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N-Butylpyridine-4-thiocarboxamide

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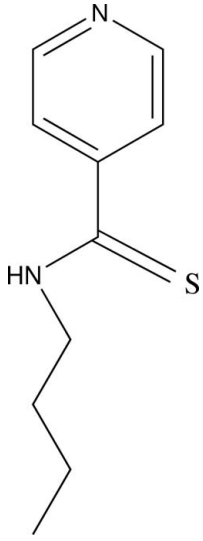
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.120; data-to-parameter ratio = 17.9.

In the title molecule, $C_{10}H_{14}N_2S$, the *n*-butyl chain assumes a *trans* zigzag conformation. The dihedral angle between the pyridine ring and the thioamide plane is 23.38 (8)°. The molecules in the crystal structure are linked by an intermolecular N—H···N hydrogen bond.

Related literature

For related literature, see: Allen *et al.* (1987); Klimsova *et al.* (1999); Ramachandran (2005); Vannelli *et al.* (2002); Desiraju (1989); Dodge *et al.* (2006).



Experimental

Crystal data

$C_{10}H_{14}N_2S$
M_r = 194.29
Monoclinic, $P2_1/c$
a = 8.0895 (3) Å
b = 13.5947 (4) Å
c = 10.4936 (3) Å
β = 111.895 (2)°
V = 1070.78 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 293 (2) K
0.26 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.935, T_{max} = 0.949
11437 measured reflections
2182 independent reflections
1744 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 1.06
2182 reflections
122 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N8—H8···N1^{i}	0.859 (19)	2.182 (19)	3.033 (2)	171 (2)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2253).

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S1. Comment

Drugs containing carbothioamide (–$CSNH_2$) functional groups are clinically effective for the treatment of *M. tuberculosis, M. leprae* and *M. avium* complex infections (Dodge *et al.,* 2006; Klimsova *et al.*, 1999). In general, the carbothioamide drugs are considered as second line drugs. The carbothioamide groups have significant effects in biological systems. Their use, especially as pyridine carbothioamides in the field of multi drug resistant systems, has increased a lot (Vannelli *et al.*, 2002). Depending on the position of the carbothioamide group at the pyridine ring and also depending on the nature of *N*-alkyl substitution at the thioamide, the pyridine carbothioamides have been found to play a vital role in their biological activities and drug action. We report here the crystal structure of a typical pyridine-carbothioamide, *viz*., 4-(*N*-1-butylcarbothioamido) pyridine.

The pyridine ring is planar. The *n*-butyl amide group assumes an extended conformation [C4—C7—N8—C9 = -178.06 (15)°, C7—N8—C9—C10 = -168.50 (16)°, N8—C9—C10—C11 = -178.86 (16)°, C9—C10—C11—C12 = -171.50 (18)°]. The C=S bond length [1.6608 (16) Å] is comparable with the literature values (Allen *et al.*, 1987). The pyridine and thioamide planes orient at an angle of 23.38 (8)° to each other.

The sum of the bond angles around N8 is 359.94 (4)° thus conforming sp^2 hybridized state of N atom. The molecules in the unit cell are stabilized by N—H···N (Desiraju, 1989) type of intermolecular interactions in addition to van der Waal's forces.

S2. Experimental

About 5 g of 4- pyridinecarbonitrile was dissolved in 15 ml of ethanol. To this about 10 ml of 1-aminobutane was added and purified and H_2S gas was passed for 3 h. The yellow solid separate was filtered, washed with ethanol and dried in vacuum desicator (yield 80%) (Ramachandran, 2005).

S3. Refinement

The H atom associated with N atom was located in a difference Fourier map and refined isotropically. Other H atoms were geometrically positioned (C—H = 0.93 - 0.97 Å) and treated as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

