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Tetrahydropyrimidin-2-ylidene-ammonium camphor-10-sulfonate

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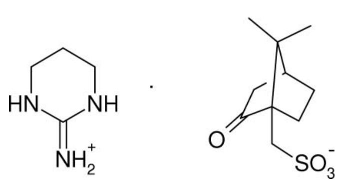
Key indicators: single-crystal X-ray study; *T* = 293 K; mean σ(C–C) = 0.004 Å; *R* factor = 0.036; *wR* factor = 0.097; data-to-parameter ratio = 14.0.

In the title molecular salt (alternative name: tetrahydropyrimidin-2-ylideneammonium 2-oxobornane-10-sulfonate), $C_4H_{10}N_3^+\cdot C_{10}H_{15}O_4S^-$, the cation and anion interact by way of N—H···O hydrogen bonds, leading to chains propagating in the polar [010] direction containing $R_2^2(8)$ supramolecular loops.

Related literature

For background, see: Bernstein *et al.* (1995). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_4H_{10}N_3^+\cdot C_{10}H_{15}O_4S^-$
M_r = 331.43
Monoclinic, $P2_1$
a = 7.4207 (4) Å
b = 7.3115 (4) Å
c = 16.421 (1) Å
β = 102.899 (1)°
V = 868.46 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 293 (2) K
0.32 × 0.26 × 0.17 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.860, T_{max} = 0.967
5301 measured reflections
3003 independent reflections
2630 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.09
3003 reflections
214 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Absolute structure: Flack (1983), with 1341 Friedel pairs
Flack parameter: 0.17 (9)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.98 (5)	1.90 (5)	2.873 (5)	173 (4)
N1—H2···O2^i	0.77 (5)	2.12 (5)	2.888 (5)	178 (6)
N2—H3···O3	0.78 (4)	2.13 (4)	2.900 (4)	169 (3)
N3—H4···O3^i	0.81 (4)	2.11 (4)	2.908 (4)	165 (3)

Symmetry code: (i) $x, y+1, z$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

The author thanks M. R. St J. Foreman and M. John Plater for supplying the sample.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RN2027).

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supplementary materials

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Tetrahydropyrimidin-2-ylideneammonium camphor-10-sulfonate

W. T. A. Harrison

Comment

The title compound, (I), is a molecular salt (Fig. 1). The C—N bond lengths in the cation [C11—N2 = 1.319 (5) Å, C11—N1 = 1.330 (3) Å, C11—N3 = 1.332 (5) Å] indicate delocalization of the electrons in the nominal C—N single bonds and C═N^+ double bond (see scheme) in a similar fashion to that seen in the $CN_3H_6^+$ guanidinium cation. The bond angle sum at C11 is exactly 360°. The conformation of the six-membered ring of the cation is well described as an envelope, with C13 displaced by 0.632 (4) Å from C11/C12/C14/N2/N3 (r.m.s. deviation for these atoms = 0.002 Å). The configurations of the chiral carbon atoms in the camphor sulfonate anion are: C2 *R* and C5 S. Otherwise, (I) displays normal geometrical parameters (Allen *et al.*, 1995).

In the crystal of (I), the components interact by way of N—H···O hydrogen bonds (Table 1) leading to infinite chains propagating in [010], with every cation and anion linked by two N—H···O bonds (Fig. 2), resulting in graph-theory (Bernstein *et al.*, 1995) $R^2_2(8)$ loops.

Experimental

Aqueous solutions of tetrahydro-pyrimidin-2-ylidene-amine and camphor-10-sulfonic acid were mixed in stoichiometric quantities leading to a clear solution. Colourless faceted chunks of (I) grew over a few days as the water slowly evaporated.

Refinement

A *PLATON*/checkcif analysis of (I) indicated pseudosymmetry at the 90% level. However, a centre of symmetry cannot be compatible with the chiral anion.

The N-bound H atoms were located in a difference map and their positions were freely refined with $U_{iso}(H) = 1.2U_{eq}(N)$.

The C-bound H atoms were placed geometrically (C—H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H)$ = $1.2U_{eq}$(carrier) or $1.5U_{eq}$(methyl C). The methyl groups were allowed to rotate, but not to tip, to best fit the electron density.

Figures

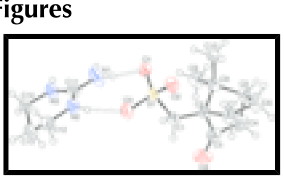

Fig. 1. The molecular structure of (I) (40% displacement ellipsoids, arbitrary spheres for the H atoms, hydrogen bonds indicated by double dashed lines).

