Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1*H*-1,2,4-Triazol-4-ium (3,4-dichlorophenyl)methanesulfonate

Ling Zhang, Guri L. V. Damu, Jing-Song Lv, Rong-Xia Geng* and Cheng-He Zhou*

Laboratory of Bioorganic & Medicinal Chemistry, School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, People's Republic of China
Correspondence e-mail: geng0712@swu.edu.cn, zhouch@swu.edu.cn

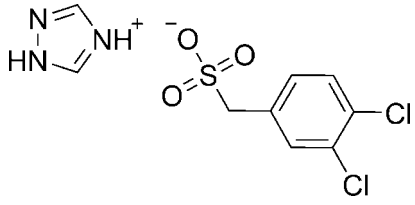
Received 4 December 2011; accepted 9 December 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.124; data-to-parameter ratio = 12.2.

In the title molecular salt, $C_2H_4N_3^+\cdot C_7H_5Cl_2O_3S^-$, C—C—S angle [112.25 (18)°] deviates slightly from that expected for ideal sp^3-hybridization geometry. In the crystal, the components are linked by N—H···O and bifurcated N—H···(O,O) hydrogen bonds into chains parallel to [110].

Related literature

For applications of triazole compounds, see: Sen *et al.* (2010); Subbaraman *et al.* (2009); Wang & Zhou (2011); Zhou *et al.* (2009); Bai *et al.* (2007); Chang *et al.*(2011).



Experimental

Crystal data

$C_2H_4N_3^+\cdot C_7H_5Cl_2O_3S^-$
M_r = 310.15
Triclinic, $P\overline{1}$
a = 5.2430 (6) Å
b = 8.2970 (8) Å
c = 14.5656 (15) Å
α = 94.330 (5)°
β = 98.387 (6)°
γ = 92.292 (5)°
V = 624.22 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.69 mm^{-1}
T = 296 K
0.30 × 0.28 × 0.25 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.820, T_{max} = 0.846
8971 measured reflections
2196 independent reflections
2000 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.124
S = 1.03
2196 reflections
180 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*M*···O1^{i}	0.85 (4)	1.96 (4)	2.709 (3)	146 (4)
N3—H4*M*···O2^{ii}	0.79 (4)	2.08 (4)	2.768 (3)	146 (3)
N3—H4*M*···O2^{iii}	0.79 (4)	2.54 (3)	3.089 (3)	128 (3)

Symmetry codes: (i) $x, y+1, z$; (ii) $x-1, y, z$; (iii) $-x, -y, -z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

This work was partially supported by the Natural Science Foundation of China (21172181), the Specialized Research Fund for the Doctoral Program of Higher Education of China (SRFDP 20110182110007) and the Fundamental Research Funds for the Central Universities (XDJK2011D007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5392).

References

Bai, X., Zhou, C.-H. & Mi, J.-L. (2007). *Chem. Res. Appl.* **19**, 721–729.
Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chang, J.-J., Wang, Y., Zhang, H.-Z., Zhou, C.-H., Geng, R.-X. & Ji, Q.-G. (2011). *Chem. J. Chin. Univ.* **32**, 1970–1985.
Sen, U., Bozkurt, A. & Ata, A. (2010). *J. Power Sources*, **195**, 7720–7726.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Subbaraman, R., Ghassemi, H. & Zawodzinski, T. Jr (2009). *Solid State Ionics*, **180**, 1143–1150.
Wang, Y. & Zhou, C.-H. (2011). *Sci. Sin. Chem.* **41**, 1429–1456.
Zhou, C.-H., Gan, L.-L., Zhang, Y.-Y., Zhang, F.-F., Wang, G.-Z., Jin, L. & Geng, R. X. (2009). *Sci. China Ser. B*, **52**, 415–458.

supplementary materials

Acta Cryst. (2012). E**68**, o131 [**doi:10.1107/S1600536811053062**]

1*H*-1,2,4-Triazol-4-ium (3,4-dichlorophenyl)methanesulfonate

L. Zhang, G. L. V. Damu, J.-S. Lv, R.-X. Geng and C.-H. Zhou

Comment

Triazole is a unique molecule which could exert diverse non-covalent interactions and endow triazole derivatives to exhibit various potential appplications in medicinal chemistry (Wang & Zhou, 2011), argrochemical and chemical fields (Bai *et al.*, 2007) and material science (Chang *et al.*, 2011). Work has shown that triazole derivatives could be used as proton transport facilitators for sulfonic acid based membranes for high temperature fuel cell operations (Sen *et al.*, 2010; Subbaraman *et al.*, 2009). Our interest is to investigate the intreractions of triazole compounds with diverse anions for the formation of supramolecular drugs (Zhou *et al.*, 2009). Herein we report the crystal structure of title compound.

