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## Structure Reports

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## 2,5-Dichloro-3,6-diisopropylcyclohexa-2,5-diene-1,4-dione

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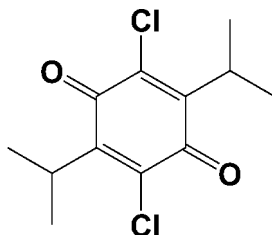
Received 17 June 2012; accepted 19 July 2012

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.059;  $wR$  factor = 0.198; data-to-parameter ratio = 14.9.

The molecule of the title compound,  $\text{C}_{12}\text{H}_{14}\text{Cl}_2\text{O}_2$ , lies about an inversion center. The six-membered ring is almost planar, with the largest deviation from the least-squares plane being 0.014 (4) Å. The molecular conformation is stabilized by a weak intramolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bond. In the crystal, molecules are packed into stacks along the  $c$ -axis direction, with an intercentroid separation of 4.811 (2) Å. Neighboring molecules within the stack are related by the  $c$ -glide plane.

### Related literature

Metal complexes of catechols, semiquinones and quinones are of general interest in the investigation of ligand centered redox reactions and as models for biochemical processes involving metal ions, see: Mostafa (1999). For standard bond lengths, see: Allen *et al.* (1987).



### Experimental

#### Crystal data

 $\text{C}_{12}\text{H}_{14}\text{Cl}_2\text{O}_2$  $M_r = 293.13$ 

Monoclinic,  $C2/c$   
 $a = 10.286$  (2) Å  
 $b = 15.034$  (3) Å  
 $c = 9.621$  (2) Å  
 $\beta = 109.022$  (4)°  
 $V = 1406.5$  (6) Å<sup>3</sup>

$Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.46$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.15 \times 0.13 \times 0.12$  mm

#### Data collection

Brucker APEXII CCD diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2007)  
 $T_{\min} = 0.925$ ,  $T_{\max} = 0.946$

3544 measured reflections  
1248 independent reflections  
676 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.079$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$   
 $wR(F^2) = 0.198$   
 $S = 1.08$   
1248 reflections  
84 parameters

12 restraints  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.41$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.24$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4}-\text{H4}\cdots\text{O1}^i$	0.98	2.34	2.926 (7)	117

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YK2064).

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## supporting information

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**2,5-Dichloro-3,6-diisopropylcyclohexa-2,5-diene-1,4-dione**

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**S1. Comment**

Metal complexes of catechols, semiquinones and quinones are of general interest in the investigation of ligand centered redox reactions and as models for biochemical processes involving metal ions (Mostafa, 1999). The title compound is the synthetic precursor for chloranilic acid, which is a simple, readily available ligand combining chelating and bridging capabilities.

In the title molecule, the six-membered ring and attached oxygen and chlorine atoms bound to every vertex of this carbon hexagon, share a same plane with the largest deviation being 0.053 (4) Å for C3. The two isopropyl groups extend from the plane, one above and one below the plane, as shown in Fig. 1. The C1=O1 bond has a lengths of 1.221 (4) Å, typical of  $Csp^2=O$  double bonds (Allen *et al.*, 1987). The C3—O2 bond, however, is a  $Csp^2-O$  single bond with the lengths of 1.346 (5) Å, which is slightly shorter than the value expected for enol ester systems [1.354 (16) Å (Allen *et al.*, 1987)]. The carbon-carbon bonds in the six-membered ring can also be divided into two groups: the C2=C3 bond is a typical double bond with the length of 1.343 (5) Å, whereas the C1—C2 and C1—C3<sup>i</sup> bonds with the lengths of 1.463 (5) Å and 1.480 (6) Å, reaspectively, are obviously the  $Csp^2-Csp^2$  single bonds.

There are weak intramolecular interactions C2—H2A $\cdots$ O2 (1 - x, 1 - y, 1 - z) [H $\cdots$ O = 2.34 Å, C $\cdots$ O = 2.926 (7) Å, and C—H $\cdots$ O = 117°], which stabilize the molecule conformation.

