

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## A polymorph of terephthalaldehyde

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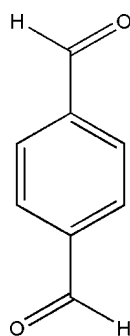
Received 15 July 2008; accepted 17 July 2008

Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  
 $R$  factor = 0.043;  $wR$  factor = 0.113; data-to-parameter ratio = 7.2.

A new orthorhombic polymorph of terephthalaldehyde,  $\text{C}_8\text{H}_6\text{O}_2$ , with a melting point of 372 K, has been obtained by recrystallization from ethanol. At room temperature, the crystals transform into the well known monoclinic form, with a melting point of 389 K. The crystal structure of the monoclinic form involves  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds, but no such bonds are observed in the orthorhombic form. The molecule is planar.

## Related literature

For the structure of the monoclinic polymorph, see: Britton (1998).



## Experimental

## Crystal data

$\text{C}_8\text{H}_6\text{O}_2$   
 $M_r = 134.13$   
Orthorhombic,  $Pca2_1$   
 $a = 12.8811$  (5) Å  
 $b = 3.8933$  (3) Å  
 $c = 13.3202$  (9) Å  
 $V = 668.01$  (7) Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 $0.20 \times 0.10 \times 0.10$  mm

## Data collection

Bruker SMART 4K CCD area-detector diffractometer  
Absorption correction: none  
3959 measured reflections  
653 independent reflections  
563 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.112$   
 $S = 1.04$   
653 reflections  
91 parameters  
1 restraint  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.10$  e Å<sup>-3</sup>

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; 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*.

This study was financially supported by a Key Project (No. Z2006zd02) of Huangshi Institute of Technology. The authors thank Dr Xiang-Gao Meng for the crystallographic data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2093).

## References

- Britton, D. (1998). *J. Chem. Crystallogr.* **28**, 601–604.  
Bruker (2001). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

## supporting information

*Acta Cryst.* (2008). E64, o1562 [doi:10.1107/S1600536808022381]

## A polymorph of terephthalaldehyde

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### S1. Comment

Terephthalaldehyde, (I), is a simple aromatic compound used in organic synthesis. It is known as a white substance, slightly soluble in water, with a melting point of 389 K. To the best of our knowledge, the only packing information of (I) in the solid state comes from the work of Britton (Britton, 1998), who investigated the intermolecular C—H···O arrangement in the structure of terephthalaldehyde and the crystals suitable for diffraction were obtained by recrystallization from an acetone/ethyl ether mixture.

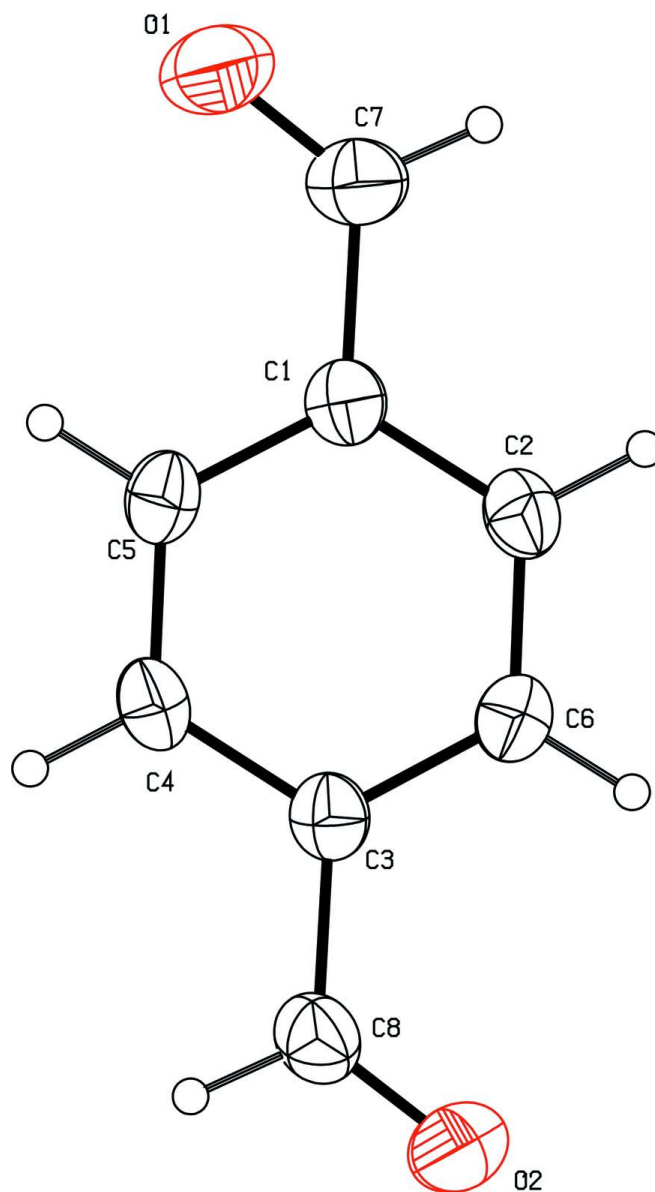
A new polymorphic form of (I) has been obtained serendipitously during cocrystallization of pyridine and terephthalaldehyde from ethanol (Fig. 1). Flat needles which precipitated first from the solution had a melting point of 372 K and were identified as a new polymorphic form of (I) by X-ray crystallography. At room temperature, the crystals transform into the well known monoclinic form, with a melting point of 389 K. The crystal structure of the monoclinic form involves C—H···O hydrogen bonds but no such bonds are observed in the orthorhombic form (Fig. 2).

