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N-(Imidazol-1-ylmethyl)phthalimide

Su-Qing Wang,^a Fang-Fang Jian^{a*} and Huan-Qiang Liu^b

^aMicroscale Science Institute, Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China, and ^bDepartment of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China

Correspondence e-mail: ffjian2008@163.com

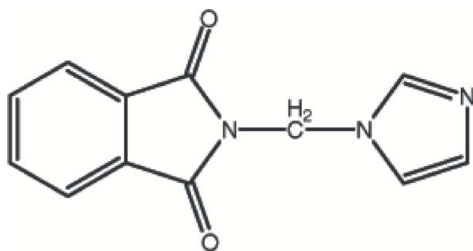
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.040; wR factor = 0.101; data-to-parameter ratio = 16.5.

The title compound [systematic name: 2-(imidazol-1-ylmethyl)isoindole-1,3-dione], $\text{C}_{12}\text{H}_9\text{N}_3\text{O}_2$, was prepared by reaction of *N*-(bromomethyl)phthalimide and imidazole in chloroform solution. The crystal structure is stabilized by weak intermolecular $\text{C}-\text{H}\cdots\pi$ interactions and intermolecular $\pi-\pi$ interactions with centroid-centroid distances in the range 3.6469 (8)–3.8831 (9) Å.

Related literature

For related literature, see: Brooks & Davidson (1960); Zhao *et al.* (2000); Barszcz *et al.* (2004); Jian *et al.* (2004).



Experimental

Crystal data

$\text{C}_{12}\text{H}_9\text{N}_3\text{O}_2$
 $M_r = 227.22$
 Monoclinic, $P2_1/c$
 $a = 7.9905$ (6) Å
 $b = 19.8096$ (15) Å
 $c = 6.9229$ (5) Å
 $\beta = 105.5540$ (10)°

$V = 1055.69$ (14) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 273$ (2) K
 $0.2 \times 0.15 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: none
 6792 measured reflections

2556 independent reflections
 1868 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.101$
 $S = 1.03$
 2556 reflections

155 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.15$ e Å⁻³

Table 1

Selected interatomic distances (Å).

$Cg1$, $Cg2$ and $Cg3$ are the centroids of the $N1/N3/C1-C3$, $N3/C5/C6/C11/C12$ and $C6-C11$ rings, respectively.

| | | | |
|----------------------|------------|-----------------------|------------|
| $Cg1\cdots Cg1^i$ | 3.8831 (9) | $Cg2\cdots Cg3^{iii}$ | 3.6469 (8) |
| $Cg2\cdots Cg3^{ii}$ | 3.6985 (8) | $Cg3\cdots Cg3^{ii}$ | 3.7214 (8) |

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

Table 2

Hydrogen-bond geometry (Å, °).

$Cg1$ is the centroid of the $N1/N3/C1-C3$ ring.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------|-------|-------------|-------------|---------------|
| $C10-H10A\cdots Cg1^{iv}$ | 0.93 | 2.94 | 3.6105 (15) | 130 |

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

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2605).

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supporting information

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***N*-(Imidazol-1-ylmethyl)phthalimide**

Su-Qing Wang, Fang-Fang Jian and Huan-Qiang Liu

S1. Comment

The imidazole and its derivatives are of considerable interest as the ligands in many biological systems in which they provide the potential binding site for metal ions (Brooks *et al.*, 1960). In our search for new ligands of this type, we have synthesized the title compound (I), and describe its structure here.

In the crystal structure of (I) (Fig. 1), the C=O bond lengths are 1.2030 (15) and 1.2026 (15) Å. The C—N bond lengths are in agreement with those observed before (Zhao *et al.*, 2000). The dihedral angles formed by the N1/N2/C1-C3 and N3/C5/C6/C11/C12 rings, with the C6-C12 ring, are 70.95 (7) and 0.44 (7)°, respectively.

