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## Structure Reports

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# (1*R*,3*S*)-Methyl 6,7-dimethoxy-1-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxylate

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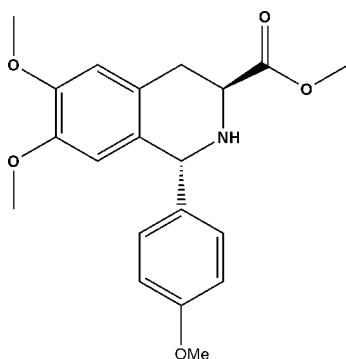
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 Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.036;  $wR$  factor = 0.090; data-to-parameter ratio = 12.0.

The title compound,  $\text{C}_{20}\text{H}_{23}\text{NO}_5$ , is the third in a series of tetrahydroisoquinoline (TIQ) compounds that are precursors to novel chiral catalysts. The N-containing six-membered ring assumes a half-boat conformation. No hydrogen bonding is observed in the crystal structure.

## Related literature

For related structures, see: Naicker *et al.* (2009, 2010); Alberach *et al.* (2004). For the synthesis of the title compound, see: Aubry *et al.* (2006).



## Experimental

## Crystal data

$\text{C}_{20}\text{H}_{23}\text{NO}_5$	$V = 1766.9(4) \text{ \AA}^3$
$M_r = 357.39$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 5.3719(7) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$b = 12.1726(14) \text{ \AA}$	$T = 173 \text{ K}$
$c = 27.021(3) \text{ \AA}$	$0.20 \times 0.12 \times 0.12 \text{ mm}$

## Data collection

Bruker Kappa DUO APEXII diffractometer	2878 independent reflections
13619 measured reflections	2538 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.032$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.090$	
$S = 1.04$	
2878 reflections	$\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$
239 parameters	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$
1 restraint	

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINTE* (Bruker, 2006); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *SHELXL97*.

The authors thank Dr Hong Su of the University of Cape-town for the data collection and structure refinement.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2711).

## References

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## supporting information

*Acta Cryst.* (2010). E66, o3105 [https://doi.org/10.1107/S1600536810044909]

## (1*R*,3*S*)-Methyl 6,7-dimethoxy-1-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxylate

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### S1. Comment

The title compound was derived from commercially available *L*-DOPA and anisaldehyde. Diastereomers formed during the first step of the synthesis were separated to yield subsequent derivatives and the title compound with the stereochemistry as illustrated in Fig. 1. The title compound is the third report in a series of molecules containing a tetrahydroisoquinoline backbone and is a precursor to one of the molecules that we previously reported ((1*R*,3*S*)-methyl 2-benzyl-6,7-dimethoxy-1-phenyl-1,2,3,4-tetrahydroisoquinoline-3-carboxylate), (Naicker *et al.*, 2009). The molecule has been reported previously and the absolute stereochemistry of the diastereomer was confirmed to be *R,S* at C4 and C2 positions respectively by proton NMR (Aubry *et al.*, 2006).

There are a number of common features found in this structure and that of the the unprotected secondary amine system. First, the *N*-containing six membered ring assumes a half boat conformation. This differs from last report for the (1*R*,3*S*)-2-benzyl-6,7-dimethoxy-1-phenyl-1,2,3,4 tetrahydroisoquinolin-3-yl diphenylmethanol structure (Naicker *et al.*, 2010) and previous reports by Alberach *et al.* (2004) and Aubry *et al.* (2006) where the heteroatomic ring adopted a half chair conformation. Second, given the presence of the secondary amine, ether and in this example ester functional groups, no hydrogen bonding is observed in any of the structures of this series, (see Fig. 2).

