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(*Z*)-5-Benzenecarbothioyl-1,11-dimethyl-6-phenyl-5*H*-dibenzo[*d*,*f*][1,3]diazepine

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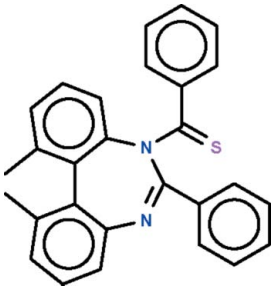
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.085; data-to-parameter ratio = 18.4.

The seven-membered ring in the title compound, $C_{28}H_{22}N_2S$, has a two-coordinate N atom as well as a three-coordinate N atom. The ring adopts a boat-shaped conformation with two C atoms of one methylphenyl ring as the stern and the three-coordinate N atom as the prow. The *N*,*N*-dimethylethanethioamide fragment is nearly planar (r.m.s. deviation = 0.049 Å); the phenyl ring of the benzenecarbothioyl unit connected to the three-coordinate N atom is aligned at 83.72 (4)° with respect to the mean plane of this fragment. Weak intermolecular C—H···S hydrogen bonding is present in the crystal structure.

Related literature

For background to the synthesis of thioamides by the reaction of 1,1′-binaphthyl-2,2′-diamine with acyl chlorides and phosphorus pentasulfide, see: Shi *et al.* (2004).



Experimental

Crystal data

$C_{28}H_{22}N_2S$
M_r = 418.54
Orthorhombic, $P2_12_12_1$
a = 8.7665 (18) Å
b = 11.605 (3) Å
c = 21.392 (5) Å
V = 2176.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 113 K
0.26 × 0.22 × 0.20 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.958, T_{max} = 0.967
21933 measured reflections
5176 independent reflections
4527 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.085
S = 0.99
5176 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983), 2775 Friedel pairs
Flack parameter: −0.03 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···S1^{i}	0.95	2.86	3.7216 (18)	152

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Beijing Normal University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5136).

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supporting information

Acta Cryst. (2011). E**67**, o364 [doi:10.1107/S1600536811000092]

(*Z*)-5-Benzenecarbothioyl-1,11-dimethyl-6-phenyl-5*H*-dibenzo[*d*,*f*][1,3]diazepine

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S1. Comment

The two amino groups of 1,1′-binaphthyl-2,2′-diamine undergo condensation with acyl chlorides and phosphorus pentasulfide to yield bis(thioamides) (Shi *et al.*, 2004). The present study represents a variation of this reaction by reacting a biphenyl dibenzamide derivative directly with phosphorus pentasulfide. The resulting compound (Scheme I) has only one carbonyl fragment replaced by a thiocarbonyl fragment as the other fragment has undergone cyclization (Scheme I). The compound features a seven-membered ring, with the two nitrogen atoms constituting members of a seven-membered ring.

S2. Experimental

N,*N*′-(6,6′-Dimethylbiphenyl-2,2′-diyl)dibenzamide (210 mg, 0.50 mmol) and phosphorus pentasulfide (111 mg, 0.5 mmol) in pyridine (2 ml) were heated at 393 K for 10 h. To the product was added 10% sodium hydroxide to a pH of about 10. The organic compound was extracted with ethyl acetate (3 *x* 20 ml). The organic phase was dried over sodium sulfate. The solvent was removed under reduced pressure and the residue was purified by column chromatography (eluent: ethyl acetate/petroleum ether 1/20) to give the title compound (46.8 mg, 20%) as a yellow solid. Single crystals were obtained upon recrystallized from a dichloromethane-hexane mixture.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95–0.98 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2–1.5U_{eq}(C).

