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1,1′-Ureylenedi-7,7-dimethylbicyclo[2.2.1]heptan-2-one

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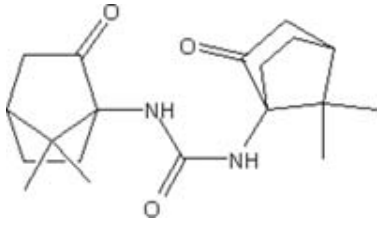
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.115; data-to-parameter ratio = 10.7.

The title compound, $C_{19}H_{28}N_2O_3$, was obtained by the acidic hydrolysis of (1*S*,4*R*)-1-isocyanato-7,7-dimethylbicyclo[2.2.1]-heptan-2-one followed by addition of aqueous sodium hydroxide. N—H···O hydrogen bonds link the molecules into chains running along the *a* axis.

Related literature

For related literature, see: Braslau *et al.* (1996); Gao *et al.* (2006).



Experimental

Crystal data

$C_{19}H_{28}N_2O_3$
M_r = 332.43
Orthorhombic, $P2_12_12_1$
a = 6.7578 (16) Å
b = 12.107 (3) Å
c = 21.269 (5) Å
V = 1740.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 223 (2) K
0.50 × 0.16 × 0.12 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.958, T_{max} = 0.990
10699 measured reflections
2418 independent reflections
2280 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.115
S = 1.11
2418 reflections
225 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.82 (3)	2.34 (2)	3.090 (2)	153 (2)
N2—H2···O3^{i}	0.83 (2)	2.32 (2)	3.061 (2)	148 (2)

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, -z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2449).

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supplementary materials

Acta Cryst. (2007). E**63**, o3994 [**doi:10.1107/S1600536807042754**]

1,1'-Ureylenedi-7,7-dimethylbicyclo[2.2.1]heptan-2-one

Y.-X. Gao, P. Liu, Y.-X. Fang, G. Tang and Y.-F. Zhao

Comment

The title compound, (I), is a byproduct in the synthesis of (1*S*,4*R*)-1-amino-7,7-dimethylbicyclo[2.2.1]heptan-2-one, which is used in the synthesis of several optically active nitroxyl radicals as a key synthetic intermediate (Braslau *et al.*, 1996). The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles in the camphor moiety are in agreement with the values reported for a related compound (Gao *et al.*, 2006). Both N—H groups are involved in hydrogen-bonding interactions with the carbonyl O atom of a neighboring molecule (Table 1). Molecules are linked into chains, running along the *a* axis, by N—H···O intermolecular hydrogen bonds.

Experimental

To a solution of (1*S*,4*R*)-1-isocyanato-7,7-dimethylbicyclo[2.2.1]heptan-2-one (0.9 g, 5 mmol) in tetrahydrofuran (10 ml) was added a 1 N aqueous HCl solution (15 ml), and the mixture was stirred at reflux for 1 h. 2 N aqueous sodium hydroxide (10 ml) was then added at room temperature and stirred for 30 min. Then the solution was extracted with ethyl acetate. The organic layer was washed with brine, dried over anhydrous $MgSO_4$, concentrated under vacuum and the crude product was purified by column chromatography (petroleum ether-ethyl acetate, 6:1) to give the title compound as a white solid (0.06 g). Single crystals of (I) were obtained by slow evaporation of a petroleum ether-ethyl acetate solution (6:1 *v*/*v*).

Refinement

N-bound H atoms were located in a difference map and refined isotropically. Methyl H atoms were placed in calculated positions, with C—H = 0.97 Å and U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in idealized positions [C—H = 0.98 Å (methine) and 0.97 Å (methylene)] and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs were merged; the absolute configuration of (I) was assigned assuming that the absolute configuration of the starting material was retained during the synthesis.