### S2. Experimental

A solution of the Cbz protected *trans*-6,7-dimethoxy-1-(4-methoxyphenyl)-TIQ methyl ester (1.0 g, 0.21 mmol) in THF (20 ml) was added to a suspension of activated 10 wt% Pd/C (500 mg) in dry MeOH (20 ml). The mixture was connected to a hydrogen source at one atmosphere and stirred at room temperature for 1 h. Completion of the reaction was monitored through TLC in hexane/ethyl acetate (50/50,  $R_f = 0.6$ ). The Pd/C was filtered through a Celite pad and washed with methanol (20 ml). The filtrate was evaporated under reduced pressure affording the crude amino ester, which was purified by column chromatography using ethyl acetate/hexane (50:50) as the eluent to yield pure title compound (0.70 g, 93%) as a yellow solid. m.p. = 392–393 K. Crystals suitable for X-ray diffraction were obtained by slow evaporation of the title compound in MeOH at room temperature.

$^1\text{H NMR}$  (600 MHz,  $\text{CDCl}_3$ , d, p.p.m.): 1.58 (broad s, 1H), 2.99 (dd, 1H), 3.09 (dd, 1H), 3.60 (s, 3H), 3.66 (s, 3H), 3.67 (s, 3H), 3.78 (m, 1H), 3.88 (s, 3H), 5.23 (s, 1H), 6.30 (s, 1H), 6.61 (s, 1H), 6.82 (d, 2H), 7.09 (d, 2H).

IR: 2946 (w), 1700 (w), 1507 (s), 1223 ( $\nu_s$ ), 832 (s), 563 (w)

### S3. Refinement

All H atoms, except H1N, were positioned geometrically with C—H distances ranging from 0.95 Å to 1.00 Å and refined as riding on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$ .

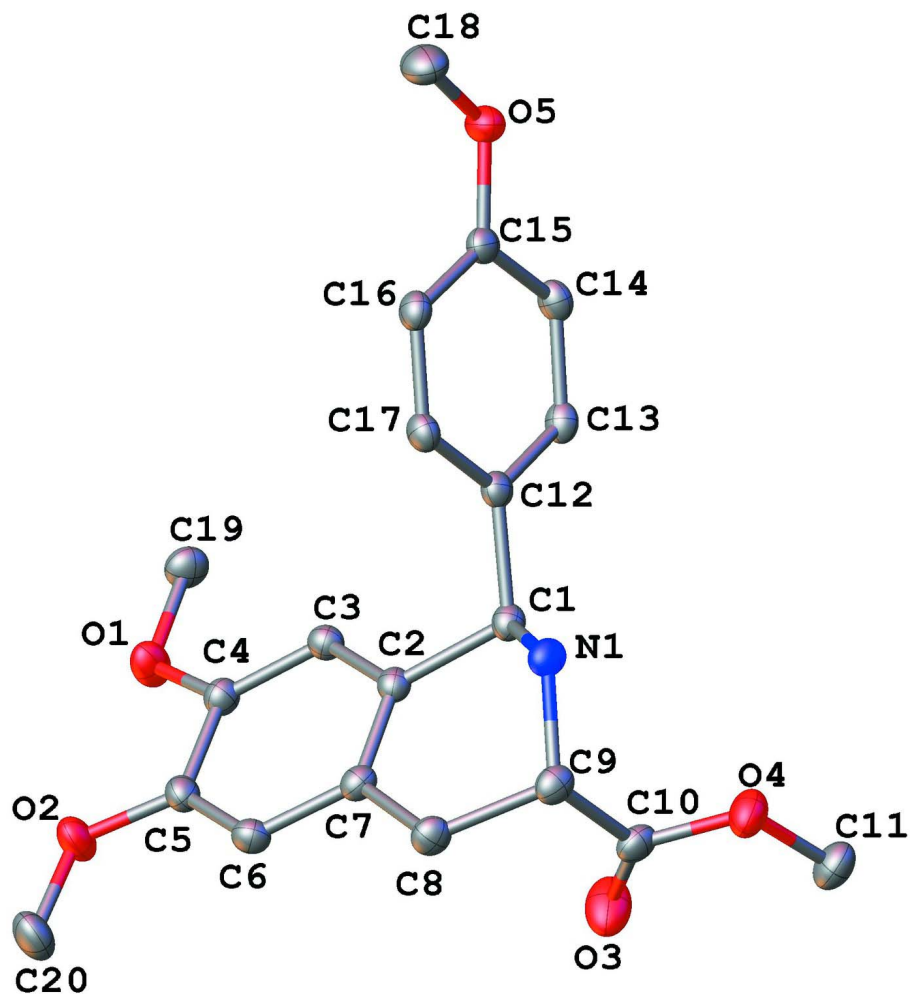


Figure 1

The title compound (all H atoms omitted for clarity). All non-H atoms are shown as ellipsoids with probability level of 50%.

