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Tetramethylammonium trifluoromethanesulfonate

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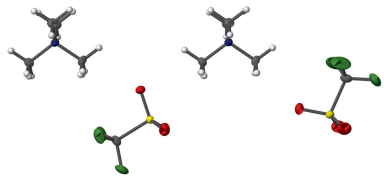
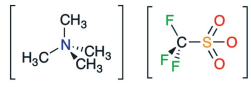
Structural data: full structural data are available from iucrdata.iucr.org

The structure of tetramethylammonium trifluoromethanesulfonate, $C_4H_{12}N^+\cdot CF_3SO_3^-$, was determined at 110 K in the monoclinic space group $P2_1/m$. The salt, which contains two cations and two anions in the asymmetric unit, has a network structure displaying C—H···O hydrogen bonding. Both the cation and the anion lie on special positions (mirror planes).

3D view



Chemical scheme



Structure description

Despite the report of the synthesis of the title compound in the literature (Sarria Toro *et al.*, 2014; and others), no structural data has been presented. The title compound has been used in various applications, such as an electrolyte for electrochemical studies and syntheses (Bond *et al.*, 1983; Ferraris *et al.*, 1998; Li *et al.*, 2002; Loveday *et al.*, 1997; Ue *et al.*, 1994), as a reagent in traditional synthesis (den Hartog *et al.*, 2014; Lei *et al.*, 2014; Sagl & Martin, 1988; Zhang *et al.*, 2014), as well as other studies (*i.e.* Bartoli & Roelens, 2002). For structures of other trifluoromethanesulfonate salts of tetraalkylammonium and ammonium cations, see: $[NBu_4][O_3SCF_3]$: Blake *et al.* (1993); $[NBu_4][O_3SCF_3]$ co-crystals: Leclercq *et al.* (2007, 2008, 2012) and $[NH_4][O_3SCF_3]$: Gänswein & Brauer (1975).

The bonding within the individual ions is as expected. The asymmetric unit is composed of two formula units (Fig. 1), with all four of the ions being positioned along a crystallographic mirror plane that is perpendicular to the [010] layer. Individual ions are connected by a three-dimensional network of hydrogen bonds (Table 1 and Fig. 2). The strongest interactions are found between C3 and O4 and C6 and O2. These generate the alternating ion types along the [010] layer. The ions are also connected by hydrogen bonds perpendicular to the [010] layer, in both the [100] and the [001] directions. These hold the ions of the asymmetric unit together along the crystallographic mirror plane. These hydrogen bonds are between C1 and O4, C1 and O3 and C6 and O4. In addition, other short contacts were discerned in the three-dimensional structure, however, it is unclear as to their nature.

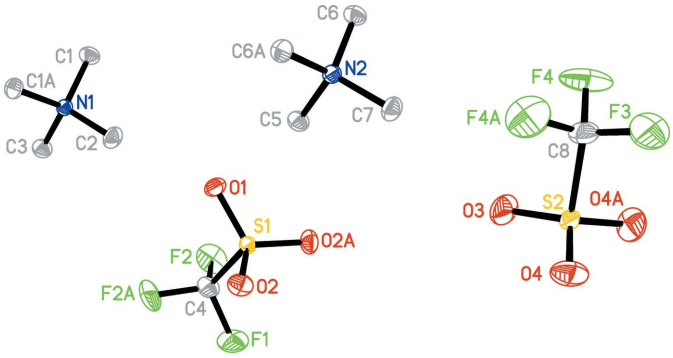


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme and with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

Synthesis and crystallization

The title compound was synthesized according to literature procedures (Sarria Toro *et al.*, 2014). Single crystals suitable for a diffraction study were serendipitously obtained from an attempted anion exchange reaction. A mixture of a $[Ga_2X_2$-(cryptand-222)$]^{2+}$ dication (Bourque *et al.*, 2015) with mixed tetrahalogallate and trifluoromethanesulfonate anions and an excess of the title compound was dissolved in acetonitrile (5 ml) and cooled to −20°C. Single crystals of the title compound were obtained after several days.

