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Bis(carboxymethyl)ammonium 4-toluenesulfonate

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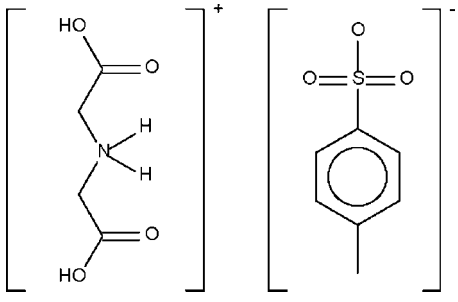
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.119; data-to-parameter ratio = 15.4.

The iminodiacetic acid component of the title salt, $C_4H_8NO_4^+\cdot C_7H_7SO_3^-$, is protonated at the N atom. The cation uses the ammonium group to form hydrogen bonds to the O atoms of two adjacent sulfonate groups. In addition, the carboxylic acid portions of the cation form hydrogen bonds to the sulfonate groups. The hydrogen-bonding interactions give rise to a layer structure.

Related literature

For the crystal structures of iminodiacetic acid hydrohalides, see: Oskarsson (1973, 1974*a*,*b*, 1976).



Experimental

Crystal data

$C_4H_8NO_4^+\cdot C_7H_7O_3S^-$
M_r = 305.30
Orthorhombic, *Pbca*
a = 9.9291 (2) Å
b = 10.3636 (2) Å
c = 25.8862 (5) Å
V = 2663.72 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 100 (2) K
0.27 × 0.27 × 0.27 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.929, T_{max} = 0.929
20842 measured reflections
3059 independent reflections
2560 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.119
S = 1.15
3059 reflections
198 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O2^{i}	0.88 (1)	2.02 (1)	2.885 (2)	167 (2)
N1—H1*N*2···O3^{ii}	0.88 (1)	2.06 (2)	2.792 (2)	140 (2)
O5—H5*O*···O1	0.84 (1)	1.79 (1)	2.607 (2)	164 (3)
O7—H7*O*···O2^{iii}	0.84 (1)	1.85 (1)	2.659 (2)	160 (3)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2187).

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supplementary materials

Acta Cryst. (2008). E**64**, o1798 [**doi:10.1107/S1600536808026214**]

Bis(carboxymethyl)ammonium 4-toluenesulfonate

K. M. Lo and S. W. Ng

Comment

(type here to add)

Experimental

Iminodiacetic acid (0.55 g, 4 mmol) and *p*-toluenesulfonic acid (0.65 g, 4 mmol) were heated in toluene (100 ml) for 1 h. Crystals were isolated from the cool solution after several days.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2 to 1.5U_{eq}(carrier C). The acid and ammonium H atoms were refined with distance restraints of O—H = 0.84 (1) and N—H = 0.88 (1) Å; their isotropic displacement parameters were freely refined.

Figures

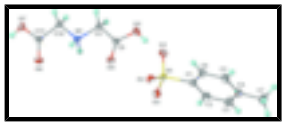

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $(C_4H_8NO_4)^+(C_7H_7O_3S)^-$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Bis(carboxymethyl)ammonium 4-toluenesulfonate

Crystal data

$C_4H_8NO_4^+ \cdot C_7H_7O_3S^-$	F_{000} = 1280
M_r = 305.30	D_x = 1.523 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 4293 reflections
a = 9.9291 (2) Å	θ = 2.9–27.2°
b = 10.3636 (2) Å	μ = 0.28 mm^{-1}
c = 25.8862 (5) Å	*T* = 100 (2) K
V = 2663.72 (9) Å^3	Triangular block, colorless
Z = 8	0.27 × 0.27 × 0.27 mm

Data collection

Bruker SMART APEX	3059 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 100(2) K

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.930, T_{max} = 0.930

20842 measured reflections

2560 reflections with $I > 2\sigma(I)$

R_{int} = 0.048

θ_{max} = 27.5º

θ_{min} = 1.6º

$h = -12 \rightarrow 7$

$k = -13 \rightarrow 13$

$l = -33 \rightarrow 33$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.038

$wR(F^2)$ = 0.119

S = 1.15

3059 reflections

198 parameters

4 restraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.8206P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.42 e Å^{-3}