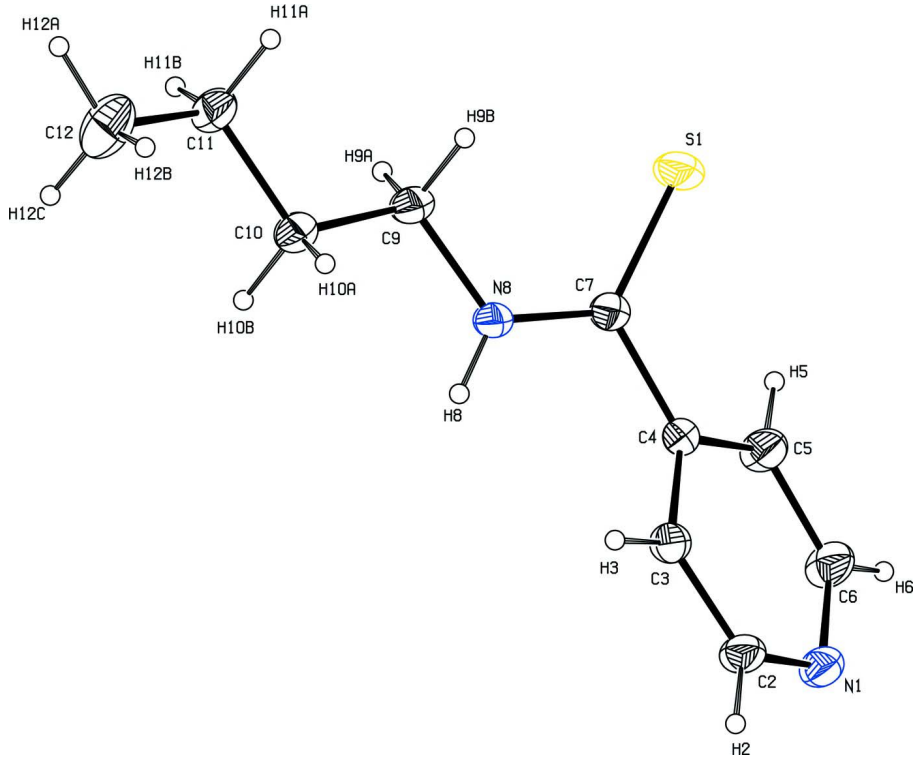

Figure 1

The molecular structure of the title compound, showing 20% probability displacement ellipsoids.

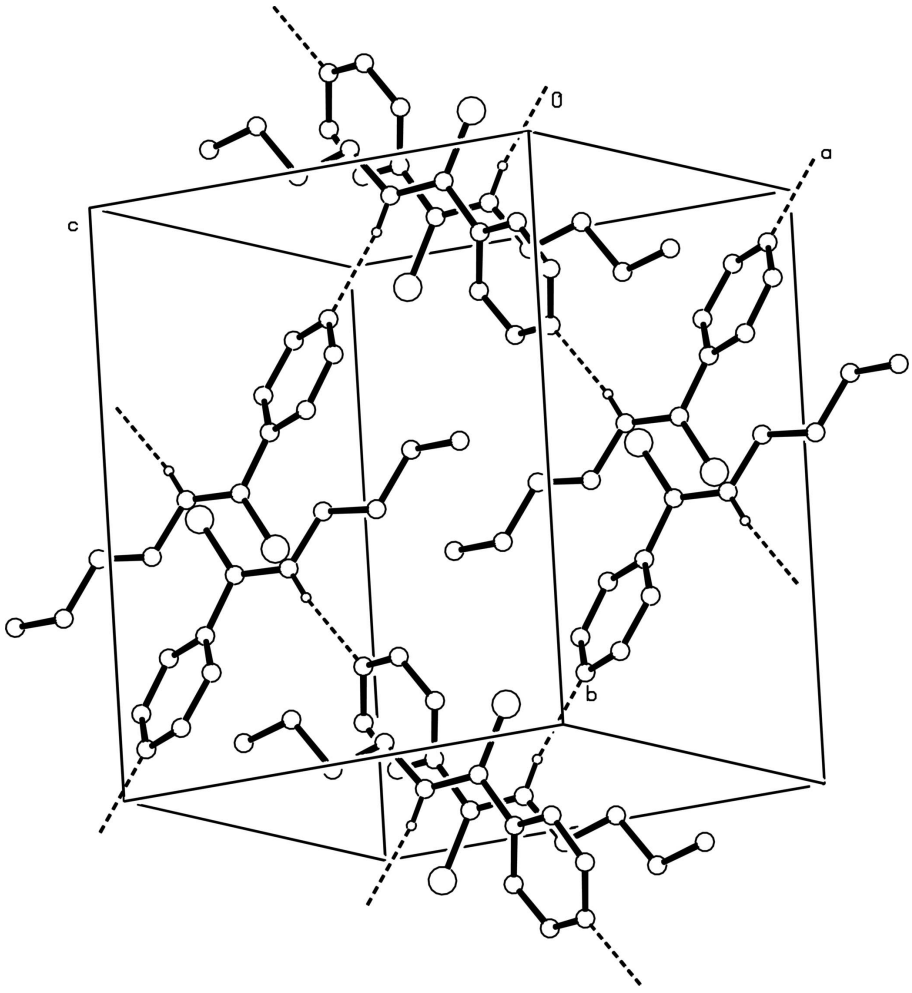

Figure 2

A packing diagram, viewed approximately along the *a* axis. Dashed lines indicated N—H···N hydrogen bonds.