Figures

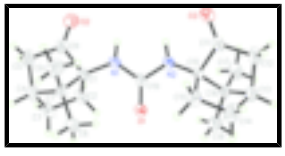


Fig. 1. The molecular structure of (I), shown with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

1,1'-Ureylenedi-7,7-dimethylbicyclo[2.2.1]heptan-2-one

Crystal data

$C_{19}H_{28}N_2O_3$ F_{000} = 720

M_r = 332.43	D_x = 1.269 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 5524 reflections
a = 6.7578 (16) Å	θ = 2.6–28.3º
b = 12.107 (3) Å	μ = 0.09 mm^{-1}
c = 21.269 (5) Å	T = 223 (2) K
V = 1740.2 (7) Å^3	Needle, colourless
Z = 4	0.50 × 0.16 × 0.12 mm

Data collection

Bruker APEX area-detector diffractometer	2418 independent reflections
Radiation source: fine-focus sealed tube	2280 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 223(2) K	θ_{max} = 28.5º
φ and ω scan	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	h = −8→9
T_{min} = 0.958, T_{max} = 0.990	k = −16→13
10699 measured reflections	l = −27→27

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.3373P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.115	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
S = 1.11	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
2418 reflections	Extinction correction: none
225 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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}
O1	0.0794 (2)	−0.00170 (12)	0.15120 (6)	0.0362 (4)
O2	−0.3852 (3)	0.30420 (16)	0.17297 (8)	0.0575 (6)
O3	0.2716 (3)	0.22757 (12)	−0.02375 (7)	0.0389 (4)
N1	−0.1005 (3)	0.15462 (15)	0.14606 (7)	0.0303 (4)
N2	0.0777 (3)	0.09851 (14)	0.06177 (7)	0.0265 (3)
C1	−0.1793 (3)	0.15398 (16)	0.20795 (8)	0.0259 (4)
C2	−0.3036 (3)	0.05390 (18)	0.22789 (9)	0.0326 (4)
H2A	−0.4341	0.0552	0.2078	0.039*
H2B	−0.2369	−0.0154	0.2171	0.039*
C3	−0.3212 (4)	0.0676 (2)	0.29920 (9)	0.0411 (5)
H3A	−0.4602	0.0699	0.3124	0.049*
H3B	−0.2542	0.0073	0.3214	0.049*
C4	−0.2196 (4)	0.1770 (2)	0.31125 (9)	0.0379 (5)
H4A	−0.1817	0.1891	0.3557	0.045*
C5	−0.3502 (4)	0.2668 (2)	0.28422 (11)	0.0490 (7)
H5A	−0.4892	0.2558	0.2958	0.059*
H5B	−0.3074	0.3402	0.2979	0.059*
C6	−0.3187 (4)	0.25094 (19)	0.21497 (10)	0.0380 (5)
C7	−0.0432 (3)	0.17393 (16)	0.26539 (9)	0.0296 (4)
C8	0.1014 (3)	0.08364 (18)	0.28097 (10)	0.0349 (5)
H8A	0.1785	0.1049	0.3175	0.052*
H8B	0.1891	0.0718	0.2455	0.052*
H8C	0.0298	0.0160	0.2900	0.052*
C9	0.0710 (4)	0.2801 (2)	0.26036 (14)	0.0504 (6)
H9A	0.1540	0.2889	0.2972	0.076*
H9B	−0.0206	0.3416	0.2576	0.076*
H9C	0.1532	0.2784	0.2230	0.076*
C10	0.2530 (3)	0.05642 (15)	0.03347 (7)	0.0227 (4)
C11	0.3229 (3)	0.13360 (16)	−0.01740 (9)	0.0292 (4)
C12	0.4655 (4)	0.07015 (19)	−0.05723 (10)	0.0390 (5)
H12A	0.5976	0.1036	−0.0565	0.047*
H12B	0.4197	0.0649	−0.1008	0.047*
C13	0.4647 (3)	−0.04173 (19)	−0.02532 (10)	0.0351 (5)
H13A	0.5125	−0.1033	−0.0519	0.042*
C14	0.5779 (4)	−0.0266 (2)	0.03588 (11)	0.0457 (6)
H14A	0.7046	0.0107	0.0287	0.055*
H14B	0.6024	−0.0978	0.0564	0.055*
C15	0.4387 (3)	0.0450 (2)	0.07487 (9)	0.0341 (5)
H15A	0.4978	0.1174	0.0834	0.041*
H15B	0.4067	0.0092	0.1149	0.041*

