

## 2-(Cyclohexa-1,4-dienyl)acetic acid

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## Key indicators

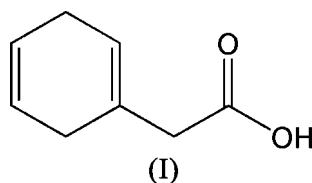
Single-crystal X-ray study  
 $T = 203$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.122  
Data-to-parameter ratio = 10.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title compound,  $\text{C}_6\text{H}_7\text{CH}_2\text{COOH}$ , is formed by a standard Birch reduction of phenylacetic acid. As expected, a centrosymmetric head-to-tail dimer is observed in the solid state, formed through  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds.

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## Comment

Dinuclear arene–ruthenium complexes are synthesized by dehydrogenation of the appropriate cyclohexadiene with  $\text{RuCl}_3$  hydrate (Bennett & Smith, 1974). The title compound, (I), has been used by Sheldrick and co-workers to synthesize the corresponding dinuclear arene ruthenium complex  $[(\eta^6\text{-C}_6\text{H}_5\text{CH}_2\text{COOH})\text{Ru}(\mu_2\text{-Cl})\text{Cl}]_2$  (Stodt *et al.*, 2003). However, it has not been characterized by X-ray crystal structure analysis before now.



The single-crystal X-ray structure analysis of (I) reveals a planar conformation of the 1,4-cyclohexadiene ring, with  $\text{C}=\text{C}$  double bonds of 1.333 (2) and 1.321 (3) Å. These values, as well as the other bond distances and angles, are similar to those found in other 1,4-cyclohexadiene derivatives, namely *N*-acetyl-D-2-(1,4-cyclohexadienyl)glycine ethyl ester (Dialer *et al.*, 2004) and 1,4-cyclohexadiene-1-glycine (Jandacek & Simonsen, 1969).

As expected, the acid function forms a centrosymmetric hydrogen-bonded dimer with a neighbouring molecule

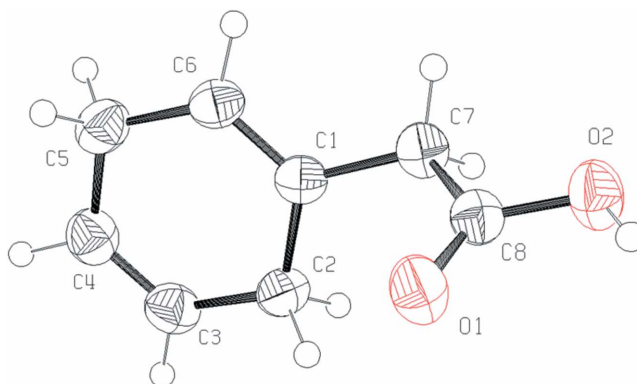


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

(Table 1, Fig. 2). A similar centrosymmetric hydrogen-bonded pair was observed in the single-crystal structure of phenylacetic acid (Hodgson & Asplund, 1991).

### Experimental

The title compound was prepared by standard Birch reduction of phenylacetic acid (Kuehne & Lambert, 1973). Colourless crystals of (I) suitable for single-crystal X-ray analysis were obtained by slow evaporation of a diethyl ether solution at 263 K.

#### Crystal data

$C_8H_{10}O_2$	$Z = 4$
$M_r = 138.16$	$D_x = 1.303 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/a$	Mo $K\alpha$ radiation
$a = 10.7111 (12) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 4.4150 (6) \text{ \AA}$	$T = 203 (2) \text{ K}$
$c = 14.9541 (18) \text{ \AA}$	Block, colourless
$\beta = 95.053 (14)^\circ$	$0.38 \times 0.28 \times 0.22 \text{ mm}$
$V = 704.42 (15) \text{ \AA}^3$	

#### Data collection

Stoe IPDS diffractometer	1336 independent reflections
$\varphi$ scans	957 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.077$
5163 measured reflections	$\theta_{\text{max}} = 26.1^\circ$

#### Refinement

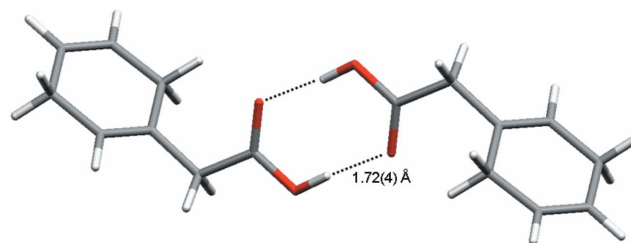
Refinement on $F^2$	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.079P)^2]$
$wR(F^2) = 0.122$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1336 reflections	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
131 parameters	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O2-H2 \cdots O1^1$	0.93 (4)	1.72 (4)	2.6436 (18)	172 (3)

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



**Figure 2**  
The hydrogen bonding (dashed lines) between pairs of molecules of (I).

The range of refined C–H distances is 0.96 (2)–1.01 (2)  $\text{\AA}$ .

Data collection: *EXPOSE* in *IPDS Software* (Stoe & Cie, 2000); cell refinement: *CELL* in *IPDS Software*; data reduction: *INTEGRATE* in *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-32* (Farrugia, 1997) and *MERCURY* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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