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

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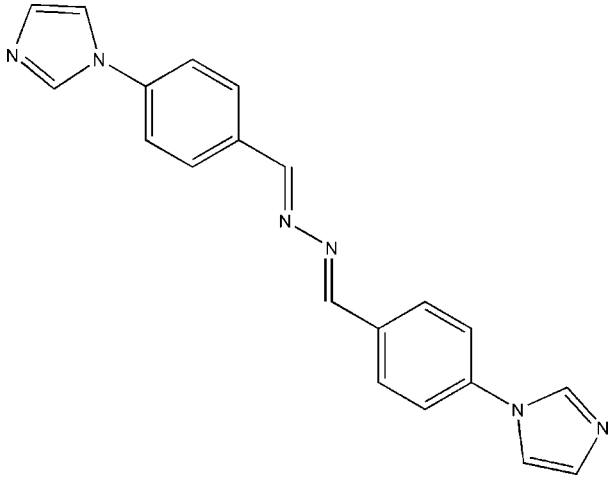
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.143; data-to-parameter ratio = 14.4.

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

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

Data collection

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

Refinement

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5536).

References

Chen, C. L., Goforth, A. M., Smith, M. D., Su, C. Y. & Loye, H. C. (2005). *Inorg. Chem.* **44**, 8762–8769.
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Rigaku/MSC (2004). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
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supplementary materials

Acta Cryst. (2012). E**68**, o1949 [doi:10.1107/S160053681202291X]

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

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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

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%.

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).

Computing details

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO* (Rigaku, 1998); 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* (Sheldrick, 2008).

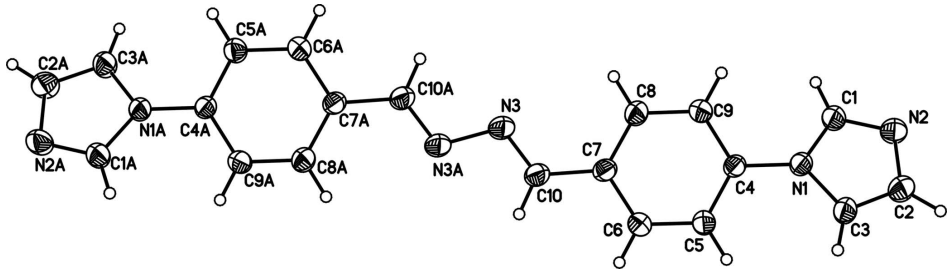

Figure 1

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

$C_{20}H_{16}N_6$
$M_r = 340.39$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.1342$ (3) Å
$b = 7.8172$ (3) Å
$c = 13.2191$ (6) Å
$\beta = 90.259$ (4)°
$V = 840.55$ (6) Å^3
$Z = 2$
$F(000) = 356$
$D_x = 1.345$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7835 reflections
$\theta = 2.9$–26.4°
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Block, yellow
0.44 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω scans
4180 measured reflections
1695 independent reflections
1249 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.9°$
$h = -10 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.143$
$S = 1.13$
1695 reflections
118 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
$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 0.0922P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.12$ 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 (Å^2)

	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.