Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-[4,5-Bis(4-methoxyphenyl)-1*H*-imidazol-2-yl]-benzonitrile

Xu-Feng Liu, Zeng-Pei Zhong* and Zun-Le Xu

School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, People's Republic of China

Correspondence e-mail: ceszzp@zsu.edu.cn

Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.054
wR factor = 0.130
Data-to-parameter ratio = 16.6

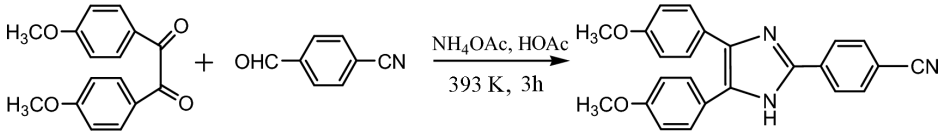
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{24}H_{19}N_3O_2$, is an analogue of lophine and exhibits two-photon induced blue fluorescent emission. It adopts a distorted T-shape.

Received 15 April 2005
Accepted 27 May 2005
Online 10 June 2005

Comment

Heterocyclic imidazoles based on a non-linear optical (NLO) chromophore have received increasing interest due to their excellent thermal stability in guest–host systems (Santos *et al.*, 2001). Previously, we found this type of compound to exhibit two-photon induced blue fluorescent emission (Huang *et al.*, 2002, 2003). In our recent research, the title compound, (I), was found to have the same property.



(I)

Compound (I) was obtained in high yield by refluxing a mixture of 4-cyanobenzaldehyde, 4,4′-dimethoxybenzil and ammonium acetate in acetic acid for 3 h (Nakashima *et al.*, 1998). The structure of (I) was also confirmed by ^{1}H NMR, elemental analysis and FAB–MS spectroscopic analysis.

Compound (I) has a distorted T-shaped molecule (Fig. 1). Adjacent molecules are arrangement in a staggered manner (Fig. 2).

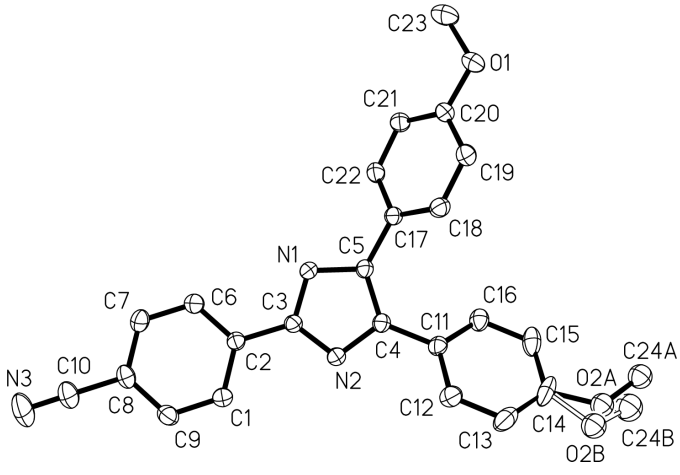


Figure 1
View of the title molecule, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. Both disorder components are shown.

Experimental

Compound (I) was obtained, in 91% yield, by refluxing 4-cyanobenzaldehyde, 4,4′-dimethoxybenzil and ammonium acetate in acetic acid for 3 h. A single crystal suitable for X-ray analysis was obtained from ethanol (m.p. 504 K). ^{1}H NMR (500 MHz in DMSO/TMS): δ 3.79 (*s*, 6H), 6.93–6.96 (*m*, 2H), 6.99–7.02 (*m*, 2H), 7.40–7.45 (*m*, 4H), 7.90 (*d, J* = 10.0 Hz, 2H), 8.21 (*d, J* = 10.0 Hz, 2H). Elemental analysis (%) calculated for $C_{24}H_{19}N_3O_2$: C 75.57, H 5.02, N 11.02; found C 75.69, H 11.11, N 10.94. FAB–MS *m*/*z* (%): 382 (M^+ + H, 8).

Crystal data

$C_{24}H_{19}N_3O_2$
M_r = 381.42
Orthorhombic, *Pbca*
a = 9.801 (3) Å
b = 15.549 (4) Å
c = 26.142 (7) Å
V = 3984.1 (19) Å^3
Z = 8
D_x = 1.272 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4326 reflections
θ = 2.6–27.0°
μ = 0.08 mm^{-1}
T = 273 (2) K
Block, colorless
0.48 × 0.37 × 0.32 mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.974
17659 measured reflections
4326 independent reflections
2563 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.1°
$h = -12 \rightarrow 12$
$k = -19 \rightarrow 19$
$l = -33 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.130
S = 1.02
4326 reflections
261 parameters
Only H-atom U's refined
$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 2.2522P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

All H atoms were included as riding atoms (C—H = 0.96 Å) and their isotropic displacement parameters were refined. One of the methoxy groups (atoms C24*A*/C24*B* and O2*A*/O2*B*) exhibits twofold disorder and these atoms were refined isotropically with site-occupancy factors 0.453 (10) and 0.547 (10).

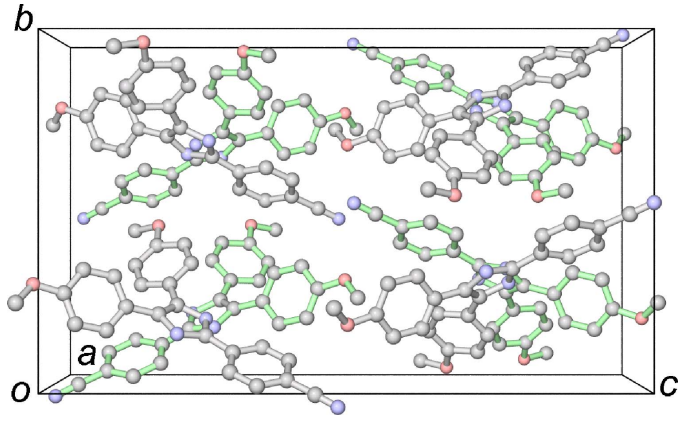


Figure 2
The molecular packing, viewed in the (001) plane. H atoms have been omitted.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

This project is supported by the Guangdong Provincial Natural Science Foundation of China.

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