Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(1,3-Benzothiazol-2-yl)-3-phenyl-2-pyrazoline

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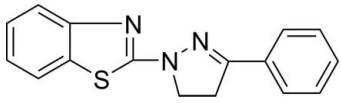
Received 6 March 2012; accepted 26 March 2012

Key indicators: single-crystal X-ray study; T = 288 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.116; data-to-parameter ratio = 17.4.

In the title compound, $C_{16}H_{13}N_3S$, the pyrazoline ring forms dihedral angles of 6.89 (14) and 4.96 (11)° with the benzene ring and the benzothiazole group, respectively. In the crystal, weak C—H···N interactions link the molecules into chains extending along the b-axis direction.

Related literature

For background to the title compound, see: Sano *et al.* (1995); Xian *et al.* (2008). For details of the synthesis, see: Xian *et al.* (2008).



Experimental

Crystal data

$C_{16}H_{13}N_3S$
M_r = 279.35
Monoclinic, $P2_1/c$
a = 16.946 (8) Å
b = 5.449 (3) Å
c = 17.306 (11) Å
β = 119.96 (2)°
V = 1384.4 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 288 K
0.54 × 0.30 × 0.28 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.887, T_{max} = 0.938
11972 measured reflections
3141 independent reflections
2227 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.14
3141 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N3^{i}	0.93	2.61	3.340 (3)	135

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (MSC & Rigaku, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge financial support from the National Natural Science Foundation of Jilin Province (grant No. 20101548).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2466).

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supporting information

Acta Cryst. (2012). E**68**, o1248 [https://doi.org/10.1107/S1600536812013219]

1-(1,3-Benzothiazol-2-yl)-3-phenyl-2-pyrazoline

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S1. Comment

Pyrazoline derivatives have been investigated in many repects due to their blue light emission with high quantum yield, accessibility. They are used as carrier transporting as well as emitting materials (Sano *et al.*, 1995). Recently, Xian reported the synthesis and optical properties of novel pyrazoline derivatives as blue light fluorescence compounds (Xian *et al.*, 2008). In this paper, we describe the crystal structure of the title compound with blue light fluorescence.

The molecular structure of title compound, $C_{16}H_{13}N_3S$, is shown in Fig. 1, all bond lengths and angles are in the normal ranges. The pyrazoline ring and benzothiazole ring are nearly coplanar and make dihedral angle of 4.96 (11)°. The molecules are linked by intermolecular C—H···N hydrogen bonds (Table 1), generating chains along the *b* direction.

S2. Experimental

The title compound was prepared according to the literature (Xian *et al.*, 2008). Single crystals suitable for X-ray diffraction were prepared by slow evaporation method from a solution in dichloromethane/petroleum (60–90 °C) at room temperature.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 and 0.97 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) = 1.2 U_{eq}(C).

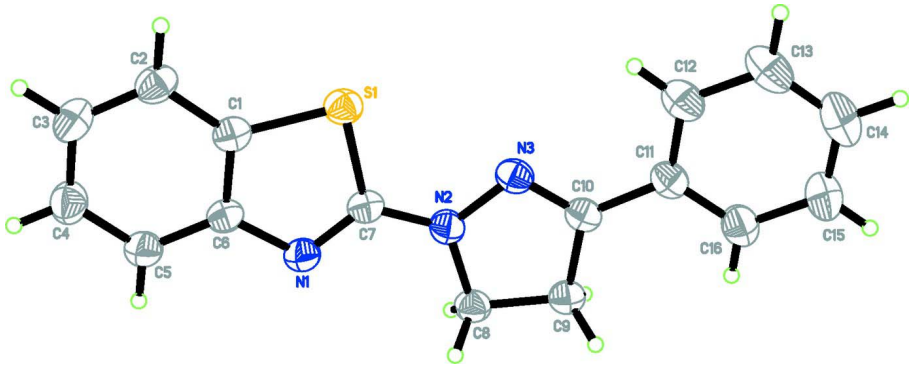

Figure 1

Molecular structure of the title compound with displacement ellipsoids drawn at the 30% probalility level.

