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N-(4-Methyl-1-piperazinyl)phthalimide

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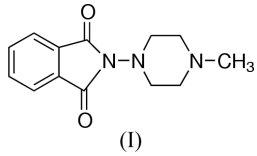
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.114
Data-to-parameter ratio = 12.2

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

The title compound, $C_{13}H_{15}N_3O_2$, (I), crystallizes in the monoclinic space group $P2_1/m$. The phthalimide rings lie in crystallographic mirror planes. Molecules are associated into columns parallel to the b-axis direction, and linked together along the a-axis direction by a two-dimensional network of hydrogen bonds involving C—H···O interactions. The molecular packing in the crystal is stabilized by the weak intermolecular C—H···O hydrogen bonds and van der Waals forces.



(I)

Experimental

The title compound was prepared by the reaction of phthalic anhydride (6.4 g) with 1-amino-4-methylpiperazine (5.0 g) under microwave irradiation for 10 min. The resulting product was heated and dissolved in ethanol (60 ml). The homogeneous solution was allowed to stand at room temperature for 12 h, after which 7.0 g of the colorless crystalline product was separated by filtration. Pure *N*-(4-methyl-1-piperazinyl)phthalimide (1.5 g) was dissolved in ethanol (20 ml). A single crystal was obtained by evaporation for 10 h at room temperature.

Crystal data

$C_{13}H_{15}N_3O_2$
M_r = 245.28
Monoclinic, $P2_1/m$
a = 8.364 (3) Å
b = 6.816 (3) Å
c = 10.972 (5) Å
β = 101.980 (6)°
V = 611.9 (4) Å^3
Z = 2
D_x = 1.331 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 853 reflections
θ = 2.8–26.4°
μ = 0.09 mm^{-1}
T = 293 (2) K
Prism, colorless
0.24 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.985
3540 measured reflections
1372 independent reflections
1064 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.4°
$h = -10 \rightarrow 10$
$k = -8 \rightarrow 8$
$l = -8 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.08
1372 reflections
112 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 0.071P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.30 (2)

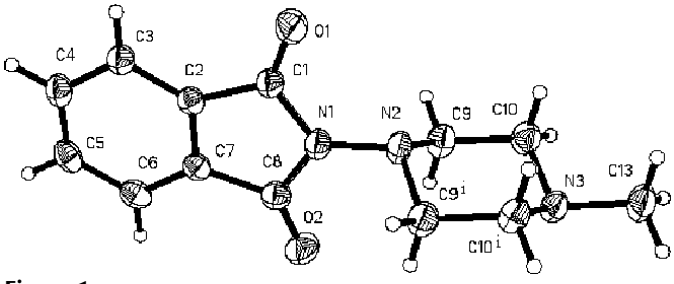


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. [Symmetry code: (i) $x, \frac{1}{2}-y, z$.]

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{ii}	0.93	2.36	3.249 (3)	161
C5—H5···O1^{iii}	0.93	2.36	3.249 (3)	161

Symmetry code: (ii) $1+x, y, z$; (iii) $1+x, \frac{1}{2}-y, z$.

H atoms were treated as riding, with C—H distances of 0.93–0.97 Å. For the H atoms attached to atom C13, U_{iso}(H) = $1.5U_{eq}$(C13); all other U_{iso}(H) values were refined.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

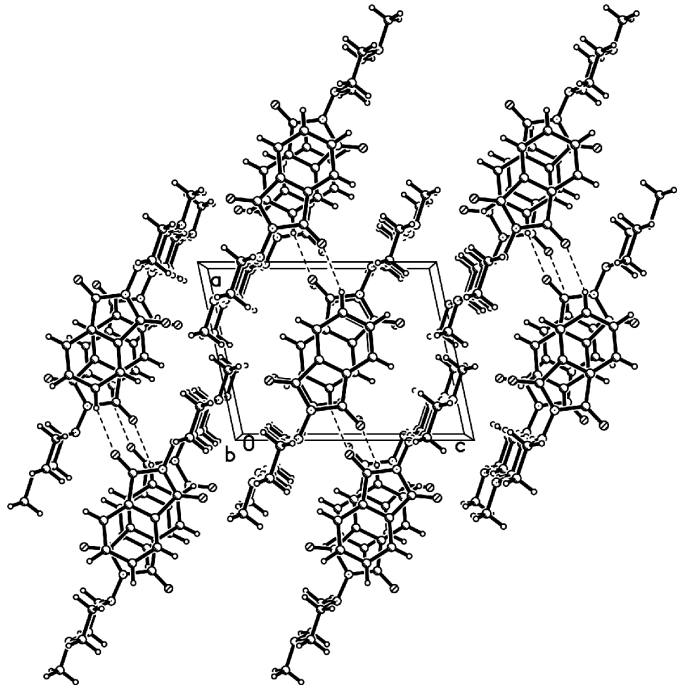


Figure 2
Packing diagram showing C—H···O interactions, viewed down the *b* axis.

References

Bruker (1997). *SMART* (Version 5.051) and *SAINT* (Version 5.A06). Bruker AXS Inc., Madison, Wisconsin, USA.
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