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N-(12-Amino-9,10-dihydro-9,10-ethanoanthracen-11-yl)-4-methylbenzenesulfonamide

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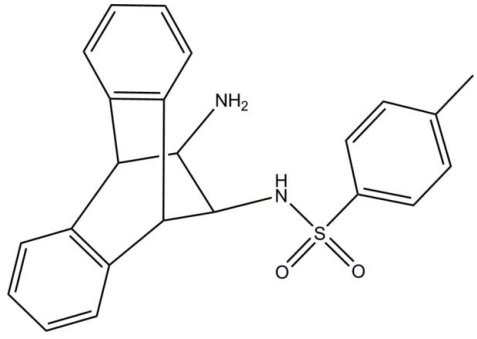
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.066; data-to-parameter ratio = 12.5.

The title compound, $C_{23}H_{22}N_2O_2S$, crystallizes with the 4-methylbenzenesulfonamide entity oriented towards the center of the bridgehead C atoms with a C—N—S—C torsion angle of −61.3 (2)°. The molecule features an intramolecular N—H···N hydrogen bond. Weak C—H···O and C—H···π interactions aid in forming the three-dimensional supramolecular structure.

Related literature

For chiral ligand devlopment, see: Abdel-Aziz *et al.* (2000, 2001, 2004); Matsunaga *et al.* (2005); Seo *et al.* (2001). For similar compounds and applications, see: Yamakuchi *et al.* (2005); Matsunaga *et al.* (2005); Abdel-Aziz *et al.* (2004). For the synthesis of the title compound, see: Matsunaga *et al.* (2005).



Experimental

Crystal data

$C_{23}H_{22}N_2O_2S$
M_r = 390.49
Monoclinic, $P2_1$
a = 8.9362 (2) Å
b = 6.8766 (2) Å
c = 15.5039 (4) Å
β = 91.540 (1)°
V = 952.38 (4) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 1.68 mm^{-1}
T = 100 K
0.25 × 0.13 × 0.03 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.83, T_{max} = 0.95
16018 measured reflections
3531 independent reflections
3255 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.066
S = 1.07
3531 reflections
282 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1582 Friedel pairs
Absolute structure parameter: 0.036 (13)

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

*Cg*1 is the centroid of the C3–C8 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···N2	0.90 (2)	2.04 (2)	2.592 (2)	117.9 (17)
C11—H11···*Cg*1^{i}	0.95	2.87	3.712 (2)	149
C5—H5···O1^{ii}	0.95	2.58	3.269 (2)	129
C12—H12···O1^{iii}	0.95	2.52	3.446 (2)	166
C23—H23*A*···O1^{iv}	0.98	2.51	3.259 (3)	133

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

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2012); software used to prepare material for publication: *SHELXTL* (Bruker, 2012).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5292).

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N-(12-Amino-9,10-dihydro-9,10-ethanoanthracen-11-yl)-4-methylbenzenesulfonamide

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S1. Experimental

S1.1. Synthesis and crystallization

The title compound was prepared by the literature method (Matsunaga *et al.*, 2005) and recrystallized from CH_2Cl_2/EtOH as colourless plates.

S1.2. Refinement

H-atoms attached to the bridgehead carbon atoms and to nitrogen were located and refined. The remainder were placed in calculated positions (C—H = 0.95 - 0.98 Å) and included as riding contributions with isotropic displacement parameters 1.2–1.5 times those of the attached carbon atoms.

S2. Results and discussion

The development of chiral ligands for asymmetric catalytic reactions is a subject of considerable interest in the field of asymmetric synthesis (Abdel-Aziz *et al.*, 2000, 2001, 2004; Matsunaga *et al.*, 2005; Seo *et al.*, 2001). As part of our onging program of drug design and discovery we report the structure of the title compound. Some applications of related compounds have been reported (Yamakuchi *et al.*, 2005; Matsunaga *et al.*, 2005; Abdel-Aziz *et al.*, 2004). The 4-methylbenzenesulfonamide entity is oriented towards the center of the bridgehead carbon atoms (C1, C16), partly due to the N1—H1N···N2 interaction, as indicated by the C1—N1—S1—C17 torsion angle of -61.3 (2)°. The dihedral angle between the benzene ring (C17–C22) and the mean plane of the C1/C2/C9/C16 unit is 87.78 (7)°. The packing of the molecules is aided by weak C—H···O hydrogen bonds as well as a C—H···π interaction between C11—H11 and the centroid of the C3–C8 ring at -*x*, -0.5 + *y*, 1 - *z* forming the three-dimensional supramolecular structure (Table 1 and Fig. 2).

