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3-Amino-1-(thiophen-2-yl)-9,10-dihydrophenanthrene-2,4-dicarbonitrile

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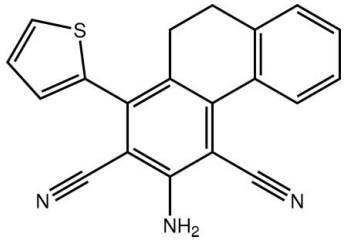
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.066; wR factor = 0.164; data-to-parameter ratio = 11.9.

In the title compound, $C_{20}H_{13}N_3S$, the partially saturated ring adopts a twisted half-boat conformation with the methylene C atom closest to the aminobenzene ring lying 0.690 (6) Å out of the plane defined by the five remaining atoms. The dihydrophenanthrene residue has a folded conformation [dihedral angle between the outer benzene rings = 26.27 (18)°]. The thiophen-2-yl ring forms a dihedral angle of 63.76 (19)° with the benzene ring to which it is attached. In the crystal, inversion dimers linked by pairs of N—H···N hydrogen bonds generate $R_2^2(12)$ loops. The dimers are linked into layers in the bc plane by weak C—H···π interactions. The thiophen-2-yl ring is disordered over two essentially coplanar but opposite orientations in a 0.918 (4):0.082 (4) ratio.

Related literature

For background to the biological activity of related dicarbonitrile compounds, see: Aly *et al.* (1991); Rostom *et al.* (2011). For related structures, see: Asiri *et al.* (2011*a*,*b*).



Experimental

Crystal data

$C_{20}H_{13}N_3S$
M_r = 327.39
Monoclinic, $P2_1/c$
a = 9.7882 (10) Å
b = 7.1199 (7) Å
c = 22.746 (3) Å
β = 93.171 (11)°
V = 1582.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 100 K
0.30 × 0.06 × 0.03 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.940, T_{max} = 0.994
5527 measured reflections
2805 independent reflections
1778 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.164
S = 1.03
2805 reflections
236 parameters
56 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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

*Cg*1 is the centroid of the C4–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···N3^{i}	0.88 (3)	2.18 (3)	3.016 (5)	160 (3)
C6—H6···*Cg*1^{ii}	0.95	2.85	3.660 (5)	144

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6670).

References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Aly, A. S., El-Ezabawy, S. R. & Abdel-Fattah, A. M. (1991). *Egypt. J. Pharm. Sci.* **32**, 827–834.
Asiri, A. M., Al-Youbi, A. O., Faidallah, H. M., Ng, S. W. & Tiekink, E. R. T. (2011*a*). *Acta Cryst.* E**67**, o2438.
Asiri, A. M., Al-Youbi, A. O., Faidallah, H. M., Ng, S. W. & Tiekink, E. R. T. (2011*b*). *Acta Cryst.* E**67**, o2449.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.

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Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Rostom, S. A. F., Faidallah, S. M. & Al Saadi, M. S. (2011). *Med. Chem. Res.* **20**, 1260–1272.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2012). E**68**, o1027–o1028 [doi:10.1107/S1600536812010033]

3-Amino-1-(thiophen-2-yl)-9,10-dihydrophenanthrene-2,4-dicarbonitrile

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Comment

The crystallographic investigation of the title compound, (I), was motivated by reports of the biological activity of related compounds (Aly *et al.*, 1991; Rostom *et al.*, 2011) and allied crystal structure investigations (Asiri *et al.*, 2011*a*; Asiri *et al.*, 2011*b*).

In (I), Fig. 1, the partially saturated ring adopts a twisted half boat conformation with the C2 atom lying 0.690 (6) Å out of the plane defined by the five remaining atoms [r.m.s. deviation = 0.1032 Å; maximum deviations = 0.076 (3) Å for the C9 atom and -0.160 (3) Å for the C10 atom]. The dihedral angle between the adjacent benzene rings = 26.27 (18)° indicating a fold in the molecule. The thiophen-2-yl ring forms a dihedral angle of 63.76 (19)° with the benzene to which it is attached.

In the crystal packing, centrosymmetric aggregates are formed *via* N—H···N hydrogen bonds leading to 12-membered $\{\cdots HNC_3N\}_2$ synthons, Table 1. These are linked into layers in the *bc* plane by C—H···π interactions, Fig. 2 and Table 1. These stack along the *a* axis with no specific interactions between them.

