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(+)-(*S*)-*N*-[(1-Benzothiophen-2-yl)methylidene]-1-(naphthalen-1-yl)ethylamine

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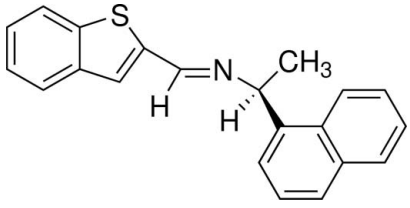
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.040; wR factor = 0.092; data-to-parameter ratio = 13.7.

In the title compound, $C_{21}H_{17}NS$, the C=N double bond shows an *E* conformation. The dihedral angle between the mean planes of the naphthyl residue and the benzothiophene residue is 89.14 (6)°. The crystal packing is stabilized by intermolecular C—H$\cdots\pi$ interactions, building a ribbon structure along the *a* axis.

Related literature

For Schiff bases, see: García *et al.* (2011); Bernès *et al.* (2010); Jeon *et al.* (2005); Noyori (2005); Tanaka & Toda (2000).



Experimental

Crystal data

$C_{21}H_{17}NS$
M_r = 315.42
Orthorhombic, $P2_12_12_1$
a = 5.6423 (3) Å
b = 8.0808 (4) Å
c = 36.3864 (19) Å
V = 1659.01 (15) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.70 mm^{-1}
T = 298 K
0.93 × 0.17 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur (Atlas, Gemini) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2006)
T_{min} = 0.665, T_{max} = 1
8690 measured reflections
2844 independent reflections
2417 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.092
S = 1.01
2844 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: Flack parameter determined using 839 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons & Flack (2004)
Absolute structure parameter: 0.021 (17)

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

*Cg*1 and *Cg*2 are the centroids of the S1/C2/C3/C4/C9, C12/C13/C18/C19/C20/C21 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C8—H8$\cdots Cg1^{i}$	0.93	2.73	3.491 (4)	139
C11—H11$B\cdots Cg2^{ii}$	0.96	2.59	3.724 (5)	149

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2006); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *SHELXL2013*; software used to prepare material for publication: *SHELXL2013*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6929).

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supporting information

Acta Cryst. (2013). E**69**, o1480 [doi:10.1107/S1600536813023611]

(+)-(*S*)-*N*-[(1-Benzothiophen-2-yl)methylidene]-1-(naphthalen-1-yl)ethylamine

Guadalupe Hernández-Téllez, Oscar Portillo-Moreno, René Gutiérrez, Francisco J. Rios-Merino and Angel Mendoza

S1. Comment

Schiff base compounds are widely studied and used, attracting much attention in both organic synthesis and metal ion complexation. Recently, we have focused our attention on the synthesis of chiral Schiff bases by using green techniques (García *et al.*, 2011; Bernès *et al.*, 2010). In continuation of this work, we synthesized the title compound using the solvent-free approach because the reactions occur under mild conditions and usually require easier workup procedures and simpler equipment. Other advantages of solvent-free reactions encompass cost saving, decreased reaction times along with reduced energy consumption, as well as increased safety (Jeon *et al.*, 2005; Noyori, 2005; Tanaka & Toda, 2000)

The C=N double bond shows an *E* configuration. The dihedral angle between the mean planes of the naphthyl residue and the benzothiophene residue is 90.86 (6)°. The crystal packing is stabilized by intermolecular C—H···π interactions (Table 2; cg1 is the centroid of the ring composed of S1, C2, C3 C4, and C9, cg2 is the centroid of the ring composed of C12, C13, C18, C19, C20, and C21).

