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Di-*tert*-butyl 7,14-dihydro-7,14-dioxoquino[2,3-*b*]acridine-5,12-dicarboxylate

Jin Mizuguchi

Department of Applied Physics, Graduate School of Engineering, Yokohama National University, 79-5 Tokiwadai, Hodogaya-ku, 240-8501 Yokohama, Japan

Correspondence e-mail: mizu-j@ynu.ac.jp

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The title compound, $C_{30}H_{28}N_2O_6$, is a soluble precursor ('latent pigment') of quinacridone pigments. The molecule has inversion symmetry. The *tert*-butoxycarbonyl group attached to the N atom of the acridine skeleton is twisted by 55.57 (8)° from the heterocyclic ring to which it is attached. The condensed ring system is not entirely planar, and the dihedral angle between the cental benzene ring and the neighboring ring is 174.56 (6)°.

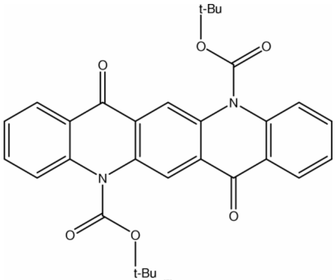
Key indicators

Single-crystal X-ray study
T = 93 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.075
Data-to-parameter ratio = 13.0

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

Comment

The title compound, (I), is a soluble yellow precursor ('latent pigment') (Zambounis *et al.*, 1994, 1997) of quinacridone pigments (QA) (Herbst & Hunger, 1997) that are known as industrially important red pigments. The soluble precursor is prepared by replacing the H atom of the NH group with a *tert*-butoxycarbonyl (*t*-BOC) group, hereafter called *t*-BOC QA. The insoluble parent QA can then be regenerated by thermochemical treatment of the precursor. The present 'latent pigment technology' is a versatile and promising technique for the preparation of nano pigment particles, as well as transparent pigmented thin films, *etc*. The crystal structure of the parent QA has previously been reported by Potts *et al.* (1994) and by us (Mizuguchi *et al.*, 2002). The present paper describes the crystal structure of *t*-BOC QA, (I).



(I)

The title compound crystallizes in space group $P2_1/n$ and the molecule has inversion symmetry (Fig. 1). Each *t*-BOC group is twisted with respect to the corresponding heterocyclic ring by 55.57 (8)° (N1/C11/O2/O3 and N1/C1/C2/C7/C8/C10). The condensed ring system is not entirely planar. The dihedral angles between two condensed rings are 174.56 (6)° [N1/C1/C2/C7/C8/C10 and C8–C10/C8^{i}–C10^{i}; symmetry code: (i) $1 - x, -y, 1 - z$] and 179.11 (8)° (N1/C1/C2/C7/C8/C10 and C2–C7). The molecules are stacked along the *a* axis.

Experimental

The title compound (I) was prepared according to the method described in the literature (Zambounis *et al.*, 1994). Single crystals of (I) were grown from an acetonitrile solution.

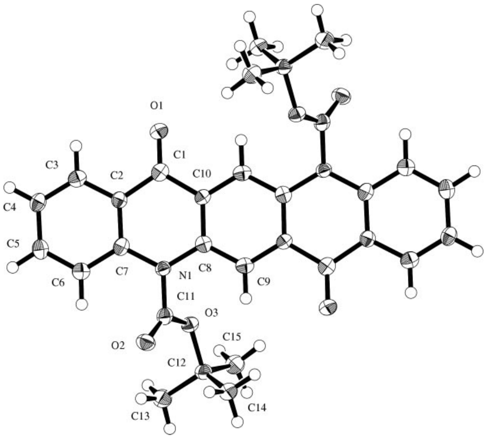


Figure 1
A view of the molecular structure of (I), showing ellipsoids at the 50% probability level for non-H atoms.

Crystal data

$C_{30}H_{28}N_2O_6$
$M_r = 512.56$
Monoclinic, $P2_1/n$
$a = 14.020$ (2) Å
$b = 6.5225$ (8) Å
$c = 14.153$ (2) Å
$\beta = 106.704$ (9)°
$V = 1239.6$ (3) Å^3
$Z = 2$

$D_x = 1.373$ Mg m^{-3}
Cu Kα radiation
Cell parameters from 8483 reflections
$\theta = 3.3$–68.1°
$\mu = 0.79$ mm^{-1}
$T = 93.2$ K
Pseudo-hexagonal prism, colorless
0.15 × 0.15 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID Imaging Plate diffractometer
ω scans; 48 frames, $\Delta\omega = 15°$
Absorption correction: multi-scan (Higashi, 1995)
$T_{\min} = 0.791$, $T_{\max} = 0.924$
10974 measured reflections

2242 independent reflections
1276 reflections with $F^2 > 2\sigma(F^2)$
$R_{\rm int} = 0.043$
$\theta_{\max} = 68.1°$
$h = -16 \rightarrow 16$
$k = -7 \rightarrow 7$
$l = -17 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.075$
$S = 1.22$
2240 reflections
172 parameters

H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.015P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.22$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.229 (3)	C2—C3	1.406 (3)
O2—C11	1.198 (3)	C2—C7	1.398 (3)
O3—C11	1.331 (3)	C3—C4	1.371 (3)
O3—C12	1.504 (3)	C4—C5	1.401 (3)
N1—C7	1.410 (3)	C5—C6	1.377 (3)
N1—C8	1.413 (3)	C6—C7	1.411 (3)
N1—C11	1.439 (3)	C8—C9	1.393 (3)
C1—C2	1.474 (3)	C8—C10	1.403 (3)
C1—C10	1.474 (3)	C9—C10$^{\rm i}$	1.384 (3)
O2—C11—N1—C7	−56.1 (3)	N1—C7—C2—C3	178.2 (2)
O2—C11—N1—C8	127.2 (2)	C1—C2—C7—C6	−176.6 (2)
O3—C11—N1—C7	122.9 (2)	C1—C10—C8—C9	−178.7 (2)
O3—C11—N1—C8	−53.7 (3)		

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

All H atoms were positioned geometrically and refined as riding.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *TEXSAN* (Molecular Structure Corporation, 2001); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985); program(s) used to refine structure: *TEXSAN*; molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *TEXSAN*.

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