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(*E*)-1-(2-Hydroxyphenyl)propan-2-one *O*-methyloxime forms hydrogen-bonded chains of edge-fused $R_4^4(16)$ and $R_4^4(24)$ rings

Christopher Glidewell,[a]* John N. Low,[b] Janet M. S. Skakle[b] and James L. Wardell[c]

[a]School of Chemistry, University of St Andrews, Fife KY16 9ST, Scotland, [b]Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB24 3UE, Scotland, and [c]Instituto de Química, Departamento de Química Inorgânica, Universidade Federal do Rio de Janeiro, 21945-970 Rio de Janeiro, RJ, Brazil
Correspondence e-mail: cg@st-andrews.ac.uk

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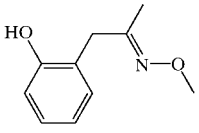
The title compound, $C_{10}H_{13}NO_2$, crystallizes with $Z' = 2$ in space group $P\overline{1}$. The molecules are linked by two O—H···N hydrogen bonds [H···O = 1.97 and 1.98 Å, O···N = 2.810 (2) and 2.815 (2) Å, and O—H···N = 175 and 174°] and by one C—H···O hydrogen bond [H···O = 2.50 Å, C···O = 3.313 (2) Å and C—H···O = 144°] into chains of edge-fused centrosymmetric rings in which $R_4^4(16)$ and $R_4^4(24)$ rings alternate.

Comment

The title compound, (I), was originally prepared as part of a study of the cyclization reactions of phenolic oximes (Forrester *et al.*, 1975). Its structure has now been determined in order to establish both the geometry at the oxime group and the nature of the supramolecular interactions.



(I)

Compound (I) crystallizes in space group $P\overline{1}$, with two independent molecules in the asymmetric unit (Fig. 1). Both molecules have the *E* configuration at the C=N bond. The intramolecular dimensions are very similar in the two molecules, and the bond distances show no unusual features. The angles at the planar C atoms C18 and C28 show considerable variation from 120° (Table 1) and both of the C—N—O angles are substantially less than 120°. As shown by the leading torsion angles, the conformations of the two molecules are very similar.

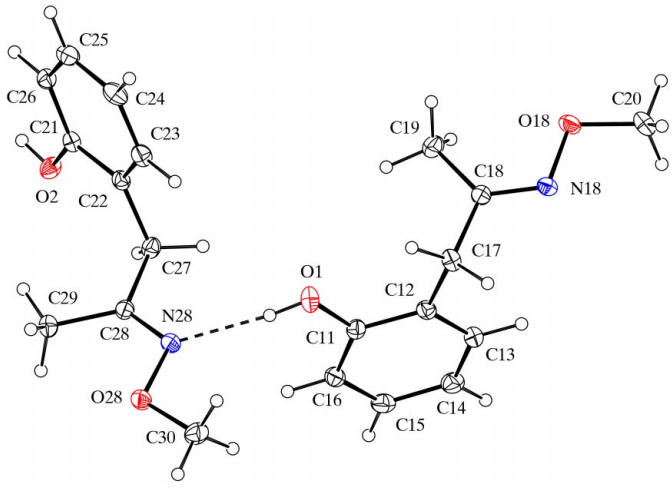


Figure 1
The two independent molecules in compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

The molecules of (I) are linked into a chain of edge-fused rings by the combination of two nearly linear O—H···N hydrogen bonds and one rather weak C—H···O hydrogen bond (Table 2). Within the asymmetric unit, phenolic atom O1 in the type 1 molecule (containing O1, *etc.*) acts as hydrogen-bond donor to oxime atom N28 in the type 2 molecule (containing O2, *etc.*) (Fig. 1), and in a similar way, phenolic atom O2 in the type 2 molecule at (x, y, z) acts as hydrogen-bond donor to oxime atom N18 in the type 1 molecule at (x, y, $z-1$). The combination of these two hydrogen bonds then generates by translation a $C_2^2(14)$ (Bernstein *et al.*, 1995) chain running parallel to the [001] direction (Fig. 2).