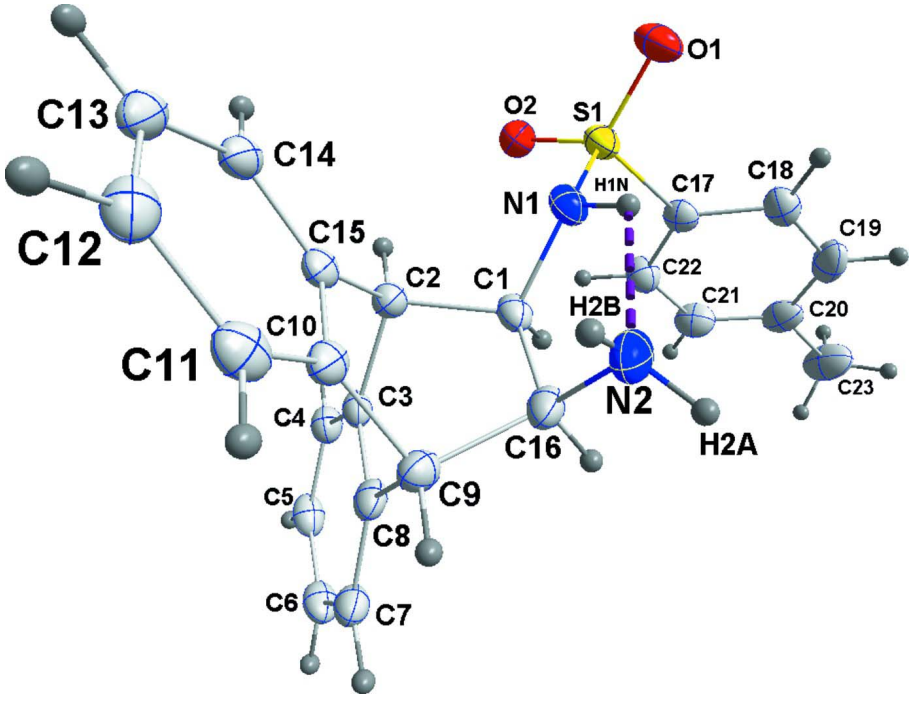

Figure 1

Perspective view of the title molecule showing the intramolecular hydrogen bond. Displacement ellipsoids are drawn at the 50% probability level.

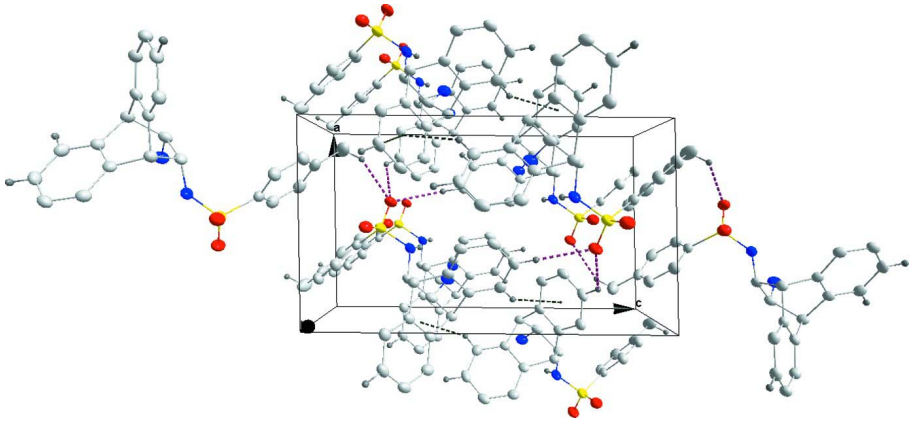

Figure 2

Packing diagram viewed down *b* with intermolecular interactions shown as dotted lines (C—H···O, purple; C—H···π, green).

