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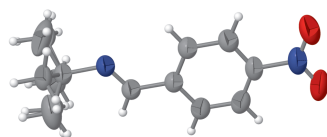
2-Methyl-*N*-[(*E*)-4-nitrobenzylidene]propan-2-amine

Eric Cyriel Hosten and Richard Betz*

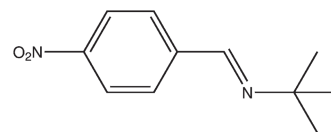
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The title compound, $C_{11}H_{14}N_2O_2$, is a Schiff base derived from *tert*-butylamine and *para*-nitrobenzaldehyde. All atoms except the methyl groups are located on a mirror plane. Thus, there is only half a molecule in the asymmetric unit. The *tert*-butyl group shows rotational disorder over four positions. The molecule is *E*-configured. In the extended structure, C—H···O contacts connect the molecules into chains along [010] in the crystal structure.

3D view



Chemical scheme



Structure description

Imines – also known as Schiff bases – are the condensation products between a primary amine and a carbonyl compound and, thus, have found application as protection group for either one of the two compounds during classical organic multi-step synthesis procedures (Becker *et al.*, 2000; Greene & Wuts, 2007). They have also found use as ligands in transition-metal chemistry for transition metals such as rhenium (Mukiza *et al.*, 2020; Yumata *et al.*, 2011*b*; Habarurema *et al.*, 2014*a,b,c*, 2015*a,b*; Potgieter *et al.*, 2013; Gerber *et al.*, 2011, 2012) or rare-earth metals (Abrahams *et al.*, 2017) and, in a structural variation, also play a role in carbohydrate chemistry in the shape of hydrazones that, in turn, give rise to osazones (Lindhorst, 2007). In a continuation of our interest in structural aspects of Schiff bases (Potgieter *et al.*, 2011; Booyesen *et al.*, 2011*a,b*; Mohamed *et al.*, 2023; Schmitt *et al.*, 2011, 2014, 2015*a,b*; Yumata *et al.*, 2011*a*; Habarurema *et al.*, 2014*a,b*; Madanhire *et al.*, 2015*a,b*) we initiated a study around the metrical parameters of Schiff bases derived from aromatic aldehydes and the influence of coordination towards transition metals on these values. An intriguing family of compounds are derivatives featuring strongly deactivating nitro groups on the aromatic aldehyde core such as the series of mononitro-substituted benzaldehydes. The literature abounds in structural information around Schiff bases derived from *ortho*-nitrobenzaldehyde (*e.g.* Cueno-Cabezas *et al.*, 2025; Shan *et al.*, 2004; Duggin *et al.*, 2024) and some derived coordination compounds with mercury (Sheikh *et al.*, 2025) and manganese (Mansour *et al.*, 2024) as well as *meta*-

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C5-H5B\cdots O1^i$	0.98	2.53	3.41 (3)	149
$C6-H6C\cdots O1^{ii}$	0.98	2.58	3.459 (19)	149
$C7-H7B\cdots O1^i$	0.98	2.56	3.35 (2)	138

Symmetry codes: (i) $-x + 1, -y, -z + 1$; (ii) $-x + 1, -y + 1, -z + 1$.

nitrobenzaldehyde (e.g. Priyadharshini *et al.*, 2025; Glidewell *et al.*, 2005; Akkurt *et al.*, 2008) and some derived coordination compounds with tin (Cui *et al.*, 2022) and antimony (Artemeva *et al.*, 2019) and *para*-nitrobenzaldehyde (e.g. Rogalewicz *et al.*, 2025; Chuskit *et al.*, 2025; Watson *et al.*, 1984) and some derived coordination compounds with nickel, copper, zinc and palladium (Rogalewicz *et al.*, 2025).

