Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

2-Chloro-3-[1-chloro-2-(2-ethynylphenyl)-ethenyl]naphthalene-1,4-dione

Hui-Ying An,[a] Jian-Hua Xu,[a] Shea-Lin Ng[b] and Hoong-Kun Fun[b]*

[a]Department of Chemistry, Nanjing University, Nanjing 210093, People's Republic of China, and [b]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

Correspondence e-mail: hkfun@usm.my

Received 4 January 2007
Accepted 8 January 2007

In the title compound, $C_{20}H_{10}Cl_2O_2$, the naphthoquinone unit is essentially planar. The dihedral angle between the naphthalene system and the benzene ring is 11.74 (6)°. The molecules are linked by intermolecular C—H$\cdots$Cl interactions, forming a chain along the *b* axis. In addition, the crystal structure is stabilized by weak intermolecular π–π interactions.

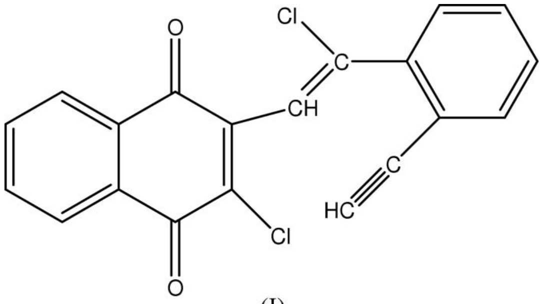
Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.051
wR factor = 0.151
Data-to-parameter ratio = 20.6

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

Comment

In continuation of our recent investigation on photoinduced reactions of quinones with alkynes (Wang *et al.*, 2005), we have investigated the photoreaction of 2,3-dichloro-1,4-naphthoquinone with 1,2-diethynylbenzene and found that this proceeded *via* the triplet excited state of the quinone to give the title compound, (I), as a minor product, together with a normal cyclobutane cycloadduct. An X-ray crystallographic analysis was undertaken to elucitate its structure.



(I)

Bond lengths and angles in (I) (Fig. 1) have normal values (Allen *et al.*, 1987). The naphthoquinone unit in the title molecule is essentially planar. The dihedral angle between the C1/C2/C7–C10 and C13–C18 planes is 11.68 (11)°. The C10—C11—C12—C13 torsion angle is 178.0 (2)°.

In the crystal structure, the molecules are linked by intermolecular C—H$\cdots$Cl interactions (Table 1), forming chains along the *b* axis (Fig. 2). The crystal packing is further stabilized by weak intermolecular π–π interactions involving the C1/C2/C7–C10 (centroid *Cg*1) and C2–C7 (centroid *Cg*2) rings, with $Cg1\cdots Cg1^{ii}$ and $Cg1\cdots Cg2^{ii}$ distances of 3.7868 (11) and 3.6508 (12) Å, respectively [symmetry code: (ii) $1 - x, -y, -z$].

Experimental

Compound (I) was prepared by photolysis of a benzene solution of 2,3-dichloro-1,4-naphthoquinone (0.05 mol) in the presence of an excess amount of 1,2-diethynylbenzene (1.5 equivalent, 4.5 mmol).

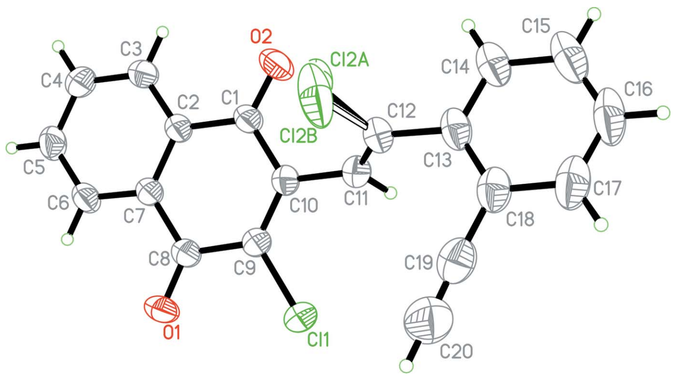


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Both disorder components are shown.

The photoreaction yielded (I) as a minor product after column chromatographic separation of the reaction mixture on a silica-gel column with petroleum ether–ethyl acetate as eluants. Single crystals suitable for X-ray diffraction studies were obtained by slow evaporation of a petroleum ether–ethyl acetate (2:1 *v*/*v*) solution.

Crystal data

$C_{20}H_{10}Cl_2O_2$
$M_r = 353.18$
Monoclinic, $P2_1/c$
$a = 13.2480$ (3) Å
$b = 8.1877$ (2) Å
$c = 15.1674$ (4) Å
$\beta = 103.965$ (1)°
$V = 1596.59$ (7) Å^3
$Z = 4$
$D_x = 1.469$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.42$ mm^{-1}
$T = 297$ (2) K
Plate, yellow
0.48 × 0.37 × 0.08 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min} = 0.802$, $T_{\max} = 0.966$
25574 measured reflections
4674 independent reflections
3064 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.054$
$\theta_{\max} = 30.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.151$
$S = 1.07$
4674 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2 + 0.0564P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.24$ e Å^{-3}
$\Delta\rho_{\min} = -0.27$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H3$A\cdots$Cl1$^{\rm i}$	0.93	2.77	3.676 (2)	164

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

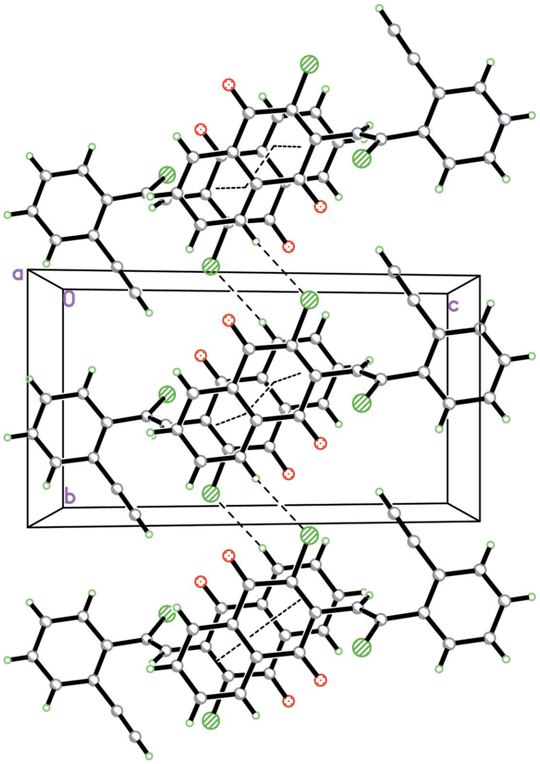


Figure 2
Packing diagram of (I), viewed down the *a* axis. Intermolecular C—H$\cdots$Cl and π–π interactions are shown as dashed lines. Only the major component of the disordered Cl atom is shown.

One of the Cl atoms is disordered over two positions (Cl2*A*/Cl2*B*) with site occupancies of 0.60 (6) and 0.40 (6). H atoms were placed in calculated positions and constrained to ride on their carrier atoms, with C—H distances in the range 0.89–0.93 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government and Universiti Sains Malaysia for the Scientific Advancement Grant Allocation (SAGA) grant No. 304/PFIZIK/653003/A118.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Wang, L., Zhang, Y., Hu, H. Y., Fun, H.-K. & Xu, J. H. (2005). *J. Org. Chem.* **70**, 3850–3858.

o698 An *et al.* • $C_{20}H_{10}Cl_2O_2$ *Acta Cryst.* (2007). E**63**, o697–o698