Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-((*Z*)-{3-[(*Z*)-(2-Hydroxy-5-methylbenzylidene)amino]-2,2-dimethylpropyl}iminomethyl)-4-methylphenol

Reza Kia,[a,b]* Hadi Kargar,[c] Valiollah Mirkhani,[d] Fatemeh Ganji[c] and Muhammad Nawaz Tahir[e]*

[a]Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran, [b]X-ray Crystallography Laboratory, Plasma Physics Research Center, Science and Research Branch, Islamic Azad University, Tehran, Iran, [c]Department of Chemistry, School of Science, Payame Noor University (PNU), Ardakan, Yazd, Iran, [d]Department of Chemistry, University of Isfahan, Isfahan, 81746-73441, Iran, and [e]Department of Physics, University of Sargodha, Punjab, Pakistan
Correspondence e-mail: rkia@srbiau.ac.ir, zsrkk@yahoo.com, dmntahir_uos@yahoo.com

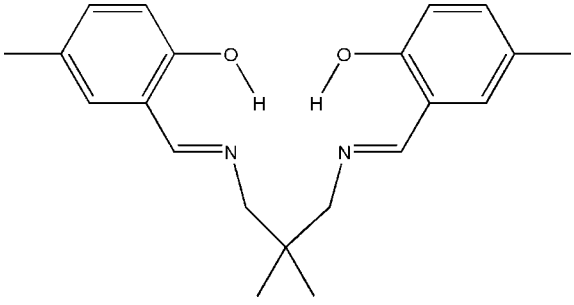
Received 4 December 2010; accepted 9 December 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.112; data-to-parameter ratio = 9.5.

In the title compound, $C_{21}H_{26}N_2O_2$, the dihedral angle between the two benzene rings is 73.47 (16)°. Strong intramolecular O—H···N hydrogen bonds generate S(6) ring motifs. The substituted benzene rings are twisted around the central quaternary C atom in opposite directions, making a vault geometry.

Related literature

For standard bond lengths, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For related structures, see: Kargar *et al.* (2009, 2010).



Experimental

Crystal data

$C_{21}H_{26}N_2O_2$
M_r = 338.44
Orthorhombic, $P2_12_12_1$
a = 5.8950 (3) Å
b = 17.8634 (10) Å
c = 18.2140 (11) Å
V = 1918.02 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.30 × 0.18 × 0.12 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.978, T_{max} = 0.991
16208 measured reflections
2199 independent reflections
1368 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.112
S = 1.03
2199 reflections
231 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1	0.82	1.89	2.620 (3)	147
O2—H2A···N2	0.82	1.88	2.609 (4)	147

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

RK thanks the Science and Research Branch, Islamic Azad University. HK and FG thank PNU for financial support. MNT thanks the University of Sargodha, Pakistan, for the research facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2096).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Kargar, H., Kia, R., Jamshidvand, A. & Fun, H.-K. (2009). *Acta Cryst.* E**65**, o776–o777.
Kargar, H., Kia, R., Ullah Khan, I. & Sahraei, A. (2010). *Acta Cryst.* E**66**, o539.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2011). E**67**, o130 [**doi:10.1107/S1600536810051688**]

2-((*Z*)-{3-[(*Z*)-(2-Hydroxy-5-methylbenzylidene)amino]-2,2-dimethylpropyl}iminomethyl)-4-methylphenol

R. Kia, H. Kargar, V. Mirkhani, F. Ganji and M. N. Tahir

Comment

Schiff base ligands are one of the most prevalent systems in coordination chemistry. As part of a general study of tetradenate Schiff bases (Kargar *et al.* 2009; Kargar *et al.* 2010), we have determined the crystal structure of the title compound.

The asymmetric unit of the title compound, Fig. 1, comprises a potentially tetradenate Schiff base ligand. The bond lengths (Allen *et al.,* 1987) and angles are within the normal ranges. The dihedral angle between the two phenyl rings is 73.47 (16)°. Strong intramolecular O—H···N hydrogen bonds generate *S(6)* ring motifs (Bernstein *et al.,* 1995). The title compound has a skew geometry. In the absence of sufficient anomalous scattering the absolute structure could not be determined.

