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Benzene-1,3-diacetic acid

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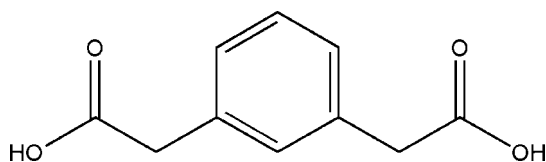
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.045; wR factor = 0.122; data-to-parameter ratio = 8.6.

Molecules of the title compound, $\text{C}_{10}\text{H}_{10}\text{O}_4$, are connected through $\text{O}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions into chains running along the c axis.

Related literature

For related literature, see Huo *et al.* (2004); Ma *et al.* (2003).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{10}\text{O}_4$	$V = 927.3$ (3) Å ³
$M_r = 194.18$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 4.9506$ (9) Å	$\mu = 0.11$ mm ⁻¹
$b = 10.0840$ (17) Å	$T = 293$ (2) K
$c = 18.576$ (3) Å	$0.31 \times 0.21 \times 0.19$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	5569 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 1998)	1094 independent reflections
$T_{\min} = 0.965$, $T_{\max} = 0.981$	970 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	127 parameters
$wR(F^2) = 0.121$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.21$ e Å ⁻³
1094 reflections	$\Delta\rho_{\text{min}} = -0.12$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O4}-\text{H4A}\cdots\text{O1}^i$	0.82	1.87	2.665 (3)	165
$\text{O2}-\text{H2}\cdots\text{O3}^{ii}$	0.82	1.87	2.673 (3)	165

 Symmetry codes: (i) $x, y - 1, z$; (ii) $x, y + 1, z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2762).

References

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Benzene-1,3-diacetic acid

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S1. Comment

The self-organization of small molecules with O—H···O and other weak intermolecular interactions is used to create one-, two-, and three-dimensional networks in crystalline solids (Huo *et al.*, 2004). Recently, aromatic di- or poly(carboxylic acids) have been investigated in the area of solid state and material science (Ma *et al.*, 2003). The title compound was synthesized from benzene-1,3-diacetic acid. In the crystal, molecules of the title compound are connected through O—H···O H-bonding interactions to chains running along the *c*-axis.

S2. Experimental

A hot aqueous solution of benzene-1,3-diacetic acid (1 mmol) was stirred until the white solids were dissolved. The clear solution was allowed to cool to room temperature and evaporated in air for 5 days. Then, colourless crystals of the title compound were obtained.

S3. Refinement

In the absence of anomalous scatterers Friedel pairs (714) were merged. H atoms were generated geometrically and refined as riding atoms with O—H = 0.82 Å, C_{aromatic}—H = 0.93 Å, C_{methylene}—H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$ or $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{O})$.

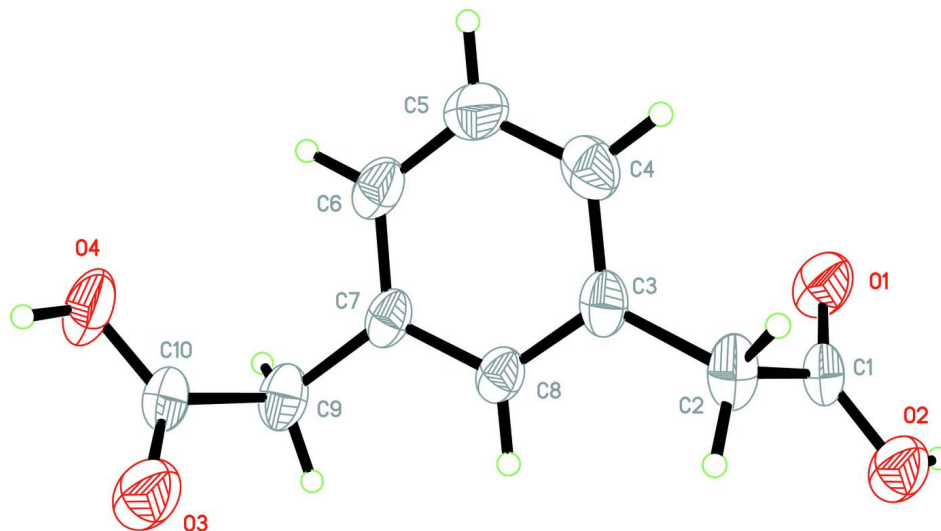


Figure 1

The structure of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Benzene-1,3-diacetic acid*Crystal data*C₁₀H₁₀O₄ $M_r = 194.18$ Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

