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2,3-Bis(3-nitrophenyl)quinoxaline

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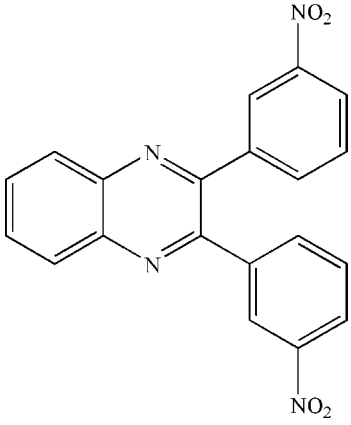
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.057; wR factor = 0.190; data-to-parameter ratio = 11.7.

The title compound, $C_{20}H_{12}N_4O_4$, contains two benzene rings *ortho* bonded to a quinoxaline nucleus. The dihedral angle between the benzene rings is 59.2 (4)°. The two benzene rings adopt a *trans* configuration with respect to the quinoxaline plane. The formal C—C σ-bond substituted by nitrophenyl groups is shorter than normal C—C bonds and the C(benzene)—C(quinoxaline) bonds. These features are consistent with electron delocalization over the whole molecule.

Related literature

For related literature, see: Cantalupo *et al.* (2006); He *et al.* (2003); Lindsley *et al.* (2005); Loriga *et al.* (1997); Rajnikant *et al.* (2006); Seitz *et al.* (2002).



Experimental

Crystal data

$C_{20}H_{12}N_4O_4$
M_r = 372.34
Orthorhombic, *Pbca*
a = 12.807 (3) Å
b = 7.6160 (15) Å
c = 34.430 (7) Å
V = 3358.2 (12) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 294 (2) K
0.22 × 0.18 × 0.12 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.977, T_{max} = 0.983
13448 measured reflections
2948 independent reflections
1533 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.190
S = 1.01
2948 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C6—C7	1.482 (5)	C14—C15	1.485 (5)
C7—C14	1.425 (5)		
N2—C7—C6	116.4 (3)	N3—C14—C15	116.4 (3)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL* (Bruker, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2119).

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supplementary materials

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2,3-Bis(3-nitrophenyl)quinoxaline

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Comment

Functionalized quinoxalines possess a wide range of biological activities, including anticancer (Lindsley *et al.*, 2005), antiviral (Loriga *et al.*, 1997), and antibacterial activity (Seitz *et al.*, 2002), and have also be reported to be kinase inhibitors (He *et al.*, 2003). Herein we report the synthesis and molecular structure of a quinoxaline derivative, (I).

In the molecular structure of (I), the two benzene rings attached to the quinoxaline nucleus make a dihedral angle of 59.2 (4)°. The quinoxaline ring is approximately planar, with a r.m.s. deviation of 0.0341 (5) Å. The two benzene rings make dihedral angles of 26.7 (4) and 58.1 (4)°, respectively, with the planar quinoxaline system. The C6—C7 and C14—C15 bond lengths linking nitrophenyl groups to the quionxaline nucleus (Table 1), are slightly shorter than the normal C—C σ bonds, as a consequence of the delocalization over the aromatic rings. Short bond length is also observed for the C7—C14 bond.

The structure of a related molecule, 2,3-diphenylquinoxaline, has been reported previously (Cantalupo *et al.*, 2006; Rajnikant *et al.*, 2006).

Experimental

A suspension of 1,2-bis(3-nitrophenyl)ethane-1,2-dione (0.8 mmol) and benzene-1,2-diamine (1.0 mmol) in acetic acid (AcOH, 3 ml) was refluxed for 0.5 h. The mixture was poured into ice-water and a white precipitate was formed. The mixture was neutralized using saturated $NaHCO_3$ solution. The resulting precipitate was filtered, washed with water, dried and purified by recrystallization using a mixture of ethyl acetate/petroleum ether, giving the target product as light yellow floccules in 35% yield. Colorless crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform/ethanol (1:15 *v*/*v*).

Refinement

All H atoms were positioned geometrically and refined as riding on their carrier atom with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(carrier C atom).

