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13-Nitrobenzo[*a*][1,4]benzothiazino[3,2-*c*]-phenoxazine

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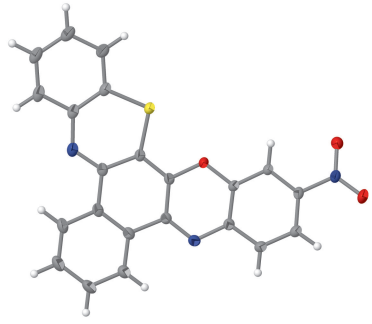
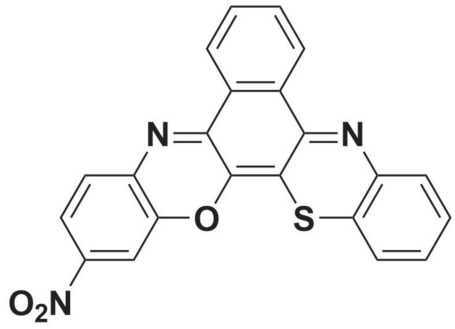
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{22}H_{11}N_3O_3S$, dihedral angle between the phenyl rings on the periphery of the molecule is 8.05 (18)°. In the crystal, aromatic π–π stacking distance and short C—H···O contacts are observed. The maximum absorption occurs at 688 nm.

3D view



Chemical scheme



Structure description

One area of interest in fused heterocyclic aromatic compounds is their potential to act as alternatives to oligoacenes for use in organic semiconducting devices (McLean *et al.*, 1989, 1990; Pham *et al.*, 2008). Surprisingly, despite this intensely researched area, structural studies of these materials are scarce. Phenothiazine systems are readily obtained by reaction of halo-*p*-benzoquinones and amino thiophenols (Agarwal *et al.*, 1980; Okafor *et al.*, 1988; Spangler *et al.*, 1989; Faleh *et al.*, 2008) The title compound, $C_{22}H_{11}N_3O_3S$, is an asymmetric molecule with sulfur and oxygen bridging atoms (Fig. 1) that was prepared in two steps.

The molecule is quasi-planar, as indicated by the torsion angles C8—C7—C22—N1 [−179.49 (19)°], S1—C7—C8—C15 [179.71 (16)°] and O2—N3—C11—C10 [−8.3 (3)°]. The nitro group subtends a dihedral angle of 8.0 (3)° with respect to its attached ring. A π–π-stacking distance of 3.290 (3) Å (Fig. 2) and close C—H···O interactions [H19···O2($1-x, \frac{3}{2}-y, \frac{1}{2}+z$) = 2.44, H12···O2($\frac{1}{4}+x, \frac{5}{4}-y, \frac{1}{4}+z$) = 2.50 and H3···O3($\frac{3}{4}-x, \frac{1}{4}+y, -\frac{1}{4}+z$) 2.63 Å] are observed.

A survey of the Cambridge Structural Database (Groom *et al.*, 2016) on March 28, 2024 revealed no hits for this compound or any closely related structure. The closest is a structure from our group of the symmetrical molecule 15,16-dithia-5,10-diazanaphtho-[2,3-*a*]benzo[*c*]anthracene, (Pham *et al.*, 2008), which crystallizes in the monoclinic space

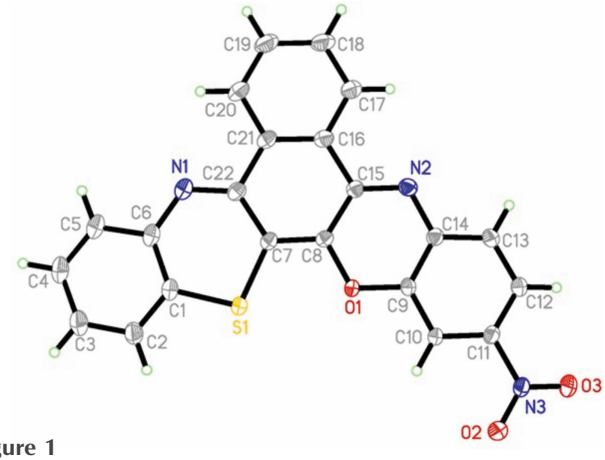


Figure 1
Structure of title compound.with displacement ellipsoids drawn at the 50% probability level.

group $P2_1/c$ with four molecules in the unit cell. This molecule is also quasi-planar with dihedral angles between the three phenyl rings on the periphery of the molecule ranging from 1.89 to 6.65° and close C—H···S and C—H···N contacts. In comparison, no C—H···S or C—H···N close contacts are observed in the title compound.

