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#### Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.064  
 $wR$  factor = 0.219  
Data-to-parameter ratio = 22.7

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

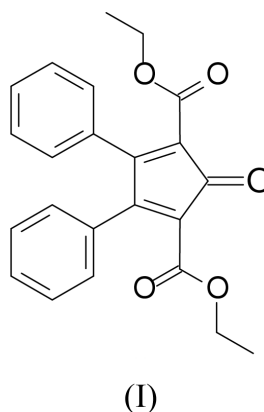
## Diethyl 2-oxo-4,5-diphenylcyclopentane-1,3-dicarboxylate

The title compound,  $\text{C}_{23}\text{H}_{20}\text{O}_5$ , is one of a series of soluble precursors to electroluminescent conjugated polymers as well as leading to helical structures. The geometries of the ring systems are within normal limits, as are those of the ethyl esters. There are few close contacts within the molecule, leading one to rationalize the overall geometry arising from pure steric interactions without any attractive forces such as hydrogen bonding.

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### Comment

Cyclopentadienones produced by a condensation reaction are the building blocks used to produce many monomers used for light emitting diodes. These cyclones can participate in Diels–Alder reactions with a large variety of internal and terminal acetylenes to generate a multitude of aromatic compounds.



The title compound, (I), reacts smoothly with alkynes to generate aromatic terephthalic esters having phenyl and alkyl substituents. Reduction of the esters to alcohols and further conversion to the corresponding chloro compounds provides poly(phenylene vinylene) (PPV) monomers (Feld *et al.*, 1998). Polymeric material produced from these monomers exhibits photoluminescence at 490 nm with an efficiency of 65%. These materials are useful for designing multicolor electroluminescent devices. In addition, the terephthalic esters are a convenient substrate for the generation of substituted 5,8-dioxo-5,8-dihydroindeno[2,1-*c*]fluorine ring systems by reaction with sulfuric acid (Lorge, 1998).

The cyclopentadienone and phenyl ring systems are themselves planar, but are not coplanar. The phenyl rings are twisted (Fig. 1) about the external bond to the five-membered ring by  $44.68$  ( $12^\circ$ ) for ring 1 (C31–C36) and  $53.91$  ( $12^\circ$ ) for ring 2 (C41–C46). The bond distances and angles around each atom are within accepted values.

## Experimental

The synthesis of 2,5-dicarboethoxy-3,4-diphenylcyclopentadienone can be carried out in a two-step process. Diethyl acetonedicarboxylate is reacted with benzil in sodium ethoxide/ethanol to provide a yellow ionic precipitate. The yellow precipitate is reacted with sulfuric acid in acetic anhydride to produce the title compound as an orange product (Reinhardt, 1974).

### Crystal data

$C_{23}H_{20}O_5$	$D_x = 1.263 \text{ Mg m}^{-3}$
$M_r = 376.39$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
$a = 10.697 (3) \text{ \AA}$	$\theta = 3.0\text{--}12.6^\circ$
$b = 18.228 (4) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 11.202 (2) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 115.02 (2)^\circ$	Trigonal prism, orange
$V = 1979.2 (9) \text{ \AA}^3$	$0.40 \times 0.35 \times 0.30 \text{ mm}$
$Z = 4$	

### Data collection

Enraf–Nonius CAD-4 diffractometer	$\theta_{\text{max}} = 30.0^\circ$
$\omega/2\theta$ scans	$h = -15 \rightarrow 13$
Absorption correction: none	$k = -6 \rightarrow 25$
6973 measured reflections	$l = -2 \rightarrow 15$
5758 independent reflections	3 standard reflections
2719 reflections with $I > 2\sigma(I)$	frequency: 120 min
$R_{\text{int}} = 0.016$	intensity decay: 1.0%