 $a = 4.9506$ (9) Å $b = 10.0840$ (17) Å $c = 18.576$ (3) Å $V = 927.3$ (3) Å³ $Z = 4$ $F(000) = 408$ $D_x = 1.391$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1094 reflections

 $\theta = 1.1$ – 26.1° $\mu = 0.11$ mm⁻¹ $T = 293$ K

Block, colorless

 $0.31 \times 0.21 \times 0.19$ mm*Data collection*Bruker SMART APEX CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scans

Absorption correction: multi-scan

(SAINT; Bruker, 1998)

 $T_{\min} = 0.965$, $T_{\max} = 0.981$

5569 measured reflections

1094 independent reflections

970 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.020$ $\theta_{\max} = 26.1^\circ$, $\theta_{\min} = 2.2^\circ$ $h = -6 \rightarrow 5$ $k = -10 \rightarrow 12$ $l = -22 \rightarrow 22$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.044$ $wR(F^2) = 0.121$ $S = 1.06$

1094 reflections

127 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 0.1185P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.21$ e Å⁻³ $\Delta\rho_{\min} = -0.12$ 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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.6445 (5)	1.3039 (2)	0.89747 (14)	0.0773 (7)
O4	0.4524 (5)	0.53787 (19)	0.85467 (15)	0.0880 (8)
H4A	0.5318	0.4677	0.8616	0.132*
O2	1.0157 (5)	1.3432 (2)	0.83572 (13)	0.0805 (7)
H2	0.9320	1.4113	0.8265	0.121*

O3	0.8315 (5)	0.5825 (3)	0.79804 (15)	0.0910 (8)
C8	0.7293 (5)	0.9447 (2)	0.85307 (14)	0.0504 (6)
H8	0.8198	0.9542	0.8095	0.060*
C1	0.8739 (6)	1.2698 (2)	0.87529 (15)	0.0524 (7)
C7	0.5408 (5)	0.8441 (2)	0.86027 (14)	0.0503 (6)
C3	0.7872 (6)	1.0315 (2)	0.90849 (15)	0.0542 (7)
C2	0.9924 (6)	1.1399 (3)	0.89799 (18)	0.0668 (8)
H2A	1.0900	1.1526	0.9427	0.080*
H2B	1.1216	1.1116	0.8619	0.080*
C10	0.5972 (6)	0.6126 (3)	0.81796 (15)	0.0557 (7)
C9	0.4895 (7)	0.7476 (3)	0.79898 (15)	0.0626 (8)
H9A	0.2971	0.7418	0.7897	0.075*
H9B	0.5771	0.7794	0.7556	0.075*
C6	0.4047 (6)	0.8332 (3)	0.92448 (16)	0.0642 (8)
H6	0.2743	0.7676	0.9300	0.077*
C5	0.4588 (7)	0.9185 (3)	0.98098 (17)	0.0751 (10)
H5	0.3660	0.9098	1.0242	0.090*
C4	0.6514 (7)	1.0169 (3)	0.97298 (15)	0.0669 (8)
H4	0.6895	1.0735	1.0112	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0676 (14)	0.0528 (11)	0.1114 (17)	0.0114 (11)	0.0163 (14)	0.0152 (11)
O4	0.0761 (15)	0.0466 (10)	0.141 (2)	0.0002 (11)	0.0161 (15)	0.0274 (13)
O2	0.0756 (14)	0.0531 (11)	0.1130 (17)	0.0032 (12)	0.0200 (13)	0.0085 (12)
O3	0.0769 (16)	0.0728 (15)	0.123 (2)	0.0130 (14)	0.0221 (15)	0.0279 (14)
C8	0.0480 (13)	0.0394 (12)	0.0637 (15)	0.0030 (11)	0.0000 (12)	0.0093 (11)
C1	0.0520 (14)	0.0367 (12)	0.0684 (16)	-0.0057 (12)	-0.0130 (14)	-0.0069 (12)
C7	0.0445 (13)	0.0378 (12)	0.0686 (16)	0.0017 (10)	-0.0042 (13)	0.0142 (11)
C3	0.0507 (15)	0.0343 (11)	0.0775 (17)	0.0080 (11)	-0.0106 (13)	0.0041 (12)
C2	0.0531 (16)	0.0452 (14)	0.102 (2)	-0.0005 (13)	-0.0150 (17)	-0.0032 (15)
C10	0.0578 (16)	0.0420 (13)	0.0674 (16)	-0.0084 (13)	-0.0140 (14)	0.0039 (12)
C9	0.0645 (17)	0.0489 (15)	0.0745 (17)	-0.0043 (14)	-0.0209 (16)	0.0103 (13)
C6	0.0559 (17)	0.0465 (14)	0.090 (2)	0.0036 (14)	0.0103 (16)	0.0181 (14)
C5	0.090 (2)	0.0599 (18)	0.0756 (19)	0.0226 (19)	0.0233 (18)	0.0163 (15)
C4	0.083 (2)	0.0498 (15)	0.0682 (17)	0.0193 (17)	-0.0042 (16)	-0.0023 (14)