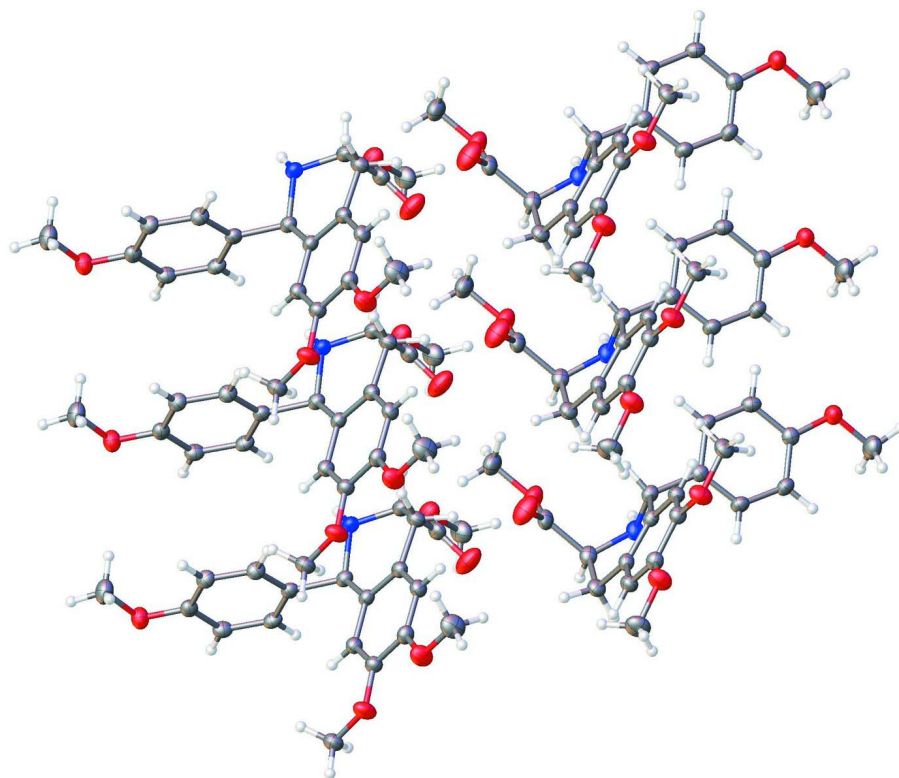


Figure 2

Projection viewed along [010].

(1*R*,3*S*)-Methyl 6,7-dimethoxy-1-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxylate

*Crystal data*

$C_{20}H_{23}NO_5$

$M_r = 357.39$

Orthorhombic,  $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 5.3719$  (7) Å

$b = 12.1726$  (14) Å

$c = 27.021$  (3) Å

$V = 1766.9$  (4) Å<sup>3</sup>

$Z = 4$

$F(000) = 760$

$D_x = 1.344$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 13619 reflections

$\theta = 2.3$ – $29.6^\circ$

$\mu = 0.10$  mm<sup>-1</sup>

$T = 173$  K

Needle, colourless

$0.20 \times 0.12 \times 0.12$  mm

*Data collection*

Bruker Kappa DUO APEXII

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$0.5^\circ$   $\varphi$  scans and  $\omega$  scans