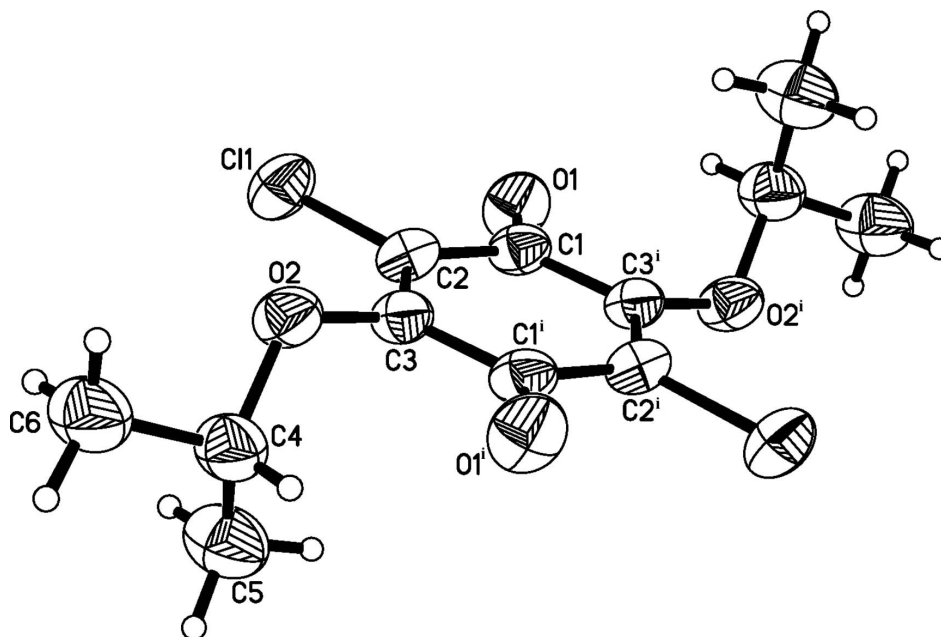
In the crystal, the molecules of the title compound are packed into stacks along the *c* direction with intercentroid separation of 4.811 (2) Å. Neighboring molecules within the stack are related by the *c* glide plane.

**S2. Experimental**

Potassium hydroxide (5.0 g) was added to a solution containing chloranil (5.0 g) in 2-propanol (100 ml). The resulting mixture was stirred under reflux for 1 h, and then the red reaction solution was cooled to 283 K. The precipitated yellow solid was collected and recrystallized in ethanol.

**S3. Refinement**

All H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.98 Å and  $U_{iso}(H) = 1.2U_{eq}(C)$  for tertiary hydrogen and with C—H = 0.96 Å and  $U_{iso}(H) = 1.5U_{eq}(C)$  for methyl group.

**Figure 1**

Molecular structure with atom labelling scheme and thermal ellipsoids drawn at the 30% probability level (symmetry code (i):  $1 - x, 1 - y, 1 - z$ ).

### 2,5-Dichloro-3,6-diisopropylcyclohexa-2,5-diene-1,4-dione

#### Crystal data

$C_{12}H_{14}Cl_2O_4$

$M_r = 293.13$

Monoclinic,  $C2/c$

Hall symbol:  $-C 2yc$

$a = 10.286 (2) \text{ \AA}$

$b = 15.034 (3) \text{ \AA}$

$c = 9.621 (2) \text{ \AA}$

$\beta = 109.022 (4)^\circ$

$V = 1406.5 (6) \text{ \AA}^3$

$Z = 4$

$F(000) = 608$

$D_x = 1.384 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71069 \text{ \AA}$

Cell parameters from 837 reflections

$\theta = 2.5\text{--}21.5^\circ$

$\mu = 0.46 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, yellow

$0.15 \times 0.13 \times 0.12 \text{ mm}$

#### Data collection

Brucker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2007)