### S2. Experimental

The title compound was purchased from Aldrich.

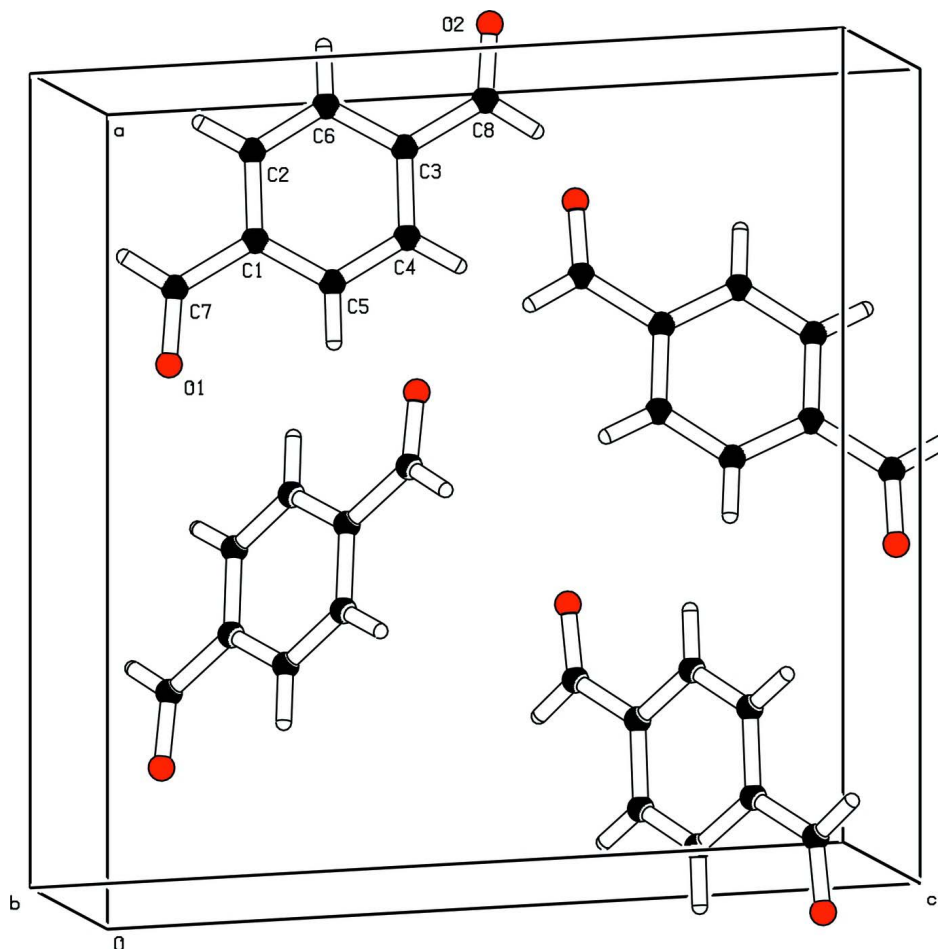
### S3. Refinement

All H atoms were initially located in a difference Fourier map and then included with constrained bond lengths and isotropic displacement parameters: C—H=0.93 Å and  $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$  for H atoms.



**Figure 1**

The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

**Figure 2**

The packing of the molecules, viewed down the *b* axis.

### terephthalaldehyde

#### Crystal data

$C_8H_6O_2$

$M_r = 134.13$

Orthorhombic,  $Pca2_1$

Hall symbol:  $P\ 2c\ -2ac$

$a = 12.8811\ (5)\ \text{\AA}$

$b = 3.8933\ (3)\ \text{\AA}$

$c = 13.3202\ (9)\ \text{\AA}$

$V = 668.01\ (7)\ \text{\AA}^3$

$Z = 4$

$F(000) = 280$

$D_x = 1.334\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1070 reflections

$\theta = 3.1\text{--}23.5^\circ$

$\mu = 0.10\ \text{mm}^{-1}$

$T = 295\ \text{K}$

Block, colorless

$0.20 \times 0.10 \times 0.10\ \text{mm}$

#### Data collection

Bruker SMART 4K CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

3959 measured reflections

653 independent reflections

563 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\text{max}} = 25.5^\circ$ ,  $\theta_{\text{min}} = 3.1^\circ$

