organic compounds

1,2-Bis[4-(1H-imidazol-1-yl)benzyl-idene]hydrazine

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The title compound, $C_{20}H_{16}N_6$, is centrosymmetric with the mid-point of the N—N bond located on an inversion center. The imidazole ring is oriented at a dihedral angle of 28.03 (6)° with respect to the attached benzene ring. In the crystal, molecules are linked via C—H⋯N interactions.

Related literature

For a related compound, see: Chen *et al.* (2005).
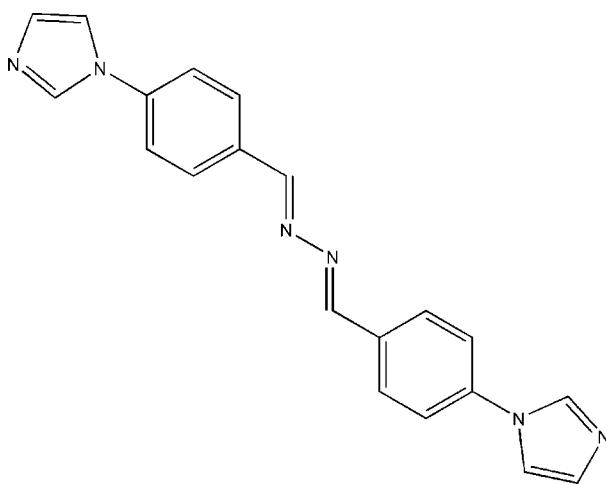
Experimental

Crystal data

$C_{20}H_{16}N_6$	V = 840.55 (6) Å^3
M_r = 340.39	Z = 2
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
a = 8.1342 (3) Å	μ = 0.09 mm^{-1}
b = 7.8172 (3) Å	T = 293 K
c = 13.2191 (6) Å	0.44 × 0.20 × 0.15 mm
β = 90.259 (4)°	

Data collection

Rigaku R-AXIS RAPID diffractometer	1695 independent reflections
	1249 reflections with $I > 2\sigma(I)$
4180 measured reflections	R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047	118 parameters
$wR(F^2)$ = 0.143	H-atom parameters constrained
S = 1.13	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
1695 reflections	$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C1—H1⋯N2^i	0.93	2.60	3.453 (2)	153
C6—H6⋯N2^{ii}	0.93	2.59	3.421 (3)	149

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2004); 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: *SHELXL97*.

References

Chen, C. L., Goforth, A. M., Smith, M. D., Su, C. Y. & Loye, H. C. (2005). *Inorg. Chem.* **44**, 8762–8769.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2004). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

1,2-Bis[4-(1*H*-imidazol-1-yl)benzylidene]hydrazine

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S1. Comment

The molecular structure of the title compound is illustrated in Fig. 1. The molecular structures is central symmetry. The bond lengths and bond angles in are within normal ranges. The N3—N3 bond length of 1.423 (3)%A is a slightly smaller than the normal length. The N3—C10 bond length is 1.273 (2)%A. The dihedral angle between the imidazole and benzene rings is 28.03 (6) Å

S2. Experimental

Hydrazine monohydrate (20 mmol, 1.08 g) and 4-imidazole benzaldehyde (40 mmol, 6.88 g) were dissolved in ethanol and the solution was refluxed for 2 h. After evaporation, a crude product was recrystallized twice from DMF and methanol to give a pure pale yellow product (Chen *et al.*, 2005). Yield: 85.2%. Calcd. for $C_{20}H_{20}N_6$: C, 69.75; H, 5.85; N, 24.40; Found: C, 69.88; H, 5.73; N, 24.67%.

S3. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms (C—H = 0.93 Å) and U_{iso}(H) values equal to $1.2U_{eq}$(C).
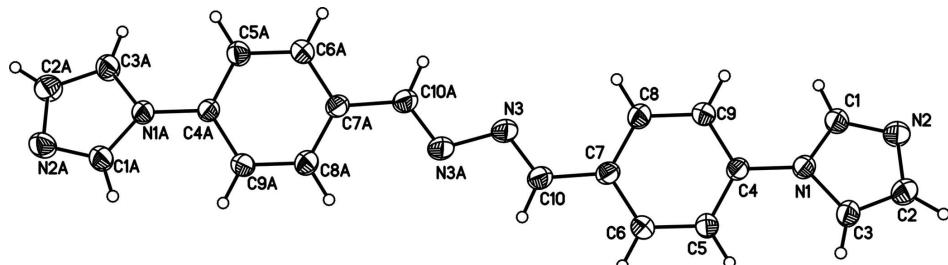
Figure 1
The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

