolte

Comment

We report here the X-ray crystal structure analysis of salicylaldehyde ethylene cyclic acetal. Recently, we have synthesized complexes with redox-active hydroquinone / quinone ligands (Lerner *et al.*, 2006; Kretz *et al.*, 2007). To get more information about ligand properties we focus our interest now on the synthesis of complexes with identical geometrical parameters but with redox-inactive ("innocent") ligands coordinate on the transition metal centers. Therefore we decided to prepare the salicylaldehyde ethylene cyclic acetal as starting material of these "innocent" ligands.

Geometric parameters of the title compound are in the usual ranges. The dioxolane ring adopts an envelope conformation with one of the ring O atoms deviating by 0.477 (4) Å from the plane of the remaining four atoms [torsion angle C11—O12—C13—C14 − 0.6 (3)°]. The molecules are linked by a O—H···O hydrogen bond to zigzag chains running along the *a* axis.

Experimental

A mixture of commercially available salicylaldehyde (2.8 g, 23 mmol), ethylene glycole (3.3 g, 53 mmol), and toluene (40 mL), and *p*-toluenesulfonic acid (0.1 g) was boiled for six hours in a flask fitted with a water-separator head. Single crystals of title compound were obtained from the reaction mixture at ambient temperature.

Refinement

H atoms bonded to C were refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C,*O*)] using a riding model with O—H = 0.84Å and C—H ranging from 0.95Å to 1.0 Å. The hydroxy group was allowed to rotate but not to tip.

Figures

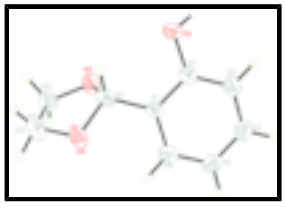

Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

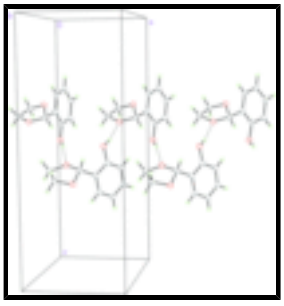

Fig. 2. Partial packing diagram of the title compound. Hydrogen bonds shown as dashed lines.

2-(1,3-Dioxolan-2-yl)phenol

Crystal data

$C_9H_{10}O_3$	F_{000} = 704
M_r = 166.17	D_x = 1.350 Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 2262 reflections
a = 7.4564 (15) Å	θ = 3.6–25.2º
b = 11.172 (2) Å	μ = 0.10 mm^{-1}
c = 19.633 (4) Å	*T* = 173 (2) K
V = 1635.5 (6) Å^3	Plate, colourless
Z = 8	0.24 × 0.12 × 0.03 mm

Data collection

Stoe IPDSII two-circle diffractometer	774 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.082
Monochromator: graphite	θ_{max} = 25.0º
T = 173(2) K	θ_{min} = 3.7º
ω scans	*h* = −8→8
Absorption correction: none	*k* = −13→13
5325 measured reflections	*l* = −22→23
1413 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H-atom parameters constrained
$wR(F^2)$ = 0.093	$w = 1/[\sigma^2(F_o^2) + (0.0241P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.86	$(\Delta/\sigma)_{max} < 0.001$
1413 reflections	$\Delta\rho_{max}$ = 0.19 e Å^{-3}

110 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. ;