1-(1,3-Benzothiazol-2-yl)-3-phenyl-2-pyrazoline

Crystal data

$C_{16}H_{13}N_3S$
M_r = 279.35

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 16.946 (8) Å
b = 5.449 (3) Å
c = 17.306 (11) Å
β = 119.96 (2)°
V = 1384.4 (14) Å^3
Z = 4
F(000) = 584
D_x = 1.340 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8759 reflections
θ = 3.6–27.6°
μ = 0.23 mm^{-1}
T = 288 K
Block, colorless
0.54 × 0.30 × 0.28 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.887, T_{max} = 0.938

11972 measured reflections
3141 independent reflections
2227 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 27.5°, θ_{min} = 3.6°
h = −21→21
k = −7→6
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.14
3141 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0607P)^2 + 0.0076P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Experimental. (See detailed section in the paper)

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 $F^2 > \sigma(F^2)$ 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}
S1	0.50225 (3)	−0.17993 (8)	0.32651 (3)	0.05497 (16)
N1	0.43537 (9)	0.1902 (2)	0.37317 (10)	0.0552 (4)
N2	0.59086 (9)	0.1280 (3)	0.46547 (10)	0.0569 (4)
N3	0.66870 (9)	0.0055 (2)	0.48121 (9)	0.0541 (3)
C1	0.38592 (10)	−0.1199 (3)	0.26333 (11)	0.0502 (4)
C2	0.32007 (12)	−0.2465 (4)	0.18951 (13)	0.0617 (5)
H2	0.3354	−0.3833	0.1677	0.074*
C3	0.23125 (12)	−0.1641 (4)	0.14930 (13)	0.0678 (5)

H3	0.1862	−0.2452	0.0994	0.081*
C4	0.20868 (12)	0.0380 (4)	0.18261 (13)	0.0690 (5)
H4	0.1485	0.0913	0.1544	0.083*
C5	0.27335 (12)	0.1621 (3)	0.25656 (13)	0.0629 (5)
H5	0.2570	0.2966	0.2786	0.075*
C6	0.36345 (10)	0.0836 (3)	0.29788 (11)	0.0509 (4)
C7	0.50936 (10)	0.0702 (3)	0.39398 (11)	0.0499 (4)
C8	0.60831 (11)	0.3438 (3)	0.52172 (12)	0.0554 (4)
H8A	0.5770	0.3329	0.5557	0.066*
H8B	0.5901	0.4934	0.4867	0.066*
C9	0.71109 (11)	0.3312 (3)	0.58214 (12)	0.0568 (4)
H9A	0.7402	0.4805	0.5784	0.068*
H9B	0.7274	0.3038	0.6437	0.068*
C10	0.73713 (11)	0.1147 (3)	0.54526 (11)	0.0493 (4)
C11	0.83120 (11)	0.0387 (3)	0.57541 (12)	0.0546 (4)
C12	0.85070 (13)	−0.1548 (4)	0.53559 (14)	0.0704 (5)
H12	0.8037	−0.2453	0.4906	0.085*
C13	0.94034 (15)	−0.2128 (5)	0.56296 (17)	0.0892 (7)
H13	0.9533	−0.3426	0.5362	0.107*
C14	1.01079 (15)	−0.0798 (5)	0.62958 (18)	0.0935 (7)
H14	1.0709	−0.1183	0.6471	0.112*
C15	0.99182 (13)	0.1075 (5)	0.66937 (17)	0.0882 (7)
H15	1.0392	0.1961	0.7147	0.106*
C16	0.90289 (12)	0.1677 (4)	0.64329 (14)	0.0725 (5)
H16	0.8909	0.2958	0.6714	0.087*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0594 (3)	0.0536 (3)	0.0590 (3)	0.00083 (18)	0.0349 (2)	−0.00678 (19)
N1	0.0564 (8)	0.0489 (8)	0.0602 (9)	−0.0009 (6)	0.0290 (7)	−0.0076 (6)
N2	0.0519 (7)	0.0566 (8)	0.0600 (9)	0.0041 (6)	0.0262 (7)	−0.0112 (7)
N3	0.0600 (8)	0.0525 (8)	0.0543 (8)	0.0057 (6)	0.0318 (7)	−0.0010 (6)
C1	0.0578 (9)	0.0483 (9)	0.0526 (9)	−0.0047 (7)	0.0336 (8)	−0.0014 (7)
C2	0.0682 (11)	0.0625 (10)	0.0650 (12)	−0.0099 (8)	0.0413 (9)	−0.0154 (9)
C3	0.0627 (10)	0.0779 (13)	0.0625 (12)	−0.0164 (9)	0.0311 (9)	−0.0172 (9)
C4	0.0552 (10)	0.0773 (13)	0.0703 (13)	−0.0026 (9)	0.0281 (9)	−0.0058 (10)
C5	0.0601 (9)	0.0554 (11)	0.0721 (12)	0.0015 (8)	0.0322 (9)	−0.0074 (9)
C6	0.0569 (9)	0.0448 (9)	0.0544 (10)	−0.0052 (7)	0.0304 (8)	−0.0018 (7)
C7	0.0570 (9)	0.0450 (9)	0.0533 (10)	−0.0026 (7)	0.0317 (8)	−0.0020 (7)
C8	0.0613 (9)	0.0485 (9)	0.0548 (10)	0.0041 (7)	0.0279 (8)	−0.0052 (7)
C9	0.0593 (9)	0.0516 (10)	0.0588 (11)	0.0004 (7)	0.0291 (8)	−0.0049 (8)
C10	0.0564 (9)	0.0482 (9)	0.0478 (9)	0.0045 (7)	0.0294 (7)	0.0060 (7)
C11	0.0592 (9)	0.0552 (10)	0.0550 (10)	0.0082 (8)	0.0327 (8)	0.0117 (8)
C12	0.0716 (11)	0.0737 (13)	0.0710 (13)	0.0159 (9)	0.0393 (10)	0.0026 (10)
C13	0.0864 (15)	0.0968 (17)	0.0963 (18)	0.0324 (13)	0.0546 (14)	0.0062 (14)
C14	0.0644 (12)	0.118 (2)	0.1009 (19)	0.0243 (13)	0.0430 (13)	0.0210 (16)
C15	0.0573 (11)	0.0989 (16)	0.0930 (17)	0.0079 (11)	0.0259 (11)	0.0044 (14)