N-(12-Amino-9,10-dihydro-9,10-ethanoanthracen-11-yl)-4-methylbenzenesulfonamide

Crystal data

$C_{23}H_{22}N_2O_2S$
M_r = 390.49
Monoclinic, $P2_1$
a = 8.9362 (2) Å
b = 6.8766 (2) Å
c = 15.5039 (4) Å
β = 91.540 (1)°
V = 952.38 (4) Å^3
Z = 2
$F(000)$ = 412
D_x = 1.362 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å

Cell parameters from 9974 reflections
θ = 2.9–69.8°
μ = 1.68 mm^{-1}
T = 100 K
Plate, colourless
0.25 × 0.13 × 0.03 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.83, T_{max} = 0.95
16018 measured reflections
3531 independent reflections
3255 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 69.8°, θ_{min} = 2.9°
h = −10→10
k = −8→8
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.066
S = 1.07
3531 reflections
282 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0302P)^2 + 0.1321P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1582 Friedel pairs
Absolute structure parameter: 0.036 (13)

Special details

Experimental. The diffraction data were obtained from 8 sets of 340 frames, each of width 0.5° in ω, collected at φ = 0.00, 90.00, 180.00 and 270.00° and at 2θ = -50.00 and -90.00° and 4 sets of 340 frames, each of width 0.5° in ω collected at 2θ = -90.00° and φ = 45.00, 135.00, 225.00 and 315.00°. The scan time was 20 sec/frame.

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. H-atoms attached to the bridgehead carbon atoms and to nitrogen were located and refined. The remainder were placed in calculated positions (C—H = 0.95 - 0.98 Å) and included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached carbon atoms.

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.47223 (4)	0.59364 (7)	0.19075 (3)	0.02581 (11)
O1	0.60539 (14)	0.4887 (2)	0.21492 (8)	0.0344 (3)
O2	0.48013 (14)	0.79099 (19)	0.16197 (8)	0.0314 (3)
N1	0.36963 (15)	0.5913 (3)	0.27530 (9)	0.0254 (3)
H1N	0.370 (2)	0.473 (3)	0.3000 (13)	0.036 (6)*