C16	0.2486 (3)	−0.05347 (16)	−0.00295 (8)	0.0279 (4)
C17	0.0970 (4)	−0.0538 (2)	−0.05517 (10)	0.0407 (5)
H17A	−0.0344	−0.0616	−0.0373	0.061*
H17B	0.1231	−0.1150	−0.0834	0.061*
H17C	0.1049	0.0151	−0.0783	0.061*
C18	0.2141 (4)	−0.15394 (18)	0.03774 (11)	0.0422 (5)
H18A	0.0760	−0.1569	0.0501	0.063*
H18B	0.2966	−0.1494	0.0750	0.063*
H18C	0.2474	−0.2200	0.0142	0.063*
C19	0.0236 (3)	0.07774 (15)	0.12232 (8)	0.0252 (4)
H1	−0.146 (4)	0.202 (2)	0.1226 (11)	0.027 (6)*
H2	0.038 (3)	0.1590 (19)	0.0484 (10)	0.023 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0492 (9)	0.0318 (7)	0.0276 (6)	0.0136 (7)	0.0129 (7)	0.0098 (6)
O2	0.0700 (13)	0.0620 (11)	0.0403 (8)	0.0400 (10)	−0.0001 (9)	0.0061 (8)
O3	0.0514 (10)	0.0307 (7)	0.0345 (7)	−0.0025 (7)	0.0111 (7)	0.0075 (6)
N1	0.0371 (9)	0.0327 (8)	0.0211 (7)	0.0111 (8)	0.0058 (7)	0.0083 (6)
N2	0.0298 (8)	0.0286 (8)	0.0210 (7)	0.0054 (7)	0.0048 (6)	0.0060 (6)
C1	0.0281 (9)	0.0299 (9)	0.0198 (8)	0.0049 (8)	0.0015 (7)	0.0000 (7)
C2	0.0309 (10)	0.0426 (11)	0.0244 (8)	−0.0071 (9)	0.0005 (8)	0.0015 (8)
C3	0.0352 (11)	0.0636 (15)	0.0244 (9)	−0.0032 (11)	0.0058 (8)	0.0047 (10)
C4	0.0386 (12)	0.0514 (13)	0.0236 (9)	0.0113 (11)	0.0003 (8)	−0.0084 (8)
C5	0.0487 (14)	0.0646 (16)	0.0338 (11)	0.0264 (13)	0.0004 (10)	−0.0122 (11)
C6	0.0371 (11)	0.0437 (12)	0.0331 (10)	0.0151 (10)	0.0017 (9)	−0.0020 (9)
C7	0.0290 (9)	0.0309 (9)	0.0289 (8)	0.0028 (8)	−0.0023 (8)	−0.0048 (7)
C8	0.0326 (10)	0.0398 (11)	0.0323 (10)	0.0059 (9)	−0.0071 (8)	−0.0014 (8)
C9	0.0512 (15)	0.0341 (11)	0.0660 (15)	−0.0066 (11)	−0.0081 (14)	−0.0043 (11)
C10	0.0251 (9)	0.0254 (8)	0.0176 (7)	−0.0009 (7)	0.0022 (6)	0.0000 (7)
C11	0.0315 (10)	0.0334 (10)	0.0225 (8)	−0.0056 (8)	0.0039 (8)	0.0006 (7)
C12	0.0418 (12)	0.0433 (12)	0.0319 (10)	−0.0048 (10)	0.0153 (9)	−0.0026 (9)
C13	0.0353 (11)	0.0379 (11)	0.0320 (9)	0.0035 (9)	0.0088 (9)	−0.0055 (9)
C14	0.0308 (12)	0.0624 (15)	0.0440 (12)	0.0094 (11)	−0.0011 (10)	−0.0046 (11)
C15	0.0281 (10)	0.0473 (12)	0.0268 (9)	−0.0006 (9)	−0.0044 (8)	−0.0037 (9)
C16	0.0332 (10)	0.0279 (9)	0.0226 (8)	−0.0012 (8)	0.0052 (8)	−0.0039 (7)
C17	0.0430 (12)	0.0502 (13)	0.0288 (10)	−0.0092 (11)	−0.0021 (9)	−0.0085 (9)
C18	0.0580 (15)	0.0269 (10)	0.0417 (11)	0.0003 (10)	0.0093 (11)	−0.0006 (9)
C19	0.0289 (9)	0.0272 (9)	0.0196 (7)	−0.0001 (8)	0.0036 (7)	0.0006 (6)

