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15-Crown-5

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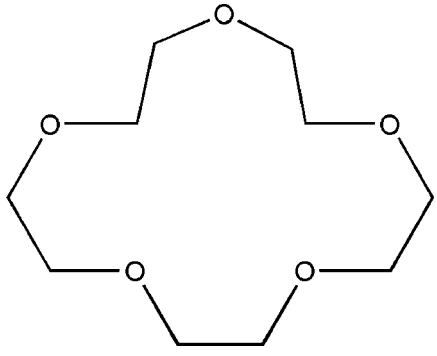
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.006 Å; R factor = 0.043; wR factor = 0.084; data-to-parameter ratio = 8.9.

15-Crown-5 (systematic name: 1,4,7,10,13-pentaoxacylopentadecane), $C_{10}H_{20}O_5$, which is liquid at room temperature, has been crystallized using *in situ* methods. It crystallizes with two different conformers in the asymmetric unit, which differ from those identified in conformational searches based on data mining and computational methods. The molecules interact through face-to-face C—H···O contacts to form layers which stack along the [001] direction.

Related literature

A crystal of the title compound was grown according to the method of Boese & Nussbaumer (1994). Hill & Feller (2000) studied conformations of the compound using *ab initio* methods, identifying 16 low-energy conformers, though none of these appear to match either of those observed here. Raithby *et al.* (1997) analysed conformers in the Cambridge Structural Database (Allen, 2002), and though regions of the uniangular conformers identified in that study resemble the conformations observed here the agreement is not complete. Hill & Feller (2000) commented that accurate prediction of low-lying conformations in floppy molecules is a challenging task, and the presence of intermolecular C—H···O interactions in the title compound, though weak, could well alter computational energy rankings derived for isolated molecules.



Experimental

Crystal data

$C_{10}H_{20}O_5$
M_r = 220.27
Tetragonal, $P4_1$
a = 8.79540 (10) Å
c = 30.0676 (10) Å
V = 2326.00 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 120 K
1.00 × 0.30 × 0.30 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.73, T_{max} = 0.97
24253 measured reflections
2414 independent reflections
1996 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.084
S = 0.95
2414 reflections
271 parameters
1 restraint
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *SMART* (Siemens, 1993); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *XP* (Sheldrick, 1997); software used to prepare material for publication: *CRYSTALS*.

The author thanks Dr Chin Fa Lee for providing the sample of 15-crown-5, Professors David Feller, Paul Raithby and Peter Tasker for helful discussions, and the EPSRC and the University of Edinburgh for funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2383).

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supplementary materials

Acta Cryst. (2007). E**63**, o3130 [**doi:10.1107/S1600536807026190**]

15-Crown-5

S. Parsons

Comment

15-crown-5 (I) is a crown ether which is often used as a ligand in coordination chemistry. It crystallizes in space group $P4_1$ with two molecules in the asymmetric unit. The conformations of the two molecules are different (Figs. 1 and 2). Hill & Feller (2000) studied conformations of I using *ab initio* methods, identifying 16 low-energy conformers, though none of these appear to match either of those observed here. Raithby *et al.* (1997) analysed conformers of I in the Cambridge Database (Allen, 2002), and though regions of the uniangular conformers identified in that study resemble the conformations observed here the agreement is not complete. Three CH···O contacts in the range 2.5–2.6 Å are formed between molecules, with a forth intramolecular interaction formed between H84 and O42 (2.51 Å). Hill & Feller (2000) commented that accurate prediction of low-lying conformations in floppy molecules is a challenging task, and the presence of intermolecular interactions, though weak, could well alter computational energy rankings derived for isolated molecules.

Experimental

15-Crown-5, which is a liquid at room temperature, was obtained from Aldrich and used as received.

A sample of 15-crown-5 was drawn into a glass capillary and mounted on the diffractometer with the low-temperature device set to 220 K. The compound supercooled at first, but solidified into a glassy mass on swabbing with liquid nitrogen. The glass was annealed into a polycrystalline mass by scanning the capillary with an IR laser (OHCD) for 4 h. The power set at half that needed to melt the sample, with the low temperature device set to 230 K. A crystal was subsequently grown over the course of 1 h by Boese's laser-assisted crystal growth method (Boese & Nussbaumer, 1994).

