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(*E*)-1-(2-Iodophenyl)-2-phenyldiazene

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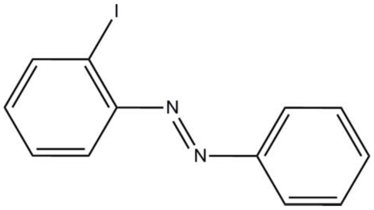
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.028; wR factor = 0.070; data-to-parameter ratio = 14.1.

The molecule of the title compound, $C_{12}H_9IN_2$, is approximately planar [maximum deviation = 0.020 (5) Å] with a *trans* arrangement of the groups around the N=N double bond. This double bond is rotated away from the iodine substiuent.

Related literature

For the synthesis, see: Badger *et al.* (1964).



Experimental

Crystal data

$C_{12}H_9IN_2$
M_r = 308.11
Orthorhombic, $P2_12_12_1$
a = 4.628 (3) Å
b = 12.801 (9) Å
c = 18.312 (12) Å
V = 1084.9 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.92 mm^{-1}
T = 296 K
1.00 × 0.07 × 0.07 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2011)
$T_{\min}$ = 0.783, $T_{\max}$ = 0.822
10050 measured reflections
1930 independent reflections
1842 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.070
S = 1.07
1930 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.57 e Å^{-3}
$\Delta\rho_{\min}$ = −0.48 e Å^{-3}
Absolute structure: Flack (1983), 763 Friedel pairs
Flack parameter: 0.08 (4)

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2011); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) in *WinGX* (Farrugia, 1999); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2021).

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supporting information

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S1. Comment

(*E*)-1-(2-iodophenyl)-2-phenyldiazene (1) was synthesized by a literature procedure (Badger *et al.* 1964) and recrystallized from absolute ethanol. The molecule is planar with a *trans* arrangement of the phenyl groups around the N—N double bond. This double bond is rotated away from the iodine substiuent on C3 (Fig. 1). There are no strong intermolecular interactions, although π-stacking interactions may exist between the phenyl rings and the N—N double bonds (Fig. 2, 3).

S2. Experimental

(1) was synthesized according to the literature procedure (Badger *et al.* 1964) and recrystallized from absolute ethanol in the form of long orange needles.

S3. Refinement

Least squares refinement was carried out with *SHELXL97* (Sheldrick, 2008) as implemented in *WinGX* (Farrugia, 1999). Hydrogen atoms were refined using a riding model the $U_{\rm iso}$ set to 1.2 times that of the heavy atom to which they are attached.

