3-Butyl-2-(piperidin-1-yl)-5,6,7,8-tetra-hydrobenzothieno[2,3-d]pyrimidin-4(3H)-one

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In the title compound, $C_{19}H_{27}N_3OS$, the central thienopyrimidine ring system is essentially planar. The cyclohexene ring adopts a half-chair conformation, while the piperidine ring is in a standard chair conformation. There is an intramolecular C—H···O hydrogen bond, which stabilizes the molecular structure. The crystal packing is stabilized by C—H···π interactions.

Related literature

For related literature, see: Ding et al. (2004); Zeng et al. (2007).
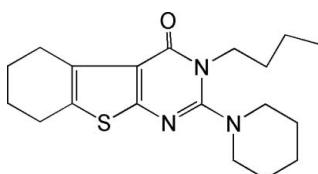
Experimental

Crystal data

$C_{19}H_{27}N_3OS$	$\gamma = 100.167 (1)°$
$M_r = 345.50$	$V = 923.97 (13)$ Å^3
Triclinic, $P\bar{1}$	$Z = 2$
$a = 9.8979 (8)$ Å	Mo $K\alpha$ radiation
$b = 10.3679 (9)$ Å	$\mu = 0.19$ mm^{-1}
$c = 10.9645 (9)$ Å	$T = 292 (2)$ K
$\alpha = 113.537 (1)°$	$0.40 \times 0.06 \times 0.02$ mm
$\beta = 107.679 (1)°$	

Data collection

Bruker SMART CCD area-detector diffractometer	3587 independent reflections
Absorption correction: none	2271 reflections with $I > 2\sigma(I)$
7700 measured reflections	$R_{int} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$	217 parameters
$wR(F^2) = 0.184$	H-atom parameters constrained
$S = 1.03$	$\Delta\rho_{max} = 0.31$ e Å^{-3}
3587 reflections	$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

$Cg1$ and $Cg2$ are the centroids of the S1/C6/C1/C8/C7 and N1/C7–C9/N2/C10 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17A···O1	0.97	2.54	3.035 (4)	112
C4—H4A···$Cg2^i$	0.97	3.00	3.854 (5)	148
C11—H11A···$Cg2^{ii}$	0.97	2.76	3.408 (3)	125
C12—H12A···$Cg1^{ii}$	0.97	2.92	3.764 (4)	146

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $-x, -y, -z$.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; 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: SHELXTL (Sheldrick, 2001).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2220).

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supplementary materials

3-Butyl-2-(piperidin-1-yl)-5,6,7,8-tetrahydrobenzothieno[2,3-*d*]pyrimidin-4(3*H*)-one

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Comment

Pyrimidine derivatives are attracting the increasing attention of the synthetic community because of the important role played by such systems in many natural products, antibiotics and drugs (Ding *et al.*, 2004). In recent years, we have been engaged in the preparation of derivatives of heterocycles *via* the aza-Wittig reaction. The title compound, (I), was synthesized and structurally characterized in this context.

In the fused heterobicyclic ring of (I), bond lengths and angles are similar to those observed in closely related structures (Zeng *et al.*, 2007). All ring atoms in the thienopyrimidine system are essentially coplanar. The cyclohexene ring adopts a half-chair conformation, while the piperidine ring is in a standard chair conformation. There is one intramolecular C—H⋯O hydrogen bond which stabilizes the molecular structure (Table 1). The crystal packing is stabilized by C—H⋯π interactions (Table 1). There exists no intermolecular hydrogen bond nor π-π stacking interaction.