The crystal grown was larger than the beam-size (0.3 mm). This often happens with low-melting compounds, as there is little experimental control over the length of a crystal grown *in situ* in a capillary. Görbitz (1999) has shown that use of a large crystal does not degrade data quality.

A data set was collected at 220 K, where the unit-cell dimensions were a = 8.8532 (5), c = 30.172 (2) Å. The crystal was then cooled to 120 K at a rate of 360 K h^{-1} for the structure determination reported here.

Following data collection a multiscan absorption correction was applied (*SADABS*, Sheldrick, 2007), though the range of transmission was more extreme than would have been calculated on crystal dimensions. *SADABS* corrects for all systematic errors that lead to disparities in the intensities of symmetry-equivalent data. These may include absorption by the mount, crystal decay, changes in the volume of the crystal illuminated, *etc*. Here the glass capillary is an obvious extra source of absorption.

One reflection (011) appears to have been obscured by the beam-stop.

Refinement

Though the space group is $P4_1$, absolute scattering effects are very slight and data were merged in point group 4/m. The abolute structure has not been established in this study.

H-atoms were placed in calculated positions with a CH bond distance of 0.99 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

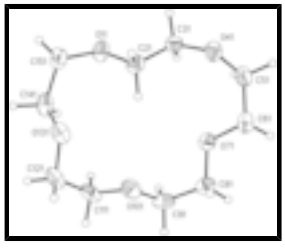


Fig. 1. : The molecular structure of the meolecule based on O11 in the crystal structure of (I). Non-H atoms are represented with 50% probability displacement ellipsoids.

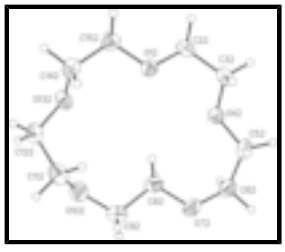


Fig. 2. : The molecular structure of the meolecule based on O12 in the crystal structure of (I). Non-H atoms are represented with 50% probability displacement ellipsoids.

1,4,7,10,13-pentaoxacylopentadecane

Crystal data

$C_{10}H_{20}O_5$	$Z = 8$
$M_r = 220.27$	$F_{000} = 960$
Tetragonal, $P4_1$	$D_x = 1.258$ Mg m^{-3}
Hall symbol: P 4w	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.79540$ (10) Å	Cell parameters from 5144 reflections
$b = 8.79540$ (10) Å	$\theta = 2$–21º
$c = 30.0676$ (10) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 90$º	$T = 120$ K
$\beta = 90$º	Cylinder, colourless
$\gamma = 90$º	1.00 × 0.30 × 0.30 mm
$V = 2326.00$ (9) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	1996 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.052$

T = 120 K

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2007)

T_{min} = 0.73, T_{max} = 0.97

24253 measured reflections

2414 independent reflections

θ_{max} = 26.4º

θ_{min} = 2.3º

h = −10→10

k = −10→10

l = −37→37

Refinement

Refinement on F^2

Least-squares matrix: full

H-atom parameters not refined

Method, part 1, Chebychev polynomial, [Watkin, D. (1994). Acta Cryst. A50, 411–437. *P*rince, E. (2004). Mathematical Techniques in Crystallography and Materials Science, 3rd ed., p. 81. Ne*w* York: Springer-Verlag] [*w*eight] = 1.0/[A_0*T_0(x) + A_1*T_1(x) ··· + A_{n-1}]*T_{n-1}(x)] where A_i are the Chebychev coefficients listed below and x = *F* /*F*max Method = Robust Weighting (*P*rince, 2004) W = [*w*eight] * [1-(delta*F*/6*sigma*F*)^2]^2 A_i are: 158. 236. 145. 57.8 14.6