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.5283 (4)	0.3479 (2)	0.62327 (12)	0.0247 (6)
C2	0.6308 (4)	0.2789 (2)	0.57795 (12)	0.0294 (7)
O2	0.6007 (3)	0.29787 (18)	0.50973 (8)	0.0396 (6)
H2	0.6481	0.2425	0.4871	0.048*
C3	0.7516 (5)	0.1944 (2)	0.60194 (13)	0.0351 (7)
H3	0.8193	0.1476	0.5708	0.042*
C4	0.7735 (5)	0.1784 (3)	0.67196 (13)	0.0394 (8)
H4	0.8556	0.1204	0.6887	0.047*
C5	0.6755 (5)	0.2469 (2)	0.71662 (14)	0.0359 (8)
H5	0.6904	0.2361	0.7643	0.043*
C6	0.5561 (4)	0.3312 (2)	0.69295 (12)	0.0306 (7)
H6	0.4914	0.3788	0.7246	0.037*
C11	0.3905 (5)	0.4325 (2)	0.59682 (13)	0.0295 (7)
H11	0.4365	0.4747	0.5554	0.035*
O12	0.2257 (3)	0.36945 (17)	0.58096 (9)	0.0373 (5)
C13	0.0756 (5)	0.4432 (3)	0.60146 (18)	0.0490 (9)
H13A	0.0010	0.4020	0.6360	0.059*
H13B	−0.0004	0.4643	0.5619	0.059*
C14	0.1629 (5)	0.5515 (3)	0.63072 (18)	0.0472 (9)
H14A	0.1635	0.6177	0.5972	0.057*
H14B	0.0986	0.5785	0.6721	0.057*
O15	0.3404 (3)	0.51632 (15)	0.64692 (10)	0.0393 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0240 (18)	0.0245 (12)	0.0255 (13)	−0.0032 (12)	−0.0018 (12)	−0.0038 (10)
C2	0.0288 (19)	0.0295 (13)	0.0298 (14)	−0.0025 (13)	0.0028 (13)	−0.0032 (11)

O2	0.0542 (17)	0.0432 (11)	0.0215 (10)	0.0140 (11)	0.0020 (9)	−0.0046 (8)
C3	0.0321 (19)	0.0335 (14)	0.0395 (15)	0.0047 (16)	0.0017 (15)	−0.0049 (12)
C4	0.036 (2)	0.0406 (16)	0.0418 (17)	0.0061 (16)	−0.0024 (15)	0.0064 (13)
C5	0.0307 (19)	0.0474 (17)	0.0297 (14)	−0.0042 (14)	−0.0040 (13)	0.0021 (12)
C6	0.0319 (19)	0.0332 (14)	0.0268 (14)	−0.0031 (14)	0.0030 (13)	−0.0059 (11)
C11	0.034 (2)	0.0244 (13)	0.0301 (14)	−0.0009 (14)	0.0057 (13)	−0.0052 (11)
O12	0.0283 (14)	0.0363 (10)	0.0473 (11)	0.0056 (10)	−0.0091 (10)	−0.0151 (9)
C13	0.039 (2)	0.0544 (19)	0.0535 (19)	0.0139 (16)	−0.0095 (17)	−0.0176 (16)
C14	0.037 (2)	0.0367 (15)	0.068 (2)	0.0049 (15)	0.0060 (19)	−0.0116 (15)
O15	0.0324 (15)	0.0324 (10)	0.0530 (12)	0.0053 (10)	−0.0044 (11)	−0.0200 (10)

Geometric parameters (Å, °)

C1—C6	1.396 (4)	C6—H6	0.9500
C1—C2	1.404 (4)	C11—O15	1.408 (3)
C1—C11	1.490 (4)	C11—O12	1.450 (4)
C2—O2	1.374 (3)	C11—H11	1.0000
C2—C3	1.387 (4)	O12—C13	1.447 (4)
O2—H2	0.8400	C13—C14	1.489 (4)
C3—C4	1.396 (4)	C13—H13A	0.9900
C3—H3	0.9500	C13—H13B	0.9900
C4—C5	1.374 (4)	C14—O15	1.417 (4)
C4—H4	0.9500	C14—H14A	0.9900
C5—C6	1.376 (4)	C14—H14B	0.9900
C5—H5	0.9500		
C6—C1—C2	117.8 (3)	O15—C11—C1	111.2 (2)
C6—C1—C11	121.9 (2)	O12—C11—C1	110.6 (2)
C2—C1—C11	120.2 (2)	O15—C11—H11	110.2
O2—C2—C3	122.8 (2)	O12—C11—H11	110.2
O2—C2—C1	116.4 (2)	C1—C11—H11	110.2
C3—C2—C1	120.8 (2)	C13—O12—C11	108.6 (2)
C2—O2—H2	109.5	O12—C13—C14	103.4 (3)
C2—C3—C4	119.8 (3)	O12—C13—H13A	111.1
C2—C3—H3	120.1	C14—C13—H13A	111.1
C4—C3—H3	120.1	O12—C13—H13B	111.1
C5—C4—C3	119.7 (3)	C14—C13—H13B	111.1
C5—C4—H4	120.2	H13A—C13—H13B	109.0
C3—C4—H4	120.2	O15—C14—C13	105.6 (2)
C4—C5—C6	120.6 (3)	O15—C14—H14A	110.6
C4—C5—H5	119.7	C13—C14—H14A	110.6
C6—C5—H5	119.7	O15—C14—H14B	110.6
C5—C6—C1	121.2 (3)	C13—C14—H14B	110.6
C5—C6—H6	119.4	H14A—C14—H14B	108.7
C1—C6—H6	119.4	C11—O15—C14	106.0 (2)
O15—C11—O12	104.4 (2)		
C6—C1—C2—O2	−179.8 (3)	C6—C1—C11—O15	19.3 (4)
C11—C1—C2—O2	2.4 (4)	C2—C1—C11—O15	−162.9 (2)
C6—C1—C2—C3	2.0 (4)	C6—C1—C11—O12	−96.2 (3)
C11—C1—C2—C3	−175.9 (3)	C2—C1—C11—O12	81.6 (3)