13619 measured reflections

2878 independent reflections

2538 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.032$

$\theta_{max} = 29.6^\circ$ ,  $\theta_{min} = 2.3^\circ$

$h = -7 \rightarrow 7$

$k = -16 \rightarrow 16$

$l = -26 \rightarrow 37$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.090$   
 $S = 1.04$   
 2878 reflections  
 239 parameters  
 1 restraint  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.3587P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.26 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.6521 (3)	0.82927 (10)	0.91879 (5)	0.0334 (3)
O2	0.3315 (3)	0.91415 (10)	0.85890 (5)	0.0351 (3)
O3	0.3734 (3)	0.44954 (13)	0.76583 (6)	0.0498 (4)
O4	0.2473 (3)	0.28121 (11)	0.78678 (5)	0.0378 (3)
O5	0.4011 (3)	0.34146 (11)	1.09674 (5)	0.0307 (3)
N1	0.0808 (3)	0.40422 (12)	0.87542 (5)	0.0253 (3)
H1N	0.078 (4)	0.3258 (5)	0.8806 (7)	0.031 (5)*
C1	0.3147 (3)	0.45361 (13)	0.89317 (6)	0.0224 (3)
H1	0.4574	0.4190	0.8752	0.027*
C2	0.3126 (3)	0.57639 (13)	0.88213 (6)	0.0211 (3)
C3	0.4841 (3)	0.64470 (14)	0.90671 (6)	0.0229 (3)
H3	0.5967	0.6136	0.9299	0.027*
C4	0.4912 (3)	0.75648 (14)	0.89759 (6)	0.0242 (3)
C5	0.3187 (4)	0.80245 (13)	0.86413 (6)	0.0250 (3)
C6	0.1543 (3)	0.73469 (14)	0.83937 (6)	0.0253 (3)
H6	0.0407	0.7657	0.8164	0.030*
C7	0.1519 (3)	0.62062 (14)	0.84759 (6)	0.0231 (3)
C8	-0.0280 (3)	0.55050 (15)	0.81826 (7)	0.0269 (4)
H8A	-0.0184	0.5713	0.7829	0.032*
H8B	-0.1997	0.5652	0.8298	0.032*
C9	0.0265 (3)	0.42813 (14)	0.82338 (6)	0.0264 (4)
H9	-0.1279	0.3871	0.8141	0.032*
C10	0.2348 (4)	0.39131 (15)	0.78851 (6)	0.0276 (4)
C11	0.4358 (4)	0.23681 (18)	0.75419 (8)	0.0383 (5)