1,2-Bis[4-(1*H*-imidazol-1-yl)benzylidene]hydrazine

Crystal data

$C_{20}H_{16}N_6$	$V = 840.55$ (6) Å³
$M_r = 340.39$	$Z = 2$
Monoclinic, $P2_1/n$	$F(000) = 356$
Hall symbol: -P 2yn	$D_x = 1.345$ Mg m⁻³
$a = 8.1342$ (3) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 7.8172$ (3) Å	Cell parameters from 7835 reflections
$c = 13.2191$ (6) Å	$\theta = 2.9–26.4°$
$\beta = 90.259$ (4)°	$\mu = 0.09$ mm⁻¹

T = 293 K

Block, yellow

0.44 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	1695 independent reflections
Radiation source: fine-focus sealed tube	1249 reflections with $I > 2\sigma(I)$
Graphite monochromator	R_{int} = 0.022
Detector resolution: 0 pixels mm⁻¹	θ_{max} = 26.4°, θ_{min} = 2.9°
ω scans	$h = -10\rightarrow8$
4180 measured reflections	$k = -9\rightarrow9$
	$l = -15\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	
$wR(F^2)$ = 0.143	
S = 1.13	H-atom parameters constrained
1695 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 0.0922P]$ where $P = (F_o^2 + 2F_c^2)/3$
118 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max}$ = 0.12 e Å⁻³
	$\Delta\rho_{min}$ = −0.17 e Å⁻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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
N1	0.03400 (17)	0.26891 (18)	0.65029 (11)	0.0443 (4)
N2	−0.1631 (2)	0.1350 (2)	0.73547 (13)	0.0605 (5)
N3	0.44959 (19)	0.9458 (2)	0.52999 (13)	0.0559 (5)
C1	−0.0938 (2)	0.2826 (2)	0.71607 (15)	0.0529 (5)
H1	−0.1281	0.3856	0.7442	0.063*
C2	−0.0742 (2)	0.0193 (3)	0.67959 (16)	0.0610 (6)
H2	−0.0941	−0.0978	0.6783	0.073*
C3	0.0454 (2)	0.0977 (2)	0.62695 (16)	0.0555 (5)
H3	0.1206	0.0465	0.5836	0.067*
C4	0.1305 (2)	0.4043 (2)	0.61009 (13)	0.0409 (4)
C5	0.1995 (2)	0.3884 (2)	0.51484 (14)	0.0471 (5)
H5	0.1838	0.2888	0.4775	0.057*
C6	0.2917 (2)	0.5209 (2)	0.47552 (15)	0.0497 (5)
H6	0.3385	0.5091	0.4118	0.060*
C7	0.3157 (2)	0.6717 (2)	0.52950 (14)	0.0447 (5)

C8	0.2452 (2)	0.6857 (2)	0.62521 (15)	0.0490 (5)
H8	0.2595	0.7857	0.6623	0.059*
C9	0.1546 (2)	0.5532 (2)	0.66558 (14)	0.0481 (5)
H9	0.1097	0.5635	0.7299	0.058*
C10	0.4159 (2)	0.8068 (2)	0.48435 (16)	0.0516 (5)
H10	0.4567	0.7903	0.4195	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0431 (8)	0.0387 (8)	0.0513 (9)	0.0015 (6)	0.0069 (7)	0.0030 (7)
N2	0.0615 (11)	0.0520 (10)	0.0681 (12)	−0.0074 (8)	0.0195 (9)	0.0048 (8)
N3	0.0572 (10)	0.0453 (9)	0.0653 (11)	−0.0046 (8)	0.0160 (8)	0.0124 (8)
C1	0.0528 (11)	0.0464 (10)	0.0597 (13)	0.0007 (8)	0.0150 (10)	0.0014 (9)
C2	0.0690 (14)	0.0436 (11)	0.0705 (15)	−0.0099 (10)	0.0131 (11)	0.0013 (10)
C3	0.0615 (12)	0.0402 (10)	0.0650 (13)	0.0000 (9)	0.0147 (10)	−0.0029 (9)
C4	0.0393 (9)	0.0370 (9)	0.0465 (11)	0.0018 (7)	0.0028 (8)	0.0040 (7)
C5	0.0493 (11)	0.0424 (10)	0.0497 (11)	0.0009 (8)	0.0063 (9)	−0.0022 (8)
C6	0.0510 (11)	0.0492 (11)	0.0490 (12)	0.0041 (8)	0.0106 (9)	0.0033 (8)
C7	0.0402 (10)	0.0433 (10)	0.0504 (11)	0.0031 (8)	0.0032 (8)	0.0099 (8)
C8	0.0543 (11)	0.0374 (9)	0.0553 (12)	−0.0006 (8)	0.0044 (9)	−0.0001 (8)
C9	0.0554 (12)	0.0434 (10)	0.0455 (11)	−0.0004 (8)	0.0101 (9)	0.0008 (8)
C10	0.0495 (11)	0.0465 (11)	0.0590 (13)	0.0030 (8)	0.0087 (10)	0.0129 (9)