Figures

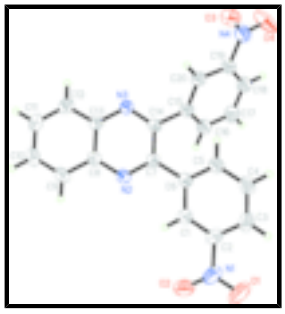


Fig. 1. View of the molecule of (I) showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 35% probability level.

2,3-Bis(3-nitrophenyl)quinoxaline

Crystal data

$C_{20}H_{12}N_4O_4$	D_x = 1.473 Mg m^{-3}
M_r = 372.34	Melting point: 484 K
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 2243 reflections
a = 12.807 (3) Å	θ = 2.3–22.5º
b = 7.6160 (15) Å	μ = 0.11 mm^{-1}
c = 34.430 (7) Å	*T* = 294 (2) K
V = 3358.2 (12) Å^3	Plate, colourless
Z = 8	0.22 × 0.18 × 0.12 mm
F_{000} = 1536	

Data collection

Bruker SMART 1000 diffractometer	2948 independent reflections
Radiation source: fine-focus sealed tube	1533 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.083
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.2º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	*h* = −12→15
T_{min} = 0.977, T_{max} = 0.983	*k* = −9→6
13448 measured reflections	*l* = −33→40

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.057	H-atom parameters constrained

$wR(F^2) = 0.190$	$w = 1/[\sigma^2(F_o^2) + (0.0892P)^2 + 1.3718P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
2948 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
253 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.7566 (4)	1.1964 (7)	−0.02595 (10)	0.1310 (17)
O2	0.8690 (3)	1.0826 (5)	0.01110 (10)	0.0870 (11)
O3	0.2285 (3)	0.8632 (5)	0.18938 (10)	0.0883 (11)
O4	0.1405 (3)	0.7078 (6)	0.14923 (13)	0.1201 (16)
N1	0.7804 (4)	1.1237 (5)	0.00377 (10)	0.0723 (12)
N2	0.7785 (2)	0.8778 (4)	0.13906 (8)	0.0410 (8)
N3	0.6311 (2)	0.7105 (4)	0.18590 (8)	0.0425 (8)
N4	0.2227 (3)	0.7670 (6)	0.16106 (13)	0.0711 (11)
C1	0.7236 (3)	0.9972 (5)	0.06500 (10)	0.0427 (9)
H1	0.7902	0.9501	0.0677	0.051*
C2	0.6987 (3)	1.0903 (5)	0.03248 (11)	0.0510 (10)
C3	0.6010 (4)	1.1591 (5)	0.02666 (13)	0.0622 (12)
H3A	0.5843	1.2163	0.0036	0.075*
C4	0.5285 (3)	1.1413 (5)	0.05580 (13)	0.0639 (12)
H4A	0.4625	1.1908	0.0531	0.077*
C5	0.5536 (3)	1.0506 (5)	0.08894 (12)	0.0532 (11)
H5	0.5040	1.0413	0.1086	0.064*
C6	0.6500 (3)	0.9724 (5)	0.09413 (10)	0.0414 (9)
C7	0.6801 (3)	0.8727 (4)	0.12936 (9)	0.0371 (9)
C8	0.8071 (3)	0.7959 (5)	0.17225 (10)	0.0410 (9)
C9	0.9120 (3)	0.7918 (5)	0.18301 (12)	0.0526 (10)
H9	0.9621	0.8434	0.1671	0.063*
C10	0.9413 (3)	0.7126 (6)	0.21664 (12)	0.0607 (12)
H10	1.0115	0.7093	0.2235	0.073*
C11	0.8674 (4)	0.6365 (6)	0.24082 (12)	0.0590 (11)
H11	0.8884	0.5825	0.2637	0.071*
C12	0.7646 (3)	0.6403 (5)	0.23127 (10)	0.0526 (11)
H12	0.7156	0.5899	0.2478	0.063*
C13	0.7320 (3)	0.7196 (5)	0.19665 (9)	0.0397 (9)
C14	0.6066 (3)	0.7777 (5)	0.15223 (10)	0.0402 (9)
C15	0.5015 (3)	0.7331 (5)	0.13689 (10)	0.0449 (9)
C16	0.4938 (3)	0.6437 (5)	0.10190 (11)	0.0560 (11)
H16	0.5544	0.6162	0.0883	0.067*
C17	0.3983 (4)	0.5947 (6)	0.08668 (12)	0.0633 (12)
H17	0.3946	0.5342	0.0633	0.076*
C18	0.3105 (4)	0.6358 (6)	0.10632 (13)	0.0610 (12)
H18	0.2456	0.6047	0.0964	0.073*