Experimental

A mixture of thiophene-2-cabaldehyde (1.1 g, 10 mmol), 1-tetralone (1.46 g, 10 mmol), malononitrile (0.66 g, 10 mmol) and ammonium acetate (6.2 g, 80 mmol) in absolute ethanol (50 ml) was refluxed for 6 h. The reaction mixture was allowed to cool, and the formed precipitate was filtered, washed with water, dried and recrystallized from ethanol as orange prisms. Yield: 69%. *M*.pt: 451–453 K.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 0.99 Å, U_{iso}(H) = 1.2U_{eq}(C)] and were included in the refinement in the riding model approximation.

The amino H-atoms were located in a difference Fourier map, and were refined with a distance restraint of N—H = 0.88±0.01 Å; U_{iso} were refined.

The thienyl ring is disordered over two positions in a 0.918 (4): 0.082 (4) ratio. The S—C distances were restrained to 1.71±0.01 Å, the formal C—C single-bond distances to 1.42±0.01 Å and the formal C═C double-bond distances to 1.42±0.01 Å. Additionally, the 1,3-related distances were restrained to within 0.01 Å of each other. Because pairs of atoms are close to each other, the U_{aniso} of the C18′ atom were equated to those of the S1 atom (as well as the C19′/C20, C20′/C19′ and C18′/S1 pairs). The anisotropic displacement parameters were tightly restrained to be nearly isotropic.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

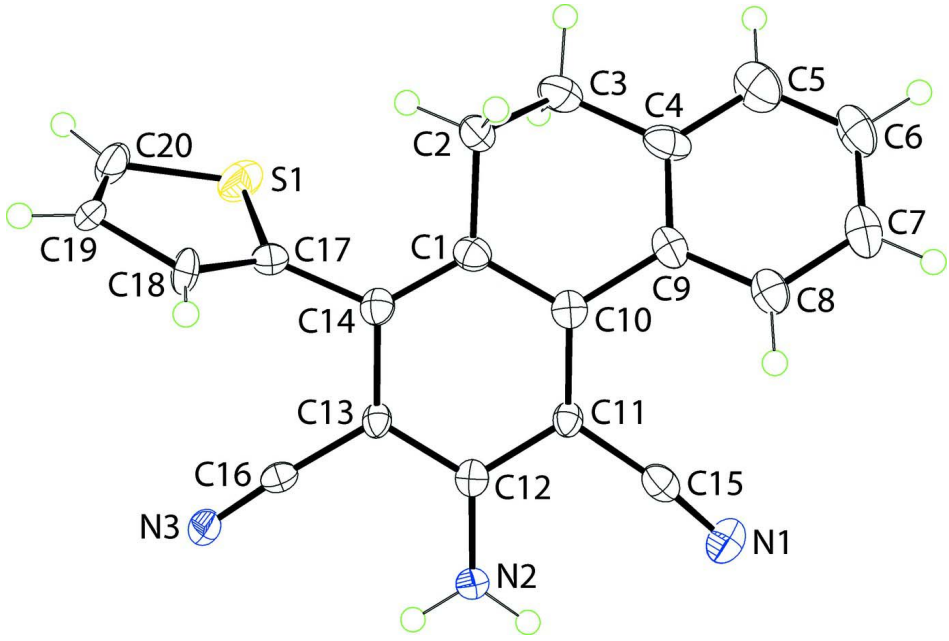

Figure 1

The molecular structure of (I) showing displacement ellipsoids at the 50% probability level.

