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N,*N*′-Bis(3-iodophenyl)ethylenediimine

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Key indicators

Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.003 Å
R factor = 0.021
wR factor = 0.056
Data-to-parameter ratio = 20.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the crystal structure of the title compound, $C_{14}H_{10}I_2N_2$, the molecule lies on a crystallographic inversion center, and hence the two imine groups are mutually *trans*.

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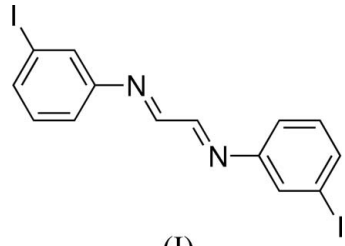
Comment

Molecules containing the 1,4-diaza-1,3-butadiene skeleton are interesting because of their versatile coordination behavior and the properties of their metal complexes (van Koten & Vrieze, 1982). The central diimine group of the title compound, (I), is planar. The angle between the planes of the diimine group and each benzene ring is 7.4 (3)°.



(I)

Experimental

The title compound was prepared by the reaction of glyoxal in water with 2 equivalents of 3-iodoaniline in propan-1-ol at room temperature (Kliegman & Barnes, 1970). The product was recrystallized from diethyl ether solution at room temperature. Single crystals suitable for X-ray diffraction were grown at room temperature by evaporation of a tetrahydrofuran solution. Spectroscopic analysis: ^{1}H NMR (500 MHz, $CDCl_3$, δ, p.p.m.): 8.30 (*s*, 2H), 7.66–7.63 (*m*, 4H), 7.24 (*s*, 2H), 7.17 (*t*, 2H). HRMS calculated for $C_{14}H_{10}I_2N_2$: 459.8933; found: 459.8933.

Crystal data

$C_{14}H_{10}I_2N_2$
M_r = 460.04
Monoclinic, *C*2/*c*
a = 16.262 (4) Å
b = 4.7074 (11) Å
c = 18.708 (4) Å
β = 98.829 (4)°
V = 1415.2 (6) Å^3
Z = 4
D_x = 2.159 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 879 reflections
θ = 2.6–28.3°
μ = 4.43 mm^{-1}
T = 193 (2) K
Tabular, yellow
0.34 × 0.24 × 0.06 mm

Data collection

Siemens SMART/Platform CCD area-detector diffractometer
ω scans
Absorption correction: integration (*XPREP* in *SHELXTL*; Bruker, 2001)
T_{min} = 0.295, T_{max} = 0.771
6991 measured reflections
1760 independent reflections
1607 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 28.3°
h = −21 → 21
k = −6 → 6
l = −24 → 24

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2 + 1.6495P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.021$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.056$	$\Delta\rho_{max} = 0.72$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.79$ e Å^{-3}
1760 reflections	Extinction correction: *SHELXTL* (Bruker, 2001)
88 parameters	Extinction coefficient: 0.0047 (2)
H-atom parameters constrained	

H atoms were included as riding idealized contributors, with C—H = 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *XCIF* (Bruker, 2001).

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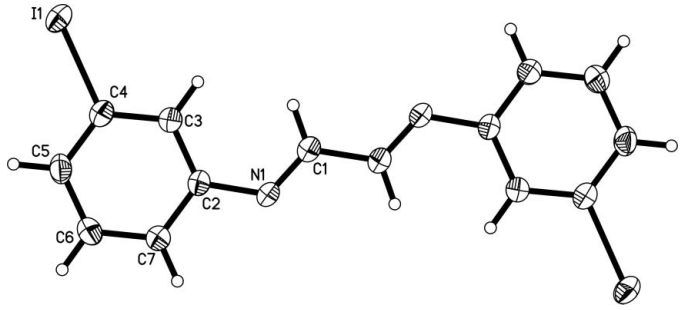

Figure 1
A plot of (I), with 50% probability displacement ellipsoids. H atoms are shown as small circles of arbitrary size. Unlabeled atoms are related to labeled atoms by the symmetry operator $(-x, 1 - y, 1 - z)$.

References

Bruker (2001). *SAINT* (Version 6.22), *SHELXTL* (Version 6.12), *SMART* (Version 5.625) and *XCIF*. Bruker AXS Inc., Madison, Wisconsin, USA.
Kliegman, J. M. & Barnes, R. K. (1970). *J. Org. Chem.* **35**, 3140–3143.
Koten, G. van & Vrieze, K. (1982). *Adv. Organomet. Chem.* **21**, 151–239.