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1,5-Bis(4-chlorophenyl)-3-(4-pyridyl)-pentane-1,5-dione

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Key indicators

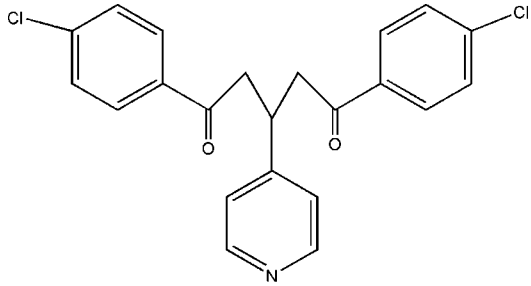
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.102
Data-to-parameter ratio = 18.8

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

The title compound, $C_{22}H_{17}Cl_2NO_2$, has been synthesized and characterized by single-crystal X-ray diffraction. In the crystal structure, the two benzene rings and the pyridyl group lie in a propeller arrangement around the central C atom, thereby minimizing the steric effects between these rings.

Comment

As part of an investigation of the structures of multi-ring compounds, we report here the structure of the title compound, (I) (Fig. 1).



(I)

In the molecule of (I), all bond lengths are within normal ranges (Allen *et al.*, 1987). The two benzene rings and the pyridyl group lie in a propeller arrangement around C9, thereby minimizing the steric effects between these rings. The dihedral angle between the two benzene rings is 15.4 (4)°. The dihedral angles between the pyridine ring and the rings C1–C6 and C12–C17 are 69.3 (4) and 89.6 (4)°, respectively.

There are no short intermolecular contacts in the crystal structure of (I).

Experimental

The title compound was synthesized by the reaction of equivalent amounts of (*E*)-1-(4-chlorophenyl)-3-(pyridin-4-yl)prop-2-en-1-one (0.1 mmol), isonicotinohydrazide (0.1 mmol) and 1-(4-chlorophenyl)ethanone (0.1 mmol) in ethanol solution (30 ml) for 3 h at 373–383 K. Single crystals suitable for X-ray diffraction analysis were obtained by evaporation of an ethanol solution.

Crystal data

$C_{22}H_{17}Cl_2NO_2$
M_r = 398.27
Orthorhombic, $P2_12_12_1$
a = 5.6553 (11) Å
b = 15.754 (3) Å
c = 21.191 (4) Å
V = 1888.0 (6) Å^3
Z = 4
D_x = 1.401 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 298 (2) K
Block, yellow
0.34 × 0.13 × 0.08 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.941, T_{max} = 0.969
17030 measured reflections
4606 independent reflections
1774 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 28.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.102
S = 0.76
4606 reflections
245 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997*a*)
Extinction coefficient: 0.0066 (10)
Absolute structure: Flack (1983), with 1918 Friedel pairs
Flack parameter: 0.01 (7)

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

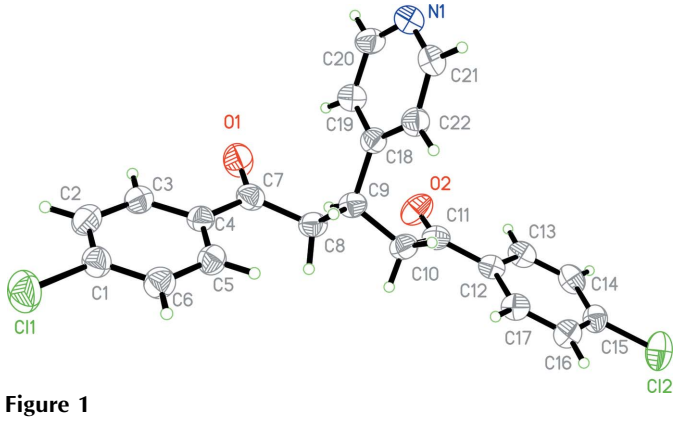


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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