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4,4′-Oxydibenzoic acid

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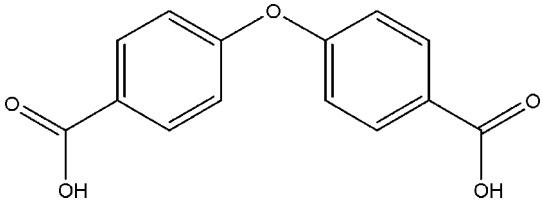
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.123; data-to-parameter ratio = 15.0.

In the title compound, $C_{14}H_{10}O_5$, each carboxyl group is coplanar with the attached aromatic ring. The dihedral angle between these planes is 72.56 (5)°. The carboxyl groups are linked by a pair of centrosymmetric O—H···O hydrogen bonds, creating a zigzag chain along the [2$\bar{3}$1] direction.

Related literature

For related literature, see: Eddaoudi *et al.* (2001); Férey *et al.* (2005).



Experimental

Crystal data

$C_{14}H_{10}O_5$
M_r = 258.22
Triclinic, $P\bar{1}$
a = 5.3654 (9) Å
b = 6.4093 (11) Å
c = 16.847 (3) Å
α = 86.848 (3)°
β = 83.106 (3)°
γ = 79.309 (3)°
V = 564.86 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 100 (2) K
0.33 × 0.24 × 0.10 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: none
6444 measured reflections
2582 independent reflections
1901 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.123
S = 1.10
2582 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001; Atwood & Barbour, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2007).

We thank Professor L. J. Barbour for helpful discussions. Financial support for this work was provided by the National Research Foundation of South Africa, as well as SASOL Industries. The data collection was undertaken on an instrument managed by the Central Analytical Facility at the University of Stellenbosch.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2104).

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supplementary materials

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4,4'-Oxydibenzoic acid

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Comment

Considerable attention is focussed on the synthesis of new ligands for the construction of metal organic frameworks (MOF's) since they add structural diversity to these materials. This study originates from our interest in U-shaped ligands of the rigid aromatics containing their coordinating groups at the terminal site. Two such ligands may coordinate two metal centers, closing the circle and thus forming a box-like aperture. Upon crystallization these boxed structures may form a porous material. Materials of this type are increasingly in demand for applications in gas storage since they are selective to the shapes and sizes of the molecules that can pass through the enclosed pore. This selectivity is dependent on their structural framework and the pore size formed therein (Férey *et al.*, 2005). It has been found that multidentate linkers such as carboxylates allow the formation of more rigid frameworks than, for example, commonly used poly-topic *N*-bound organic linkers. This functionality is due to their ability to incorporate metal ions into M—O—C clusters (Eddaoudi *et al.*, 2001). To this end the dicarboxylic acid had been selected as an organic linker.

One such linker that was selected is 4,4'-oxydibenzoic acid, (**I**), commercially available from Sigma-Aldrich. However, its crystal structure has not been reported.

In the crystal structure, the respective acid groups are co-planar with their aromatic rings (Fig. 1). The angle subtended at the central oxygen atom, O3, is 117.97 (12)°. This is higher than the average C—O—C angle of 115° owing to the steric interactions between H6 and H13.

The angle between the least squares planes defined by the 6 carbon atoms of each benzene ring is 72.56 (0.05) °.

This structure forms a one-dimensional zig-zag chain that is linked via the H-bonds between the acid proton of one molecule and the carbonyl oxygen of another. The infinite chain of intermolecular H-bonded molecules packs along [2 -3 1].

Experimental

The compound was purchased from Sigma-Aldrich [CAS 2215-89-6] and recrystallised from ethanol without further purification.

Refinement

Structure solution and refinement was performed using the *SHELX-97* suite of programs. Hydrogen atoms were refined in calculated positions, using a riding model (C–H = 0.95 Å; O–H = 0.84 Å).

Figures

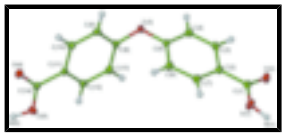

Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius.

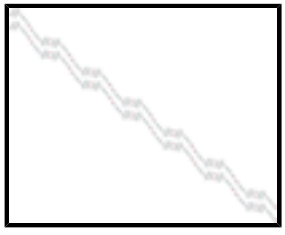

Fig. 2. The crystal packing of (I) viewed along [010] showing zig-zag chain. H-bonds are displayed as dashed lines.