C16	0.0586 (10)	0.0765 (13)	0.0736 (14)	0.0073 (9)	0.0264 (10)	0.0004 (10)

Geometric parameters (Å, º)

S1—C1	1.7424 (18)	C8—C9	1.521 (2)
S1—C7	1.7591 (18)	C8—H8A	0.9700
N1—C7	1.296 (2)	C8—H8B	0.9700
N1—C6	1.391 (2)	C9—C10	1.508 (2)
N2—C7	1.353 (2)	C9—H9A	0.9700
N2—N3	1.3788 (18)	C9—H9B	0.9700
N2—C8	1.459 (2)	C10—C11	1.468 (2)
N3—C10	1.282 (2)	C11—C12	1.387 (3)
C1—C2	1.389 (2)	C11—C16	1.387 (3)
C1—C6	1.400 (2)	C12—C13	1.383 (3)
C2—C3	1.380 (3)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.380 (3)
C3—C4	1.382 (3)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.356 (4)
C4—C5	1.377 (2)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.379 (3)
C5—C6	1.391 (2)	C15—H15	0.9300
C5—H5	0.9300	C16—H16	0.9300
C1—S1—C7	87.26 (8)	N2—C8—H8B	111.4
C7—N1—C6	108.86 (14)	C9—C8—H8B	111.4
C7—N2—N3	120.46 (14)	H8A—C8—H8B	109.3
C7—N2—C8	124.87 (14)	C10—C9—C8	102.76 (13)
N3—N2—C8	113.78 (13)	C10—C9—H9A	111.2
C10—N3—N2	108.00 (14)	C8—C9—H9A	111.2
C2—C1—C6	121.40 (15)	C10—C9—H9B	111.2
C2—C1—S1	128.44 (14)	C8—C9—H9B	111.2
C6—C1—S1	110.15 (12)	H9A—C9—H9B	109.1
C3—C2—C1	118.38 (17)	N3—C10—C11	121.95 (15)
C3—C2—H2	120.8	N3—C10—C9	113.54 (13)
C1—C2—H2	120.8	C11—C10—C9	124.44 (15)
C2—C3—C4	120.52 (17)	C12—C11—C16	118.72 (16)
C2—C3—H3	119.7	C12—C11—C10	121.59 (17)
C4—C3—H3	119.7	C16—C11—C10	119.65 (16)
C5—C4—C3	121.41 (17)	C13—C12—C11	119.8 (2)
C5—C4—H4	119.3	C13—C12—H12	120.1
C3—C4—H4	119.3	C11—C12—H12	120.1
C4—C5—C6	119.12 (16)	C14—C13—C12	120.7 (2)
C4—C5—H5	120.4	C14—C13—H13	119.7
C6—C5—H5	120.4	C12—C13—H13	119.7
N1—C6—C5	125.20 (15)	C15—C14—C13	119.6 (2)
N1—C6—C1	115.65 (14)	C15—C14—H14	120.2
C5—C6—C1	119.14 (15)	C13—C14—H14	120.2
N1—C7—N2	122.74 (15)	C14—C15—C16	120.7 (2)

