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(*E*)-1-(3,3′-Dimethoxy-4′-{[(*E*)-4-nitrobenzylidene]-amino}-[1,1′-biphenyl]-4-yl)-*N*-(4-nitrophenyl)-methanimine

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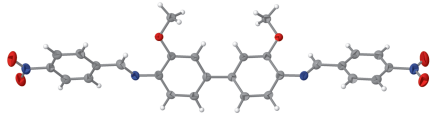
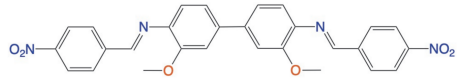
The title compound, $C_{28}H_{22}N_4O_6$, crystallizes with one half-molecule in the asymmetric unit centered on a twofold rotation axis located at the midpoint of the central C—C bond. The structure is non-planar overall, with nearly planar anisole-imine and nitrophenyl-methanimine fragments. In the crystal, a cooperative network of intermolecular C—H···O hydrogen bonds organizes the molecules into layers parallel to the (101) plane, which are further consolidated by offset π–π stacking between centrosymmetrically related phenyl rings and C—H···π interactions. Collectively, these non-covalent interactions contribute to the cohesion of the three-dimensional supramolecular framework.

3D view



Chemical scheme



Structure description

The title Schiff base was synthesized as part of a broader search for multifunctional imine-based molecules, whose tunable π-conjugation underpins applications in catalysis, sensing, materials science and medicinal chemistry. The title compound crystallizes in the monoclinic space group *I*2/*a*, with one half-molecule in the asymmetric unit. The molecule is centered on a crystallographic twofold rotation axis located at the midpoint of the C11—C11^{i} bond of the amine molecule [symmetry code: (i) $\frac{3}{2} - x, 1 - y, 1 - z$] (Fig. 1). The molecule is not planar. Within the asymmetric unit, the two Schiff base moieties are also non-planar, whereas the anisole-imine and nitrophenyl-methanimine are each individually nearly planar (C1—C6 and N, O1, O2, C7 are planar with a maximum

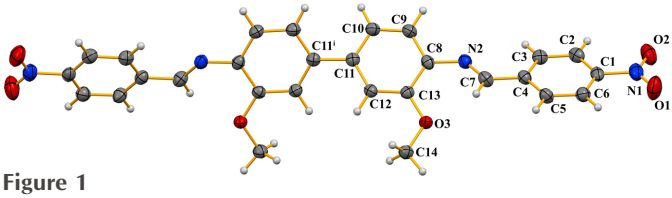


Figure 1
View of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. Symmetry code (i): $\frac{3}{2} - x, 1 - y, 1 - z$.

deviation of 0.045 (2) Å for the azomethine carbon atom C7; and C8–C13, N2, O3 and C14 are planar with a maximum deviation of 0.148 (1) Å for the azomethine nitrogen atom N2). In the two six-membered rings, the largest distance between atom and the mean plane is 0.005 (2) Å, and 0.018 (2) Å in the nearly planar parts, respectively. Bond length analysis indicates an extended network of π bonds across the molecule, consistent with pronounced electronic delocalization. The N2—C7 bond length of 1.266 (2) Å is characteristic of a C═N double bond, confirming significant π character within the imine fragment. The C7—N2—C8 bond angle of 122.82 (14)° shows that atom N2 adopts an essentially trigonal–planar geometry, in agreement with sp^2 hybridization and conjugation with the adjacent aromatic ring system. The imine unit adopts an almost perfectly *trans* arrangement, with the atoms around the C=N bond being essentially coplanar as indicated by the C8—N2—C7—C4 torsion angle of −179.82(14°). The bond distances and angles are normal and are in good agreement with those in analogous structures (Hernández Téllez *et al.*, 2025; Adam *et al.*, 2015; Madhuprasad *et al.*, 2014). The dihedral angle between the aromatic rings in the asymmetric unit is 35.68 (7)° and is largely controlled by the cooperative effect of the intramolecular C7—H7···O3 and the intermolecular C2—H2···O3 hydrogen bonds (Table 1). The latter interaction links neighboring molecules, forming layers parallel to the (101) plane (Fig. 2). In the crystal, slightly offset π–π stacking interactions are present between centrosymmetrically related phenyl rings with a $Cg1\cdots Cg1(\frac{1}{2} - x, \frac{3}{2} - y, \frac{3}{2} - z)$ separation of 3.5385 (10) Å, slippage = 1.235 Å, where $Cg1$ is the centroid of the C1–C6 ring. The overall crystal cohesion is reinforced by C—H···π interactions involving C5—H5···$Cg2(-\frac{1}{2} + x, 1 - y, z)$ and C14—H14A···$Cg2(1 - x, 1 - y, 1 - z)$ interactions,

