Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

8-Amino-11-hydroxypentacyclo-undecane-8,11-lactam

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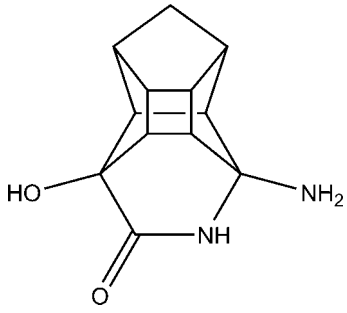
Received 31 July 2007; accepted 10 August 2007

Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.113; data-to-parameter ratio = 15.0.

The title compound, $C_{12}H_{14}N_2O_2$, is a δ-lactam derived from the pentacycloundecane skeleton. The compound displays C—C bond lengths that deviate from the normal value, ranging from very short [1.5154 (17) Å] to long [1.5691 (18) Å]. The molecules are arranged in a bilayer conformation consisting of a hydrophobic cage moiety and a polar lactam region. These polar lactam regions are linked by N—H···O and O—H···O intermolecular hydrogen bonds.

Related literature

Related structures: Flippen-Anderson *et al.* (1991); Kruger *et al.* (1996, 2005, 2006); Martins *et al.* (1993, 1994).



Experimental

Crystal data

$C_{12}H_{14}N_2O_2$
M_r = 218.25
Monoclinic, $P2_1/c$
a = 12.8324 (6) Å
b = 7.3821 (4) Å
c = 10.8437 (5) Å
β = 103.449 (3)°
V = 999.05 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 223 (2) K
0.48 × 0.27 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
13512 measured reflections
2418 independent reflections
1955 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.113
S = 1.03
2418 reflections
161 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O2^{i}	0.903 (19)	1.976 (19)	2.8741 (14)	172.9 (17)
N2—H2NB···O2^{ii}	0.92 (2)	2.37 (2)	3.2469 (18)	158.6 (15)
O1—H1O···O2^{iii}	0.89 (2)	1.90 (2)	2.7619 (14)	163.2 (19)

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

We thank Dr Manuel Fernandes of the Jan Boeyens Structural Chemistry Laboratory at the University of the Witwatersrand for his assistance in the acquisition of the crystallographic data. This work was supported by grants from the National Research Foundation (South Africa), GUN 2046819, and the University of KwaZulu-Natal.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2154).

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supplementary materials

Acta Cryst. (2007). E**63**, o3906 [**doi:10.1107/S1600536807039827**]

8-Amino-11-hydroxypentacycloundecane-8,11-lactam

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Comment

The structure of the title compound(I) was obtained as part of an investigation into the biological activity of cage compound derivatives. The 8,11-dihydroxy-pentacycloundecane-8, 11-lactam has been previously reported (Martins *et al.*, 1993) as has the crystal structure of the dihydroxy derivative (Kruger, *et al.*, 1996; Kruger *et al.*, 2006).

It has been reported earlier that the molecular structure of pentacylcloundecane derivatives exhibit C—C single bond lengths that deviate from the normal value of 1.54 Å (for example Flippen-Anderson *et al.*, 1991; Kruger *et al.*, 2005). The C9—C10 bond is typically longer than expected in most derivatives whereas the C11—C12 is commonly shorter.

In (I) longer than normal bonds include C9—C10(1.569 Å), C2—C6 (1.569 Å), C1—C2 (1.560 Å) and C1—C7 (1.558 Å). The bonds involving the bridge atom C4 are shorter than normal with C11—C12 being the shortest at 1.5144 Å). Fig. 1 shows the molecular geometry and labeling scheme employed.

In the crystal structure the molecules are arranged in a bilayer conformation involving the hydrophobic cage moiety and the polar lactam region. This is typical for these types of molecules (Kruger *et al.*, 2006). Intermolecular hydrogen bonding is observed in the polar lactam region. This complex hydrogen bonding network involves atoms N, O1 and O2 as hydrogen bond donors and O2 as a hydrogen bond acceptor. Fig. 2 shows the packing and intermolecular hydrogen bonding.

