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Methyl 5-methyl-3,4-diphenyl-1*H*-pyrrole-2-carboxylate

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The title compound, $C_{19}H_{17}NO_2$, forms dimeric aggregates in the solid state due to the pyrrole-NH–carboxyl-O hydrogen bonds.

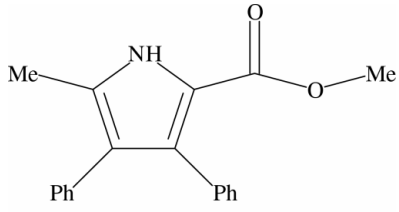
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.060
wR factor = 0.171
Data-to-parameter ratio = 13.7

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

Comment

The title compound, (I), forms dimeric aggregates in the solid state in a similar fashion to 2-amidopyrroles and 2,5-diamidopyrroles (Gale *et al.*, 2001) due to the pyrrole-NH–carboxyl-O hydrogen bonds.



(I)

Experimental

For the preparation of the title compound, ethyl 3,4-diphenyl-5-methyl-1*H*-pyrrole-2-carboxylate (1 g, 3.3 mmol) was suspended in dry methanol (30 ml) and a catalytic amount of sodium cyanide (18 mg, 0.4 mmol) was added. After refluxing for 7 d, the solvent was removed *in vacuo* and acetonitrile (5 ml) was added. The brown suspension was heated until the solid dissolved and overnight recrystallization led to the formation of a white crystalline compound (yield 0.63 g, 67%).

Crystal data

$C_{19}H_{17}NO_2$
M_r = 291.34
Monoclinic, $C2/c$
a = 34.1913 (12) Å
b = 10.7042 (4) Å
c = 19.1129 (9) Å
β = 118.186 (2)°
V = 6165.6 (4) Å^3
Z = 16
D_x = 1.255 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 28010 reflections
θ = 3.3–25.0°
μ = 0.08 mm^{-1}
T = 120 (2) K
Plate, colourless
0.10 × 0.10 × 0.05 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.992, T_{max} = 0.996
28010 measured reflections
5420 independent reflections
3071 reflections with $I > 2\sigma(I)$
R_{int} = 0.102
θ_{max} = 25.0°
$h = -40 \rightarrow 40$
$k = -12 \rightarrow 12$
$l = -22 \rightarrow 22$

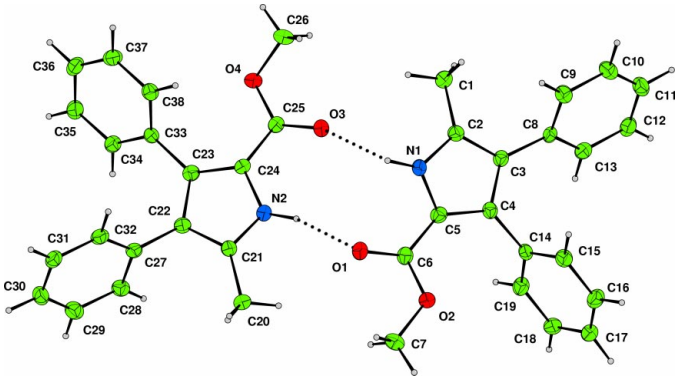


Figure 1
A view of the asymmetric unit of the title compound showing the atomic numbering scheme and the hydrogen bonding. Displacement ellipsoids are drawn at the 30% probability level.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0881P)^2 + 0.4211P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.060$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.171$	$\Delta\rho_{max} = 0.37$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.36$ e Å^{-3}
5420 reflections	
397 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.88	2.05	2.875 (3)	157
N2—H2···O1	0.88	1.99	2.829 (3)	158

H atoms were placed in calculated positions and included in the final refinement in the riding-model approximation with U_{iso} constrained to be $1.5U_{eq}$ of the carrier atom for the methyl–H atoms and $1.2U_{eq}$ for the remaining H atoms.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* (Otwinowski & Minor, 1997), *COLLECT* and *maXus* (Mackay *et al.*, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1998).

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