In the molecular structure the title compound (Fig. 1) there is a slight deviation of the C2—C1—S1 angle (112.25°) in terms ideal sp^3 hybridization geometry. In the crystal, the components are linked by N—H···O hydrogen bonds and bifurcated N—H···(O,O) into one dimensional chains along [110].

Experimental

A crystal of title the compound suitable for X-ray analysis was grown from the solution of 1,2,4-triazole and (3,4-dichlorophenyl)methanesulfonic acid in methanol by slow evaporation at room temperature.

Refinement

The H atoms of the anion were placed in calculated positions with C—H = 0.93Å (aromatic) and 0.97Å (methylene) and refined in a riding-motion approximation with $U_{iso}(H) = 1.2U_{eq}(C)$. All H atoms in the cation were refined independently with isotropic displacement parameters.

Figures

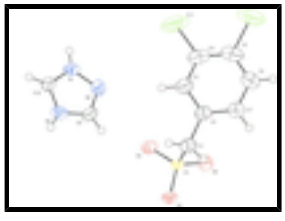


Fig. 1. The molecular structure of (I) showing displacement ellipsoids drawn at the 50% probability level.

1*H*-1,2,4-Triazol-4-ium (3,4-dichlorophenyl)methanesulfonate

Crystal data

$C_2H_4N_3^+ \cdot C_7H_5Cl_2O_3S^-$ $Z = 2$

M_r = 310.15	F(000) = 316
Triclinic, $P\overline{1}$	D_x = 1.650 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 5.2430 (6) Å	Cell parameters from 4951 reflections
b = 8.2970 (8) Å	θ = 2.8–27.5°
c = 14.5656 (15) Å	μ = 0.69 mm^{-1}
α = 94.330 (5)°	T = 296 K
β = 98.387 (6)°	Block, colorless
γ = 92.292 (5)°	0.30 × 0.28 × 0.25 mm
V = 624.22 (11) Å^3	

Data collection

Bruker SMART CCD diffractometer	2196 independent reflections
Radiation source: fine-focus sealed tube	2000 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.030
φ scans and ω scans with κ offsets	θ_{max} = 25.0°, θ_{min} = 2.5°
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −6→6
T_{min} = 0.820, T_{max} = 0.846	k = −9→9
8971 measured reflections	l = −17→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.124	$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 0.6305P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
2196 reflections	$\Delta\rho_{max}$ = 0.69 e Å^{-3}
180 parameters	$\Delta\rho_{min}$ = −0.60 e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.064 (7)