$\Delta\rho_{min}$ = −0.50 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}
S1	0.49041 (5)	0.84948 (4)	0.358654 (17)	0.01248 (14)
O1	0.55419 (15)	0.74172 (13)	0.38508 (5)	0.0195 (3)
O2	0.56209 (14)	0.88382 (13)	0.31102 (5)	0.0163 (3)
O3	0.34727 (14)	0.83294 (13)	0.35029 (5)	0.0190 (3)
O4	0.40223 (14)	0.52637 (13)	0.30853 (5)	0.0171 (3)
O5	0.51261 (16)	0.49339 (13)	0.38301 (5)	0.0199 (3)
H5O	0.510 (3)	0.5747 (10)	0.3841 (10)	0.034 (7)*
O6	0.20627 (14)	0.17528 (13)	0.21695 (5)	0.0176 (3)
O7	0.29656 (14)	−0.02406 (13)	0.22217 (5)	0.0163 (3)
H7O	0.229 (2)	−0.047 (3)	0.2048 (10)	0.051 (9)*
N1	0.37466 (17)	0.27383 (15)	0.28845 (6)	0.0129 (3)
H1N1	0.402 (3)	0.316 (2)	0.2610 (7)	0.031 (7)*
H1N2	0.2899 (11)	0.296 (2)	0.2924 (8)	0.014 (5)*
C1	0.50864 (19)	0.98391 (18)	0.40013 (7)	0.0141 (4)
C2	0.3995 (2)	1.02980 (19)	0.42797 (8)	0.0187 (4)
H2	0.3146	0.9879	0.4256	0.022*
C3	0.4152 (2)	1.1376 (2)	0.45941 (8)	0.0212 (4)
H3	0.3404	1.1681	0.4788	0.025*
C4	0.5374 (2)	1.20164 (19)	0.46306 (7)	0.0183 (4)

C5	0.6471 (2)	1.15329 (19)	0.43556 (8)	0.0191 (4)
H5	0.7319	1.1952	0.4380	0.023*
C6	0.6335 (2)	1.04440 (19)	0.40462 (7)	0.0171 (4)
H6	0.7093	1.0112	0.3866	0.021*
C7	0.5517 (2)	1.3217 (2)	0.49545 (8)	0.0247 (5)
H7A	0.4636	1.3631	0.4993	0.037*
H7B	0.6142	1.3815	0.4785	0.037*
H7C	0.5868	1.2985	0.5296	0.037*
C8	0.45172 (19)	0.45546 (18)	0.34029 (7)	0.0137 (4)
C9	0.45326 (19)	0.31071 (18)	0.33494 (7)	0.0137 (4)
H9A	0.5472	0.2798	0.3315	0.016*
H9B	0.4132	0.2705	0.3660	0.016*
C10	0.3811 (2)	0.13288 (17)	0.27813 (7)	0.0142 (4)
H10A	0.3570	0.0845	0.3098	0.017*
H10B	0.4738	0.1085	0.2680	0.017*
C11	0.28461 (19)	0.09925 (18)	0.23534 (7)	0.0132 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0104 (2)	0.0118 (2)	0.0153 (2)	−0.00084 (17)	−0.00072 (16)	0.00057 (16)
O1	0.0240 (8)	0.0125 (7)	0.0221 (7)	−0.0013 (6)	−0.0072 (6)	0.0031 (5)
O2	0.0164 (7)	0.0158 (7)	0.0168 (7)	−0.0021 (6)	0.0028 (5)	−0.0016 (5)
O3	0.0109 (7)	0.0226 (8)	0.0233 (7)	−0.0016 (6)	−0.0006 (6)	−0.0024 (5)
O4	0.0169 (7)	0.0148 (7)	0.0197 (7)	0.0007 (6)	−0.0025 (5)	0.0007 (5)
O5	0.0293 (9)	0.0111 (7)	0.0192 (7)	−0.0007 (6)	−0.0092 (6)	−0.0014 (5)
O6	0.0156 (7)	0.0155 (7)	0.0217 (7)	−0.0016 (6)	−0.0030 (5)	0.0033 (5)
O7	0.0134 (7)	0.0143 (7)	0.0211 (7)	−0.0023 (6)	−0.0006 (6)	−0.0043 (5)
N1	0.0123 (8)	0.0109 (8)	0.0154 (8)	0.0011 (6)	−0.0002 (6)	0.0000 (6)
C1	0.0144 (9)	0.0131 (9)	0.0149 (8)	−0.0001 (7)	−0.0003 (7)	0.0010 (7)
C2	0.0148 (10)	0.0198 (10)	0.0215 (9)	−0.0019 (8)	0.0032 (8)	0.0004 (8)
C3	0.0190 (11)	0.0217 (10)	0.0228 (10)	0.0025 (8)	0.0066 (8)	−0.0020 (8)
C4	0.0237 (11)	0.0162 (10)	0.0150 (9)	0.0007 (8)	−0.0001 (8)	0.0004 (7)
C5	0.0145 (10)	0.0225 (10)	0.0202 (9)	−0.0045 (8)	0.0002 (8)	−0.0023 (8)
C6	0.0130 (9)	0.0199 (10)	0.0183 (9)	0.0004 (8)	0.0014 (7)	−0.0027 (7)
C7	0.0276 (12)	0.0219 (11)	0.0247 (10)	−0.0011 (9)	0.0010 (9)	−0.0067 (8)
C8	0.0102 (9)	0.0150 (9)	0.0161 (8)	−0.0005 (7)	0.0005 (7)	0.0004 (7)
C9	0.0125 (9)	0.0133 (9)	0.0152 (9)	0.0002 (7)	−0.0026 (7)	0.0000 (7)
C10	0.0132 (9)	0.0095 (8)	0.0200 (9)	0.0004 (7)	−0.0017 (7)	−0.0009 (7)
C11	0.0108 (9)	0.0132 (9)	0.0157 (8)	−0.0019 (7)	0.0028 (7)	0.0012 (7)