$R[F^2 > 2\sigma(F^2)]$ = 0.043

$wR(F^2)$ = 0.084

S = 0.95

2414 reflections

271 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

$(\Delta/\sigma)_{max}$ = 0.005

$\Delta\rho_{max}$ = 0.20 e Å^{-3}

$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Extinction correction: None

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O11	0.8585 (3)	0.1125 (3)	0.65682 (10)	0.0359
C21	0.7737 (4)	0.2441 (4)	0.64577 (13)	0.0315
C31	0.6206 (4)	0.2220 (4)	0.66747 (13)	0.0313
O41	0.5287 (3)	0.3540 (3)	0.66244 (10)	0.0332
C51	0.3923 (4)	0.3337 (4)	0.63720 (13)	0.0345
C61	0.4052 (4)	0.3894 (4)	0.59059 (14)	0.0356
O71	0.5012 (3)	0.2899 (3)	0.56624 (9)	0.0333
C81	0.5226 (5)	0.3386 (4)	0.52185 (13)	0.0368
C91	0.6388 (5)	0.2377 (4)	0.50020 (13)	0.0373
O101	0.7829 (3)	0.2746 (3)	0.51751 (10)	0.0370
C111	0.8965 (5)	0.1651 (4)	0.50746 (14)	0.0371
C121	1.0431 (4)	0.2156 (4)	0.52836 (15)	0.0387
O131	1.0336 (3)	0.2323 (3)	0.57526 (11)	0.0340
C141	1.0566 (4)	0.0962 (4)	0.59932 (15)	0.0363

C151	1.0171 (4)	0.1225 (4)	0.64738 (14)	0.0349
O12	0.6696 (3)	0.8020 (3)	0.39743 (9)	0.0293
C22	0.7388 (4)	0.7345 (4)	0.43517 (12)	0.0286
C32	0.7435 (4)	0.5657 (4)	0.42843 (12)	0.0293
O42	0.8383 (3)	0.5346 (3)	0.39138 (9)	0.0298
C52	0.8145 (4)	0.3873 (4)	0.37354 (14)	0.0316
C62	0.8974 (4)	0.3728 (4)	0.32991 (14)	0.0341
O72	0.8270 (3)	0.4512 (3)	0.29374 (10)	0.0378
C82	0.8440 (4)	0.6116 (4)	0.29590 (13)	0.0345
C92	0.8089 (5)	0.6733 (5)	0.25020 (14)	0.0427
O102	0.8080 (3)	0.8351 (3)	0.25098 (10)	0.0396
C112	0.6627 (4)	0.8981 (5)	0.25936 (14)	0.0377
C122	0.6797 (4)	1.0472 (4)	0.28319 (13)	0.0332
O132	0.7249 (3)	1.0262 (3)	0.32812 (10)	0.0303
C142	0.6008 (4)	1.0242 (4)	0.35831 (13)	0.0306
C152	0.6532 (4)	0.9617 (4)	0.40185 (13)	0.0302
H21	0.8243	0.3363	0.6577	0.0383*
H22	0.7629	0.2531	0.6132	0.0383*
H31	0.6353	0.2012	0.6996	0.0374*
H32	0.5687	0.1346	0.6534	0.0374*
H51	0.3095	0.3900	0.6524	0.0414*
H52	0.3678	0.2239	0.6369	0.0414*
H61	0.4490	0.4931	0.5904	0.0424*
H62	0.3032	0.3915	0.5767	0.0424*
H81	0.5586	0.4452	0.5217	0.0437*
H82	0.4250	0.3316	0.5056	0.0437*
H91	0.6152	0.1298	0.5067	0.0445*
H92	0.6381	0.2542	0.4677	0.0445*
H111	0.8668	0.0650	0.5197	0.0441*
H112	0.9095	0.1575	0.4749	0.0441*
H121	1.1227	0.1391	0.5216	0.0477*
H122	1.0728	0.3147	0.5153	0.0477*
H141	1.1644	0.0648	0.5969	0.0441*
H142	0.9907	0.0152	0.5870	0.0441*
H151	1.0707	0.0453	0.6656	0.0422*
H152	1.0526	0.2252	0.6559	0.0422*
H23	0.8433	0.7743	0.4389	0.0338*
H24	0.6785	0.7587	0.4623	0.0338*
H33	0.7855	0.5157	0.4555	0.0359*
H34	0.6397	0.5267	0.4229	0.0359*
H53	0.8532	0.3097	0.3947	0.0389*
H54	0.7043	0.3706	0.3687	0.0389*
H63	1.0012	0.4142	0.3340	0.0411*
H64	0.9037	0.2636	0.3222	0.0411*
H83	0.9494	0.6378	0.3046	0.0420*
H84	0.7723	0.6544	0.3181	0.0420*
H93	0.8872	0.6375	0.2291	0.0510*
H94	0.7078	0.6360	0.2407	0.0510*
H113	0.6029	0.8274	0.2781	0.0460*