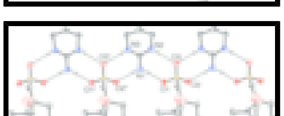

Fig. 2. Detail of (I) showing an [010] hydrogen-bonded chain containing $R^2_2(8)$ loops. Atoms marked with a * suffix are at the symmetry position (x, $y - 1$, z).

Tetrahydropyrimidin-2-ylideneammonium 2-oxobornane-10-sulfonate

Crystal data

$C_4H_{10}N_3^+\cdot C_{10}H_{15}O_4S^-$	F_{000} = 356
M_r = 331.43	D_x = 1.267 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 3004 reflections
a = 7.4207 (4) Å	θ = 2.8–25.0º
b = 7.3115 (4) Å	μ = 0.21 mm^{-1}
c = 16.421 (1) Å	T = 293 (2) K
β = 102.899 (1)º	Faceted chunk, colourless
V = 868.46 (9) Å^3	0.32 × 0.26 × 0.17 mm
Z = 2	

Data collection

Bruker SMART 1000 CCD diffractometer	3003 independent reflections
Radiation source: fine-focus sealed tube	2630 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 293(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.3º
Absorption correction: multi-scan (SADABS; Bruker, 1999)	$h = -8 \rightarrow 8$
T_{min} = 0.860, T_{max} = 0.967	$k = -8 \rightarrow 8$
5301 measured reflections	$l = -16 \rightarrow 19$

Refinement

Refinement on F^2	Hydrogen site location: difmap and geom
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2 + 0.0964P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.097	$(\Delta/\sigma)_{max}$ < 0.001
S = 1.09	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
3003 reflections	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
214 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with 1341 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.17 (9)
Secondary atom site location: difference Fourier map	

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	0.5794 (3)	0.3098 (6)	0.20808 (13)	0.0443 (5)
H1A	0.4756	0.2258	0.1970	0.053*
H1B	0.5307	0.4301	0.1904	0.053*
C2	0.7072 (3)	0.2553 (3)	0.15159 (16)	0.0429 (6)
C3	0.6026 (4)	0.2795 (4)	0.06007 (18)	0.0592 (9)
C4	0.7455 (5)	0.2783 (7)	0.00768 (19)	0.0804 (13)
H41	0.7483	0.3941	−0.0209	0.096*
H42	0.7233	0.1802	−0.0331	0.096*
C5	0.9240 (5)	0.2470 (4)	0.07361 (19)	0.0636 (8)
H51	1.0374	0.2795	0.0557	0.062 (8)*
C6	0.9151 (5)	0.0456 (5)	0.1020 (2)	0.0736 (10)
H61	0.8800	−0.0355	0.0543	0.088*
H62	1.0330	0.0063	0.1359	0.088*
C7	0.7654 (5)	0.0506 (4)	0.1535 (2)	0.0567 (7)
H71	0.8148	0.0100	0.2104	0.068*
H72	0.6612	−0.0263	0.1285	0.068*
C8	0.8908 (4)	0.3566 (4)	0.14960 (17)	0.0496 (8)
C9	0.8664 (5)	0.5612 (4)	0.1348 (3)	0.0729 (10)
H91	0.9728	0.6098	0.1181	0.109*
H92	0.8529	0.6199	0.1854	0.109*
H93	0.7581	0.5833	0.0916	0.109*
C10	1.0493 (3)	0.3306 (7)	0.22651 (17)	0.0639 (7)
H101	1.1640	0.3649	0.2130	0.096*
H102	1.0550	0.2046	0.2434	0.096*
H103	1.0280	0.4059	0.2713	0.096*
S1	0.66387 (7)	0.31798 (11)	0.31831 (3)	0.03870 (15)
O1	0.7694 (3)	0.4848 (3)	0.33660 (15)	0.0523 (6)
O2	0.7726 (3)	0.1533 (3)	0.34393 (14)	0.0505 (6)
O3	0.4966 (2)	0.3208 (4)	0.35201 (10)	0.0505 (4)
O4	0.4382 (3)	0.2951 (6)	0.03598 (13)	0.0893 (8)
C11	0.4246 (3)	0.8182 (6)	0.38435 (16)	0.0498 (5)
C12	0.1889 (5)	0.6527 (5)	0.4365 (2)	0.0538 (9)
H12A	0.2267	0.6427	0.4969	0.065*

