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4-Aminophthalimide

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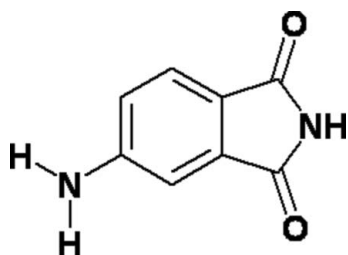
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.064; wR factor = 0.126; data-to-parameter ratio = 9.0.

The molecules in the title compound (systematic name: 5-aminoisindole-1,3-dione), $\text{C}_8\text{H}_6\text{N}_2\text{O}_2$, are packed through $\text{N}-\text{H}\cdots\text{O}$ intermolecular hydrogen-bonding interactions. Two types of hydrogen bonds are observed: one, involving the imide group, forms molecular chains along the c axis and another two, involving the amino group, connect the molecular chains.

Related literature

For related literature, see Paul & Samanta (2007).



Experimental

Crystal data

 $\text{C}_8\text{H}_6\text{N}_2\text{O}_2$ $M_r = 162.15$ Orthorhombic, $Pna2_1$ $a = 14.5786$ (19) Å $b = 13.0728$ (17) Å $c = 3.7216$ (5) Å $V = 709.27$ (16) Å³ $Z = 4$ Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹ $T = 298$ K
 $0.25 \times 0.08 \times 0.06$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.97$, $T_{\max} = 0.99$ 7856 measured reflections
978 independent reflections
636 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.086$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.063$ $wR(F^2) = 0.126$ $S = 1.09$

978 reflections

109 parameters

1 restraint

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^{\text{i}}$	0.86	2.09	2.924 (4)	164
$\text{N2}-\text{H2B}\cdots\text{O1}^{\text{ii}}$	0.86	2.28	3.122 (5)	167
$\text{N2}-\text{H2A}\cdots\text{O2}^{\text{iii}}$	0.86	2.17	2.996 (4)	161

Symmetry codes: (i) $-x + 1, -y + 1, z + \frac{1}{2}$; (ii) $-x + \frac{3}{2}, y + \frac{1}{2}, z - \frac{1}{2}$; (iii) $-x + 1, -y + 2, z - \frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

MS thanks the National Institute of Science Education and Research (NISER), Bhubaneswar for financial support. The structure determination was performed at the National Single Crystal Diffractometer Facility (funded by the DST), School of Chemistry, University of Hyderabad.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2195).

References

- Bruker (1997). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Paul, A. & Samanta, A. (2007). *J. Phys. Chem. B*, **111**, 4724–4731.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

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4-Aminophthalimide

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S1. Comment

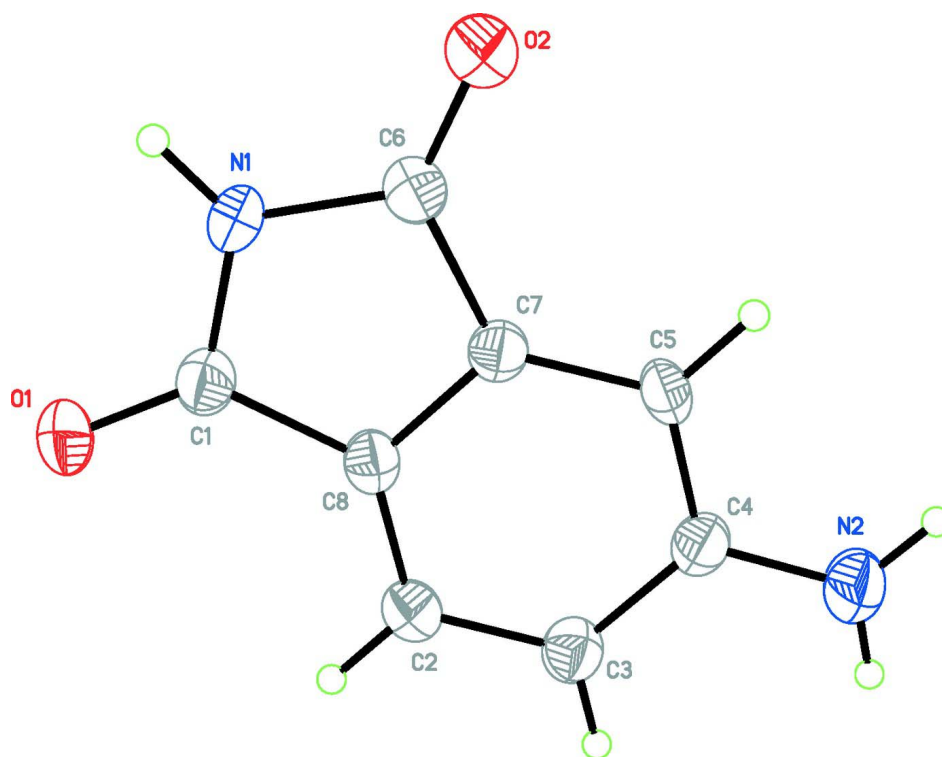
Fluorescent electron donor-acceptor (EDA) systems, 4-aminophthalimide and its derivatives in particular, are found to be attractive candidates for the study of various photophysical processes both in conventional and non-conventional media. Very recently, 4-aminophthalimide has been used in order to investigate specific hydrogen bonding interactions in the solvation and rotational dynamics in room temperature ionic liquids (Paul and Samanta, 2007). Since the ground state structure also influences considerably the photophysical properties of the EDA molecules, we have determined the crystal structure of the title compound $C_8H_6N_2O_2$, (I), shown in Fig. 1. We observe that the imide group forms N—H \cdots O hydrogen bonds (Table 1) in a helical pattern to form molecular chains along *c* axis (Figure 2). The molecules in the chains are further stabilized by π - π stacking (centroid-to-centroid distance = 3.722 Å). These chains are connected through another type of N—H \cdots O hydrogen bonds (Table 1) involving the amino hydrogen and the unused oxygen of the phthalimide group (Figure 3).