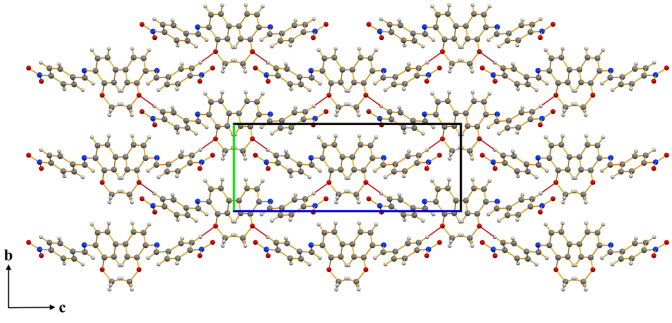


Figure 2
Extended packing arrangement viewed in the [010] direction of the unit cell showing C—H···O intermolecular interactions (red line).

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O3^{i}	0.95	2.59	3.3833 (19)	141
C7—H7···O3	0.95	2.25	2.7783 (19)	114

Symmetry code: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$.

with H···Cg separations of 3.4898 (18) and 3.6757 (17) Å, respectively, and C—H···Cg angles of 140 and 129°, respectively, where $Cg2$ is the centroid of the C8–C13 ring (Fig. 3). Collectively, these non-covalent interactions contribute to the cohesion of the three-dimensional supramolecular framework.

Synthesis and crystallization

An ethanolic solution of 4-nitrosalicylaldehyde (0.02 mmol, 3.34 mg) was added dropwise to a methanolic solution of *O*-dianisidine (0.01 mmol, 2.44 mg) under constant magnetic stirring at room temperature. The reaction mixture was stirred for 1 h, during which the solution gradually turned orange. The product was obtained as brown crystals suitable for X-ray diffraction analysis after slow evaporation of the solvent, washed with cold ethanol, and dried in a desiccator. Yield: 76.24%. m.p 529.15 K.

FTIR (ATR, cm^{-1}): 3100–3000 (*w*) (aromatic/sp^2 C—H stretching), 2924 (*w*) (asymmetric aliphatic C—H stretching), 2857 (*w*) (symmetric aliphatic C—H stretching), 1687 (*w*)–1630 (*vs*) (azomethine stretching vibration C═N), 1599 (*s*) (N—O asymmetric stretching), 1371 (*w*) (N—O symmetric stretching).

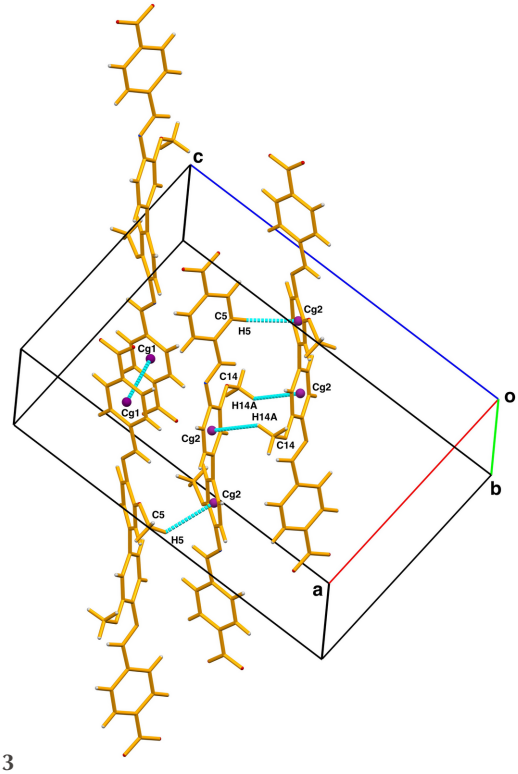


Figure 3
Graphical view of C—H···π and π-π stacking interactions.

