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2-Phenyl-1*H*-imidazole

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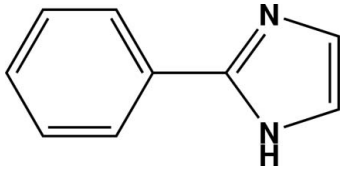
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.056; wR factor = 0.095; data-to-parameter ratio = 10.9.

In the title compound, $C_9H_8N_2$, a mirror plane lies perpendicular to the phenyl and imidazole rings and passes through the bridging C—C bond, so that the imidazole ring is disordered over two sites about the mirror plane with the equal site occupancy; the asymmetric unit contains one half-molecule. In the crystal, adjacent molecules are linked *via* N—H···N hydrogen bonds.

Related literature

For structures of 2-phenyl-1*H*-imidazolium salts, see: Xia *et al.* (2009); Xia & Yao (2010).



Experimental

Crystal data

$C_9H_8N_2$ M_r = 144.17
Orthorhombic, *Ama*2
a = 10.0740 (15) Å
b = 18.151 (4) Å
c = 4.1562 (10) Å
V = 760.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.17 × 0.12 × 0.10 mm

Data collection

Stoe IPDS 2T diffractometer
1776 measured reflections
609 independent reflections
304 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.095
S = 0.98
609 reflections
56 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.09 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···N1^{i}	0.86	2.05	2.891 (3)	165

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5367).

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Xia, D.-C., Li, W.-C. & Han, S. (2009). *Acta Cryst.* E**65**, o3283.
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supporting information

Acta Cryst. (2011). E**67**, o3248 [https://doi.org/10.1107/S160053681104699X]

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S1. Comment

2-Phenylimidazole, as an important compound with potential N donor atom that may contribute in classical hydrogen bonding in generation of supramolecular assemblies. There are some crystal structure reports that show 2-phenyl-imidazole can be protonated (Xia *et al.*, 2009; Xia & Yao, 2010).

The asymmetric unit of the title compound contains one half-molecule, a mirror plane passes through the C—C connecting two rings (Fig. 1). In this molecule the bond lengths and angles are within normal ranges. The imidazole and phenyl rings are nearly co-planar. The intermolecular N—H···N hydrogen bonds (Table 1) occurs in the crystal structure (Table 1).

S2. Experimental

The title compound has been obtained during the stirring of 2-phenyl-1*H*-imidazole and aniline in 1:1 molar ration in methanol for synthesis of co-crystal of reagents. The suitable crystals for X-ray analysis were obtained by slow evaporation from methanol solution after one week (yield; 86.5%).

S3. Refinement

All of the H atoms were positioned geometrically with C—H = 0.93 and N—H = 0.86 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,N). The molecule is disordered over two sites in the crystal structure and H1B atom is in 50% occupancy. Friedel pairs were merged as no significant anomalous scatterings.

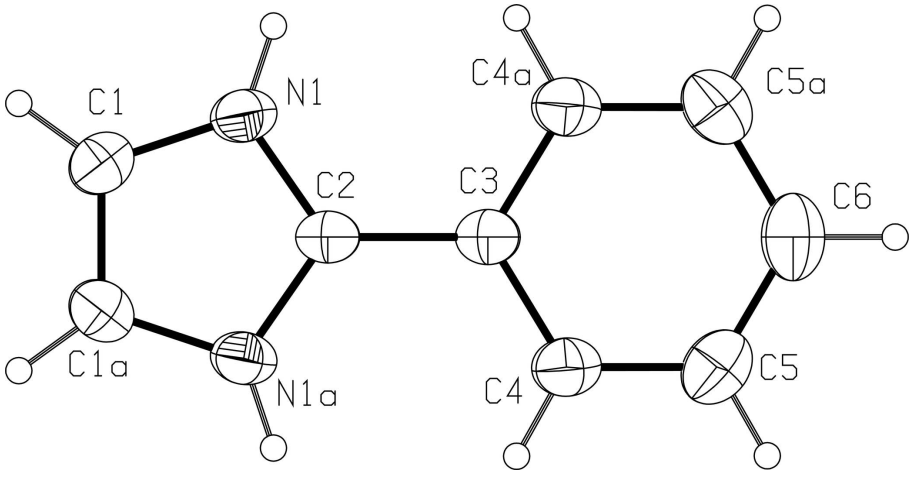

Figure 1

The molecular structure with the atom-numbering scheme. Displacement ellipsoids are drawn at 30% probability level.