N2	0.19878 (19)	0.4067 (2)	0.38013 (13)	0.0310 (4)
H2A	0.149 (3)	0.296 (4)	0.3825 (16)	0.053 (7)*
H2B	0.228 (2)	0.440 (3)	0.4308 (15)	0.036 (6)*
C1	0.21944 (19)	0.6768 (3)	0.27202 (12)	0.0239 (4)
H1	0.1753 (18)	0.667 (3)	0.2111 (11)	0.020 (5)*
C2	0.22327 (19)	0.8966 (3)	0.29742 (11)	0.0223 (4)
H2	0.295 (2)	0.963 (3)	0.2608 (12)	0.024 (5)*
C3	0.06161 (19)	0.9626 (2)	0.28635 (11)	0.0213 (4)
C4	0.00777 (18)	1.1038 (3)	0.22989 (10)	0.0253 (4)
H4	0.0742	1.1748	0.1949	0.03*
C5	−0.1461 (2)	1.1400 (3)	0.22537 (11)	0.0276 (4)
H5	−0.1842	1.2399	0.1886	0.033*
C6	−0.2433 (2)	1.0319 (3)	0.27387 (12)	0.0280 (4)
H6	−0.348	1.0544	0.2683	0.034*
C7	−0.18973 (19)	0.8909 (3)	0.33066 (12)	0.0252 (4)
H7	−0.257	0.8172	0.364	0.03*
C8	−0.03595 (19)	0.8586 (2)	0.33827 (11)	0.0224 (4)
C9	0.04146 (19)	0.7098 (3)	0.39548 (12)	0.0229 (4)
H9	−0.0255 (19)	0.644 (3)	0.4339 (11)	0.021 (5)*
C10	0.16898 (18)	0.8096 (2)	0.44541 (11)	0.0208 (4)
C11	0.1950 (2)	0.8058 (3)	0.53355 (11)	0.0246 (4)
H11	0.1301	0.7354	0.5697	0.03*
C12	0.3175 (2)	0.9060 (3)	0.56923 (11)	0.0254 (4)
H12	0.3357	0.9047	0.6299	0.03*
C13	0.41273 (19)	1.0076 (3)	0.51641 (12)	0.0254 (4)
H13	0.4947	1.0779	0.5412	0.03*
C14	0.38929 (19)	1.0075 (3)	0.42748 (12)	0.0232 (4)
H14	0.4565	1.0744	0.3914	0.028*
C15	0.26676 (18)	0.9089 (2)	0.39163 (11)	0.0208 (4)
C16	0.1156 (2)	0.5601 (3)	0.33479 (12)	0.0258 (4)
H16	0.0421 (19)	0.500 (3)	0.2966 (11)	0.016 (4)*
C17	0.37770 (19)	0.4609 (3)	0.10866 (11)	0.0242 (4)
C18	0.4012 (2)	0.2615 (3)	0.10068 (12)	0.0299 (4)
H18	0.47	0.1958	0.1383	0.036*
C19	0.3221 (2)	0.1610 (3)	0.03665 (13)	0.0366 (5)
H19	0.338	0.0251	0.0306	0.044*
C20	0.2202 (2)	0.2533 (3)	−0.01897 (12)	0.0346 (5)
C21	0.1995 (2)	0.4513 (3)	−0.00981 (12)	0.0352 (5)
H21	0.1302	0.5167	−0.0472	0.042*
C22	0.2777 (2)	0.5561 (3)	0.05282 (12)	0.0315 (4)
H22	0.2632	0.6925	0.0577	0.038*
C23	0.1345 (3)	0.1440 (4)	−0.08860 (15)	0.0525 (7)
H23A	0.1836	0.1615	−0.1438	0.079*
H23B	0.0319	0.1941	−0.0932	0.079*
H23C	0.1322	0.0054	−0.074	0.079*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0225 (2)	0.0273 (2)	0.0275 (2)	0.0056 (2)	−0.00269 (16)	−0.0029 (2)
O1	0.0248 (7)	0.0437 (8)	0.0345 (7)	0.0115 (6)	−0.0042 (5)	−0.0040 (6)
O2	0.0285 (7)	0.0281 (7)	0.0377 (7)	−0.0004 (6)	−0.0011 (6)	−0.0022 (6)
N1	0.0255 (7)	0.0255 (8)	0.0250 (7)	0.0081 (8)	−0.0050 (6)	−0.0017 (8)
N2	0.0301 (9)	0.0185 (8)	0.0440 (11)	0.0015 (7)	−0.0045 (8)	0.0020 (8)
C1	0.0222 (9)	0.0221 (8)	0.0270 (10)	0.0063 (8)	−0.0060 (8)	−0.0029 (8)
C2	0.0213 (9)	0.0206 (9)	0.0249 (9)	0.0007 (7)	−0.0010 (7)	−0.0006 (7)
C3	0.0229 (9)	0.0188 (9)	0.0221 (9)	0.0036 (7)	−0.0037 (7)	−0.0054 (7)
C4	0.0286 (9)	0.0226 (8)	0.0244 (8)	0.0038 (9)	−0.0022 (7)	−0.0028 (9)
C5	0.0338 (10)	0.0244 (10)	0.0241 (9)	0.0094 (8)	−0.0068 (8)	−0.0024 (7)
C6	0.0243 (9)	0.0288 (10)	0.0304 (10)	0.0078 (8)	−0.0058 (8)	−0.0068 (8)
C7	0.0233 (9)	0.0224 (9)	0.0298 (10)	0.0002 (7)	−0.0024 (7)	−0.0058 (8)
C8	0.0230 (9)	0.0195 (9)	0.0242 (9)	−0.0003 (7)	−0.0053 (7)	−0.0051 (7)
C9	0.0211 (9)	0.0194 (9)	0.0283 (10)	−0.0017 (7)	0.0001 (8)	0.0016 (7)
C10	0.0199 (8)	0.0152 (8)	0.0271 (10)	0.0028 (7)	−0.0019 (7)	0.0003 (7)
C11	0.0262 (9)	0.0194 (9)	0.0283 (10)	0.0053 (7)	0.0023 (7)	0.0032 (7)
C12	0.0302 (10)	0.0229 (9)	0.0226 (9)	0.0070 (8)	−0.0061 (7)	−0.0026 (7)
C13	0.0227 (9)	0.0187 (8)	0.0343 (10)	0.0034 (7)	−0.0078 (8)	−0.0058 (8)
C14	0.0208 (9)	0.0175 (8)	0.0311 (9)	0.0022 (7)	−0.0012 (7)	−0.0003 (7)
C15	0.0198 (8)	0.0154 (8)	0.0270 (9)	0.0050 (7)	−0.0014 (7)	−0.0013 (7)
C16	0.0229 (9)	0.0193 (10)	0.0347 (10)	0.0000 (7)	−0.0070 (7)	−0.0028 (8)
C17	0.0237 (9)	0.0275 (10)	0.0216 (9)	0.0007 (8)	0.0027 (7)	−0.0010 (8)
C18	0.0323 (11)	0.0269 (10)	0.0305 (10)	0.0032 (8)	0.0039 (8)	0.0019 (9)
C19	0.0434 (12)	0.0263 (10)	0.0407 (12)	−0.0041 (9)	0.0135 (10)	−0.0067 (9)
C20	0.0315 (11)	0.0439 (12)	0.0287 (10)	−0.0074 (9)	0.0082 (8)	−0.0082 (9)
C21	0.0342 (11)	0.0448 (13)	0.0265 (10)	−0.0002 (10)	−0.0030 (8)	−0.0008 (9)
C22	0.0343 (10)	0.0309 (11)	0.0291 (10)	0.0044 (8)	−0.0022 (8)	0.0010 (8)
C23	0.0447 (12)	0.0670 (19)	0.0459 (13)	−0.0138 (12)	0.0058 (10)	−0.0235 (12)