Synthesis and crystallization

The target molecule was synthesized in a two-step process following published procedures (Agarwal *et al.*, 1980; Okafor *et al.*, 1988; Fiester *et al.*, 2023; Spangler *et al.*, 1989) as shown in Fig. 3.

*Synthesis of the precursor 6-chloro-9-nitro-5-oxo-5H-benzo-[a]phenoxazine (**1**)*

2-Amino-5-nitrophenol (5 mmol, 0.7612 g) and potassium acetate (5 mmol, 0.7740 g) were combined in 25 mL of ethanol. 2,3-Dichloro-1,4-napthophenol (5 mmol, 1.120 g) was added to the solution, which was then heated gently for 2 h. The solution was cooled and filtered, resulting in an orange–red solid (1.0028 g, 77%), m.p. 255°C.

Synthesis of the title compound 13-nitrobenzo[a][1,4]-benzothiazino[3,2-c]phenoxazine

2-Aminothiophenol (excess) and potassium acetate were combined in 10 mL of ethanol. Precursor **1** (0.9781 g, 3.7 mmol) was added to the solution, which was then heated at 60°C for approximately 5 h. The solution was cooled and filtered, resulting in a dark-blue solid (0.4136 g, 33% yield), m.p. 340°C. The product was crystallized by slow evaporation from dichloromethane solution.

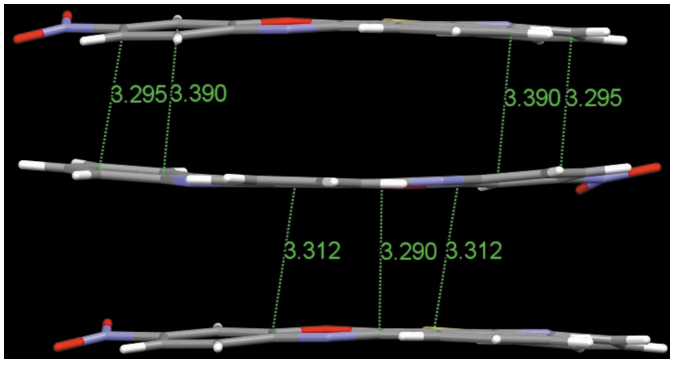


Figure 2
Stacking of molecules with shortest observed distances (atom to atom).

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{11}N_3O_3S$
M_r	397.40
Crystal system, space group	Orthorhombic, *Fdd*2
Temperature (K)	130
a, *b*, *c* (Å)	6.7497 (9), 52.478 (7), 18.832 (3)
V (Å^3)	6670.5 (16)
Z	16
Radiation type	Mo *Kα*
μ (mm^{-1})	0.23
Crystal size (mm)	0.20 × 0.13 × 0.05
Data collection	
Diffractometer	Bruker PHOTON-III CPAD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.681, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22321, 5093, 4718
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.714
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.033, 0.087, 1.03
No. of reflections	5093
No. of parameters	262
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.23
Absolute structure	Flack *x* determined using 2109 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.01 (3)

Computer programs: *APEX4* and *SAINT* (Bruker, 2014), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

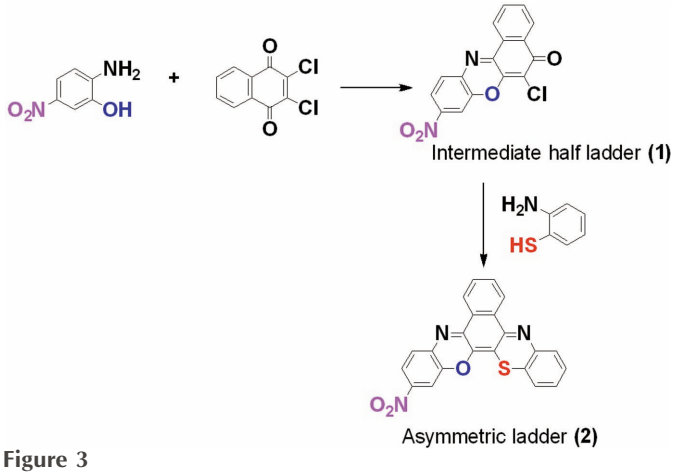


Figure 3
Reaction scheme for the preparation of the title compound.