O2—C2—C3—C4	−178.9 (3)	O15—C11—O12—C13	21.0 (3)
C1—C2—C3—C4	−0.7 (5)	C1—C11—O12—C13	140.6 (2)
C2—C3—C4—C5	−0.3 (5)	C11—O12—C13—C14	−0.6 (3)
C3—C4—C5—C6	0.0 (5)	O12—C13—C14—O15	−19.9 (3)
C4—C5—C6—C1	1.3 (5)	O12—C11—O15—C14	−33.9 (3)
C2—C1—C6—C5	−2.2 (4)	C1—C11—O15—C14	−153.1 (2)
C11—C1—C6—C5	175.6 (3)	C13—C14—O15—C11	34.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O12^{i}	0.84	1.92	2.745 (3)	167

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*+1.

Fig. 1

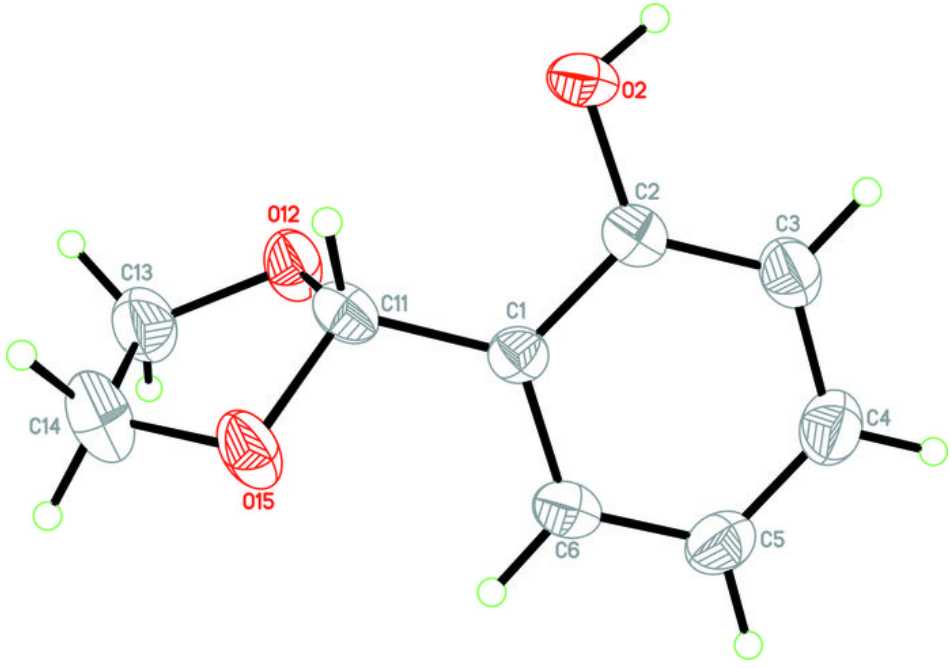

Fig. 2