4,4'-Oxydibenzoic acid

Crystal data

$C_{14}H_{10}O_5$	$Z = 2$
$M_r = 258.22$	$F_{000} = 268$
Triclinic, $P\bar{1}$	$D_x = 1.518$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.3654$ (9) Å	Cell parameters from 2085 reflections
$b = 6.4093$ (11) Å	$\theta = 2.4$–27.7º
$c = 16.847$ (3) Å	$\mu = 0.12$ mm^{-1}
$\alpha = 86.848$ (3)º	$T = 100$ (2) K
$\beta = 83.106$ (3)º	Needle, colourless
$\gamma = 79.309$ (3)º	0.33 × 0.24 × 0.10 mm
$V = 564.86$ (16) Å^3	

Data collection

Bruker APEX CCD area-detector diffractometer	1901 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.053$
Monochromator: graphite	$\theta_{max} = 28.3$º
$T = 100(2)$ K	$\theta_{min} = 2.4$º
ω scans	$h = -7 \rightarrow 6$
Absorption correction: none	$k = -8 \rightarrow 8$
6444 measured reflections	$l = -22 \rightarrow 22$
2582 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.0103P]$

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.123$

$S = 1.10$

2582 reflections

172 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.009$

$\Delta\rho_{max} = 0.38$ e Å^{-3}

$\Delta\rho_{min} = -0.35$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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}
O1	0.1763 (2)	1.24541 (18)	0.02374 (7)	0.0251 (3)
H1	0.0651	1.3129	−0.0037	0.030*
C1	0.2712 (3)	1.3777 (3)	0.06123 (10)	0.0176 (4)
O2	0.2019 (2)	1.57409 (18)	0.05702 (7)	0.0242 (3)
C2	0.4720 (3)	1.2816 (3)	0.11236 (10)	0.0171 (4)
O3	1.0046 (2)	1.03887 (17)	0.26827 (7)	0.0196 (3)
C3	0.5979 (3)	1.4139 (3)	0.14919 (10)	0.0179 (4)
H3	0.5621	1.5629	0.1385	0.022*
O4	1.1999 (2)	0.12156 (17)	0.43485 (7)	0.0206 (3)
C4	0.7753 (3)	1.3304 (3)	0.20139 (10)	0.0187 (4)
H4	0.8604	1.4211	0.2268	0.022*
O5	0.7865 (2)	0.22879 (18)	0.47782 (7)	0.0219 (3)
H5	0.8076	0.1086	0.5012	0.026*
C5	0.8262 (3)	1.1128 (3)	0.21581 (10)	0.0166 (4)
C6	0.7121 (3)	0.9777 (3)	0.17638 (10)	0.0199 (4)
H6	0.7564	0.8282	0.1845	0.024*
C7	0.5332 (3)	1.0625 (3)	0.12509 (10)	0.0194 (4)
H7	0.4522	0.9711	0.0986	0.023*
C8	0.9921 (3)	0.8447 (3)	0.30857 (10)	0.0167 (4)
C9	1.2095 (3)	0.6890 (3)	0.30130 (10)	0.0186 (4)
H9	1.3571	0.7134	0.2676	0.022*