Experimental

The title compound was synthesized by adding 5-methyl-salicylaldehyde (4 mmol) to a solution of 2,2'-dimethylpropylene-diamine (2 mmol) in ethanol (20 ml). The mixture was refluxed with stirring for half an hour. The resultant yellow solution was filtered. Yellow single crystals of the title compound suitable for *X*-ray structure determination were recrystallized from ethanol by slow evaporation of the solvents at room temperature over several days.

Refinement

H atoms of the hydroxy groups were located by a rotating O–H group and constraied to refine with the parent atoms with U_{iso}(H) = 1.5 U_{eq}(O), see Table 1. The remaining H atoms were positioned geometrically with C—H = 0.93-0.97 Å and included in a riding model approximation with U_{iso} (H) = 1.2 or 1.5 U_{eq} (C). A rotating group model was used for the methyl groups of the benzene rings. In the absence of sufficient anomalous scattering the absolute structure could not be determined and 1580 Friedel pairs were merged.

Figures

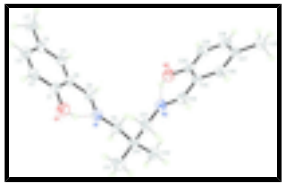


Fig. 1. The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids and the atomic numbering. Intramolecular hydrogen bonds are drawn as dashed lines.

2-((*Z*)-{3-[(*Z*)-(2-Hydroxy-5-methylbenzylidene)amino]- 2,2-dimethylpropyl}iminomethyl)-4-methylphenol

Crystal data

$C_{21}H_{26}N_2O_2$	$F(000) = 728$
$M_r = 338.44$	$D_x = 1.172$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 2150 reflections
$a = 5.8950$ (3) Å	$\theta = 2.5$–$29.8°$
$b = 17.8634$ (10) Å	$\mu = 0.08$ mm^{-1}
$c = 18.2140$ (11) Å	$T = 296$ K
$V = 1918.02$ (19) Å^3	Plate, yellow
$Z = 4$	0.30 × 0.18 × 0.12 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	2199 independent reflections
Radiation source: fine-focus sealed tube	1368 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.062$
φ and ω scans	$\theta_{max} = 26.0°$, $\theta_{min} = 2.2°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$h = -7\rightarrow7$
$T_{min} = 0.978$, $T_{max} = 0.991$	$k = -22\rightarrow22$
16208 measured reflections	$l = -22\rightarrow22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.112$	$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.082P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
2199 reflections	$\Delta\rho_{max} = 0.15$ e Å^{-3}
231 parameters	$\Delta\rho_{min} = -0.12$ e Å^{-3}
0 restraints	Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.013 (2)

