Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(4-Nitrophenyl)-2-(3-phenylallylidene)-hydrazine

Feng-Yu Bao

Department of Applied Chemistry, College of Sciences, Henan Agricultural University, Zhengzhou 450002, People's Republic of China
Correspondence e-mail: bfyu2008@yahoo.com.cn

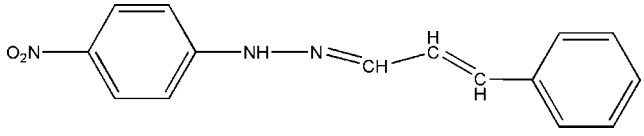
Received 3 July 2008; accepted 10 July 2008

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.039; wR factor = 0.101; data-to-parameter ratio = 8.1.

In the title compound, $C_{15}H_{13}N_3O_2$, the nitrobenzene and benzene rings make a dihedral angle of 9.1 (2)°. The crystal structure is consolidated by intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Okabe *et al.* (1993).



Experimental

Crystal data

$C_{15}H_{13}N_3O_2$
M_r = 267.28
Monoclinic, Pc
a = 6.1011 (3) Å
b = 12.4505 (6) Å
c = 9.0076 (4) Å
β = 93.273 (3)°
V = 683.12 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 (2) K
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.982
5992 measured reflections
1502 independent reflections
783 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.101
S = 0.94
1502 reflections
185 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.10 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.89 (3)	2.20 (3)	3.082 (4)	169 (3)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2421).

References

Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Okabe, N., Nakamura, T. & Fukuda, H. (1993). *Acta Cryst.* C**49**, 1678–1680.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, o1531 [doi:10.1107/S1600536808021429]

1-(4-Nitrophenyl)-2-(3-phenylallylidene)hydrazine

Feng-Yu Bao

S1. Comment

4-Nitrophenylhydrazine has applications in organic synthesis and some of its derivatives have been shown to be potentially DNA-damaging and mutagenic agents (Okabe *et al.*, 1993). As part of our interest in the study of the coordination chemistry, we report the synthesis and crystal structure of the title compound (I).

The 4-nitrophenyl group and the benzene ring are slightly twisted, making a dihedral angle of 9.1 (2)°. The dihedral angle between the N1/O1/O2 and its attached benzene ring is 7.4 (2)° (Fig. 1).

The molecules are linked by N—H···O hydrogen bonds to form a zigzag like chain (Fig. 2).

S2. Experimental

4-Nitrophenylhydrazine (1 mmol, 0.153 g) was dissolved in anhydrous methanol and H_2SO_4 (98% 0.5 ml) was added. The resultant solution was stirred for several minutes at 351 K. Cinnamaldehyde (1 mmol 0.132 g) in methanol (8 ml) was added dropwise and the mixture was stirred at refluxing temperature for 2 h. The product was isolated and recrystallized in dichloromethane. Brown single crystals of (I) were obtained after 6 d.

S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.93Å (aromatic) with U_{iso}(H) = 1.2U_{eq}(C). H2A was located from a difference Fourier map and refined isotropically, with N–H distance restrained to 0.89 (3)Å.

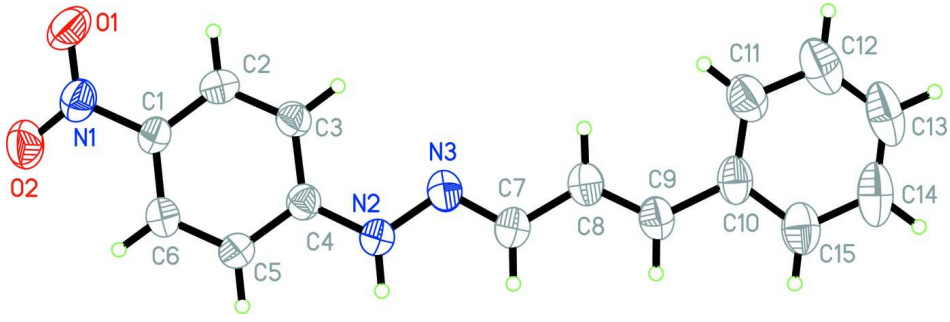


Figure 1

the *ORTEP* plot of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as small spheres of arbitrary radii.