N-Butylpyridine-4-thiocarboxamide

Crystal data

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$M_r = 194.29$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.0895\ (3)$ Å
$b = 13.5947\ (4)$ Å
$c = 10.4936\ (3)$ Å
$\beta = 111.895\ (2)°$
$V = 1070.78\ (6)$ Å^3
$Z = 4$
$F(000) = 416$
$D_x = 1.205$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2182 reflections
$\theta = 2.6–26.3°$
$\mu = 0.26$ mm^{-1}
$T = 293$ K
Block, brown
0.26 × 0.20 × 0.20 mm

Data collection

Bruker APEXII kappa diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.935$, $T_{max} = 0.949$

11437 measured reflections
2182 independent reflections
1744 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 26.3°$, $\theta_{min} = 2.6°$
$h = -9 \rightarrow 10$
$k = -15 \rightarrow 16$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.120$
$S = 1.06$
2182 reflections
122 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.2939P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
H8	0.753 (2)	−0.0813 (14)	0.501 (2)	0.055 (5)*
C2	0.6652 (3)	−0.27758 (12)	0.74847 (18)	0.0533 (4)
H2	0.5953	−0.3302	0.7016	0.064*
C3	0.6682 (2)	−0.19391 (12)	0.67438 (17)	0.0461 (4)
H3	0.6041	−0.1917	0.5802	0.055*
C4	0.7670 (2)	−0.11385 (11)	0.74138 (15)	0.0406 (4)
C5	0.8613 (3)	−0.12389 (14)	0.88113 (18)	0.0561 (5)
H5	0.9304	−0.0721	0.9312	0.067*
C6	0.8525 (3)	−0.21036 (14)	0.94534 (19)	0.0606 (5)
H6	0.9185	−0.2154	1.0390	0.073*
C7	0.7739 (2)	−0.01937 (11)	0.67065 (17)	0.0446 (4)
C9	0.7746 (3)	0.06103 (12)	0.46367 (18)	0.0519 (4)
H9A	0.8954	0.0864	0.5005	0.062*
H9B	0.6965	0.1116	0.4748	0.062*
C10	0.7241 (3)	0.04039 (12)	0.31368 (18)	0.0514 (4)
H10A	0.6022	0.0168	0.2754	0.062*
H10B	0.8008	−0.0107	0.3017	0.062*
C11	0.7414 (3)	0.13253 (14)	0.23755 (19)	0.0590 (5)
H11A	0.6797	0.1862	0.2618	0.071*
H11B	0.8663	0.1503	0.2673	0.071*

C12	0.6671 (4)	0.1204 (2)	0.0840 (2)	0.0914 (8)
H12A	0.6822	0.1806	0.0417	0.137*
H12B	0.5427	0.1046	0.0533	0.137*
H12C	0.7292	0.0683	0.0590	0.137*
N1	0.7559 (2)	−0.28736 (10)	0.88235 (15)	0.0544 (4)
N8	0.7638 (2)	−0.02581 (10)	0.54257 (14)	0.0450 (3)
S1	0.79203 (10)	0.08676 (3)	0.75316 (5)	0.0775 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0742 (12)	0.0386 (9)	0.0445 (10)	−0.0106 (8)	0.0193 (9)	−0.0039 (7)
C3	0.0591 (10)	0.0420 (8)	0.0351 (8)	−0.0019 (7)	0.0152 (7)	−0.0010 (6)
C4	0.0507 (9)	0.0356 (8)	0.0393 (9)	−0.0011 (7)	0.0212 (7)	−0.0016 (6)
C5	0.0744 (13)	0.0482 (10)	0.0396 (9)	−0.0177 (9)	0.0143 (9)	−0.0047 (7)
C6	0.0829 (14)	0.0548 (11)	0.0359 (9)	−0.0104 (9)	0.0126 (9)	0.0045 (8)
C7	0.0563 (10)	0.0371 (8)	0.0420 (9)	−0.0009 (7)	0.0201 (8)	−0.0013 (6)
C9	0.0716 (12)	0.0354 (8)	0.0507 (10)	0.0021 (8)	0.0253 (9)	0.0062 (7)
C10	0.0649 (11)	0.0424 (9)	0.0485 (10)	0.0035 (8)	0.0228 (8)	0.0079 (7)
C11	0.0721 (13)	0.0510 (11)	0.0593 (12)	0.0064 (9)	0.0307 (10)	0.0166 (8)
C12	0.1018 (19)	0.107 (2)	0.0593 (14)	−0.0033 (15)	0.0234 (13)	0.0293 (13)
N1	0.0776 (11)	0.0426 (8)	0.0432 (8)	−0.0073 (7)	0.0227 (8)	0.0025 (6)
N8	0.0662 (9)	0.0316 (7)	0.0405 (7)	0.0033 (6)	0.0235 (7)	0.0021 (6)
S1	0.1429 (6)	0.0376 (3)	0.0602 (4)	−0.0080 (3)	0.0474 (4)	−0.0114 (2)