Geometric parameters (Å, º)

S1—O2	1.4309 (14)	C9—C16	1.555 (3)
S1—O1	1.4328 (13)	C9—H9	0.968 (18)
S1—N1	1.6197 (15)	C10—C11	1.380 (2)
S1—C17	1.7631 (18)	C10—C15	1.401 (2)
N1—C1	1.465 (2)	C11—C12	1.395 (3)
N1—H1N	0.90 (2)	C11—H11	0.95
N2—C16	1.460 (2)	C12—C13	1.386 (3)
N2—H2A	0.88 (3)	C12—H12	0.95
N2—H2B	0.85 (2)	C13—C14	1.389 (2)
C1—C2	1.562 (2)	C13—H13	0.95
C1—C16	1.581 (3)	C14—C15	1.391 (2)
C1—H1	1.015 (17)	C14—H14	0.95
C2—C15	1.504 (2)	C16—H16	0.967 (17)
C2—C3	1.520 (2)	C17—C22	1.391 (2)

C2—H2	0.982 (19)	C17—C18	1.393 (3)
C3—C4	1.385 (3)	C18—C19	1.388 (3)
C3—C8	1.399 (3)	C18—H18	0.95
C4—C5	1.397 (2)	C19—C20	1.390 (3)
C4—H4	0.95	C19—H19	0.95
C5—C6	1.381 (3)	C20—C21	1.382 (3)
C5—H5	0.95	C20—C23	1.508 (3)
C6—C7	1.386 (3)	C21—C22	1.384 (3)
C6—H6	0.95	C21—H21	0.95
C7—C8	1.394 (2)	C22—H22	0.95
C7—H7	0.95	C23—H23A	0.98
C8—C9	1.510 (2)	C23—H23B	0.98
C9—C10	1.524 (2)	C23—H23C	0.98