C10	1.2098 (3)	0.4977 (3)	0.34358 (10)	0.0185 (4)
H10	1.3584	0.3903	0.3391	0.022*
C11	0.9941 (3)	0.4623 (2)	0.39243 (9)	0.0155 (4)
C12	0.7761 (3)	0.6215 (2)	0.39935 (10)	0.0174 (4)
H12	0.6280	0.5976	0.4329	0.021*
C13	0.7753 (3)	0.8134 (3)	0.35746 (10)	0.0184 (4)
H13	0.6280	0.9219	0.3622	0.022*
C14	0.9955 (3)	0.2569 (3)	0.43785 (10)	0.0153 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0253 (7)	0.0267 (7)	0.0242 (7)	0.0004 (6)	−0.0133 (6)	−0.0030 (6)
C1	0.0180 (9)	0.0188 (9)	0.0151 (8)	−0.0022 (7)	−0.0004 (7)	−0.0008 (7)
O2	0.0258 (7)	0.0194 (7)	0.0262 (7)	0.0009 (5)	−0.0077 (6)	0.0036 (5)
C2	0.0160 (9)	0.0213 (9)	0.0131 (8)	−0.0024 (7)	−0.0003 (7)	0.0000 (7)
O3	0.0204 (7)	0.0165 (6)	0.0236 (7)	−0.0055 (5)	−0.0086 (5)	0.0050 (5)
C3	0.0207 (9)	0.0132 (8)	0.0185 (9)	−0.0003 (7)	−0.0013 (7)	0.0003 (7)
O4	0.0185 (7)	0.0183 (7)	0.0236 (7)	0.0011 (5)	−0.0034 (5)	−0.0004 (5)
C4	0.0209 (9)	0.0189 (9)	0.0171 (9)	−0.0057 (7)	−0.0024 (7)	−0.0007 (7)
O5	0.0215 (7)	0.0182 (6)	0.0249 (7)	−0.0045 (5)	0.0007 (5)	0.0047 (5)
C5	0.0138 (8)	0.0203 (9)	0.0149 (8)	−0.0018 (7)	−0.0016 (7)	0.0016 (7)
C6	0.0212 (9)	0.0166 (9)	0.0215 (9)	−0.0018 (7)	−0.0044 (7)	0.0002 (7)
C7	0.0211 (9)	0.0180 (9)	0.0202 (9)	−0.0047 (7)	−0.0042 (7)	−0.0009 (7)
C8	0.0215 (9)	0.0136 (8)	0.0164 (9)	−0.0049 (7)	−0.0058 (7)	−0.0003 (7)
C9	0.0146 (9)	0.0226 (9)	0.0190 (9)	−0.0047 (7)	−0.0015 (7)	0.0002 (7)
C10	0.0165 (9)	0.0165 (9)	0.0216 (9)	−0.0005 (7)	−0.0022 (7)	−0.0015 (7)
C11	0.0182 (9)	0.0157 (9)	0.0137 (8)	−0.0036 (7)	−0.0053 (7)	−0.0008 (7)
C12	0.0147 (8)	0.0204 (9)	0.0174 (9)	−0.0035 (7)	−0.0022 (7)	−0.0023 (7)
C13	0.0175 (9)	0.0167 (9)	0.0203 (9)	0.0006 (7)	−0.0046 (7)	−0.0024 (7)
C14	0.0168 (9)	0.0147 (8)	0.0160 (8)	−0.0038 (7)	−0.0049 (7)	−0.0033 (7)

Geometric parameters (Å, °)

O1—C1	1.2933 (19)	C5—C6	1.386 (2)
O1—H1	0.8400	C6—C7	1.385 (2)
C1—O2	1.2455 (19)	C6—H6	0.9500
C1—C2	1.484 (2)	C7—H7	0.9500
C2—C7	1.392 (2)	C8—C13	1.382 (2)
C2—C3	1.390 (2)	C8—C9	1.385 (2)
O3—C5	1.3820 (19)	C9—C10	1.384 (2)
O3—C8	1.3930 (19)	C9—H9	0.9500
C3—C4	1.388 (2)	C10—C11	1.384 (2)
C3—H3	0.9500	C10—H10	0.9500
O4—C14	1.2633 (19)	C11—C12	1.400 (2)
C4—C5	1.385 (2)	C11—C14	1.485 (2)
C4—H4	0.9500	C12—C13	1.383 (2)
O5—C14	1.274 (2)	C12—H12	0.9500
O5—H5	0.8400	C13—H13	0.9500

