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ISSN 2414-3146

(*E*)-4-Nitro-2-[(phenylimino)methyl]phenol

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Received 3 October 2016
Accepted 9 October 2016

Edited by P. C. Healy, Griffith University, Australia

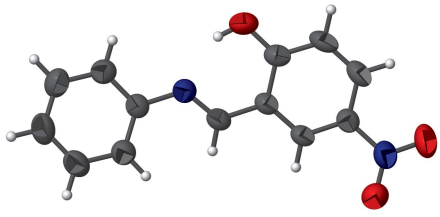
Keywords: crystal structure; salicylaldehyde derivative; O—H···N; C—H···O hydrogen bonding.

CCDC reference: 1508947

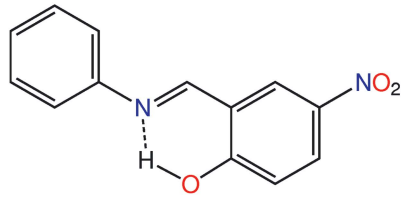
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{13}H_{10}N_2O_3$, the dihedral angle between the planes of the two aryl rings is 7.42 (10)°. An intramolecular O—H···N hydrogen bond generates an *S*(6) ring. The crystal structure features C—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

We report here the synthesis and characterization of the title Schiff base derivative (Fig. 1)) prepared from the condensation reaction of an equimolar proportion of 5-nitrosalicylaldehyde and aniline in CCl_4. The diversified nature of salicylaldehyde derivatives containing Schiff bases as an integral part of the structure exhibit a variety of important biological properties, including anti-bacterial, anti-cancer and anti-tumor activities (Ida Malarselvi *et al.*, 2016).

The benzene and phenyl rings are inclined at 7.42 (10)° to one another. The molecule has an *E* conformation about the C=N bond, and the C5—C7=N2—C8 torsion angle is −177.03 (16)°. The 4-nitro group is slightly tilted away from the benzene ring to which it is attached [O1—N1—C1—C2 = −5.8 (3)° and O2—N1—C1—C6 = −2.7 (3)°]. The strong intramolecular O3—H3*A*···N2 hydrogen bond (N···H distance of 1.83 Å) generates an S(6) ring. The strong band in the IR at 1632 cm^{-1} is assigned to the C7=N2 stretching frequency of the imine group of Schiff base with the C7=N2 bond distance of 1.276 (2) Å indicative of double-bond character. The crystal structure features C2—H2···O1 and C7—H7···O2 hydrogen bonds (Table 1, Fig. 2).

Yan *et al.*, (2014) have reported the crystal structure of 4-bromo-2-[(phenylimino)-methyl]phenol, in which the molecule is essentially planar (r.m.s. deviation = 0.026 Å).

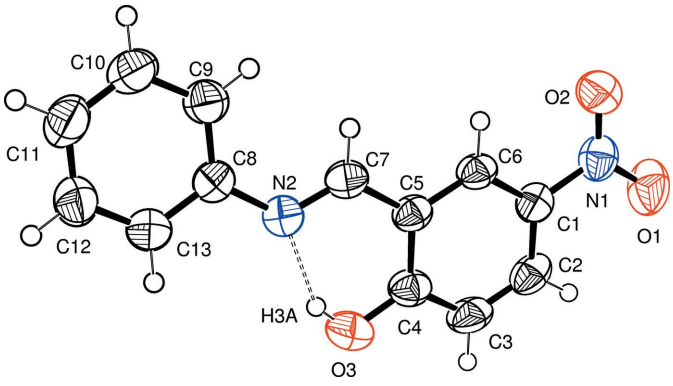


Figure 1
A view of the title molecule with displacement ellipsoids drawn at the 50% probability level. A dashed line indicates the hydrogen-bonding interaction.