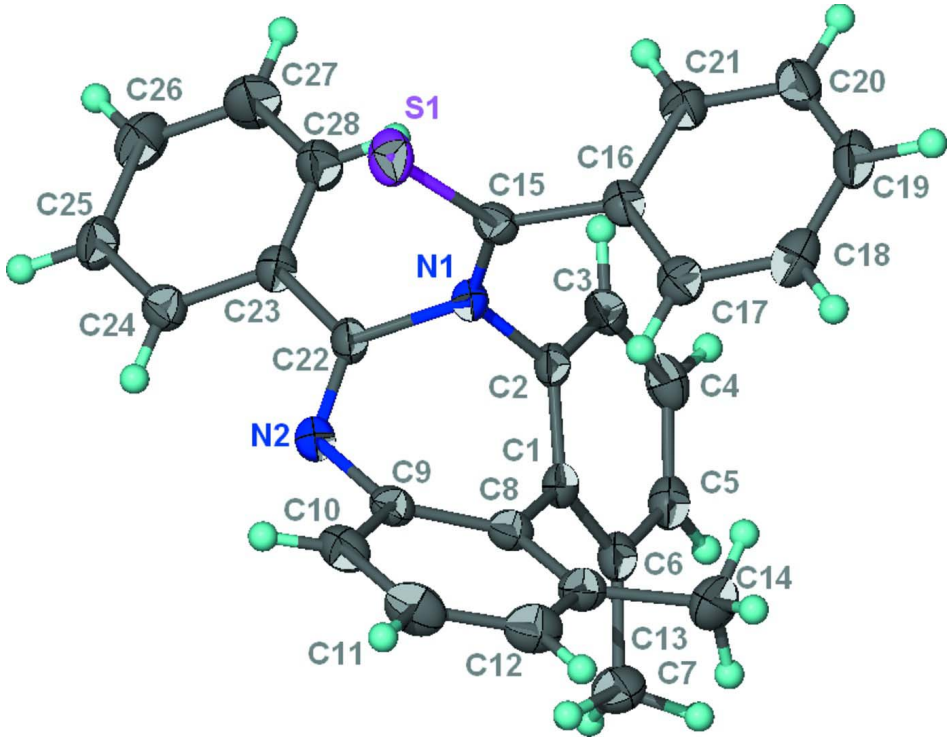

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{28}H_{22}N_2S$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

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Crystal data

$C_{28}H_{22}N_2S$
$M_r = 418.54$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 8.7665\ (18)$ Å
$b = 11.605\ (3)$ Å
$c = 21.392\ (5)$ Å
$V = 2176.4\ (8)$ Å^3
$Z = 4$

$F(000) = 880$
$D_x = 1.277$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Cell parameters from 7653 reflections
$\theta = 1.9$–$27.9°$
$\mu = 0.17$ mm^{-1}
$T = 113$ K
Block, yellow
0.26 × 0.22 × 0.20 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.958$, $T_{max} = 0.967$

21933 measured reflections
5176 independent reflections
4527 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 27.9°$, $\theta_{min} = 1.9°$
$h = -11 \rightarrow 9$
$k = -15 \rightarrow 15$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.085$
$S = 0.99$
5176 reflections
282 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
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Absolute structure: Flack (1983), 2775 Friedel pairs
Absolute structure parameter: −0.03 (6)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	1.09723 (5)	0.47544 (4)	0.76793 (2)	0.02825 (11)
N1	0.95131 (14)	0.56476 (11)	0.67231 (6)	0.0178 (3)
N2	0.76743 (15)	0.41503 (11)	0.66647 (6)	0.0200 (3)
C1	0.88897 (18)	0.55478 (13)	0.56264 (7)	0.0187 (3)
C2	0.92563 (17)	0.62439 (13)	0.61387 (7)	0.0178 (3)
C3	0.91869 (17)	0.74326 (13)	0.61224 (7)	0.0209 (3)
H3	0.9482	0.7880	0.6474	0.025*
C4	0.86735 (18)	0.79547 (14)	0.55772 (8)	0.0240 (4)
H4	0.8658	0.8771	0.5546	0.029*
C5	0.81855 (18)	0.72897 (15)	0.50809 (8)	0.0237 (4)
H5	0.7770	0.7660	0.4723	0.028*
C6	0.82841 (18)	0.60889 (14)	0.50890 (7)	0.0214 (3)
C7	0.7658 (2)	0.54265 (15)	0.45397 (8)	0.0288 (4)
H7A	0.6619	0.5690	0.4449	0.043*
H7B	0.7641	0.4602	0.4640	0.043*
H7C	0.8307	0.5556	0.4173	0.043*
C8	0.91836 (18)	0.42900 (13)	0.56802 (7)	0.0194 (3)
C9	0.85781 (17)	0.36525 (13)	0.61850 (7)	0.0197 (3)
C10	0.88359 (19)	0.24726 (13)	0.62336 (8)	0.0248 (4)
H10	0.8367	0.2042	0.6559	0.030*
C11	0.9777 (2)	0.19306 (15)	0.58068 (8)	0.0293 (4)
H11	0.9968	0.1128	0.5843	0.035*
C12	1.0442 (2)	0.25546 (14)	0.53263 (8)	0.0270 (4)
H12	1.1099	0.2175	0.5039	0.032*
C13	1.01628 (18)	0.37322 (14)	0.52574 (7)	0.0221 (3)
C14	1.1039 (2)	0.43886 (15)	0.47629 (8)	0.0291 (4)
H14A	1.1978	0.3970	0.4660	0.044*
H14B	1.1298	0.5156	0.4921	0.044*
H14C	1.0409	0.4464	0.4387	0.044*
C15	1.08502 (18)	0.54891 (12)	0.70153 (7)	0.0193 (3)
C16	1.22481 (18)	0.59577 (13)	0.67023 (7)	0.0192 (3)
C17	1.29579 (18)	0.52874 (14)	0.62485 (7)	0.0228 (3)

