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N,*N*′-Bis[(*E*)-2-Benzylidenepropylidene]-ethane-1,2-diamine

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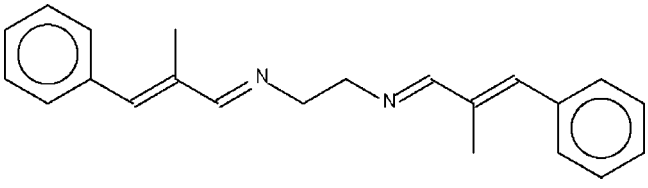
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.069; wR factor = 0.228; data-to-parameter ratio = 13.8.

The two independent molecules in the asymmetric unit of the title Schiff base, $C_{22}H_{24}N_2$, lie across centers of inversion. The C=N double bonds are in a *trans* configuration.

Related literature

There are many examples of similar Schiff bases in the current (2008) Cambrige Structural Database; for example, see: Khalaji *et al.* (2007). For the structure of bis[(*E*)-3-phenylpropen-1-al]-1,2-diiminoethane, see: Khalaji & Weil (2007).



Experimental

Crystal data

$C_{22}H_{24}N_2$
M_r = 316.43
Triclinic, $P\overline{1}$
a = 9.524 (2) Å
b = 9.576 (2) Å
c = 10.202 (2) Å
α = 88.160 (3)°
β = 76.865 (2)°
γ = 78.651 (3)°
V = 888.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 100 (2) K
0.24 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
4114 measured reflections
3015 independent reflections
2186 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.228
S = 1.13
3015 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2448).

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supplementary materials

Acta Cryst. (2008). E**64**, o1771 [**doi:10.1107/S1600536808025919**]

N,*N*'-Bis[(*E*)-2-Benzylidenepropylidene]ethane-1,2-diamine

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Comment

(type here to add)

Experimental

Ethylenediamine (1 mmol, 60 mg) and α-methylcinnamaldehyde (2 mmol, 292 mg) were dissolved in methanol (10 ml) to give a colorless solution. Slow evaporation of the solvent yielded colorless crystals in about 85% yield.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with *U*(H) fixed at 1.2 to 1.5*U*(C).

Figures

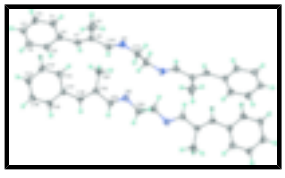


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of the two independent molecules of the title compound; probability ellipsoids are set at the 70% level, and H atoms are drawn as spheres of arbitrary radius. The two molecules lie about centers of inversion.

N,N'-Bis[(*E*)-2-Benzylidenepropylidene]ethane-1,2-diamine

Crystal data

$C_{22}H_{24}N_2$	$Z = 2$
$M_r = 316.43$	$F_{000} = 340$
Triclinic, $P\overline{1}$	$D_x = 1.183$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.524$ (2) Å	Cell parameters from 1031 reflections
$b = 9.576$ (2) Å	$\theta = 3.2$–28.0º
$c = 10.202$ (2) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 88.160$ (3)º	$T = 100$ (2) K
$\beta = 76.865$ (2)º	Block, colorless
$\gamma = 78.651$ (3)º	0.24 × 0.12 × 0.08 mm
$V = 888.3$ (3) Å^3	