Refinement

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

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{22}N_4O_6$
M_r	510.49
Crystal system, space group	Monoclinic, *I*2/*a*
Temperature (K)	150
a, *b*, *c* (Å)	14.2099 (14), 8.0341 (8), 20.899 (2)
β (°)	92.171 (9)
V (Å^3)	2384.2 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.85
Crystal size (mm)	0.28 × 0.15 × 0.07
Data collection	
Diffractometer	Xcalibur, Atlas, Gemini ultra
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.729, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9789, 2120, 1821
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.121, 1.06
No. of reflections	2120
No. of parameters	173
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.23

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *OLEX2.solve* (Dolomanov *et al.*, 2009), *SHELXL2019/3* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

full crystallographic data

IUCrData (2026). **11**, x260220 [https://doi.org/10.1107/S2414314626002208]

(*E*)-1-(3,3′-Dimethoxy-4′-{[(*E*)-4-nitrobenzylidene]amino}-[1,1′-biphenyl]-4-yl)-*N*-(4-nitrophenyl)methanimine

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(*E*)-1-(3,3′-Dimethoxy-4′-{[(*E*)-4-nitrobenzylidene]amino}-[1,1′-biphenyl]-4-yl)-*N*-(4-nitrophenyl)methanimine

Crystal data

$C_{28}H_{22}N_4O_6$
M_r = 510.49
Monoclinic, *I*2/*a*
Hall symbol: -I 2ya
a = 14.2099 (14) Å
b = 8.0341 (8) Å
c = 20.899 (2) Å
β = 92.171 (9)°
V = 2384.2 (4) Å^3
Z = 4
F(000) = 1064
D_x = 1.422 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 5072 reflections
θ = 4.1–66.9°
μ = 0.85 mm^{-1}
T = 150 K
Plate, brown
0.28 × 0.15 × 0.07 mm

Data collection

Xcalibur, Atlas, Gemini ultra diffractometer
Mirror monochromator
Detector resolution: 10.4685 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
T_{min} = 0.729, T_{max} = 1.000
9789 measured reflections
2120 independent reflections
1821 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 67.0°, θ_{min} = 4.2°
h = −16→16
k = −9→9
l = −24→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.121
S = 1.06
2120 reflections
173 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$W = 1/[\Sigma^2(FO^2) + (0.068P)^2 + 1.2673P]$ WHERE $P = (FO^2 + 2FC^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95–0.98 Å with U_{iso}(H) values of 1.2 or 1.5 U_{eq} of the parent atoms.

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.08857 (11)	0.4892 (2)	0.84954 (7)	0.0664 (6)
O2	0.18453 (10)	0.64173 (19)	0.90565 (6)	0.0538 (5)
O3	0.53245 (7)	0.32934 (13)	0.58125 (5)	0.0311 (3)
N1	0.16324 (11)	0.56187 (19)	0.85733 (7)	0.0409 (5)
N2	0.50068 (9)	0.61140 (16)	0.66003 (6)	0.0305 (4)
C1	0.23150 (11)	0.55294 (19)	0.80633 (7)	0.0313 (5)
C2	0.31525 (12)	0.6393 (2)	0.81402 (7)	0.0330 (5)
C3	0.37976 (11)	0.6307 (2)	0.76630 (7)	0.0318 (5)
C4	0.35916 (11)	0.53793 (19)	0.71097 (7)	0.0297 (5)
C5	0.27422 (11)	0.4534 (2)	0.70499 (8)	0.0339 (5)
C6	0.20921 (11)	0.4594 (2)	0.75260 (8)	0.0345 (5)
C7	0.42422 (11)	0.5304 (2)	0.65778 (8)	0.0327 (5)
C8	0.56487 (10)	0.60829 (19)	0.61024 (7)	0.0280 (4)
C9	0.61697 (11)	0.75257 (19)	0.60148 (7)	0.0298 (5)
C10	0.68751 (11)	0.76153 (19)	0.55758 (7)	0.0298 (5)
C11	0.71028 (10)	0.62133 (19)	0.52197 (7)	0.0271 (4)
C12	0.65722 (11)	0.47610 (18)	0.52939 (7)	0.0272 (4)
C13	0.58502 (10)	0.46875 (18)	0.57190 (7)	0.0261 (4)
C14	0.54558 (11)	0.19137 (19)	0.53924 (7)	0.0331 (5)
H2	0.32825	0.70356	0.85148	0.0400*
H3	0.43814	0.68782	0.77112	0.0380*
H5	0.26035	0.39003	0.66742	0.0410*
H6	0.15118	0.40094	0.74839	0.0410*
H7	0.40857	0.46390	0.62132	0.0390*
H9	0.60377	0.84807	0.62640	0.0360*
H10	0.72033	0.86310	0.55175	0.0360*
H12	0.67113	0.38055	0.50469	0.0330*
H14A	0.53360	0.22693	0.49482	0.0500*
H14B	0.50174	0.10202	0.54958	0.0500*
H14C	0.61042	0.15064	0.54454	0.0500*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0501 (9)	0.0891 (12)	0.0617 (9)	−0.0142 (8)	0.0233 (7)	−0.0021 (8)
O2	0.0611 (9)	0.0675 (9)	0.0334 (7)	0.0152 (7)	0.0106 (6)	−0.0032 (6)
O3	0.0330 (6)	0.0246 (5)	0.0364 (6)	−0.0020 (4)	0.0089 (4)	−0.0027 (4)
N1	0.0429 (9)	0.0456 (8)	0.0348 (8)	0.0107 (7)	0.0093 (6)	0.0070 (7)
N2	0.0283 (7)	0.0316 (7)	0.0317 (7)	0.0034 (5)	0.0039 (5)	0.0007 (5)
C1	0.0335 (8)	0.0320 (8)	0.0287 (8)	0.0090 (6)	0.0054 (6)	0.0059 (6)