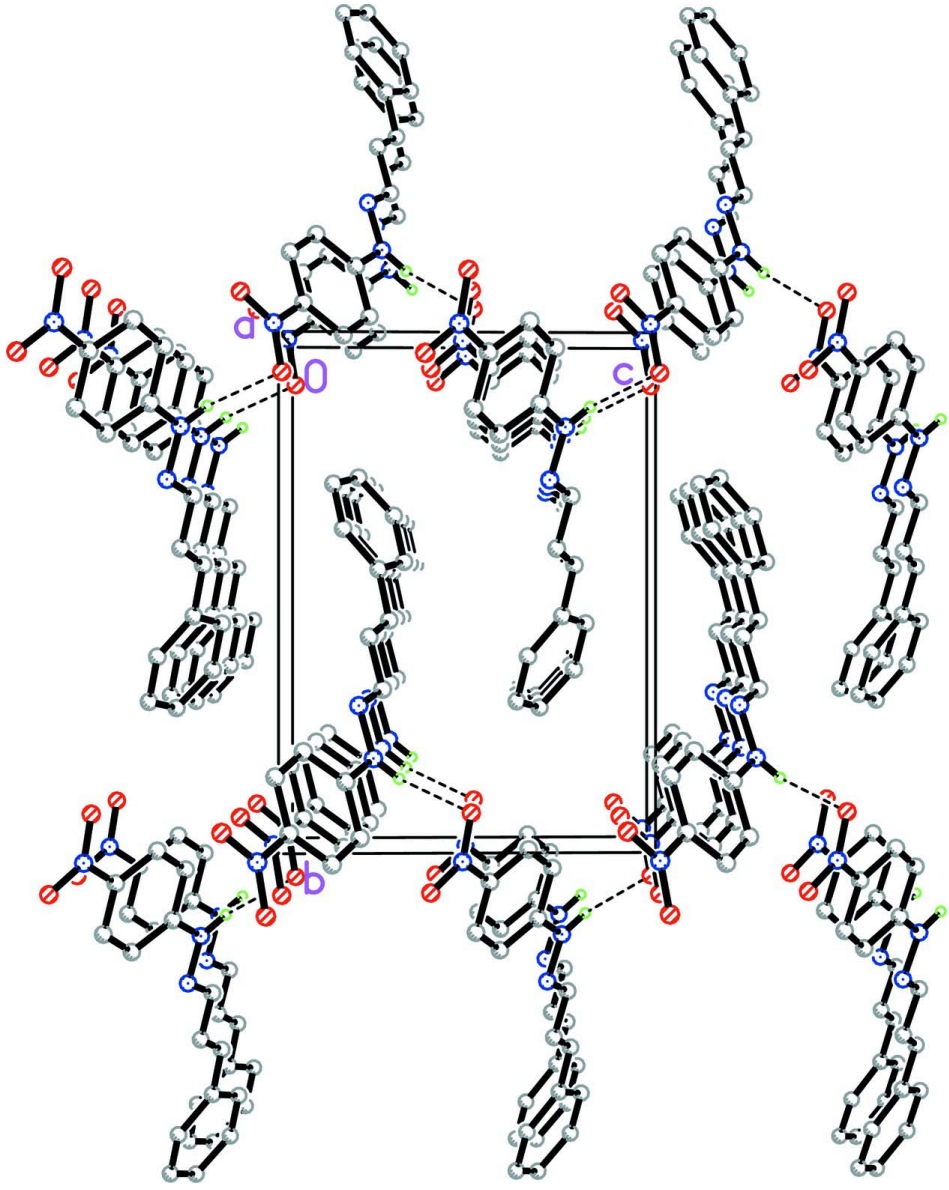


Figure 2

Packing of (I), showing the intermolecular hydrogen bonds as dashed lines.

1-(4-Nitrophenyl)-2-(3-phenylallylidene)hydrazine

Crystal data

$C_{15}H_{13}N_3O_2$
$M_r = 267.28$
Monoclinic, *Pc*
Hall symbol: P -2yc
$a = 6.1011\ (3)$ Å
$b = 12.4505\ (6)$ Å
$c = 9.0076\ (4)$ Å
$\beta = 93.273\ (3)°$
$V = 683.12\ (6)$ Å^3
$Z = 2$

$F(000) = 280$
$D_x = 1.299$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1143 reflections
$\theta = 2.1–25.6°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Block, brown
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.982
5992 measured reflections
1502 independent reflections
783 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.0°, θ_{min} = 1.6°
$h = -7 \rightarrow 7$
$k = -14 \rightarrow 15$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.101
S = 0.95
1502 reflections
185 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.10 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.027 (6)