Data collection

Bruker SMART APEX diffractometer	2186 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.023$
Monochromator: graphite	$\theta_{max} = 25.0°$
$T = 100(2)$ K	$\theta_{min} = 2.1°$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: None	$k = -11 \rightarrow 7$
4114 measured reflections	$l = -12 \rightarrow 12$
3015 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.069$	H-atom parameters constrained
$wR(F^2) = 0.228$	$w = 1/[\sigma^2(F_o^2) + (0.0966P)^2 + 1.385P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} = 0.001$
3015 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
219 parameters	$\Delta\rho_{min} = -0.30$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.3982 (3)	1.1256 (3)	0.1398 (3)	0.0221 (7)
N2	0.3642 (3)	0.5970 (3)	0.1443 (3)	0.0220 (7)
C1	0.1158 (4)	1.3426 (4)	0.6498 (4)	0.0242 (8)
H1	0.0674	1.3700	0.5785	0.029*
C2	0.0423 (4)	1.3777 (4)	0.7810 (4)	0.0268 (9)
H2	−0.0567	1.4279	0.7993	0.032*
C3	0.1114 (4)	1.3405 (4)	0.8862 (4)	0.0238 (8)
H3	0.0597	1.3646	0.9762	0.029*
C4	0.2550 (4)	1.2685 (4)	0.8602 (4)	0.0238 (8)
H4	0.3026	1.2428	0.9322	0.029*
C5	0.3297 (4)	1.2335 (4)	0.7291 (3)	0.0218 (8)
H5	0.4296	1.1860	0.7118	0.026*
C6	0.2613 (4)	1.2668 (4)	0.6210 (3)	0.0209 (8)
C7	0.3478 (4)	1.2169 (4)	0.4872 (3)	0.0211 (8)
H7	0.4501	1.1871	0.4819	0.025*
C8	0.3067 (4)	1.2062 (4)	0.3699 (3)	0.0198 (8)
C9	0.1543 (4)	1.2473 (5)	0.3469 (4)	0.0358 (10)
H9A	0.0849	1.2137	0.4217	0.054*

H9B	0.1502	1.2039	0.2625	0.054*
H9C	0.1279	1.3512	0.3415	0.054*
C10	0.4227 (4)	1.1443 (4)	0.2552 (3)	0.0209 (8)
H10	0.5204	1.1169	0.2671	0.025*
C11	0.5216 (4)	1.0601 (4)	0.0345 (3)	0.0224 (8)
H11A	0.6070	1.0211	0.0738	0.027*
H11B	0.5500	1.1325	−0.0326	0.027*
C12	0.1872 (4)	0.8841 (4)	0.6385 (4)	0.0234 (8)
H12	0.1826	0.9391	0.5599	0.028*
C13	0.1387 (4)	0.9502 (4)	0.7643 (4)	0.0235 (8)
H13	0.1002	1.0497	0.7709	0.028*
C14	0.1461 (4)	0.8727 (4)	0.8798 (4)	0.0252 (8)
H14	0.1117	0.9184	0.9656	0.030*
C15	0.2040 (4)	0.7277 (4)	0.8698 (4)	0.0238 (8)
H15	0.2112	0.6740	0.9488	0.029*
C16	0.2510 (4)	0.6617 (4)	0.7450 (4)	0.0224 (8)
H16	0.2901	0.5622	0.7394	0.027*
C17	0.2427 (3)	0.7372 (4)	0.6261 (3)	0.0188 (8)
C18	0.2977 (4)	0.6565 (4)	0.4993 (4)	0.0210 (8)
H18	0.3495	0.5626	0.5085	0.025*
C19	0.2885 (4)	0.6906 (4)	0.3718 (3)	0.0201 (8)
C20	0.2131 (4)	0.8296 (4)	0.3247 (4)	0.0260 (9)
H20A	0.1151	0.8581	0.3833	0.039*
H20B	0.2041	0.8184	0.2320	0.039*
H20C	0.2711	0.9028	0.3282	0.039*
C21	0.3610 (4)	0.5804 (4)	0.2695 (3)	0.0207 (8)
H21	0.4084	0.4915	0.2977	0.025*
C22	0.4398 (4)	0.4776 (4)	0.0556 (3)	0.0245 (8)
H22A	0.3687	0.4421	0.0145	0.029*
H22B	0.4845	0.3993	0.1079	0.029*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0217 (15)	0.0204 (16)	0.0237 (17)	−0.0038 (12)	−0.0043 (13)	−0.0017 (12)
N2	0.0225 (15)	0.0213 (16)	0.0224 (17)	−0.0058 (12)	−0.0041 (12)	0.0005 (12)
C1	0.0238 (18)	0.026 (2)	0.0222 (19)	−0.0025 (15)	−0.0076 (15)	0.0024 (15)
C2	0.0238 (19)	0.027 (2)	0.028 (2)	−0.0021 (16)	−0.0043 (16)	−0.0027 (16)
C3	0.0293 (19)	0.0191 (19)	0.0221 (19)	−0.0049 (15)	−0.0035 (15)	−0.0022 (15)
C4	0.030 (2)	0.0163 (18)	0.027 (2)	−0.0048 (15)	−0.0112 (16)	0.0010 (15)
C5	0.0228 (18)	0.0181 (18)	0.026 (2)	−0.0040 (15)	−0.0085 (15)	0.0012 (15)
C6	0.0238 (18)	0.0178 (18)	0.0226 (19)	−0.0077 (14)	−0.0054 (15)	0.0012 (14)
C7	0.0198 (17)	0.0186 (18)	0.0239 (19)	−0.0034 (14)	−0.0031 (15)	−0.0003 (15)
C8	0.0233 (18)	0.0190 (18)	0.0191 (18)	−0.0075 (15)	−0.0062 (15)	0.0033 (14)
C9	0.028 (2)	0.053 (3)	0.025 (2)	0.0003 (19)	−0.0093 (17)	−0.0110 (19)
C10	0.0200 (17)	0.0176 (18)	0.026 (2)	−0.0054 (14)	−0.0064 (15)	0.0046 (14)
C11	0.0220 (18)	0.026 (2)	0.0196 (18)	−0.0063 (15)	−0.0036 (15)	0.0001 (15)
C12	0.0253 (19)	0.023 (2)	0.026 (2)	−0.0094 (15)	−0.0108 (16)	0.0056 (15)

