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## Structure Reports

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## 3,3-Dimethyl-2-benzofuran-1(3H)-one

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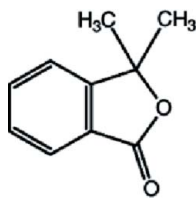
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Key indicators: single-crystal X-ray study;  $T = 123$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.052;  $wR$  factor = 0.133; data-to-parameter ratio = 25.9.

In the title compound,  $\text{C}_{10}\text{H}_{10}\text{O}_2$ , all the non-H atoms except the methyl C atoms lie on a crystallographic mirror plane. In the crystal,  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into zigzag chains running parallel to [100]. Weak  $\pi-\pi$  stacking interactions between the benzene rings [centroid-centroid distance = 3.9817 (5) Å] link the chains in the [010] direction.

## Related literature

For related structures, see: Fun *et al.* (2010, 2011).

## Experimental

## Crystal data

$\text{C}_{10}\text{H}_{10}\text{O}_2$   
 $M_r = 162.18$   
 Orthorhombic,  $Pnma$   
 $a = 14.3537$  (9) Å

$b = 7.0069$  (5) Å  
 $c = 8.2605$  (5) Å  
 $V = 830.80$  (9) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>

$T = 123$  K  
 $0.55 \times 0.44 \times 0.30$  mm

## Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer  
 Absorption correction: refined from  $\Delta F$  (XABS2; Parkin *et al.*, 1995)  
 $T_{\min} = 0.952$ ,  $T_{\max} = 0.974$

1840 measured reflections  
 1840 independent reflections  
 1454 reflections with  $I > 2\sigma(I)$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.133$   
 $S = 1.09$   
 1840 reflections

71 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.34$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.30$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C2}-\text{H2}\cdots\text{O2}^i$	0.93	2.43	3.3072 (17)	158

Symmetry code: (i)  $x - \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{1}{2}$ .

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

MSS thanks the University of Mysore for research facilities. RJB wishes to acknowledge the NSF-MRI program (grant CHE-0619278) for funds to purchase the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6560).

## References

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**supplementary materials**

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### 3,3-Dimethyl-2-benzofuran-1(3*H*)-one

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#### Comment

3,3-Dimethylisobenzofuran-1(3*H*)-one, (I), is used to synthesize 10,10-dimethylanthrone (Fun *et al.*, 2010). It is a one of the intermediate for melitraceniun chloride (Fun *et al.*, 2011). We now report its structure.

In the title molecule (I), (Fig. 1), a mirror plane passes through the remaining atoms of the molecule, except the atoms of two methyl groups which are *mirror images of each other*.

In the crystal, intermolecular C—H...O hydrogen bonds link molecules forming zigzag chains in the layer parallel to the (101) plane and along the *a* axis (Table 1, Fig. 2a,b,c). Furthermore, there exist weak  $\pi$ - $\pi$  stacking interactions [ $Cg2 \cdots Cg2(2-x, -1/2+y, -z) = 3.9817(5) \text{ \AA}$ ,  $Cg2 \cdots Cg2(2-x, 1/2+y, -z) = 3.9817(5) \text{ \AA}$ ,  $Cg2 \cdots Cg2(2-x, -y, -z) = 3.9817(5) \text{ \AA}$ ,  $Cg2 \cdots Cg2(2-x, 1-y, -z) = 3.9817(5) \text{ \AA}$ ] between the C1–C6 benzene rings along the [010] direction.

#### Experimental

The title compound was obtained as a gift sample from R. L. Fine Chemicals, Bengaluru, India. Colourless prisms of (I) were grown from toluene solution by slow evaporation (m.p.: 337–340 K).

#### Refinement

All H atoms were added in calculated positions and refined as riding with C–H distances of 0.93 and 0.96  $\text{\AA}$ . The isotropic atomic displacement parameters of H atoms were fixed to 1.2 or 1.5  $\times U_{eq}$  of the parent atom.