Special details

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4633 (4)	0.71477 (13)	0.18637 (14)	0.0691 (7)
H1A	0.3887	0.6786	0.1999	0.104*
O2	−0.1798 (4)	0.44857 (14)	0.02145 (14)	0.0769 (7)
H2A	−0.0936	0.4643	0.0533	0.115*
N1	0.1130 (4)	0.62471 (14)	0.19160 (15)	0.0576 (7)
N2	0.1758 (5)	0.44863 (14)	0.10671 (15)	0.0589 (7)
C1	0.3362 (5)	0.75772 (18)	0.14103 (17)	0.0513 (8)
C2	0.4215 (5)	0.82499 (18)	0.11644 (19)	0.0593 (9)
H2	0.5650	0.8401	0.1316	0.071*
C3	0.2994 (6)	0.87012 (19)	0.07010 (18)	0.0593 (9)
H3	0.3614	0.9153	0.0545	0.071*
C4	0.0828 (5)	0.84926 (18)	0.04596 (18)	0.0558 (9)
C5	−0.0004 (6)	0.78143 (17)	0.07017 (17)	0.0544 (8)
H5	−0.1421	0.7659	0.0537	0.065*
C6	0.1183 (5)	0.73540 (17)	0.11802 (17)	0.0487 (8)
C7	−0.0504 (7)	0.90009 (19)	−0.0039 (2)	0.0777 (11)
H7A	0.0048	0.8952	−0.0533	0.117*
H7B	−0.0332	0.9510	0.0120	0.117*
H7C	−0.2079	0.8865	−0.0023	0.117*
C8	0.0162 (6)	0.66623 (17)	0.14440 (18)	0.0562 (9)
H8	−0.1246	0.6520	0.1261	0.067*
C9	−0.0035 (6)	0.55714 (17)	0.21706 (19)	0.0641 (10)
H9A	−0.1067	0.5401	0.1791	0.077*
H9B	−0.0929	0.5693	0.2601	0.077*
C10	0.1605 (6)	0.49409 (17)	0.23599 (18)	0.0615 (9)
C11	0.3201 (7)	0.5184 (2)	0.2980 (2)	0.0892 (13)
H11A	0.2336	0.5276	0.3417	0.134*
H11B	0.3982	0.5633	0.2838	0.134*
H11C	0.4286	0.4794	0.3072	0.134*
C12	0.0218 (8)	0.4259 (2)	0.2593 (2)	0.0891 (13)
H12A	0.1216	0.3842	0.2673	0.134*
H12B	−0.0850	0.4136	0.2214	0.134*
H12C	−0.0582	0.4370	0.3039	0.134*
C13	0.3085 (6)	0.47518 (18)	0.16952 (19)	0.0640 (10)
H13A	0.3929	0.5194	0.1551	0.077*
H13B	0.4171	0.4369	0.1833	0.077*
C14	0.2562 (6)	0.39671 (18)	0.06619 (18)	0.0571 (9)
H14	0.3962	0.3762	0.0784	0.069*