H17	1.2494	0.4592	0.6111	0.027*
C18	1.43445 (19)	0.56342 (15)	0.59970 (8)	0.0271 (4)
H18	1.4845	0.5166	0.5696	0.032*
C19	1.49930 (19)	0.66606 (16)	0.61859 (8)	0.0272 (4)
H19	1.5942	0.6898	0.6015	0.033*
C20	1.4268 (2)	0.73423 (15)	0.66218 (8)	0.0284 (4)
H20A	1.4712	0.8055	0.6743	0.034*
C21	1.28956 (19)	0.69967 (14)	0.68849 (8)	0.0249 (4)
H21A	1.2403	0.7467	0.7187	0.030*
C22	0.81179 (17)	0.50720 (13)	0.69330 (7)	0.0196 (3)
C23	0.72239 (18)	0.56611 (13)	0.74184 (7)	0.0200 (3)
C24	0.58133 (17)	0.52104 (14)	0.75993 (7)	0.0226 (3)
H24	0.5459	0.4509	0.7423	0.027*
C25	0.4935 (2)	0.57849 (15)	0.80349 (8)	0.0269 (4)
H25	0.3987	0.5467	0.8164	0.032*
C26	0.5424 (2)	0.68208 (16)	0.82853 (8)	0.0312 (4)
H26	0.4804	0.7219	0.8579	0.037*
C27	0.6819 (2)	0.72744 (16)	0.81069 (9)	0.0348 (4)
H27	0.7159	0.7983	0.8280	0.042*
C28	0.7718 (2)	0.66969 (15)	0.76768 (8)	0.0279 (4)
H28	0.8677	0.7009	0.7557	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0262 (2)	0.0317 (2)	0.0269 (2)	−0.00369 (19)	−0.00223 (19)	0.01130 (18)
N1	0.0185 (7)	0.0179 (6)	0.0171 (6)	−0.0035 (5)	0.0025 (5)	0.0004 (5)
N2	0.0197 (7)	0.0204 (7)	0.0198 (6)	−0.0026 (5)	0.0019 (6)	0.0006 (5)
C1	0.0164 (8)	0.0212 (8)	0.0183 (7)	−0.0023 (6)	0.0034 (6)	0.0007 (6)
C2	0.0147 (8)	0.0211 (8)	0.0177 (7)	−0.0017 (6)	0.0023 (6)	0.0025 (6)
C3	0.0175 (8)	0.0197 (7)	0.0256 (8)	−0.0021 (6)	0.0024 (7)	−0.0020 (6)
C4	0.0205 (9)	0.0187 (8)	0.0328 (9)	0.0001 (6)	0.0026 (7)	0.0050 (7)
C5	0.0193 (9)	0.0281 (9)	0.0236 (8)	−0.0005 (7)	0.0018 (7)	0.0069 (7)
C6	0.0184 (8)	0.0241 (8)	0.0215 (8)	−0.0019 (6)	0.0028 (7)	0.0036 (7)
C7	0.0318 (9)	0.0323 (10)	0.0223 (8)	−0.0020 (8)	−0.0047 (8)	0.0015 (7)
C8	0.0181 (8)	0.0200 (7)	0.0202 (7)	−0.0006 (6)	−0.0016 (7)	−0.0020 (6)
C9	0.0163 (8)	0.0213 (8)	0.0214 (8)	−0.0020 (6)	−0.0018 (6)	−0.0025 (7)
C10	0.0255 (9)	0.0204 (8)	0.0285 (8)	−0.0034 (7)	−0.0046 (7)	0.0006 (7)
C11	0.0301 (9)	0.0186 (8)	0.0391 (10)	0.0029 (7)	−0.0038 (8)	−0.0032 (7)
C12	0.0239 (8)	0.0270 (9)	0.0300 (9)	0.0048 (7)	−0.0011 (7)	−0.0068 (7)
C13	0.0208 (8)	0.0240 (8)	0.0214 (8)	−0.0006 (7)	−0.0011 (7)	−0.0029 (7)
C14	0.0282 (9)	0.0339 (9)	0.0253 (8)	0.0005 (8)	0.0068 (8)	−0.0031 (7)
C15	0.0191 (8)	0.0158 (7)	0.0229 (8)	−0.0012 (6)	0.0002 (7)	−0.0030 (6)
C16	0.0161 (8)	0.0207 (7)	0.0208 (7)	0.0002 (6)	−0.0024 (7)	0.0054 (6)
C17	0.0238 (8)	0.0217 (8)	0.0230 (8)	0.0002 (7)	−0.0016 (7)	0.0035 (7)
C18	0.0269 (9)	0.0321 (9)	0.0223 (8)	0.0078 (7)	0.0042 (7)	0.0056 (7)
C19	0.0186 (8)	0.0374 (10)	0.0257 (9)	−0.0021 (7)	0.0009 (7)	0.0106 (8)
C20	0.0284 (10)	0.0289 (8)	0.0280 (9)	−0.0103 (7)	−0.0028 (8)	0.0061 (7)