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}
O1	1.0954 (5)	0.9273 (2)	−0.0961 (4)	0.1019 (9)
O2	1.0374 (5)	1.0780 (3)	0.0100 (3)	0.1053 (11)
N1	0.9922 (5)	0.9832 (3)	−0.0132 (3)	0.0768 (9)
N2	0.2734 (4)	0.8124 (2)	0.2572 (3)	0.0689 (8)
N3	0.1907 (4)	0.7139 (2)	0.2171 (3)	0.0718 (8)
C1	0.8094 (5)	0.9377 (3)	0.0590 (4)	0.0595 (8)
C2	0.7374 (5)	0.8364 (3)	0.0209 (4)	0.0663 (10)
H2	0.8096	0.7967	−0.0488	0.080*
C3	0.5603 (5)	0.7940 (3)	0.0852 (4)	0.0644 (9)
H3	0.5116	0.7255	0.0585	0.077*
C4	0.4516 (5)	0.8519 (3)	0.1903 (4)	0.0593 (8)
C5	0.5270 (6)	0.9545 (3)	0.2290 (4)	0.0689 (10)
H5	0.4567	0.9941	0.2998	0.083*
C6	0.7040 (5)	0.9972 (3)	0.1631 (4)	0.0695 (9)
H6	0.7532	1.0659	0.1882	0.083*

C7	0.0126 (6)	0.6853 (3)	0.2753 (4)	0.0717 (9)
H7	−0.0511	0.7305	0.3429	0.086*
C8	−0.0884 (6)	0.5852 (3)	0.2375 (4)	0.0742 (10)
H8	−0.0170	0.5393	0.1747	0.089*
C9	−0.2781 (6)	0.5539 (3)	0.2868 (4)	0.0757 (10)
H9	−0.3443	0.6017	0.3497	0.091*
C10	−0.3973 (6)	0.4540 (3)	0.2553 (4)	0.0781 (11)
C11	−0.3260 (8)	0.3749 (4)	0.1614 (5)	0.0973 (13)
H11	−0.1919	0.3827	0.1184	0.117*
C12	−0.4506 (11)	0.2854 (4)	0.1313 (6)	0.1188 (19)
H12	−0.4012	0.2338	0.0664	0.143*
C13	−0.6461 (12)	0.2703 (5)	0.1945 (7)	0.128 (2)
H13	−0.7300	0.2094	0.1724	0.153*
C14	−0.7170 (8)	0.3456 (5)	0.2905 (7)	0.1205 (19)
H14	−0.8479	0.3346	0.3363	0.145*
C15	−0.5968 (7)	0.4385 (4)	0.3210 (5)	0.0968 (13)
H15	−0.6488	0.4901	0.3849	0.116*
H2A	0.205 (5)	0.852 (2)	0.323 (3)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0786 (17)	0.127 (2)	0.1032 (19)	−0.0004 (17)	0.0351 (16)	−0.0009 (18)
O2	0.104 (2)	0.104 (2)	0.109 (2)	−0.040 (2)	0.0197 (18)	−0.0008 (18)
N1	0.068 (2)	0.094 (3)	0.0691 (19)	−0.012 (2)	0.0059 (17)	0.008 (2)
N2	0.0610 (19)	0.070 (2)	0.077 (2)	−0.0064 (16)	0.0103 (16)	−0.0075 (15)
N3	0.0674 (19)	0.0658 (19)	0.082 (2)	−0.0096 (16)	0.0027 (17)	0.0023 (16)
C1	0.0512 (18)	0.070 (2)	0.0578 (19)	−0.0043 (18)	0.0033 (16)	0.0044 (17)
C2	0.069 (2)	0.069 (2)	0.062 (2)	0.0083 (19)	0.0106 (19)	−0.0015 (18)
C3	0.062 (2)	0.055 (2)	0.076 (2)	0.0008 (18)	0.0037 (19)	−0.0048 (19)
C4	0.0539 (19)	0.064 (2)	0.0598 (19)	−0.0012 (17)	0.0007 (17)	0.0004 (17)
C5	0.061 (2)	0.072 (2)	0.074 (2)	−0.0022 (18)	0.0110 (19)	−0.0102 (19)
C6	0.067 (2)	0.065 (2)	0.076 (2)	−0.011 (2)	0.0021 (19)	−0.0015 (19)
C7	0.062 (2)	0.075 (2)	0.077 (2)	−0.007 (2)	0.0044 (19)	0.0044 (19)
C8	0.074 (2)	0.068 (2)	0.080 (3)	−0.008 (2)	0.000 (2)	0.0086 (19)
C9	0.077 (3)	0.074 (2)	0.076 (2)	−0.016 (2)	−0.003 (2)	0.0047 (19)
C10	0.073 (3)	0.080 (3)	0.079 (3)	−0.018 (2)	−0.014 (2)	0.018 (2)
C11	0.123 (3)	0.086 (3)	0.082 (3)	−0.024 (3)	−0.002 (3)	−0.001 (2)
C12	0.169 (6)	0.082 (3)	0.102 (4)	−0.034 (4)	−0.022 (4)	0.011 (3)
C13	0.157 (6)	0.098 (4)	0.122 (4)	−0.061 (4)	−0.042 (4)	0.025 (4)
C14	0.096 (3)	0.119 (4)	0.144 (5)	−0.045 (4)	−0.022 (3)	0.045 (4)
C15	0.077 (3)	0.093 (3)	0.119 (3)	−0.014 (3)	−0.009 (3)	0.019 (2)