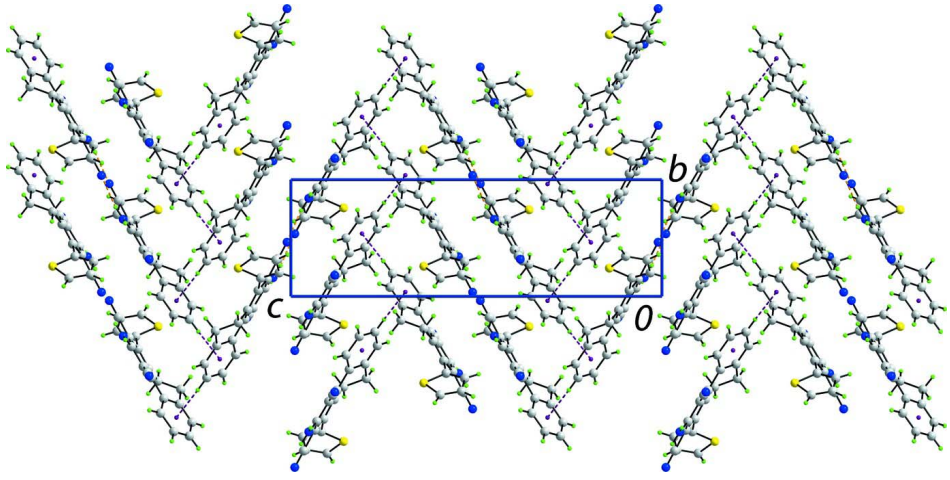

Figure 2

A view of the supramolecular layer in the *bc* plane in (I). The C—H···O and C—H···π interactions are shown as orange and purple dashed lines, respectively.

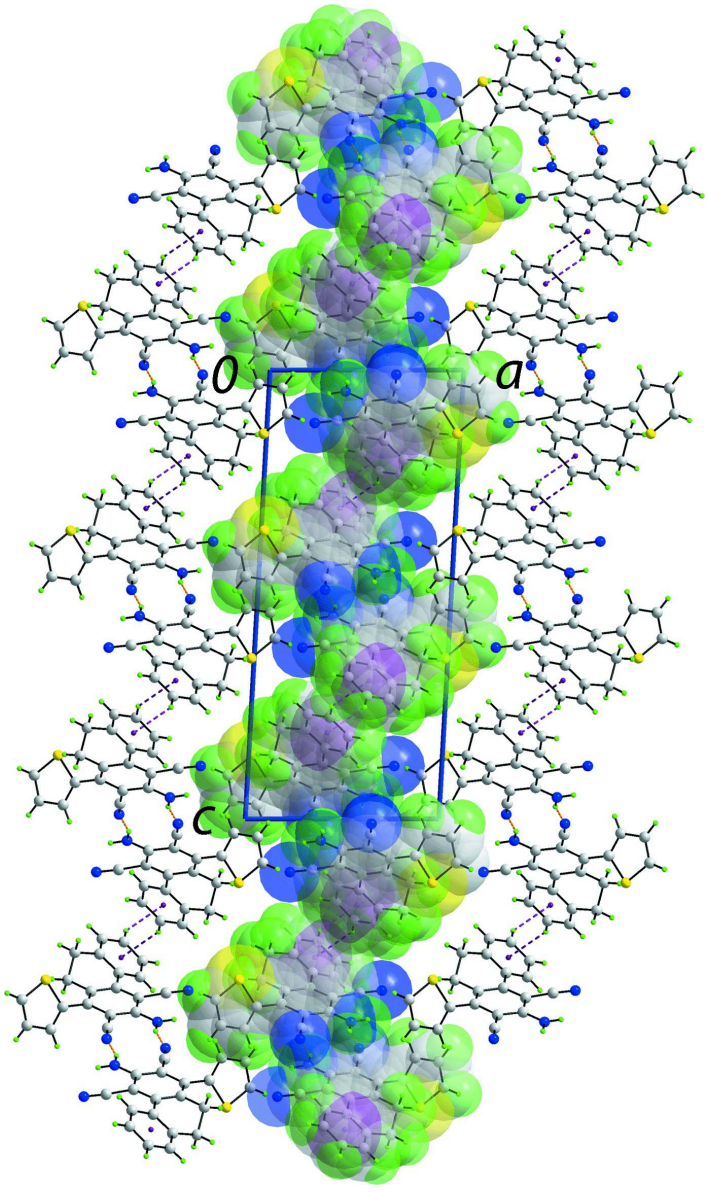

Figure 3

A view in projection down the *b* axis of the unit-cell contents of (I) showing the stacking of layers. The C—H···O and C—H···π interactions are shown as orange and purple dashed lines, respectively. One layer is highlighted in space-filling mode.