S2. Experimental

Under solvent-free conditions, (*S*)-(-)-(1-naphthyl)ethylamine (0.21 g, 1.2 mmol) and benzo[*b*]thiophene-2-carboxaldehyde (0.20 g, 1.2 mmol) were mixed at room temperature obtaining a white solid. The crude was recrystallized from CH_2Cl_2 affording colorless crystals of the title compound. Yield 94%; mp 125–127 °C. Analysis: $[\alpha]_D^{25}$ = +318 (cL, $CHCl_3$). FT—IR (KBr): 1621 cm-1 (C=N). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ = 1.76, 1.78 (d, 3H, CHCH3,), 5.40, 5.42, 5.44, 5.45(q, ^{1}H, CH), 7.32–7.89 (m, 12 H Ar), 8.20, 8.23 (d, 1H *cyclo* S), 8.54 (s, 1 H, HC=N). ^{13}C NMR (100 MHz, $CDCl_3$/TMS) δ = 24.20 (CCH_3), 64.87 ($CHCH_3$), 122.66 (Ar), 123.58 (Ar), 124.14 (Ar), 124.43(Ar), 125.36 (Ar), 125.66 (Ar), 125.90 (Ar), 127.47 (Ar), 127.62 (Ar), 128.91 (Ar), 130.58(Ar), 133.93 (Ar), 139.31 (Ar),140.57 (Ar), 143.16 (Ar), 153.61 (HC=N). MS—EI: *m/z*= 315 (*M*+).

S3. Refinement

H atoms linked to C atoms were placed in geometrical idealized positions and refined as riding on their parent atoms, with C—H = 0.93–0.96 Å and with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(methyl C).

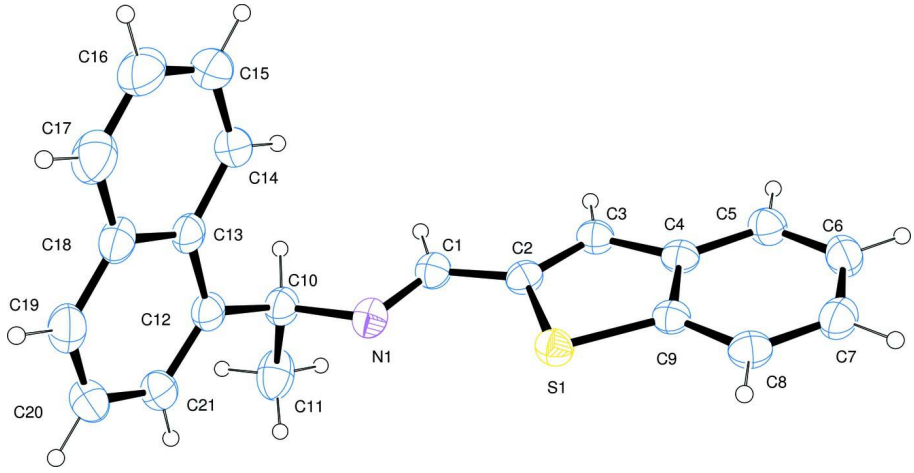

Figure 1

The molecular structure of title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