Two such chains, related to one another by inversion, pass through each unit cell, and these two chains are weakly linked by the C—H···O hydrogen bond. Aryl atom C23 in the type 2 molecule at (x, y, z) acts as hydrogen-bond donor to phenolic atom O1 in the type 1 molecule at ($1-x$, $1-y$, $1-z$), so

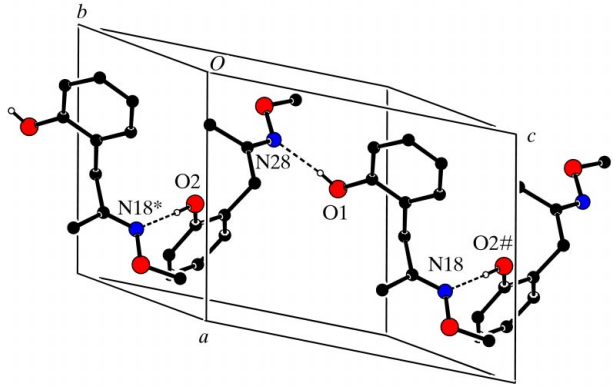


Figure 2
Part of the crystal structure of (I), showing the formation of a $C_2^2(14)$ chain along [001]. For the sake of clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions (x, y, $z-1$) and (x, y, $1+z$), respectively.

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generating by inversion an $R_4^4(16)$ ring centred at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. Propagation by translation and inversion of the $R_4^4(16)$ motif linking antiparallel $C_2^2(14)$ chains then generates an [001] chain of edge-fused rings, with $R_4^4(16)$ rings centred at $(\frac{1}{2},\frac{1}{2},\frac{1}{2}+n)$ (n = zero or integer) alternating with $R_4^4(24)$ rings centred at $(\frac{1}{2},\frac{1}{2},n)$ (n = zero or integer) (Fig. 3).

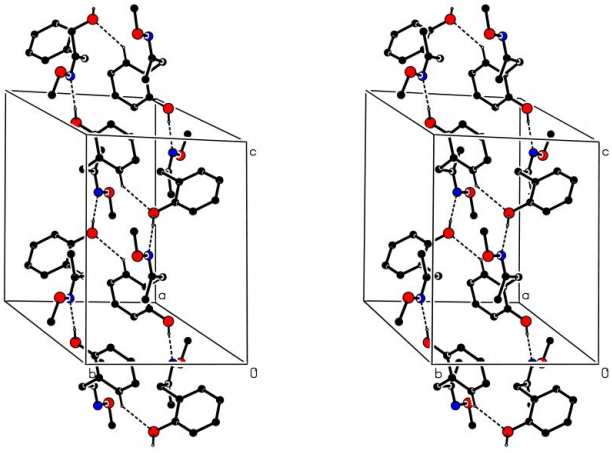

Figure 3
A stereoview of part of the crystal structure of (I), showing the formation of a chain of alternating and edge-fused $R_4^4(16)$ and $R_4^4(24)$ rings. For the sake of clarity, H atoms bonded to C atoms have been omitted.

There are no direction-specific interactions between adjacent chains of rings in (I). In particular, there are neither C—H···π(arene) hydrogen bonds nor aromatic π–π stacking interactions present in the structure.

Experimental

The title compound, (I), was prepared (Forrester *et al.*, 1975) from 2-hydroxyphenylpropanone (Tinsley, 1959) and *O*-methylhydroxylamine. Crystals of (I) suitable for single-crystal X-ray diffraction were grown by slow evaporation of a solution in ethanol (m.p. 350–352 K).

Crystal data

$C_{10}H_{13}NO_2$
M_r = 179.21
Triclinic, $P\overline{1}$
a = 9.3723 (2) Å
b = 9.4254 (2) Å
c = 12.3080 (3) Å
α = 89.7146 (12)°
β = 68.5508 (11)°
γ = 77.0903 (10)°
V = 982.85 (4) Å^3
Z = 4
D_x = 1.211 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4492 reflections
θ = 3.0–27.6°
μ = 0.09 mm^{-1}
T = 120 (2) K
Plate, colourless
0.20 × 0.20 × 0.04 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.978, T_{max} = 0.997
8474 measured reflections
4492 independent reflections
3441 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.6°
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.154
S = 1.09
4492 reflections
240 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0707P)^2 + 0.2766P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.034 (6)

Table 1
Selected geometric parameters (Å, °).