#### Figures

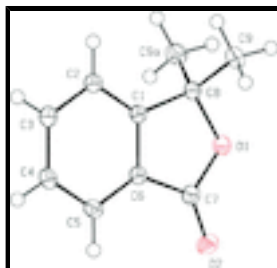


Fig. 1. The title molecule (I) showing displacement ellipsoids for non-H atoms drawn at the 50% probability level.

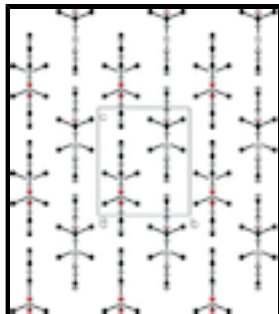


Fig. 2. View of the packing and hydrogen bonding of (I) down *a* axis.

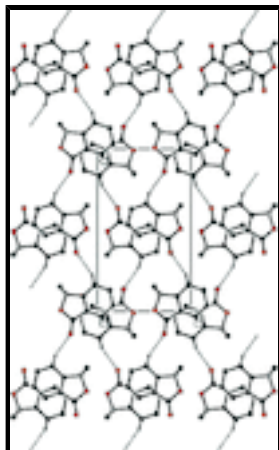


Fig. 3. View of the packing and hydrogen bonding of (I) down *b* axis.

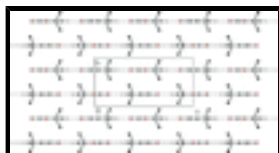


Fig. 4. View of the packing and hydrogen bonding of (I) down *c* axis.

### 3,3-Dimethyl-2-benzofuran-1(3H)-one

#### Crystal data

$C_{10}H_{10}O_2$

$M_r = 162.18$

Orthorhombic, *Pnma*

Hall symbol: -P 2ac 2n

$a = 14.3537$  (9) Å

$b = 7.0069$  (5) Å

$c = 8.2605$  (5) Å

$V = 830.80$  (9) Å<sup>3</sup>

$Z = 4$

$F(000) = 344$

$D_x = 1.297$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1444 reflections

$\theta = 2.8$ – $35.2^\circ$

$\mu = 0.09$  mm<sup>-1</sup>

$T = 123$  K

Prism, colourless

$0.55 \times 0.44 \times 0.30$  mm

#### Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer

Radiation source: Enhance (Mo) X-ray Source graphite

1840 independent reflections

1454 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.000$

Detector resolution: 10.5081 pixels mm<sup>-1</sup>       $\theta_{\max} = 35.2^\circ$ ,  $\theta_{\min} = 2.8^\circ$   
 $\omega$  scans       $h = 0 \rightarrow 22$   
Absorption correction: part of the refinement model  
( $\Delta F$ )       $k = 0 \rightarrow 11$   
(XABS2; Parkin *et al.*, 1995)  
 $T_{\min} = 0.952$ ,  $T_{\max} = 0.974$        $l = 0 \rightarrow 13$   
1840 measured reflections

### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.052$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.133$	H-atom parameters constrained
$S = 1.09$	$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.0987P]$
1840 reflections	where $P = (F_o^2 + 2F_c^2)/3$
71 parameters	$(\Delta/\sigma)_{\max} < 0.001$
0 restraints	$\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$

### Special details

**Experimental.** Absorption correction: XABS2 (Parkin *et al.*, 1995); cubic fit to  $\sin\theta/\lambda$  - 24 parameters

**Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement.** Refinement on  $F^2$  for ALL reflections except those flagged by the user for potential systematic errors. Weighted  $R$ -factors  $wR$  and all goodnesses 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 observed criterion of  $F^2 > \sigma(F^2)$  is used only for calculating  $-R$ -factor-obs *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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.99217 (7)	0.25000	0.38584 (11)	0.0216 (3)
O2	1.13652 (7)	0.25000	0.28045 (13)	0.0260 (3)
C1	0.90567 (9)	0.25000	0.14603 (15)	0.0159 (3)
C2	0.83829 (9)	0.25000	0.02623 (16)	0.0193 (3)
C3	0.86910 (10)	0.25000	-0.13404 (16)	0.0211 (3)
C4	0.96384 (10)	0.25000	-0.17273 (16)	0.0208 (3)
C5	1.03071 (9)	0.25000	-0.05143 (16)	0.0192 (3)
C6	0.99948 (9)	0.25000	0.10807 (15)	0.0165 (3)
C7	1.05334 (9)	0.25000	0.25962 (15)	0.0189 (3)
C8	0.89464 (9)	0.25000	0.32851 (15)	0.0175 (3)

