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A new polymorph of *N*-phenylphthalimide

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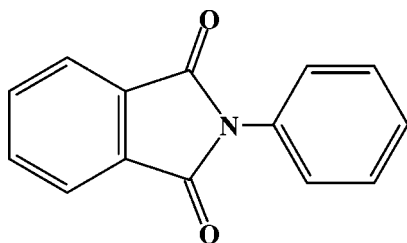
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.067; wR factor = 0.137; data-to-parameter ratio = 13.0.

During an attempt to prepare a cocrystal of *N*-phenylphthalimide, $\text{C}_{14}\text{H}_9\text{NO}_2$, with *N*-(2,3,4,5,6-pentafluorophenyl)phthalimide, a new orthorhombic polymorph of the first component was obtained. This new form has $Z' = 0.5$ and the molecule is located around a twofold axis, whereas in the previously reported polymorph (space group *Pbca*), the molecule has no crystallographically imposed symmetry. Pairs of $\text{C}-\text{H}\cdots\text{O}$ interactions between inversion-related phthalimide units arrange molecules into tapes that are further assembled into (010) layers *via* stacking interactions between phthalimide fragments [interplanar distance = 3.37 (5) Å].

Related literature

For the crystal structure of another polymorph of *N*-phenylphthalimide, see: Magomedova *et al.* (1981); Schwarzer & Weber (2008).



Experimental

Crystal data

$\text{C}_{14}\text{H}_9\text{NO}_2$	$V = 1059.7$ (4) Å ³
$M_r = 223.22$	$Z = 4$
Orthorhombic, <i>Pbcn</i>	Mo $K\alpha$ radiation
$a = 5.5480$ (11) Å	$\mu = 0.10$ mm ⁻¹
$b = 23.801$ (5) Å	$T = 293$ K
$c = 8.0250$ (16) Å	$0.2 \times 0.05 \times 0.05$ mm

Data collection

Stoe Stadi-4 diffractometer	662 reflections with $I > 2\sigma(I)$
Absorption correction: none	3 standard reflections
1039 measured reflections	every 60 reflections
1039 independent reflections	intensity decay: 3.9%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$	80 parameters
$wR(F^2) = 0.137$	H-atom parameters constrained
$S = 1.17$	$\Delta\rho_{\text{max}} = 0.17$ e Å ⁻³
1039 reflections	$\Delta\rho_{\text{min}} = -0.15$ e Å ⁻³

Data collection: *STADI4* (Stoe & Cie, 1997); cell refinement: *STADI4*; data reduction: *X-RED* (Stoe & Cie, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2189).

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supporting information

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S1. Comment

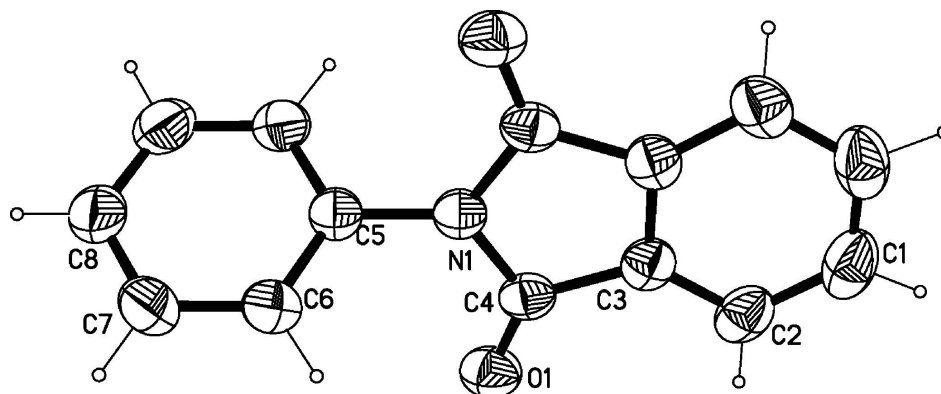
The crystal structure of the polymorph I of the title compound has previously been reported [Magomedova *et al.*, 1981; Schwarzer & Weber, 2008]. In the course of our studies on the crystal-engineering behaviour of *N*-aryl substituted phthalimides (Schwarzer & Weber, 2008) and on polymorphism in general a new polymorph of *N*-phenylphthalimide (designated as II), was obtained. The molecular structure of *N*-phenylphthalimide (Fig. 1) is similar to that in the polymorph I, except the twist angle between the phenyl and phthalimide units which is larger in polymorph II [64.09 (10)°] than in polymorph I [56.73 (4)°] owing to differences in the crystal packing and intermolecular interactions. The most prominent interactions in the polymorph I are carbonyl-carbonyl interaction leading to a short C1=O1...C2=O2 contact (3.08 Å) and a weak C3—H1...O1 interaction (2.65 Å, 137°). In the form II molecules of *N*-phenylphthalimide related by inversion interact *via* C2—H2...O1ⁱ hydrogen bonds (2.66 Å, 145°; symmetry code: (i) 1 - x, 1 - y, -z) forming zigzag tapes parallel to the crystallographic (102) plane (Fig. 2). These tapes are arranged into (010) layers *via* stacking interactions between phthalimide units. Within the stacks, the distance between planes of phthalimide units of consecutive molecules is 3.37 (5) Å.