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 $F^2 > \sigma(F^2)$ 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}
H4M	−0.257 (7)	0.126 (5)	0.067 (2)	0.059 (10)*
C1	0.5971 (5)	−0.1996 (3)	0.24949 (19)	0.0405 (6)
H1A	0.4222	−0.1654	0.2491	0.049*
H1B	0.6118	−0.2993	0.2801	0.049*
C2	0.7822 (5)	−0.0722 (3)	0.30368 (18)	0.0393 (6)
C3	0.7467 (7)	0.0915 (4)	0.2965 (2)	0.0522 (8)
H3	0.6021	0.1240	0.2589	0.063*
C4	0.9246 (8)	0.2072 (4)	0.3449 (2)	0.0577 (9)
C5	1.1357 (8)	0.1603 (4)	0.4029 (2)	0.0634 (9)
C6	1.1715 (8)	−0.0016 (5)	0.4095 (3)	0.0751 (11)
H6	1.3146	−0.0343	0.4478	0.090*
C7	0.9978 (7)	−0.1156 (4)	0.3600 (2)	0.0560 (8)
H7	1.0266	−0.2248	0.3647	0.067*
C8	0.1007 (6)	0.1330 (3)	0.1058 (2)	0.0448 (7)
C10	−0.1080 (5)	0.3440 (3)	0.0826 (2)	0.0404 (6)
Cl1	0.8778 (3)	0.40861 (12)	0.33114 (10)	0.1080 (5)
Cl2	1.3556 (3)	0.30086 (16)	0.46816 (10)	0.1064 (5)
N1	0.1333 (4)	0.3833 (3)	0.10869 (16)	0.0393 (6)
N2	0.2733 (4)	0.2507 (3)	0.12354 (19)	0.0476 (6)
N3	−0.1339 (4)	0.1855 (3)	0.08066 (18)	0.0423 (6)
O1	0.4994 (3)	−0.3828 (2)	0.09619 (13)	0.0383 (5)
O2	0.5688 (4)	−0.0964 (2)	0.08476 (13)	0.0417 (5)
O3	0.9286 (3)	−0.2589 (2)	0.13509 (14)	0.0446 (5)
S1	0.65640 (11)	−0.23697 (7)	0.13202 (4)	0.0291 (2)
H3M	0.132 (7)	0.035 (5)	0.108 (3)	0.070 (11)*
H2M	−0.232 (8)	0.408 (5)	0.070 (3)	0.069 (11)*
H1M	0.197 (8)	0.480 (5)	0.111 (3)	0.069 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0418 (15)	0.0362 (14)	0.0448 (15)	−0.0018 (11)	0.0112 (12)	0.0037 (11)
C2	0.0474 (16)	0.0346 (14)	0.0369 (13)	0.0005 (11)	0.0119 (12)	0.0001 (11)
C3	0.067 (2)	0.0388 (16)	0.0495 (16)	0.0047 (14)	0.0037 (14)	0.0031 (13)
C4	0.089 (3)	0.0335 (16)	0.0525 (18)	−0.0047 (16)	0.0240 (18)	−0.0040 (13)
C5	0.069 (2)	0.057 (2)	0.060 (2)	−0.0170 (17)	0.0137 (17)	−0.0196 (16)
C6	0.069 (2)	0.061 (2)	0.083 (3)	0.0053 (18)	−0.020 (2)	−0.0160 (19)
C7	0.060 (2)	0.0419 (17)	0.0606 (19)	0.0051 (14)	−0.0021 (15)	−0.0072 (14)
C8	0.0402 (16)	0.0259 (14)	0.0685 (19)	0.0036 (11)	0.0082 (13)	0.0052 (13)

C10	0.0316 (14)	0.0324 (14)	0.0553 (16)	0.0028 (11)	0.0013 (12)	0.0011 (12)
Cl1	0.1756 (14)	0.0328 (5)	0.1118 (9)	−0.0042 (6)	0.0125 (9)	0.0028 (5)
Cl2	0.1059 (10)	0.0813 (8)	0.1162 (10)	−0.0352 (7)	−0.0009 (7)	−0.0397 (7)
N1	0.0373 (13)	0.0243 (12)	0.0543 (14)	−0.0071 (9)	0.0030 (10)	0.0023 (10)
N2	0.0283 (12)	0.0420 (14)	0.0704 (16)	0.0012 (10)	0.0000 (11)	0.0059 (12)
N3	0.0267 (12)	0.0332 (12)	0.0651 (16)	−0.0091 (10)	0.0086 (11)	−0.0048 (11)
O1	0.0332 (10)	0.0229 (9)	0.0571 (11)	−0.0051 (7)	0.0052 (8)	−0.0026 (8)
O2	0.0462 (11)	0.0250 (9)	0.0518 (11)	−0.0040 (8)	−0.0012 (8)	0.0092 (8)
O3	0.0264 (10)	0.0443 (11)	0.0617 (12)	−0.0004 (8)	0.0071 (8)	−0.0051 (9)
S1	0.0251 (4)	0.0196 (3)	0.0417 (4)	−0.0026 (2)	0.0042 (2)	0.0009 (2)

Geometric parameters (Å, °)