C15	0.1397 (5)	0.36831 (16)	0.00220 (18)	0.0512 (8)
C16	0.2388 (6)	0.31298 (17)	−0.04090 (17)	0.0542 (8)
H16	0.3790	0.2940	−0.0267	0.065*
C17	0.1400 (6)	0.28490 (17)	−0.10341 (18)	0.0570 (9)
C18	−0.0714 (6)	0.3128 (2)	−0.1220 (2)	0.0638 (10)
H18	−0.1438	0.2943	−0.1636	0.077*
C19	−0.1782 (6)	0.3673 (2)	−0.08042 (19)	0.0648 (9)
H19	−0.3205	0.3850	−0.0941	0.078*
C20	−0.0727 (5)	0.39531 (18)	−0.01880 (19)	0.0542 (9)
C21	0.2588 (7)	0.22644 (19)	−0.14975 (19)	0.0775 (12)
H21A	0.3779	0.2497	−0.1775	0.116*
H21B	0.1517	0.2039	−0.1827	0.116*
H21C	0.3222	0.1886	−0.1184	0.116*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0584 (15)	0.0711 (17)	0.0778 (17)	0.0012 (12)	−0.0145 (14)	0.0031 (14)
O2	0.0690 (16)	0.0818 (17)	0.0798 (19)	0.0272 (15)	0.0009 (14)	−0.0003 (14)
N1	0.0590 (17)	0.0501 (16)	0.0636 (18)	0.0000 (13)	0.0014 (15)	−0.0032 (14)
N2	0.0615 (17)	0.0523 (17)	0.0629 (18)	0.0032 (14)	−0.0008 (16)	0.0023 (15)
C1	0.0439 (18)	0.0545 (19)	0.056 (2)	0.0055 (16)	−0.0042 (16)	−0.0062 (16)
C2	0.0503 (19)	0.060 (2)	0.068 (2)	−0.0066 (17)	−0.0024 (18)	−0.0138 (18)
C3	0.057 (2)	0.056 (2)	0.065 (2)	−0.0064 (17)	0.0018 (18)	−0.0047 (18)
C4	0.056 (2)	0.054 (2)	0.058 (2)	0.0018 (16)	0.0007 (17)	−0.0054 (16)
C5	0.0467 (18)	0.055 (2)	0.061 (2)	−0.0020 (16)	−0.0037 (17)	−0.0096 (17)
C6	0.0423 (17)	0.0497 (18)	0.0540 (19)	−0.0008 (14)	0.0011 (16)	−0.0062 (16)
C7	0.078 (3)	0.070 (2)	0.085 (3)	−0.0059 (19)	−0.015 (2)	0.014 (2)
C8	0.0485 (19)	0.057 (2)	0.063 (2)	−0.0020 (16)	0.0052 (17)	−0.0098 (17)
C9	0.067 (2)	0.061 (2)	0.064 (2)	−0.0107 (19)	0.0100 (19)	−0.0015 (17)
C10	0.072 (2)	0.052 (2)	0.060 (2)	−0.0139 (19)	−0.0039 (19)	0.0081 (17)
C11	0.109 (3)	0.080 (3)	0.079 (3)	−0.012 (2)	−0.027 (3)	−0.002 (2)
C12	0.116 (3)	0.077 (3)	0.074 (3)	−0.032 (3)	−0.009 (3)	0.016 (2)
C13	0.060 (2)	0.052 (2)	0.080 (3)	−0.0010 (17)	−0.006 (2)	−0.0061 (18)
C14	0.0495 (19)	0.054 (2)	0.068 (2)	0.0020 (16)	−0.0012 (18)	0.0062 (18)
C15	0.0506 (19)	0.0491 (18)	0.0538 (19)	0.0021 (15)	0.0049 (17)	0.0105 (16)
C16	0.0496 (19)	0.0534 (19)	0.059 (2)	0.0028 (15)	0.0031 (17)	0.0083 (17)
C17	0.063 (2)	0.055 (2)	0.053 (2)	−0.0015 (17)	0.0069 (18)	0.0096 (17)
C18	0.064 (2)	0.072 (2)	0.055 (2)	−0.0100 (19)	−0.0029 (19)	0.0109 (18)
C19	0.0495 (19)	0.079 (3)	0.066 (2)	0.0022 (19)	−0.002 (2)	0.018 (2)
C20	0.051 (2)	0.0555 (19)	0.057 (2)	0.0067 (16)	0.0082 (17)	0.0106 (17)
C21	0.099 (3)	0.068 (2)	0.065 (2)	0.011 (2)	0.006 (2)	−0.0031 (19)

Geometric parameters (Å, °)

O1—C1	1.354 (3)	C10—C12	1.527 (5)
O1—H1A	0.8200	C10—C13	1.530 (4)
O2—C20	1.357 (4)	C10—C11	1.533 (5)
O2—H2A	0.8200	C11—H11A	0.9600