N1—C7—S1	118.07 (12)	C14—C15—H15	119.7
N2—C7—S1	119.18 (12)	C16—C15—H15	119.7
N2—C8—C9	101.73 (12)	C15—C16—C11	120.6 (2)
N2—C8—H8A	111.4	C15—C16—H16	119.7
C9—C8—H8A	111.4	C11—C16—H16	119.7
C7—N2—N3—C10	171.82 (15)	C8—N2—C7—S1	173.69 (13)
C8—N2—N3—C10	2.14 (19)	C1—S1—C7—N1	−0.77 (13)
C7—S1—C1—C2	−178.47 (17)	C1—S1—C7—N2	178.58 (14)
C7—S1—C1—C6	0.79 (12)	C7—N2—C8—C9	−173.15 (16)
C6—C1—C2—C3	1.2 (3)	N3—N2—C8—C9	−4.01 (18)
S1—C1—C2—C3	−179.59 (14)	N2—C8—C9—C10	3.99 (16)
C1—C2—C3—C4	−0.7 (3)	N2—N3—C10—C11	−176.45 (14)
C2—C3—C4—C5	−0.3 (3)	N2—N3—C10—C9	0.87 (19)
C3—C4—C5—C6	0.7 (3)	C8—C9—C10—N3	−3.27 (19)
C7—N1—C6—C5	179.52 (15)	C8—C9—C10—C11	173.97 (15)
C7—N1—C6—C1	0.2 (2)	N3—C10—C11—C12	0.4 (3)
C4—C5—C6—N1	−179.49 (17)	C9—C10—C11—C12	−176.66 (16)
C4—C5—C6—C1	−0.2 (3)	N3—C10—C11—C16	178.12 (17)
C2—C1—C6—N1	178.56 (15)	C9—C10—C11—C16	1.1 (2)
S1—C1—C6—N1	−0.76 (18)	C16—C11—C12—C13	−1.0 (3)
C2—C1—C6—C5	−0.8 (3)	C10—C11—C12—C13	176.74 (18)
S1—C1—C6—C5	179.88 (13)	C11—C12—C13—C14	0.0 (3)
C6—N1—C7—N2	−178.85 (15)	C12—C13—C14—C15	0.9 (4)
C6—N1—C7—S1	0.47 (18)	C13—C14—C15—C16	−0.6 (4)
N3—N2—C7—N1	−175.46 (14)	C14—C15—C16—C11	−0.4 (4)
C8—N2—C7—N1	−7.0 (3)	C12—C11—C16—C15	1.3 (3)
N3—N2—C7—S1	5.2 (2)	C10—C11—C16—C15	−176.54 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N3^{i}	0.93	2.61	3.340 (3)	135

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