H11A	0.4304	0.1564	0.7553	0.057*
H11B	0.6003	0.2623	0.7649	0.057*
H11C	0.4044	0.2617	0.7203	0.057*
C12	0.3392 (3)	0.42874 (12)	0.94812 (6)	0.0216 (3)
C13	0.5433 (3)	0.37117 (13)	0.96620 (6)	0.0239 (3)
H13	0.6727	0.3501	0.9442	0.029*
C14	0.5606 (3)	0.34403 (14)	1.01604 (7)	0.0256 (3)
H14	0.7007	0.3045	1.0280	0.031*
C15	0.3716 (3)	0.37499 (13)	1.04827 (6)	0.0238 (3)
C16	0.1682 (3)	0.43478 (13)	1.03116 (6)	0.0250 (3)
H16	0.0406	0.4574	1.0533	0.030*
C17	0.1551 (3)	0.46090 (13)	0.98113 (6)	0.0245 (3)
H17	0.0167	0.5017	0.9692	0.029*
C18	0.1949 (4)	0.35863 (18)	1.12932 (7)	0.0399 (5)
H18A	0.2374	0.3319	1.1625	0.060*
H18B	0.0496	0.3185	1.1169	0.060*
H18C	0.1563	0.4372	1.1309	0.060*
C19	0.8323 (4)	0.78695 (16)	0.95244 (7)	0.0317 (4)
H19A	0.9354	0.8473	0.9650	0.047*
H19B	0.9380	0.7334	0.9353	0.047*
H19C	0.7474	0.7510	0.9802	0.047*
C20	0.1569 (4)	0.96322 (17)	0.82600 (8)	0.0419 (5)
H20A	0.1835	1.0429	0.8252	0.063*
H20B	-0.0125	0.9477	0.8375	0.063*
H20C	0.1797	0.9329	0.7927	0.063*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0349 (7)	0.0253 (6)	0.0399 (7)	-0.0042 (6)	-0.0127 (6)	-0.0019 (5)
O2	0.0433 (8)	0.0212 (6)	0.0409 (8)	-0.0014 (6)	-0.0095 (7)	0.0042 (5)
O3	0.0537 (10)	0.0375 (8)	0.0581 (10)	-0.0089 (8)	0.0274 (9)	-0.0036 (7)
O4	0.0463 (8)	0.0301 (7)	0.0370 (7)	-0.0025 (6)	0.0121 (7)	-0.0065 (6)
O5	0.0360 (7)	0.0309 (6)	0.0252 (6)	0.0054 (6)	0.0012 (5)	0.0018 (5)
N1	0.0265 (7)	0.0241 (7)	0.0253 (7)	-0.0065 (6)	0.0018 (6)	-0.0012 (6)
C1	0.0226 (7)	0.0205 (7)	0.0242 (7)	-0.0020 (6)	0.0033 (6)	-0.0014 (6)
C2	0.0214 (7)	0.0201 (7)	0.0218 (7)	-0.0015 (6)	0.0032 (6)	-0.0004 (6)
C3	0.0221 (7)	0.0237 (7)	0.0229 (7)	0.0002 (6)	-0.0005 (6)	0.0009 (6)
C4	0.0246 (8)	0.0236 (7)	0.0246 (8)	-0.0022 (7)	-0.0007 (7)	-0.0023 (6)
C5	0.0292 (8)	0.0207 (7)	0.0252 (8)	-0.0003 (7)	0.0020 (7)	0.0014 (6)
C6	0.0256 (8)	0.0268 (8)	0.0235 (8)	0.0008 (7)	-0.0023 (7)	0.0023 (6)
C7	0.0229 (7)	0.0254 (7)	0.0211 (7)	-0.0019 (7)	0.0015 (7)	-0.0027 (6)
C8	0.0242 (8)	0.0296 (8)	0.0269 (8)	-0.0021 (7)	-0.0041 (7)	-0.0024 (7)
C9	0.0256 (8)	0.0276 (8)	0.0261 (8)	-0.0063 (7)	0.0012 (7)	-0.0034 (7)
C10	0.0302 (9)	0.0302 (9)	0.0223 (8)	-0.0047 (7)	-0.0004 (7)	-0.0057 (7)
C11	0.0400 (11)	0.0407 (11)	0.0342 (10)	0.0036 (9)	0.0033 (9)	-0.0115 (9)
C12	0.0226 (7)	0.0175 (7)	0.0248 (8)	-0.0022 (6)	0.0006 (7)	-0.0006 (6)
C13	0.0198 (7)	0.0214 (7)	0.0304 (8)	0.0000 (6)	0.0042 (7)	-0.0027 (6)

C14	0.0214 (7)	0.0225 (7)	0.0329 (9)	0.0021 (6)	-0.0017 (7)	0.0004 (7)
C15	0.0281 (8)	0.0185 (7)	0.0247 (8)	-0.0027 (6)	-0.0004 (7)	-0.0006 (6)
C16	0.0252 (7)	0.0220 (7)	0.0278 (8)	0.0027 (7)	0.0041 (7)	-0.0028 (6)
C17	0.0235 (7)	0.0211 (7)	0.0289 (8)	0.0036 (7)	0.0012 (7)	0.0006 (6)
C18	0.0469 (12)	0.0432 (11)	0.0296 (9)	0.0033 (10)	0.0082 (9)	0.0042 (8)
C19	0.0302 (9)	0.0348 (9)	0.0300 (9)	-0.0043 (8)	-0.0062 (8)	-0.0030 (7)
C20	0.0488 (12)	0.0272 (9)	0.0498 (12)	0.0069 (10)	-0.0084 (11)	0.0058 (8)