C2	0.0383 (9)	0.0329 (8)	0.0274 (7)	0.0048 (6)	−0.0034 (6)	−0.0012 (6)
C3	0.0297 (8)	0.0330 (8)	0.0323 (8)	0.0014 (6)	−0.0024 (6)	0.0011 (6)
C4	0.0286 (8)	0.0294 (8)	0.0312 (8)	0.0041 (6)	0.0012 (6)	−0.0006 (6)
C5	0.0317 (8)	0.0341 (9)	0.0360 (8)	0.0011 (6)	0.0022 (6)	−0.0083 (7)
C6	0.0301 (8)	0.0320 (8)	0.0414 (9)	0.0006 (6)	0.0020 (7)	0.0003 (7)
C7	0.0305 (8)	0.0359 (8)	0.0315 (8)	0.0043 (7)	−0.0004 (6)	−0.0052 (7)
C8	0.0261 (7)	0.0313 (8)	0.0265 (7)	0.0047 (6)	0.0001 (6)	−0.0004 (6)
C9	0.0311 (8)	0.0263 (8)	0.0319 (8)	0.0025 (6)	0.0004 (6)	−0.0039 (6)
C10	0.0300 (8)	0.0252 (8)	0.0342 (8)	−0.0006 (6)	−0.0005 (6)	−0.0012 (6)
C11	0.0267 (7)	0.0284 (8)	0.0261 (7)	0.0011 (6)	−0.0012 (6)	0.0012 (6)
C12	0.0292 (7)	0.0254 (7)	0.0271 (7)	0.0022 (6)	0.0008 (6)	−0.0010 (6)
C13	0.0248 (7)	0.0254 (7)	0.0278 (7)	0.0011 (6)	−0.0009 (6)	0.0021 (6)
C14	0.0383 (9)	0.0282 (8)	0.0330 (8)	−0.0032 (6)	0.0037 (6)	−0.0025 (6)

Geometric parameters (Å, º)

