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N-Benzyl-*N*-[(*E*)-(3,4,5-trimethoxyphenyl)-methylidene]amine

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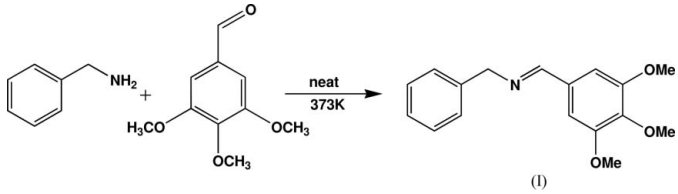
In the title molecule, $C_{17}H_{19}NO_3$, the dihedral angle formed by the planes of the two benzene rings is 62.3 (1)°. There are no direction-specific interactions in the supramolecular structure.

Comment

The bond lengths and angles in the title compound, (I), show no unusual features. The central part of the molecule is essentially planar, with only the methyl group at C241 and the phenyl group attached to atom C1 tilted out of the plane. This is shown by the leading torsion angles given in Table 1. The dihedral angle formed by the planes of the two benzene rings is 62.3 (1)°.



(I)

Experimental

A neat mixture of benzylamine (3.17 mmol) and 3,4,5-trimethoxybenzaldehyde (3.11 mmol) was heated at 373 K for five minutes. After cooling, a white solid was obtained in quantitative yield. Crystals suitable for single-crystal X-ray diffraction were grown from ethanol (m.p. 367 K).

Crystal data

$C_{17}H_{19}NO_3$
M_r = 285.33
Monoclinic, $P2_1/c$
a = 22.1302 (10) Å
b = 5.3140 (2) Å
c = 12.4571 (5) Å
β = 98.447 (2)°
V = 1449.06 (10) Å^3
Z = 4
D_x = 1.308 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 120 (2) K
Plate, colourless
0.42 × 0.34 × 0.03 mm

Data collection

Bruker-Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.963, T_{max} = 0.997
14669 measured reflections
3317 independent reflections
2627 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 27.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.154
S = 1.14
3317 reflections
193 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 1.1271P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.154
Data-to-parameter ratio = 17.2

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

Table 1
Selected torsion angles (°).

C2—N1—C1—C11	125.0 (2)	C22—C23—O23—C231	3.5 (3)
C1—N1—C2—C21	175.79 (18)	C24—C23—O23—C231	−176.53 (16)
N1—C1—C11—C16	89.1 (2)	C25—C24—O24—C241	72.8 (2)
N1—C1—C11—C12	−91.1 (2)	C23—C24—O24—C241	−110.4 (2)
N1—C2—C21—C26	172.26 (19)	C26—C25—O25—C251	3.7 (3)
N1—C2—C21—C22	−9.6 (3)	C24—C25—O25—C251	−176.98 (17)

H atoms were treated as riding, with C—H = 0.95, 0.99 and 0.98 Å for aromatic, methylene and methyl C, respectively; U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl and 1.2 for other H atoms.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97*; molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *WORDPERFECT* macro *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. The authors thank the staff for all their help and advice. JC thanks the Consejería de Innovacíon, Ciencia y Empresa (Junta de Andalucía, Spain) and the Universidad de Jaén for financial support. RA and LS thank COLCIENCIAS, UNIVALLE (Universidad del Valle, Colombia), and RA also thanks AUIP for supporting a research fellowship.

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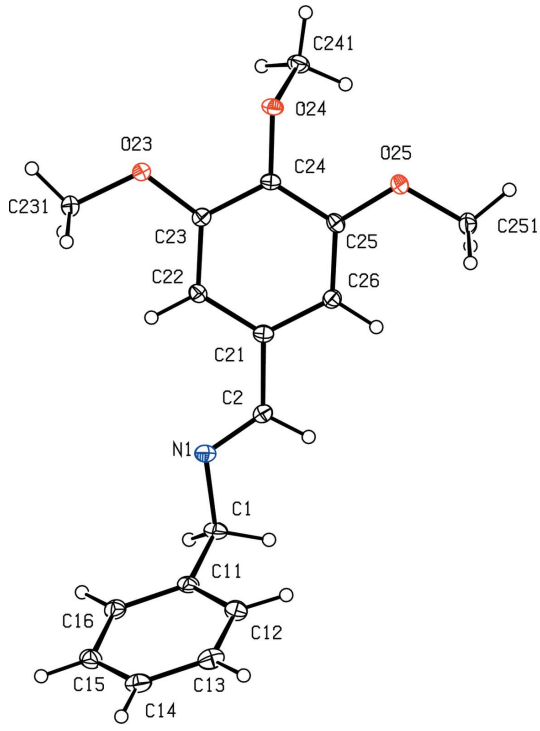