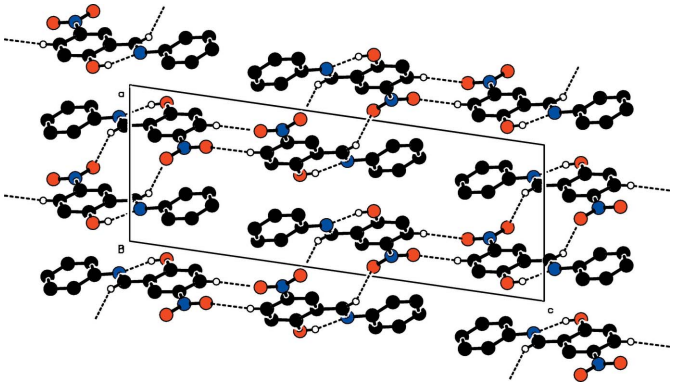


Figure 2
The crystal packing of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines (see Table 1). H atoms not involved in hydrogen bonding have been omitted for clarity.

Synthesis and crystallization

0.2 g (0.001 mol) of 5-nitrosalicylaldehyde was dissolved in 5 ml of CCl_4. To this solution, 0.1 g (0.111 mol) of aniline was added dropwise with constant stirring for 1 h. During this time, the solution turned deep yellow. On standing for two weeks with slow evaporation of the solvent, yellow crystals of the title compound were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors would like to acknowledge the University Grants Commission (UGC), New Delhi, for providing funds under Minor Research Project Scheme No. FERP5150/14 (SERO/UGC). The authors are grateful to the Sophisticated Analytical Instrument Facility (SAIF), IITM, Chennai 600 036, Tamilnadu, India, for the single-crystal X-ray diffraction data.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93	2.60	3.278 (2)	130
C7—H7···O2^{ii}	0.93	2.41	3.252 (2)	150
O3—H3A···N2	0.82	1.83	2.5637 (19)	149

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{10}N_2O_3$
M_r	242.23
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	8.0774 (10), 6.5801 (6), 21.668 (3)
β (°)	98.240 (5)
V (Å^3)	1139.8 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.95, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15249, 2857, 1645
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.135, 1.04
No. of reflections	2857
No. of parameters	164
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.22

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SIR92* (Altomare *et al.*, 1993), *ORTEP-3 for Windows* (Farrugia, 2012), *SHELXL2016* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2016). **1**, x161595 [https://doi.org/10.1107/S2414314616015959]