The structure solution shows the presence of a Schiff base derived from 4-nitrobenzaldehyde and *tert*-butylamine. The $C=N$ double bond is (*E*)-configured ($C2-N1-C1-C11 = 180$ and $N1-C1-C11-C12 = 0^\circ$) (Fig. 1). The *tert*-butyl group shows rotational disorder. Except for the methyl groups, the molecule is exactly planar. Intracyclic $C-C-C$ angles cover a range of $118.48(19)$ – $122.28(18)^\circ$ with the largest angle located on the carbon atom bearing the nitro group and the smallest angle on one of the CH groups directly adjacent to the latter carbon atom. All other bond lengths and angles are in good agreement with comparable values reported for other Schiff bases whose molecular and crystal structures have been determined on grounds of diffraction studies carried out on single crystals and whose metrical parameters have been deposited with the Cambridge Structural Database (Groom *et al.*, 2016).

In the crystal, $C-H\cdots O$ contacts (Table 1) whose range falls by more than 0.1 \AA below the sum of the van der Waals radii of the atoms participating in them are observed. These are established between one hydrogen atom each of two methyl groups as donors and one of the nitro group's oxygen atoms as acceptor. In terms of graph-set analysis (Etter *et al.*, 1990; Bernstein *et al.*, 1995), the descriptor for these contacts is $C_1^1(11)$. π -Stacking is not a prominent consolidating feature in the crystal structure of the title compound, with the shortest intercentroid distance in between two centers of gravity measured at $4.0640(6) \text{ \AA}$.

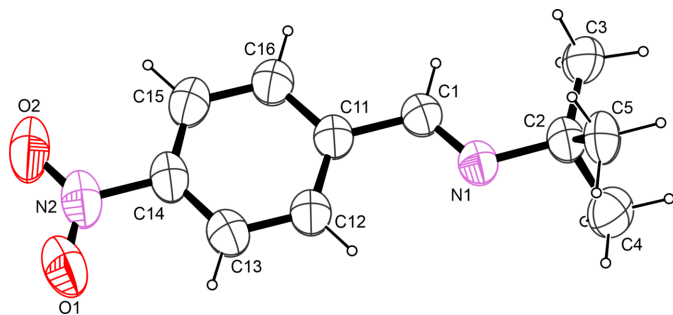


Figure 1

The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level). Only one of the four positions of the disordered methyl groups is shown.

Table 2

Experimental details.

Crystal data	
Chemical formula	$C_{11}H_{14}N_2O_2$
M_r	206.24
Crystal system, space group	Orthorhombic, $Pnma$
Temperature (K)	200
a, b, c (Å)	9.5110 (4), 7.2400 (3), 16.2386 (7)
V (Å ³)	1118.18 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.09
Crystal size (mm)	$0.39 \times 0.25 \times 0.14$
Data collection	
Diffractionmeter	Bruker APEXII CCD
Absorption correction	Numerical (SADABS; Krause <i>et al.</i> , 2015)
T_{min}, T_{max}	0.951, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38579, 1388, 1087
R_{int}	0.027
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.051, 0.168, 1.17
No. of reflections	1388
No. of parameters	127
No. of restraints	30
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.14, -0.28

Computer programs: APEX2 and SAINT (Bruker, 2014), SHELXS97 (Sheldrick 2008), ORTEP-3 for Windows (Farrugia, 2012), Mercury (Macrae *et al.*, 2020), SHELXL2019/3 (Sheldrick, 2015) and PLATON (Spek, 2020).

Synthesis and crystallization

The compound was obtained following a standard procedure by reacting *para*-nitrobenzaldehyde with *tert*-butylamine (Becker *et al.*, 2000). Crystals suitable for the diffraction study were obtained straight from the solidified isolated product.

Refinement

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

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full crystallographic data

IUCrData (2025). **10**, x251136 [<https://doi.org/10.1107/S2414314625011368>]

2-Methyl-*N*-[(*E*)-4-nitrobenzylidene]propan-2-amine

Eric Cyriel Hosten and Richard Betz

2-Methyl-*N*-[(*E*)-4-nitrobenzylidene]propan-2-amine*Crystal data*

$C_{11}H_{14}N_2O_2$

$M_r = 206.24$

Orthorhombic, *Pnma*

$a = 9.5110$ (4) Å

$b = 7.2400$ (3) Å

$c = 16.2386$ (7) Å

$V = 1118.18$ (8) Å³

$Z = 4$

$F(000) = 440$

$D_x = 1.225$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9822 reflections