S2. Experimental

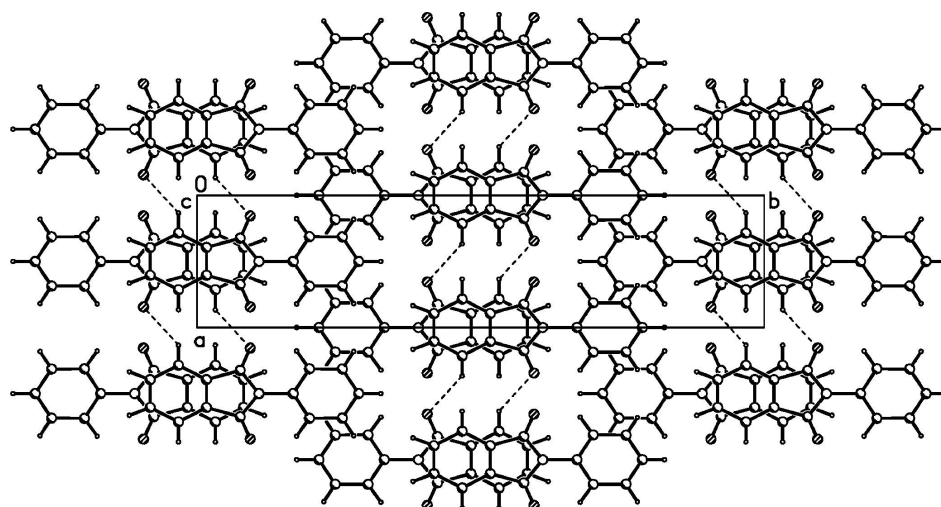
N-Phenylphthalimide was synthesized from aniline and phthalic anhydride according to the procedure described by Schwarzer & Weber (2008). After evaporation of solvent from an acetone solution containing equimolar mixture of *N*-phenylphthalimide and *N*-(2,3,4,5,6,-pentafluorophenyl)phthalimide two types of crystals have deposited. The crystals of the plate form (m.p. 456.5 K) appeared to be the polymorph I of *N*-phenylphthalimide whereas bulky needles the polymorph II (m.p. 485 K). Both types of crystals were stable in the air.

S3. Refinement

All H-atoms were positioned geometrically (C—H 0.93 Å) and refined as riding on their carrier atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

**Figure 1**

Perspective view of the molecule showing 40% probability displacement ellipsoids for the non-hydrogen atoms.

**Figure 2**

Packing diagram for polymorph II; viewed down the *c* axis. Hydrogen bonds are shown as dashed lines.

***N*-phenylphthalimide**

Crystal data

$C_{14}H_9NO_2$

$M_r = 223.22$

Orthorhombic, *Pbcn*

Hall symbol: $-P\ 2n\ 2ab$

$a = 5.5480\ (11)\ \text{\AA}$

$b = 23.801\ (5)\ \text{\AA}$

$c = 8.0250\ (16)\ \text{\AA}$

$V = 1059.7\ (4)\ \text{\AA}^3$

$Z = 4$

$F(000) = 464$

$D_x = 1.399\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 25 reflections

$\theta = 10\text{--}25^\circ$

$\mu = 0.10\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Needle, colourless

$0.2 \times 0.05 \times 0.05\ \text{mm}$

Data collection

Stoe Stadi-4

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω - 2τ scans

1039 measured reflections

1039 independent reflections

662 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.000$
 $\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 1.7^\circ$
 $h = 0 \rightarrow 6$
 $k = -29 \rightarrow 0$

$l = 0 \rightarrow 9$
 3 standard reflections every 60 reflections
 intensity decay: 3.9%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.137$
 $S = 1.17$
 1039 reflections
 80 parameters
 0 restraints
 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
 $w = 1/[\sigma^2(F_o^2) + (0.0266P)^2 + 0.8879P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.17 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.15 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0123 (18)