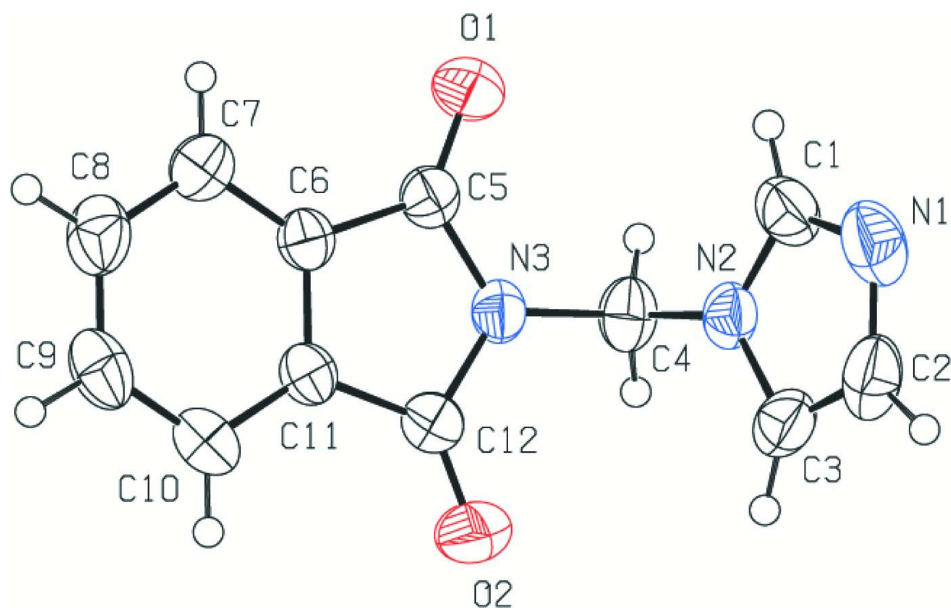
The crystal structure is stabilized by weak intermolecular C—H \cdots π interactions and intermolecular π – π interactions with centroid-to-centroid distances of 3.6469 (8)–3.8831 (9) Å (Table 1). The crystal packing of the title compound is shown in Fig. 2, viewed down the *a* axis.

S2. Experimental

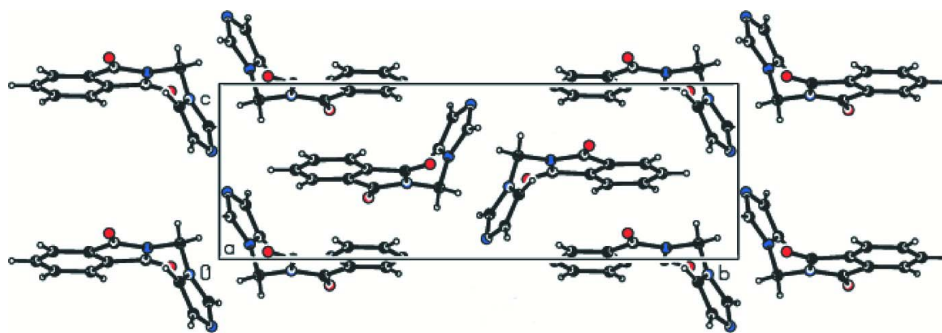
N-bromomethyl phthalic imidine 7.2 g (0.03 mol) and imidazole 2.04 g (0.03 mol) were dissolved in 20 ml chloroform. The solution was cooled to 283 K. Then, 3 g (0.03 mol) triethylamine was added dropwise *via* cannula into the well stirred solution. The reaction mixture was stirred at 283 K for 6 h. Then the solution was continued to stir at room temperature about 17 h. 20 ml water was added into the solution, the organic phase was separated and dried with anhydrous potassium carbonate. The colourless organic phase was evaporated. The title compound is afforded in 65% yield. The colourless crystals of suitable for X-ray determination were obtained from anhydrous ethanol at room temperature after two days.

S3. Refinement

H atoms were fixed geometrically and allowed to ride on their parent atoms, with C—H distance of 0.93 Å, respectively, and with $U_{\text{iso}}=1.2U_{\text{eq}}$ of the parent atoms.

**Figure 1**

The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 50% probability level.

**Figure 2**

The crystal packing of (I), viewed down the *a* axis.

2-(Imidazol-1-ylmethyl)isoindole-1,3-dione

Crystal data

$C_{12}H_9N_3O_2$

$M_r = 227.22$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 7.9905$ (6) Å

$b = 19.8096$ (15) Å

$c = 6.9229$ (5) Å

$\beta = 105.554$ (1)°

$V = 1055.69$ (14) Å³

$Z = 4$

$F(000) = 472$

$D_x = 1.430$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2256 reflections

$\theta = 2.1$ – 28.3 °

$\mu = 0.10$ mm⁻¹

$T = 273$ K

Bar, colourless

$0.2 \times 0.15 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
6792 measured reflections
2556 independent reflections

1868 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 2.1^\circ$
 $h = -7 \rightarrow 10$
 $k = -25 \rightarrow 26$
 $l = -8 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.101$
 $S = 1.03$
2556 reflections
155 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
 $w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 0.1392P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.24 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.15 \text{ e } \text{\AA}^{-3}$
Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kFc[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.008 (2)