H114	0.6093	0.9149	0.2309	0.0460*
H123	0.7572	1.1091	0.2678	0.0407*
H124	0.5808	1.1012	0.2827	0.0407*
H143	0.5620	1.1292	0.3627	0.0381*
H144	0.5182	0.9596	0.3463	0.0381*
H153	0.7526	1.0074	0.4100	0.0368*
H154	0.5780	0.9850	0.4254	0.0368*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O11	0.0300 (14)	0.0283 (13)	0.0495 (17)	0.0026 (11)	0.0000 (12)	0.0089 (12)
C21	0.0331 (19)	0.0276 (18)	0.034 (2)	0.0014 (15)	−0.0017 (16)	0.0081 (16)
C31	0.034 (2)	0.032 (2)	0.0275 (19)	0.0016 (15)	0.0009 (15)	0.0021 (15)
O41	0.0312 (14)	0.0290 (14)	0.0395 (15)	0.0036 (11)	−0.0031 (12)	−0.0071 (11)
C51	0.0281 (19)	0.036 (2)	0.039 (2)	0.0010 (15)	0.0017 (17)	−0.0070 (17)
C61	0.0284 (19)	0.0310 (19)	0.047 (2)	0.0067 (15)	−0.0006 (17)	−0.0013 (17)
O71	0.0343 (14)	0.0338 (13)	0.0317 (15)	0.0054 (11)	−0.0007 (11)	0.0006 (11)
C81	0.040 (2)	0.041 (2)	0.029 (2)	0.0003 (17)	−0.0054 (17)	0.0026 (17)
C91	0.051 (2)	0.034 (2)	0.0268 (19)	−0.0097 (18)	−0.0036 (18)	0.0001 (16)
O101	0.0411 (16)	0.0331 (15)	0.0369 (15)	−0.0011 (12)	0.0060 (12)	−0.0056 (12)
C111	0.049 (2)	0.031 (2)	0.032 (2)	−0.0005 (17)	0.0170 (18)	−0.0028 (16)
C121	0.035 (2)	0.037 (2)	0.044 (2)	0.0009 (17)	0.0172 (18)	−0.0007 (18)
O131	0.0335 (15)	0.0270 (13)	0.0416 (15)	−0.0028 (11)	0.0078 (12)	−0.0040 (12)
C141	0.0276 (19)	0.0260 (19)	0.055 (3)	0.0007 (15)	0.0000 (17)	−0.0028 (18)
C151	0.0246 (18)	0.036 (2)	0.044 (2)	0.0012 (15)	−0.0046 (17)	0.0054 (18)
O12	0.0377 (14)	0.0237 (12)	0.0264 (12)	−0.0021 (10)	−0.0039 (11)	0.0010 (10)
C22	0.0276 (18)	0.035 (2)	0.0231 (18)	−0.0006 (15)	0.0007 (14)	0.0031 (15)
C32	0.0279 (18)	0.0331 (19)	0.0270 (18)	−0.0012 (15)	−0.0004 (15)	0.0068 (15)
O42	0.0324 (14)	0.0278 (13)	0.0291 (14)	−0.0025 (11)	0.0047 (11)	−0.0004 (10)
C52	0.0315 (19)	0.0218 (17)	0.042 (2)	−0.0010 (15)	−0.0030 (16)	0.0050 (15)
C62	0.038 (2)	0.0271 (19)	0.038 (2)	−0.0002 (16)	−0.0059 (17)	−0.0051 (16)
O72	0.0486 (16)	0.0257 (13)	0.0392 (16)	−0.0030 (12)	−0.0123 (13)	−0.0065 (12)
C82	0.045 (2)	0.0305 (19)	0.028 (2)	−0.0049 (16)	−0.0020 (17)	−0.0052 (17)
C92	0.057 (3)	0.040 (2)	0.031 (2)	0.0015 (19)	0.001 (2)	−0.0050 (18)
O102	0.0442 (16)	0.0380 (16)	0.0367 (15)	0.0009 (12)	0.0084 (13)	0.0070 (12)
C112	0.034 (2)	0.045 (2)	0.034 (2)	−0.0028 (17)	−0.0038 (17)	0.0067 (18)
C122	0.033 (2)	0.032 (2)	0.035 (2)	−0.0012 (16)	−0.0039 (16)	0.0074 (16)
O132	0.0247 (12)	0.0374 (14)	0.0289 (13)	0.0004 (10)	−0.0019 (11)	0.0068 (11)
C142	0.0242 (18)	0.0271 (18)	0.040 (2)	−0.0018 (14)	0.0000 (16)	0.0002 (16)
C152	0.0273 (18)	0.0282 (18)	0.035 (2)	−0.0007 (15)	0.0042 (15)	−0.0045 (15)