Figure 1
Molecular structure of (I) with the numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

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supporting information

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$c = 12.4571$ (5) Å
$\beta = 98.447$ (2)°
$V = 1449.06$ (10) Å^3
$Z = 4$
$F(000) = 608$
$D_x = 1.308$ Mg m^{-3}
Melting point: 367 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3317 reflections
$\theta = 3.3$–27.6°
$\mu = 0.09$ mm^{-1}
$T = 120$ K
Plate, colourless
0.42 × 0.34 × 0.03 mm

Data collection

Bruker-Nonius KappaCCD diffractometer
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Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ & ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.963$, $T_{max} = 0.997$
14669 measured reflections
3317 independent reflections
2627 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.3°$
$h = -28 \rightarrow 28$
$k = -6 \rightarrow 6$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.154$
$S = 1.14$
3317 reflections
193 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
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 1.1271P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Special details

Experimental. The scale factors in the experimental table are calculated from the 'size' command in the *SHELXL97* input file.
MS (IE 70 eV): m/*z* (%) 285 (45), 270 (6), 254 (5), 91 (100).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.17303 (7)	0.3758 (3)	0.49211 (13)	0.0216 (4)
C1	0.12212 (9)	0.2916 (4)	0.54614 (17)	0.0243 (4)
C2	0.21935 (9)	0.2331 (4)	0.50281 (15)	0.0201 (4)
C11	0.10308 (8)	0.4877 (4)	0.62221 (16)	0.0210 (4)
C12	0.12924 (9)	0.4898 (4)	0.73129 (17)	0.0264 (5)
C13	0.11283 (10)	0.6721 (4)	0.80159 (18)	0.0298 (5)
C14	0.06916 (10)	0.8502 (4)	0.76425 (19)	0.0297 (5)
C15	0.04209 (10)	0.8478 (4)	0.65706 (19)	0.0277 (5)
C16	0.05928 (9)	0.6690 (4)	0.58604 (17)	0.0241 (4)
C21	0.27357 (8)	0.2747 (4)	0.44917 (15)	0.0187 (4)
C22	0.27406 (8)	0.4577 (4)	0.36889 (15)	0.0183 (4)
C23	0.32533 (9)	0.4804 (4)	0.31665 (15)	0.0181 (4)
O23	0.33080 (6)	0.6491 (3)	0.23613 (11)	0.0216 (3)
C231	0.28149 (9)	0.8224 (4)	0.20817 (17)	0.0228 (4)
C24	0.37622 (8)	0.3231 (4)	0.34585 (15)	0.0179 (4)
O24	0.42718 (6)	0.3559 (3)	0.29596 (11)	0.0211 (3)
C241	0.43719 (9)	0.1529 (4)	0.22369 (17)	0.0244 (4)
C25	0.37572 (8)	0.1454 (4)	0.42831 (15)	0.0186 (4)
O25	0.42793 (6)	0.0090 (3)	0.45386 (11)	0.0241 (3)
C251	0.42837 (9)	−0.1839 (4)	0.53421 (17)	0.0235 (4)
C26	0.32410 (9)	0.1194 (4)	0.47905 (15)	0.0201 (4)
H1A	0.1342	0.1361	0.5876	0.029*
H1B	0.0868	0.2504	0.4905	0.029*
H2	0.2191	0.0899	0.5484	0.024*
H12	0.1585	0.3654	0.7577	0.032*
H13	0.1316	0.6745	0.8752	0.036*
H14	0.0578	0.9743	0.8124	0.036*
H15	0.0117	0.9687	0.6318	0.033*
H16	0.0410	0.6702	0.5121	0.029*
H22	0.2399	0.5653	0.3501	0.022*
H23A	0.2757	0.9214	0.2723	0.034*
H23B	0.2440	0.7292	0.1823	0.034*
H23C	0.2910	0.9354	0.1508	0.034*
H24A	0.4049	0.1541	0.1608	0.037*
H24B	0.4365	−0.0079	0.2620	0.037*
H24C	0.4770	0.1747	0.1992	0.037*
H25A	0.3958	−0.3053	0.5107	0.035*
H25B	0.4217	−0.1082	0.6033	0.035*
H25C	0.4679	−0.2702	0.5437	0.035*
H26	0.3233	−0.0040	0.5340	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0199 (8)	0.0253 (9)	0.0207 (8)	−0.0002 (7)	0.0066 (6)	−0.0010 (7)