O1—C11	1.367 (2)	O2—C21	1.368 (2)
C18—N18	1.278 (2)	C28—N28	1.280 (2)
N18—O18	1.422 (2)	N28—O28	1.420 (2)
C17—C18—N18	116.52 (14)	C27—C28—N28	115.95 (13)
C17—C18—C19	118.82 (14)	C27—C28—C29	119.00 (14)
N18—C18—C19	124.62 (15)	N28—C28—C29	125.01 (15)
C18—N18—O18	111.66 (13)	C28—N28—O28	112.21 (12)
N18—O18—C20	108.27 (12)	N28—O28—C30	107.86 (12)
C11—C12—C17—C18	−117.67 (16)	C21—C22—C27—C28	−109.88 (16)
C17—C18—N18—O18	178.57 (12)	C27—C28—N28—O28	179.05 (12)
C18—N18—O18—C20	−171.79 (13)	C28—N28—O28—C30	179.96 (14)
C19—C18—N18—O18	1.0 (2)	C29—C28—N28—O28	1.4 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N28	0.84	1.98	2.815 (2)	174
O2—H2···N18^{i}	0.84	1.97	2.810 (2)	175
C23—H23···O1^{ii}	0.95	2.50	3.313 (2)	144

Symmetry codes: (i) $x, y, z-1$; (ii) $1-x, 1-y, 1-z$.

Crystals of compound (I) are triclinic; space group $P\overline{1}$ was selected and confirmed by the successful structure analysis. All H atoms were located from difference maps and subsequently treated as riding atoms, with C—H distances of 0.95 (aromatic), 0.98 (CH_3) or 0.99 Å (CH_2), and O—H distances of 0.84 Å, and with U_{iso}(H) = 1.2U_{eq}(C,O) or 1.5U_{eq}(methyl C).

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England; the authors thank the staff for all their help and advice. JNL thanks NCR Self-Service, Dundee, for grants which have provided computing facilities for this work, and JLW thanks CNPq and FAPERJ for financial support.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1704). Services for accessing these data are described at the back of the journal.

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supporting information

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Computing details

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
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$\alpha = 89.7146\ (12)°$
$\beta = 68.5508\ (11)°$
$\gamma = 77.0903\ (10)°$
$V = 982.85\ (4)$ Å^3
$Z = 4$
$F(000) = 384$
$D_x = 1.211$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4492 reflections
$\theta = 3.0–27.6°$
$\mu = 0.09$ mm^{-1}
$T = 120$ K
Plate, colourless
0.20 × 0.20 × 0.04 mm

Data collection

Kappa-CCD diffractometer
Radiation source: rotating anode
Graphite monochromator
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing 1995, 1997)
$T_{min} = 0.978$, $T_{max} = 0.997$
8474 measured reflections
4492 independent reflections
3441 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.0°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.154$
$S = 1.09$
4492 reflections
240 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

$w = 1/[\sigma^2(F_o^2) + (0.0707P)^2 + 0.2766P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.034 (6)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.39534 (15)	0.36002 (12)	0.57489 (10)	0.0303 (3)
O2	0.55460 (14)	0.17204 (13)	0.03400 (10)	0.0289 (3)
C11	0.32061 (19)	0.26467 (17)	0.64453 (13)	0.0235 (3)
C12	0.38170 (19)	0.20224 (17)	0.72650 (14)	0.0242 (3)
C13	0.3119 (2)	0.09933 (19)	0.79440 (15)	0.0290 (4)
C14	0.1839 (2)	0.0602 (2)	0.78326 (16)	0.0337 (4)
C15	0.1214 (2)	0.1258 (2)	0.70438 (15)	0.0320 (4)
C16	0.1889 (2)	0.22874 (18)	0.63541 (14)	0.0275 (4)
C17	0.5215 (2)	0.24310 (17)	0.74141 (15)	0.0264 (4)
C18	0.65818 (19)	0.11186 (17)	0.71219 (14)	0.0234 (3)
C19	0.7379 (2)	0.0466 (2)	0.58836 (14)	0.0320 (4)
N18	0.69418 (15)	0.06114 (14)	0.79775 (12)	0.0236 (3)
O18	0.82216 (13)	−0.06457 (12)	0.76048 (10)	0.0292 (3)
C20	0.8404 (2)	−0.1266 (2)	0.86204 (17)	0.0340 (4)
C21	0.64437 (19)	0.24590 (17)	0.06690 (14)	0.0235 (3)
C22	0.58684 (19)	0.30253 (16)	0.18393 (14)	0.0235 (3)
C23	0.6739 (2)	0.38166 (18)	0.21835 (15)	0.0285 (4)
C24	0.8157 (2)	0.40444 (19)	0.14040 (17)	0.0322 (4)
C25	0.8737 (2)	0.34384 (18)	0.02540 (16)	0.0312 (4)
C26	0.7887 (2)	0.26469 (18)	−0.01102 (14)	0.0269 (4)
C27	0.4323 (2)	0.28037 (17)	0.27188 (14)	0.0254 (4)
C28	0.30726 (19)	0.42157 (17)	0.30663 (13)	0.0236 (3)
C29	0.2531 (2)	0.4943 (2)	0.21552 (15)	0.0310 (4)
N28	0.25907 (16)	0.47231 (14)	0.41354 (12)	0.0247 (3)
O28	0.14343 (14)	0.60645 (13)	0.43818 (10)	0.0302 (3)
C30	0.0975 (2)	0.6536 (2)	0.55899 (15)	0.0357 (4)
H1	0.3482	0.3917	0.5301	0.036*
H13	0.3532	0.0551	0.8496	0.035*
H14	0.1391	−0.0114	0.8295	0.040*
H15	0.0323	0.1006	0.6973	0.038*
H16	0.1451	0.2746	0.5820	0.033*
H17A	0.5533	0.3202	0.6893	0.032*
H17B	0.4910	0.2824	0.8233	0.032*
H19A	0.8470	0.0571	0.5573	0.048*
H19B	0.6813	0.0970	0.5409	0.048*
H19C	0.7377	−0.0573	0.5857	0.048*
H20A	0.8600	−0.0541	0.9082	0.051*
H20B	0.9298	−0.2123	0.8380	0.051*
H20C	0.7439	−0.1561	0.9096	0.051*
H2	0.6009	0.1418	−0.0371	0.035*