C13	0.0176 (17)	0.0210 (19)	0.031 (2)	−0.0011 (14)	−0.0054 (15)	−0.0033 (15)
C14	0.0189 (18)	0.030 (2)	0.0243 (19)	−0.0042 (15)	0.0006 (15)	−0.0064 (16)
C15	0.0227 (18)	0.030 (2)	0.0179 (18)	−0.0043 (16)	−0.0046 (15)	0.0036 (15)
C16	0.0208 (17)	0.0196 (19)	0.027 (2)	−0.0033 (15)	−0.0076 (15)	0.0042 (15)
C17	0.0143 (16)	0.0236 (19)	0.0185 (18)	−0.0059 (14)	−0.0021 (13)	0.0023 (14)
C18	0.0196 (17)	0.0153 (18)	0.028 (2)	−0.0020 (14)	−0.0057 (15)	0.0013 (14)
C19	0.0190 (17)	0.0210 (19)	0.0215 (19)	−0.0072 (14)	−0.0043 (14)	0.0018 (14)
C20	0.028 (2)	0.0214 (19)	0.025 (2)	0.0013 (16)	−0.0037 (16)	0.0007 (16)
C21	0.0236 (18)	0.0176 (18)	0.0222 (19)	−0.0061 (15)	−0.0059 (14)	0.0014 (14)
C22	0.031 (2)	0.0207 (19)	0.0220 (19)	−0.0058 (16)	−0.0067 (16)	−0.0025 (15)