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Crystal data

$C_{20}H_{13}N_3S$
M_r = 327.39
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 9.7882 (10) Å
b = 7.1199 (7) Å
c = 22.746 (3) Å
β = 93.171 (11)°
V = 1582.8 (3) Å^3
Z = 4
F(000) = 680
D_x = 1.374 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1132 reflections

θ = 2.7–25.0°
μ = 0.21 mm^{-1}
T = 100 K

Prism, orange
0.30 × 0.06 × 0.03 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)

T_{min} = 0.940, T_{max} = 0.994
5527 measured reflections
2805 independent reflections
1778 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 25.1°, θ_{min} = 2.7°
h = −9→11
k = −8→6
l = −19→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.164
S = 1.03
2805 reflections
236 parameters
56 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
$w = 1/[\sigma^2(F_o^2) + (0.0559P)^2 + 1.2744P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.98458 (11)	0.25812 (17)	0.64193 (6)	0.0331 (4)	0.918 (4)
S1′	0.976 (2)	0.275 (3)	0.5229 (7)	0.0358 (13)	0.082 (4)
N1	0.2456 (3)	0.6816 (5)	0.61810 (16)	0.0329 (9)	
N2	0.3958 (3)	0.3401 (5)	0.54813 (14)	0.0213 (7)	
H1	0.402 (4)	0.236 (3)	0.5276 (15)	0.026*	
H2	0.3108 (16)	0.373 (5)	0.5535 (17)	0.026*	
N3	0.6533 (3)	0.0358 (5)	0.51041 (15)	0.0255 (8)	
C1	0.7477 (4)	0.6177 (5)	0.61652 (16)	0.0213 (9)	
C2	0.8711 (4)	0.7249 (5)	0.64154 (18)	0.0262 (9)	
H2A	0.8904	0.8322	0.6156	0.031*	
H2B	0.9523	0.6418	0.6438	0.031*	
C3	0.8422 (4)	0.7966 (6)	0.70321 (18)	0.0329 (11)	
H3A	0.8278	0.6888	0.7297	0.039*	
H3B	0.9215	0.8696	0.7196	0.039*	
C4	0.7144 (4)	0.9209 (5)	0.69949 (19)	0.0295 (10)	
C5	0.7052 (5)	1.0784 (6)	0.73318 (19)	0.0380 (11)	
H5	0.7768	1.1082	0.7615	0.046*	
C6	0.5919 (4)	1.1956 (6)	0.72634 (19)	0.0329 (11)	
H6	0.5848	1.3024	0.7510	0.040*	
C7	0.4905 (4)	1.1578 (5)	0.68423 (18)	0.0289 (10)	
H7	0.4145	1.2402	0.6792	0.035*	
C8	0.4980 (4)	0.9990 (5)	0.64865 (18)	0.0260 (10)	