Geometric parameters (Å, °)

O11—C21	1.416 (4)	O12—C22	1.418 (4)
O11—C151	1.427 (4)	O12—C152	1.419 (4)
C21—C31	1.509 (5)	C22—C32	1.499 (5)
C21—H21	0.992	C22—H23	0.990
C21—H22	0.987	C22—H24	0.995

C31—O41	1.423 (4)	C32—O42	1.418 (4)
C31—H31	0.991	C32—H33	0.995
C31—H32	0.989	C32—H34	0.990
O41—C51	1.430 (4)	O42—C52	1.418 (4)
C51—C61	1.489 (5)	C52—C62	1.507 (5)
C51—H51	0.992	C52—H53	0.992
C51—H52	0.990	C52—H54	0.991
C61—O71	1.420 (4)	C62—O72	1.429 (5)
C61—H61	0.991	C62—H63	0.990
C61—H62	0.990	C62—H64	0.989
O71—C81	1.415 (4)	O72—C82	1.420 (4)
C81—C91	1.502 (6)	C82—C92	1.509 (6)
C81—H81	0.989	C82—H83	0.990
C81—H82	0.989	C82—H84	0.992
C91—O101	1.409 (5)	C92—O102	1.424 (5)
C91—H91	0.991	C92—H93	0.988
C91—H92	0.987	C92—H94	0.990
O101—C111	1.420 (5)	O102—C112	1.416 (5)
C111—C121	1.502 (6)	C112—C122	1.502 (6)
C111—H111	0.989	C112—H113	0.990
C111—H112	0.988	C112—H114	0.988
C121—O131	1.420 (5)	C122—O132	1.420 (4)
C121—H121	0.992	C122—H123	0.988
C121—H122	0.991	C122—H124	0.991
O131—C141	1.413 (5)	O132—C142	1.420 (4)
C141—C151	1.504 (6)	C142—C152	1.493 (5)
C141—H141	0.990	C142—H143	0.992
C141—H142	0.990	C142—H144	0.990
C151—H151	0.992	C152—H153	0.993
C151—H152	0.989	C152—H154	0.990
C21—O11—C151	114.7 (3)	C22—O12—C152	112.5 (3)
O11—C21—C31	105.3 (3)	O12—C22—C32	108.6 (3)
O11—C21—H21	110.3	O12—C22—H23	109.9
C31—C21—H21	110.5	C32—C22—H23	109.9
O11—C21—H22	110.4	O12—C22—H24	109.7
C31—C21—H22	110.7	C32—C22—H24	109.7
H21—C21—H22	109.5	H23—C22—H24	109.1
C21—C31—O41	110.8 (3)	C22—C32—O42	108.3 (3)
C21—C31—H31	109.2	C22—C32—H33	109.7
O41—C31—H31	109.2	O42—C32—H33	109.8
C21—C31—H32	109.1	C22—C32—H34	109.9
O41—C31—H32	109.0	O42—C32—H34	110.1
H31—C31—H32	109.4	H33—C32—H34	109.1
C31—O41—C51	115.5 (3)	C32—O42—C52	112.7 (3)
O41—C51—C61	113.3 (3)	O42—C52—C62	109.6 (3)
O41—C51—H51	108.0	O42—C52—H53	109.6
C61—C51—H51	109.0	C62—C52—H53	109.5
O41—C51—H52	108.1	O42—C52—H54	109.6
C61—C51—H52	109.2	C62—C52—H54	109.4