H12B	0.1168	0.5452	0.4156	0.065*
C13	0.0735 (3)	0.8206 (6)	0.41374 (18)	0.0586 (6)
H13A	−0.0258	0.8211	0.4435	0.070*
H13B	0.0185	0.8195	0.3543	0.070*
C14	0.1890 (4)	0.9908 (4)	0.4354 (2)	0.0505 (8)
H14A	0.1171	1.0976	0.4131	0.061*
H14B	0.2262	1.0039	0.4956	0.061*
N1	0.5722 (3)	0.8172 (6)	0.3510 (2)	0.0822 (9)
H1	0.629 (6)	0.699 (7)	0.345 (3)	0.099*
H2	0.627 (7)	0.906 (7)	0.350 (3)	0.099*
N2	0.3515 (4)	0.6619 (4)	0.4010 (2)	0.0517 (8)
H3	0.378 (4)	0.570 (5)	0.383 (2)	0.062*
N3	0.3521 (4)	0.9775 (4)	0.4001 (2)	0.0527 (8)
H4	0.408 (5)	1.070 (5)	0.394 (2)	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0366 (10)	0.0506 (13)	0.0443 (11)	0.0004 (17)	0.0063 (9)	−0.0012 (17)
C2	0.0437 (13)	0.0438 (14)	0.0405 (13)	0.0009 (10)	0.0080 (10)	−0.0017 (10)
C3	0.0616 (17)	0.063 (3)	0.0484 (15)	−0.0021 (15)	0.0024 (12)	−0.0016 (14)
C4	0.093 (2)	0.106 (4)	0.0437 (15)	−0.007 (2)	0.0184 (15)	−0.0050 (19)
C5	0.0656 (18)	0.077 (2)	0.0562 (17)	−0.0009 (15)	0.0305 (15)	0.0032 (15)
C6	0.095 (3)	0.065 (2)	0.073 (2)	0.012 (2)	0.045 (2)	−0.0148 (18)
C7	0.0696 (19)	0.0443 (16)	0.0607 (19)	−0.0002 (15)	0.0238 (15)	−0.0062 (14)
C8	0.0461 (13)	0.052 (2)	0.0529 (14)	0.0002 (12)	0.0152 (11)	0.0028 (12)
C9	0.080 (2)	0.0486 (19)	0.093 (3)	−0.0117 (18)	0.024 (2)	0.0163 (19)
C10	0.0382 (12)	0.089 (2)	0.0655 (16)	0.007 (2)	0.0128 (11)	0.001 (2)
S1	0.0374 (3)	0.0358 (3)	0.0450 (3)	0.0025 (4)	0.0135 (2)	−0.0019 (4)
O1	0.0490 (14)	0.0429 (12)	0.0678 (16)	−0.0062 (11)	0.0189 (11)	−0.0168 (11)
O2	0.0507 (14)	0.0494 (13)	0.0523 (13)	0.0151 (11)	0.0134 (11)	0.0076 (10)
O3	0.0512 (8)	0.0438 (8)	0.0642 (10)	0.0014 (14)	0.0293 (7)	−0.0024 (13)
O4	0.0631 (12)	0.134 (2)	0.0595 (12)	−0.004 (2)	−0.0109 (10)	−0.0016 (19)
C11	0.0422 (11)	0.0410 (11)	0.0669 (14)	−0.003 (2)	0.0134 (10)	−0.004 (2)
C12	0.054 (2)	0.053 (2)	0.057 (2)	−0.0091 (17)	0.0194 (17)	−0.0034 (17)
C13	0.0465 (12)	0.0590 (15)	0.0738 (16)	0.000 (2)	0.0210 (11)	−0.002 (2)
C14	0.047 (2)	0.045 (2)	0.060 (2)	0.0069 (15)	0.0136 (16)	−0.0022 (16)
N1	0.0653 (14)	0.0459 (13)	0.153 (3)	−0.001 (2)	0.0619 (16)	−0.001 (3)
N2	0.0480 (18)	0.0379 (17)	0.072 (2)	0.0020 (14)	0.0194 (15)	−0.0073 (14)
N3	0.051 (2)	0.0336 (16)	0.078 (2)	0.0030 (14)	0.0253 (16)	−0.0037 (14)

Geometric parameters (Å, °)

C1—C2	1.520 (3)	C9—H93	0.9600
C1—S1	1.779 (2)	C10—H101	0.9600
C1—H1A	0.9700	C10—H102	0.9600
C1—H1B	0.9700	C10—H103	0.9600
C2—C3	1.540 (4)	S1—O1	1.444 (2)
C2—C7	1.556 (4)	S1—O2	1.458 (2)