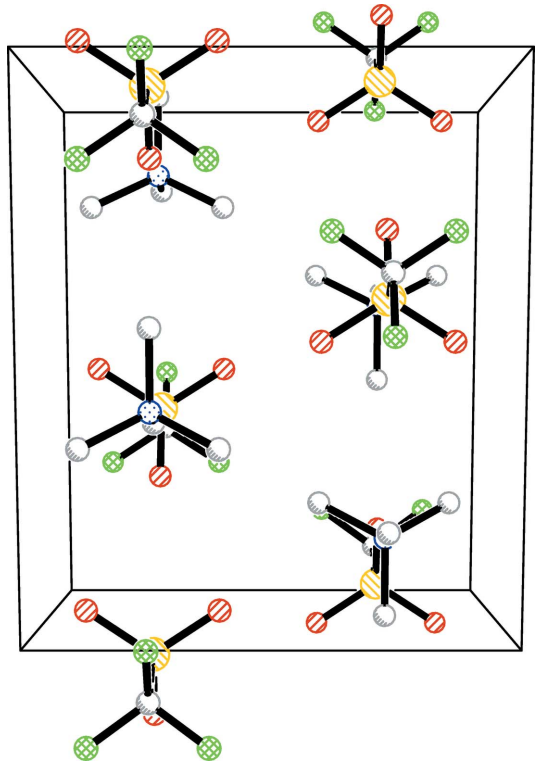


Figure 2
Crystal packing of the title compound viewed along the *c* axis. H atoms have been omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···O4^{i}	0.98	2.53	3.4075 (16)	149
C1—H1*C*···O3^{ii}	0.98	2.52	3.4038 (18)	150
C3—H3*A*···O4^{i}	0.98	2.48	3.3536 (13)	149
C3—H3*C*···O4^{iii}	0.98	2.45	3.3536 (13)	152
C5—H5*A*···O2^{i}	0.98	2.50	3.3734 (12)	148
C5—H5*C*···O2^{iii}	0.98	2.52	3.3734 (12)	145
C6—H6*A*···O4^{iv}	0.98	2.56	3.4594 (17)	153
C6—H6*B*···O2^{i}	0.98	2.47	3.3463 (15)	149

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_4H_{12}N^+\cdot CF_3O_3S^-$
M_r	223.22
Crystal system, space group	Monoclinic, $P2_1/m$
Temperature (K)	110
a, *b*, *c* (Å)	10.216 (3), 8.507 (2), 11.445 (4)
β (°)	101.807 (17)
V (Å^3)	973.6 (5)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.36
Crystal size (mm)	0.22 × 0.16 × 0.07
Data collection	
Diffractometer	Bruker Kappa-axis APEXII
Absorption correction	Multi-scan (*TWINABS*; Bruker, 2012)
T_{min}, T_{max}	0.225, 0.438
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4962, 4962, 3766
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.835
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.040, 0.106, 1.06
No. of reflections	4962
No. of parameters	145
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.54

Computer programs: *APEX2* (Bruker, 2013), *CELL_NOW* (Bruker, 2008), *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *XP* in *SHELXTL* (Sheldrick, 2008), *cif2tables.py* (Boyle, 2008).

Refinement

Crystal data, data collection and refinement details are shown in Table 2.

Acknowledgements

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full crystallographic data

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Crystal data

$C_4H_{12}N^+·CF_3O_3S^-$
M_r = 223.22
Monoclinic, $P2_1/m$
a = 10.216 (3) Å
b = 8.507 (2) Å
c = 11.445 (4) Å
β = 101.807 (17)°
V = 973.6 (5) Å^3
Z = 4
$F(000)$ = 464
D_x = 1.523 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7184 reflections
θ = 3.1–35.8°
μ = 0.36 mm^{-1}
T = 110 K
Plate, colourless
0.22 × 0.16 × 0.07 mm