## supplementary materials

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C9	0.84773 (7)	0.07067 (15)	0.39183 (12)	0.0229 (3)
H2	0.77510	0.25000	0.05140	0.0230*
H3	0.82540	0.25000	-0.21720	0.0250*
H4	0.98220	0.25000	-0.28070	0.0250*
H5	1.09400	0.25000	-0.07580	0.0230*
H9A	0.88010	-0.03960	0.35190	0.0340*
H9B	0.78420	0.06740	0.35560	0.0340*
H9C	0.84920	0.07080	0.50800	0.0340*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0185 (4)	0.0326 (5)	0.0136 (4)	0.0000	-0.0019 (4)	0.0000
O2	0.0169 (4)	0.0368 (6)	0.0242 (5)	0.0000	-0.0042 (4)	0.0000
C1	0.0169 (5)	0.0170 (5)	0.0137 (5)	0.0000	0.0004 (4)	0.0000
C2	0.0176 (5)	0.0251 (6)	0.0153 (5)	0.0000	-0.0002 (5)	0.0000
C3	0.0220 (6)	0.0270 (6)	0.0143 (5)	0.0000	-0.0021 (5)	0.0000
C4	0.0246 (6)	0.0248 (6)	0.0131 (5)	0.0000	0.0025 (5)	0.0000
C5	0.0185 (5)	0.0213 (5)	0.0177 (5)	0.0000	0.0031 (5)	0.0000
C6	0.0176 (5)	0.0173 (5)	0.0147 (5)	0.0000	0.0003 (4)	0.0000
C7	0.0182 (6)	0.0214 (5)	0.0172 (5)	0.0000	-0.0011 (5)	0.0000
C8	0.0164 (5)	0.0232 (6)	0.0130 (5)	0.0000	-0.0007 (4)	0.0000
C9	0.0259 (5)	0.0244 (4)	0.0185 (4)	-0.0011 (4)	0.0028 (3)	0.0028 (3)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

O1—C7	1.3631 (16)	C6—C7	1.4714 (18)
O1—C8	1.4779 (16)	C8—C9	1.5185 (13)
O2—C7	1.2063 (16)	C8—C9 <sup>i</sup>	1.5185 (13)
C1—C2	1.3837 (18)	C2—H2	0.9300
C1—C6	1.3826 (18)	C3—H3	0.9300
C1—C8	1.5157 (18)	C4—H4	0.9300
C2—C3	1.3958 (19)	C5—H5	0.9300
C3—C4	1.397 (2)	C9—H9A	0.9600
C4—C5	1.3875 (19)	C9—H9B	0.9600
C5—C6	1.3917 (18)	C9—H9C	0.9600
C7—O1—C8	111.41 (9)	C1—C8—C9	112.89 (7)
C2—C1—C6	121.23 (12)	C1—C8—C9 <sup>i</sup>	112.89 (7)
C2—C1—C8	129.66 (12)	C9—C8—C9 <sup>i</sup>	111.68 (10)
C6—C1—C8	109.11 (11)	C1—C2—H2	121.00
C1—C2—C3	117.19 (12)	C3—C2—H2	121.00
C2—C3—C4	121.70 (12)	C2—C3—H3	119.00
C3—C4—C5	120.54 (12)	C4—C3—H3	119.00
C4—C5—C6	117.44 (12)	C3—C4—H4	120.00
C1—C6—C5	121.90 (12)	C5—C4—H4	120.00
C1—C6—C7	108.59 (11)	C4—C5—H5	121.00
C5—C6—C7	129.51 (12)	C6—C5—H5	121.00
O1—C7—O2	121.90 (12)	C8—C9—H9A	109.00