Experimental

To an ice-cooled solution of 25% ammonia (15 cm^3), dione (1 g) was added followed by the addition of NH_4Cl (0.4 g) and NaCN (0.4 g). The mixture was left to stir in a sealed vessel immersed in an ice-water bath for 6hrs. The resulting white precipitate was filtered and washed with acetone (2 *x* 15 ml) and the product (0.75 g) was recrystallized from methanol to yield crystals suitable for crystallography (Martins *et al.*, 1994).

Refinement

With the exception of those involved in H-bonding, all hydrogen atoms were first located in the difference map then positioned geometrically and allowed to ride on their respective parent atoms. Hydrogen atoms attached to O or N were placed using the Fourier difference map and allowed to refine freely.

Figures

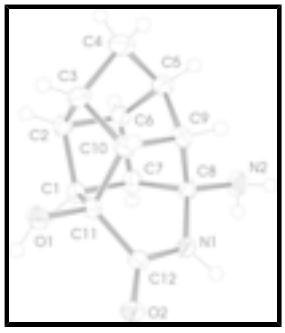

Fig. 1. Molecular structure of (I) showing the atomic numbering scheme and displacement ellipsoids at the 50% probability level

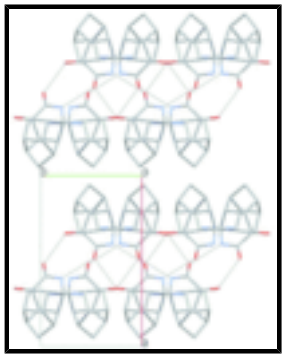

Fig. 2. Packing diagram of (I), illustrating the layered structure and hydrogen bond interactions. Hydrogen atoms have been omitted.

8-Amino-11-hydroxypentacycloundecane-8,11-lactam

Crystal data

$C_{12}H_{14}N_2O_2$	F_{000} = 464
M_r = 218.25	D_x = 1.451 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1018 reflections
a = 12.8324 (6) Å	θ = 3.2–28.2º
b = 7.3821 (4) Å	μ = 0.10 mm^{-1}
c = 10.8437 (5) Å	T = 223 (2) K
β = 103.449 (3)º	Plate, colourless
V = 999.05 (9) Å^3	0.48 × 0.27 × 0.12 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	1955 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.049
Monochromator: graphite	θ_{max} = 28.0º
T = 223(2) K	θ_{min} = 1.6º
φ and ω scans	h = −16→16
Absorption correction: none	k = −7→9

13512 measured reflections
2418 independent reflections

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.113$
$S = 1.03$
2418 reflections
161 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.324P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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}
C1	0.66746 (11)	1.11198 (17)	0.07351 (12)	0.0232 (3)
H1	0.6108	1.1929	0.0255	0.028*
C2	0.78494 (11)	1.16318 (18)	0.07122 (14)	0.0279 (3)
H2	0.7957	1.2741	0.0244	0.033*
C3	0.85446 (11)	1.14034 (19)	0.20586 (14)	0.0287 (3)
H3	0.8766	1.2543	0.2528	0.034*
C4	0.94594 (12)	1.0186 (2)	0.18706 (17)	0.0373 (4)
H4A	0.9909	0.9751	0.2674	0.045*
H4B	0.9904	1.0762	0.1360	0.045*
C5	0.87304 (11)	0.87066 (19)	0.11453 (15)	0.0300 (3)
H5	0.9102	0.7658	0.0872	0.036*
C6	0.79718 (12)	0.97639 (18)	0.00700 (13)	0.0288 (3)
H6	0.8154	0.9789	−0.0768	0.035*
C7	0.68036 (11)	0.92648 (17)	0.01022 (12)	0.0244 (3)
H7	0.6307	0.9033	−0.0729	0.029*