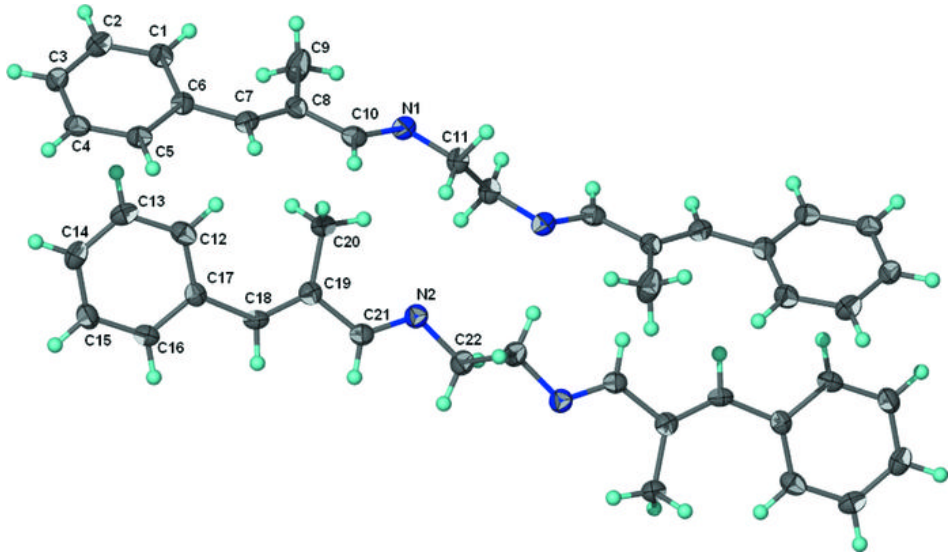
Geometric parameters (Å, °)

N1—C10	1.276 (5)	C11—H11A	0.9900
N1—C11	1.452 (5)	C11—H11B	0.9900
N2—C21	1.276 (5)	C12—C13	1.389 (5)
N2—C22	1.446 (5)	C12—C17	1.401 (5)
C1—C2	1.380 (5)	C12—H12	0.9500
C1—C6	1.403 (5)	C13—C14	1.380 (5)
C1—H1	0.9500	C13—H13	0.9500
C2—C3	1.384 (5)	C14—C15	1.388 (5)
C2—H2	0.9500	C14—H14	0.9500
C3—C4	1.375 (5)	C15—C16	1.380 (5)
C3—H3	0.9500	C15—H15	0.9500
C4—C5	1.382 (5)	C16—C17	1.401 (5)
C4—H4	0.9500	C16—H16	0.9500
C5—C6	1.401 (5)	C17—C18	1.464 (5)
C5—H5	0.9500	C18—C19	1.349 (5)
C6—C7	1.465 (5)	C18—H18	0.9500
C7—C8	1.354 (5)	C19—C21	1.462 (5)
C7—H7	0.9500	C19—C20	1.502 (5)
C8—C10	1.463 (5)	C20—H20A	0.9800
C8—C9	1.497 (5)	C20—H20B	0.9800
C9—H9A	0.9800	C20—H20C	0.9800
C9—H9B	0.9800	C21—H21	0.9500
C9—H9C	0.9800	C22—C22^{ii}	1.534 (7)
C10—H10	0.9500	C22—H22A	0.9900
C11—C11^{i}	1.536 (7)	C22—H22B	0.9900
C10—N1—C11	117.7 (3)	H11A—C11—H11B	108.2
C21—N2—C22	117.0 (3)	C13—C12—C17	120.8 (3)
C2—C1—C6	120.5 (3)	C13—C12—H12	119.6
C2—C1—H1	119.8	C17—C12—H12	119.6
C6—C1—H1	119.8	C14—C13—C12	120.6 (3)
C1—C2—C3	120.7 (3)	C14—C13—H13	119.7
C1—C2—H2	119.7	C12—C13—H13	119.7
C3—C2—H2	119.7	C13—C14—C15	119.6 (3)
C4—C3—C2	119.9 (3)	C13—C14—H14	120.2
C4—C3—H3	120.0	C15—C14—H14	120.2