C19	0.3170 (3)	0.7230 (5)	0.14073 (12)	0.0514 (10)
C20	0.4127 (3)	0.7711 (5)	0.15701 (11)	0.0487 (10)
H20	0.4158	0.8274	0.1809	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.141 (3)	0.177 (4)	0.075 (2)	0.057 (3)	0.027 (2)	0.065 (3)
O2	0.077 (2)	0.101 (3)	0.083 (2)	0.012 (2)	0.027 (2)	0.022 (2)
O3	0.071 (3)	0.119 (3)	0.075 (2)	0.018 (2)	0.0175 (19)	0.005 (2)
O4	0.036 (2)	0.145 (4)	0.180 (4)	−0.012 (2)	0.004 (2)	−0.018 (3)
N1	0.093 (3)	0.074 (3)	0.050 (2)	0.020 (2)	0.012 (2)	0.015 (2)
N2	0.036 (2)	0.0402 (18)	0.0466 (18)	0.0011 (14)	0.0006 (15)	−0.0021 (14)
N3	0.041 (2)	0.0475 (18)	0.0390 (17)	−0.0006 (15)	−0.0014 (14)	−0.0019 (15)
N4	0.053 (3)	0.077 (3)	0.083 (3)	0.006 (2)	0.003 (2)	0.020 (2)
C1	0.042 (2)	0.040 (2)	0.046 (2)	−0.0001 (17)	−0.0010 (19)	−0.0046 (17)
C2	0.065 (3)	0.046 (2)	0.042 (2)	−0.003 (2)	0.005 (2)	0.0032 (19)
C3	0.068 (3)	0.056 (3)	0.063 (3)	0.002 (2)	−0.014 (3)	0.012 (2)
C4	0.048 (3)	0.057 (3)	0.086 (3)	0.007 (2)	−0.004 (3)	0.017 (2)
C5	0.041 (2)	0.051 (2)	0.068 (3)	0.004 (2)	0.005 (2)	0.012 (2)
C6	0.040 (2)	0.039 (2)	0.045 (2)	−0.0027 (17)	−0.0007 (18)	−0.0040 (17)
C7	0.037 (2)	0.035 (2)	0.039 (2)	0.0015 (16)	0.0018 (17)	−0.0036 (16)
C8	0.041 (2)	0.040 (2)	0.042 (2)	0.0037 (17)	−0.0023 (18)	−0.0055 (17)
C9	0.037 (3)	0.056 (2)	0.065 (3)	0.0005 (19)	0.000 (2)	0.000 (2)
C10	0.047 (3)	0.068 (3)	0.068 (3)	0.006 (2)	−0.020 (2)	0.003 (2)
C11	0.067 (3)	0.061 (3)	0.049 (2)	0.003 (2)	−0.013 (2)	0.000 (2)
C12	0.062 (3)	0.052 (3)	0.043 (2)	−0.004 (2)	−0.001 (2)	−0.0020 (18)
C13	0.042 (2)	0.041 (2)	0.0358 (19)	0.0015 (17)	0.0007 (18)	−0.0053 (16)
C14	0.035 (2)	0.040 (2)	0.046 (2)	0.0023 (16)	0.0030 (18)	−0.0037 (17)
C15	0.043 (3)	0.045 (2)	0.047 (2)	−0.0008 (18)	0.0039 (19)	0.0084 (18)
C16	0.049 (3)	0.063 (3)	0.056 (3)	−0.002 (2)	−0.002 (2)	−0.004 (2)
C17	0.068 (3)	0.066 (3)	0.056 (3)	−0.003 (2)	−0.008 (3)	−0.008 (2)
C18	0.051 (3)	0.066 (3)	0.066 (3)	−0.006 (2)	−0.007 (2)	0.013 (2)
C19	0.040 (3)	0.052 (2)	0.062 (3)	0.000 (2)	0.007 (2)	0.014 (2)
C20	0.049 (3)	0.047 (2)	0.050 (2)	0.0025 (19)	0.004 (2)	0.0062 (18)