C21	0.0252 (9)	0.0239 (8)	0.0256 (8)	−0.0021 (7)	0.0011 (7)	0.0000 (7)
C22	0.0176 (8)	0.0219 (8)	0.0193 (7)	−0.0036 (6)	0.0020 (6)	0.0032 (6)
C23	0.0190 (8)	0.0217 (7)	0.0192 (7)	0.0003 (6)	0.0019 (7)	0.0024 (6)
C24	0.0217 (8)	0.0244 (7)	0.0217 (7)	−0.0028 (7)	−0.0017 (7)	0.0025 (7)
C25	0.0189 (8)	0.0394 (10)	0.0226 (8)	−0.0012 (7)	0.0036 (7)	0.0034 (7)
C26	0.0304 (10)	0.0368 (9)	0.0265 (9)	0.0057 (8)	0.0071 (8)	−0.0022 (8)
C27	0.0392 (11)	0.0298 (10)	0.0353 (10)	−0.0039 (8)	0.0088 (9)	−0.0118 (8)
C28	0.0267 (9)	0.0279 (9)	0.0290 (9)	−0.0056 (7)	0.0070 (8)	−0.0052 (8)

Geometric parameters (Å, º)

S1—C15	1.6601 (16)	C13—C14	1.513 (2)
N1—C15	1.341 (2)	C14—H14A	0.9800
N1—C2	1.4465 (19)	C14—H14B	0.9800
N1—C22	1.4642 (19)	C14—H14C	0.9800
N2—C22	1.275 (2)	C15—C16	1.499 (2)
N2—C9	1.419 (2)	C16—C21	1.389 (2)
C1—C2	1.399 (2)	C16—C17	1.391 (2)
C1—C6	1.413 (2)	C17—C18	1.389 (2)
C1—C8	1.487 (2)	C17—H17	0.9500
C2—C3	1.381 (2)	C18—C19	1.380 (2)
C3—C4	1.389 (2)	C18—H18	0.9500
C3—H3	0.9500	C19—C20	1.378 (2)
C4—C5	1.381 (2)	C19—H19	0.9500
C4—H4	0.9500	C20—C21	1.388 (2)
C5—C6	1.396 (2)	C20—H20A	0.9500
C5—H5	0.9500	C21—H21A	0.9500
C6—C7	1.508 (2)	C22—C23	1.470 (2)
C7—H7A	0.9800	C23—C24	1.397 (2)
C7—H7B	0.9800	C23—C28	1.392 (2)
C7—H7C	0.9800	C24—C25	1.380 (2)
C8—C13	1.405 (2)	C24—H24	0.9500
C8—C9	1.413 (2)	C25—C26	1.384 (3)
C9—C10	1.392 (2)	C25—H25	0.9500
C10—C11	1.382 (2)	C26—C27	1.385 (3)
C10—H10	0.9500	C26—H26	0.9500
C11—C12	1.386 (2)	C27—C28	1.385 (2)
C11—H11	0.9500	C27—H27	0.9500
C12—C13	1.396 (2)	C28—H28	0.9500
C12—H12	0.9500		

C15—N1—C2	127.19 (12)	C13—C14—H14B	109.5
C15—N1—C22	121.64 (12)	H14A—C14—H14B	109.5
C2—N1—C22	110.69 (12)	C13—C14—H14C	109.5
C22—N2—C9	119.79 (13)	H14A—C14—H14C	109.5