Experimental

To a solution of iminophosphorane (*a*) (1.45 g, 3 mmol) in anhydrous dichloromethane (15 ml) was added butyl isocyanate (3 mmol) under dry nitrogen at room temperature (Fig. 2). The reaction mixture was left unstirred for 48 h at room temperature, then the solvent was removed under reduced pressure and an ether/petroleum ether (1:3 *v/v*, 20 ml) mixture was added to precipitate triphenylphosphine oxide. After filtration the solvent was removed to give carbodiimide, which was used directly without further purification. To the solution of carbodiimide (15 ml), piperidine (3 mmol) was added. After the mixture was stirred for 6 h, the solvent was removed and anhydrous ethanol (10 ml) containing several drops of EtONa in EtOH was added. The mixture was stirred for 12 h at room temperature. The solution was condensed and the residue was recrystallized from ethanol to give the title compound, (I), in a yield of 47% (m.p. 362 K). Spectroscopic analysis: IR (KBr, cm^{-1}): 1655 (C=O); ^{1}H NMR (CDCl$_3$, 400 MHz): δ 4.07–4.04 (*t*, J=7.2 Hz, 2H, NCH$_2$), 3.06–2.72 (*m*, 8H, 4CH$_2$), 1.85–1.63 (*m*, 12H, 6CH$_2$), 1.36–1.31 (*m*, 2H, CH$_2$), 0.96–0.92 (*t*, J=7.4 Hz, 3H, CH$_3$); MS (EI, 70 eV) m/*z*(%): 349 (21), 345 (*M*+, 94), 328 (42), 289 (100), 261 (99), 205 (92), 179 (69), 83 (97); Anal. Calcd. for C$_{19}$H$_{27}$N$_3$OS: C 66.05, H 7.88, N 12.16; Found: C 66.31, H 6.23, N 9.41%. Crystals suitable for single-crystal X-ray diffraction analysis were obtained by vapour diffusion of a hexane/dichloromethane solution (1:3 *v/v*) at room temperature.

Refinement

All H atoms were located in difference maps and then treated as riding atoms, with C—H = 0.97 Å (CH$_2$) or 0.96 (CH$_3$), and with U_{iso}(H) = 1.2U_{eq}(C), or 1.5U_{eq}(methyl C).

supplementary materials

Figures
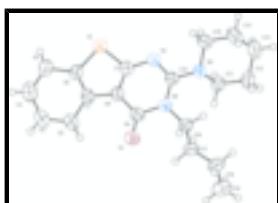
Fig. 1. The molecular structure of the title compound, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H-atoms are represented by circles of arbitrary size.
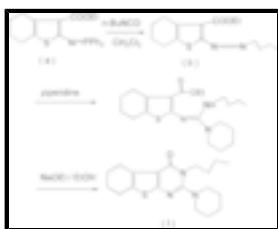
Fig. 2. Reaction scheme of the title compound, (I).

3-Butyl-2-(piperidin-1-yl)-5,6,7,8-tetrahydrobenzothieno[2,3-*d*]pyrimidin- 4(3*H*)-one

Crystal data

$C_{19}H_{27}N_3OS$	$Z = 2$
$M_r = 345.50$	$F_{000} = 372$
Triclinic, $P\bar{1}$	$D_x = 1.242$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.8979$ (8) Å	Cell parameters from 1934 reflections
$b = 10.3679$ (9) Å	$\theta = 2.2–22.4º$
$c = 10.9645$ (9) Å	$\mu = 0.19$ mm^{-1}
$\alpha = 113.537$ (1)º	$T = 292$ (2) K
$\beta = 107.679$ (1)º	Block, colorless
$\gamma = 100.167$ (1)º	$0.40 \times 0.06 \times 0.02$ mm
$V = 923.97$ (13) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2271 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.044$
Monochromator: graphite	$\theta_{max} = 26.0º$
$T = 292(2)$ K	$\theta_{min} = 2.2º$
φ and ω scans	$h = -11 \rightarrow 12$
Absorption correction: none	$k = -12 \rightarrow 9$
7700 measured reflections	$l = -13 \rightarrow 13$
3587 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

$R[F^2 > 2\sigma(F^2)] = 0.059$

H-atom parameters constrained

$wR(F^2) = 0.184$

$w = 1/[\sigma^2(F_o^2) + (0.0975P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.03$