Geometric parameters (Å, °)

O1—C19	1.202 (2)	C8—H8C	0.97
O2—C6	1.190 (3)	C9—H9A	0.97
O3—C11	1.197 (3)	C9—H9B	0.97
N1—C19	1.351 (2)	C9—H9C	0.97
N1—C1	1.420 (2)	C10—C11	1.506 (3)
N1—H1	0.82 (3)	C10—C15	1.539 (3)

N2—C19	1.362 (2)	C10—C16	1.540 (2)
N2—C10	1.423 (2)	C11—C12	1.495 (3)
N2—H2	0.83 (2)	C12—C13	1.515 (3)
C1—C6	1.513 (3)	C12—H12A	0.98
C1—C2	1.534 (3)	C12—H12B	0.98
C1—C7	1.548 (3)	C13—C14	1.521 (3)
C2—C3	1.530 (3)	C13—C16	1.543 (3)
C2—H2A	0.98	C13—H13A	0.99
C2—H2B	0.98	C14—C15	1.525 (3)
C3—C4	1.514 (3)	C14—H14A	0.98
C3—H3A	0.98	C14—H14B	0.98
C3—H3B	0.98	C15—H15A	0.98
C4—C5	1.513 (3)	C15—H15B	0.98
C4—C7	1.541 (3)	C16—C17	1.511 (3)
C4—H4A	0.99	C16—C18	1.511 (3)
C5—C6	1.500 (3)	C17—H17A	0.97
C5—H5A	0.98	C17—H17B	0.97
C5—H5B	0.98	C17—H17C	0.97
C7—C8	1.503 (3)	C18—H18A	0.97
C7—C9	1.504 (3)	C18—H18B	0.97
C8—H8A	0.97	C18—H18C	0.97
C8—H8B	0.97		
C19—N1—C1	125.14 (16)	H9B—C9—H9C	109.5
C19—N1—H1	119.3 (16)	N2—C10—C11	110.05 (16)
C1—N1—H1	115.1 (16)	N2—C10—C15	117.95 (14)
C19—N2—C10	123.87 (16)	C11—C10—C15	102.19 (16)
C19—N2—H2	113.6 (15)	N2—C10—C16	120.39 (16)
C10—N2—H2	116.0 (16)	C11—C10—C16	100.42 (14)
N1—C1—C6	108.71 (16)	C15—C10—C16	103.08 (15)
N1—C1—C2	117.77 (16)	O3—C11—C12	127.66 (19)
C6—C1—C2	104.15 (17)	O3—C11—C10	125.45 (19)
N1—C1—C7	120.53 (18)	C12—C11—C10	106.89 (17)
C6—C1—C7	99.85 (15)	C11—C12—C13	101.71 (16)
C2—C1—C7	103.32 (15)	C11—C12—H12A	111.4
C3—C2—C1	103.36 (17)	C13—C12—H12A	111.4
C3—C2—H2A	111.1	C11—C12—H12B	111.4
C1—C2—H2A	111.1	C13—C12—H12B	111.4
C3—C2—H2B	111.1	H12A—C12—H12B	109.3
C1—C2—H2B	111.1	C12—C13—C14	105.91 (19)
H2A—C2—H2B	109.1	C12—C13—C16	102.95 (18)
C4—C3—C2	103.12 (18)	C14—C13—C16	102.90 (17)
C4—C3—H3A	111.1	C12—C13—H13A	114.6
C2—C3—H3A	111.1	C14—C13—H13A	114.6
C4—C3—H3B	111.1	C16—C13—H13A	114.6
C2—C3—H3B	111.1	C13—C14—C15	102.93 (18)
H3A—C3—H3B	109.1	C13—C14—H14A	111.2
C5—C4—C3	107.4 (2)	C15—C14—H14A	111.2
C5—C4—C7	103.20 (18)	C13—C14—H14B	111.2
C3—C4—C7	102.86 (16)	C15—C14—H14B	111.2