H23	0.6353	0.4213	0.2974	0.034*
H24	0.8723	0.4607	0.1653	0.039*
H25	0.9719	0.3567	−0.0284	0.037*
H26	0.8292	0.2231	−0.0896	0.032*
H27A	0.3962	0.2074	0.2373	0.031*
H27B	0.4489	0.2419	0.3424	0.031*
H29A	0.2626	0.5958	0.2146	0.046*
H29B	0.1427	0.4924	0.2338	0.046*
H29C	0.3186	0.4423	0.1385	0.046*
H30A	0.1888	0.6717	0.5727	0.054*
H30B	0.0584	0.5776	0.6078	0.054*
H30C	0.0140	0.7438	0.5792	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0409 (7)	0.0296 (6)	0.0294 (6)	−0.0130 (5)	−0.0207 (6)	0.0091 (5)
O2	0.0307 (7)	0.0358 (7)	0.0212 (6)	−0.0106 (5)	−0.0091 (5)	−0.0026 (5)
C11	0.0275 (8)	0.0199 (7)	0.0204 (7)	−0.0023 (6)	−0.0078 (6)	−0.0015 (6)
C12	0.0245 (8)	0.0218 (7)	0.0239 (8)	−0.0005 (6)	−0.0093 (7)	−0.0022 (6)
C13	0.0274 (9)	0.0313 (9)	0.0266 (8)	−0.0029 (7)	−0.0104 (7)	0.0057 (7)
C14	0.0271 (9)	0.0359 (9)	0.0353 (10)	−0.0095 (8)	−0.0074 (8)	0.0081 (8)
C15	0.0224 (9)	0.0378 (10)	0.0333 (9)	−0.0063 (7)	−0.0080 (7)	−0.0023 (8)
C16	0.0262 (9)	0.0303 (8)	0.0252 (8)	−0.0019 (7)	−0.0112 (7)	−0.0023 (7)
C17	0.0315 (9)	0.0225 (8)	0.0283 (8)	−0.0047 (7)	−0.0159 (7)	0.0018 (6)
C18	0.0230 (8)	0.0251 (8)	0.0246 (8)	−0.0085 (6)	−0.0100 (6)	0.0020 (6)
C19	0.0328 (10)	0.0369 (10)	0.0233 (8)	−0.0068 (8)	−0.0081 (7)	−0.0008 (7)
N18	0.0212 (7)	0.0225 (7)	0.0263 (7)	−0.0023 (5)	−0.0098 (6)	−0.0010 (5)
O18	0.0243 (6)	0.0278 (6)	0.0315 (6)	0.0029 (5)	−0.0110 (5)	−0.0013 (5)
C20	0.0332 (10)	0.0317 (9)	0.0430 (10)	−0.0040 (7)	−0.0230 (8)	0.0077 (8)
C21	0.0263 (8)	0.0220 (7)	0.0248 (8)	−0.0047 (6)	−0.0131 (7)	0.0037 (6)
C22	0.0255 (8)	0.0201 (7)	0.0241 (8)	−0.0009 (6)	−0.0110 (7)	0.0017 (6)
C23	0.0330 (9)	0.0240 (8)	0.0291 (9)	−0.0008 (7)	−0.0156 (7)	−0.0025 (7)
C24	0.0295 (9)	0.0269 (8)	0.0458 (10)	−0.0060 (7)	−0.0209 (8)	0.0006 (8)
C25	0.0244 (9)	0.0284 (9)	0.0402 (10)	−0.0057 (7)	−0.0118 (7)	0.0077 (7)
C26	0.0276 (9)	0.0262 (8)	0.0242 (8)	−0.0020 (7)	−0.0093 (7)	0.0030 (6)
C27	0.0306 (9)	0.0235 (8)	0.0210 (8)	−0.0057 (7)	−0.0088 (7)	0.0012 (6)
C28	0.0234 (8)	0.0263 (8)	0.0219 (8)	−0.0072 (6)	−0.0087 (6)	0.0031 (6)
C29	0.0322 (9)	0.0362 (9)	0.0247 (8)	−0.0043 (8)	−0.0133 (7)	0.0040 (7)
N28	0.0241 (7)	0.0225 (7)	0.0258 (7)	−0.0022 (5)	−0.0092 (6)	0.0023 (5)
O28	0.0288 (6)	0.0288 (6)	0.0269 (6)	0.0041 (5)	−0.0096 (5)	−0.0005 (5)
C30	0.0360 (10)	0.0335 (9)	0.0279 (9)	0.0003 (8)	−0.0057 (8)	−0.0046 (7)