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 | 0.38144 (13) | 0.59386 (5) | 0.45690 (16) | 0.0582 (3) |
| O2 | 0.88708 (13) | 0.71264 (5) | 0.64832 (19) | 0.0713 (3) |
| N1 | 0.79858 (19) | 0.51519 (6) | 0.1175 (2) | 0.0656 (4) |
| N2 | 0.80767 (14) | 0.55831 (5) | 0.41391 (16) | 0.0424 (3) |
| N3 | 0.65627 (13) | 0.63862 (5) | 0.56497 (15) | 0.0407 (3) |
| C1 | 0.7178 (2) | 0.52112 (7) | 0.2578 (2) | 0.0535 (4) |
| H1B | 0.6103 | 0.5018 | 0.2505 | 0.064* |
| C2 | 0.9506 (2) | 0.55038 (7) | 0.1900 (3) | 0.0604 (4) |
| H2A | 1.0367 | 0.5550 | 0.1234 | 0.073* |
| C3 | 0.95804 (18) | 0.57721 (7) | 0.3700 (2) | 0.0518 (4) |
| H3A | 1.0472 | 0.6033 | 0.4488 | 0.062* |
| C4 | 0.75385 (19) | 0.57605 (6) | 0.5912 (2) | 0.0471 (3) |
| H4A | 0.8558 | 0.5806 | 0.7042 | 0.057* |
| H4B | 0.6827 | 0.5400 | 0.6216 | 0.057* |
| C5 | 0.47554 (17) | 0.64220 (6) | 0.49665 (18) | 0.0402 (3) |

| | | | | |
|------|--------------|-------------|--------------|------------|
| C6 | 0.43317 (15) | 0.71539 (6) | 0.48572 (17) | 0.0382 (3) |
| C7 | 0.27516 (18) | 0.74781 (7) | 0.4294 (2) | 0.0510 (3) |
| H7A | 0.1717 | 0.7237 | 0.3900 | 0.061* |
| C8 | 0.2764 (2) | 0.81774 (8) | 0.4338 (2) | 0.0582 (4) |
| H8A | 0.1715 | 0.8410 | 0.3980 | 0.070* |
| C9 | 0.4295 (2) | 0.85355 (7) | 0.4899 (2) | 0.0540 (4) |
| H9A | 0.4259 | 0.9005 | 0.4911 | 0.065* |
| C10 | 0.58863 (18) | 0.82107 (7) | 0.54462 (18) | 0.0476 (3) |
| H10A | 0.6922 | 0.8452 | 0.5817 | 0.057* |
| C11 | 0.58717 (16) | 0.75136 (6) | 0.54189 (17) | 0.0387 (3) |
| C12 | 0.73314 (17) | 0.70263 (6) | 0.59332 (19) | 0.0441 (3) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|------------|-------------|-------------|------------|-------------|
| O1 | 0.0538 (6) | 0.0424 (6) | 0.0806 (8) | -0.0112 (4) | 0.0217 (5) | -0.0014 (5) |
| O2 | 0.0410 (6) | 0.0627 (7) | 0.1006 (9) | -0.0031 (5) | 0.0027 (6) | -0.0102 (6) |
| N1 | 0.0894 (10) | 0.0504 (7) | 0.0696 (9) | -0.0025 (7) | 0.0429 (8) | -0.0105 (6) |
| N2 | 0.0453 (6) | 0.0332 (5) | 0.0525 (6) | 0.0058 (4) | 0.0200 (5) | 0.0031 (5) |
| N3 | 0.0417 (6) | 0.0354 (6) | 0.0464 (6) | 0.0046 (4) | 0.0141 (5) | -0.0016 (4) |
| C1 | 0.0633 (9) | 0.0393 (7) | 0.0639 (9) | -0.0074 (6) | 0.0273 (7) | -0.0080 (6) |
| C2 | 0.0676 (10) | 0.0490 (8) | 0.0787 (11) | 0.0133 (7) | 0.0439 (9) | 0.0093 (8) |
| C3 | 0.0412 (8) | 0.0447 (7) | 0.0723 (10) | 0.0066 (6) | 0.0200 (7) | 0.0079 (7) |
| C4 | 0.0543 (8) | 0.0416 (7) | 0.0480 (7) | 0.0114 (6) | 0.0184 (6) | 0.0063 (6) |
| C5 | 0.0440 (7) | 0.0390 (7) | 0.0411 (7) | -0.0014 (5) | 0.0173 (5) | 0.0002 (5) |
| C6 | 0.0425 (7) | 0.0377 (6) | 0.0353 (6) | 0.0014 (5) | 0.0122 (5) | -0.0005 (5) |
| C7 | 0.0437 (8) | 0.0503 (8) | 0.0565 (8) | 0.0053 (6) | 0.0090 (6) | -0.0003 (6) |
| C8 | 0.0590 (9) | 0.0540 (9) | 0.0558 (9) | 0.0200 (7) | 0.0054 (7) | 0.0026 (7) |
| C9 | 0.0767 (11) | 0.0362 (7) | 0.0453 (7) | 0.0095 (7) | 0.0095 (7) | 0.0013 (6) |
| C10 | 0.0610 (9) | 0.0378 (7) | 0.0421 (7) | -0.0048 (6) | 0.0109 (6) | -0.0034 (5) |
| C11 | 0.0448 (7) | 0.0378 (7) | 0.0339 (6) | 0.0002 (5) | 0.0111 (5) | -0.0029 (5) |
| C12 | 0.0428 (7) | 0.0439 (7) | 0.0444 (7) | -0.0018 (6) | 0.0095 (6) | -0.0055 (5) |