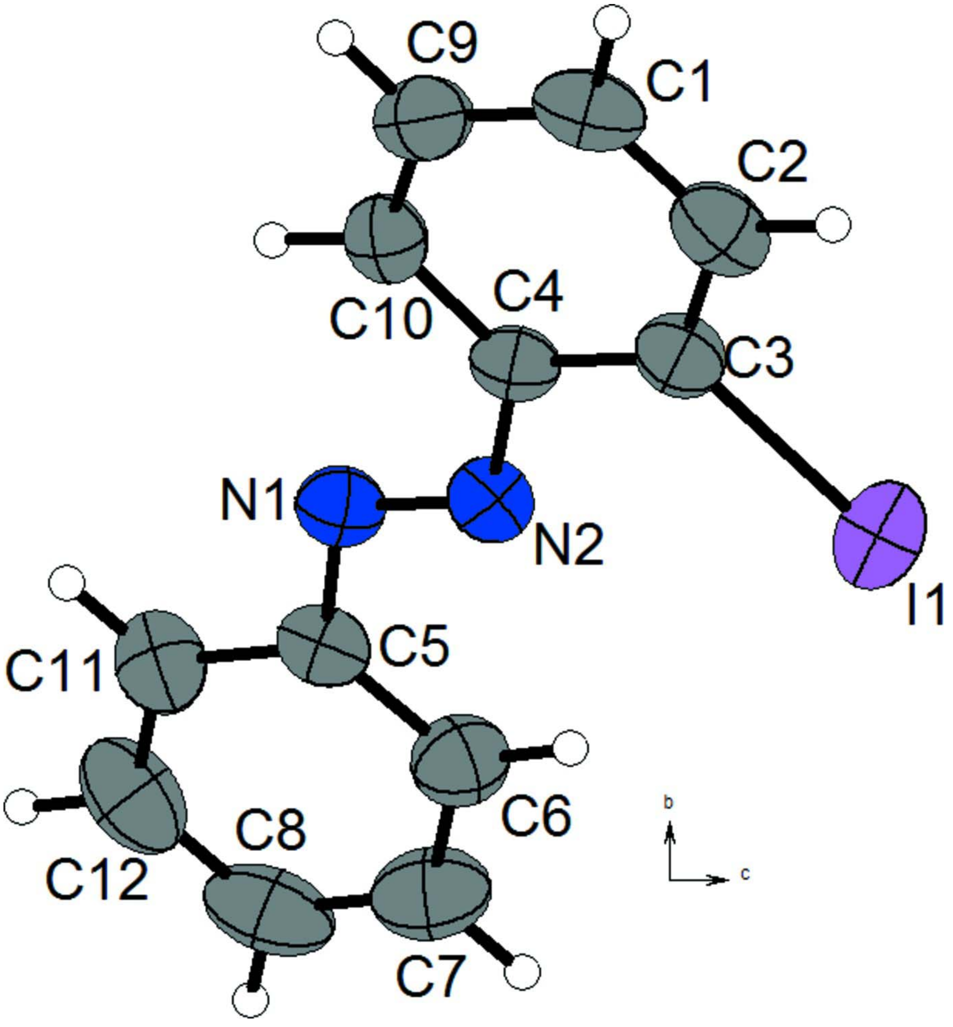

Figure 1

The asymmetric unit of (1) shown with thermal ellipsoids at 50% probability. Hydrogen atoms unlabelled for clarity.

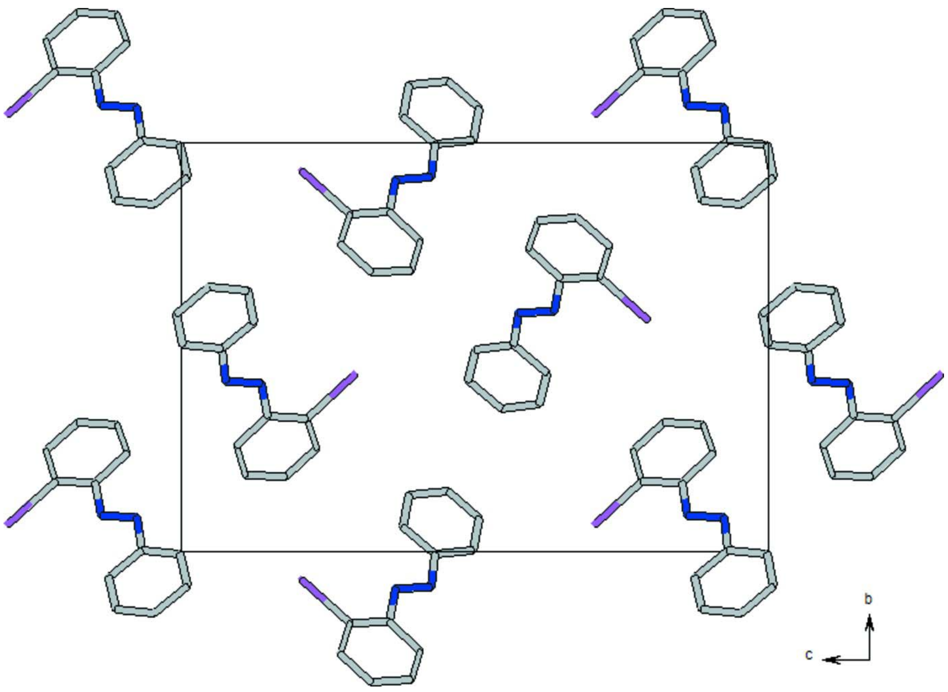

Figure 2

Packing diagram of (1) viewed along the *a*-axis.

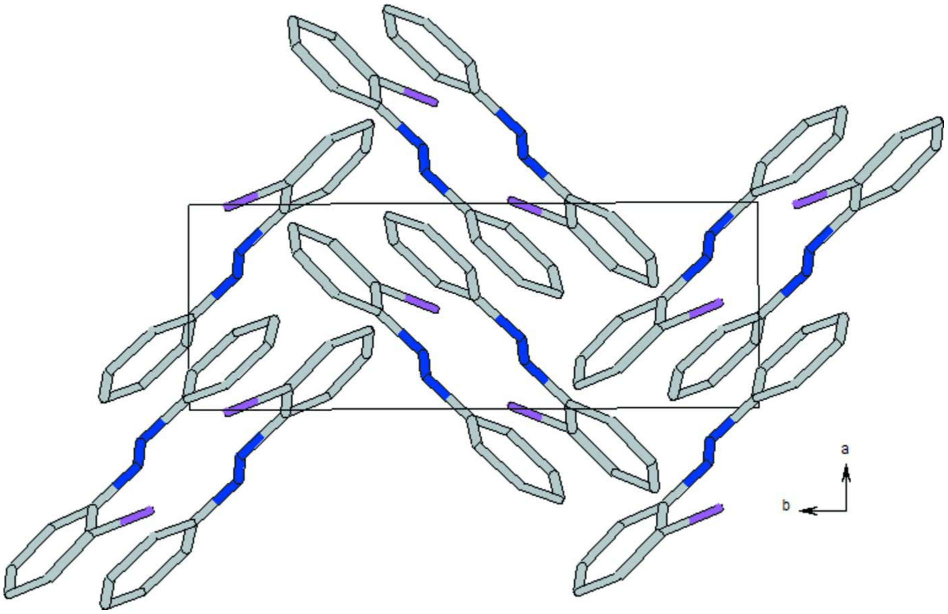

Figure 3

Packing diagram of (1) viewed along the *c*-axis.