C2—C8	1.558 (3)	S1—O3	1.4678 (14)
C3—O4	1.201 (3)	C11—N2	1.319 (5)
C3—C4	1.507 (4)	C11—N1	1.330 (3)
C4—C5	1.529 (5)	C11—N3	1.332 (5)
C4—H41	0.9700	C12—N2	1.454 (4)
C4—H42	0.9700	C12—C13	1.496 (5)
C5—C8	1.548 (4)	C12—H12A	0.9700
C5—C6	1.550 (5)	C12—H12B	0.9700
C5—H51	0.9800	C13—C14	1.508 (5)
C6—C7	1.540 (4)	C13—H13A	0.9700
C6—H61	0.9700	C13—H13B	0.9700
C6—H62	0.9700	C14—N3	1.458 (4)
C7—H71	0.9700	C14—H14A	0.9700
C7—H72	0.9700	C14—H14B	0.9700
C8—C9	1.520 (4)	N1—H1	0.98 (5)
C8—C10	1.533 (4)	N1—H2	0.77 (5)
C9—H91	0.9600	N2—H3	0.78 (4)
C9—H92	0.9600	N3—H4	0.81 (4)

C2—C1—S1	120.23 (15)	H91—C9—H92	109.5
C2—C1—H1A	107.3	C8—C9—H93	109.5
S1—C1—H1A	107.3	H91—C9—H93	109.5
C2—C1—H1B	107.3	H92—C9—H93	109.5
S1—C1—H1B	107.3	C8—C10—H101	109.5
H1A—C1—H1B	106.9	C8—C10—H102	109.5
C1—C2—C3	108.6 (2)	H101—C10—H102	109.5
C1—C2—C7	116.6 (2)	C8—C10—H103	109.5
C3—C2—C7	102.0 (2)	H101—C10—H103	109.5
C1—C2—C8	123.8 (2)	H102—C10—H103	109.5
C3—C2—C8	100.2 (2)	O1—S1—O2	113.46 (10)
C7—C2—C8	102.6 (2)	O1—S1—O3	112.00 (13)
O4—C3—C4	127.2 (3)	O2—S1—O3	111.28 (14)
O4—C3—C2	125.9 (3)	O1—S1—C1	106.94 (16)
C4—C3—C2	106.9 (2)	O2—S1—C1	108.20 (15)
C3—C4—C5	101.8 (2)	O3—S1—C1	104.38 (10)
C3—C4—H41	111.4	N2—C11—N1	119.7 (4)
C5—C4—H41	111.4	N2—C11—N3	120.9 (2)
C3—C4—H42	111.4	N1—C11—N3	119.4 (4)
C5—C4—H42	111.4	N2—C12—C13	110.0 (3)
H41—C4—H42	109.3	N2—C12—H12A	109.7
C4—C5—C8	103.0 (3)	C13—C12—H12A	109.7
C4—C5—C6	105.5 (3)	N2—C12—H12B	109.7
C8—C5—C6	103.0 (2)	C13—C12—H12B	109.7
C4—C5—H51	114.7	H12A—C12—H12B	108.2
C8—C5—H51	114.7	C12—C13—C14	110.76 (19)
C6—C5—H51	114.7	C12—C13—H13A	109.5
C7—C6—C5	103.1 (2)	C14—C13—H13A	109.5
C7—C6—H61	111.1	C12—C13—H13B	109.5
C5—C6—H61	111.1	C14—C13—H13B	109.5
C7—C6—H62	111.1	H13A—C13—H13B	108.1

C5—C6—H62	111.1	N3—C14—C13	109.3 (2)
H61—C6—H62	109.1	N3—C14—H14A	109.8
C6—C7—C2	104.0 (2)	C13—C14—H14A	109.8
C6—C7—H71	111.0	N3—C14—H14B	109.8
C2—C7—H71	111.0	C13—C14—H14B	109.8
C6—C7—H72	111.0	H14A—C14—H14B	108.3
C2—C7—H72	111.0	C11—N1—H1	118 (3)
H71—C7—H72	109.0	C11—N1—H2	120 (4)
C9—C8—C10	107.2 (3)	H1—N1—H2	120 (3)
C9—C8—C5	114.6 (3)	C11—N2—C12	122.7 (3)
C10—C8—C5	111.6 (3)	C11—N2—H3	121 (3)
C9—C8—C2	113.4 (2)	C12—N2—H3	114 (3)
C10—C8—C2	115.9 (2)	C11—N3—C14	122.9 (3)
C5—C8—C2	93.9 (2)	C11—N3—H4	118 (3)
C8—C9—H91	109.5	C14—N3—H4	119 (3)
C8—C9—H92	109.5		

