Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Di-*tert*-butyl 3,6-bis(2-methylphenyl)-1,4-dioxo-1,2,4,5-tetrahydropyrrolo[3,4-*c*]pyrrole-2,5-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

Received 21 February 2003
Accepted 5 March 2003
Online 21 March 2003

The title compound, $C_{30}H_{32}N_2O_6$, is a soluble precursor ('latent pigment') of diketopyrrolopyrrole pigments. The molecule has inversion symmetry. The aryl ring and *tert*-butoxycarbonyl group are twisted with respect to the heterocyclic ring by 64.5 (1) and 30.7 (1)°, respectively.

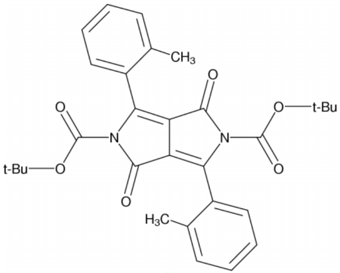
Key indicators

Single-crystal X-ray study
T = 93 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.107
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 diketopyrrolopyrrole pigments (DPP) (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 DPP. The insoluble parent DPP 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*. We have previously reported the crystal structures of the α and β forms of unsubstituted DPP (Mizuguchi, 2003*a*,*b*). The present paper deals with the crystal structure of the *o*-methylphenyl derivative, (I).



(I)

The title compound crystallizes in space group $P2_1/c$ and the molecule has inversion symmetry (Fig. 1). Each aryl ring is twisted from the heterocyclic system by 64.5 (1)° [N1/C1/C2/C3/C3^i and C4–C9; symmetry code: (i) $1-x$, $1-y$, $1-z$]. Each *t*-BOC group is also twisted from the heterocyclic system by 30.7 (1)° (N1/C1/C2/C3/C3^i and N1/C11/O2/O3). The heterocyclic ring system is entirely planar. 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.

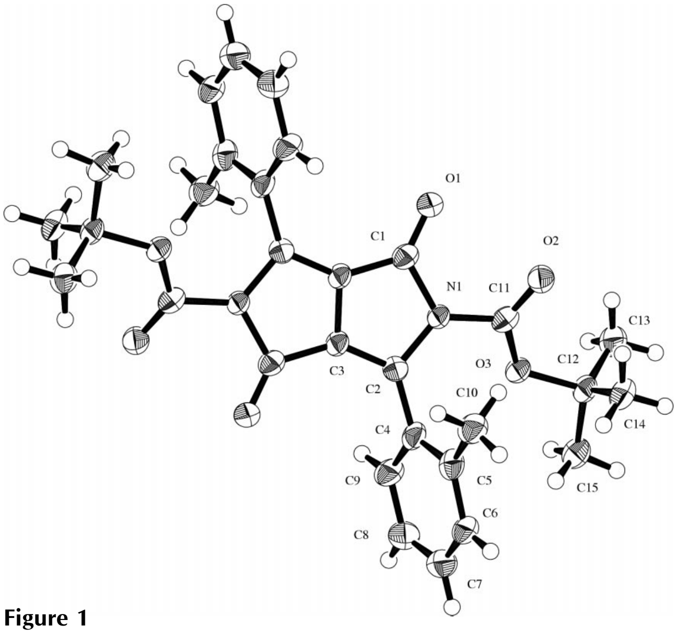


Figure 1
A view of the molecular structure of (I), showing ellipsoids at the 50% probability level for non-H atoms.

Crystal data

$C_{30}H_{32}N_2O_6$
$M_r = 516.59$
Monoclinic, $P2_1/n$
$a = 7.148$ (1) Å
$b = 14.148$ (3) Å
$c = 13.065$ (2) Å
$\beta = 95.729$ (8)°
$V = 1314.7$ (4) Å^3
$Z = 2$

$D_x = 1.305$ Mg m^{-3}
Cu Kα radiation
Cell parameters from 5184 reflections
$\theta = 4.6$–68.2°
$\mu = 0.75$ mm^{-1}
$T = 93.2$ K
Block, colorless
0.30 × 0.10 × 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)
$T_{\min} = 0.841$, $T_{\max} = 0.928$
12159 measured reflections

2243 independent reflections
1226 reflections with $F^2 > 2\sigma(F^2)$
$R_{\rm int} = 0.051$
$\theta_{\max} = 68.3°$
$h = -7 \rightarrow 7$
$k = -16 \rightarrow 17$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.107$
$S = 0.87$
2241 reflections
172 parameters

H atoms not refined
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.005$
$\Delta\rho_{\max} = 0.57$ e Å^{-3}
$\Delta\rho_{\min} = -0.33$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.214 (3)	N1—C11	1.428 (3)
O2—C11	1.205 (3)	C1—C3$^{\text{i}}$	1.456 (4)
O3—C11	1.320 (3)	C2—C3	1.350 (3)
O3—C12	1.492 (3)	C2—C4	1.473 (4)
N1—C1	1.452 (3)	C3—C3$^{\text{i}}$	1.420 (5)
N1—C2	1.430 (3)		
O2—C11—N1—C1	32.9 (4)	N1—C2—C4—C5	65.3 (4)
O2—C11—N1—C2	−152.9 (3)	N1—C2—C4—C9	−118.1 (3)
O3—C11—N1—C1	−146.8 (2)	C3—C2—C4—C5	−113.3 (3)
O3—C11—N1—C2	27.4 (3)	C3—C2—C4—C9	63.3 (4)

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

All H atoms were positioned geometrically, but not refined.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *TEXSAN* (Molecular Structure Corporation, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *TEXSAN*; molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *TEXSAN*.

References

Burnett, M. N. & Johnson, C. K. (1996). *ORTEP*III. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Herbst, W. & Hunger, K. (1997). *Industrial Organic Pigments*, 2nd ed. Weinheim: VCH.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Mizuguchi, J. (2003*a*). *Acta Cryst.* E**59**, o469–o471.
Mizuguchi, J. (2003*b*). *Z. Kristallogr. New Cryst. Struct.* **218**. In the press.
Molecular Structure Corporation (2001). *TEXSAN*. Version 1.11. MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXS*97. University of Göttingen, Germany.
Zambounis, J., Hao, H. & Iqbal, A. (1994). US Patent 5 484 943.
Zambounis, J., Hao, H. & Iqbal, A. (1997). *Nature (London)*, **388**, 131–132.