C1—C2	1.500 (4)	C7—H7	0.9300
C1—S1	1.790 (3)	C8—N2	1.289 (4)
C1—H1A	0.9700	C8—N3	1.332 (4)
C1—H1B	0.9700	C8—H3M	0.84 (4)
C2—C7	1.374 (4)	C10—N1	1.288 (4)
C2—C3	1.388 (4)	C10—N3	1.314 (4)
C3—C4	1.387 (5)	C10—H2M	0.86 (4)
C3—H3	0.9300	N1—N2	1.360 (3)
C4—C5	1.378 (6)	N1—H1M	0.86 (4)
C4—Cl1	1.721 (3)	N3—H4M	0.79 (4)
C5—C6	1.373 (6)	O1—S1	1.4538 (17)
C5—Cl2	1.732 (3)	O2—S1	1.4550 (19)
C6—C7	1.371 (5)	O3—S1	1.4405 (19)
C6—H6	0.9300		
C2—C1—S1	112.25 (18)	C6—C7—H7	119.3
C2—C1—H1A	109.2	C2—C7—H7	119.3
S1—C1—H1A	109.2	N2—C8—N3	111.8 (3)
C2—C1—H1B	109.2	N2—C8—H3M	124 (3)
S1—C1—H1B	109.2	N3—C8—H3M	124 (3)
H1A—C1—H1B	107.9	N1—C10—N3	106.9 (3)
C7—C2—C3	118.1 (3)	N1—C10—H2M	128 (3)
C7—C2—C1	120.3 (3)	N3—C10—H2M	126 (3)
C3—C2—C1	121.6 (3)	C10—N1—N2	111.6 (2)
C4—C3—C2	120.7 (3)	C10—N1—H1M	123 (3)
C4—C3—H3	119.7	N2—N1—H1M	125 (3)
C2—C3—H3	119.7	C8—N2—N1	103.0 (2)
C5—C4—C3	120.0 (3)	C10—N3—C8	106.8 (2)
C5—C4—Cl1	120.9 (3)	C10—N3—H4M	131 (3)
C3—C4—Cl1	119.0 (3)	C8—N3—H4M	122 (3)
C6—C5—C4	119.2 (3)	O3—S1—O1	112.59 (11)
C6—C5—Cl2	119.2 (3)	O3—S1—O2	113.48 (12)
C4—C5—Cl2	121.6 (3)	O1—S1—O2	111.99 (11)
C7—C6—C5	120.5 (4)	O3—S1—C1	107.50 (13)
C7—C6—H6	119.7	O1—S1—C1	104.86 (12)
C5—C6—H6	119.7	O2—S1—C1	105.69 (13)
C6—C7—C2	121.4 (3)		

S1—C1—C2—C7	−96.9 (3)	C5—C6—C7—C2	−0.9 (6)
S1—C1—C2—C3	81.1 (3)	C3—C2—C7—C6	1.2 (5)
C7—C2—C3—C4	0.1 (5)	C1—C2—C7—C6	179.3 (3)
C1—C2—C3—C4	−177.9 (3)	N3—C10—N1—N2	0.8 (3)
C2—C3—C4—C5	−1.8 (5)	N3—C8—N2—N1	0.4 (3)
C2—C3—C4—Cl1	178.0 (2)	C10—N1—N2—C8	−0.7 (3)
C3—C4—C5—C6	2.2 (5)	N1—C10—N3—C8	−0.5 (3)
Cl1—C4—C5—C6	−177.7 (3)	N2—C8—N3—C10	0.0 (4)
C3—C4—C5—Cl2	−177.3 (3)	C2—C1—S1—O3	48.8 (2)
Cl1—C4—C5—Cl2	2.8 (4)	C2—C1—S1—O1	168.79 (19)
C4—C5—C6—C7	−0.8 (6)	C2—C1—S1—O2	−72.7 (2)
Cl2—C5—C6—C7	178.7 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1M···O1^{i}	0.85 (4)	1.96 (4)	2.709 (3)	146 (4)
N3—H4M···O2^{ii}	0.79 (4)	2.08 (4)	2.768 (3)	146 (3)
N3—H4M···O2^{iii}	0.79 (4)	2.54 (3)	3.089 (3)	128 (3)

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

Fig. 1