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2-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)isoindoline-1,3-dione

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In the title compound, $C_{19}H_{15}N_3O_3$, the phthalimide group, dihydropyrazole ring and phenyl ring are all essentially planar. The dihedral angles between the phthalimide group and dihydropyrazole ring, and the phthalimide group and phenyl ring are 57.0 (2) and 46.3 (3)°, respectively.

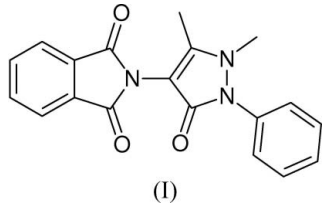
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.115
Data-to-parameter ratio = 14.2

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

Comment

Phthalimides and *N*-substituted phthalimides are an important class of compounds because of their interesting biological activities (Lima *et al.*, 2002). In the title phthalimide derivative, (I) (Fig. 1), the phthalimide group is essentially planar to within 0.015 (3) Å, and its geometry is closely comparable to that in the related compounds 2-(4-hydroxyphenyl)isoindoline-1,3-dione (Liang & Li, 2006*a*) and 2-ethylisoindoline-1,3-dione (Liang & Li, 2006*b*). The dihydropyrazole ring is planar to within 0.032 (3) Å and the phenyl ring is planar to within 0.009 (4) Å. The dihedral angles between the phthalimide group and dihydropyrazole ring, and the phthalimide group and phenyl ring are 57.0 (2) and 46.3 (3)°, respectively.



(I)

Experimental

A mixture of phthalimide (0.1 mol) and 4-amino-1,2-dihydro-2,3-dimethyl-1-phenylpyrazol-5-one (0.1 mol) in acetic acid (90 ml) was refluxed for 4 h. After cooling, filtration and drying, the title compound was obtained. A sample of (I) (10 mg) was dissolved in acetone (13 ml) and the solution kept at room temperature for 5 d. Natural evaporation gave light-yellow single crystals suitable for X-ray analysis.

Crystal data

$C_{19}H_{15}N_3O_3$
M_r = 333.34
Monoclinic, $P2_1/c$
a = 13.960 (3) Å
b = 15.948 (3) Å
c = 7.3536 (14) Å
β = 102.358 (3)°
V = 1599.2 (5) Å^3
Z = 4
D_x = 1.385 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, light yellow
0.22 × 0.18 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.979, T_{max} = 0.989
8874 measured reflections
3257 independent reflections
2109 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.115
S = 1.05
3257 reflections
229 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.256P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0184 (19)

H atoms were visible in difference Fourier maps, but were placed in idealized positions and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(aromatic C) or C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate about their local threefold axes.

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

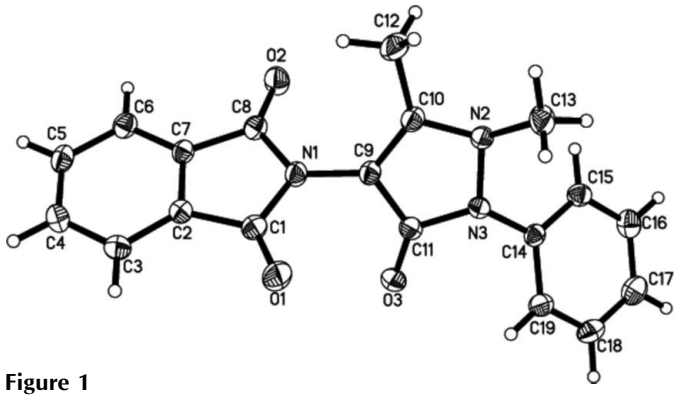


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level for non-H atoms.

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