S2. Experimental

The title compound was purchased from Aldrich. Tiny single crystals suitable for X-ray diffraction were obtained by slow evaporation from a solution of the compound in ethanol:water (9:1).

S3. Refinement

All H atoms were placed geometrically at idealized positions and refined in the riding-model approximation with the following constraints: C—H = 0.93 Å, N—H = 0.86 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$, $U_{iso}(H) = 1.2U_{eq}(N)$. In the absence of any significant anomalous effect, the data set was merged.

**Figure 1**

The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level for non-H atoms.

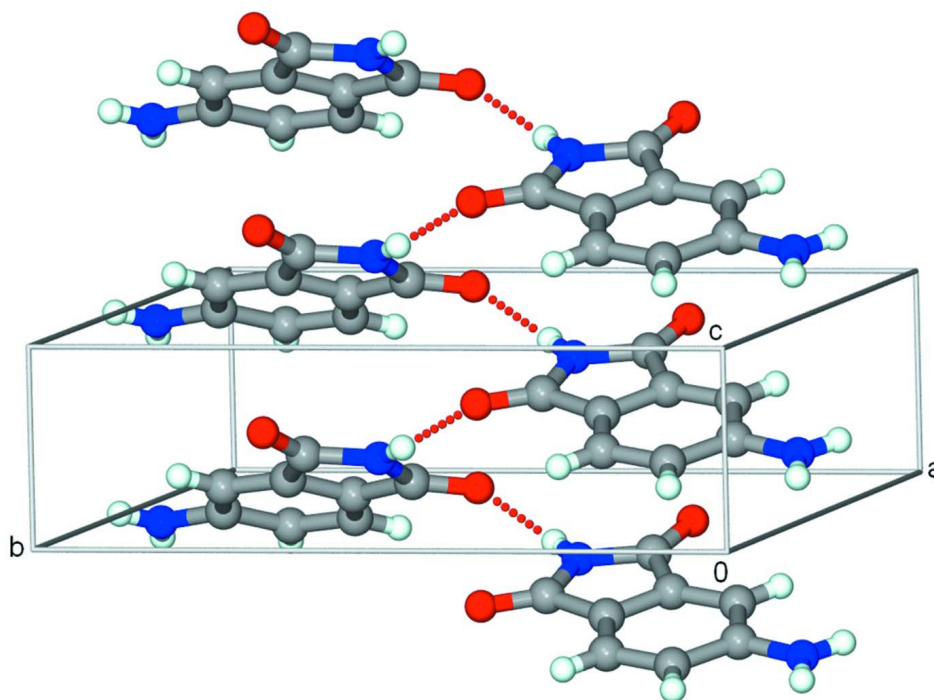


Figure 2

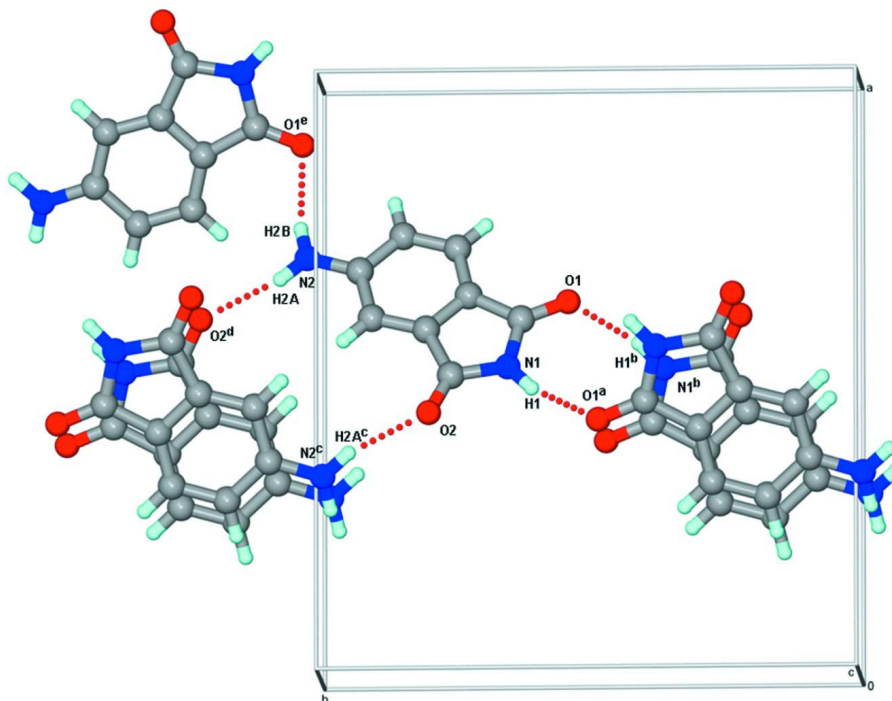
Molecular chain along the *c* axis.

Figure 3

Packing diagram showing N—H \cdots O intermolecular hydrogen bonds. [(1) N1—H1 \cdots O1^a, (2) N1^b—H1^b \cdots O1, (3) N2^c—H2A^c \cdots O2, (4) N2—H2A \cdots