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4-Phthalimidobenzoic acid *N*,*N*-dimethylformamide solvate

Zu-Pei Liang,* Jian Li and Ben-Yu Huang

Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China

Correspondence e-mail: zupeiliang@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.127
Data-to-parameter ratio = 12.3

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

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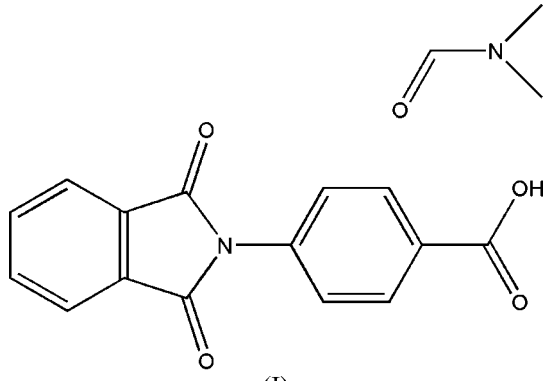
The crystal structure of the title compound, $C_{15}H_9NO_4\cdot C_3H_7NO$, comprises 4-phthalimidobenzoic acid and *N*,*N*-dimethylformamide (DMF) molecules, which are held together by an O—H···O hydrogen bond. The dihedral angle between the phthalimide group and the benzene ring is 53.5 (2)°.

Comment

Phthalimides and N-substituted phthalimides are an important class of compounds because of their interesting biological activities (Lima *et al.*, 2002; Orzeszka *et al.*, 2000; Bailleux *et al.*, 1993). Phthalimides are also used as starting materials and intermediates for the syntheses of alkaloids (Couture *et al.*, 1998) and pharmacophores (Couture *et al.*, 1997).



(I)

The asymmetric unit of (I) contains one 4-phthalimidobenzoic acid molecule and one DMF molecule (Fig. 1). The phthalimide group is essentially planar, with a mean deviation of 0.027 (2) Å. The dihedral angle between the phthalimide group and the benzene C9–C14 ring is 53.5 (2)°. The DMF molecule is planar, within 0.006 (2) Å, for all non-H atoms. The crystal structure is stabilized by an O—H···O hydrogen bond which connects the benzoic acid and DMF molecules and by a C—H···O hydrogen bond which links the DMF molecules (Fig. 2 and Table 1).

Experimental

A mixture of phthalimide (0.1 mol) and 4-aminobenzoic acid (0.1 mol) in acetic acid (40 ml) was refluxed for 3 h. After cooling, filtration and drying, 4-phthalimidobenzoic acid was obtained (m.p. 562–563 K). This compound (10 mg) was dissolved in acetic acid / DMF (2.5:1 *v*/*v*; 12 ml) and the solution was allowed to evaporate at room temperature. Colourless single crystals of the title compound were formed after 20 d.

Crystal data

$C_{15}H_9NO_4{\cdot}C_3H_7NO$
M_r = 340.33
Triclinic, $P\overline{1}$
a = 5.926 (2) Å
b = 8.398 (3) Å
c = 17.518 (7) Å
α = 95.986 (7)°
β = 90.837 (7)°
γ = 109.706 (6)°
V = 815.1 (5) Å^3
Z = 2
D_x = 1.387 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, colourless
0.34 × 0.30 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.966, T_{max} = 0.978
4122 measured reflections
2819 independent reflections
1777 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.127
S = 1.02
2819 reflections
230 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.084 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O5^{i}	0.82	1.76	2.573 (3)	169
C17—H17A···O5^{ii}	0.96	2.52	3.269 (4)	135

Symmetry codes: (i) $x+1, y+1, z$; (ii) $x+1, y, z$.

H atoms were positioned geometrically (C—H = 0.93–0.96 and O—H = 0.82 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C, O).

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*.

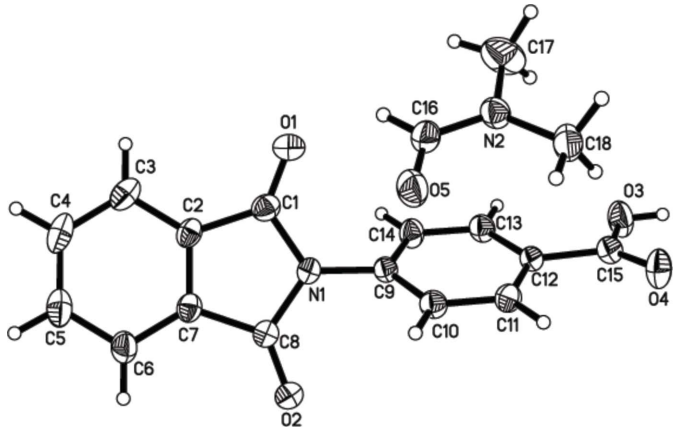


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids.

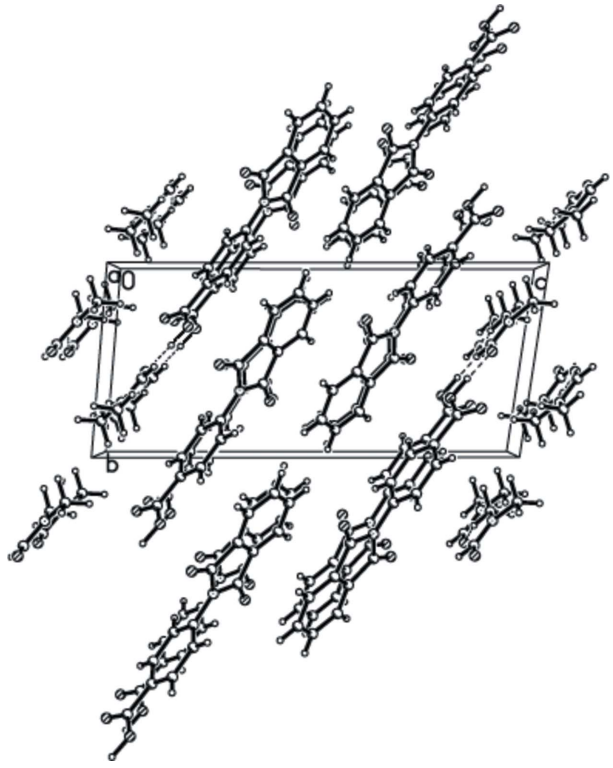


Figure 2
The packing of (I), viewed along the *a* axis. Dashed lines indicate O—H···O hydrogen bonds.

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