*Geometric parameters (Å, °)*

O1—C4	1.364 (2)	C8—H8B	0.9900
O1—C19	1.425 (2)	C9—C10	1.530 (3)
O2—C5	1.369 (2)	C9—H9	1.0000
O2—C20	1.424 (2)	C11—H11A	0.9800
O3—C10	1.197 (2)	C11—H11B	0.9800
O4—C10	1.343 (2)	C11—H11C	0.9800
O4—C11	1.446 (2)	C12—C17	1.388 (2)
O5—C15	1.381 (2)	C12—C13	1.390 (2)
O5—C18	1.430 (2)	C13—C14	1.390 (2)
N1—C9	1.465 (2)	C13—H13	0.9500
N1—C1	1.473 (2)	C14—C15	1.390 (2)
N1—H1N	0.965 (5)	C14—H14	0.9500
C1—C12	1.521 (2)	C15—C16	1.392 (2)
C1—C2	1.524 (2)	C16—C17	1.391 (2)
C1—H1	1.0000	C16—H16	0.9500
C2—C7	1.381 (2)	C17—H17	0.9500
C2—C3	1.407 (2)	C18—H18A	0.9800
C3—C4	1.383 (2)	C18—H18B	0.9800
C3—H3	0.9500	C18—H18C	0.9800
C4—C5	1.410 (2)	C19—H19A	0.9800
C5—C6	1.381 (2)	C19—H19B	0.9800
C6—C7	1.406 (2)	C19—H19C	0.9800
C6—H6	0.9500	C20—H20A	0.9800
C7—C8	1.514 (2)	C20—H20B	0.9800
C8—C9	1.524 (3)	C20—H20C	0.9800
C8—H8A	0.9900		
C4—O1—C19	117.63 (14)	O3—C10—C9	126.64 (17)
C5—O2—C20	116.62 (16)	O4—C10—C9	110.53 (15)
C10—O4—C11	115.43 (16)	O4—C11—H11A	109.5
C15—O5—C18	116.85 (15)	O4—C11—H11B	109.5
C9—N1—C1	113.65 (13)	H11A—C11—H11B	109.5
C9—N1—H1N	109.5 (12)	O4—C11—H11C	109.5
C1—N1—H1N	111.7 (13)	H11A—C11—H11C	109.5
N1—C1—C12	108.07 (13)	H11B—C11—H11C	109.5
N1—C1—C2	109.28 (14)	C17—C12—C13	118.58 (15)
C12—C1—C2	112.76 (13)	C17—C12—C1	120.63 (15)
N1—C1—H1	108.9	C13—C12—C1	120.77 (15)