O2^d, (5) N2—H2B \cdots O1^e; symmetry codes: (a) 1 - *x*, 1 - *y*, 1/2 + *z*; (b) 1 - *x*, 1 - *y*, -1/2 + *z*; (c) 1 - *x*, 2 - *y*, 1/2 + *z*; (d) 1 - *x*, 2 - *y*, -1/2 + *z*; (e) 3/2 - *x*, 1/2 + *y*, -1/2 + *z*; (1) and (2), (3) and (4) are symmetry related hydrogen bonds].

5-aminoisindole-1,3-dione

Crystal data

C₈H₆N₂O₂*M_r* = 162.15Orthorhombic, *Pna*2₁

Hall symbol: P 2c -2n

a = 14.5786 (19) Å*b* = 13.0728 (17) Å*c* = 3.7216 (5) Å*V* = 709.27 (16) Å³*Z* = 4*F*(000) = 336*D_x* = 1.518 Mg m⁻³Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 704 reflections

θ = 2.8–18.3°

μ = 0.11 mm⁻¹*T* = 298 K

Needle, yellow

0.25 × 0.08 × 0.06 mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 2003)*T_{min}* = 0.97, *T_{max}* = 0.99

7856 measured reflections

978 independent reflections

636 reflections with *I* > 2σ(*I*)

$R_{\text{int}} = 0.086$
 $\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 2.1^\circ$
 $h = -19 \rightarrow 19$