Geometric parameters (Å, º)

N1—C1	1.362 (2)	C4—C9	1.389 (2)
N1—C3	1.377 (2)	C5—C6	1.382 (2)
N1—C4	1.422 (2)	C5—H5	0.9300
N2—C1	1.311 (2)	C6—C7	1.391 (3)
N2—C2	1.375 (3)	C6—H6	0.9300
N3—C10	1.273 (2)	C7—C8	1.396 (3)
N3—N3^i	1.423 (3)	C7—C10	1.463 (2)
C1—H1	0.9300	C8—C9	1.380 (2)
C2—C3	1.346 (3)	C8—H8	0.9300
C2—H2	0.9300	C9—H9	0.9300
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.386 (2)		
C1—N1—C3	105.79 (15)	C6—C5—H5	120.1
C1—N1—C4	127.14 (15)	C4—C5—H5	120.1
C3—N1—C4	127.01 (16)	C5—C6—C7	121.14 (18)
C1—N2—C2	104.24 (17)	C5—C6—H6	119.4
C10—N3—N3^i	111.6 (2)	C7—C6—H6	119.4
N2—C1—N1	112.69 (17)	C6—C7—C8	118.32 (16)
N2—C1—H1	123.7	C6—C7—C10	118.64 (18)
N1—C1—H1	123.7	C8—C7—C10	123.03 (18)
C3—C2—N2	111.20 (18)	C9—C8—C7	120.93 (17)

C3—C2—H2	124.4	C9—C8—H8	119.5
N2—C2—H2	124.4	C7—C8—H8	119.5
C2—C3—N1	106.07 (18)	C8—C9—C4	119.92 (18)
C2—C3—H3	127.0	C8—C9—H9	120.0
N1—C3—H3	127.0	C4—C9—H9	120.0
C5—C4—C9	119.88 (16)	N3—C10—C7	122.85 (19)
C5—C4—N1	119.93 (16)	N3—C10—H10	118.6
C9—C4—N1	120.19 (16)	C7—C10—H10	118.6
C6—C5—C4	119.80 (17)		
C2—N2—C1—N1	0.5 (2)	N1—C4—C5—C6	179.29 (15)
C3—N1—C1—N2	−0.2 (2)	C4—C5—C6—C7	−0.6 (3)
C4—N1—C1—N2	177.01 (17)	C5—C6—C7—C8	0.5 (3)
C1—N2—C2—C3	−0.6 (2)	C5—C6—C7—C10	179.37 (16)
N2—C2—C3—N1	0.5 (2)	C6—C7—C8—C9	0.3 (3)
C1—N1—C3—C2	−0.2 (2)	C10—C7—C8—C9	−178.54 (16)
C4—N1—C3—C2	−177.38 (16)	C7—C8—C9—C4	−1.0 (3)
C1—N1—C4—C5	−150.06 (18)	C5—C4—C9—C8	0.9 (3)
C3—N1—C4—C5	26.6 (3)	N1—C4—C9—C8	−178.52 (16)
C1—N1—C4—C9	29.3 (3)	N3^i—N3—C10—C7	179.27 (17)
C3—N1—C4—C9	−154.04 (18)	C6—C7—C10—N3	−177.13 (17)
C9—C4—C5—C6	−0.1 (3)	C8—C7—C10—N3	1.7 (3)

Symmetry code: (i) −x+1, −y+2, −z+1.

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···N2^{ii}	0.93	2.60	3.453 (2)	153
C6—H6···N2^{iii}	0.93	2.59	3.421 (3)	149

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