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# (1*E*,2*E*)-1,2-Bis[(*E*)-3-phenylallylidene]-hydrazine

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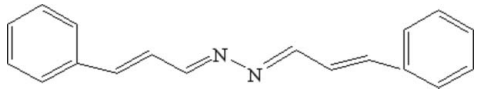
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.041; $wR$ factor = 0.094; data-to-parameter ratio = 15.2.

The title compound [alternatively called (*E*)-3-phenylprop-2-enal azine], $C_{18}H_{16}N_2$, was synthesized by the reaction of hydrocinnamaldehyde with hydrazine hydrate. The nearly planar molecule is centrosymmetric, with the mid-point of the N—N bond lying at an inversion center.

## Related literature

For related literature, see: Jiang & Hu (2004); Kundu *et al.* (2005); Trujillo *et al.* (1997); Zheng & Zhao (2006); Zhao *et al.* (2006).



## Experimental

### *Crystal data*

$C_{18}H_{16}N_2$
$M_r$ = 260.33
Monoclinic, $P2_1/c$
$a$ = 17.11 (2) Å
$b$ = 5.456 (5) Å
$c$ = 7.988 (7) Å
$\beta$ = 98.25 (4)°
$V$ = 738.0 (13) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 293 (2) K
0.55 × 0.21 × 0.12 mm

### *Data collection*

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: none
5393 measured reflections
1381 independent reflections
844 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.094
$S$ = 0.95
1381 reflections
91 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.09 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2335).

## References

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o4443 [ **doi:10.1107/S1600536807051707** ]

# (1*E*,2*E*)-1,2-Bis[(*E*)-3-phenylallylidene]hydrazine

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## Comment

The azine derivatives have been investigated in terms of their coordination chemistry and their special properties (Zheng & Zhao, 2006; Kundu *et al.*, 2005; Jiang & Hu, 2004; Trujillo *et al.*, 1997). The synthesis and crystal structure of the title compound (Fig. 1) is reported here.

In the molecule of title molecule, there is an inversion center at the midpoint of the N1—N1A single bond [symmetry code A, −*x*, −*y*, −*z* + 1], and all of the atoms are approximately coplanar. The single N—N bond length is 1.398 (3)Å (Table 1), which is consistent with those found in related azine compounds (Zheng & Zhao, 2006; Zhao *et al.*, 2006). The bond angle of N(1)—C(9)—C(8) is 120.9 (2)°, showing the atom C9 is of $sp^2$ hybridization.

## Experimental

The title compound was prepared by the reaction of hydrocinncmaladehyde and hydrazine hydrate with a ratio of 2:1 under reflux in the mixture of ethanol and DMF for 2 h. After one week, yellow prismatic crystals were obtained by slow evaporation at room temperature.

## Refinement

All H atoms were placed in calculated positions and treated using a riding model with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C).

## Figures

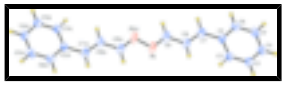


Fig. 1. View of the molecular structure with displacement ellipsoids drawn at the 30% probability level for non-H atoms. [Symmetry code: (A) −*x*, −*y*, −*z* + 1.]

## (1E,2E)-1,2-Bis[(*E*)-3-phenylallylidene]hydrazine

*Crystal data*

| | |
|---|---|
| $C_{18}H_{16}N_2$ | $F_{000}$ = 276 |
| $M_r$ = 260.33 | $D_x$ = 1.172 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 1381 reflections |
| *a* = 17.11 (2) Å | θ = 3.6–26.0º |
| *b* = 5.456 (5) Å | μ = 0.07 mm$^{-1}$ |