Geometric parameters (Å, °)

O1—C1	1.256 (4)	C3—C4	1.382 (4)
O4—C10	1.244 (4)	C3—C2	1.505 (4)
O4—H4A	0.8200	C2—H2A	0.9700
O2—C1	1.258 (3)	C2—H2B	0.9700
O2—H2	0.8200	C10—C9	1.503 (4)
O3—C10	1.255 (4)	C9—H9A	0.9700
C8—C3	1.381 (3)	C9—H9B	0.9700
C8—C7	1.385 (3)	C6—C5	1.383 (4)

C8—H8	0.9300	C6—H6	0.9300
C1—C2	1.496 (4)	C5—C4	1.384 (5)
C7—C6	1.375 (4)	C5—H5	0.9300
C7—C9	1.519 (4)	C4—H4	0.9300
C10—O4—H4A	109.5	H2A—C2—H2B	107.6
C1—O2—H2	109.5	O4—C10—O3	123.2 (3)
C3—C8—C7	122.1 (2)	O4—C10—C9	118.2 (3)
C3—C8—H8	118.9	O3—C10—C9	118.6 (3)
C7—C8—H8	118.9	C10—C9—C7	110.2 (2)
O1—C1—O2	122.3 (3)	C10—C9—H9A	109.6
O1—C1—C2	120.2 (3)	C7—C9—H9A	109.6
O2—C1—C2	117.5 (3)	C10—C9—H9B	109.6
C6—C7—C8	118.2 (3)	C7—C9—H9B	109.6
C6—C7—C9	121.1 (3)	H9A—C9—H9B	108.1
C8—C7—C9	120.6 (2)	C7—C6—C5	120.9 (3)
C8—C3—C4	118.5 (3)	C7—C6—H6	119.5
C8—C3—C2	120.2 (3)	C5—C6—H6	119.5
C4—C3—C2	121.2 (3)	C6—C5—C4	119.9 (3)
C1—C2—C3	114.1 (2)	C6—C5—H5	120.1
C1—C2—H2A	108.7	C4—C5—H5	120.1
C3—C2—H2A	108.7	C3—C4—C5	120.3 (3)
C1—C2—H2B	108.7	C3—C4—H4	119.8
C3—C2—H2B	108.7	C5—C4—H4	119.8

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4A \cdots O1 ⁱ	0.82	1.87	2.665 (3)	165
O2—H2 \cdots O3 ⁱⁱ	0.82	1.87	2.673 (3)	165

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.