Geometric parameters (Å, °)

S1—O3	1.4478 (14)	C2—H2	0.9500
S1—O1	1.4547 (14)	C3—C4	1.386 (3)
S1—O2	1.4675 (13)	C3—H3	0.9500
S1—C1	1.768 (2)	C4—C5	1.394 (3)
O4—C8	1.207 (2)	C4—C7	1.507 (3)
O5—C8	1.320 (2)	C5—C6	1.390 (3)

O5—H5o	0.84 (1)	C5—H5	0.9500
O6—C11	1.205 (2)	C6—H6	0.9500
O7—C11	1.328 (2)	C7—H7A	0.9800
O7—H7o	0.84 (1)	C7—H7B	0.9800
N1—C9	1.484 (2)	C7—H7C	0.9800
N1—C10	1.486 (2)	C8—C9	1.507 (3)
N1—H1n1	0.88 (1)	C9—H9A	0.9900
N1—H1n2	0.88 (1)	C9—H9B	0.9900
C1—C2	1.385 (3)	C10—C11	1.505 (3)
C1—C6	1.394 (3)	C10—H10A	0.9900
C2—C3	1.391 (3)	C10—H10B	0.9900
O3—S1—O1	114.00 (9)	C4—C5—H5	119.7
O3—S1—O2	112.28 (8)	C5—C6—C1	119.93 (18)
O1—S1—O2	111.72 (8)	C5—C6—H6	120.0
O3—S1—C1	106.53 (9)	C1—C6—H6	120.0
O1—S1—C1	105.95 (9)	C4—C7—H7A	109.5
O2—S1—C1	105.63 (8)	C4—C7—H7B	109.5
C8—O5—H5O	108.2 (18)	H7A—C7—H7B	109.5
C11—O7—H7O	110 (2)	C4—C7—H7C	109.5
C9—N1—C10	112.10 (14)	H7A—C7—H7C	109.5
C9—N1—H1N1	111.7 (17)	H7B—C7—H7C	109.5
C10—N1—H1N1	109.4 (16)	O4—C8—O5	125.13 (18)
C9—N1—H1N2	110.2 (14)	O4—C8—C9	123.20 (17)
C10—N1—H1N2	108.3 (15)	O5—C8—C9	111.66 (15)
H1N1—N1—H1N2	105 (2)	N1—C9—C8	109.01 (15)
C2—C1—C6	119.85 (18)	N1—C9—H9A	109.9
C2—C1—S1	120.41 (15)	C8—C9—H9A	109.9
C6—C1—S1	119.73 (15)	N1—C9—H9B	109.9
C1—C2—C3	119.53 (19)	C8—C9—H9B	109.9
C1—C2—H2	120.2	H9A—C9—H9B	108.3
C3—C2—H2	120.2	N1—C10—C11	109.43 (15)
C4—C3—C2	121.46 (18)	N1—C10—H10A	109.8
C4—C3—H3	119.3	C11—C10—H10A	109.8
C2—C3—H3	119.3	N1—C10—H10B	109.8
C3—C4—C5	118.49 (18)	C11—C10—H10B	109.8
C3—C4—C7	121.06 (19)	H10A—C10—H10B	108.2
C5—C4—C7	120.4 (2)	O6—C11—O7	125.83 (17)
C6—C5—C4	120.68 (19)	O6—C11—C10	123.36 (17)
C6—C5—H5	119.7	O7—C11—C10	110.79 (16)
O3—S1—C1—C2	16.35 (19)	C3—C4—C5—C6	0.9 (3)
O1—S1—C1—C2	−105.40 (17)	C7—C4—C5—C6	−178.42 (18)
O2—S1—C1—C2	135.94 (16)	C4—C5—C6—C1	1.2 (3)
O3—S1—C1—C6	−163.36 (15)	C2—C1—C6—C5	−2.3 (3)
O1—S1—C1—C6	74.89 (17)	S1—C1—C6—C5	177.39 (15)
O2—S1—C1—C6	−43.77 (18)	C10—N1—C9—C8	175.26 (15)
C6—C1—C2—C3	1.3 (3)	O4—C8—C9—N1	−5.4 (3)
S1—C1—C2—C3	−178.42 (15)	O5—C8—C9—N1	175.76 (15)
C1—C2—C3—C4	0.9 (3)	C9—N1—C10—C11	172.17 (15)

C2—C3—C4—C5	−1.9 (3)	N1—C10—C11—O6	−6.8 (3)
C2—C3—C4—C7	177.37 (19)	N1—C10—C11—O7	174.56 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N1···O2^{i}	0.88 (1)	2.02 (1)	2.885 (2)	167 (2)
N1—H1N2···O3^{ii}	0.88 (1)	2.06 (2)	2.792 (2)	140 (2)
O5—H5O···O1	0.84 (1)	1.79 (1)	2.607 (2)	164 (3)
O7—H7O···O2^{iii}	0.84 (1)	1.85 (1)	2.659 (2)	160 (3)

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

Fig. 1