$h = -15 \rightarrow 12$   
 $k = -4 \rightarrow 4$

$l = -16 \rightarrow 15$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.112$   
 $S = 1.04$   
 653 reflections  
 91 parameters  
 1 restraint  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0755P)^2 + 0.0133P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.014$   
 $\Delta\rho_{\max} = 0.16 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.10 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.8164 (2)	0.3463 (7)	0.2145 (2)	0.0509 (7)
C2	0.9236 (2)	0.3850 (7)	0.2147 (3)	0.0545 (7)
H2	0.9566	0.4847	0.1599	0.065*
C3	0.9315 (2)	0.1279 (7)	0.3776 (2)	0.0515 (7)
C4	0.8239 (2)	0.0894 (7)	0.3770 (3)	0.0547 (7)
H4	0.7907	-0.0106	0.4316	0.066*
C5	0.7668 (2)	0.1993 (6)	0.2955 (3)	0.0543 (7)
H5	0.6950	0.1744	0.2953	0.065*
C6	0.9805 (2)	0.2776 (7)	0.2951 (3)	0.0547 (6)
H6	1.0523	0.3040	0.2949	0.066*
C7	0.7563 (4)	0.4635 (8)	0.1269 (4)	0.0707 (10)
H7	0.7934	0.5547	0.0733	0.085*
C8	0.9916 (3)	0.0084 (8)	0.4657 (4)	0.0627 (9)
H8	0.9550	-0.0874	0.5190	0.075*
O1	0.6637 (2)	0.4514 (7)	0.1187 (3)	0.0930 (10)
O2	1.0834 (2)	0.0266 (7)	0.4731 (4)	0.0876 (9)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0535 (16)	0.0494 (14)	0.0498 (17)	0.0041 (11)	0.0057 (14)	-0.0068 (13)
C2	0.0564 (18)	0.0551 (15)	0.0520 (17)	0.0022 (13)	0.0123 (15)	0.0015 (15)
C3	0.0547 (16)	0.0509 (14)	0.0490 (17)	-0.0008 (12)	0.0064 (15)	-0.0078 (13)

## supporting information

C4	0.0593 (19)	0.0573 (14)	0.0476 (17)	-0.0067 (14)	0.0140 (16)	0.0002 (14)
C5	0.0463 (13)	0.0570 (14)	0.0595 (15)	-0.0016 (12)	0.0102 (17)	-0.0083 (14)
C6	0.0448 (13)	0.0582 (14)	0.0610 (15)	-0.0003 (12)	0.0043 (18)	-0.0008 (14)
C7	0.071 (2)	0.077 (2)	0.063 (3)	0.0121 (16)	-0.006 (2)	-0.0016 (18)
C8	0.067 (2)	0.0704 (19)	0.0508 (19)	0.0030 (13)	0.009 (2)	0.0003 (14)
O1	0.075 (2)	0.129 (2)	0.075 (2)	0.0162 (14)	-0.0158 (19)	-0.0026 (18)
O2	0.0617 (17)	0.125 (2)	0.0761 (19)	0.0064 (12)	-0.0077 (16)	0.0074 (15)

### Geometric parameters (Å, °)

C1—C5	1.378 (4)	C4—C5	1.379 (5)
C1—C2	1.389 (4)	C4—H4	0.9300
C1—C7	1.473 (6)	C5—H5	0.9300
C2—C6	1.363 (5)	C6—H6	0.9300
C2—H2	0.9300	C7—O1	1.199 (5)
C3—C4	1.393 (4)	C7—H7	0.9300
C3—C6	1.395 (4)	C8—O2	1.188 (4)
C3—C8	1.482 (6)	C8—H8	0.9300
C5—C1—C2	120.2 (3)	C1—C5—C4	119.9 (3)
C5—C1—C7	120.4 (3)	C1—C5—H5	120.1
C2—C1—C7	119.4 (3)	C4—C5—H5	120.1
C6—C2—C1	120.2 (3)	C2—C6—C3	120.2 (2)
C6—C2—H2	119.9	C2—C6—H6	119.9
C1—C2—H2	119.9	C3—C6—H6	119.9
C4—C3—C6	119.4 (3)	O1—C7—C1	125.6 (5)
C4—C3—C8	119.4 (3)	O1—C7—H7	117.2
C6—C3—C8	121.2 (3)	C1—C7—H7	117.2
C5—C4—C3	120.1 (3)	O2—C8—C3	124.5 (4)
C5—C4—H4	120.0	O2—C8—H8	117.7
C3—C4—H4	120.0	C3—C8—H8	117.7
C5—C1—C2—C6	0.1 (4)	C1—C2—C6—C3	0.0 (4)
C7—C1—C2—C6	-179.9 (3)	C4—C3—C6—C2	0.0 (4)
C6—C3—C4—C5	-0.2 (4)	C8—C3—C6—C2	179.9 (3)
C8—C3—C4—C5	180.0 (3)	C5—C1—C7—O1	1.8 (5)
C2—C1—C5—C4	-0.2 (4)	C2—C1—C7—O1	-178.2 (3)
C7—C1—C5—C4	179.7 (3)	C4—C3—C8—O2	179.2 (3)
C3—C4—C5—C1	0.2 (4)	C6—C3—C8—O2	-0.6 (5)