(+)-(*S*)-*N*-[(1-Benzothiophen-2-yl)methylidene]-1-(naphthalen-1-yl)ethylamine

Crystal data

$C_{21}H_{17}NS$
$M_r = 315.42$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.6423$ (3) Å
$b = 8.0808$ (4) Å
$c = 36.3864$ (19) Å
$V = 1659.01$ (15) Å^3
$Z = 4$
$F(000) = 664$
$D_x = 1.263$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2302 reflections
$\theta = 4.8$–$73.7°$
$\mu = 1.70$ mm^{-1}
$T = 298$ K
Plate, translucent colourless
0.93 × 0.17 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur (Atlas, Gemini) diffractometer
Graphite monochromator
Detector resolution: 10.5564 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2006)
$T_{min} = 0.665$, $T_{max} = 1$
8690 measured reflections
2844 independent reflections
2417 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 66.1°$, $\theta_{min} = 4.9°$
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -43 \rightarrow 43$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.092$
$S = 1.01$
2844 reflections
208 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Absolute structure: Flack parameter determined using 839 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons & Flack (2004)
Absolute structure parameter: 0.021 (17)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.66160 (15)	0.33795 (10)	0.20762 (2)	0.0504 (2)
C13	0.8326 (7)	0.6220 (4)	0.07300 (9)	0.0526 (8)
C5	0.8422 (8)	0.4832 (4)	0.30726 (10)	0.0559 (8)
H5	0.9665	0.5439	0.3173	0.067*
C9	0.6413 (6)	0.3627 (4)	0.25514 (9)	0.0453 (7)
C3	0.9946 (6)	0.4998 (4)	0.24067 (10)	0.0492 (8)
H3	1.1323	0.5599	0.2451	0.059*
C4	0.8335 (6)	0.4527 (4)	0.26915 (10)	0.0467 (7)
C2	0.9289 (5)	0.4490 (4)	0.20692 (11)	0.0485 (7)
C1	1.0499 (6)	0.4771 (4)	0.17269 (10)	0.0506 (8)
H1	1.182	0.546	0.1725	0.061*
C6	0.6675 (8)	0.4233 (5)	0.32929 (11)	0.0612 (9)
H6	0.6735	0.4435	0.3544	0.073*
N1	0.9833 (5)	0.4116 (4)	0.14263 (9)	0.0557 (7)
C12	0.9580 (6)	0.4687 (4)	0.07747 (10)	0.0524 (8)
C8	0.4653 (6)	0.3017 (4)	0.27776 (11)	0.0553 (9)
H8	0.3398	0.2412	0.2681	0.066*
C10	1.1270 (7)	0.4460 (5)	0.10929 (10)	0.0563 (9)
H10	1.2155	0.549	0.113	0.068*
C19	0.6218 (8)	0.5002 (6)	0.02083 (11)	0.0696 (11)
H19	0.51	0.5086	0.0021	0.083*
C18	0.6615 (8)	0.6360 (5)	0.04455 (10)	0.0626 (9)
C11	1.3029 (8)	0.3034 (6)	0.10488 (12)	0.0797 (13)
H11A	1.4038	0.2983	0.1261	0.12*
H11B	1.3975	0.3214	0.0833	0.12*
H11C	1.2177	0.2012	0.1025	0.12*
C17	0.5403 (10)	0.7867 (6)	0.04014 (15)	0.0848 (15)
H17	0.4272	0.7966	0.0217	0.102*
C7	0.4790 (7)	0.3319 (5)	0.31476 (11)	0.0611 (10)
H7	0.362	0.2913	0.3303	0.073*
C14	0.8719 (9)	0.7621 (5)	0.09573 (12)	0.0659 (11)
H14	0.9816	0.7552	0.1147	0.079*
C15	0.7523 (10)	0.9062 (6)	0.09026 (14)	0.0851 (15)
H15	0.7825	0.997	0.1052	0.102*
C20	0.7450 (8)	0.3587 (6)	0.02515 (12)	0.0700 (11)
H20	0.7182	0.2704	0.0093	0.084*
C16	0.5852 (10)	0.9180 (6)	0.06237 (15)	0.0950 (18)
H16	0.5034	1.0167	0.0589	0.114*
C21	0.9123 (7)	0.3431 (5)	0.05316 (10)	0.0610 (9)

H21	0.9956	0.2443	0.0554	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0487 (4)	0.0531 (4)	0.0493 (4)	−0.0025 (4)	−0.0075 (4)	−0.0035 (4)
C13	0.0587 (19)	0.0561 (19)	0.0431 (17)	0.0004 (18)	0.0125 (17)	0.0075 (14)
C5	0.059 (2)	0.0567 (19)	0.0522 (19)	−0.002 (2)	−0.0078 (19)	−0.0037 (16)
C9	0.0447 (16)	0.0411 (14)	0.0501 (17)	0.0052 (15)	−0.0051 (16)	0.0011 (13)
C3	0.0460 (19)	0.0482 (17)	0.054 (2)	−0.0028 (15)	−0.0055 (16)	−0.0030 (15)
C4	0.0446 (17)	0.0415 (14)	0.0541 (18)	0.0071 (16)	−0.0046 (18)	−0.0002 (14)
C2	0.0472 (17)	0.0431 (16)	0.0552 (19)	0.0040 (13)	−0.0013 (17)	0.0042 (16)
C1	0.0484 (18)	0.0518 (18)	0.051 (2)	0.0041 (15)	−0.0027 (17)	0.0030 (16)
C6	0.070 (2)	0.065 (2)	0.0485 (19)	0.005 (2)	0.002 (2)	−0.0040 (18)
N1	0.0539 (17)	0.0614 (17)	0.0517 (18)	0.0019 (15)	0.0030 (14)	0.0063 (15)
C12	0.055 (2)	0.0558 (18)	0.0461 (19)	0.0009 (17)	0.0109 (17)	0.0041 (16)
C8	0.0486 (19)	0.0497 (19)	0.068 (2)	−0.0031 (16)	−0.0031 (18)	−0.0008 (17)
C10	0.058 (2)	0.061 (2)	0.0497 (19)	−0.0035 (18)	0.0073 (18)	0.0045 (16)
C19	0.077 (3)	0.082 (3)	0.049 (2)	−0.005 (2)	−0.004 (2)	0.006 (2)
C18	0.067 (2)	0.070 (2)	0.0502 (19)	0.007 (2)	0.008 (2)	0.0127 (18)
C11	0.070 (3)	0.103 (4)	0.066 (3)	0.022 (3)	0.012 (2)	0.017 (3)
C17	0.093 (3)	0.090 (3)	0.072 (3)	0.025 (3)	−0.001 (3)	0.015 (3)
C7	0.061 (2)	0.060 (2)	0.062 (2)	0.003 (2)	0.0126 (19)	0.009 (2)
C14	0.085 (3)	0.059 (2)	0.054 (2)	0.003 (2)	0.010 (2)	0.0002 (17)
C15	0.127 (4)	0.060 (2)	0.069 (3)	0.007 (3)	0.022 (3)	0.000 (2)
C20	0.087 (3)	0.070 (3)	0.053 (2)	−0.009 (2)	0.003 (2)	−0.009 (2)
C16	0.128 (5)	0.073 (3)	0.084 (4)	0.039 (3)	0.020 (3)	0.016 (3)
C21	0.073 (2)	0.0584 (19)	0.052 (2)	0.0054 (18)	0.0099 (18)	−0.0017 (19)