Acknowledgements

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full crystallographic data

IUCrData (2024). **9**, x240299 [https://doi.org/10.1107/S2414314624002992]

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Crystal data

$C_{22}H_{11}N_3O_3S$
M_r = 397.40
Orthorhombic, *Fdd*2
a = 6.7497 (9) Å
b = 52.478 (7) Å
c = 18.832 (3) Å
V = 6670.5 (16) Å^3
Z = 16
F(000) = 3264
D_x = 1.583 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 2857 reflections
θ = 2.3–30.0°
μ = 0.23 mm^{-1}
T = 130 K
Needle, brown
0.20 × 0.13 × 0.05 mm

Data collection

Bruker PHOTON-III CPAD diffractometer
Radiation source: micro-focus
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.681, T_{max} = 0.746
22321 measured reflections
5093 independent reflections
4718 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 30.5°, θ_{min} = 2.3°
h = −6→9
k = −74→73
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
S = 1.03
5093 reflections
262 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack *x* determined using 2109 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.01 (3)

Special details

Experimental. Prof. M. Bader/C. Fiester

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.51936 (8)	0.77762 (2)	0.36455 (3)	0.02344 (12)
O1	0.4662 (2)	0.73153 (2)	0.43558 (7)	0.0198 (3)
O2	0.3593 (2)	0.64760 (3)	0.32680 (8)	0.0293 (3)
O3	0.4057 (3)	0.62015 (3)	0.41134 (8)	0.0338 (4)
N1	0.5694 (3)	0.82016 (3)	0.48286 (9)	0.0227 (3)
N2	0.4745 (3)	0.72228 (3)	0.58474 (9)	0.0209 (3)
N3	0.3919 (3)	0.64213 (3)	0.38935 (9)	0.0225 (3)
C1	0.5695 (3)	0.81010 (4)	0.35380 (11)	0.0223 (4)
C2	0.5942 (3)	0.81878 (4)	0.28432 (12)	0.0273 (4)
H2	0.581985	0.807310	0.245538	0.033*
C3	0.6371 (3)	0.84436 (4)	0.27226 (13)	0.0312 (4)
H3	0.655028	0.850328	0.225073	0.037*
C4	0.6537 (3)	0.86123 (4)	0.32886 (13)	0.0306 (5)
H4	0.683467	0.878653	0.320257	0.037*
C5	0.6269 (3)	0.85268 (4)	0.39781 (13)	0.0271 (4)
H5	0.637067	0.864410	0.436066	0.033*
C6	0.5849 (3)	0.82691 (4)	0.41212 (11)	0.0227 (4)
C7	0.5201 (3)	0.77476 (3)	0.45674 (10)	0.0189 (3)
C8	0.4934 (3)	0.75094 (3)	0.48421 (10)	0.0180 (3)
C9	0.4496 (3)	0.70709 (3)	0.46210 (9)	0.0177 (3)
C10	0.4258 (3)	0.68769 (3)	0.41332 (9)	0.0181 (3)
H10	0.416843	0.691018	0.363837	0.022*
C11	0.4155 (3)	0.66298 (3)	0.44028 (10)	0.0198 (3)
C12	0.4311 (3)	0.65728 (4)	0.51177 (10)	0.0225 (4)
H12	0.429063	0.640118	0.527818	0.027*
C13	0.4499 (3)	0.67737 (4)	0.55959 (10)	0.0223 (4)
H13	0.457868	0.673908	0.609021	0.027*
C14	0.4573 (3)	0.70262 (4)	0.53568 (10)	0.0192 (4)
C15	0.4910 (3)	0.74534 (4)	0.55893 (10)	0.0184 (3)
C16	0.5132 (3)	0.76694 (4)	0.60727 (11)	0.0212 (4)
C17	0.5121 (3)	0.76263 (4)	0.68082 (11)	0.0283 (4)
H17	0.492764	0.745872	0.698569	0.034*
C18	0.5391 (4)	0.78256 (5)	0.72745 (12)	0.0370 (5)
H18	0.536487	0.779604	0.777212	0.044*
C19	0.5703 (4)	0.80725 (5)	0.70113 (12)	0.0355 (5)
H19	0.591278	0.820946	0.733259	0.043*
C20	0.5707 (4)	0.81181 (4)	0.62893 (11)	0.0280 (4)
H20	0.591466	0.828616	0.611690	0.034*
C21	0.5408 (3)	0.79174 (4)	0.58094 (10)	0.0214 (4)
C22	0.5444 (3)	0.79669 (4)	0.50355 (10)	0.0202 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0338 (3)	0.01553 (18)	0.02103 (19)	−0.00169 (18)	0.00096 (19)	0.00055 (17)