Data collection

Bruker Kappa-axis APEXII diffractometer
Radiation source: sealed tube
phi and ω scans
Absorption correction: multi-scan (*TWINABS*; Bruker, 2012)
T_{min} = 0.225, T_{max} = 0.438
4962 measured reflections
4962 independent reflections
3766 reflections with $I > 2\sigma(I)$
θ_{max} = 36.4°, θ_{min} = 2.4°
h = −17→16
k = 0→14
l = 0→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.106
S = 1.06
4962 reflections
145 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.1452P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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. The structural model was fit to the data using full matrix least-squares based on F^2. The calculated structure factors included corrections for anomalous dispersion from the usual tabulation. The initial indexing indicated the sample crystal was a non-merohedral twin. The twin law was determined to be:
Twin Law,
Sample 1 of 1 Transforms h1.1(1)->h1.2(2)
0.08833 − 0.00004 0.90535
0.00561 − 0.99998 0.00058
1.09590 0.00873 − 0.08833
which corresponds to an approximately −179.7° rotation about the [101] vector in reciprocal space. The data demonstrated that the minor component refined to a normalized occupancy value of 0.02379 (22). Due to the small size of the secondary domain, the larger R_1 value obtained when including all the data, and increased levels of noise observed in the difference map, the structural model was refined using only data from the dominant component of the twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	−0.16040 (11)	0.7500	0.59284 (10)	0.01428 (19)	
C1	−0.22304 (11)	0.60593 (11)	0.53007 (10)	0.02051 (19)	
H1A	−0.3190	0.6053	0.5302	0.031*	
H1B	−0.1811	0.5122	0.5714	0.031*	
H1C	−0.2101	0.6060	0.4476	0.031*	
C2	−0.01370 (14)	0.7500	0.59337 (15)	0.0225 (3)	
H2A	0.0293	0.6627	0.6426	0.034*	0.5
H2B	0.0257	0.8496	0.6264	0.034*	0.5
H2C	−0.0001	0.7377	0.5116	0.034*	0.5
C3	−0.17984 (16)	0.7500	0.71906 (13)	0.0205 (3)	
H3A	−0.1312	0.6613	0.7623	0.031*	0.5
H3B	−0.2753	0.7400	0.7195	0.031*	0.5
H3C	−0.1458	0.8487	0.7580	0.031*	0.5
C4	0.35549 (17)	0.7500	0.79047 (14)	0.0233 (3)	
F1	0.46663 (13)	0.7500	0.87653 (9)	0.0399 (3)	
F2	0.28477 (9)	0.62388 (10)	0.80708 (7)	0.0381 (2)	
S1	0.39742 (3)	0.7500	0.64268 (3)	0.01368 (7)	
O1	0.26921 (11)	0.7500	0.56276 (10)	0.0209 (2)	
O2	0.47442 (8)	0.89272 (9)	0.64345 (8)	0.02385 (16)	
N2	0.40095 (11)	0.7500	0.20271 (10)	0.01435 (19)	
C5	0.37919 (15)	0.7500	0.32830 (12)	0.0183 (2)	
H5A	0.4104	0.6501	0.3668	0.027*	0.5
H5B	0.2837	0.7630	0.3275	0.027*	0.5
H5C	0.4293	0.8369	0.3727	0.027*	0.5
C6	0.33803 (11)	0.60648 (11)	0.13956 (9)	0.01936 (18)	
H6A	0.2419	0.6067	0.1388	0.029*	
H6B	0.3789	0.5124	0.1812	0.029*	
H6C	0.3520	0.6062	0.0574	0.029*	
C7	0.54785 (14)	0.7500	0.20474 (15)	0.0210 (3)	
H7A	0.5885	0.6554	0.2457	0.032*	0.5
H7B	0.5888	0.8435	0.2471	0.032*	0.5
H7C	0.5624	0.7511	0.1227	0.032*	0.5
S2	0.96358 (3)	0.7500	0.22288 (3)	0.01601 (7)	

O3	0.84541 (13)	0.7500	0.27165 (12)	0.0369 (3)
O4	1.04184 (10)	0.89119 (11)	0.24164 (9)	0.0366 (2)
C8	0.89895 (18)	0.7500	0.06244 (15)	0.0276 (3)
F3	0.99738 (16)	0.7500	0.00278 (12)	0.0579 (4)
F4	0.82365 (12)	0.62540 (14)	0.02824 (9)	0.0650 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0133 (4)	0.0133 (4)	0.0159 (5)	0.000	0.0022 (4)	0.000
C1	0.0234 (5)	0.0161 (4)	0.0210 (5)	−0.0036 (3)	0.0023 (4)	−0.0028 (3)
C2	0.0132 (6)	0.0275 (7)	0.0273 (7)	0.000	0.0054 (5)	0.000
C3	0.0237 (7)	0.0212 (6)	0.0169 (6)	0.000	0.0045 (5)	0.000
C4	0.0288 (7)	0.0256 (7)	0.0167 (6)	0.000	0.0075 (5)	0.000
F1	0.0435 (7)	0.0592 (8)	0.0139 (5)	0.000	−0.0017 (4)	0.000
F2	0.0503 (5)	0.0366 (4)	0.0330 (4)	−0.0112 (4)	0.0219 (4)	0.0064 (3)
S1	0.01419 (13)	0.01330 (13)	0.01369 (14)	0.000	0.00323 (10)	0.000
O1	0.0156 (4)	0.0273 (5)	0.0183 (5)	0.000	0.0000 (4)	0.000
O2	0.0249 (4)	0.0208 (3)	0.0263 (4)	−0.0082 (3)	0.0063 (3)	−0.0009 (3)
N2	0.0138 (5)	0.0143 (4)	0.0147 (5)	0.000	0.0023 (4)	0.000
C5	0.0220 (6)	0.0191 (6)	0.0142 (6)	0.000	0.0047 (5)	0.000
C6	0.0224 (4)	0.0160 (4)	0.0189 (4)	−0.0023 (3)	0.0025 (3)	−0.0032 (3)
C7	0.0137 (5)	0.0242 (6)	0.0258 (7)	0.000	0.0054 (5)	0.000
S2	0.01404 (14)	0.01859 (15)	0.01491 (15)	0.000	0.00181 (11)	0.000
O3	0.0216 (6)	0.0640 (9)	0.0276 (6)	0.000	0.0107 (5)	0.000
O4	0.0382 (5)	0.0324 (5)	0.0368 (5)	−0.0163 (4)	0.0019 (4)	−0.0090 (4)
C8	0.0267 (8)	0.0349 (8)	0.0180 (7)	0.000	−0.0027 (6)	0.000
F3	0.0515 (8)	0.1044 (12)	0.0205 (5)	0.000	0.0138 (5)	0.000
F4	0.0755 (8)	0.0681 (7)	0.0412 (6)	−0.0331 (6)	−0.0116 (5)	−0.0202 (5)