$\theta = 2.5$ – 27.5°

$\mu = 0.09$ mm⁻¹

$T = 200$ K

Block, colourless

$0.39 \times 0.25 \times 0.14$ mm

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

Absorption correction: numerical
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.951$, $T_{\max} = 1.000$

38579 measured reflections

1388 independent reflections

1087 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.5^\circ$

$h = -12 \rightarrow 12$

$k = -9 \rightarrow 9$

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.168$

$S = 1.17$

1388 reflections

127 parameters

30 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

$w = 1/[\sigma^2(F_o^2) + (0.0741P)^2 + 0.2341P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.14$ e Å⁻³

$\Delta\rho_{\min} = -0.28$ 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.

Refinement. H atoms were placed in calculated positions (C–H 0.95 Å for aromatic and vinylic carbon atoms, C–H 0.98 Å for the methyl groups) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$ (aromatic and vinylic carbon atoms) and $U(\text{H})$ set to $1.5U_{\text{eq}}(\text{C})$ (methyl carbon atoms).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.80982 (18)	0.250000	0.41353 (13)	0.0882 (6)	
O2	0.7034 (2)	0.250000	0.29689 (12)	0.0958 (7)	
N1	0.16773 (16)	0.250000	0.61550 (10)	0.0528 (4)	
N2	0.7029 (2)	0.250000	0.37195 (13)	0.0682 (6)	
C1	0.1760 (2)	0.250000	0.53874 (12)	0.0519 (5)	
H1	0.091886	0.250000	0.507196	0.062*	
C2	0.0296 (2)	0.250000	0.65746 (12)	0.0536 (5)	
C11	0.31255 (19)	0.250000	0.49559 (12)	0.0484 (5)	
C12	0.4375 (2)	0.250000	0.53988 (13)	0.0542 (5)	
H12	0.435145	0.250000	0.598363	0.065*	
C13	0.5655 (2)	0.250000	0.49924 (14)	0.0574 (5)	
H13	0.651108	0.250000	0.529340	0.069*	
C14	0.5664 (2)	0.250000	0.41468 (13)	0.0539 (5)	
C15	0.4456 (2)	0.250000	0.36931 (13)	0.0611 (6)	
H15	0.448969	0.250000	0.310839	0.073*	
C16	0.3178 (2)	0.250000	0.41056 (13)	0.0591 (5)	
H16	0.232716	0.250000	0.379898	0.071*	
C3	-0.0973 (5)	0.265 (4)	0.6039 (3)	0.068 (3)	0.25
H3A	-0.182003	0.263914	0.638266	0.102*	0.25
H3B	-0.093343	0.381236	0.572847	0.102*	0.25
H3C	-0.099806	0.160966	0.565549	0.102*	0.25
C4	0.031 (2)	0.409 (3)	0.7219 (14)	0.065 (5)	0.25
H4A	-0.059907	0.412007	0.750737	0.098*	0.25
H4B	0.106252	0.387595	0.761811	0.098*	0.25
H4C	0.046114	0.526941	0.693901	0.098*	0.25
C5	0.025 (2)	0.067 (3)	0.7079 (13)	0.059 (4)	0.25
H5A	-0.064623	0.058891	0.737398	0.089*	0.25
H5B	0.034319	-0.038276	0.670486	0.089*	0.25
H5C	0.102642	0.065927	0.747639	0.089*	0.25
C6	-0.062 (2)	0.4163 (17)	0.6252 (12)	0.056 (3)	0.25
H6A	-0.082575	0.398370	0.566662	0.084*	0.25
H6B	-0.149716	0.422350	0.656392	0.084*	0.25
H6C	-0.009376	0.531863	0.632479	0.084*	0.25
C7	-0.047 (2)	0.073 (2)	0.6354 (16)	0.100 (8)	0.25
H7A	-0.062591	0.069305	0.575825	0.150*	0.25
H7B	0.010265	-0.032942	0.652070	0.150*	0.25
H7C	-0.137343	0.069667	0.664117	0.150*	0.25
C8	0.0610 (8)	0.276 (4)	0.7447 (4)	0.120 (7)	0.25
H8A	-0.026868	0.277721	0.776207	0.180*	0.25
H8B	0.120741	0.175117	0.764160	0.180*	0.25
H8C	0.110222	0.394110	0.752281	0.180*	0.25