C1—O1—H1	109.5	C2—C7—H7	120.0
O2—C1—O1	124.03 (15)	C13—C8—C9	121.36 (16)
O2—C1—C2	120.17 (15)	C13—C8—O3	121.04 (15)
O1—C1—C2	115.80 (15)	C9—C8—O3	117.50 (15)
C7—C2—C3	119.63 (16)	C10—C9—C8	119.44 (16)
C7—C2—C1	121.30 (15)	C10—C9—H9	120.3
C3—C2—C1	119.06 (15)	C8—C9—H9	120.3
C5—O3—C8	117.97 (12)	C9—C10—C11	120.15 (15)
C4—C3—C2	120.62 (16)	C9—C10—H10	119.9
C4—C3—H3	119.7	C11—C10—H10	119.9
C2—C3—H3	119.7	C10—C11—C12	119.74 (15)
C5—C4—C3	118.89 (16)	C10—C11—C14	119.96 (15)
C5—C4—H4	120.6	C12—C11—C14	120.29 (15)
C3—C4—H4	120.6	C13—C12—C11	120.30 (16)
C14—O5—H5	109.5	C13—C12—H12	119.9
O3—C5—C4	116.30 (14)	C11—C12—H12	119.9
O3—C5—C6	122.47 (15)	C8—C13—C12	119.01 (16)
C4—C5—C6	121.16 (16)	C8—C13—H13	120.5
C7—C6—C5	119.48 (16)	C12—C13—H13	120.5
C7—C6—H6	120.3	O4—C14—O5	123.99 (15)
C5—C6—H6	120.3	O4—C14—C11	119.03 (15)
C6—C7—C2	120.07 (16)	O5—C14—C11	116.98 (14)
C6—C7—H7	120.0		
O2—C1—C2—C7	172.85 (16)	C5—O3—C8—C13	−59.0 (2)
O1—C1—C2—C7	−6.4 (2)	C5—O3—C8—C9	124.55 (16)
O2—C1—C2—C3	−6.1 (2)	C13—C8—C9—C10	0.2 (3)
O1—C1—C2—C3	174.68 (15)	O3—C8—C9—C10	176.70 (14)
C7—C2—C3—C4	−3.0 (3)	C8—C9—C10—C11	0.3 (2)
C1—C2—C3—C4	175.93 (15)	C9—C10—C11—C12	−0.5 (2)
C2—C3—C4—C5	0.4 (3)	C9—C10—C11—C14	−179.86 (14)
C8—O3—C5—C4	155.32 (15)	C10—C11—C12—C13	0.2 (2)
C8—O3—C5—C6	−27.7 (2)	C14—C11—C12—C13	179.56 (14)
C3—C4—C5—O3	179.98 (14)	C9—C8—C13—C12	−0.5 (2)
C3—C4—C5—C6	3.0 (3)	O3—C8—C13—C12	−176.87 (14)
O3—C5—C6—C7	179.47 (15)	C11—C12—C13—C8	0.3 (2)
C4—C5—C6—C7	−3.7 (3)	C10—C11—C14—O4	4.2 (2)
C5—C6—C7—C2	1.1 (3)	C12—C11—C14—O4	−175.22 (15)
C3—C2—C7—C6	2.3 (3)	C10—C11—C14—O5	−175.75 (14)
C1—C2—C7—C6	−176.65 (15)	C12—C11—C14—O5	4.9 (2)

Fig. 1

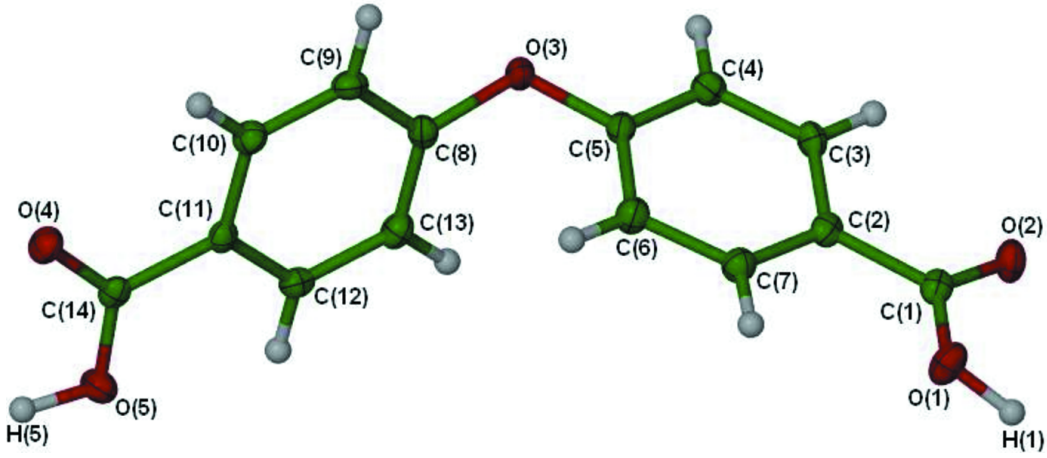

Fig. 2