C8	0.68967 (10)	0.77508 (16)	0.10950 (12)	0.0213 (3)
C9	0.79613 (10)	0.82542 (17)	0.20091 (12)	0.0236 (3)
H9	0.8238	0.7285	0.2630	0.028*
C10	0.78383 (10)	1.01202 (17)	0.26537 (12)	0.0223 (3)
H10	0.8058	1.0075	0.3591	0.027*
C11	0.66954 (10)	1.08606 (16)	0.21535 (12)	0.0194 (3)
C12	0.58789 (10)	0.94538 (16)	0.23194 (12)	0.0203 (3)
N1	0.60055 (9)	0.79045 (14)	0.17415 (11)	0.0233 (2)
N2	0.69531 (11)	0.59827 (16)	0.05535 (13)	0.0303 (3)
O1	0.66090 (8)	1.25102 (12)	0.27785 (10)	0.0265 (2)
O2	0.51744 (7)	0.97022 (13)	0.29291 (9)	0.0264 (2)
H1N	0.5586 (15)	0.694 (2)	0.1800 (17)	0.035 (4)*
H2NB	0.6332 (15)	0.572 (2)	−0.0045 (18)	0.037 (5)*
H2NA	0.7070 (14)	0.517 (3)	0.1203 (18)	0.038 (5)*
H1O	0.5986 (17)	1.305 (3)	0.2435 (19)	0.043 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0274 (7)	0.0182 (6)	0.0244 (6)	0.0013 (5)	0.0068 (5)	0.0023 (5)
C2	0.0322 (7)	0.0195 (6)	0.0368 (7)	−0.0002 (5)	0.0178 (6)	0.0037 (5)
C3	0.0215 (6)	0.0260 (6)	0.0399 (8)	−0.0037 (5)	0.0098 (6)	−0.0062 (6)
C4	0.0226 (7)	0.0350 (8)	0.0563 (10)	0.0003 (6)	0.0134 (7)	−0.0055 (7)
C5	0.0251 (7)	0.0234 (6)	0.0447 (8)	0.0040 (5)	0.0151 (6)	−0.0018 (6)
C6	0.0363 (8)	0.0257 (6)	0.0293 (7)	−0.0013 (5)	0.0176 (6)	0.0000 (5)
C7	0.0324 (7)	0.0215 (6)	0.0200 (6)	−0.0004 (5)	0.0073 (5)	−0.0010 (5)
C8	0.0257 (6)	0.0164 (5)	0.0241 (6)	0.0001 (4)	0.0104 (5)	−0.0025 (5)
C9	0.0234 (6)	0.0197 (6)	0.0281 (6)	0.0048 (5)	0.0066 (5)	0.0006 (5)
C10	0.0194 (6)	0.0223 (6)	0.0246 (6)	0.0017 (5)	0.0034 (5)	−0.0028 (5)
C11	0.0199 (6)	0.0165 (5)	0.0220 (6)	0.0004 (4)	0.0052 (5)	−0.0026 (4)
C12	0.0193 (6)	0.0200 (6)	0.0214 (6)	0.0014 (4)	0.0044 (5)	0.0003 (5)
N1	0.0243 (6)	0.0183 (5)	0.0297 (6)	−0.0029 (4)	0.0114 (4)	−0.0021 (4)
N2	0.0388 (7)	0.0189 (5)	0.0365 (7)	−0.0012 (5)	0.0155 (6)	−0.0059 (5)
O1	0.0246 (5)	0.0202 (4)	0.0349 (5)	0.0009 (4)	0.0075 (4)	−0.0095 (4)
O2	0.0234 (5)	0.0251 (5)	0.0340 (5)	0.0003 (4)	0.0136 (4)	−0.0019 (4)

Geometric parameters (Å, °)

C1—C11	1.5440 (17)	C7—C8	1.5370 (17)
C1—C7	1.5577 (17)	C7—H7	0.9900
C1—C2	1.5601 (18)	C8—N2	1.4400 (15)
C1—H1	0.9900	C8—N1	1.4782 (16)
C2—C3	1.533 (2)	C8—C9	1.5353 (18)
C2—C6	1.5691 (18)	C9—C10	1.5692 (17)
C2—H2	0.9900	C9—H9	0.9900
C3—C4	1.5293 (19)	C10—C11	1.5406 (17)
C3—C10	1.5516 (18)	C10—H10	0.9900
C3—H3	0.9900	C11—O1	1.4104 (14)
C4—C5	1.531 (2)	C11—C12	1.5154 (17)