C5—C4—H4A	114.1	H14A—C14—H14B	109.1
C3—C4—H4A	114.1	C14—C15—C10	104.04 (16)
C7—C4—H4A	114.1	C14—C15—H15A	110.9
C6—C5—C4	101.45 (18)	C10—C15—H15A	110.9
C6—C5—H5A	111.5	C14—C15—H15B	110.9
C4—C5—H5A	111.5	C10—C15—H15B	110.9
C6—C5—H5B	111.5	H15A—C15—H15B	109.0
C4—C5—H5B	111.5	C17—C16—C18	108.32 (18)
H5A—C5—H5B	109.3	C17—C16—C10	112.65 (17)
O2—C6—C5	127.9 (2)	C18—C16—C10	114.24 (15)
O2—C6—C1	125.57 (19)	C17—C16—C13	114.54 (16)
C5—C6—C1	106.52 (18)	C18—C16—C13	113.39 (19)
C8—C7—C9	107.70 (19)	C10—C16—C13	93.27 (15)
C8—C7—C4	112.41 (17)	C16—C17—H17A	109.5
C9—C7—C4	114.92 (19)	C16—C17—H17B	109.5
C8—C7—C1	116.53 (16)	H17A—C17—H17B	109.5
C9—C7—C1	112.47 (18)	C16—C17—H17C	109.5
C4—C7—C1	92.50 (16)	H17A—C17—H17C	109.5
C7—C8—H8A	109.5	H17B—C17—H17C	109.5
C7—C8—H8B	109.5	C16—C18—H18A	109.5
H8A—C8—H8B	109.5	C16—C18—H18B	109.5
C7—C8—H8C	109.5	H18A—C18—H18B	109.5
H8A—C8—H8C	109.5	C16—C18—H18C	109.5
H8B—C8—H8C	109.5	H18A—C18—H18C	109.5
C7—C9—H9A	109.5	H18B—C18—H18C	109.5
C7—C9—H9B	109.5	O1—C19—N1	123.73 (17)
H9A—C9—H9B	109.5	O1—C19—N2	123.13 (18)
C7—C9—H9C	109.5	N1—C19—N2	113.13 (17)
H9A—C9—H9C	109.5		
C19—N1—C1—C6	−177.4 (2)	C19—N2—C10—C16	92.3 (2)
C19—N1—C1—C2	−59.3 (3)	N2—C10—C11—O3	16.8 (3)
C19—N1—C1—C7	68.4 (3)	C15—C10—C11—O3	−109.3 (2)
N1—C1—C2—C3	167.25 (19)	C16—C10—C11—O3	144.7 (2)
C6—C1—C2—C3	−72.3 (2)	N2—C10—C11—C12	−163.16 (16)
C7—C1—C2—C3	31.6 (2)	C15—C10—C11—C12	70.73 (19)
C1—C2—C3—C4	4.1 (2)	C16—C10—C11—C12	−35.2 (2)
C2—C3—C4—C5	69.8 (2)	O3—C11—C12—C13	−179.5 (2)
C2—C3—C4—C7	−38.7 (2)	C10—C11—C12—C13	0.4 (2)
C3—C4—C5—C6	−73.0 (2)	C11—C12—C13—C14	−72.8 (2)
C7—C4—C5—C6	35.2 (3)	C11—C12—C13—C16	34.9 (2)
C4—C5—C6—O2	−177.4 (3)	C12—C13—C14—C15	69.8 (2)
C4—C5—C6—C1	1.2 (3)	C16—C13—C14—C15	−37.9 (2)
N1—C1—C6—O2	15.0 (3)	C13—C14—C15—C10	4.0 (2)
C2—C1—C6—O2	−111.3 (3)	N2—C10—C15—C14	166.56 (18)
C7—C1—C6—O2	142.1 (3)	C11—C10—C15—C14	−72.7 (2)
N1—C1—C6—C5	−163.6 (2)	C16—C10—C15—C14	31.2 (2)
C2—C1—C6—C5	70.0 (2)	N2—C10—C16—C17	55.8 (2)
C7—C1—C6—C5	−36.5 (2)	C11—C10—C16—C17	−65.0 (2)
C5—C4—C7—C8	−176.07 (19)	C15—C10—C16—C17	−170.25 (17)