O1—C7—C6	108.20 (11)	C8—C9—H9B	109.00
O2—C7—C6	129.90 (12)	C8—C9—H9C	110.00
O1—C8—C1	102.69 (10)	H9A—C9—H9B	109.00
O1—C8—C9	108.04 (7)	H9A—C9—H9C	109.00
O1—C8—C9 <sup>i</sup>	108.04 (7)	H9B—C9—H9C	109.00
C7—O1—C8—C9	119.51 (7)	C8—C1—C6—C5	180.00
C8—O1—C7—O2	180.00	C2—C1—C8—C9	63.92 (8)
C8—O1—C7—C6	0.00	C1—C2—C3—C4	0.00
C7—O1—C8—C1	0.00	C2—C3—C4—C5	0.00
C8—C1—C2—C3	180.00	C3—C4—C5—C6	0.00
C2—C1—C6—C5	0.00	C4—C5—C6—C1	0.00
C2—C1—C6—C7	180.00	C4—C5—C6—C7	180.00
C6—C1—C2—C3	0.00	C1—C6—C7—O2	180.00
C6—C1—C8—O1	0.00	C5—C6—C7—O1	180.00
C6—C1—C8—C9	-116.08 (8)	C5—C6—C7—O2	0.00
C8—C1—C6—C7	0.00	C1—C6—C7—O1	0.00
C2—C1—C8—O1	180.00		

Symmetry codes: (i)  $x, -y+1/2, z$ .

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 $\cdots$ O2 <sup>ii</sup>	0.93	2.43	3.3072 (17)	158

Symmetry codes: (ii)  $x-1/2, -y+1/2, -z+1/2$ .