O1	0.0289 (7)	0.0131 (5)	0.0174 (6)	−0.0013 (5)	−0.0005 (5)	0.0009 (5)
O2	0.0431 (9)	0.0224 (7)	0.0225 (7)	−0.0040 (7)	−0.0027 (6)	−0.0007 (5)
O3	0.0555 (10)	0.0147 (6)	0.0313 (8)	−0.0026 (7)	0.0011 (7)	0.0011 (6)
N1	0.0214 (8)	0.0178 (7)	0.0289 (8)	0.0004 (6)	−0.0017 (7)	−0.0013 (6)
N2	0.0239 (8)	0.0210 (8)	0.0178 (7)	0.0016 (6)	−0.0014 (6)	0.0003 (6)
N3	0.0279 (9)	0.0159 (7)	0.0236 (7)	−0.0029 (6)	0.0024 (7)	−0.0003 (6)
C1	0.0208 (9)	0.0172 (8)	0.0289 (10)	−0.0003 (7)	−0.0003 (7)	0.0031 (7)
C2	0.0299 (10)	0.0229 (9)	0.0291 (10)	−0.0020 (8)	−0.0007 (8)	0.0042 (7)
C3	0.0312 (11)	0.0244 (9)	0.0380 (11)	−0.0032 (8)	−0.0025 (9)	0.0089 (8)
C4	0.0281 (11)	0.0201 (9)	0.0437 (12)	−0.0024 (8)	−0.0029 (9)	0.0073 (8)
C5	0.0230 (10)	0.0175 (8)	0.0409 (11)	0.0015 (7)	−0.0027 (8)	−0.0002 (8)
C6	0.0182 (8)	0.0175 (8)	0.0323 (10)	0.0002 (7)	−0.0011 (8)	0.0011 (7)
C7	0.0193 (9)	0.0164 (8)	0.0209 (8)	0.0007 (6)	−0.0008 (6)	−0.0012 (6)
C8	0.0185 (8)	0.0166 (8)	0.0190 (8)	0.0012 (6)	−0.0009 (6)	−0.0022 (6)
C9	0.0192 (8)	0.0147 (7)	0.0191 (8)	0.0010 (6)	−0.0004 (6)	0.0022 (6)
C10	0.0215 (8)	0.0145 (7)	0.0185 (7)	−0.0005 (6)	0.0001 (7)	0.0009 (6)
C11	0.0214 (9)	0.0154 (7)	0.0226 (8)	−0.0013 (7)	0.0007 (7)	−0.0011 (6)
C12	0.0276 (9)	0.0174 (8)	0.0223 (9)	0.0000 (7)	−0.0002 (7)	0.0030 (6)
C13	0.0277 (10)	0.0198 (9)	0.0193 (8)	0.0007 (7)	−0.0003 (7)	0.0030 (6)
C14	0.0202 (8)	0.0176 (8)	0.0198 (8)	0.0008 (6)	−0.0003 (6)	−0.0002 (6)
C15	0.0183 (8)	0.0177 (8)	0.0193 (8)	0.0017 (6)	−0.0015 (6)	−0.0005 (6)
C16	0.0218 (9)	0.0215 (8)	0.0202 (8)	0.0026 (7)	−0.0026 (7)	−0.0031 (7)
C17	0.0381 (11)	0.0242 (10)	0.0227 (9)	0.0014 (8)	−0.0020 (8)	−0.0032 (8)
C18	0.0572 (15)	0.0331 (11)	0.0208 (9)	0.0032 (11)	−0.0047 (10)	−0.0081 (9)
C19	0.0500 (14)	0.0286 (11)	0.0280 (10)	0.0029 (10)	−0.0051 (10)	−0.0108 (8)
C20	0.0322 (11)	0.0218 (9)	0.0302 (10)	0.0005 (8)	−0.0026 (8)	−0.0082 (8)
C21	0.0202 (9)	0.0198 (8)	0.0244 (9)	0.0032 (7)	−0.0022 (7)	−0.0049 (7)
C22	0.0178 (8)	0.0184 (8)	0.0242 (8)	0.0011 (6)	−0.0006 (6)	−0.0028 (6)