$T_{\min} = 0.925$ ,  $T_{\max} = 0.946$

3544 measured reflections

1248 independent reflections

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

$R_{\text{int}} = 0.079$

$\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 2.5^\circ$

$h = -12 \rightarrow 9$

$k = -17 \rightarrow 17$

$l = -10 \rightarrow 11$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.059$   
 $wR(F^2) = 0.198$   
 $S = 1.08$   
 1248 reflections  
 84 parameters  
 12 restraints  
 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  
 $w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.41 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'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 s.u.'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	0.4914 (5)	0.5935 (3)	0.5241 (4)	0.0672 (11)
C2	0.5842 (4)	0.5580 (3)	0.4504 (4)	0.0686 (12)
C3	0.5968 (4)	0.4704 (3)	0.4308 (4)	0.0632 (11)
C4	0.7787 (5)	0.3702 (3)	0.4212 (5)	0.0903 (13)
H4	0.7285	0.3149	0.4223	0.108*
C5	0.8654 (6)	0.3916 (4)	0.5744 (6)	0.1146 (16)
H5A	0.9196	0.4436	0.5740	0.172*
H5B	0.9252	0.3424	0.6150	0.172*
H5C	0.8075	0.4027	0.6331	0.172*
C6	0.8576 (7)	0.3595 (4)	0.3175 (6)	0.1114 (16)
H6A	0.7949	0.3508	0.2198	0.167*
H6B	0.9173	0.3089	0.3459	0.167*
H6C	0.9115	0.4120	0.3198	0.167*
Cl1	0.68016 (14)	0.63397 (8)	0.39265 (14)	0.0914 (7)
O1	0.4891 (4)	0.6728 (2)	0.5509 (4)	0.0948 (11)
O2	0.6789 (3)	0.4409 (2)	0.3567 (3)	0.0789 (10)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.085 (3)	0.052 (3)	0.065 (3)	0.012 (2)	0.025 (2)	0.007 (2)
C2	0.086 (3)	0.061 (3)	0.058 (2)	-0.001 (2)	0.022 (2)	0.007 (2)
C3	0.075 (3)	0.059 (3)	0.057 (2)	0.010 (2)	0.023 (2)	0.0061 (19)
C4	0.095 (3)	0.100 (3)	0.079 (3)	0.027 (2)	0.033 (2)	0.006 (2)
C5	0.114 (3)	0.124 (3)	0.094 (3)	0.026 (3)	0.018 (3)	-0.006 (3)

C6	0.124 (3)	0.121 (3)	0.092 (3)	0.044 (3)	0.040 (3)	0.004 (3)
C11	0.1161 (12)	0.0720 (9)	0.0961 (10)	-0.0080 (6)	0.0484 (8)	0.0120 (6)
O1	0.125 (3)	0.055 (2)	0.119 (3)	0.0052 (18)	0.059 (2)	-0.0032 (18)
O2	0.102 (2)	0.0689 (19)	0.075 (2)	0.0238 (16)	0.0414 (18)	0.0111 (14)

*Geometric parameters (Å, °)*

C1—O1	1.221 (4)	C4—C5	1.489 (7)
C1—C2	1.463 (5)	C4—H4	0.9800
C1—C3 <sup>i</sup>	1.480 (6)	C5—H5A	0.9600
C2—C3	1.343 (5)	C5—H5B	0.9600
C2—C11	1.715 (4)	C5—H5C	0.9600
C3—O2	1.346 (5)	C6—H6A	0.9600
C4—O2	1.468 (5)	C6—H6B	0.9600
C4—C6	1.486 (7)	C6—H6C	0.9600
O1—C1—C2	121.2 (4)	C5—C4—H4	108.7
O1—C1—C3 <sup>i</sup>	121.0 (4)	C4—C5—H5A	109.5
C2—C1—C3 <sup>i</sup>	117.7 (4)	C4—C5—H5B	109.5
C3—C2—C1	122.2 (4)	H5A—C5—H5B	109.5
C3—C2—C11	121.1 (3)	C4—C5—H5C	109.5
C1—C2—C11	116.7 (3)	H5A—C5—H5C	109.5
C2—C3—O2	120.2 (4)	H5B—C5—H5C	109.5
C2—C3—C1 <sup>i</sup>	120.0 (4)	C4—C6—H6A	109.5
O2—C3—C1 <sup>i</sup>	119.5 (4)	C4—C6—H6B	109.5
O2—C4—C6	104.7 (4)	H6A—C6—H6B	109.5
O2—C4—C5	111.9 (4)	C4—C6—H6C	109.5
C6—C4—C5	114.0 (5)	H6A—C6—H6C	109.5
O2—C4—H4	108.7	H6B—C6—H6C	109.5
C6—C4—H4	108.7	C3—O2—C4	119.2 (3)
O1—C1—C2—C3	174.3 (4)	C1—C2—C3—C1 <sup>i</sup>	4.0 (6)
C3 <sup>i</sup> —C1—C2—C3	-3.9 (6)	C11—C2—C3—C1 <sup>i</sup>	-177.4 (3)
O1—C1—C2—C11	-4.3 (5)	C2—C3—O2—C4	130.7 (4)
C3 <sup>i</sup> —C1—C2—C11	177.4 (3)	C1 <sup>i</sup> —C3—O2—C4	-56.2 (5)
C1—C2—C3—O2	177.1 (3)	C6—C4—O2—C3	-175.7 (4)
C11—C2—C3—O2	-4.4 (5)	C5—C4—O2—C3	-51.8 (6)

Symmetry code: (i)  $-x+1, -y+1, -z+1$ .*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C4—H4 $\cdots$ O1 <sup>i</sup>	0.98	2.34	2.926 (7)	117

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