$(\Delta/\sigma)_{max} = 0.002$

3587 reflections

$\Delta\rho_{max} = 0.31$ e Å^{-3}

217 parameters

$\Delta\rho_{min} = -0.29$ 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*	$U_{iso}*/U_{eq}$
S1	0.40177 (10)	0.46312 (8)	0.21177 (8)	0.0609 (3)
N1	0.3069 (2)	0.1715 (2)	0.1435 (2)	0.0465 (6)
N2	0.1870 (2)	0.1033 (2)	0.2765 (2)	0.0434 (5)
C8	0.2699 (3)	0.3619 (3)	0.3400 (3)	0.0439 (7)
N3	0.2303 (2)	−0.0775 (2)	0.0898 (2)	0.0456 (6)
O1	0.1534 (3)	0.2739 (2)	0.4653 (2)	0.0698 (7)
C16	0.1233 (3)	−0.0109 (3)	0.3111 (3)	0.0484 (7)
H16A	0.1728	0.0261	0.4155	0.058*
H16B	0.1451	−0.1005	0.2622	0.058*
C9	0.1995 (3)	0.2514 (3)	0.3694 (3)	0.0486 (7)
C10	0.2415 (3)	0.0708 (3)	0.1690 (3)	0.0417 (6)
C1	0.2966 (3)	0.5199 (3)	0.4082 (3)	0.0453 (7)
C7	0.3202 (3)	0.3150 (3)	0.2314 (3)	0.0456 (7)
C6	0.3667 (3)	0.5875 (3)	0.3505 (3)	0.0494 (7)
C11	0.0765 (3)	−0.1862 (3)	−0.0144 (3)	0.0496 (7)
H11A	0.0417	−0.1704	−0.0984	0.060*
H11B	0.0077	−0.1703	0.0325	0.060*
C17	−0.0465 (3)	−0.0517 (3)	0.2656 (3)	0.0520 (7)
H17A	−0.0666	0.0299	0.3320	0.062*
H17B	−0.0941	−0.0642	0.1683	0.062*
C2	0.2488 (4)	0.6038 (3)	0.5266 (3)	0.0595 (8)
H2A	0.3113	0.6105	0.6178	0.071*

H2B	0.1449	0.5502	0.5003	0.071*
C15	0.3358 (3)	−0.0959 (3)	0.0196 (3)	0.0571 (8)
H15A	0.4361	−0.0251	0.0891	0.069*
H15B	0.3044	−0.0759	−0.0620	0.069*
C12	0.0763 (4)	−0.3444 (3)	−0.0643 (3)	0.0644 (9)
H12A	−0.0248	−0.4141	−0.1324	0.077*
H12B	0.1072	−0.3617	0.0190	0.077*
C18	−0.1149 (3)	−0.1924 (4)	0.2660 (4)	0.0645 (9)
H18A	−0.0679	−0.1798	0.3635	0.077*
H18B	−0.0941	−0.2739	0.2002	0.077*
C5	0.4085 (4)	0.7505 (3)	0.3967 (3)	0.0626 (8)
H5A	0.5133	0.7899	0.4151	0.075*
H5B	0.3472	0.7643	0.3183	0.075*
C14	0.3392 (4)	−0.2539 (4)	−0.0343 (4)	0.0725 (10)
H14A	0.3794	−0.2700	0.0488	0.087*
H14B	0.4061	−0.2661	−0.0838	0.087*
C13	0.1840 (4)	−0.3699 (4)	−0.1381 (4)	0.0768 (10)
H13A	0.1892	−0.4695	−0.1644	0.092*
H13B	0.1478	−0.3622	−0.2268	0.092*
C3	0.2643 (5)	0.7599 (4)	0.5461 (5)	0.1045 (15)
H3A	0.1719	0.7538	0.4765	0.125*
H3B	0.2716	0.8223	0.6431	0.125*
C4	0.3868 (5)	0.8343 (4)	0.5298 (4)	0.0913 (13)
H4A	0.4786	0.8629	0.6139	0.110*
H4B	0.3737	0.9257	0.5323	0.110*
C19	−0.2845 (4)	−0.2338 (4)	0.2196 (4)	0.0811 (11)
H19A	−0.3059	−0.1533	0.2839	0.122*
H19B	−0.3224	−0.3228	0.2242	0.122*
H19C	−0.3323	−0.2514	0.1212	0.122*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0750 (6)	0.0451 (5)	0.0729 (5)	0.0160 (4)	0.0478 (5)	0.0270 (4)
N1	0.0518 (14)	0.0402 (13)	0.0494 (12)	0.0145 (11)	0.0279 (11)	0.0187 (11)
N2	0.0454 (13)	0.0426 (13)	0.0483 (11)	0.0153 (11)	0.0250 (10)	0.0232 (10)
C8	0.0480 (17)	0.0401 (16)	0.0414 (13)	0.0137 (13)	0.0174 (12)	0.0189 (12)
N3	0.0401 (13)	0.0422 (13)	0.0517 (12)	0.0151 (11)	0.0219 (10)	0.0177 (10)
O1	0.1052 (18)	0.0561 (13)	0.0683 (12)	0.0268 (12)	0.0617 (13)	0.0296 (11)
C16	0.0526 (18)	0.0486 (17)	0.0551 (15)	0.0170 (14)	0.0280 (14)	0.0311 (14)
C9	0.0568 (19)	0.0464 (17)	0.0439 (13)	0.0192 (14)	0.0244 (13)	0.0198 (13)
C10	0.0381 (15)	0.0428 (16)	0.0439 (13)	0.0150 (12)	0.0187 (12)	0.0192 (12)
C1	0.0423 (16)	0.0420 (16)	0.0427 (13)	0.0126 (13)	0.0145 (12)	0.0156 (12)
C7	0.0472 (17)	0.0401 (16)	0.0469 (13)	0.0130 (13)	0.0212 (12)	0.0182 (12)
C6	0.0464 (17)	0.0389 (16)	0.0548 (15)	0.0097 (13)	0.0203 (14)	0.0178 (13)
C11	0.0431 (17)	0.0446 (17)	0.0525 (15)	0.0118 (13)	0.0159 (13)	0.0197 (13)
C17	0.0505 (18)	0.0549 (19)	0.0659 (17)	0.0218 (15)	0.0342 (15)	0.0341 (15)
C2	0.070 (2)	0.0511 (19)	0.0530 (15)	0.0242 (16)	0.0302 (15)	0.0163 (14)