Geometric parameters (Å, º)

S1—C7	1.743 (2)	C8—C15	1.437 (2)
S1—C1	1.750 (2)	C9—C10	1.381 (2)
O1—C9	1.381 (2)	C9—C14	1.407 (2)
O1—C8	1.382 (2)	C10—C11	1.395 (2)
O2—N3	1.232 (2)	C10—H10	0.9500
O3—N3	1.229 (2)	C11—C12	1.383 (3)
N1—C22	1.303 (3)	C12—C13	1.392 (3)
N1—C6	1.382 (3)	C12—H12	0.9500
N2—C15	1.309 (2)	C13—C14	1.400 (3)
N2—C14	1.390 (2)	C13—H13	0.9500
N3—C11	1.464 (2)	C15—C16	1.461 (3)
C1—C2	1.396 (3)	C16—C17	1.403 (3)
C1—C6	1.412 (3)	C16—C21	1.405 (3)
C2—C3	1.392 (3)	C17—C18	1.378 (3)
C2—H2	0.9500	C17—H17	0.9500
C3—C4	1.390 (3)	C18—C19	1.403 (4)
C3—H3	0.9500	C18—H18	0.9500

C4—C5	1.385 (3)	C19—C20	1.381 (3)
C4—H4	0.9500	C19—H19	0.9500
C5—C6	1.408 (3)	C20—C21	1.403 (3)
C5—H5	0.9500	C20—H20	0.9500
C7—C8	1.365 (2)	C21—C22	1.480 (3)
C7—C22	1.459 (3)		

C7—S1—C1	101.44 (9)	C12—C11—C10	123.48 (17)
C9—O1—C8	117.11 (14)	C12—C11—N3	118.98 (16)
C22—N1—C6	122.71 (17)	C10—C11—N3	117.52 (16)
C15—N2—C14	116.53 (17)	C11—C12—C13	118.21 (18)
O3—N3—O2	123.65 (18)	C11—C12—H12	120.9
O3—N3—C11	118.20 (17)	C13—C12—H12	120.9
O2—N3—C11	118.16 (17)	C12—C13—C14	120.79 (18)
C2—C1—C6	121.09 (18)	C12—C13—H13	119.6
C2—C1—S1	116.71 (16)	C14—C13—H13	119.6
C6—C1—S1	122.20 (15)	N2—C14—C13	119.46 (17)
C3—C2—C1	119.5 (2)	N2—C14—C9	122.28 (17)
C3—C2—H2	120.2	C13—C14—C9	118.26 (17)
C1—C2—H2	120.2	N2—C15—C8	123.61 (17)
C4—C3—C2	120.4 (2)	N2—C15—C16	119.62 (18)
C4—C3—H3	119.8	C8—C15—C16	116.75 (17)
C2—C3—H3	119.8	C17—C16—C21	119.87 (19)
C5—C4—C3	120.12 (19)	C17—C16—C15	119.31 (19)
C5—C4—H4	119.9	C21—C16—C15	120.80 (18)
C3—C4—H4	119.9	C18—C17—C16	120.4 (2)
C4—C5—C6	121.1 (2)	C18—C17—H17	119.8
C4—C5—H5	119.4	C16—C17—H17	119.8
C6—C5—H5	119.4	C17—C18—C19	119.7 (2)
N1—C6—C5	116.49 (18)	C17—C18—H18	120.1
N1—C6—C1	125.70 (17)	C19—C18—H18	120.1
C5—C6—C1	117.77 (19)	C20—C19—C18	120.6 (2)
C8—C7—C22	120.54 (18)	C20—C19—H19	119.7
C8—C7—S1	117.13 (14)	C18—C19—H19	119.7
C22—C7—S1	122.32 (14)	C19—C20—C21	120.3 (2)
C7—C8—O1	116.19 (16)	C19—C20—H20	119.9
C7—C8—C15	124.04 (17)	C21—C20—H20	119.9
O1—C8—C15	119.76 (16)	C20—C21—C16	119.16 (19)
C10—C9—O1	116.98 (16)	C20—C21—C22	120.02 (19)
C10—C9—C14	122.47 (16)	C16—C21—C22	120.79 (17)
O1—C9—C14	120.55 (16)	N1—C22—C7	125.41 (18)
C9—C10—C11	116.70 (16)	N1—C22—C21	117.54 (18)
C9—C10—H10	121.6	C7—C22—C21	117.06 (17)
C11—C10—H10	121.6		