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0537 (10)	0.1050 (15)	0.1060 (15)	0.000	0.0215 (9)	0.000
O2	0.0840 (13)	0.1273 (18)	0.0762 (12)	0.000	0.0377 (10)	0.000
N1	0.0448 (8)	0.0618 (10)	0.0518 (9)	0.000	0.0050 (7)	0.000
N2	0.0630 (11)	0.0611 (11)	0.0805 (14)	0.000	0.0266 (10)	0.000
C1	0.0457 (9)	0.0615 (11)	0.0486 (10)	0.000	0.0014 (7)	0.000
C2	0.0440 (9)	0.0643 (12)	0.0525 (10)	0.000	0.0078 (8)	0.000
C11	0.0477 (10)	0.0472 (10)	0.0502 (10)	0.000	0.0060 (7)	0.000
C12	0.0513 (11)	0.0587 (12)	0.0526 (10)	0.000	0.0061 (8)	0.000
C13	0.0489 (10)	0.0589 (12)	0.0644 (12)	0.000	0.0055 (8)	0.000
C14	0.0523 (10)	0.0449 (10)	0.0645 (12)	0.000	0.0183 (9)	0.000
C15	0.0657 (12)	0.0674 (13)	0.0502 (11)	0.000	0.0120 (9)	0.000
C16	0.0531 (11)	0.0740 (14)	0.0502 (10)	0.000	0.0036 (8)	0.000
C3	0.049 (2)	0.095 (9)	0.060 (3)	0.013 (7)	0.0064 (19)	-0.024 (7)
C4	0.079 (8)	0.060 (6)	0.057 (7)	-0.014 (5)	0.011 (5)	0.006 (5)
C5	0.057 (5)	0.064 (7)	0.057 (7)	-0.004 (5)	0.020 (5)	0.008 (7)
C6	0.045 (4)	0.045 (5)	0.079 (6)	0.010 (4)	0.012 (4)	0.001 (4)
C7	0.067 (9)	0.109 (13)	0.124 (16)	0.003 (7)	0.040 (9)	0.017 (9)
C8	0.084 (5)	0.23 (2)	0.049 (3)	0.065 (12)	0.017 (3)	0.017 (10)

Geometric parameters (Å, °)

O1—N2	1.221 (3)	C15—H15	0.9500
O2—N2	1.219 (3)	C16—H16	0.9500
N1—C1	1.249 (2)	C3—H3A	0.9800
N1—C2	1.480 (2)	C3—H3B	0.9800
N2—C14	1.472 (2)	C3—H3C	0.9800
C1—C11	1.476 (2)	C4—H4A	0.9800
C1—H1	0.9500	C4—H4B	0.9800
C2—C8	1.460 (7)	C4—H4C	0.9800
C2—C3	1.491 (5)	C5—H5A	0.9800
C2—C7	1.513 (11)	C5—H5B	0.9800
C2—C4	1.555 (11)	C5—H5C	0.9800
C2—C5	1.557 (10)	C6—H6A	0.9800
C2—C6	1.574 (8)	C6—H6B	0.9800
C11—C16	1.382 (3)	C6—H6C	0.9800
C11—C12	1.389 (3)	C7—H7A	0.9800
C12—C13	1.384 (3)	C7—H7B	0.9800
C12—H12	0.9500	C7—H7C	0.9800
C13—C14	1.373 (3)	C8—H8A	0.9800
C13—H13	0.9500	C8—H8B	0.9800
C14—C15	1.365 (3)	C8—H8C	0.9800
C15—C16	1.388 (3)		
C1—N1—C2	121.03 (17)	C2—C3—H3A	109.5
O2—N2—O1	123.4 (2)	C2—C3—H3B	109.5