C15	0.0510 (18)	0.0562 (19)	0.0608 (16)	0.0195 (15)	0.0310 (15)	0.0190 (15)
C12	0.063 (2)	0.0397 (18)	0.0693 (18)	0.0085 (15)	0.0203 (16)	0.0165 (15)
C18	0.054 (2)	0.070 (2)	0.086 (2)	0.0175 (16)	0.0401 (17)	0.0470 (18)
C5	0.063 (2)	0.0448 (19)	0.0776 (19)	0.0149 (16)	0.0323 (17)	0.0268 (16)
C14	0.074 (2)	0.063 (2)	0.085 (2)	0.0379 (19)	0.0450 (19)	0.0251 (18)
C13	0.085 (3)	0.046 (2)	0.088 (2)	0.0257 (19)	0.040 (2)	0.0170 (17)
C3	0.129 (4)	0.057 (2)	0.139 (3)	0.038 (2)	0.095 (3)	0.026 (2)
C4	0.130 (4)	0.053 (2)	0.095 (3)	0.033 (2)	0.060 (3)	0.029 (2)
C19	0.062 (2)	0.082 (3)	0.100 (3)	0.014 (2)	0.042 (2)	0.042 (2)

Geometric parameters (Å, °)

S1—C7	1.728 (3)	C2—H2A	0.9700
S1—C6	1.735 (3)	C2—H2B	0.9700
N1—C10	1.302 (3)	C15—C14	1.513 (4)
N1—C7	1.367 (3)	C15—H15A	0.9700
N2—C10	1.388 (3)	C15—H15B	0.9700
N2—C9	1.420 (3)	C12—C13	1.521 (5)
N2—C16	1.477 (3)	C12—H12A	0.9700
C8—C7	1.373 (3)	C12—H12B	0.9700
C8—C9	1.433 (4)	C18—C19	1.521 (4)
C8—C1	1.436 (4)	C18—H18A	0.9700
N3—C10	1.394 (3)	C18—H18B	0.9700
N3—C15	1.470 (3)	C5—C4	1.475 (4)
N3—C11	1.485 (3)	C5—H5A	0.9700
O1—C9	1.225 (3)	C5—H5B	0.9700
C16—C17	1.524 (4)	C14—C13	1.515 (5)
C16—H16A	0.9700	C14—H14A	0.9700
C16—H16B	0.9700	C14—H14B	0.9700
C1—C6	1.350 (4)	C13—H13A	0.9700
C1—C2	1.510 (3)	C13—H13B	0.9700
C6—C5	1.492 (4)	C3—C4	1.417 (5)
C11—C12	1.506 (4)	C3—H3A	0.9700
C11—H11A	0.9700	C3—H3B	0.9700
C11—H11B	0.9700	C4—H4A	0.9700
C17—C18	1.498 (4)	C4—H4B	0.9700
C17—H17A	0.9700	C19—H19A	0.9600
C17—H17B	0.9700	C19—H19B	0.9600
C2—C3	1.518 (5)	C19—H19C	0.9600
C7—S1—C6	91.25 (13)	C14—C15—H15A	109.7
C10—N1—C7	115.3 (2)	N3—C15—H15B	109.7
C10—N2—C9	122.3 (2)	C14—C15—H15B	109.7
C10—N2—C16	122.7 (2)	H15A—C15—H15B	108.2
C9—N2—C16	114.9 (2)	C11—C12—C13	109.7 (3)
C7—C8—C9	117.7 (2)	C11—C12—H12A	109.7
C7—C8—C1	113.0 (2)	C13—C12—H12A	109.7
C9—C8—C1	129.3 (2)	C11—C12—H12B	109.7
C10—N3—C15	114.1 (2)	C13—C12—H12B	109.7
C10—N3—C11	116.6 (2)	H12A—C12—H12B	108.2