O1—N1	1.217 (2)	C9—C10	1.386 (2)
O2—N1	1.225 (2)	C10—C11	1.395 (2)
O3—C13	1.3645 (18)	C11—C12	1.401 (2)
O3—C14	1.4306 (18)	C11—C11^{i}	1.482 (2)
N1—C1	1.470 (2)	C12—C13	1.384 (2)
N2—C7	1.266 (2)	C2—H2	0.9500
N2—C8	1.4097 (19)	C3—H3	0.9500
C1—C2	1.382 (2)	C5—H5	0.9500
C1—C6	1.378 (2)	C6—H6	0.9500
C2—C3	1.382 (2)	C7—H7	0.9500
C3—C4	1.397 (2)	C9—H9	0.9500
C4—C5	1.386 (2)	C10—H10	0.9500
C4—C7	1.474 (2)	C12—H12	0.9500
C5—C6	1.384 (2)	C14—H14A	0.9800
C8—C9	1.391 (2)	C14—H14B	0.9800
C8—C13	1.414 (2)	C14—H14C	0.9800
C13—O3—C14	117.60 (11)	O3—C13—C8	116.49 (13)
O1—N1—O2	123.28 (16)	O3—C13—C12	123.39 (13)
O1—N1—C1	118.41 (14)	C8—C13—C12	120.08 (13)
O2—N1—C1	118.32 (15)	C1—C2—H2	121.00
C7—N2—C8	122.82 (14)	C3—C2—H2	121.00
N1—C1—C2	118.71 (13)	C2—C3—H3	120.00
N1—C1—C6	118.68 (14)	C4—C3—H3	120.00
C2—C1—C6	122.62 (14)	C4—C5—H5	119.00
C1—C2—C3	118.88 (14)	C6—C5—H5	119.00
C2—C3—C4	120.01 (15)	C1—C6—H6	121.00
C3—C4—C5	119.36 (14)	C5—C6—H6	121.00
C3—C4—C7	121.89 (14)	N2—C7—H7	120.00
C5—C4—C7	118.73 (14)	C4—C7—H7	120.00
C4—C5—C6	121.38 (15)	C8—C9—H9	119.00
C1—C6—C5	117.76 (15)	C10—C9—H9	119.00

N2—C7—C4	120.86 (15)	C9—C10—H10	120.00
N2—C8—C9	116.41 (13)	C11—C10—H10	120.00
N2—C8—C13	125.67 (13)	C11—C12—H12	119.00
C9—C8—C13	117.77 (13)	C13—C12—H12	119.00
C8—C9—C10	122.15 (14)	O3—C14—H14A	109.00
C9—C10—C11	119.96 (14)	O3—C14—H14B	109.00
C10—C11—C12	118.48 (13)	O3—C14—H14C	109.00
C10—C11—C11^{i}	121.88 (14)	H14A—C14—H14B	109.00
C11^{i}—C11—C12	119.63 (13)	H14A—C14—H14C	109.00
C11—C12—C13	121.46 (13)	H14B—C14—H14C	109.00
C14—O3—C13—C8	174.58 (12)	C5—C4—C7—N2	176.96 (15)
C14—O3—C13—C12	−7.9 (2)	C4—C5—C6—C1	0.2 (2)
O1—N1—C1—C2	178.07 (16)	N2—C8—C9—C10	174.91 (14)
O1—N1—C1—C6	−1.6 (2)	C13—C8—C9—C10	−0.9 (2)
O2—N1—C1—C2	−2.2 (2)	N2—C8—C13—O3	5.0 (2)
O2—N1—C1—C6	178.16 (15)	N2—C8—C13—C12	−172.64 (14)
C8—N2—C7—C4	−179.82 (14)	C9—C8—C13—O3	−179.61 (13)
C7—N2—C8—C9	148.63 (15)	C9—C8—C13—C12	2.7 (2)
C7—N2—C8—C13	−36.0 (2)	C8—C9—C10—C11	−2.1 (2)
N1—C1—C2—C3	179.75 (14)	C9—C10—C11—C12	3.2 (2)
C6—C1—C2—C3	−0.6 (2)	C9—C10—C11—C11^{i}	−175.41 (14)
N1—C1—C6—C5	179.64 (14)	C10—C11—C12—C13	−1.4 (2)
C2—C1—C6—C5	0.0 (2)	C11^{i}—C11—C12—C13	177.27 (14)
C1—C2—C3—C4	1.0 (2)	C10—C11—C11^{i}—C10^{i}	−36.0 (2)
C2—C3—C4—C5	−0.8 (2)	C10—C11—C11^{i}—C12^{i}	145.35 (15)
C2—C3—C4—C7	177.62 (15)	C12—C11—C11^{i}—C10^{i}	145.35 (15)
C3—C4—C5—C6	0.2 (2)	C12—C11—C11^{i}—C12^{i}	−33.3 (2)
C7—C4—C5—C6	−178.29 (15)	C11—C12—C13—O3	−179.10 (13)
C3—C4—C7—N2	−1.5 (2)	C11—C12—C13—C8	−1.6 (2)

Symmetry code: (i) −*x*+3/2, *y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O3^{ii}	0.95	2.59	3.3833 (19)	141
C7—H7···O3	0.95	2.25	2.7783 (19)	114

Symmetry code: (ii) −*x*+1, *y*+1/2, −*z*+3/2.