Geometric parameters (Å, º)

S1—C9	1.744 (3)	C8—H8	0.93
S1—C2	1.755 (3)	C10—C11	1.529 (6)
C13—C14	1.419 (5)	C10—H10	0.98
C13—C18	1.420 (6)	C19—C20	1.347 (6)
C13—C12	1.436 (5)	C19—C18	1.414 (6)
C5—C6	1.359 (6)	C19—H19	0.93
C5—C4	1.409 (5)	C18—C17	1.406 (6)
C5—H5	0.93	C11—H11A	0.96
C9—C8	1.380 (5)	C11—H11B	0.96
C9—C4	1.402 (5)	C11—H11C	0.96
C3—C2	1.347 (5)	C17—C16	1.358 (7)
C3—C4	1.430 (5)	C17—H17	0.93
C3—H3	0.93	C7—H7	0.93
C2—C1	1.438 (5)	C14—C15	1.361 (6)
C1—N1	1.272 (5)	C14—H14	0.93
C1—H1	0.93	C15—C16	1.388 (7)
C6—C7	1.399 (6)	C15—H15	0.93

C6—H6	0.93	C20—C21	1.395 (6)
N1—C10	1.485 (5)	C20—H20	0.93
C12—C21	1.371 (6)	C16—H16	0.93
C12—C10	1.511 (6)	C21—H21	0.93
C8—C7	1.371 (6)		