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Crystal data

$C_{13}H_{10}N_2O_3$
M_r = 242.23
Monoclinic, $P2_1/n$
a = 8.0774 (10) Å
b = 6.5801 (6) Å
c = 21.668 (3) Å
β = 98.240 (5)°
V = 1139.8 (2) Å^3
Z = 4
$F(000)$ = 504
D_x = 1.412 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3323 reflections
θ = 4.0–24.5°
μ = 0.10 mm^{-1}
T = 296 K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: Sealed tube
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.95, T_{max} = 0.96
15249 measured reflections
2857 independent reflections
1645 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 28.4°, θ_{min} = 2.6°
h = −10→9
k = −8→8
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
S = 1.04
2857 reflections
164 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.3112P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2784 (2)	0.1044 (3)	−0.11963 (7)	0.0468 (4)
C2	0.1930 (3)	0.2130 (3)	−0.16876 (8)	0.0563 (5)
H2	0.179342	0.159614	−0.208907	0.068*
C3	0.1293 (3)	0.3986 (3)	−0.15790 (8)	0.0608 (5)
H3	0.072527	0.472297	−0.190992	0.073*
C4	0.1474 (2)	0.4797 (3)	−0.09835 (8)	0.0508 (5)
C5	0.2374 (2)	0.3697 (3)	−0.04848 (7)	0.0450 (4)
C6	0.3016 (2)	0.1809 (3)	−0.06025 (7)	0.0464 (4)
H6	0.360524	0.106126	−0.027877	0.056*
C7	0.2662 (2)	0.4542 (3)	0.01343 (8)	0.0506 (5)
H7	0.323271	0.377170	0.045658	0.061*
C8	0.2495 (2)	0.7204 (3)	0.08524 (8)	0.0464 (4)
C9	0.3526 (2)	0.6347 (3)	0.13497 (8)	0.0565 (5)
H9	0.403539	0.509943	0.130314	0.068*
C10	0.3796 (3)	0.7343 (3)	0.19118 (9)	0.0643 (6)
H10	0.449407	0.677035	0.224503	0.077*
C11	0.3043 (3)	0.9175 (4)	0.19849 (10)	0.0705 (6)
H11	0.322110	0.983561	0.236820	0.085*
C12	0.2030 (3)	1.0033 (3)	0.14949 (10)	0.0696 (6)
H12	0.151911	1.127794	0.154403	0.083*
C13	0.1768 (2)	0.9057 (3)	0.09319 (9)	0.0567 (5)
H13	0.108938	0.965574	0.059827	0.068*
N1	0.3522 (2)	−0.0902 (2)	−0.13139 (7)	0.0586 (4)
N2	0.21561 (19)	0.6317 (2)	0.02536 (6)	0.0486 (4)
O1	0.3253 (2)	−0.1609 (2)	−0.18406 (7)	0.0843 (5)
O2	0.4381 (2)	−0.1762 (2)	−0.08827 (7)	0.0723 (5)
O3	0.08189 (19)	0.6599 (2)	−0.08898 (6)	0.0665 (4)
H3A	0.106727	0.692303	−0.052274	0.100*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0517 (11)	0.0475 (10)	0.0416 (9)	−0.0074 (8)	0.0083 (8)	0.0025 (7)
C2	0.0634 (13)	0.0679 (13)	0.0357 (9)	−0.0131 (10)	0.0005 (8)	0.0027 (8)
C3	0.0643 (13)	0.0672 (13)	0.0456 (10)	−0.0038 (10)	−0.0102 (9)	0.0162 (9)
C4	0.0474 (11)	0.0519 (11)	0.0518 (10)	−0.0024 (9)	0.0028 (8)	0.0111 (8)
C5	0.0453 (10)	0.0492 (10)	0.0396 (9)	−0.0041 (8)	0.0027 (7)	0.0052 (7)
C6	0.0494 (11)	0.0506 (10)	0.0378 (9)	−0.0009 (8)	0.0009 (7)	0.0072 (7)
C7	0.0540 (12)	0.0545 (11)	0.0422 (9)	0.0021 (9)	0.0032 (8)	0.0063 (8)
C8	0.0416 (10)	0.0518 (10)	0.0465 (9)	−0.0046 (8)	0.0091 (8)	0.0000 (8)
C9	0.0554 (12)	0.0619 (12)	0.0525 (11)	0.0060 (9)	0.0087 (9)	−0.0016 (9)
C10	0.0556 (13)	0.0841 (15)	0.0515 (11)	0.0048 (11)	0.0018 (9)	−0.0030 (10)
C11	0.0585 (14)	0.0892 (16)	0.0627 (13)	−0.0009 (12)	0.0048 (10)	−0.0242 (11)
C12	0.0649 (15)	0.0666 (13)	0.0758 (14)	0.0072 (11)	0.0056 (11)	−0.0184 (11)
C13	0.0511 (12)	0.0586 (12)	0.0590 (11)	0.0041 (9)	0.0029 (9)	−0.0009 (9)

N1	0.0688 (12)	0.0590 (10)	0.0495 (9)	−0.0078 (9)	0.0134 (8)	−0.0047 (8)
N2	0.0477 (9)	0.0506 (9)	0.0483 (8)	−0.0002 (7)	0.0091 (7)	0.0006 (7)
O1	0.1271 (16)	0.0753 (10)	0.0519 (8)	−0.0080 (9)	0.0177 (9)	−0.0165 (7)
O2	0.0777 (11)	0.0665 (9)	0.0702 (10)	0.0142 (8)	0.0022 (8)	−0.0039 (7)
O3	0.0689 (10)	0.0614 (9)	0.0662 (9)	0.0136 (7)	−0.0008 (7)	0.0115 (7)

Geometric parameters (Å, º)