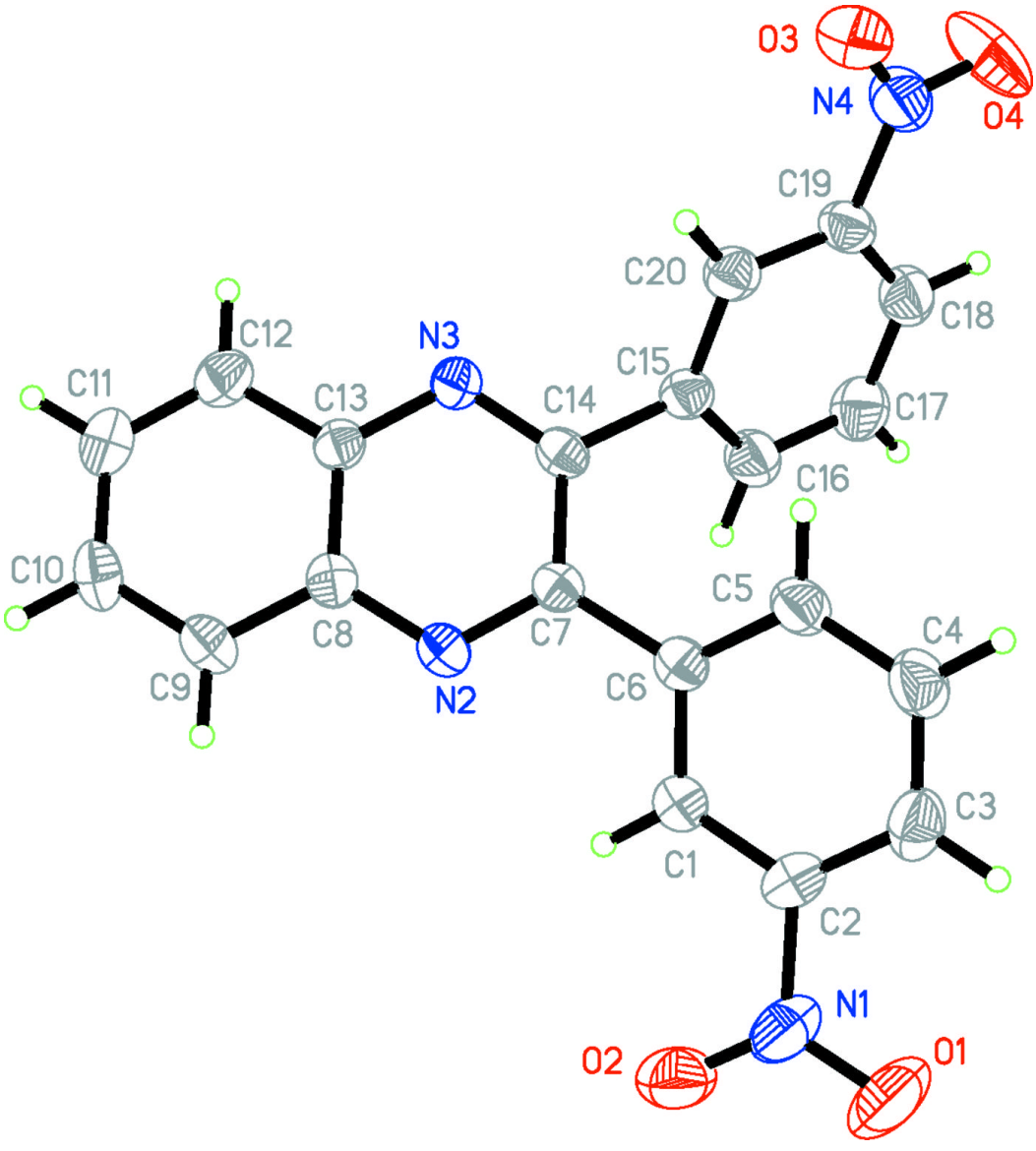
Geometric parameters (Å, °)

