

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

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

 Aliakbar Dehno Khalaji<sup>a</sup> and Seik Weng Ng<sup>b\*</sup>
<sup>a</sup>Department of Science, Gorgan University of Agricultural Sciences and Natural Resources, Gorgan 49189-43464, Iran, and <sup>b</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

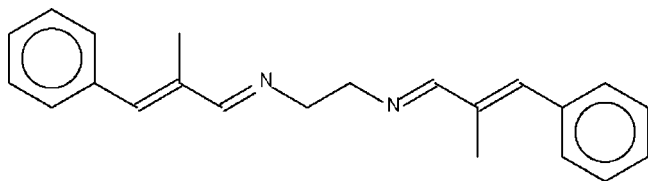
Received 11 August 2008; accepted 11 August 2008

 Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  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,  $\text{C}_{22}\text{H}_{24}\text{N}_2$ , lie across centers of inversion. The  $\text{C}=\text{N}$  double bonds are in a *trans* configuration.

## Related literature

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



## Experimental

## Crystal data

$\text{C}_{22}\text{H}_{24}\text{N}_2$	$\gamma = 78.651$ (3)°
$M_r = 316.43$	$V = 888.3$ (3) Å <sup>3</sup>
Triclinic, $P\bar{1}$	$Z = 2$
$a = 9.524$ (2) Å	Mo $K\alpha$ radiation
$b = 9.576$ (2) Å	$\mu = 0.07$ mm <sup>-1</sup>
$c = 10.202$ (2) Å	$T = 100$ (2) K
$\alpha = 88.160$ (3)°	$0.24 \times 0.12 \times 0.08$ mm
$\beta = 76.865$ (2)°	

## Data collection

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

## Refinement

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

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).

We thank Gorgan University of Agricultural Sciences and Natural Resources and the University of Malaya for supporting this study.

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

## References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.  
 Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Khalaji, A. D., Brad, K. & Zhang, Y. (2007). *Acta Cryst.* **E63**, o4389.  
 Khalaji, A. D. & Weil, M. (2007). *Anal. Sci.* **23**, x187–x188.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Westrip, S. P. (2008). *publCIF*. In preparation.

**supplementary materials**

*Acta Cryst.* (2008). E64, o1771 [ doi:10.1107/S1600536808025919 ]

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

**A. D. Khalaji and S. W. Ng**

**Comment**

(type here to add)

**Experimental**

Ethylenediamine (1 mmol, 60 mg) and  $\alpha$ -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  $U(\text{H})$  fixed at 1.2 to 1.5 $U(\text{C})$ .

**Figures**

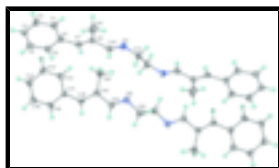


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of the two independent molecules of the title compound; probability ellipsoids are set at the 70% level, and H atoms are drawn as spheres of arbitrary radius. The two molecules lie about centers of inversion.

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

*Crystal data*

$\text{C}_{22}\text{H}_{24}\text{N}_2$	$Z = 2$
$M_r = 316.43$	$F_{000} = 340$
Triclinic, $P\bar{1}$	$D_x = 1.183 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 9.524 (2) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 9.576 (2) \text{ \AA}$	Cell parameters from 1031 reflections
$c = 10.202 (2) \text{ \AA}$	$\theta = 3.2\text{--}28.0^\circ$
$\alpha = 88.160 (3)^\circ$	$\mu = 0.07 \text{ mm}^{-1}$
$\beta = 76.865 (2)^\circ$	$T = 100 (2) \text{ K}$
$\gamma = 78.651 (3)^\circ$	Block, colorless
$V = 888.3 (3) \text{ \AA}^3$	$0.24 \times 0.12 \times 0.08 \text{ mm}$

# supplementary materials

---

## Data collection

Bruker SMART APEX diffractometer	2186 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.023$
Monochromator: graphite	$\theta_{\text{max}} = 25.0^\circ$
$T = 100(2)$ K	$\theta_{\text{min}} = 2.1^\circ$
$\omega$ 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
$wR(F^2) = 0.228$	$w = 1/[\sigma^2(F_o^2) + (0.0966P)^2 + 1.385P]$
$S = 1.13$	where $P = (F_o^2 + 2F_c^2)/3$
3015 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
219 parameters	$\Delta\rho_{\text{max}} = 0.34 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.30 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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)

## supplementary materials

---

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 <sup>ii</sup>	1.534 (7)
C10—H10	0.9500	C22—H22A	0.9900
C11—C11 <sup>i</sup>	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 <sup>ii</sup>	110.4 (4)
N1—C11—C11 <sup>i</sup>	109.5 (3)	N2—C22—H22A	109.6
N1—C11—H11A	109.8	C22 <sup>ii</sup> —C22—H22A	109.6
C11 <sup>i</sup> —C11—H11A	109.8	N2—C22—H22B	109.6
N1—C11—H11B	109.8	C22 <sup>ii</sup> —C22—H22B	109.6
C11 <sup>i</sup> —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 <sup>i</sup>	131.7 (4)	C21—N2—C22—C22 <sup>ii</sup>	-124.0 (4)

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

Fig. 1