H8	0.4288	0.9752	0.6187	0.031*	
C9	0.6089 (4)	0.8743 (5)	0.65742 (16)	0.0221 (9)	
C10	0.6174 (4)	0.6957 (5)	0.62403 (16)	0.0201 (9)	
C11	0.5006 (3)	0.5995 (5)	0.60216 (16)	0.0173 (8)	
C12	0.5094 (4)	0.4290 (5)	0.57009 (16)	0.0184 (8)	
C13	0.6410 (3)	0.3549 (5)	0.56377 (16)	0.0170 (8)	
C14	0.7610 (3)	0.4495 (5)	0.58825 (16)	0.0202 (9)	
C15	0.3602 (4)	0.6548 (5)	0.61278 (17)	0.0237 (9)	
C16	0.6518 (3)	0.1773 (5)	0.53443 (16)	0.0193 (9)	
C17	0.8889 (3)	0.3421 (4)	0.58171 (17)	0.0234 (9)	
C18	0.9449 (5)	0.2974 (7)	0.5317 (2)	0.0358 (13)	0.918 (4)
H18	0.9073	0.3340	0.4940	0.043*	0.918 (4)
C18′	0.953 (2)	0.282 (3)	0.6333 (6)	0.0331 (4)	0.08
H18′	0.9194	0.3055	0.6710	0.040*	0.082 (4)
C19	1.0686 (4)	0.1878 (6)	0.5402 (2)	0.0325 (13)	0.918 (4)
H19	1.1203	0.1430	0.5089	0.039*	0.918 (4)
C19′	1.0749 (19)	0.179 (3)	0.6240 (13)	0.0361 (13)	0.082 (4)
H19′	1.1321	0.1274	0.6549	0.043*	0.082 (4)
C20	1.1022 (4)	0.1564 (6)	0.5979 (2)	0.0361 (13)	0.918 (4)
H20	1.1802	0.0875	0.6122	0.043*	0.918 (4)
C20′	1.1006 (14)	0.1645 (15)	0.5660 (15)	0.0325 (13)	0.08
H20′	1.1771	0.1011	0.5514	0.039*	0.082 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0230 (7)	0.0336 (7)	0.0420 (8)	0.0037 (5)	−0.0030 (5)	0.0073 (6)
S1′	0.021 (3)	0.045 (3)	0.043 (3)	0.005 (2)	0.015 (2)	−0.020 (2)
N1	0.025 (2)	0.035 (2)	0.038 (2)	0.0062 (16)	0.0029 (17)	0.0003 (17)
N2	0.0165 (16)	0.0228 (17)	0.0244 (19)	−0.0001 (15)	−0.0003 (14)	−0.0056 (15)
N3	0.0169 (17)	0.0238 (19)	0.036 (2)	0.0003 (14)	0.0039 (15)	−0.0071 (17)
C1	0.022 (2)	0.021 (2)	0.021 (2)	−0.0035 (17)	0.0023 (16)	0.0002 (17)
C2	0.024 (2)	0.023 (2)	0.032 (2)	−0.0028 (18)	0.0044 (18)	−0.0083 (19)
C3	0.032 (2)	0.035 (2)	0.031 (3)	−0.005 (2)	−0.0030 (19)	−0.010 (2)
C4	0.034 (2)	0.021 (2)	0.032 (3)	−0.0097 (19)	−0.0055 (19)	0.0035 (19)
C5	0.047 (3)	0.041 (3)	0.026 (3)	−0.004 (2)	0.012 (2)	−0.006 (2)
C6	0.047 (3)	0.027 (2)	0.026 (2)	−0.002 (2)	0.018 (2)	−0.007 (2)
C7	0.040 (2)	0.020 (2)	0.029 (2)	0.0020 (19)	0.016 (2)	0.0036 (19)
C8	0.033 (2)	0.022 (2)	0.023 (2)	−0.0007 (19)	0.0085 (18)	−0.0005 (18)
C9	0.030 (2)	0.0173 (19)	0.020 (2)	−0.0026 (18)	0.0090 (17)	0.0006 (17)
C10	0.023 (2)	0.019 (2)	0.018 (2)	−0.0003 (17)	0.0038 (16)	0.0037 (16)
C11	0.0177 (19)	0.0141 (18)	0.021 (2)	0.0009 (16)	0.0038 (16)	0.0016 (16)
C12	0.021 (2)	0.0190 (19)	0.015 (2)	0.0010 (17)	0.0041 (16)	0.0029 (16)
C13	0.0161 (19)	0.0154 (18)	0.020 (2)	0.0000 (16)	0.0063 (15)	0.0004 (16)
C14	0.020 (2)	0.020 (2)	0.021 (2)	−0.0004 (16)	0.0051 (16)	0.0016 (17)
C15	0.032 (2)	0.018 (2)	0.020 (2)	−0.0007 (18)	−0.0020 (18)	−0.0004 (17)
C16	0.0144 (19)	0.022 (2)	0.021 (2)	−0.0030 (16)	0.0006 (16)	0.0018 (18)
C17	0.0176 (19)	0.023 (2)	0.030 (2)	−0.0044 (17)	0.0021 (17)	−0.0049 (18)
C18	0.021 (3)	0.045 (3)	0.043 (3)	0.005 (2)	0.015 (2)	−0.020 (2)

C18′	0.0230 (7)	0.0336 (7)	0.0420 (8)	0.0037 (5)	−0.0030 (5)	0.0073 (6)
C19	0.011 (2)	0.033 (2)	0.053 (3)	0.0018 (19)	0.000 (2)	−0.021 (2)
C19′	0.018 (2)	0.027 (2)	0.064 (4)	0.0064 (19)	0.004 (2)	−0.008 (3)
C20	0.018 (2)	0.027 (2)	0.064 (4)	0.0064 (19)	0.004 (2)	−0.008 (3)
C20′	0.011 (2)	0.033 (2)	0.053 (3)	0.0018 (19)	0.000 (2)	−0.021 (2)

Geometric parameters (Å, º)