| | |
|---|---|
| $c$ = 7.988 (7) Å | $T$ = 293 (2) K |
| β = 98.25 (4)º | Prism, yellow |
| $V$ = 738.0 (13) Å$^3$ | 0.55 × 0.21 × 0.12 mm |
| $Z$ = 2 | |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID IP diffractometer | 844 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.034 |
| Monochromator: graphite | $\theta_{max}$ = 26.0º |
| $T$ = 293(2) K | $\theta_{min}$ = 3.6º |
| ω scans | $h$ = −21→21 |
| Absorption correction: none | $k$ = −6→6 |
| 5393 measured reflections | $l$ = −9→9 |
| 1381 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 |
| $R[F^2 > 2\sigma(F^2)]$ = 0.041 | H-atom parameters constrained |
| $wR(F^2)$ = 0.094 | $w = 1/[\sigma^2(F_o^2) + (0.0491P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 0.95 | $(\Delta/\sigma)_{max} < 0.001$ |
| 1381 reflections | $\Delta\rho_{max}$ = 0.09 e Å$^{-3}$ |
| 91 parameters | $\Delta\rho_{min}$ = −0.14 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on $F^2$, conventional *R*-factors *R* are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.04070 (6) | −0.0045 (3) | 0.49829 (15) | 0.0722 (4) |
| C1 | 0.26140 (7) | 0.4619 (2) | 0.34602 (14) | 0.0481 (3) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.32091 (8) | 0.3004 (2) | 0.41067 (17) | 0.0517 (4) |
| H2A | 0.3085 | 0.1627 | 0.4701 | 0.062* |
| C3 | 0.39765 (8) | 0.3412 (3) | 0.38813 (17) | 0.0568 (4) |
| H3A | 0.4367 | 0.2307 | 0.4321 | 0.068* |
| C4 | 0.41760 (9) | 0.5435 (3) | 0.30128 (17) | 0.0608 (4) |
| H4A | 0.4698 | 0.5701 | 0.2863 | 0.073* |
| C5 | 0.35992 (9) | 0.7059 (3) | 0.23671 (19) | 0.0626 (4) |
| H5A | 0.3731 | 0.8428 | 0.1773 | 0.075* |
| C6 | 0.28275 (8) | 0.6675 (3) | 0.25939 (16) | 0.0562 (4) |
| H6A | 0.2443 | 0.7802 | 0.2164 | 0.067* |
| C7 | 0.17886 (8) | 0.4207 (3) | 0.36486 (16) | 0.0579 (4) |
| H7A | 0.1439 | 0.5477 | 0.3309 | 0.070* |
| C8 | 0.14843 (8) | 0.2210 (3) | 0.42545 (18) | 0.0609 (4) |
| H8A | 0.1825 | 0.0927 | 0.4619 | 0.073* |
| C9 | 0.06635 (8) | 0.1918 (3) | 0.43782 (18) | 0.0657 (4) |
| H9A | 0.0312 | 0.3173 | 0.4014 | 0.079* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0402 (6) | 0.0995 (10) | 0.0762 (8) | −0.0123 (7) | 0.0061 (6) | 0.0094 (8) |
| C1 | 0.0463 (8) | 0.0529 (8) | 0.0449 (7) | −0.0053 (6) | 0.0062 (5) | −0.0037 (7) |
| C2 | 0.0490 (8) | 0.0503 (8) | 0.0561 (8) | −0.0049 (6) | 0.0086 (6) | 0.0018 (7) |
| C3 | 0.0481 (8) | 0.0587 (9) | 0.0638 (9) | 0.0000 (7) | 0.0090 (6) | −0.0045 (7) |
| C4 | 0.0531 (9) | 0.0677 (11) | 0.0644 (9) | −0.0145 (8) | 0.0178 (7) | −0.0093 (8) |
| C5 | 0.0723 (11) | 0.0556 (9) | 0.0622 (9) | −0.0185 (8) | 0.0178 (8) | 0.0014 (7) |
| C6 | 0.0616 (9) | 0.0504 (9) | 0.0561 (8) | −0.0006 (7) | 0.0064 (7) | 0.0009 (7) |
| C7 | 0.0467 (8) | 0.0688 (10) | 0.0573 (8) | 0.0001 (7) | 0.0039 (6) | 0.0010 (8) |
| C8 | 0.0433 (9) | 0.0803 (11) | 0.0588 (9) | −0.0071 (7) | 0.0059 (6) | 0.0042 (8) |
| C9 | 0.0456 (9) | 0.0900 (12) | 0.0606 (9) | −0.0084 (8) | 0.0042 (6) | 0.0028 (9) |