C2—C1—C6	117.83 (14)	H14B—C14—H14C	109.5
C2—C1—C8	117.81 (13)	N1—C15—C16	117.18 (13)
C6—C1—C8	124.35 (14)	N1—C15—S1	121.71 (11)

C3—C2—C1	123.16 (14)	C16—C15—S1	121.06 (12)
C3—C2—N1	120.42 (14)	C21—C16—C17	119.94 (15)
C1—C2—N1	115.88 (13)	C21—C16—C15	121.58 (14)
C2—C3—C4	118.10 (15)	C17—C16—C15	118.34 (14)
C2—C3—H3	120.9	C18—C17—C16	119.99 (16)
C4—C3—H3	120.9	C18—C17—H17	120.0
C5—C4—C3	120.14 (15)	C16—C17—H17	120.0
C5—C4—H4	119.9	C19—C18—C17	119.80 (16)
C3—C4—H4	119.9	C19—C18—H18	120.1
C4—C5—C6	121.95 (16)	C17—C18—H18	120.1
C4—C5—H5	119.0	C18—C19—C20	120.25 (16)
C6—C5—H5	119.0	C18—C19—H19	119.9
C5—C6—C1	118.48 (15)	C20—C19—H19	119.9
C5—C6—C7	118.46 (15)	C19—C20—C21	120.55 (16)
C1—C6—C7	122.97 (14)	C19—C20—H20A	119.7
C6—C7—H7A	109.5	C21—C20—H20A	119.7
C6—C7—H7B	109.5	C16—C21—C20	119.43 (16)
H7A—C7—H7B	109.5	C16—C21—H21A	120.3
C6—C7—H7C	109.5	C20—C21—H21A	120.3
H7A—C7—H7C	109.5	N2—C22—N1	119.97 (14)
H7B—C7—H7C	109.5	N2—C22—C23	123.08 (14)
C13—C8—C9	118.71 (14)	N1—C22—C23	116.74 (13)
C13—C8—C1	120.56 (14)	C24—C23—C28	119.25 (15)
C9—C8—C1	120.55 (14)	C24—C23—C22	119.57 (14)
C10—C9—C8	120.75 (15)	C28—C23—C22	121.08 (14)
C10—C9—N2	115.93 (15)	C25—C24—C23	119.98 (15)
C8—C9—N2	123.32 (14)	C25—C24—H24	120.0
C11—C10—C9	119.71 (16)	C23—C24—H24	120.0
C11—C10—H10	120.1	C24—C25—C26	120.54 (16)
C9—C10—H10	120.1	C24—C25—H25	119.7
C10—C11—C12	120.21 (16)	C26—C25—H25	119.7
C10—C11—H11	119.9	C25—C26—C27	119.79 (17)
C12—C11—H11	119.9	C25—C26—H26	120.1
C11—C12—C13	121.07 (16)	C27—C26—H26	120.1
C11—C12—H12	119.5	C28—C27—C26	120.12 (17)
C13—C12—H12	119.5	C28—C27—H27	119.9
C12—C13—C8	119.35 (15)	C26—C27—H27	119.9
C12—C13—C14	118.53 (15)	C27—C28—C23	120.30 (16)
C8—C13—C14	121.89 (14)	C27—C28—H28	119.8
C13—C14—H14A	109.5	C23—C28—H28	119.8