O2—S1—O1	120.76 (9)	C11—C10—C15	120.47 (16)
O2—S1—N1	107.20 (9)	C11—C10—C9	126.75 (16)
O1—S1—N1	105.51 (8)	C15—C10—C9	112.76 (15)
O2—S1—C17	107.00 (8)	C10—C11—C12	119.52 (17)
O1—S1—C17	107.86 (8)	C10—C11—H11	120.2
N1—S1—C17	107.96 (8)	C12—C11—H11	120.2
C1—N1—S1	120.39 (12)	C13—C12—C11	120.17 (16)
C1—N1—H1N	111.6 (13)	C13—C12—H12	119.9
S1—N1—H1N	111.1 (13)	C11—C12—H12	119.9
C16—N2—H2A	113.1 (16)	C12—C13—C14	120.51 (16)
C16—N2—H2B	113.2 (16)	C12—C13—H13	119.7
H2A—N2—H2B	109 (2)	C14—C13—H13	119.7
N1—C1—C2	111.46 (14)	C13—C14—C15	119.52 (17)
N1—C1—C16	109.09 (14)	C13—C14—H14	120.2
C2—C1—C16	110.19 (15)	C15—C14—H14	120.2
N1—C1—H1	109.8 (10)	C14—C15—C10	119.77 (16)
C2—C1—H1	107.7 (10)	C14—C15—C2	126.55 (16)
C16—C1—H1	108.6 (10)	C10—C15—C2	113.69 (15)
C15—C2—C3	108.25 (14)	N2—C16—C9	113.99 (15)
C15—C2—C1	107.61 (14)	N2—C16—C1	111.32 (14)
C3—C2—C1	104.26 (14)	C9—C16—C1	107.66 (14)
C15—C2—H2	112.3 (11)	N2—C16—H16	108.2 (11)
C3—C2—H2	115.5 (11)	C9—C16—H16	111.2 (10)
C1—C2—H2	108.3 (11)	C1—C16—H16	104.0 (10)
C4—C3—C8	120.72 (16)	C22—C17—C18	120.25 (17)
C4—C3—C2	126.44 (16)	C22—C17—S1	119.53 (14)
C8—C3—C2	112.80 (15)	C18—C17—S1	120.20 (14)
C3—C4—C5	118.77 (17)	C19—C18—C17	118.60 (18)
C3—C4—H4	120.6	C19—C18—H18	120.7
C5—C4—H4	120.6	C17—C18—H18	120.7
C6—C5—C4	120.62 (16)	C18—C19—C20	121.91 (18)
C6—C5—H5	119.7	C18—C19—H19	119.0
C4—C5—H5	119.7	C20—C19—H19	119.0
C5—C6—C7	120.72 (17)	C21—C20—C19	118.26 (18)

C5—C6—H6	119.6	C21—C20—C23	119.9 (2)
C7—C6—H6	119.6	C19—C20—C23	121.9 (2)
C6—C7—C8	119.20 (17)	C20—C21—C22	121.26 (19)
C6—C7—H7	120.4	C20—C21—H21	119.4
C8—C7—H7	120.4	C22—C21—H21	119.4
C7—C8—C3	119.86 (16)	C21—C22—C17	119.70 (18)
C7—C8—C9	126.36 (16)	C21—C22—H22	120.2
C3—C8—C9	113.69 (15)	C17—C22—H22	120.2
C8—C9—C10	108.52 (14)	C20—C23—H23A	109.5
C8—C9—C16	106.81 (14)	C20—C23—H23B	109.5
C10—C9—C16	106.30 (14)	H23A—C23—H23B	109.5
C8—C9—H9	113.4 (10)	C20—C23—H23C	109.5
C10—C9—H9	111.4 (10)	H23A—C23—H23C	109.5
C16—C9—H9	110.0 (11)	H23B—C23—H23C	109.5