O2—N2—C14	118.4 (2)	H3A—C3—H3B	109.5
O1—N2—C14	118.3 (2)	C2—C3—H3C	109.5
N1—C1—C11	121.96 (18)	H3A—C3—H3C	109.5
N1—C1—H1	119.0	H3B—C3—H3C	109.5
C11—C1—H1	119.0	C2—C4—H4A	109.5
C8—C2—N1	105.4 (3)	C2—C4—H4B	109.5
N1—C2—C3	116.7 (3)	H4A—C4—H4B	109.5
C8—C2—C7	116.0 (9)	C2—C4—H4C	109.5
N1—C2—C7	108.5 (10)	H4A—C4—H4C	109.5
N1—C2—C4	107.7 (9)	H4B—C4—H4C	109.5
C3—C2—C4	110.0 (8)	C2—C5—H5A	109.5
N1—C2—C5	105.5 (7)	C2—C5—H5B	109.5
C3—C2—C5	110.3 (8)	H5A—C5—H5B	109.5
C4—C2—C5	105.9 (5)	C2—C5—H5C	109.5
C8—C2—C6	109.6 (8)	H5A—C5—H5C	109.5
N1—C2—C6	109.6 (8)	H5B—C5—H5C	109.5
C7—C2—C6	107.6 (5)	C2—C6—H6A	109.5
C16—C11—C12	119.11 (17)	C2—C6—H6B	109.5
C16—C11—C1	120.41 (18)	H6A—C6—H6B	109.5
C12—C11—C1	120.48 (17)	C2—C6—H6C	109.5
C13—C12—C11	120.36 (19)	H6A—C6—H6C	109.5
C13—C12—H12	119.8	H6B—C6—H6C	109.5
C11—C12—H12	119.8	C2—C7—H7A	109.5
C14—C13—C12	118.9 (2)	C2—C7—H7B	109.5
C14—C13—H13	120.6	H7A—C7—H7B	109.5
C12—C13—H13	120.6	C2—C7—H7C	109.5
C15—C14—C13	122.28 (18)	H7A—C7—H7C	109.5
C15—C14—N2	119.19 (19)	H7B—C7—H7C	109.5
C13—C14—N2	118.5 (2)	C2—C8—H8A	109.5
C14—C15—C16	118.48 (19)	C2—C8—H8B	109.5
C14—C15—H15	120.8	H8A—C8—H8B	109.5
C16—C15—H15	120.8	C2—C8—H8C	109.5
C11—C16—C15	120.91 (19)	H8A—C8—H8C	109.5
C11—C16—H16	119.5	H8B—C8—H8C	109.5
C15—C16—H16	119.5		
C2—N1—C1—C11	180.000 (1)	C12—C13—C14—C15	0.000 (1)
C1—N1—C2—C8	-172.2 (12)	C12—C13—C14—N2	180.000 (1)
C1—N1—C2—C3	-4.8 (12)	O2—N2—C14—C15	0.000 (1)
C1—N1—C2—C7	63.0 (10)	O1—N2—C14—C15	180.000 (1)
C1—N1—C2—C4	-129.1 (11)	O2—N2—C14—C13	180.000 (1)
C1—N1—C2—C5	118.1 (10)	O1—N2—C14—C13	0.000 (1)
C1—N1—C2—C6	-54.3 (8)	C13—C14—C15—C16	0.000 (1)
N1—C1—C11—C16	180.000 (1)	N2—C14—C15—C16	180.000 (1)
N1—C1—C11—C12	0.000 (1)	C12—C11—C16—C15	0.000 (1)
C16—C11—C12—C13	0.000 (1)	C1—C11—C16—C15	180.000 (1)
C1—C11—C12—C13	180.000 (1)	C14—C15—C16—C11	0.000 (1)
C11—C12—C13—C14	0.000 (1)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C5—H5 <i>B</i> \cdots O1 ⁱ	0.98	2.53	3.41 (3)	149
C6—H6 <i>C</i> \cdots O1 ⁱⁱ	0.98	2.58	3.459 (19)	149
C7—H7 <i>B</i> \cdots O1 ⁱ	0.98	2.56	3.35 (2)	138

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z+1$.