C9—S1—C2	90.70 (18)	C12—C10—H10	108.9
C14—C13—C18	117.9 (4)	C11—C10—H10	108.9
C14—C13—C12	123.0 (4)	C20—C19—C18	120.4 (4)
C18—C13—C12	119.1 (3)	C20—C19—H19	119.8
C6—C5—C4	119.5 (4)	C18—C19—H19	119.8
C6—C5—H5	120.2	C17—C18—C19	121.7 (4)
C4—C5—H5	120.2	C17—C18—C13	118.9 (4)
C8—C9—C4	121.6 (3)	C19—C18—C13	119.4 (4)
C8—C9—S1	126.7 (3)	C10—C11—H11A	109.5
C4—C9—S1	111.7 (3)	C10—C11—H11B	109.5
C2—C3—C4	113.9 (3)	H11A—C11—H11B	109.5
C2—C3—H3	123.1	C10—C11—H11C	109.5
C4—C3—H3	123.1	H11A—C11—H11C	109.5
C9—C4—C5	118.4 (4)	H11B—C11—H11C	109.5
C9—C4—C3	111.5 (3)	C16—C17—C18	121.2 (5)
C5—C4—C3	130.1 (4)	C16—C17—H17	119.4
C3—C2—C1	127.6 (3)	C18—C17—H17	119.4
C3—C2—S1	112.3 (3)	C8—C7—C6	120.5 (4)
C1—C2—S1	120.1 (3)	C8—C7—H7	119.7
N1—C1—C2	122.6 (3)	C6—C7—H7	119.7
N1—C1—H1	118.7	C15—C14—C13	121.3 (5)
C2—C1—H1	118.7	C15—C14—H14	119.3
C5—C6—C7	121.1 (4)	C13—C14—H14	119.3
C5—C6—H6	119.5	C14—C15—C16	120.2 (5)
C7—C6—H6	119.5	C14—C15—H15	119.9
C1—N1—C10	117.6 (3)	C16—C15—H15	119.9
C21—C12—C13	118.2 (3)	C19—C20—C21	120.7 (4)
C21—C12—C10	121.5 (3)	C19—C20—H20	119.6
C13—C12—C10	120.2 (3)	C21—C20—H20	119.6
C7—C8—C9	118.8 (4)	C17—C16—C15	120.6 (4)
C7—C8—H8	120.6	C17—C16—H16	119.7
C9—C8—H8	120.6	C15—C16—H16	119.7
N1—C10—C12	107.7 (3)	C12—C21—C20	122.1 (4)
N1—C10—C11	107.4 (3)	C12—C21—H21	118.9
C12—C10—C11	114.9 (3)	C20—C21—H21	118.9
N1—C10—H10	108.9		

C2—S1—C9—C8	−178.8 (3)	C1—N1—C10—C11	95.0 (4)
C2—S1—C9—C4	0.0 (2)	C21—C12—C10—N1	−99.0 (4)
C8—C9—C4—C5	−1.2 (5)	C13—C12—C10—N1	78.2 (4)
S1—C9—C4—C5	179.9 (3)	C21—C12—C10—C11	20.6 (5)
C8—C9—C4—C3	178.8 (3)	C13—C12—C10—C11	−162.1 (3)

S1—C9—C4—C3	−0.1 (3)	C20—C19—C18—C17	178.3 (4)
C6—C5—C4—C9	0.9 (5)	C20—C19—C18—C13	0.0 (6)
C6—C5—C4—C3	−179.1 (3)	C14—C13—C18—C17	0.2 (6)
C2—C3—C4—C9	0.2 (4)	C12—C13—C18—C17	−179.6 (4)
C2—C3—C4—C5	−179.9 (4)	C14—C13—C18—C19	178.5 (4)
C4—C3—C2—C1	179.4 (3)	C12—C13—C18—C19	−1.2 (6)
C4—C3—C2—S1	−0.2 (4)	C19—C18—C17—C16	−177.9 (5)
C9—S1—C2—C3	0.1 (3)	C13—C18—C17—C16	0.4 (7)
C9—S1—C2—C1	−179.5 (3)	C9—C8—C7—C6	0.2 (6)
C3—C2—C1—N1	173.8 (4)	C5—C6—C7—C8	−0.5 (6)
S1—C2—C1—N1	−6.7 (5)	C18—C13—C14—C15	−0.9 (6)
C4—C5—C6—C7	0.0 (6)	C12—C13—C14—C15	178.9 (4)
C2—C1—N1—C10	−178.2 (3)	C13—C14—C15—C16	1.0 (7)
C14—C13—C12—C21	−177.7 (4)	C18—C19—C20—C21	0.4 (7)
C18—C13—C12—C21	2.0 (5)	C18—C17—C16—C15	−0.3 (8)
C14—C13—C12—C10	5.0 (5)	C14—C15—C16—C17	−0.4 (8)
C18—C13—C12—C10	−175.3 (3)	C13—C12—C21—C20	−1.7 (6)
C4—C9—C8—C7	0.7 (5)	C10—C12—C21—C20	175.6 (3)
S1—C9—C8—C7	179.4 (3)	C19—C20—C21—C12	0.4 (6)
C1—N1—C10—C12	−140.7 (3)		

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the S1/C2/C3/C4/C9, C12/C13/C18/C19/C20/C21 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···*Cg*1^{i}	0.93	2.73	3.491 (4)	139
C11—H11*B*···*Cg*2^{ii}	0.96	2.59	3.724 (5)	149

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