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

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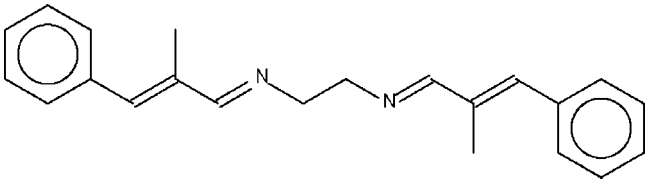
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.069; $wR$ factor = 0.228; data-to-parameter ratio = 13.8.

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
$\alpha$ = 88.160 (3)°
$\beta$ = 76.865 (2)°
$\gamma$ = 78.651 (3)°
$V$ = 888.3 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 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).

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

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# supporting information

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

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

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### S1. 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.

### S2. 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).

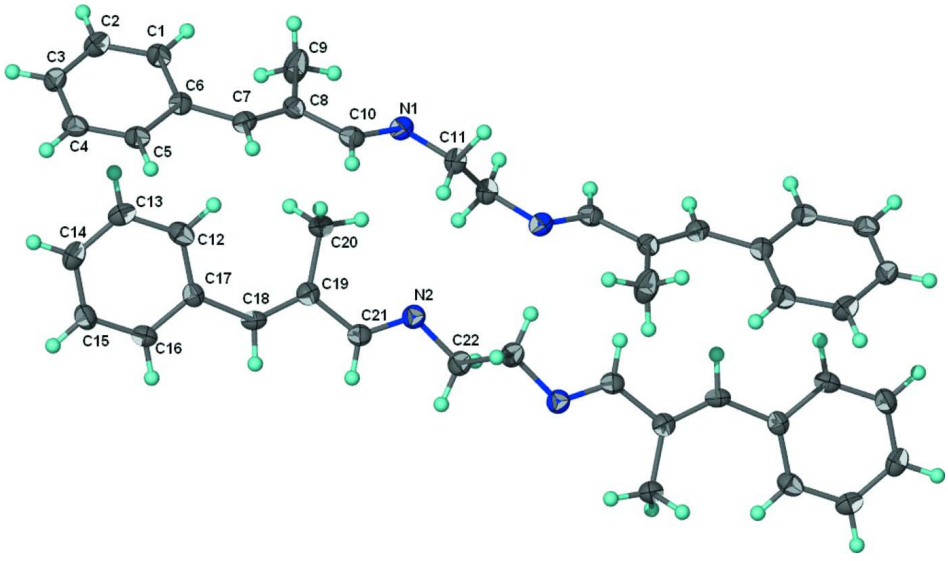


**Figure 1**

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*

$C_{22}H_{24}N_2$
$M_r = 316.43$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.524$ (2) Å
$b = 9.576$ (2) Å
$c = 10.202$ (2) Å
$\alpha = 88.160$ (3)°
$\beta = 76.865$ (2)°
$\gamma = 78.651$ (3)°
$V = 888.3$ (3) Å$^3$
$Z = 2$
$F(000) = 340$
$D_x = 1.183$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1031 reflections
$\theta$ = 3.2–28.0°
$\mu$ = 0.07 mm$^{-1}$
$T$ = 100 K
Block, colorless
0.24 × 0.12 × 0.08 mm

*Data collection*

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
4114 measured reflections
3015 independent reflections
2186 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.1°
$h$ = −11→11
$k$ = −11→7
$l$ = −12→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.228
$S$ = 1.13
3015 reflections
219 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
$w = 1/[\sigma^2(F_o^2) + (0.0966P)^2 + 1.385P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

*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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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*.