C4—H4A	0.9800	C12—O2	1.2514 (15)
C4—H4B	0.9800	C12—N1	1.3321 (16)
C5—C6	1.546 (2)	N1—H1N	0.903 (19)
C5—C9	1.5469 (18)	N2—H2NB	0.92 (2)
C5—H5	0.9900	N2—H2NA	0.913 (19)
C6—C7	1.5520 (19)	O1—H1O	0.89 (2)
C6—H6	0.9900		
C11—C1—C7	110.55 (10)	C6—C7—C1	90.19 (10)
C11—C1—C2	104.65 (11)	C8—C7—H7	116.2
C7—C1—C2	90.22 (10)	C6—C7—H7	116.2
C11—C1—H1	116.1	C1—C7—H7	116.2
C7—C1—H1	116.1	N2—C8—N1	112.38 (10)
C2—C1—H1	116.1	N2—C8—C9	111.17 (11)
C3—C2—C1	107.98 (10)	N1—C8—C9	110.22 (10)
C3—C2—C6	103.29 (11)	N2—C8—C7	112.12 (11)
C1—C2—C6	89.48 (10)	N1—C8—C7	109.49 (10)
C3—C2—H2	117.3	C9—C8—C7	100.88 (10)
C1—C2—H2	117.3	C8—C9—C5	104.99 (11)
C6—C2—H2	117.3	C8—C9—C10	109.48 (10)
C4—C3—C2	103.44 (12)	C5—C9—C10	102.98 (10)
C4—C3—C10	103.73 (11)	C8—C9—H9	112.9
C2—C3—C10	101.33 (10)	C5—C9—H9	112.9
C4—C3—H3	115.5	C10—C9—H9	112.9
C2—C3—H3	115.5	C11—C10—C3	103.73 (10)
C10—C3—H3	115.5	C11—C10—C9	109.92 (10)
C3—C4—C5	95.24 (11)	C3—C10—C9	102.80 (10)
C3—C4—H4A	112.7	C11—C10—H10	113.2
C5—C4—H4A	112.7	C3—C10—H10	113.2
C3—C4—H4B	112.7	C9—C10—H10	113.2
C5—C4—H4B	112.7	O1—C11—C12	113.63 (10)
H4A—C4—H4B	110.2	O1—C11—C10	108.17 (10)
C4—C5—C6	103.29 (12)	C12—C11—C10	110.06 (10)
C4—C5—C9	104.04 (12)	O1—C11—C1	112.74 (10)
C6—C5—C9	100.79 (10)	C12—C11—C1	110.54 (10)
C4—C5—H5	115.6	C10—C11—C1	100.91 (10)
C6—C5—H5	115.6	O2—C12—N1	123.82 (11)
C9—C5—H5	115.6	O2—C12—C11	124.52 (11)
C5—C6—C7	107.78 (10)	N1—C12—C11	111.66 (10)
C5—C6—C2	102.67 (11)	C12—N1—C8	118.78 (10)
C7—C6—C2	90.10 (10)	C12—N1—H1N	120.2 (11)
C5—C6—H6	117.4	C8—N1—H1N	120.8 (11)
C7—C6—H6	117.4	C8—N2—H2NB	111.0 (11)
C2—C6—H6	117.4	C8—N2—H2NA	107.4 (11)
C8—C7—C6	105.68 (11)	H2NB—N2—H2NA	111.4 (16)
C8—C7—C1	109.24 (10)	C11—O1—H1O	110.2 (13)
C11—C1—C2—C3	7.72 (13)	N1—C8—C9—C10	−50.48 (13)
C7—C1—C2—C3	−103.61 (11)	C7—C8—C9—C10	65.17 (12)
C11—C1—C2—C6	111.54 (10)	C4—C5—C9—C8	147.14 (11)