Geometric parameters (Å, º)

C2—N1	1.327 (2)	C9—C10	1.498 (2)
C2—C3	1.383 (2)	C9—H9A	0.9700
C2—H2	0.9300	C9—H9B	0.9700
C3—C4	1.378 (2)	C10—C11	1.520 (2)
C3—H3	0.9300	C10—H10A	0.9700
C4—C5	1.384 (2)	C10—H10B	0.9700
C4—C7	1.495 (2)	C11—C12	1.504 (3)
C5—C6	1.370 (3)	C11—H11A	0.9700
C5—H5	0.9300	C11—H11B	0.9700
C6—N1	1.326 (2)	C12—H12A	0.9600
C6—H6	0.9300	C12—H12B	0.9600
C7—N8	1.318 (2)	C12—H12C	0.9600
C7—S1	1.6608 (16)	N8—H8	0.86 (2)
C9—N8	1.463 (2)		
N1—C2—C3	123.97 (16)	H9A—C9—H9B	107.8
N1—C2—H2	118.0	C9—C10—C11	110.82 (15)
C3—C2—H2	118.0	C9—C10—H10A	109.5
C4—C3—C2	119.42 (15)	C11—C10—H10A	109.5
C4—C3—H3	120.3	C9—C10—H10B	109.5
C2—C3—H3	120.3	C11—C10—H10B	109.5

C3—C4—C5	116.63 (15)	H10A—C10—H10B	108.1
C3—C4—C7	123.18 (14)	C12—C11—C10	113.24 (19)
C5—C4—C7	120.18 (15)	C12—C11—H11A	108.9
C6—C5—C4	119.76 (16)	C10—C11—H11A	108.9
C6—C5—H5	120.1	C12—C11—H11B	108.9
C4—C5—H5	120.1	C10—C11—H11B	108.9
N1—C6—C5	124.15 (17)	H11A—C11—H11B	107.7
N1—C6—H6	117.9	C11—C12—H12A	109.5
C5—C6—H6	117.9	C11—C12—H12B	109.5
N8—C7—C4	116.70 (13)	H12A—C12—H12B	109.5
N8—C7—S1	123.30 (12)	C11—C12—H12C	109.5
C4—C7—S1	120.00 (12)	H12A—C12—H12C	109.5
N8—C9—C10	113.15 (14)	H12B—C12—H12C	109.5
N8—C9—H9A	108.9	C6—N1—C2	116.05 (15)
C10—C9—H9A	108.9	C7—N8—C9	121.94 (14)
N8—C9—H9B	108.9	C7—N8—H8	122.2 (13)
C10—C9—H9B	108.9	C9—N8—H8	115.8 (13)
N1—C2—C3—C4	−1.5 (3)	C5—C4—C7—S1	−33.5 (2)
C2—C3—C4—C5	1.2 (2)	N8—C9—C10—C11	−178.86 (16)
C2—C3—C4—C7	−178.13 (16)	C9—C10—C11—C12	−171.50 (18)
C3—C4—C5—C6	−0.1 (3)	C5—C6—N1—C2	0.6 (3)
C7—C4—C5—C6	179.24 (18)	C3—C2—N1—C6	0.6 (3)
C4—C5—C6—N1	−0.9 (3)	C4—C7—N8—C9	−178.06 (15)
C3—C4—C7—N8	−33.7 (2)	S1—C7—N8—C9	2.4 (3)
C5—C4—C7—N8	146.99 (17)	C10—C9—N8—C7	−168.50 (16)
C3—C4—C7—S1	145.88 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N8—H8···N1^{i}	0.859 (19)	2.182 (19)	3.033 (2)	171 (2)

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