Geometric parameters (Å, º)

O1—C11	1.367 (2)	O2—C21	1.368 (2)
O1—H1	0.84	O2—H2	0.84
C11—C16	1.393 (2)	C21—C26	1.392 (2)

C11—C12	1.399 (2)	C21—C22	1.401 (2)
C12—C13	1.394 (2)	C22—C23	1.389 (2)
C12—C17	1.517 (2)	C22—C27	1.516 (2)
C13—C14	1.383 (2)	C23—C24	1.388 (3)
C13—H13	0.95	C23—H23	0.95
C14—C15	1.384 (2)	C24—C25	1.390 (3)
C14—H14	0.95	C24—H24	0.95
C15—C16	1.391 (2)	C25—C26	1.387 (2)
C15—H15	0.95	C25—H25	0.95
C16—H16	0.95	C26—H26	0.95
C17—C18	1.503 (2)	C27—C28	1.507 (2)
C17—H17A	0.99	C27—H27A	0.99
C17—H17B	0.99	C27—H27B	0.99
C18—N18	1.278 (2)	C28—N28	1.280 (2)
C18—C19	1.494 (2)	C28—C29	1.496 (2)
C19—H19A	0.98	C29—H29A	0.98
C19—H19B	0.98	C29—H29B	0.98
C19—H19C	0.98	C29—H29C	0.98
N18—O18	1.422 (2)	N28—O28	1.420 (2)
O18—C20	1.428 (2)	O28—C30	1.431 (2)
C20—H20A	0.98	C30—H30A	0.98
C20—H20B	0.98	C30—H30B	0.98
C20—H20C	0.98	C30—H30C	0.98