$k = -17 \rightarrow 17$
 $l = -4 \rightarrow 4$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.063$
 $wR(F^2) = 0.126$
 $S = 1.09$
 978 reflections
 109 parameters
 1 restraint
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 0.1098P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.22 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.17 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.60766 (19)	0.53133 (19)	1.0695 (10)	0.0556 (10)
O2	0.41159 (18)	0.7846 (2)	1.4175 (11)	0.0559 (9)
N1	0.4932 (2)	0.6407 (2)	1.2599 (11)	0.0445 (9)
H1	0.4542	0.5954	1.3284	0.053*
N2	0.6919 (2)	1.0180 (2)	0.8617 (13)	0.0599 (12)
H2A	0.6551	1.0669	0.9164	0.072*
H2B	0.7443	1.0315	0.7663	0.072*
C1	0.5777 (3)	0.6181 (3)	1.1116 (14)	0.0411 (10)
C2	0.7055 (3)	0.7394 (3)	0.8804 (12)	0.0400 (10)
H2	0.7459	0.6875	0.8153	0.048*
C3	0.7288 (3)	0.8405 (3)	0.8309 (11)	0.0423 (11)
H3	0.7857	0.8569	0.7338	0.051*
C4	0.6676 (3)	0.9196 (3)	0.9256 (12)	0.0386 (10)
C5	0.5831 (3)	0.8952 (3)	1.0800 (12)	0.0359 (10)
H5	0.5424	0.9464	1.1489	0.043*
C6	0.4787 (3)	0.7455 (3)	1.2853 (12)	0.0402 (10)
C7	0.5613 (2)	0.7937 (3)	1.1281 (12)	0.0346 (9)
C8	0.6212 (3)	0.7165 (3)	1.0282 (11)	0.0350 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.054 (2)	0.0267 (15)	0.086 (3)	0.0020 (13)	-0.0039 (19)	-0.0037 (18)
O2	0.0478 (17)	0.0435 (17)	0.076 (2)	0.0027 (14)	0.0124 (18)	0.0012 (19)
N1	0.0401 (19)	0.0284 (17)	0.065 (2)	-0.0068 (15)	0.0033 (19)	0.005 (2)
N2	0.056 (2)	0.038 (2)	0.086 (3)	-0.0050 (17)	0.012 (3)	0.001 (2)
C1	0.042 (2)	0.033 (2)	0.049 (3)	-0.0026 (19)	-0.005 (2)	0.000 (2)
C2	0.039 (2)	0.037 (2)	0.044 (3)	0.0043 (17)	0.002 (2)	-0.002 (2)
C3	0.045 (2)	0.039 (2)	0.043 (3)	-0.0019 (18)	0.002 (2)	0.001 (2)
C4	0.040 (2)	0.034 (2)	0.041 (2)	-0.0048 (17)	-0.003 (2)	0.002 (2)
C5	0.041 (2)	0.025 (2)	0.041 (2)	0.0078 (16)	-0.004 (2)	-0.003 (2)
C6	0.039 (2)	0.036 (2)	0.047 (3)	0.0022 (18)	-0.002 (2)	-0.001 (2)
C7	0.035 (2)	0.033 (2)	0.036 (2)	-0.0011 (16)	-0.0067 (19)	0.0014 (19)
C8	0.040 (2)	0.030 (2)	0.035 (3)	0.0012 (18)	-0.0032 (18)	0.0008 (19)

Geometric parameters (Å, °)

O1—C1	1.226 (4)	C2—C8	1.380 (5)
O2—C6	1.209 (4)	C2—H2	0.9300
N1—C1	1.381 (5)	C3—C4	1.411 (5)
N1—C6	1.389 (5)	C3—H3	0.9300
N1—H1	0.8600	C4—C5	1.396 (5)
N2—C4	1.356 (5)	C5—C7	1.377 (5)
N2—H2A	0.8600	C5—H5	0.9300
N2—H2B	0.8600	C6—C7	1.479 (5)
C1—C8	1.467 (5)	C7—C8	1.385 (5)
C2—C3	1.378 (6)		
C1—N1—C6	112.0 (3)	N2—C4—C5	121.3 (4)
C1—N1—H1	124.0	N2—C4—C3	119.0 (4)
C6—N1—H1	124.0	C5—C4—C3	119.6 (3)
C4—N2—H2A	120.0	C7—C5—C4	118.5 (3)
C4—N2—H2B	120.0	C7—C5—H5	120.8
H2A—N2—H2B	120.0	C4—C5—H5	120.8
O1—C1—N1	124.6 (4)	O2—C6—N1	124.6 (4)
O1—C1—C8	129.0 (4)	O2—C6—C7	129.8 (4)
N1—C1—C8	106.4 (3)	N1—C6—C7	105.6 (3)
C3—C2—C8	118.8 (4)	C5—C7—C8	121.5 (4)
C3—C2—H2	120.6	C5—C7—C6	130.5 (4)
C8—C2—H2	120.6	C8—C7—C6	108.0 (3)
C2—C3—C4	120.9 (4)	C2—C8—C7	120.7 (3)
C2—C3—H3	119.5	C2—C8—C1	131.3 (4)
C4—C3—H3	119.5	C7—C8—C1	108.0 (4)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1 \cdots O1 ⁱ	0.86	2.09	2.924 (4)	164
N2—H2B \cdots O1 ⁱⁱ	0.86	2.28	3.122 (5)	167
N2—H2A \cdots O2 ⁱⁱⁱ	0.86	2.17	2.996 (4)	161

Symmetry codes: (i) $-x+1, -y+1, z+1/2$; (ii) $-x+3/2, y+1/2, z-1/2$; (iii) $-x+1, -y+2, z-1/2$.