H51—C51—H52	109.3	H53—C52—H54	109.2
C51—C61—O71	109.1 (3)	C52—C62—O72	114.3 (3)
C51—C61—H61	109.8	C52—C62—H63	107.9
O71—C61—H61	109.4	O72—C62—H63	108.4
C51—C61—H62	109.6	C52—C62—H64	108.2
O71—C61—H62	109.4	O72—C62—H64	108.4
H61—C61—H62	109.4	H63—C62—H64	109.5
C61—O71—C81	112.3 (3)	C62—O72—C82	113.5 (3)
O71—C81—C91	108.7 (3)	O72—C82—C92	107.1 (3)
O71—C81—H81	109.4	O72—C82—H83	110.0
C91—C81—H81	109.9	C92—C82—H83	110.3
O71—C81—H82	109.3	O72—C82—H84	109.9
C91—C81—H82	109.9	C92—C82—H84	110.3
H81—C81—H82	109.6	H83—C82—H84	109.3
C81—C91—O101	108.4 (3)	C82—C92—O102	110.2 (3)
C81—C91—H91	109.8	C82—C92—H93	109.2
O101—C91—H91	109.6	O102—C92—H93	109.4
C81—C91—H92	109.7	C82—C92—H94	109.1
O101—C91—H92	109.7	O102—C92—H94	109.3
H91—C91—H92	109.6	H93—C92—H94	109.6
C91—O101—C111	113.5 (3)	C92—O102—C112	113.5 (3)
O101—C111—C121	108.3 (3)	O102—C112—C122	109.7 (3)
O101—C111—H111	109.8	O102—C112—H113	109.6
C121—C111—H111	109.5	C122—C112—H113	109.2
O101—C111—H112	109.8	O102—C112—H114	109.5
C121—C111—H112	109.6	C122—C112—H114	109.3
H111—C111—H112	109.8	H113—C112—H114	109.6
C111—C121—O131	113.3 (3)	C112—C122—O132	111.6 (3)
C111—C121—H121	108.6	C112—C122—H123	109.0
O131—C121—H121	108.3	O132—C122—H123	109.0
C111—C121—H122	108.8	C112—C122—H124	108.9
O131—C121—H122	108.5	O132—C122—H124	108.8
H121—C121—H122	109.3	H123—C122—H124	109.5
C121—O131—C141	114.4 (3)	C122—O132—C142	113.2 (3)
O131—C141—C151	109.2 (3)	O132—C142—C152	109.1 (3)
O131—C141—H141	109.6	O132—C142—H143	109.7
C151—C141—H141	109.5	C152—C142—H143	109.5
O131—C141—H142	109.5	O132—C142—H144	109.8
C151—C141—H142	109.6	C152—C142—H144	109.5
H141—C141—H142	109.4	H143—C142—H144	109.3
C141—C151—O11	114.0 (3)	C142—C152—O12	108.3 (3)
C141—C151—H151	108.4	C142—C152—H153	109.8
O11—C151—H151	108.2	O12—C152—H153	109.5
C141—C151—H152	108.5	C142—C152—H154	110.1
O11—C151—H152	108.2	O12—C152—H154	109.8
H151—C151—H152	109.4	H153—C152—H154	109.3
C151—O11—C21—C31	−167.9 (3)	C152—O12—C22—C32	177.0 (3)
C31—O41—C51—C61	−100.8 (4)	C32—O42—C52—C62	169.9 (3)
C111—O101—C91—C81	166.4 (3)	C112—O102—C92—C82	−91.7 (4)