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	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.0000	0.39051 (14)	0.2500	0.0475 (9)
O1	0.3444 (4)	0.40588 (9)	0.0909 (3)	0.0624 (7)
C1	0.1048 (7)	0.58237 (14)	0.2026 (4)	0.0740 (12)
H1	0.1731	0.6164	0.1709	0.089*
C2	0.2140 (6)	0.53244 (14)	0.1544 (4)	0.0626 (10)
H2	0.3548	0.5324	0.0916	0.075*
C3	0.1056 (5)	0.48304 (12)	0.2034 (3)	0.0491 (8)
C4	0.1752 (6)	0.42378 (12)	0.1702 (4)	0.0479 (8)
C5	0.0000	0.33042 (18)	0.2500	0.0498 (11)
C6	0.1868 (6)	0.30175 (13)	0.3253 (4)	0.0601 (9)
H6	0.3125	0.3213	0.3754	0.072*
C7	0.1855 (6)	0.24375 (14)	0.3257 (5)	0.0765 (12)
H7	0.3099	0.2241	0.3771	0.092*
C8	0.0000	0.2150 (2)	0.2500	0.0820 (19)
H8	0.0000	0.1759	0.2500	0.098*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.044 (2)	0.049 (2)	0.049 (2)	0.000	0.0052 (18)	0.000

O1	0.0502 (13)	0.0738 (15)	0.0631 (15)	0.0017 (12)	0.0078 (12)	0.0049 (12)
C1	0.088 (3)	0.0545 (19)	0.079 (3)	-0.0123 (18)	-0.033 (2)	0.0080 (18)
C2	0.063 (2)	0.066 (2)	0.059 (2)	-0.0128 (18)	-0.0198 (18)	0.0059 (18)
C3	0.0502 (17)	0.0543 (18)	0.0427 (18)	-0.0033 (14)	-0.0134 (15)	0.0018 (14)
C4	0.0409 (16)	0.0589 (19)	0.0438 (17)	-0.0017 (16)	-0.0061 (15)	0.0036 (15)
C5	0.048 (2)	0.050 (3)	0.052 (3)	0.000	0.003 (2)	0.000
C6	0.0476 (18)	0.062 (2)	0.070 (2)	0.0027 (17)	-0.0001 (18)	0.0049 (18)
C7	0.057 (2)	0.067 (2)	0.106 (3)	0.013 (2)	0.011 (2)	0.018 (2)
C8	0.058 (3)	0.057 (3)	0.130 (5)	0.000	0.033 (4)	0.000

Geometric parameters (Å, °)

N1—C4 ⁱ	1.408 (3)	C3—C4	1.487 (4)
N1—C4	1.408 (3)	C5—C6	1.380 (4)
N1—C5	1.430 (5)	C5—C6 ⁱ	1.380 (4)
O1—C4	1.211 (3)	C6—C7	1.380 (4)
C1—C2	1.389 (4)	C6—H6	0.9300
C1—C1 ⁱ	1.389 (8)	C7—C8	1.378 (4)
C1—H1	0.9300	C7—H7	0.9300
C2—C3	1.378 (4)	C8—C7 ⁱ	1.378 (4)
C2—H2	0.9300	C8—H8	0.9300
C3—C3 ⁱ	1.389 (6)		
C4 ⁱ —N1—C4	111.6 (4)	N1—C4—C3	105.8 (3)
C4 ⁱ —N1—C5	124.22 (18)	C6—C5—C6 ⁱ	120.7 (4)
C4—N1—C5	124.22 (18)	C6—C5—N1	119.6 (2)
C2—C1—C1 ⁱ	121.2 (2)	C6 ⁱ —C5—N1	119.6 (2)
C2—C1—H1	119.4	C7—C6—C5	119.5 (4)
C1 ⁱ —C1—H1	119.4	C7—C6—H6	120.3
C3—C2—C1	117.4 (3)	C5—C6—H6	120.3
C3—C2—H2	121.3	C8—C7—C6	120.0 (4)
C1—C2—H2	121.3	C8—C7—H7	120.0
C2—C3—C3 ⁱ	121.4 (2)	C6—C7—H7	120.0
C2—C3—C4	130.2 (3)	C7—C8—C7 ⁱ	120.3 (5)
C3 ⁱ —C3—C4	108.40 (16)	C7—C8—H8	119.8
O1—C4—N1	125.2 (3)	C7 ⁱ —C8—H8	119.8
O1—C4—C3	129.0 (3)		

Symmetry code: (i) $-x, y, -z+1/2$.