O2—S1—N1—C1	53.66 (16)	C12—C13—C14—C15	1.8 (3)
O1—S1—N1—C1	−176.43 (14)	C13—C14—C15—C10	−0.4 (2)
C17—S1—N1—C1	−61.31 (17)	C13—C14—C15—C2	178.89 (16)
S1—N1—C1—C2	−90.01 (17)	C11—C10—C15—C14	−1.3 (2)
S1—N1—C1—C16	148.09 (14)	C9—C10—C15—C14	−179.93 (15)
N1—C1—C2—C15	−67.85 (18)	C11—C10—C15—C2	179.27 (15)
C16—C1—C2—C15	53.41 (18)	C9—C10—C15—C2	0.7 (2)
N1—C1—C2—C3	177.35 (14)	C3—C2—C15—C14	−126.01 (18)
C16—C1—C2—C3	−61.39 (17)	C1—C2—C15—C14	121.86 (18)
C15—C2—C3—C4	127.49 (18)	C3—C2—C15—C10	53.35 (19)
C1—C2—C3—C4	−118.15 (18)	C1—C2—C15—C10	−58.78 (18)
C15—C2—C3—C8	−54.95 (19)	C8—C9—C16—N2	178.79 (14)
C1—C2—C3—C8	59.40 (18)	C10—C9—C16—N2	63.07 (19)
C8—C3—C4—C5	−0.3 (2)	C8—C9—C16—C1	54.78 (16)
C2—C3—C4—C5	177.07 (16)	C10—C9—C16—C1	−60.94 (17)
C3—C4—C5—C6	−2.4 (3)	N1—C1—C16—N2	2.1 (2)
C4—C5—C6—C7	2.7 (3)	C2—C1—C16—N2	−120.58 (16)
C5—C6—C7—C8	−0.2 (3)	N1—C1—C16—C9	127.70 (15)
C6—C7—C8—C3	−2.6 (3)	C2—C1—C16—C9	5.03 (18)
C6—C7—C8—C9	−178.97 (16)	O2—S1—C17—C22	−25.90 (17)
C4—C3—C8—C7	2.8 (3)	O1—S1—C17—C22	−157.23 (14)
C2—C3—C8—C7	−174.90 (15)	N1—S1—C17—C22	89.20 (16)
C4—C3—C8—C9	179.66 (15)	O2—S1—C17—C18	155.12 (14)
C2—C3—C8—C9	1.9 (2)	O1—S1—C17—C18	23.79 (17)
C7—C8—C9—C10	−131.40 (18)	N1—S1—C17—C18	−89.78 (16)
C3—C8—C9—C10	52.0 (2)	C22—C17—C18—C19	−0.5 (3)
C7—C8—C9—C16	114.37 (19)	S1—C17—C18—C19	178.43 (13)
C3—C8—C9—C16	−62.23 (18)	C17—C18—C19—C20	−0.3 (3)
C8—C9—C10—C11	127.94 (18)	C18—C19—C20—C21	0.6 (3)
C16—C9—C10—C11	−117.50 (18)	C18—C19—C20—C23	179.92 (19)
C8—C9—C10—C15	−53.57 (19)	C19—C20—C21—C22	0.1 (3)
C16—C9—C10—C15	60.99 (18)	C23—C20—C21—C22	−179.28 (19)
C15—C10—C11—C12	1.8 (2)	C20—C21—C22—C17	−0.9 (3)

C9—C10—C11—C12	−179.86 (16)	C18—C17—C22—C21	1.2 (3)
C10—C11—C12—C13	−0.4 (3)	S1—C17—C22—C21	−177.80 (15)
C11—C12—C13—C14	−1.3 (3)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C3–C8 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···N2	0.90 (2)	2.04 (2)	2.592 (2)	117.9 (17)
C11—H11···*Cg*1^{i}	0.95	2.87	3.712 (2)	149
C5—H5···O1^{ii}	0.95	2.58	3.269 (2)	129
C12—H12···O1^{iii}	0.95	2.52	3.446 (2)	166
C23—H23*A*···O1^{iv}	0.98	2.51	3.259 (3)	133

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