O1—N1	1.202 (4)	C8—C9	1.394 (5)
O2—N1	1.204 (4)	C8—C13	1.403 (5)
O3—N4	1.222 (5)	C9—C10	1.358 (5)
O4—N4	1.215 (5)	C9—H9	0.9300
N1—C2	1.462 (5)	C10—C11	1.387 (6)
N2—C7	1.304 (4)	C10—H10	0.9300
N2—C8	1.353 (4)	C11—C12	1.357 (5)
N3—C14	1.305 (4)	C11—H11	0.9300
N3—C13	1.346 (4)	C12—C13	1.401 (5)
N4—C19	1.435 (5)	C12—H12	0.9300
C1—C2	1.363 (5)	C14—C15	1.485 (5)

C1—C6	1.389 (5)	C15—C20	1.363 (5)
C1—H1	0.9300	C15—C16	1.387 (5)
C2—C3	1.372 (5)	C16—C17	1.382 (5)
C3—C4	1.373 (6)	C16—H16	0.9300
C3—H3A	0.9300	C17—C18	1.349 (5)
C4—C5	1.372 (5)	C17—H17	0.9300
C4—H4A	0.9300	C18—C19	1.361 (6)
C5—C6	1.383 (5)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.397 (5)
C6—C7	1.482 (5)	C20—H20	0.9300
C7—C14	1.425 (5)		
O1—N1—O2	122.5 (4)	C8—C9—H9	119.9
O1—N1—C2	118.3 (4)	C9—C10—C11	120.6 (4)
O2—N1—C2	119.2 (4)	C9—C10—H10	119.7
C7—N2—C8	117.7 (3)	C11—C10—H10	119.7
C14—N3—C13	117.0 (3)	C12—C11—C10	120.5 (4)
O4—N4—O3	122.9 (4)	C12—C11—H11	119.7
O4—N4—C19	118.6 (5)	C10—C11—H11	119.7
O3—N4—C19	118.5 (4)	C11—C12—C13	120.3 (4)
C2—C1—C6	120.3 (4)	C11—C12—H12	119.8
C2—C1—H1	119.8	C13—C12—H12	119.8
C6—C1—H1	119.8	N3—C13—C12	119.9 (3)
C1—C2—C3	122.2 (4)	N3—C13—C8	121.0 (3)
C1—C2—N1	118.6 (4)	C12—C13—C8	118.9 (4)
C3—C2—N1	119.2 (4)	N3—C14—C7	122.1 (3)
C2—C3—C4	118.2 (4)	N3—C14—C15	116.4 (3)
C2—C3—H3A	120.9	C7—C14—C15	121.2 (3)
C4—C3—H3A	120.9	C20—C15—C16	119.1 (4)
C5—C4—C3	120.0 (4)	C20—C15—C14	121.8 (3)
C5—C4—H4A	120.0	C16—C15—C14	119.1 (3)
C3—C4—H4A	120.0	C17—C16—C15	121.7 (4)
C4—C5—C6	122.2 (4)	C17—C16—H16	119.2
C4—C5—H5	118.9	C15—C16—H16	119.2
C6—C5—H5	118.9	C18—C17—C16	119.0 (4)
C5—C6—C1	117.0 (3)	C18—C17—H17	120.5
C5—C6—C7	124.0 (3)	C16—C17—H17	120.5
C1—C6—C7	119.0 (3)	C17—C18—C19	119.9 (4)
N2—C7—C14	120.8 (3)	C17—C18—H18	120.0
N2—C7—C6	116.4 (3)	C19—C18—H18	120.0
C14—C7—C6	122.8 (3)	C18—C19—C20	122.1 (4)
N2—C8—C9	119.8 (3)	C18—C19—N4	119.1 (4)
N2—C8—C13	120.7 (3)	C20—C19—N4	118.8 (4)
C9—C8—C13	119.5 (3)	C15—C20—C19	118.2 (4)
C10—C9—C8	120.2 (4)	C15—C20—H20	120.9
C10—C9—H9	119.9	C19—C20—H20	120.9
C6—C1—C2—C3	−1.5 (6)	C11—C12—C13—C8	−0.4 (5)
C6—C1—C2—N1	175.8 (3)	N2—C8—C13—N3	6.7 (5)
O1—N1—C2—C1	175.5 (4)	C9—C8—C13—N3	−175.4 (3)