(*E*)-1-(2-Iodophenyl)-2-phenyldiazene

Crystal data

$C_{12}H_9IN_2$	Orthorhombic, $P2_12_12_1$
$M_r = 308.11$	Hall symbol: P 2ac 2ab

$a = 4.628$ (3) Å
$b = 12.801$ (9) Å
$c = 18.312$ (12) Å
$V = 1084.9$ (13) Å^3
$Z = 4$
$F(000) = 592$
$D_x = 1.886$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4258 reflections
$\theta = 2.2–25.0°$
$\mu = 2.92$ mm^{-1}
$T = 296$ K
Needle, orange
1.00 × 0.07 × 0.07 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2011)
$T_{\rm min} = 0.783$, $T_{\rm max} = 0.822$
10050 measured reflections
1930 independent reflections
1842 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
$\theta_{\rm max} = 25.1°$, $\theta_{\rm min} = 1.9°$
$h = -5 \rightarrow 5$
$k = -15 \rightarrow 15$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.070$
$S = 1.07$
1930 reflections
137 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
$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.6387P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.57$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.48$ e Å^{-3}
Absolute structure: Flack (1983), 763 Friedel pairs
Absolute structure parameter: 0.08 (4)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	$U_{\rm iso}$*/$U_{\rm eq}$
C1	0.1092 (10)	0.3166 (4)	0.1768 (3)	0.0549 (12)
H1	−0.0297	0.3672	0.1865	0.066*
C2	0.1881 (10)	0.2473 (3)	0.2300 (3)	0.0521 (11)
H2	0.1032	0.2496	0.2760	0.062*
C3	0.3968 (9)	0.1737 (3)	0.2138 (2)	0.0450 (10)
C4	0.5235 (10)	0.1691 (3)	0.1465 (2)	0.0389 (8)
C5	1.0496 (8)	0.0040 (3)	0.0680 (2)	0.0407 (9)
C6	1.1155 (10)	−0.0629 (3)	0.1240 (3)	0.0530 (10)

H6	1.0261	−0.0561	0.1693	0.064*
C7	1.3160 (11)	−0.1401 (4)	0.1121 (3)	0.0643 (13)
H7	1.3637	−0.1860	0.1495	0.077*
C8	1.4446 (10)	−0.1497 (4)	0.0459 (3)	0.0637 (14)
H8	1.5794	−0.2025	0.0383	0.076*
C9	0.2346 (10)	0.3116 (3)	0.1090 (3)	0.0523 (11)
H9	0.1763	0.3584	0.0731	0.063*
C10	0.4372 (8)	0.2417 (3)	0.0934 (2)	0.0420 (10)
H10	0.5218	0.2408	0.0473	0.050*
C11	1.1796 (10)	−0.0058 (4)	0.0017 (3)	0.0550 (12)
H11	1.1331	0.0400	−0.0360	0.066*
C12	1.3793 (10)	−0.0833 (4)	−0.0095 (3)	0.0638 (14)
H12	1.4693	−0.0903	−0.0546	0.077*
N1	0.8420 (7)	0.0855 (3)	0.07490 (19)	0.0433 (8)
N2	0.7314 (7)	0.0892 (3)	0.13658 (19)	0.0422 (8)
I1	0.51175 (8)	0.06841 (2)	0.294862 (15)	0.06222 (13)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.050 (2)	0.039 (2)	0.075 (3)	0.0054 (19)	0.000 (2)	−0.010 (2)
C2	0.048 (3)	0.052 (3)	0.056 (3)	−0.006 (2)	0.009 (2)	−0.013 (2)
C3	0.045 (2)	0.042 (2)	0.048 (2)	−0.0057 (17)	−0.0028 (18)	−0.0042 (18)
C4	0.036 (2)	0.0332 (16)	0.0476 (19)	0.003 (2)	0.000 (2)	−0.0029 (13)
C5	0.032 (2)	0.039 (2)	0.051 (2)	0.0013 (18)	−0.0029 (18)	−0.0058 (15)
C6	0.051 (2)	0.050 (2)	0.058 (3)	0.005 (2)	0.001 (2)	0.002 (2)
C7	0.056 (3)	0.051 (3)	0.086 (4)	0.011 (2)	−0.006 (3)	0.006 (3)
C8	0.043 (3)	0.048 (2)	0.100 (4)	0.008 (2)	−0.007 (3)	−0.021 (2)
C9	0.055 (3)	0.042 (2)	0.060 (3)	−0.002 (2)	−0.013 (2)	0.003 (2)
C10	0.038 (2)	0.047 (2)	0.041 (2)	−0.0067 (18)	−0.0007 (17)	−0.0027 (16)
C11	0.054 (3)	0.063 (3)	0.049 (3)	0.004 (2)	−0.001 (2)	−0.005 (2)
C12	0.046 (2)	0.079 (4)	0.066 (3)	0.005 (3)	0.003 (2)	−0.025 (3)
N1	0.0426 (18)	0.040 (2)	0.047 (2)	0.0022 (16)	0.0011 (16)	−0.0016 (15)
N2	0.0394 (17)	0.044 (2)	0.0433 (19)	−0.0003 (15)	0.0006 (15)	−0.0031 (15)
I1	0.0674 (2)	0.0688 (2)	0.05044 (18)	−0.0007 (2)	0.0006 (2)	0.01231 (12)