C7—C1—C2—C6	0.21 (10)	C6—C5—C9—C8	40.36 (12)
C1—C2—C3—C4	127.45 (11)	C4—C5—C9—C10	32.56 (13)
C6—C2—C3—C4	33.62 (12)	C6—C5—C9—C10	−74.22 (12)
C1—C2—C3—C10	20.19 (13)	C4—C3—C10—C11	−148.27 (11)
C6—C2—C3—C10	−73.65 (11)	C2—C3—C10—C11	−41.23 (12)
C2—C3—C4—C5	−53.01 (13)	C4—C3—C10—C9	−33.73 (13)
C10—C3—C4—C5	52.43 (14)	C2—C3—C10—C9	73.30 (11)
C3—C4—C5—C6	52.83 (13)	C8—C9—C10—C11	−0.65 (14)
C3—C4—C5—C9	−52.09 (13)	C5—C9—C10—C11	110.63 (11)
C4—C5—C6—C7	−127.61 (11)	C8—C9—C10—C3	−110.60 (11)
C9—C5—C6—C7	−20.22 (13)	C5—C9—C10—C3	0.68 (13)
C4—C5—C6—C2	−33.37 (12)	C3—C10—C11—O1	−72.18 (12)
C9—C5—C6—C2	74.02 (12)	C9—C10—C11—O1	178.48 (9)
C3—C2—C6—C5	−0.11 (12)	C3—C10—C11—C12	163.14 (10)
C1—C2—C6—C5	−108.47 (11)	C9—C10—C11—C12	53.80 (13)
C3—C2—C6—C7	108.15 (11)	C3—C10—C11—C1	46.35 (11)
C1—C2—C6—C7	−0.21 (10)	C9—C10—C11—C1	−62.99 (12)
C5—C6—C7—C8	−6.51 (13)	C7—C1—C11—O1	178.46 (10)
C2—C6—C7—C8	−109.86 (10)	C2—C1—C11—O1	82.59 (12)
C5—C6—C7—C1	103.56 (11)	C7—C1—C11—C12	−53.13 (13)
C2—C6—C7—C1	0.21 (10)	C2—C1—C11—C12	−149.01 (10)
C11—C1—C7—C8	0.73 (14)	C7—C1—C11—C10	63.30 (12)
C2—C1—C7—C8	106.49 (11)	C2—C1—C11—C10	−32.57 (11)
C11—C1—C7—C6	−105.97 (11)	O1—C11—C12—O2	1.13 (17)
C2—C1—C7—C6	−0.21 (10)	C10—C11—C12—O2	122.61 (13)
C6—C7—C8—N2	−87.67 (13)	C1—C11—C12—O2	−126.79 (13)
C1—C7—C8—N2	176.49 (11)	O1—C11—C12—N1	−178.45 (10)
C6—C7—C8—N1	146.88 (10)	C10—C11—C12—N1	−56.97 (13)
C1—C7—C8—N1	51.05 (13)	C1—C11—C12—N1	53.63 (14)
C6—C7—C8—C9	30.69 (12)	O2—C12—N1—C8	−177.47 (12)
C1—C7—C8—C9	−65.15 (12)	C11—C12—N1—C8	2.12 (16)
N2—C8—C9—C5	74.27 (12)	N2—C8—N1—C12	178.00 (12)
N1—C8—C9—C5	−160.44 (10)	C9—C8—N1—C12	53.40 (15)
C7—C8—C9—C5	−44.79 (11)	C7—C8—N1—C12	−56.71 (15)
N2—C8—C9—C10	−175.77 (10)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O2^{i}	0.903 (19)	1.976 (19)	2.8741 (14)	172.9 (17)
N2—H2NB···O2^{ii}	0.92 (2)	2.37 (2)	3.2469 (18)	158.6 (15)
O1—H1O···O2^{iii}	0.89 (2)	1.90 (2)	2.7619 (14)	163.2 (19)