S1—C17	1.723 (4)	C7—C8	1.395 (5)
S1—C20	1.727 (5)	C7—H7	0.9500
S1′—C17	1.695 (9)	C8—C9	1.408 (5)
S1′—C20′	1.713 (10)	C8—H8	0.9500
N1—C15	1.150 (5)	C9—C10	1.486 (5)
N2—C12	1.351 (5)	C10—C11	1.400 (5)
N2—H1	0.882 (10)	C11—C12	1.422 (5)
N2—H2	0.880 (10)	C11—C15	1.462 (5)
N3—C16	1.146 (5)	C12—C13	1.407 (5)
C1—C14	1.369 (5)	C13—C16	1.437 (5)
C1—C10	1.410 (5)	C13—C14	1.439 (5)
C1—C2	1.513 (5)	C14—C17	1.481 (5)
C2—C3	1.534 (5)	C17—C18	1.329 (6)
C2—H2A	0.9900	C17—C18′	1.367 (9)
C2—H2B	0.9900	C18—C19	1.445 (6)
C3—C4	1.531 (6)	C18—H18	0.9500
C3—H3A	0.9900	C18′—C19′	1.427 (9)
C3—H3B	0.9900	C18′—H18′	0.9500
C4—C5	1.364 (6)	C19—C20	1.354 (6)
C4—C9	1.408 (5)	C19—H19	0.9500
C5—C6	1.390 (6)	C19′—C20′	1.360 (9)
C5—H5	0.9500	C19′—H19′	0.9500
C6—C7	1.367 (6)	C20—H20	0.9500
C6—H6	0.9500	C20′—H20′	0.9500
C17—S1—C20	92.0 (2)	C1—C10—C9	118.4 (3)
C17—S1′—C20′	93.0 (5)	C10—C11—C12	121.9 (3)
C12—N2—H1	121 (2)	C10—C11—C15	124.5 (3)
C12—N2—H2	126 (3)	C12—C11—C15	113.5 (3)
H1—N2—H2	113 (4)	N2—C12—C13	121.8 (3)
C14—C1—C10	120.8 (3)	N2—C12—C11	121.2 (3)
C14—C1—C2	121.6 (3)	C13—C12—C11	117.0 (3)
C10—C1—C2	117.7 (3)	C12—C13—C16	117.9 (3)
C1—C2—C3	109.1 (3)	C12—C13—C14	121.2 (3)
C1—C2—H2A	109.9	C16—C13—C14	120.9 (3)
C3—C2—H2A	109.9	C1—C14—C13	119.6 (3)
C1—C2—H2B	109.9	C1—C14—C17	127.0 (3)
C3—C2—H2B	109.9	C13—C14—C17	113.3 (3)
H2A—C2—H2B	108.3	N1—C15—C11	172.9 (4)
C4—C3—C2	109.5 (3)	N3—C16—C13	176.6 (4)
C4—C3—H3A	109.8	C18—C17—C14	126.9 (4)
C2—C3—H3A	109.8	C18′—C17—C14	115.1 (11)

C4—C3—H3B	109.8	C18′—C17—S1′	111.3 (7)
C2—C3—H3B	109.8	C14—C17—S1′	133.6 (8)
H3A—C3—H3B	108.2	C18—C17—S1	111.5 (3)
C5—C4—C9	120.4 (4)	C14—C17—S1	121.6 (3)
C5—C4—C3	121.6 (4)	C17—C18—C19	113.4 (4)
C9—C4—C3	117.9 (4)	C17—C18—H18	123.3
C4—C5—C6	120.5 (4)	C19—C18—H18	123.3
C4—C5—H5	119.7	C17—C18′—C19′	112.4 (6)
C6—C5—H5	119.7	C17—C18′—H18′	123.8
C7—C6—C5	120.2 (4)	C19′—C18′—H18′	123.8
C7—C6—H6	119.9	C20—C19—C18	112.1 (4)
C5—C6—H6	119.9	C20—C19—H19	124.0
C6—C7—C8	120.5 (4)	C18—C19—H19	124.0
C6—C7—H7	119.8	C20′—C19′—C18′	112.7 (7)
C8—C7—H7	119.8	C20′—C19′—H19′	123.7
C7—C8—C9	119.6 (4)	C18′—C19′—H19′	123.7
C7—C8—H8	120.2	C19—C20—S1	111.1 (3)
C9—C8—H8	120.2	C19—C20—H20	124.5
C8—C9—C4	118.6 (4)	S1—C20—H20	124.5
C8—C9—C10	122.1 (3)	C19′—C20′—S1′	110.8 (8)
C4—C9—C10	119.3 (3)	C19′—C20′—H20′	124.6
C11—C10—C1	119.4 (3)	S1′—C20′—H20′	124.6
C11—C10—C9	122.2 (3)		