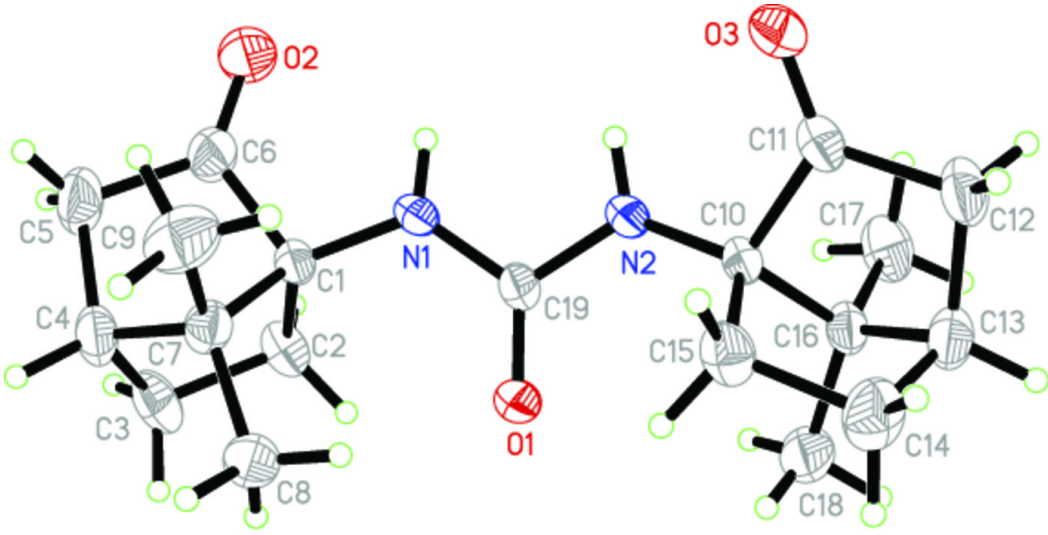
C3—C4—C7—C8	−64.4 (2)	N2—C10—C16—C18	−68.4 (2)
C5—C4—C7—C9	60.3 (2)	C11—C10—C16—C18	170.8 (2)
C3—C4—C7—C9	171.92 (19)	C15—C10—C16—C18	65.6 (2)
C5—C4—C7—C1	−55.97 (19)	N2—C10—C16—C13	174.14 (16)
C3—C4—C7—C1	55.68 (18)	C11—C10—C16—C13	53.35 (16)
N1—C1—C7—C8	−70.1 (2)	C15—C10—C16—C13	−51.91 (16)
C6—C1—C7—C8	171.19 (18)	C12—C13—C16—C17	61.9 (2)
C2—C1—C7—C8	64.0 (2)	C14—C13—C16—C17	171.84 (18)
N1—C1—C7—C9	54.9 (3)	C12—C13—C16—C18	−173.08 (17)
C6—C1—C7—C9	−63.8 (2)	C14—C13—C16—C18	−63.1 (2)
C2—C1—C7—C9	−171.00 (18)	C12—C13—C16—C10	−54.87 (17)
N1—C1—C7—C4	173.26 (19)	C14—C13—C16—C10	55.09 (18)
C6—C1—C7—C4	54.55 (17)	C1—N1—C19—O1	1.2 (3)
C2—C1—C7—C4	−52.67 (17)	C1—N1—C19—N2	−179.62 (19)
C19—N2—C10—C11	−151.76 (18)	C10—N2—C19—O1	−23.8 (3)
C19—N2—C10—C15	−35.1 (3)	C10—N2—C19—N1	156.98 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.82 (3)	2.34 (2)	3.090 (2)	153 (2)
N2—H2···O3^{i}	0.83 (2)	2.32 (2)	3.061 (2)	148 (2)

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

Fig. 1


O2
O3
C6
C11
C5
C9
C10
C17
C12
N1
N2
C1
C19
C4
C7
C2
C16
C13
C15
C3
O1
C14
C8
C18