C1	0.0197 (9)	0.0266 (11)	0.0281 (11)	−0.0033 (8)	0.0092 (8)	−0.0024 (9)
C2	0.0219 (10)	0.0207 (10)	0.0183 (9)	−0.0010 (8)	0.0045 (7)	0.0008 (8)
C11	0.0158 (9)	0.0226 (10)	0.0259 (10)	−0.0043 (7)	0.0070 (7)	−0.0001 (8)
C12	0.0211 (10)	0.0291 (12)	0.0293 (11)	−0.0012 (8)	0.0049 (8)	0.0008 (9)
C13	0.0307 (11)	0.0354 (13)	0.0240 (11)	−0.0077 (9)	0.0068 (9)	−0.0029 (9)
C14	0.0338 (12)	0.0250 (11)	0.0341 (12)	−0.0054 (9)	0.0174 (9)	−0.0038 (9)
C15	0.0235 (10)	0.0231 (11)	0.0385 (12)	0.0000 (8)	0.0118 (9)	0.0027 (9)
C16	0.0213 (9)	0.0247 (11)	0.0268 (10)	−0.0044 (8)	0.0053 (8)	0.0028 (8)
C21	0.0192 (9)	0.0200 (10)	0.0171 (9)	−0.0016 (7)	0.0039 (7)	−0.0041 (8)
C22	0.0175 (9)	0.0189 (9)	0.0184 (9)	0.0018 (7)	0.0018 (7)	−0.0018 (8)
C23	0.0210 (9)	0.0168 (9)	0.0166 (9)	−0.0014 (7)	0.0032 (7)	−0.0017 (7)
O23	0.0212 (7)	0.0220 (7)	0.0229 (7)	0.0033 (5)	0.0072 (5)	0.0049 (6)
C231	0.0240 (10)	0.0206 (10)	0.0237 (10)	0.0039 (8)	0.0035 (8)	0.0032 (8)
C24	0.0154 (9)	0.0204 (10)	0.0185 (9)	−0.0024 (7)	0.0043 (7)	−0.0022 (8)
O24	0.0174 (7)	0.0218 (7)	0.0257 (7)	−0.0015 (5)	0.0084 (5)	−0.0016 (6)
C241	0.0235 (10)	0.0245 (11)	0.0271 (10)	0.0027 (8)	0.0099 (8)	−0.0022 (9)
C25	0.0156 (9)	0.0196 (10)	0.0197 (9)	0.0013 (7)	−0.0003 (7)	−0.0021 (8)
O25	0.0170 (7)	0.0289 (8)	0.0265 (7)	0.0051 (6)	0.0033 (5)	0.0078 (6)
C251	0.0223 (10)	0.0228 (10)	0.0244 (10)	0.0026 (8)	−0.0003 (8)	0.0041 (8)
C26	0.0202 (9)	0.0211 (10)	0.0189 (9)	−0.0003 (7)	0.0029 (7)	0.0019 (8)

Geometric parameters (Å, º)

N1—C2	1.266 (3)	C22—H22	0.95
N1—C1	1.465 (2)	C23—O23	1.364 (2)
C1—C11	1.510 (3)	C23—C24	1.407 (3)
C1—H1A	0.99	O23—C231	1.431 (2)
C1—H1B	0.99	C231—H23A	0.98
C2—C21	1.473 (3)	C231—H23B	0.98
C2—H2	0.95	C231—H23C	0.98
C11—C16	1.394 (3)	C24—O24	1.376 (2)
C11—C12	1.397 (3)	C24—C25	1.397 (3)
C12—C13	1.390 (3)	O24—C241	1.443 (2)
C12—H12	0.95	C241—H24A	0.98
C13—C14	1.384 (3)	C241—H24B	0.98
C13—H13	0.95	C241—H24C	0.98
C14—C15	1.381 (3)	C25—O25	1.361 (2)
C14—H14	0.95	C25—C26	1.391 (3)
C15—C16	1.389 (3)	O25—C251	1.432 (2)
C15—H15	0.95	C251—H25A	0.98
C16—H16	0.95	C251—H25B	0.98
C21—C26	1.395 (3)	C251—H25C	0.98
C21—C22	1.396 (3)	C26—H26	0.95
C22—C23	1.394 (3)		
C2—N1—C1	115.73 (17)	O23—C23—C22	124.54 (17)
N1—C1—C11	112.45 (17)	O23—C23—C24	115.24 (16)
N1—C1—H1A	109.1	C22—C23—C24	120.23 (17)