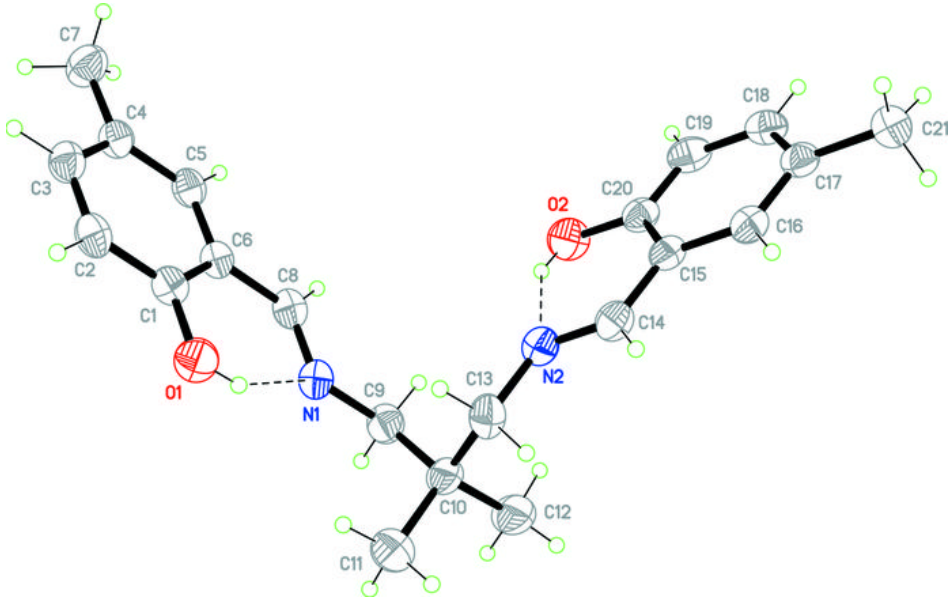
N1—C8	1.271 (4)	C11—H11B	0.9600
N1—C9	1.464 (4)	C11—H11C	0.9600
N2—C14	1.276 (4)	C12—H12A	0.9600
N2—C13	1.465 (4)	C12—H12B	0.9600
C1—C2	1.377 (4)	C12—H12C	0.9600
C1—C6	1.409 (4)	C13—H13A	0.9700
C2—C3	1.371 (4)	C13—H13B	0.9700
C2—H2	0.9300	C14—C15	1.445 (4)
C3—C4	1.401 (4)	C14—H14	0.9300
C3—H3	0.9300	C15—C16	1.391 (4)
C4—C5	1.380 (4)	C15—C20	1.395 (4)
C4—C7	1.506 (4)	C16—C17	1.374 (4)
C5—C6	1.388 (4)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.384 (5)
C6—C8	1.456 (4)	C17—C21	1.515 (4)
C7—H7A	0.9600	C18—C19	1.386 (5)
C7—H7B	0.9600	C18—H18	0.9300
C7—H7C	0.9600	C19—C20	1.377 (4)
C8—H8	0.9300	C19—H19	0.9300
C9—C10	1.524 (5)	C21—H21A	0.9600
C9—H9A	0.9700	C21—H21B	0.9600
C9—H9B	0.9700	C21—H21C	0.9600
C1—O1—H1A	109.5	C10—C11—H11B	109.5
C20—O2—H2A	109.5	H11A—C11—H11B	109.5
C8—N1—C9	119.0 (3)	C10—C11—H11C	109.5
C14—N2—C13	119.3 (3)	H11A—C11—H11C	109.5
O1—C1—C2	119.4 (3)	H11B—C11—H11C	109.5
O1—C1—C6	121.7 (3)	C10—C12—H12A	109.5
C2—C1—C6	118.9 (3)	C10—C12—H12B	109.5
C3—C2—C1	121.4 (3)	H12A—C12—H12B	109.5
C3—C2—H2	119.3	C10—C12—H12C	109.5
C1—C2—H2	119.3	H12A—C12—H12C	109.5
C2—C3—C4	121.0 (3)	H12B—C12—H12C	109.5
C2—C3—H3	119.5	N2—C13—C10	112.6 (3)
C4—C3—H3	119.5	N2—C13—H13A	109.1
C5—C4—C3	117.2 (3)	C10—C13—H13A	109.1
C5—C4—C7	122.5 (3)	N2—C13—H13B	109.1
C3—C4—C7	120.3 (3)	C10—C13—H13B	109.1
C4—C5—C6	122.8 (3)	H13A—C13—H13B	107.8
C4—C5—H5	118.6	N2—C14—C15	123.0 (3)
C6—C5—H5	118.6	N2—C14—H14	118.5
C5—C6—C1	118.6 (3)	C15—C14—H14	118.5
C5—C6—C8	120.1 (3)	C16—C15—C20	117.9 (3)
C1—C6—C8	121.3 (3)	C16—C15—C14	120.4 (3)
C4—C7—H7A	109.5	C20—C15—C14	121.7 (3)
C4—C7—H7B	109.5	C17—C16—C15	123.3 (3)
H7A—C7—H7B	109.5	C17—C16—H16	118.3
C4—C7—H7C	109.5	C15—C16—H16	118.3
H7A—C7—H7C	109.5	C16—C17—C18	117.0 (3)