C121—O131—C141—C151	−170.2 (3)	C122—O132—C142—C152	165.2 (3)
O71—C81—C91—O101	−73.1 (4)	O72—C82—C92—O102	173.9 (3)
C21—O11—C151—C141	−79.7 (4)	C22—O12—C152—C142	171.9 (3)
C81—O71—C61—C51	−178.1 (3)	C82—O72—C62—C52	73.5 (4)
C91—O101—C111—C121	−178.9 (3)	C92—O102—C112—C122	149.8 (3)
O11—C21—C31—O41	174.4 (3)	O12—C22—C32—O42	64.0 (3)
O101—C111—C121—O131	59.1 (4)	O102—C112—C122—O132	−72.8 (4)
C51—O41—C31—C21	116.9 (3)	C52—O42—C32—C22	−161.6 (3)
C61—O71—C81—C91	173.6 (3)	C62—O72—C82—C92	162.9 (3)
C141—O131—C121—C111	84.8 (4)	C142—O132—C122—C112	−94.9 (3)
O41—C51—C61—O71	71.4 (4)	O42—C52—C62—O72	−74.6 (4)
O131—C141—C151—O11	82.0 (4)	O132—C142—C152—O12	−75.2 (3)

Fig. 1

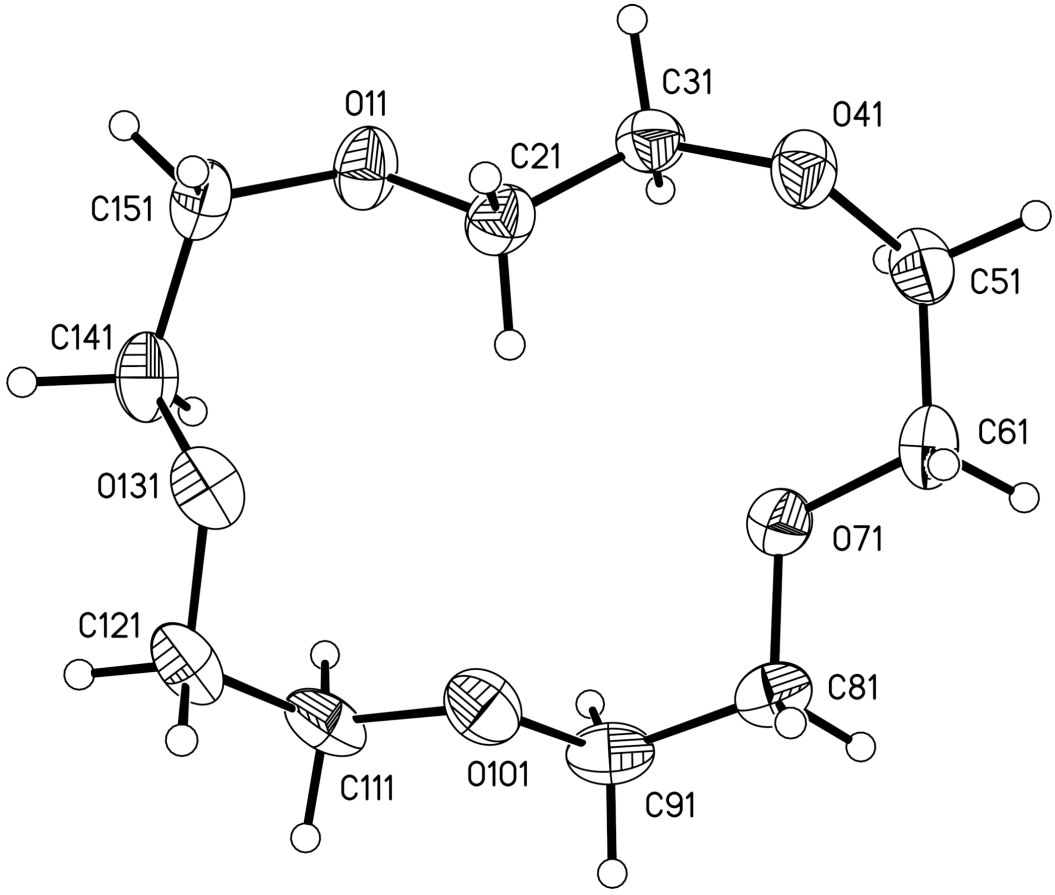
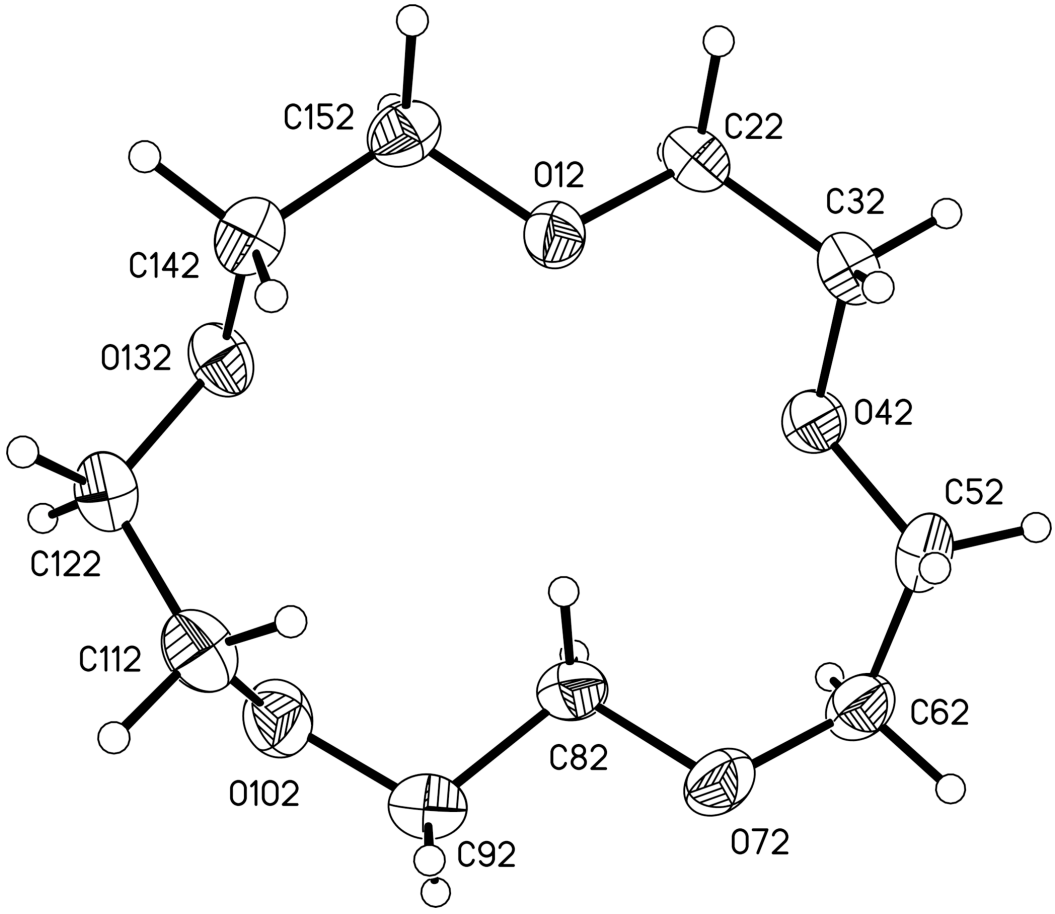

C31
O11
O41
C21
C151
C51
C141
C61
O131
O71
C121
C81
C111
O101
C91

Fig. 2


C152
C22
O12
C32
C142
O132
O42
C52
C122
C112
C62
C82
O102
O72
C92