C15—N3—C11	110.6 (2)	C17—C18—C19	112.7 (3)
N2—C16—C17	113.6 (2)	C17—C18—H18A	109.1
N2—C16—H16A	108.8	C19—C18—H18A	109.1
C17—C16—H16A	108.8	C17—C18—H18B	109.1
N2—C16—H16B	108.8	C19—C18—H18B	109.1
C17—C16—H16B	108.8	H18A—C18—H18B	107.8
H16A—C16—H16B	107.7	C4—C5—C6	111.5 (3)
O1—C9—N2	119.4 (3)	C4—C5—H5A	109.3
O1—C9—C8	126.5 (2)	C6—C5—H5A	109.3
N2—C9—C8	114.1 (2)	C4—C5—H5B	109.3
N1—C10—N2	123.5 (2)	C6—C5—H5B	109.3
N1—C10—N3	119.2 (2)	H5A—C5—H5B	108.0
N2—C10—N3	117.2 (2)	C15—C14—C13	112.1 (3)
C6—C1—C8	111.9 (2)	C15—C14—H14A	109.2
C6—C1—C2	122.5 (3)	C13—C14—H14A	109.2
C8—C1—C2	125.6 (3)	C15—C14—H14B	109.2
N1—C7—C8	127.0 (3)	C13—C14—H14B	109.2
N1—C7—S1	121.77 (19)	H14A—C14—H14B	107.9
C8—C7—S1	111.2 (2)	C14—C13—C12	109.3 (3)
C1—C6—C5	124.8 (3)	C14—C13—H13A	109.8
C1—C6—S1	112.6 (2)	C12—C13—H13A	109.8
C5—C6—S1	122.5 (2)	C14—C13—H13B	109.8
N3—C11—C12	110.6 (2)	C12—C13—H13B	109.8
N3—C11—H11A	109.5	H13A—C13—H13B	108.3
C12—C11—H11A	109.5	C4—C3—C2	117.9 (3)
N3—C11—H11B	109.5	C4—C3—H3A	107.8
C12—C11—H11B	109.5	C2—C3—H3A	107.8
H11A—C11—H11B	108.1	C4—C3—H3B	107.8
C18—C17—C16	112.7 (2)	C2—C3—H3B	107.8
C18—C17—H17A	109.1	H3A—C3—H3B	107.2
C16—C17—H17A	109.1	C3—C4—C5	116.9 (3)
C18—C17—H17B	109.1	C3—C4—H4A	108.1
C16—C17—H17B	109.1	C5—C4—H4A	108.1
H17A—C17—H17B	107.8	C3—C4—H4B	108.1
C1—C2—C3	110.0 (3)	C5—C4—H4B	108.1
C1—C2—H2A	109.7	H4A—C4—H4B	107.3
C3—C2—H2A	109.7	C18—C19—H19A	109.5
C1—C2—H2B	109.7	C18—C19—H19B	109.5
C3—C2—H2B	109.7	H19A—C19—H19B	109.5
H2A—C2—H2B	108.2	C18—C19—H19C	109.5
N3—C15—C14	109.8 (3)	H19A—C19—H19C	109.5
N3—C15—H15A	109.7	H19B—C19—H19C	109.5
C10—N2—C16—C17	−110.2 (3)	C9—C8—C7—S1	−179.9 (2)
C9—N2—C16—C17	74.5 (3)	C1—C8—C7—S1	0.4 (3)
C10—N2—C9—O1	−177.9 (2)	C6—S1—C7—N1	178.1 (2)
C16—N2—C9—O1	−2.6 (4)	C6—S1—C7—C8	−0.1 (2)
C10—N2—C9—C8	1.2 (4)	C8—C1—C6—C5	179.3 (3)
C16—N2—C9—C8	176.4 (2)	C2—C1—C6—C5	1.4 (4)
C7—C8—C9—O1	177.1 (3)	C8—C1—C6—S1	0.4 (3)