Fig. 1

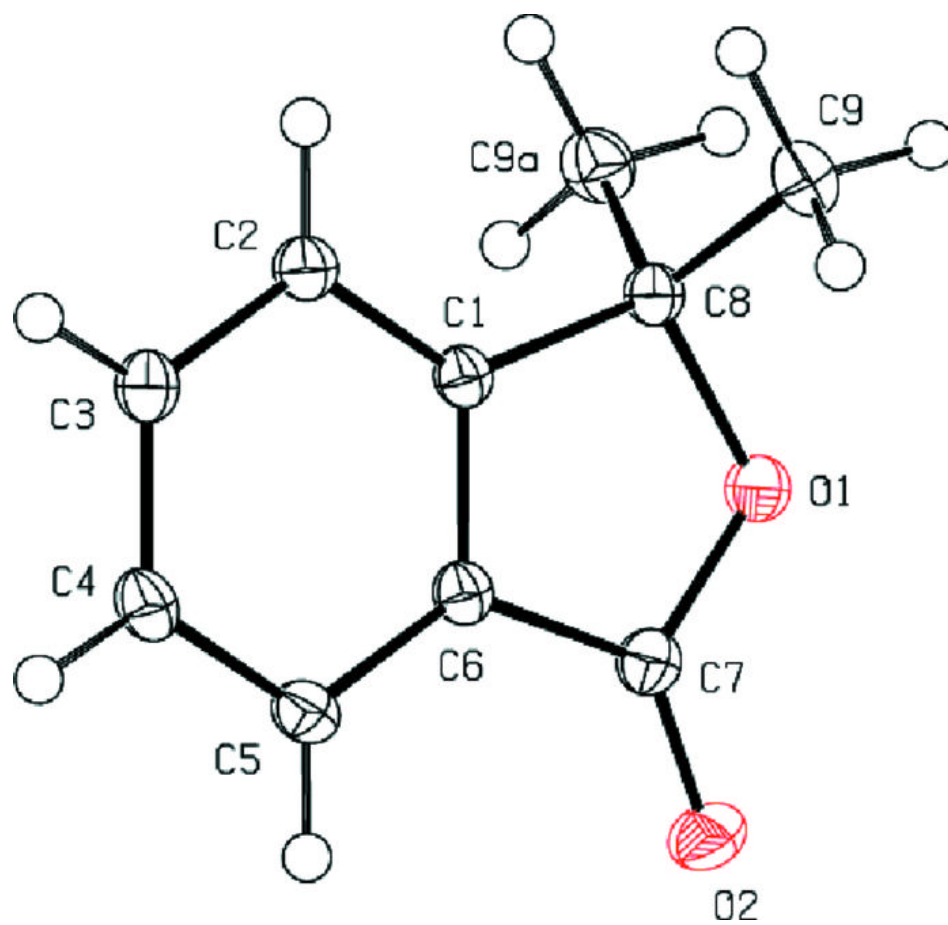




Fig. 2

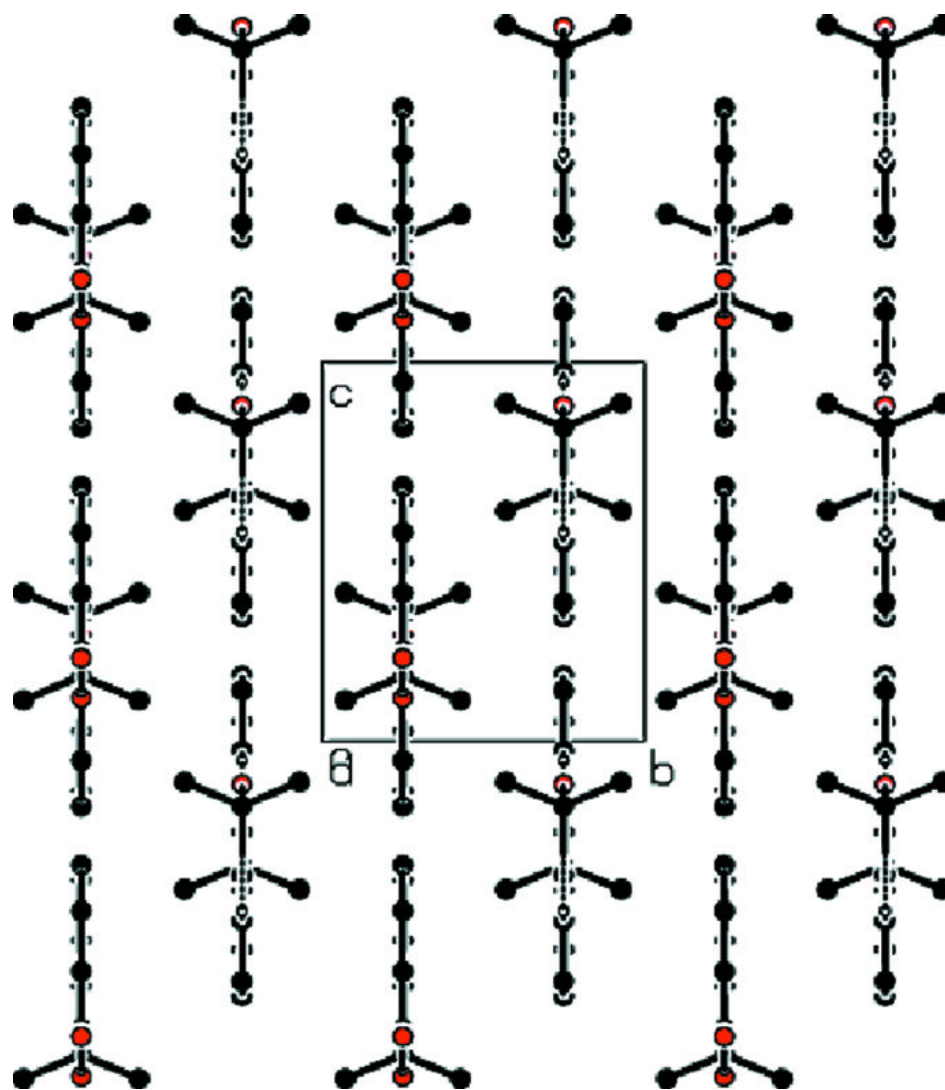