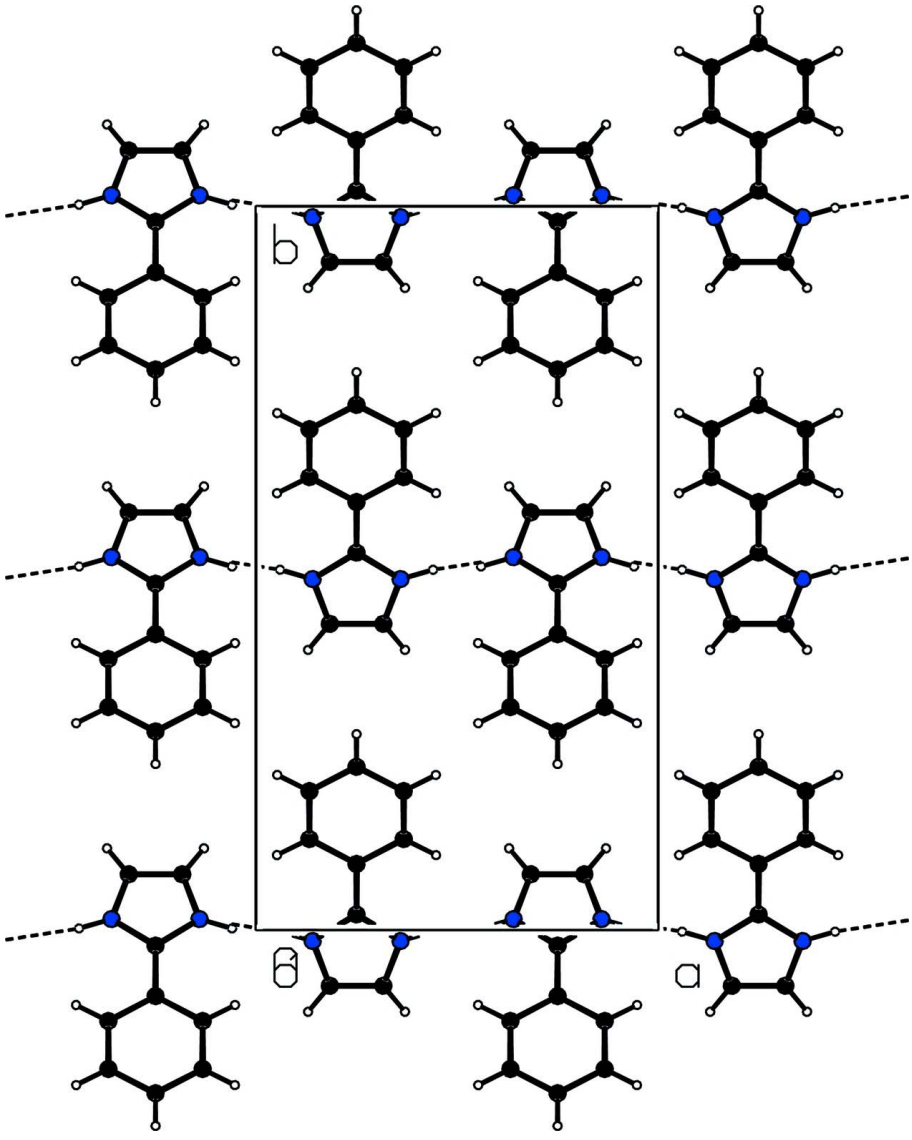

Figure 2

Packing diagram.

2-Phenyl-1*H*-imidazole

Crystal data

$C_9H_8N_2$
M_r = 144.17
Orthorhombic, *Ama*2
Hall symbol: A 2 -2a
a = 10.0740 (15) Å
b = 18.151 (4) Å
c = 4.1562 (10) Å
V = 760.0 (3) Å^3
Z = 4
F(000) = 304
D_x = 1.26 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 1776 reflections
θ = 3.0–29.1°
μ = 0.08 mm^{-1}
T = 298 K
Prism, colorless
0.17 × 0.12 × 0.10 mm