C7—S1—C1—C2	175.38 (16)	C12—C13—C14—N2	179.45 (19)
C7—S1—C1—C6	−4.46 (19)	C12—C13—C14—C9	−1.4 (3)
C6—C1—C2—C3	0.7 (3)	C10—C9—C14—N2	−177.73 (18)

S1—C1—C2—C3	−179.14 (16)	O1—C9—C14—N2	2.4 (3)
C1—C2—C3—C4	−0.5 (3)	C10—C9—C14—C13	3.1 (3)
C2—C3—C4—C5	−0.2 (3)	O1—C9—C14—C13	−176.79 (17)
C3—C4—C5—C6	0.7 (3)	C14—N2—C15—C8	−0.4 (3)
C22—N1—C6—C5	−175.21 (19)	C14—N2—C15—C16	−178.93 (16)
C22—N1—C6—C1	2.4 (3)	C7—C8—C15—N2	−176.72 (19)
C4—C5—C6—N1	177.30 (19)	O1—C8—C15—N2	3.7 (3)
C4—C5—C6—C1	−0.5 (3)	C7—C8—C15—C16	1.9 (3)
C2—C1—C6—N1	−177.8 (2)	O1—C8—C15—C16	−177.73 (16)
S1—C1—C6—N1	2.0 (3)	N2—C15—C16—C17	−1.3 (3)
C2—C1—C6—C5	−0.2 (3)	C8—C15—C16—C17	−179.96 (19)
S1—C1—C6—C5	179.61 (15)	N2—C15—C16—C21	176.93 (18)
C1—S1—C7—C8	−177.22 (15)	C8—C15—C16—C21	−1.7 (3)
C1—S1—C7—C22	3.86 (19)	C21—C16—C17—C18	−0.3 (3)
C22—C7—C8—O1	178.25 (16)	C15—C16—C17—C18	177.9 (2)
S1—C7—C8—O1	−0.7 (2)	C16—C17—C18—C19	−0.8 (4)
C22—C7—C8—C15	−1.4 (3)	C17—C18—C19—C20	1.2 (4)
S1—C7—C8—C15	179.71 (16)	C18—C19—C20—C21	−0.3 (4)
C9—O1—C8—C7	176.59 (17)	C19—C20—C21—C16	−0.9 (3)
C9—O1—C8—C15	−3.8 (2)	C19—C20—C21—C22	−179.1 (2)
C8—O1—C9—C10	−178.95 (17)	C17—C16—C21—C20	1.2 (3)
C8—O1—C9—C14	1.0 (2)	C15—C16—C21—C20	−177.03 (19)
O1—C9—C10—C11	178.00 (16)	C17—C16—C21—C22	179.4 (2)
C14—C9—C10—C11	−1.9 (3)	C15—C16—C21—C22	1.1 (3)
C9—C10—C11—C12	−1.1 (3)	C6—N1—C22—C7	−3.1 (3)
C9—C10—C11—N3	−179.50 (16)	C6—N1—C22—C21	176.77 (18)
O3—N3—C11—C12	−6.8 (3)	C8—C7—C22—N1	−179.49 (19)
O2—N3—C11—C12	173.20 (19)	S1—C7—C22—N1	−0.6 (3)
O3—N3—C11—C10	171.68 (18)	C8—C7—C22—C21	0.6 (3)
O2—N3—C11—C10	−8.3 (3)	S1—C7—C22—C21	179.50 (15)
C10—C11—C12—C13	2.7 (3)	C20—C21—C22—N1	−2.3 (3)
N3—C11—C12—C13	−178.88 (18)	C16—C21—C22—N1	179.57 (18)
C11—C12—C13—C14	−1.4 (3)	C20—C21—C22—C7	177.60 (19)
C15—N2—C14—C13	176.55 (18)	C16—C21—C22—C7	−0.5 (3)
C15—N2—C14—C9	−2.6 (3)		