C12—C1—H1	108.9	C14—C13—C12	120.87 (16)
C2—C1—H1	108.9	C14—C13—H13	119.6
C7—C2—C3	119.86 (15)	C12—C13—H13	119.6
C7—C2—C1	121.29 (15)	C15—C14—C13	119.62 (16)
C3—C2—C1	118.82 (15)	C15—C14—H14	120.2
C4—C3—C2	121.00 (16)	C13—C14—H14	120.2
C4—C3—H3	119.5	O5—C15—C14	115.50 (16)
C2—C3—H3	119.5	O5—C15—C16	124.03 (16)
O1—C4—C3	125.56 (16)	C14—C15—C16	120.46 (16)
O1—C4—C5	115.32 (15)	C17—C16—C15	118.84 (16)
C3—C4—C5	119.11 (16)	C17—C16—H16	120.6
O2—C5—C6	125.13 (16)	C15—C16—H16	120.6
O2—C5—C4	115.30 (16)	C12—C17—C16	121.60 (16)
C6—C5—C4	119.57 (15)	C12—C17—H17	119.2
C5—C6—C7	121.27 (16)	C16—C17—H17	119.2
C5—C6—H6	119.4	O5—C18—H18A	109.5
C7—C6—H6	119.4	O5—C18—H18B	109.5
C2—C7—C6	119.08 (16)	H18A—C18—H18B	109.5
C2—C7—C8	122.23 (15)	O5—C18—H18C	109.5
C6—C7—C8	118.69 (16)	H18A—C18—H18C	109.5
C7—C8—C9	112.38 (15)	H18B—C18—H18C	109.5
C7—C8—H8A	109.1	O1—C19—H19A	109.5
C9—C8—H8A	109.1	O1—C19—H19B	109.5
C7—C8—H8B	109.1	H19A—C19—H19B	109.5
C9—C8—H8B	109.1	O1—C19—H19C	109.5
H8A—C8—H8B	107.9	H19A—C19—H19C	109.5
N1—C9—C8	108.63 (14)	H19B—C19—H19C	109.5
N1—C9—C10	112.79 (15)	O2—C20—H20A	109.5
C8—C9—C10	111.78 (15)	O2—C20—H20B	109.5
N1—C9—H9	107.8	H20A—C20—H20B	109.5
C8—C9—H9	107.8	O2—C20—H20C	109.5
C10—C9—H9	107.8	H20A—C20—H20C	109.5
O3—C10—O4	122.83 (18)	H20B—C20—H20C	109.5
C9—N1—C1—C12	176.36 (14)	C6—C7—C8—C9	168.41 (16)
C9—N1—C1—C2	53.33 (17)	C1—N1—C9—C8	-67.42 (18)
N1—C1—C2—C7	-18.3 (2)	C1—N1—C9—C10	57.07 (19)
C12—C1—C2—C7	-138.55 (16)	C7—C8—C9—N1	43.2 (2)
N1—C1—C2—C3	163.71 (14)	C7—C8—C9—C10	-81.93 (18)
C12—C1—C2—C3	43.5 (2)	C11—O4—C10—O3	-1.9 (3)
C7—C2—C3—C4	1.4 (2)	C11—O4—C10—C9	179.03 (15)
C1—C2—C3—C4	179.36 (15)	N1—C9—C10—O3	-110.1 (2)
C19—O1—C4—C3	1.4 (3)	C8—C9—C10—O3	12.7 (3)
C19—O1—C4—C5	-179.25 (15)	N1—C9—C10—O4	68.92 (19)
C2—C3—C4—O1	-178.92 (16)	C8—C9—C10—O4	-168.34 (16)
C2—C3—C4—C5	1.8 (3)	N1—C1—C12—C17	-57.33 (19)
C20—O2—C5—C6	1.4 (3)	C2—C1—C12—C17	63.6 (2)
C20—O2—C5—C4	-178.97 (16)	N1—C1—C12—C13	121.18 (16)



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O1—C4—C5—O2	-2.1 (2)	C2—C1—C12—C13	-117.93 (17)
C3—C4—C5—O2	177.27 (16)	C17—C12—C13—C14	1.5 (2)
O1—C4—C5—C6	177.55 (16)	C1—C12—C13—C14	-177.06 (15)
C3—C4—C5—C6	-3.1 (3)	C12—C13—C14—C15	-0.1 (3)
O2—C5—C6—C7	-179.09 (17)	C18—O5—C15—C14	-171.63 (16)
C4—C5—C6—C7	1.3 (3)	C18—O5—C15—C16	7.7 (2)
C3—C2—C7—C6	-3.2 (2)	C13—C14—C15—O5	178.05 (15)
C1—C2—C7—C6	178.92 (15)	C13—C14—C15—C16	-1.3 (2)
C3—C2—C7—C8	177.06 (15)	O5—C15—C16—C17	-177.95 (16)
C1—C2—C7—C8	-0.9 (2)	C14—C15—C16—C17	1.3 (2)
C5—C6—C7—C2	1.9 (3)	C13—C12—C17—C16	-1.4 (2)
C5—C6—C7—C8	-178.36 (16)	C1—C12—C17—C16	177.10 (15)
C2—C7—C8—C9	-11.8 (2)	C15—C16—C17—C12	0.0 (3)

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