C1—C8—C9—O1	−3.2 (5)	C2—C1—C6—S1	−177.6 (2)
C7—C8—C9—N2	−1.8 (4)	C7—S1—C6—C1	−0.1 (2)
C1—C8—C9—N2	177.9 (2)	C7—S1—C6—C5	−179.1 (3)
C7—N1—C10—N2	0.4 (4)	C10—N3—C11—C12	−166.3 (2)
C7—N1—C10—N3	−176.6 (2)	C15—N3—C11—C12	61.1 (3)
C9—N2—C10—N1	−0.5 (4)	N2—C16—C17—C18	165.4 (2)
C16—N2—C10—N1	−175.4 (2)	C6—C1—C2—C3	10.6 (4)
C9—N2—C10—N3	176.6 (2)	C8—C1—C2—C3	−167.1 (3)
C16—N2—C10—N3	1.7 (4)	C10—N3—C15—C14	167.6 (2)
C15—N3—C10—N1	18.8 (3)	C11—N3—C15—C14	−58.6 (3)
C11—N3—C10—N1	−112.1 (3)	N3—C11—C12—C13	−59.2 (3)
C15—N3—C10—N2	−158.4 (2)	C16—C17—C18—C19	−179.6 (2)
C11—N3—C10—N2	70.7 (3)	C1—C6—C5—C4	9.4 (5)
C7—C8—C1—C6	−0.5 (3)	S1—C6—C5—C4	−171.8 (3)
C9—C8—C1—C6	179.8 (3)	N3—C15—C14—C13	56.7 (4)
C7—C8—C1—C2	177.4 (2)	C15—C14—C13—C12	−55.1 (4)
C9—C8—C1—C2	−2.3 (5)	C11—C12—C13—C14	55.6 (4)
C10—N1—C7—C8	−1.2 (4)	C1—C2—C3—C4	−35.9 (5)
C10—N1—C7—S1	−179.1 (2)	C2—C3—C4—C5	50.3 (6)
C9—C8—C7—N1	2.0 (4)	C6—C5—C4—C3	−34.3 (5)
C1—C8—C7—N1	−177.7 (2)		

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C17—H17A⋯O1	0.97	2.54	3.035 (4)	112
C4—H4A⋯Cg2[i]	0.97	3.00	3.854 (5)	148
C11—H11A⋯Cg2[ii]	0.97	2.76	3.408 (3)	125
C12—H12A⋯Cg1[ii]	0.97	2.92	3.764 (4)	146

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

Fig. 1

Fig. 2

(a) n-BuNCO / CH₂Cl₂ (b)

piperidine

NaOEt / EtOH

(I)