Geometric parameters (Å, º)

C1—C2	1.367 (7)	C6—H6	0.9300
C1—C9	1.371 (7)	C7—C8	1.356 (7)
C1—H1	0.9300	C7—H7	0.9300
C2—C3	1.381 (6)	C8—C12	1.357 (7)
C2—H2	0.9300	C8—H8	0.9300
C3—C4	1.367 (6)	C9—C10	1.328 (6)
C3—I1	2.075 (4)	C9—H9	0.9300
C4—C10	1.403 (5)	C10—H10	0.9300
C4—N2	1.416 (5)	C11—C12	1.371 (7)
C5—C11	1.361 (6)	C11—H11	0.9300

C5—C6	1.370 (6)	C12—H12	0.9300
C5—N1	1.424 (5)	N1—N2	1.241 (5)
C6—C7	1.374 (6)		

C2—C1—C9	120.1 (4)	C8—C7—H7	119.9
C2—C1—H1	120.0	C6—C7—H7	119.9
C9—C1—H1	120.0	C7—C8—C12	120.9 (4)
C1—C2—C3	118.5 (4)	C7—C8—H8	119.5
C1—C2—H2	120.8	C12—C8—H8	119.5
C3—C2—H2	120.8	C10—C9—C1	121.7 (4)
C4—C3—C2	121.5 (4)	C10—C9—H9	119.1
C4—C3—I1	120.5 (3)	C1—C9—H9	119.1
C2—C3—I1	118.0 (3)	C9—C10—C4	119.9 (4)
C3—C4—C10	118.3 (4)	C9—C10—H10	120.1
C3—C4—N2	116.0 (3)	C4—C10—H10	120.1
C10—C4—N2	125.7 (4)	C5—C11—C12	119.8 (5)
C11—C5—C6	120.8 (4)	C5—C11—H11	120.1
C11—C5—N1	116.4 (4)	C12—C11—H11	120.1
C6—C5—N1	122.8 (4)	C8—C12—C11	119.5 (5)
C5—C6—C7	118.7 (5)	C8—C12—H12	120.3
C5—C6—H6	120.6	C11—C12—H12	120.3
C7—C6—H6	120.6	N2—N1—C5	112.8 (3)
C8—C7—C6	120.3 (5)	N1—N2—C4	115.1 (3)

C9—C1—C2—C3	0.6 (7)	C1—C9—C10—C4	1.3 (7)
C1—C2—C3—C4	−0.1 (6)	C3—C4—C10—C9	−0.8 (6)
C1—C2—C3—I1	−179.5 (3)	N2—C4—C10—C9	178.5 (4)
C2—C3—C4—C10	0.3 (6)	C6—C5—C11—C12	−0.1 (7)
I1—C3—C4—C10	179.6 (3)	N1—C5—C11—C12	−179.2 (4)
C2—C3—C4—N2	−179.1 (4)	C7—C8—C12—C11	−0.3 (8)
I1—C3—C4—N2	0.2 (5)	C5—C11—C12—C8	0.1 (7)
C11—C5—C6—C7	0.1 (7)	C11—C5—N1—N2	179.6 (4)
N1—C5—C6—C7	179.1 (4)	C6—C5—N1—N2	0.5 (5)
C5—C6—C7—C8	−0.2 (7)	C5—N1—N2—C4	179.9 (3)
C6—C7—C8—C12	0.3 (8)	C3—C4—N2—N1	179.3 (4)
C2—C1—C9—C10	−1.2 (7)	C10—C4—N2—N1	0.0 (6)