Geometric parameters (Å, °)

| | | | |
|--------|-------------|----------|-------------|
| O1—C5 | 1.2030 (15) | C4—H4A | 0.9700 |
| O2—C12 | 1.2026 (15) | C4—H4B | 0.9700 |
| N1—C1 | 1.3075 (18) | C5—C6 | 1.4861 (17) |
| N1—C2 | 1.373 (2) | C6—C7 | 1.3764 (18) |
| N2—C1 | 1.3455 (17) | C6—C11 | 1.3843 (17) |
| N2—C3 | 1.3683 (16) | C7—C8 | 1.386 (2) |
| N2—C4 | 1.4487 (16) | C7—H7A | 0.9300 |
| N3—C5 | 1.3957 (17) | C8—C9 | 1.377 (2) |
| N3—C12 | 1.3996 (16) | C8—H8A | 0.9300 |
| N3—C4 | 1.4496 (15) | C9—C10 | 1.3845 (19) |
| C1—H1B | 0.9300 | C9—H9A | 0.9300 |
| C2—C3 | 1.341 (2) | C10—C11 | 1.3810 (18) |
| C2—H2A | 0.9300 | C10—H10A | 0.9300 |

| | | | |
|--------------------------|-------------|--------------------------|-------------|
| C3—H3A | 0.9300 | C11—C12 | 1.4820 (18) |
| Cg1...Cg1 ⁱ | 3.8831 (9) | Cg3...Cg2 ⁱⁱⁱ | 3.6985 (8) |
| Cg2...Cg3 ⁱⁱ | 3.6985 (8) | Cg3...Cg3 ⁱⁱ | 3.7214 (8) |
| Cg2...Cg3 ⁱⁱⁱ | 3.6469 (8) | Cg3...Cg3 ⁱⁱⁱ | 3.7214 (8) |
| Cg3...Cg2 ⁱⁱ | 3.6469 (8) | | |
| C1—N1—C2 | 104.28 (13) | O1—C5—C6 | 130.18 (13) |
| C1—N2—C3 | 106.40 (12) | N3—C5—C6 | 105.53 (10) |
| C1—N2—C4 | 126.73 (12) | C7—C6—C11 | 121.21 (12) |
| C3—N2—C4 | 126.86 (12) | C7—C6—C5 | 130.44 (12) |
| C5—N3—C12 | 112.14 (10) | C11—C6—C5 | 108.34 (11) |
| C5—N3—C4 | 123.97 (11) | C6—C7—C8 | 117.36 (13) |
| C12—N3—C4 | 123.78 (11) | C6—C7—H7A | 121.3 |
| N1—C1—N2 | 112.51 (13) | C8—C7—H7A | 121.3 |
| N1—C1—H1B | 123.7 | C9—C8—C7 | 121.47 (13) |
| N2—C1—H1B | 123.7 | C9—C8—H8A | 119.3 |
| C3—C2—N1 | 110.84 (13) | C7—C8—H8A | 119.3 |
| C3—C2—H2A | 124.6 | C8—C9—C10 | 121.27 (13) |
| N1—C2—H2A | 124.6 | C8—C9—H9A | 119.4 |
| C2—C3—N2 | 105.96 (13) | C10—C9—H9A | 119.4 |
| C2—C3—H3A | 127.0 | C11—C10—C9 | 117.21 (13) |
| N2—C3—H3A | 127.0 | C11—C10—H10A | 121.4 |
| N2—C4—N3 | 111.91 (10) | C9—C10—H10A | 121.4 |
| N2—C4—H4A | 109.2 | C10—C11—C6 | 121.47 (12) |
| N3—C4—H4A | 109.2 | C10—C11—C12 | 130.15 (12) |
| N2—C4—H4B | 109.2 | C6—C11—C12 | 108.38 (11) |
| N3—C4—H4B | 109.2 | O2—C12—N3 | 124.54 (12) |
| H4A—C4—H4B | 107.9 | O2—C12—C11 | 129.87 (13) |
| O1—C5—N3 | 124.30 (12) | N3—C12—C11 | 105.59 (11) |

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

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|------------------------------|-------------|---------------|-----------------------|-------------------------|
| C10—H10A...Cg1 ^{iv} | 0.93 | 2.94 | 3.6105 (15) | 130 |

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