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) *x*, −*y*+3/2, *z*−1/2; (iii) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

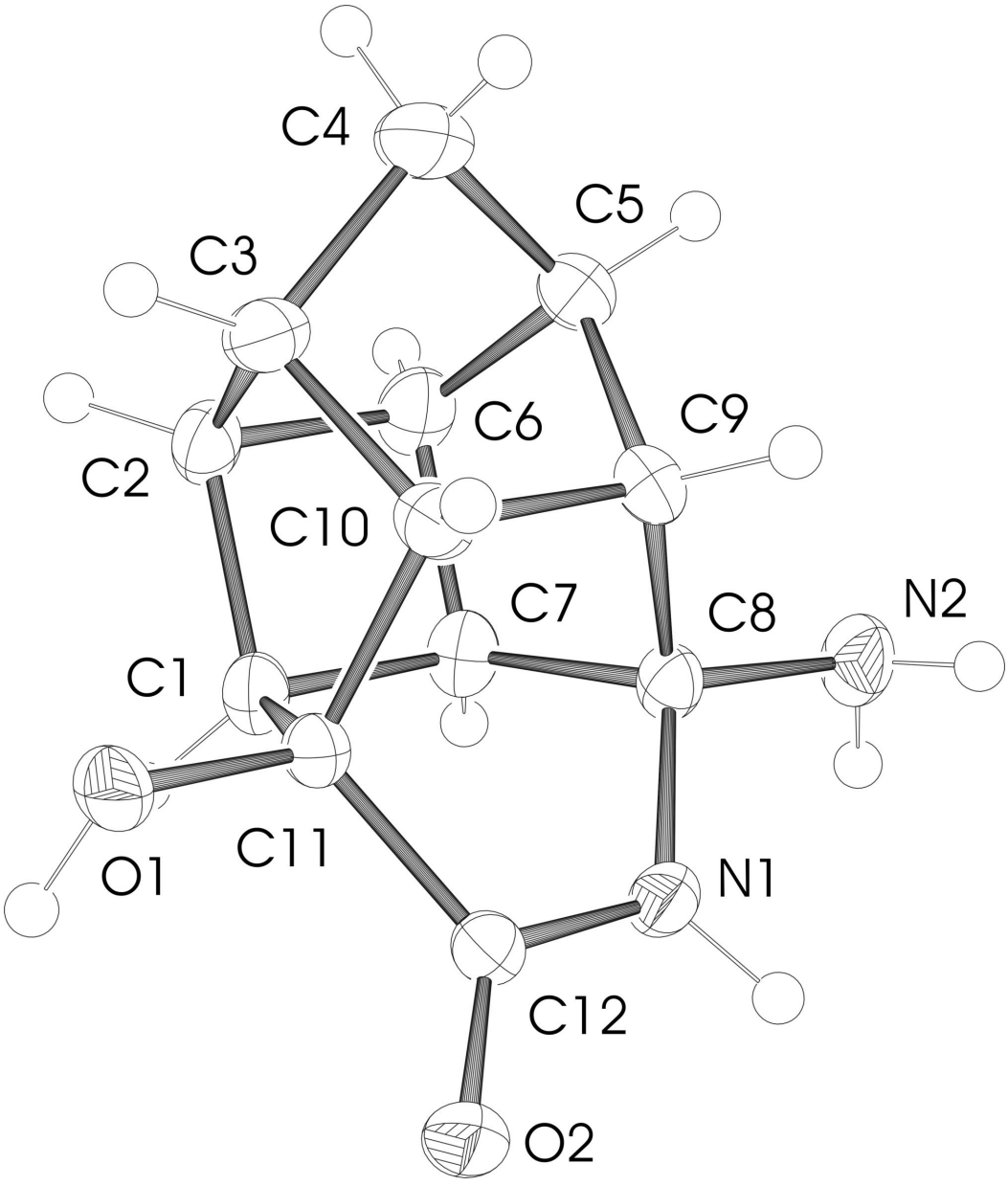

Fig. 2