H7B—C7—H7C	109.5	C16—C17—C21	121.2 (3)
N1—C8—C6	122.2 (3)	C18—C17—C21	121.9 (3)
N1—C8—H8	118.9	C17—C18—C19	121.9 (4)
C6—C8—H8	118.9	C17—C18—H18	119.0
N1—C9—C10	112.6 (3)	C19—C18—H18	119.0
N1—C9—H9A	109.1	C20—C19—C18	119.7 (3)
C10—C9—H9A	109.1	C20—C19—H19	120.2
N1—C9—H9B	109.1	C18—C19—H19	120.2
C10—C9—H9B	109.1	O2—C20—C19	119.0 (3)
H9A—C9—H9B	107.8	O2—C20—C15	120.8 (3)
C9—C10—C12	108.2 (3)	C19—C20—C15	120.2 (3)
C9—C10—C13	110.2 (3)	C17—C21—H21A	109.5
C12—C10—C13	110.4 (3)	C17—C21—H21B	109.5
C9—C10—C11	110.3 (3)	H21A—C21—H21B	109.5
C12—C10—C11	110.5 (3)	C17—C21—H21C	109.5
C13—C10—C11	107.2 (3)	H21A—C21—H21C	109.5
C10—C11—H11A	109.5	H21B—C21—H21C	109.5
O1—C1—C2—C3	179.6 (3)	C14—N2—C13—C10	−142.8 (3)
C6—C1—C2—C3	−0.3 (5)	C9—C10—C13—N2	−61.8 (4)
C1—C2—C3—C4	−0.1 (5)	C12—C10—C13—N2	57.8 (4)
C2—C3—C4—C5	−0.6 (5)	C11—C10—C13—N2	178.1 (3)
C2—C3—C4—C7	179.0 (3)	C13—N2—C14—C15	−178.5 (3)
C3—C4—C5—C6	1.7 (5)	N2—C14—C15—C16	178.3 (3)
C7—C4—C5—C6	−177.9 (3)	N2—C14—C15—C20	−1.2 (5)
C4—C5—C6—C1	−2.1 (4)	C20—C15—C16—C17	1.3 (4)
C4—C5—C6—C8	176.9 (3)	C14—C15—C16—C17	−178.3 (3)
O1—C1—C6—C5	−178.6 (3)	C15—C16—C17—C18	−1.7 (5)
C2—C1—C6—C5	1.3 (4)	C15—C16—C17—C21	177.9 (3)
O1—C1—C6—C8	2.4 (4)	C16—C17—C18—C19	1.0 (5)
C2—C1—C6—C8	−177.7 (3)	C21—C17—C18—C19	−178.7 (3)
C9—N1—C8—C6	178.2 (3)	C17—C18—C19—C20	0.2 (5)
C5—C6—C8—N1	−175.7 (3)	C18—C19—C20—O2	−179.8 (3)
C1—C6—C8—N1	3.3 (5)	C18—C19—C20—C15	−0.7 (5)
C8—N1—C9—C10	147.8 (3)	C16—C15—C20—O2	179.1 (3)
N1—C9—C10—C12	−178.1 (3)	C14—C15—C20—O2	−1.3 (5)
N1—C9—C10—C13	−57.2 (4)	C16—C15—C20—C19	0.0 (4)
N1—C9—C10—C11	60.9 (4)	C14—C15—C20—C19	179.5 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···N1	0.82	1.89	2.620 (3)	147
O2—H2A···N2	0.82	1.88	2.609 (4)	147

Fig. 1


C7
C4
C5
C3
C6
C2
C8
C1
O1
N1
C9
C13
N2
C10
C12
C11
O2
C20
C19
C18
C21
C17
C16
C15
C14