Data collection

Stoe IPDS 2T diffractometer
Graphite monochromator
rotation method scans
1776 measured reflections
609 independent reflections
304 reflections with $I > 2\sigma(I)$
$R_{int} = 0.082$
$\theta_{max} = 29.1°$, $\theta_{min} = 3.0°$
$h = -13 \rightarrow 11$
$k = -19 \rightarrow 24$
$l = -5 \rightarrow 4$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.095$
$S = 0.98$
609 reflections
56 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
$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.09$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008)
Extinction coefficient: 0.009 (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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.8165 (3)	0.57694 (18)	0.2820 (10)	0.0683 (10)	
H1	0.8705	0.6129	0.1911	0.082*	
C2	0.75	0.4784 (3)	0.5302 (10)	0.0489 (13)	
C3	0.75	0.4087 (3)	0.7033 (11)	0.0484 (12)	
C4	0.6328 (3)	0.3743 (2)	0.7893 (9)	0.0650 (9)	
H4	0.5523	0.3965	0.7387	0.078*	
C5	0.6329 (4)	0.3080 (2)	0.9474 (10)	0.0778 (12)	
H5	0.5528	0.2858	1.0015	0.093*	
C6	0.75	0.2743 (3)	1.0264 (15)	0.0799 (17)	
H6	0.75	0.2292	1.1323	0.096*	
N1	0.8591 (2)	0.51510 (13)	0.4384 (6)	0.0592 (8)	
H1B	0.9402	0.5022	0.4716	0.071*	0.5

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0563 (17)	0.0625 (19)	0.086 (3)	−0.0063 (15)	0.0075 (18)	0.007 (2)

C2	0.038 (3)	0.054 (3)	0.055 (4)	0	0	−0.010 (3)
C3	0.044 (3)	0.047 (2)	0.054 (3)	0	0	−0.014 (3)
C4	0.0494 (18)	0.069 (2)	0.077 (2)	−0.0027 (18)	−0.001 (2)	0.000 (2)
C5	0.080 (2)	0.071 (2)	0.082 (3)	−0.018 (2)	0.002 (2)	0.003 (3)
C6	0.111 (5)	0.053 (3)	0.076 (4)	0	0	0.001 (3)
N1	0.0398 (15)	0.0607 (16)	0.0771 (18)	−0.0022 (14)	0.0056 (15)	−0.0011 (19)

Geometric parameters (Å, º)

C1—C1^{i}	1.339 (6)	C4—C5	1.370 (5)
C1—N1	1.367 (4)	C4—H4	0.93
C1—H1	0.93	C5—C6	1.369 (4)
C2—N1^{i}	1.341 (3)	C5—H5	0.93
C2—N1	1.341 (3)	C6—C5^{i}	1.369 (4)
C2—C3	1.456 (6)	C6—H6	0.93
C3—C4^{i}	1.383 (4)	N1—H1B	0.86
C3—C4	1.383 (4)		
C1^{i}—C1—N1	108.34 (16)	C3—C4—H4	119.4
C1^{i}—C1—H1	125.8	C6—C5—C4	120.6 (4)
N1—C1—H1	125.8	C6—C5—H5	119.7
N1^{i}—C2—N1	110.2 (4)	C4—C5—H5	119.7
N1^{i}—C2—C3	124.9 (2)	C5—C6—C5^{i}	119.0 (5)
N1—C2—C3	124.9 (2)	C5—C6—H6	120.5
C4^{i}—C3—C4	117.3 (4)	C5^{i}—C6—H6	120.5
C4^{i}—C3—C2	121.4 (2)	C2—N1—C1	106.6 (3)
C4—C3—C2	121.4 (2)	C2—N1—H1B	126.7
C5—C4—C3	121.3 (4)	C1—N1—H1B	126.7
C5—C4—H4	119.4		
N1^{i}—C2—C3—C4^{i}	180.0 (4)	C3—C4—C5—C6	0.4 (6)
N1—C2—C3—C4^{i}	0.2 (6)	C4—C5—C6—C5^{i}	0.5 (8)
N1^{i}—C2—C3—C4	−0.2 (6)	N1^{i}—C2—N1—C1	−0.3 (5)
N1—C2—C3—C4	−180.0 (4)	C3—C2—N1—C1	179.5 (4)
C4^{i}—C3—C4—C5	−1.3 (6)	C1^{i}—C1—N1—C2	0.2 (3)
C2—C3—C4—C5	178.9 (4)		

Symmetry code: (i) −*x*+3/2, *y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···N1^{ii}	0.86	2.05	2.891 (3)	165

Symmetry code: (ii) −*x*+2, −*y*+1, *z*.