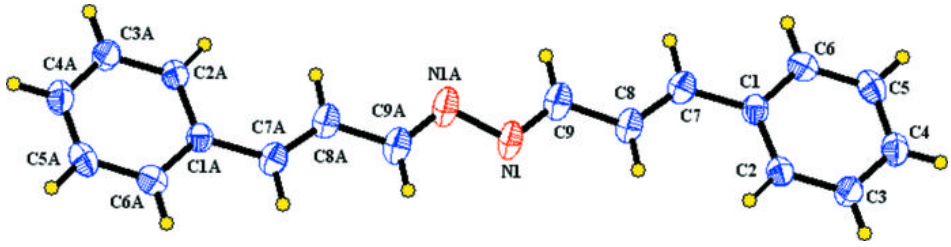
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C9 | 1.278 (2) | C4—H4A | 0.9300 |
| N1—N1$^{i}$ | 1.398 (3) | C5—C6 | 1.374 (2) |
| C1—C2 | 1.389 (2) | C5—H5A | 0.9300 |
| C1—C6 | 1.3944 (19) | C6—H6A | 0.9300 |
| C1—C7 | 1.459 (2) | C7—C8 | 1.329 (2) |
| C2—C3 | 1.369 (2) | C7—H7A | 0.9300 |
| C2—H2A | 0.9300 | C8—C9 | 1.431 (2) |
| C3—C4 | 1.373 (2) | C8—H8A | 0.9300 |
| C3—H3A | 0.9300 | C9—H9A | 0.9300 |
| C4—C5 | 1.371 (2) | | |
| C9—N1—N1$^{i}$ | 112.04 (17) | C4—C5—H5A | 119.8 |
| C2—C1—C6 | 117.70 (14) | C6—C5—H5A | 119.8 |
| C2—C1—C7 | 122.21 (14) | C5—C6—C1 | 120.87 (14) |
| C6—C1—C7 | 120.09 (13) | C5—C6—H6A | 119.6 |
| C3—C2—C1 | 120.92 (14) | C1—C6—H6A | 119.6 |

| | | | |
|---|---|---|---|
| C3—C2—H2A | 119.5 | C8—C7—C1 | 126.82 (14) |
| C1—C2—H2A | 119.5 | C8—C7—H7A | 116.6 |
| C2—C3—C4 | 120.66 (14) | C1—C7—H7A | 116.6 |
| C2—C3—H3A | 119.7 | C7—C8—C9 | 123.78 (15) |
| C4—C3—H3A | 119.7 | C7—C8—H8A | 118.1 |
| C5—C4—C3 | 119.49 (15) | C9—C8—H8A | 118.1 |
| C5—C4—H4A | 120.3 | N1—C9—C8 | 120.86 (16) |
| C3—C4—H4A | 120.3 | N1—C9—H9A | 119.6 |
| C4—C5—C6 | 120.34 (15) | C8—C9—H9A | 119.6 |
| C6—C1—C2—C3 | −0.73 (18) | C7—C1—C6—C5 | −178.33 (12) |
| C7—C1—C2—C3 | 178.68 (12) | C2—C1—C7—C8 | −8.1 (2) |
| C1—C2—C3—C4 | 0.2 (2) | C6—C1—C7—C8 | 171.33 (13) |
| C2—C3—C4—C5 | 0.0 (2) | C1—C7—C8—C9 | −178.97 (12) |
| C3—C4—C5—C6 | 0.3 (2) | $N1^{i}$—N1—C9—C8 | 179.17 (13) |
| C4—C5—C6—C1 | −0.9 (2) | C7—C8—C9—N1 | −179.57 (14) |
| C2—C1—C6—C5 | 1.08 (19) | | |

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

**Fig. 1**


C3A
C4A
C2A
C5A
C1A
C6A
C7A
C8A
C9A
N1A
N1
C9
C8
C7
C1
C6
C5
C4
C2
C3