C11—O1—H1	109.5	C21—O2—H2	109.5
O1—C11—C16	122.20 (14)	O2—C21—C26	122.37 (14)
O1—C11—C12	117.53 (14)	O2—C21—C22	117.59 (14)
C16—C11—C12	120.26 (14)	C26—C21—C22	120.04 (15)
C13—C12—C11	118.40 (14)	C23—C22—C21	118.52 (15)
C13—C12—C17	120.10 (14)	C23—C22—C27	120.09 (14)
C11—C12—C17	121.50 (14)	C21—C22—C27	121.39 (14)
C14—C13—C12	121.51 (15)	C24—C23—C22	121.78 (16)
C14—C13—H13	119.2	C24—C23—H23	119.1
C12—C13—H13	119.2	C22—C23—H23	119.1
C13—C14—C15	119.62 (16)	C23—C24—C25	119.06 (15)
C13—C14—H14	120.2	C23—C24—H24	120.5
C15—C14—H14	120.2	C25—C24—H24	120.5
C14—C15—C16	120.05 (16)	C26—C25—C24	120.16 (16)
C14—C15—H15	120.0	C26—C25—H25	119.9
C16—C15—H15	120.0	C24—C25—H25	119.9
C15—C16—C11	120.09 (15)	C25—C26—C21	120.38 (16)
C15—C16—H16	120.0	C25—C26—H26	119.8
C11—C16—H16	120.0	C21—C26—H26	119.8
C18—C17—C12	110.43 (13)	C28—C27—C22	111.11 (13)
C18—C17—H17A	109.6	C28—C27—H27A	109.4
C12—C17—H17A	109.6	C22—C27—H27A	109.4
C18—C17—H17B	109.6	C28—C27—H27B	109.4
C12—C17—H17B	109.6	C22—C27—H27B	109.4

H17A—C17—H17B	108.1	H27A—C27—H27B	108.0
C17—C18—N18	116.52 (14)	C27—C28—N28	115.95 (13)
C17—C18—C19	118.82 (14)	C27—C28—C29	119.00 (14)
N18—C18—C19	124.62 (15)	N28—C28—C29	125.01 (15)
C18—C19—H19A	109.5	C28—C29—H29A	109.5
C18—C19—H19B	109.5	C28—C29—H29B	109.5
H19A—C19—H19B	109.5	H29A—C29—H29B	109.5
C18—C19—H19C	109.5	C28—C29—H29C	109.5
H19A—C19—H19C	109.5	H29A—C29—H29C	109.5
H19B—C19—H19C	109.5	H29B—C29—H29C	109.5
C18—N18—O18	111.66 (13)	C28—N28—O28	112.21 (12)
N18—O18—C20	108.27 (12)	N28—O28—C30	107.86 (12)
O18—C20—H20A	109.5	O28—C30—H30A	109.5
O18—C20—H20B	109.5	O28—C30—H30B	109.5
H20A—C20—H20B	109.5	H30A—C30—H30B	109.5
O18—C20—H20C	109.5	O28—C30—H30C	109.5
H20A—C20—H20C	109.5	H30A—C30—H30C	109.5
H20B—C20—H20C	109.5	H30B—C30—H30C	109.5
O1—C11—C12—C13	−176.92 (14)	O2—C21—C22—C23	−178.10 (13)
C16—C11—C12—C13	2.8 (2)	C26—C21—C22—C23	2.4 (2)
O1—C11—C12—C17	2.5 (2)	O2—C21—C22—C27	1.2 (2)
C16—C11—C12—C17	−177.87 (15)	C26—C21—C22—C27	−178.27 (14)
C11—C12—C13—C14	−0.9 (3)	C21—C22—C23—C24	−0.6 (2)
C17—C12—C13—C14	179.72 (16)	C27—C22—C23—C24	−179.92 (15)
C12—C13—C14—C15	−1.0 (3)	C22—C23—C24—C25	−1.3 (3)
C13—C14—C15—C16	1.1 (3)	C23—C24—C25—C26	1.5 (2)
C14—C15—C16—C11	0.8 (3)	C24—C25—C26—C21	0.3 (2)
O1—C11—C16—C15	176.94 (15)	O2—C21—C26—C25	178.22 (14)
C12—C11—C16—C15	−2.7 (2)	C22—C21—C26—C25	−2.3 (2)
C13—C12—C17—C18	61.69 (19)	C23—C22—C27—C28	69.43 (18)
C11—C12—C17—C18	−117.67 (16)	C21—C22—C27—C28	−109.88 (16)
C12—C17—C18—N18	−110.41 (16)	C22—C27—C28—N28	−114.08 (16)
C12—C17—C18—C19	67.29 (18)	C22—C27—C28—C29	63.76 (18)
C17—C18—N18—O18	178.57 (12)	C27—C28—N28—O28	179.05 (12)
C18—N18—O18—C20	−171.79 (13)	C28—N28—O28—C30	179.96 (14)
C19—C18—N18—O18	1.0 (2)	C29—C28—N28—O28	1.4 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N28	0.84	1.98	2.815 (2)	174
O2—H2···N18^{i}	0.84	1.97	2.810 (2)	175
C23—H23···O1^{ii}	0.95	2.50	3.313 (2)	144

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