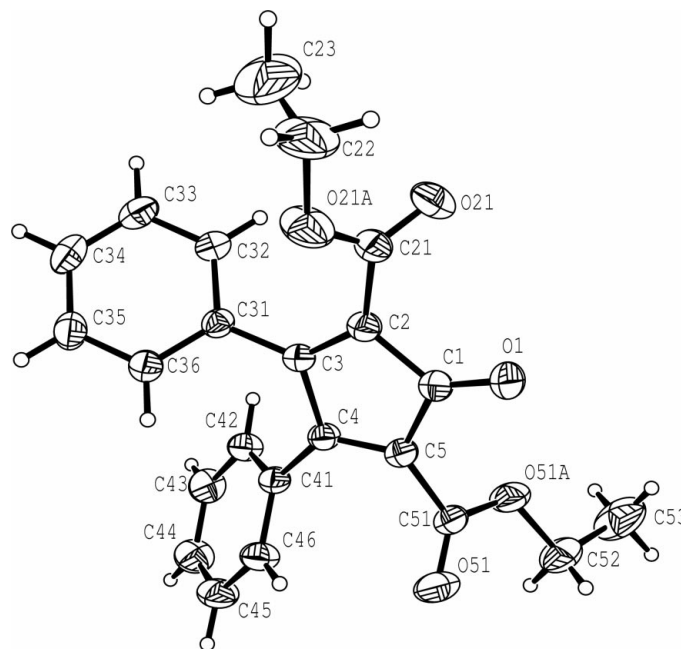
### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.122P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.064$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.219$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.98$	$\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$
5758 reflections	$\Delta\rho_{\text{min}} = -0.30 \text{ e \AA}^{-3}$
254 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.009 (2)

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O1–C1	1.208 (2)	C2–C3	1.344 (3)
O21–C21	1.191 (3)	C2–C21	1.482 (3)
O51–C51	1.190 (2)	C3–C31	1.466 (3)
O21A–C21	1.312 (3)	C3–C4	1.529 (2)
O21A–C22	1.472 (3)	C4–C5	1.341 (3)
O51A–C51	1.305 (3)	C4–C41	1.473 (2)
O51A–C52	1.466 (3)	C5–C51	1.486 (3)
C1–C5	1.497 (3)	C22–C23	1.396 (8)
C1–C2	1.498 (3)	C52–C53	1.453 (4)
C21–O21A–C22	117.9 (2)	C41–C4–C3	124.14 (16)
C51–O51A–C52	117.05 (19)	C4–C5–C51	128.24 (17)
O1–C1–C5	127.19 (18)	C4–C5–C1	108.51 (16)
O1–C1–C2	127.04 (18)	C51–C5–C1	123.20 (16)
C5–C1–C2	105.67 (15)	O21–C21–O21A	123.0 (2)
C3–C2–C21	130.07 (17)	O21–C21–C2	123.6 (2)
C3–C2–C1	108.55 (16)	O21A–C21–C2	113.45 (18)
C21–C2–C1	121.34 (17)	C23–C22–O21A	111.3 (4)
C2–C3–C31	127.68 (16)	O51–C51–O51A	123.5 (2)
C2–C3–C4	108.45 (15)	O51–C51–C5	124.8 (2)
C31–C3–C4	123.87 (15)	O51A–C51–C5	111.68 (17)
C5–C4–C41	126.93 (17)	C53–C52–O51A	108.4 (2)
C5–C4–C3	108.81 (15)		
O1–C1–C5–C51	–5.9 (4)	C5–C4–C41–C42	–123.7 (2)
C22–O21A–C21–C2	–178.1 (3)	C52–O51A–C51–C5	179.0 (2)
C3–C2–C21–O21	–132.6 (3)	C4–C5–C51–O51	–62.3 (4)
C21–O21A–C22–C23	86.2 (5)	C51–O51A–C52–C53	–176.5 (3)
C2–C3–C31–C36	–133.9 (2)		



**Figure 1**

Molecular structure diagram with probability ellipsoids for all non-H atoms shown at the 30% probability level.

H-atom positions were calculated at the beginning of each least-squares refinement cycle, using geometric considerations, and were constrained. Methyl, methylene, and aromatic H atoms had fixed C–H bond lengths of 0.96, 0.97, and 0.93  $\text{\AA}$ , respectively. In all cases, the H-atom  $U_{\text{iso}}$  is 1.3 times  $U_{\text{iso}}$  of the parent atom. Atom C23 is observed to have large thermal motion in all directions, which at first was thought to be due to disorder. An extensive effort was made to resolve this situation, but without success. Residual electron density is present in the vicinity of C23; however, the position of this density does not lend itself to the required geometry for an alternative C23 atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD* (McArdle, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *OSCAIL* (McArdle, 1995).

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