O2—N1—C2—C1	−6.6 (6)	N2—C8—C13—C12	−178.3 (3)
O1—N1—C2—C3	−7.2 (6)	C9—C8—C13—C12	−0.3 (5)
O2—N1—C2—C3	170.7 (4)	C13—N3—C14—C7	−6.3 (5)
C1—C2—C3—C4	3.8 (6)	C13—N3—C14—C15	167.0 (3)
N1—C2—C3—C4	−173.5 (4)	N2—C7—C14—N3	8.5 (5)
C2—C3—C4—C5	−2.5 (6)	C6—C7—C14—N3	−170.5 (3)
C3—C4—C5—C6	−1.0 (6)	N2—C7—C14—C15	−164.5 (3)
C4—C5—C6—C1	3.3 (6)	C6—C7—C14—C15	16.5 (5)
C4—C5—C6—C7	−179.7 (4)	N3—C14—C15—C20	58.2 (5)
C2—C1—C6—C5	−2.0 (5)	C7—C14—C15—C20	−128.4 (4)
C2—C1—C6—C7	−179.2 (3)	N3—C14—C15—C16	−119.1 (4)
C8—N2—C7—C14	−2.6 (5)	C7—C14—C15—C16	54.4 (5)
C8—N2—C7—C6	176.5 (3)	C20—C15—C16—C17	1.0 (6)
C5—C6—C7—N2	−148.7 (3)	C14—C15—C16—C17	178.3 (4)
C1—C6—C7—N2	28.2 (5)	C15—C16—C17—C18	0.4 (6)
C5—C6—C7—C14	30.3 (5)	C16—C17—C18—C19	−0.6 (6)
C1—C6—C7—C14	−152.8 (3)	C17—C18—C19—C20	−0.6 (6)
C7—N2—C8—C9	177.5 (3)	C17—C18—C19—N4	179.5 (4)
C7—N2—C8—C13	−4.6 (5)	O4—N4—C19—C18	8.2 (6)
N2—C8—C9—C10	178.8 (3)	O3—N4—C19—C18	−171.3 (4)
C13—C8—C9—C10	0.8 (6)	O4—N4—C19—C20	−171.6 (4)
C8—C9—C10—C11	−0.6 (6)	O3—N4—C19—C20	8.8 (6)
C9—C10—C11—C12	−0.1 (6)	C16—C15—C20—C19	−2.1 (5)
C10—C11—C12—C13	0.6 (6)	C14—C15—C20—C19	−179.3 (3)
C14—N3—C13—C12	−176.0 (3)	C18—C19—C20—C15	2.0 (6)
C14—N3—C13—C8	−1.0 (5)	N4—C19—C20—C15	−178.1 (3)
C11—C12—C13—N3	174.7 (3)		

Fig. 1


O3
N4
O4
C19
C20
C18
C12
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C15
C11
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C14
C17
C16
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C5
C4
C8
C7
C9
N2
C6
C3
C1
C2
N1
O2
O1