Geometric parameters (Å, º)

O1—N1	1.221 (4)	C7—C8	1.423 (5)
O2—N1	1.228 (4)	C7—H7	0.9300
N1—C1	1.438 (4)	C8—C9	1.322 (5)

N2—C4	1.365 (4)	C8—H8	0.9300
N2—N3	1.366 (4)	C9—C10	1.461 (5)
N2—H2A	0.89 (3)	C9—H9	0.9300
N3—C7	1.284 (4)	C10—C11	1.384 (6)
C1—C2	1.373 (4)	C10—C15	1.397 (5)
C1—C6	1.382 (4)	C11—C12	1.368 (6)
C2—C3	1.361 (4)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.364 (8)
C3—C4	1.388 (4)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.362 (8)
C4—C5	1.396 (4)	C13—H13	0.9300
C5—C6	1.369 (4)	C14—C15	1.389 (7)
C5—H5	0.9300	C14—H14	0.9300
C6—H6	0.9300	C15—H15	0.9300
O1—N1—O2	122.2 (3)	N3—C7—H7	119.7
O1—N1—C1	119.5 (4)	C8—C7—H7	119.7
O2—N1—C1	118.3 (3)	C9—C8—C7	123.6 (4)
C4—N2—N3	119.9 (3)	C9—C8—H8	118.2
C4—N2—H2A	120 (2)	C7—C8—H8	118.2
N3—N2—H2A	120 (2)	C8—C9—C10	128.4 (4)
C7—N3—N2	116.7 (3)	C8—C9—H9	115.8
C2—C1—C6	120.5 (3)	C10—C9—H9	115.8
C2—C1—N1	119.6 (3)	C11—C10—C15	118.2 (4)
C6—C1—N1	119.9 (3)	C11—C10—C9	123.7 (4)
C3—C2—C1	120.1 (3)	C15—C10—C9	118.1 (4)
C3—C2—H2	120.0	C12—C11—C10	120.7 (5)
C1—C2—H2	120.0	C12—C11—H11	119.6
C2—C3—C4	120.7 (3)	C10—C11—H11	119.6
C2—C3—H3	119.7	C13—C12—C11	121.2 (5)
C4—C3—H3	119.7	C13—C12—H12	119.4
N2—C4—C3	122.5 (3)	C11—C12—H12	119.4
N2—C4—C5	118.6 (3)	C14—C13—C12	119.2 (5)
C3—C4—C5	118.8 (3)	C14—C13—H13	120.4
C6—C5—C4	120.3 (3)	C12—C13—H13	120.4
C6—C5—H5	119.9	C13—C14—C15	121.0 (6)
C4—C5—H5	119.9	C13—C14—H14	119.5
C5—C6—C1	119.7 (3)	C15—C14—H14	119.5
C5—C6—H6	120.2	C14—C15—C10	119.6 (5)
C1—C6—H6	120.2	C14—C15—H15	120.2
N3—C7—C8	120.7 (4)	C10—C15—H15	120.2

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{i}	0.89 (3)	2.20 (3)	3.082 (4)	169 (3)

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