Fig. 3

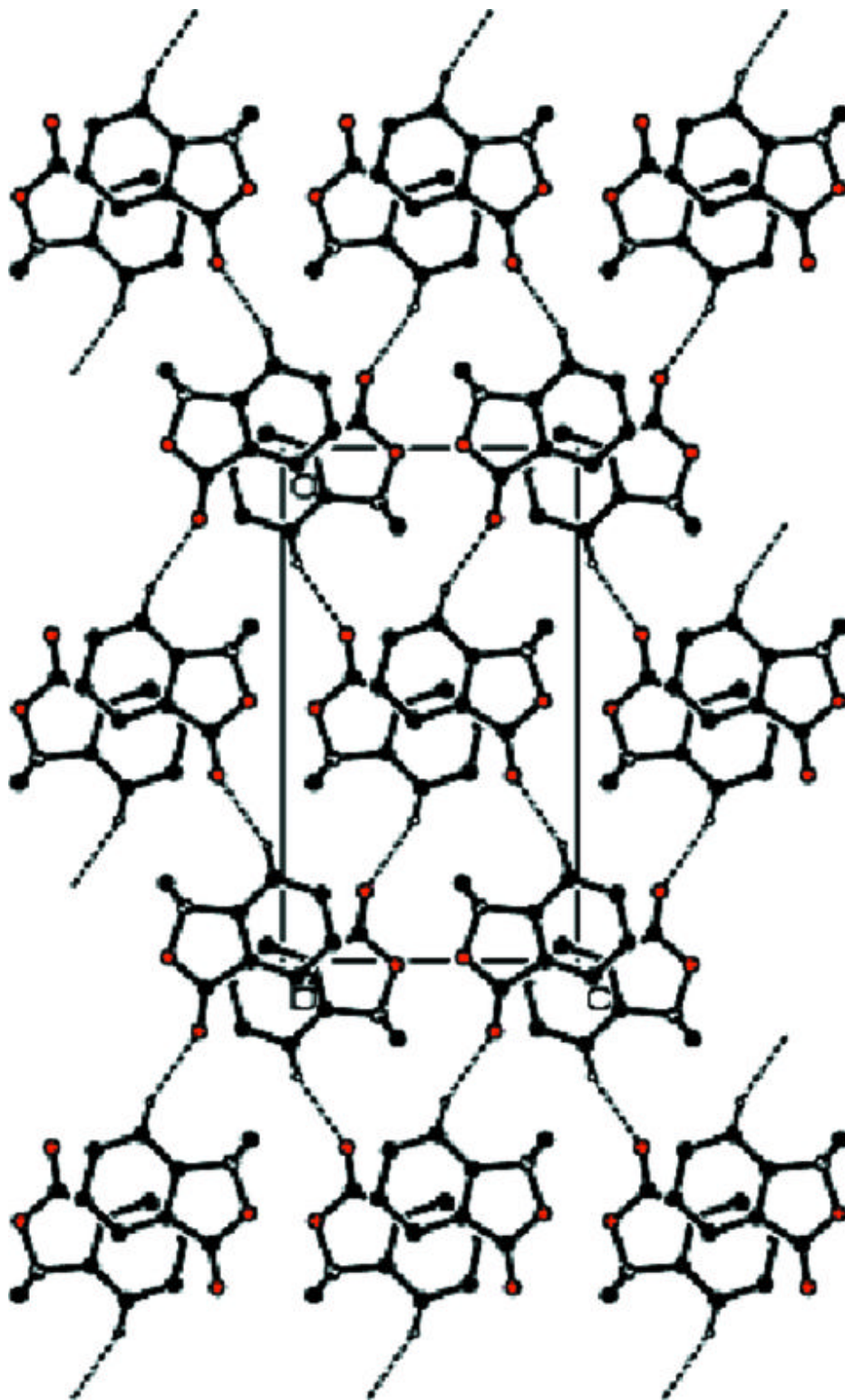


Fig. 4

