Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

p-Phenylene diacetate

Juan Men,[a]* Fengcai Gu[a] and Huifang Sun[b]

[a]Department of Chemistry, Tianjin University, Tianjin 300072, People's Republic of China, and [b]College of Science, Tianjin University of Science and Technology, Tianjin 300457, People's Republic of China

Correspondence e-mail: menanlan@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.116
Data-to-parameter ratio = 18.0

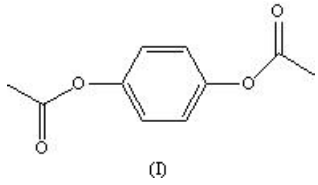
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 11 January 2005
Accepted 20 January 2005
Online 29 January 2005

The molecule of the title compound, $C_{10}H_{10}O_4$, is centrosymmetric.

Comment

The title compound, (I), can be prepared readily (Mohammadpoor-Baltork *et al.*, 2001; Chakraborti & Gulhane, 2003) and is also commercially available. In spite of this ready availability, the crystal structure is not known yet. We report it here.



(I)

As shown in Fig. 1, the molecule is centrosymmetric, with the two acetyl groups on opposite sides of the central benzene ring.

Experimental

Single crystals suitable for X-ray diffraction analysis were obtained by recrystallization from ethanol (m.p. 397 K). IR (KBr, ν cm^{-1}): 1763, 1505, 1369, 1215 1175, 920; ^{1}H NMR ($CDCl_3$): δ 6.97 (*d*, 4H), 2.255 (*s*, 6H).

Crystal data

$C_{10}H_{10}O_4$
M_r = 194.18
Monoclinic, $P2_1/c$
a = 7.740 (2) Å
b = 5.6749 (13) Å
c = 11.484 (2) Å
β = 101.055 (2)°
V = 495.1 (2) Å^3
Z = 2
D_x = 1.303 Mg m^{-3}
Mo Kα radiation
Cell parameters from 682 reflections
θ = 2.7–22.6°
μ = 0.10 mm^{-1}
T = 293 (2) K
Plate, colourless
0.24 × 0.20 × 0.08 mm

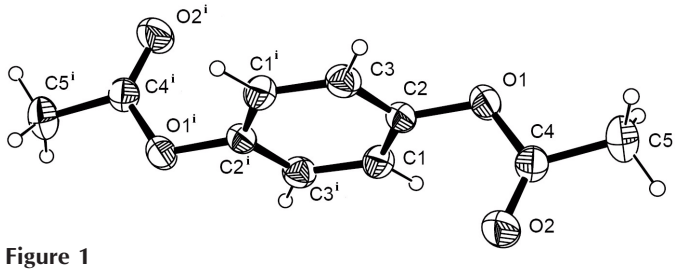


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) 2 − *x*, −*y*, 2 − *z*.]

Data collection

Bruker SMART CCD area-detector diffractometer	769 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.019$
Absorption correction: none	$\theta_{max} = 27.9^\circ$
3186 measured reflections	$h = -10 \rightarrow 8$
1188 independent reflections	$k = -7 \rightarrow 6$
	$l = -15 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.0732P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.039$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.116$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
$S = 1.07$	$\Delta\rho_{min} = -0.13$ e Å^{-3}
1188 reflections	Extinction correction: *SHELXL*
66 parameters	Extinction coefficient: 0.053 (10)
H-atom parameters constrained	

All H atoms were positioned geometrically and refined as riding (C—H = 0.93 or 0.96 Å), with $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}(C)$ for methyl groups.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

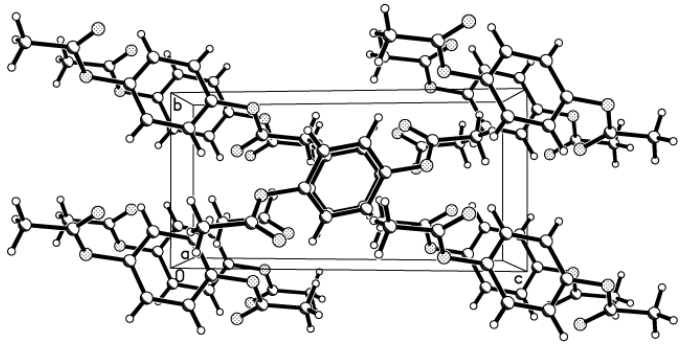


Figure 2
A packing diagram for (I), viewed along the *a* axis.

References

Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chakraborti, A. K. & Gulhane, R. (2003). *Tetrahedron Lett.* **44**, 6749–6753.
Mohammadpoor-Baltork, I., Aliyan, H. & Khosropour, A. R. (2001). *Tetrahedron*, **57**, 5851–5854.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.