C6—C1—C2—C3	−6.1 (2)	C9—C8—C13—C14	−170.84 (15)
C8—C1—C2—C3	173.00 (15)	C1—C8—C13—C14	4.3 (2)
C6—C1—C2—N1	165.46 (13)	C2—N1—C15—C16	−1.2 (2)
C8—C1—C2—N1	−15.4 (2)	C22—N1—C15—C16	170.10 (13)
C15—N1—C2—C3	−80.0 (2)	C2—N1—C15—S1	−178.48 (11)
C22—N1—C2—C3	107.88 (16)	C22—N1—C15—S1	−7.2 (2)
C15—N1—C2—C1	108.11 (17)	N1—C15—C16—C21	99.88 (18)

C22—N1—C2—C1	−63.97 (16)	S1—C15—C16—C21	−82.82 (18)
C1—C2—C3—C4	2.5 (2)	N1—C15—C16—C17	−84.55 (18)
N1—C2—C3—C4	−168.78 (13)	S1—C15—C16—C17	92.75 (16)
C2—C3—C4—C5	2.9 (2)	C21—C16—C17—C18	2.6 (2)
C3—C4—C5—C6	−4.4 (2)	C15—C16—C17—C18	−173.01 (14)
C4—C5—C6—C1	0.6 (2)	C16—C17—C18—C19	−1.8 (2)
C4—C5—C6—C7	177.21 (15)	C17—C18—C19—C20	−0.1 (3)
C2—C1—C6—C5	4.5 (2)	C18—C19—C20—C21	1.2 (3)
C8—C1—C6—C5	−174.62 (15)	C17—C16—C21—C20	−1.5 (2)
C2—C1—C6—C7	−171.95 (14)	C15—C16—C21—C20	173.97 (15)
C8—C1—C6—C7	9.0 (2)	C19—C20—C21—C16	−0.4 (3)
C2—C1—C8—C13	−121.05 (16)	C9—N2—C22—N1	3.3 (2)
C6—C1—C8—C13	58.0 (2)	C9—N2—C22—C23	177.90 (14)
C2—C1—C8—C9	54.0 (2)	C15—N1—C22—N2	−97.74 (18)
C6—C1—C8—C9	−126.86 (16)	C2—N1—C22—N2	74.85 (17)
C13—C8—C9—C10	−5.5 (2)	C15—N1—C22—C23	87.33 (17)
C1—C8—C9—C10	179.28 (15)	C2—N1—C22—C23	−100.07 (15)
C13—C8—C9—N2	175.05 (14)	N2—C22—C23—C24	−0.4 (2)
C1—C8—C9—N2	−0.1 (2)	N1—C22—C23—C24	174.33 (14)
C22—N2—C9—C10	132.30 (16)	N2—C22—C23—C28	−176.79 (16)
C22—N2—C9—C8	−48.3 (2)	N1—C22—C23—C28	−2.0 (2)
C8—C9—C10—C11	4.3 (2)	C28—C23—C24—C25	−0.7 (2)
N2—C9—C10—C11	−176.25 (15)	C22—C23—C24—C25	−177.15 (14)
C9—C10—C11—C12	−1.0 (3)	C23—C24—C25—C26	1.4 (2)
C10—C11—C12—C13	−0.9 (3)	C24—C25—C26—C27	−1.3 (3)
C11—C12—C13—C8	−0.4 (2)	C25—C26—C27—C28	0.4 (3)
C11—C12—C13—C14	174.18 (16)	C26—C27—C28—C23	0.4 (3)
C9—C8—C13—C12	3.6 (2)	C24—C23—C28—C27	−0.2 (2)
C1—C8—C13—C12	178.74 (15)	C22—C23—C28—C27	176.20 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···S1^{i}	0.95	2.86	3.7216 (18)	152

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