C2—C3—H3	120.0	C16—C15—C14	119.8 (3)
C3—C4—C5	119.8 (3)	C16—C15—H15	120.1
C3—C4—H4	120.1	C14—C15—H15	120.1
C5—C4—H4	120.1	C15—C16—C17	121.8 (3)
C4—C5—C6	121.4 (3)	C15—C16—H16	119.1
C4—C5—H5	119.3	C17—C16—H16	119.1
C6—C5—H5	119.3	C12—C17—C16	117.3 (3)
C5—C6—C1	117.6 (3)	C12—C17—C18	125.6 (3)
C5—C6—C7	116.9 (3)	C16—C17—C18	117.1 (3)
C1—C6—C7	125.5 (3)	C19—C18—C17	132.0 (3)
C8—C7—C6	131.0 (3)	C19—C18—H18	114.0
C8—C7—H7	114.5	C17—C18—H18	114.0
C6—C7—H7	114.5	C18—C19—C21	116.0 (3)
C7—C8—C10	116.5 (3)	C18—C19—C20	126.8 (3)
C7—C8—C9	126.6 (3)	C21—C19—C20	117.2 (3)
C10—C8—C9	116.9 (3)	C19—C20—H20A	109.5
C8—C9—H9A	109.5	C19—C20—H20B	109.5
C8—C9—H9B	109.5	H20A—C20—H20B	109.5
H9A—C9—H9B	109.5	C19—C20—H20C	109.5
C8—C9—H9C	109.5	H20A—C20—H20C	109.5
H9A—C9—H9C	109.5	H20B—C20—H20C	109.5
H9B—C9—H9C	109.5	N2—C21—C19	123.5 (3)
N1—C10—C8	122.7 (3)	N2—C21—H21	118.2
N1—C10—H10	118.6	C19—C21—H21	118.2
C8—C10—H10	118.6	N2—C22—C22^{ii}	110.4 (4)
N1—C11—C11^{i}	109.5 (3)	N2—C22—H22A	109.6
N1—C11—H11A	109.8	C22^{ii}—C22—H22A	109.6
C11^{i}—C11—H11A	109.8	N2—C22—H22B	109.6
N1—C11—H11B	109.8	C22^{ii}—C22—H22B	109.6
C11^{i}—C11—H11B	109.8	H22A—C22—H22B	108.1
C6—C1—C2—C3	0.9 (6)	C17—C12—C13—C14	0.8 (5)
C1—C2—C3—C4	0.4 (6)	C12—C13—C14—C15	0.7 (5)
C2—C3—C4—C5	0.0 (5)	C13—C14—C15—C16	−1.2 (5)
C3—C4—C5—C6	−1.6 (5)	C14—C15—C16—C17	0.2 (5)
C4—C5—C6—C1	2.8 (5)	C13—C12—C17—C16	−1.8 (5)
C4—C5—C6—C7	−176.2 (3)	C13—C12—C17—C18	−179.5 (3)
C2—C1—C6—C5	−2.4 (5)	C15—C16—C17—C12	1.3 (5)
C2—C1—C6—C7	176.5 (3)	C15—C16—C17—C18	179.2 (3)
C5—C6—C7—C8	165.1 (4)	C12—C17—C18—C19	−12.3 (6)
C1—C6—C7—C8	−13.8 (6)	C16—C17—C18—C19	169.9 (4)
C6—C7—C8—C10	−177.0 (3)	C17—C18—C19—C21	178.9 (3)
C6—C7—C8—C9	1.1 (6)	C17—C18—C19—C20	−0.6 (6)
C11—N1—C10—C8	−178.6 (3)	C22—N2—C21—C19	−179.8 (3)
C7—C8—C10—N1	178.6 (3)	C18—C19—C21—N2	−178.9 (3)
C9—C8—C10—N1	0.2 (5)	C20—C19—C21—N2	0.6 (5)
C10—N1—C11—C11^{i}	131.7 (4)	C21—N2—C22—C22^{ii}	−124.0 (4)

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*; (ii) −*x*+1, −*y*+1, −*z*.

Fig. 1


C2
C1
C3
C6
C9
C7
C8
C10
N1
C11
C4
C5
C13
C14
C12
C20
C17
C18
C19
N2
C21
C22
C15
C16