C11—C1—H1A	109.1	C23—O23—C231	117.07 (14)
N1—C1—H1B	109.1	O23—C231—H23A	109.5
C11—C1—H1B	109.1	O23—C231—H23B	109.5
H1A—C1—H1B	107.8	H23A—C231—H23B	109.5
N1—C2—C21	124.27 (18)	O23—C231—H23C	109.5
N1—C2—H2	117.9	H23A—C231—H23C	109.5
C21—C2—H2	117.9	H23B—C231—H23C	109.5
C16—C11—C12	118.58 (19)	O24—C24—C25	120.88 (17)
C16—C11—C1	121.29 (18)	O24—C24—C23	119.08 (17)
C12—C11—C1	120.14 (19)	C25—C24—C23	119.96 (16)
C13—C12—C11	120.6 (2)	C24—O24—C241	113.47 (15)
C13—C12—H12	119.7	O24—C241—H24A	109.5
C11—C12—H12	119.7	O24—C241—H24B	109.5
C14—C13—C12	120.0 (2)	H24A—C241—H24B	109.5
C14—C13—H13	120.0	O24—C241—H24C	109.5
C12—C13—H13	120.0	H24A—C241—H24C	109.5
C15—C14—C13	120.1 (2)	H24B—C241—H24C	109.5
C15—C14—H14	120.0	O25—C25—C26	124.48 (17)
C13—C14—H14	120.0	O25—C25—C24	115.71 (16)
C14—C15—C16	120.1 (2)	C26—C25—C24	119.81 (17)
C14—C15—H15	119.9	C25—O25—C251	117.58 (15)
C16—C15—H15	119.9	O25—C251—H25A	109.5
C15—C16—C11	120.6 (2)	O25—C251—H25B	109.5
C15—C16—H16	119.7	H25A—C251—H25B	109.5
C11—C16—H16	119.7	O25—C251—H25C	109.5
C26—C21—C22	120.85 (17)	H25A—C251—H25C	109.5
C26—C21—C2	117.68 (17)	H25B—C251—H25C	109.5
C22—C21—C2	121.45 (17)	C25—C26—C21	119.95 (18)
C23—C22—C21	119.17 (17)	C25—C26—H26	120.0
C23—C22—H22	120.4	C21—C26—H26	120.0
C21—C22—H22	120.4		

C2—N1—C1—C11	125.0 (2)	C22—C23—O23—C231	3.5 (3)
C1—N1—C2—C21	175.79 (18)	C24—C23—O23—C231	−176.53 (16)
N1—C1—C11—C16	89.1 (2)	O23—C23—C24—O24	2.5 (3)
N1—C1—C11—C12	−91.1 (2)	C22—C23—C24—O24	−177.52 (17)
C16—C11—C12—C13	−1.4 (3)	O23—C23—C24—C25	179.29 (17)
C1—C11—C12—C13	178.87 (18)	C22—C23—C24—C25	−0.8 (3)
C11—C12—C13—C14	1.5 (3)	C25—C24—O24—C241	72.8 (2)
C12—C13—C14—C15	−0.4 (3)	C23—C24—O24—C241	−110.4 (2)
C13—C14—C15—C16	−1.0 (3)	O24—C24—C25—O25	−0.7 (3)
C14—C15—C16—C11	1.1 (3)	C23—C24—C25—O25	−177.41 (17)
C12—C11—C16—C15	0.0 (3)	O24—C24—C25—C26	178.67 (17)
C1—C11—C16—C15	179.81 (18)	C23—C24—C25—C26	2.0 (3)
N1—C2—C21—C26	172.26 (19)	C26—C25—O25—C251	3.7 (3)
N1—C2—C21—C22	−9.6 (3)	C24—C25—O25—C251	−176.98 (17)
C26—C21—C22—C23	1.5 (3)	O25—C25—C26—C21	177.84 (18)
C2—C21—C22—C23	−176.64 (17)	C24—C25—C26—C21	−1.5 (3)

C21—C22—C23—O23	179.02 (17)	C22—C21—C26—C25	−0.2 (3)
C21—C22—C23—C24	−0.9 (3)	C2—C21—C26—C25	177.91 (17)