S1—C1—C2—C3	−174.3 (2)	C4—C5—C8—C2	55.4 (3)
S1—C1—C2—C7	71.4 (3)	C6—C5—C8—C2	−54.1 (3)
S1—C1—C2—C8	−57.5 (4)	C1—C2—C8—C9	−53.8 (3)
C1—C2—C3—O4	−16.5 (5)	C3—C2—C8—C9	66.8 (3)
C7—C2—C3—O4	107.2 (4)	C7—C2—C8—C9	171.7 (3)
C8—C2—C3—O4	−147.5 (4)	C1—C2—C8—C10	70.9 (3)
C1—C2—C3—C4	163.9 (3)	C3—C2—C8—C10	−168.5 (3)
C7—C2—C3—C4	−72.5 (3)	C7—C2—C8—C10	−63.6 (3)
C8—C2—C3—C4	32.8 (3)	C1—C2—C8—C5	−172.8 (2)
O4—C3—C4—C5	−177.9 (4)	C3—C2—C8—C5	−52.1 (2)
C2—C3—C4—C5	1.8 (4)	C7—C2—C8—C5	52.7 (2)
C3—C4—C5—C8	−36.4 (3)	C2—C1—S1—O1	77.3 (3)
C3—C4—C5—C6	71.2 (3)	C2—C1—S1—O2	−45.2 (3)
C4—C5—C6—C7	−71.9 (3)	C2—C1—S1—O3	−163.9 (3)
C8—C5—C6—C7	35.8 (3)	N2—C12—C13—C14	−51.8 (3)
C5—C6—C7—C2	−1.5 (3)	C12—C13—C14—N3	51.3 (3)
C1—C2—C7—C6	−171.4 (2)	N1—C11—N2—C12	−179.2 (3)
C3—C2—C7—C6	70.6 (3)	N3—C11—N2—C12	0.4 (4)
C8—C2—C7—C6	−32.9 (3)	C13—C12—N2—C11	26.5 (4)
C4—C5—C8—C9	−62.6 (3)	N2—C11—N3—C14	−0.6 (4)
C6—C5—C8—C9	−172.1 (3)	N1—C11—N3—C14	179.0 (3)
C4—C5—C8—C10	175.3 (3)	C13—C14—N3—C11	−25.8 (4)
C6—C5—C8—C10	65.7 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.98 (5)	1.90 (5)	2.873 (5)	173 (4)
N1—H2···O2^{i}	0.77 (5)	2.12 (5)	2.888 (5)	178 (6)
N2—H3···O3	0.78 (4)	2.13 (4)	2.900 (4)	169 (3)
N3—H4···O3^{i}	0.81 (4)	2.11 (4)	2.908 (4)	165 (3)

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

Fig. 1

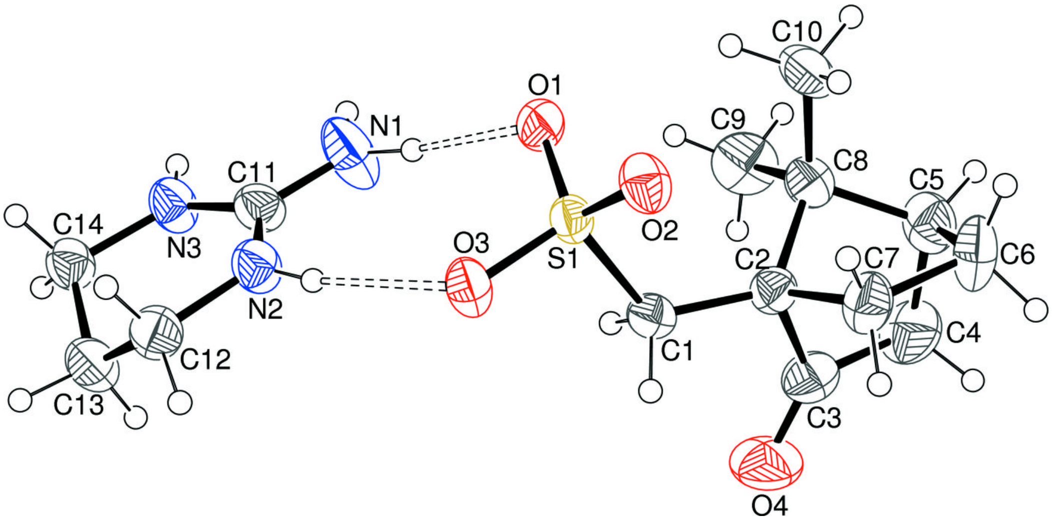

Fig. 2