C1—C6	1.369 (2)	C8—C9	1.384 (2)
C1—C2	1.382 (2)	C8—N2	1.413 (2)
C1—N1	1.450 (2)	C9—C10	1.373 (3)
C2—C3	1.359 (3)	C9—H9	0.9300
C2—H2	0.9300	C10—C11	1.370 (3)
C3—C4	1.385 (3)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.366 (3)
C4—O3	1.326 (2)	C11—H11	0.9300
C4—C5	1.412 (2)	C12—C13	1.368 (3)
C5—C6	1.384 (2)	C12—H12	0.9300
C5—C7	1.440 (2)	C13—H13	0.9300
C6—H6	0.9300	N1—O2	1.220 (2)
C7—N2	1.276 (2)	N1—O1	1.2228 (19)
C7—H7	0.9300	O3—H3A	0.8200
C8—C13	1.375 (3)		
C6—C1—C2	121.32 (17)	C13—C8—N2	116.85 (16)
C6—C1—N1	119.04 (15)	C9—C8—N2	124.19 (16)
C2—C1—N1	119.58 (16)	C10—C9—C8	119.81 (19)
C3—C2—C1	119.42 (17)	C10—C9—H9	120.1
C3—C2—H2	120.3	C8—C9—H9	120.1
C1—C2—H2	120.3	C11—C10—C9	120.4 (2)
C2—C3—C4	121.04 (17)	C11—C10—H10	119.8
C2—C3—H3	119.5	C9—C10—H10	119.8
C4—C3—H3	119.5	C12—C11—C10	120.01 (19)
O3—C4—C3	119.74 (16)	C12—C11—H11	120.0
O3—C4—C5	120.94 (16)	C10—C11—H11	120.0
C3—C4—C5	119.31 (17)	C11—C12—C13	119.9 (2)
C6—C5—C4	118.98 (15)	C11—C12—H12	120.1
C6—C5—C7	120.24 (15)	C13—C12—H12	120.1
C4—C5—C7	120.76 (16)	C12—C13—C8	120.93 (19)
C1—C6—C5	119.92 (16)	C12—C13—H13	119.5
C1—C6—H6	120.0	C8—C13—H13	119.5
C5—C6—H6	120.0	O2—N1—O1	122.93 (18)
N2—C7—C5	121.91 (16)	O2—N1—C1	118.55 (15)
N2—C7—H7	119.0	O1—N1—C1	118.52 (17)
C5—C7—H7	119.0	C7—N2—C8	122.60 (15)
C13—C8—C9	118.95 (17)	C4—O3—H3A	109.5
C6—C1—C2—C3	−0.7 (3)	C13—C8—C9—C10	0.5 (3)

N1—C1—C2—C3	−177.65 (18)	N2—C8—C9—C10	179.08 (18)
C1—C2—C3—C4	−0.5 (3)	C8—C9—C10—C11	0.4 (3)
C2—C3—C4—O3	−179.07 (19)	C9—C10—C11—C12	−0.7 (3)
C2—C3—C4—C5	1.6 (3)	C10—C11—C12—C13	0.1 (3)
O3—C4—C5—C6	179.13 (17)	C11—C12—C13—C8	0.8 (3)
C3—C4—C5—C6	−1.6 (3)	C9—C8—C13—C12	−1.1 (3)
O3—C4—C5—C7	−2.6 (3)	N2—C8—C13—C12	−179.80 (18)
C3—C4—C5—C7	176.72 (17)	C6—C1—N1—O2	−2.7 (3)
C2—C1—C6—C5	0.7 (3)	C2—C1—N1—O2	174.36 (17)
N1—C1—C6—C5	177.68 (16)	C6—C1—N1—O1	177.16 (17)
C4—C5—C6—C1	0.4 (3)	C2—C1—N1—O1	−5.8 (3)
C7—C5—C6—C1	−177.87 (16)	C5—C7—N2—C8	−177.03 (16)
C6—C5—C7—N2	176.63 (17)	C13—C8—N2—C7	−174.99 (17)
C4—C5—C7—N2	−1.7 (3)	C9—C8—N2—C7	6.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.93	2.60	3.278 (2)	130
C7—H7···O2^{ii}	0.93	2.41	3.252 (2)	150
O3—H3*A*···N2	0.82	1.83	2.5637 (19)	149

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