C14—C1—C2—C3	−135.7 (4)	C2—C1—C14—C13	−178.3 (3)
C10—C1—C2—C3	43.4 (5)	C10—C1—C14—C17	−174.1 (3)
C1—C2—C3—C4	−58.1 (4)	C2—C1—C14—C17	5.0 (6)
C2—C3—C4—C5	−142.1 (4)	C12—C13—C14—C1	−2.2 (5)
C2—C3—C4—C9	34.1 (5)	C16—C13—C14—C1	−179.3 (3)
C9—C4—C5—C6	−0.3 (6)	C12—C13—C14—C17	174.9 (3)
C3—C4—C5—C6	175.8 (4)	C16—C13—C14—C17	−2.2 (5)
C4—C5—C6—C7	−2.3 (6)	C1—C14—C17—C18	−118.5 (4)
C5—C6—C7—C8	1.5 (6)	C13—C14—C17—C18	64.6 (3)
C6—C7—C8—C9	1.8 (6)	C1—C14—C17—C18′	62.6 (12)
C7—C8—C9—C4	−4.3 (5)	C13—C14—C17—C18′	−114.3 (11)
C7—C8—C9—C10	175.3 (3)	C1—C14—C17—S1′	−117.4 (11)
C5—C4—C9—C8	3.6 (6)	C13—C14—C17—S1′	65.7 (11)
C3—C4—C9—C8	−172.7 (4)	C1—C14—C17—S1	61.6 (4)
C5—C4—C9—C10	−176.1 (4)	C13—C14—C17—S1	−115.3 (3)
C3—C4—C9—C10	7.6 (5)	C20′—S1′—C17—C18	−173 (8)
C14—C1—C10—C11	−0.1 (5)	C20′—S1′—C17—C18′	0.1 (3)
C2—C1—C10—C11	−179.2 (3)	C20′—S1′—C17—C14	−179.92 (19)
C14—C1—C10—C9	177.3 (3)	C20′—S1′—C17—S1	1.0 (10)
C2—C1—C10—C9	−1.8 (5)	C20—S1—C17—C18	−0.9 (2)
C8—C9—C10—C11	−28.0 (6)	C20—S1—C17—C18′	171 (9)
C4—C9—C10—C11	151.7 (4)	C20—S1—C17—C14	178.99 (15)
C8—C9—C10—C1	154.7 (4)	C20—S1—C17—S1′	−1.8 (8)
C4—C9—C10—C1	−25.6 (5)	C18′—C17—C18—C19	0.2 (14)
C1—C10—C11—C12	−3.0 (5)	C14—C17—C18—C19	−178.7 (2)

C9—C10—C11—C12	179.8 (3)	S1′—C17—C18—C19	8 (7)
C1—C10—C11—C15	172.9 (3)	S1—C17—C18—C19	1.2 (3)
C9—C10—C11—C15	−4.3 (6)	C18—C17—C18′—C19′	1.0 (12)
C10—C11—C12—N2	−178.5 (3)	C14—C17—C18′—C19′	180.0 (3)
C15—C11—C12—N2	5.2 (5)	S1′—C17—C18′—C19′	0.0 (3)
C10—C11—C12—C13	3.3 (5)	S1—C17—C18′—C19′	−8 (9)
C15—C11—C12—C13	−173.0 (3)	C17—C18—C19—C20	−1.0 (4)
N2—C12—C13—C16	−1.7 (5)	C17—C18′—C19′—C20′	−0.1 (5)
C11—C12—C13—C16	176.5 (3)	C18—C19—C20—S1	0.2 (4)
N2—C12—C13—C14	−178.9 (3)	C17—S1—C20—C19	0.4 (3)
C11—C12—C13—C14	−0.7 (5)	C18′—C19′—C20′—S1′	0.1 (6)
C10—C1—C14—C13	2.6 (6)	C17—S1′—C20′—C19′	−0.1 (5)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1···N3^{i}	0.88 (3)	2.18 (3)	3.016 (5)	160 (3)
C6—H6···*Cg*1^{ii}	0.95	2.85	3.660 (5)	144

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, *y*+1/2, −*z*+3/2.