Geometric parameters (Å, º)

N1—C1	1.4965 (12)	N2—C6^{i}	1.4953 (12)
N1—C1^{i}	1.4965 (12)	N2—C6	1.4954 (12)
N1—C2	1.4974 (18)	N2—C7	1.4960 (18)
N1—C3	1.4979 (19)	N2—C5	1.4988 (18)
C1—H1A	0.9800	C5—H5A	0.9800
C1—H1B	0.9800	C5—H5B	0.9800
C1—H1C	0.9800	C5—H5C	0.9800
C2—H2A	0.9800	C6—H6A	0.9800
C2—H2B	0.9800	C6—H6B	0.9800
C2—H2C	0.9800	C6—H6C	0.9800
C3—H3A	0.9800	C7—H7A	0.9800
C3—H3B	0.9800	C7—H7B	0.9800
C3—H3C	0.9800	C7—H7C	0.9800
C4—F2^{i}	1.3286 (12)	S2—O3	1.4299 (13)
C4—F2	1.3286 (12)	S2—O4^{i}	1.4344 (9)
C4—F1	1.342 (2)	S2—O4	1.4344 (9)

C4—S1	1.8279 (16)	S2—C8	1.8198 (18)
S1—O1	1.4360 (12)	C8—F4	1.3210 (14)
S1—O2^{i}	1.4457 (8)	C8—F4^{i}	1.3210 (14)
S1—O2	1.4457 (8)	C8—F3	1.326 (2)
C1—N1—C1^{i}	109.96 (11)	C6^{i}—N2—C6	109.47 (11)
C1—N1—C2	109.34 (7)	C6^{i}—N2—C7	109.76 (7)
C1^{i}—N1—C2	109.35 (7)	C6—N2—C7	109.76 (7)
C1—N1—C3	109.57 (7)	C6^{i}—N2—C5	109.27 (7)
C1^{i}—N1—C3	109.57 (7)	C6—N2—C5	109.27 (7)
C2—N1—C3	109.03 (12)	C7—N2—C5	109.29 (11)
N1—C1—H1A	109.5	N2—C5—H5A	109.5
N1—C1—H1B	109.5	N2—C5—H5B	109.5
H1A—C1—H1B	109.5	H5A—C5—H5B	109.5
N1—C1—H1C	109.5	N2—C5—H5C	109.5
H1A—C1—H1C	109.5	H5A—C5—H5C	109.5
H1B—C1—H1C	109.5	H5B—C5—H5C	109.5
N1—C2—H2A	109.5	N2—C6—H6A	109.5
N1—C2—H2B	109.5	N2—C6—H6B	109.5
H2A—C2—H2B	109.5	H6A—C6—H6B	109.5
N1—C2—H2C	109.5	N2—C6—H6C	109.5
H2A—C2—H2C	109.5	H6A—C6—H6C	109.5
H2B—C2—H2C	109.5	H6B—C6—H6C	109.5
N1—C3—H3A	109.5	N2—C7—H7A	109.5
N1—C3—H3B	109.5	N2—C7—H7B	109.5
H3A—C3—H3B	109.5	H7A—C7—H7B	109.5
N1—C3—H3C	109.5	N2—C7—H7C	109.5
H3A—C3—H3C	109.5	H7A—C7—H7C	109.5
H3B—C3—H3C	109.5	H7B—C7—H7C	109.5
F2^{i}—C4—F2	107.70 (14)	O3—S2—O4^{i}	115.51 (5)
F2^{i}—C4—F1	107.34 (9)	O3—S2—O4	115.51 (5)
F2—C4—F1	107.34 (9)	O4^{i}—S2—O4	113.72 (9)
F2^{i}—C4—S1	111.69 (8)	O3—S2—C8	103.47 (9)
F2—C4—S1	111.69 (8)	O4^{i}—S2—C8	103.13 (5)
F1—C4—S1	110.85 (11)	O4—S2—C8	103.13 (5)
O1—S1—O2^{i}	115.35 (4)	F4—C8—F4^{i}	106.70 (16)
O1—S1—O2	115.35 (4)	F4—C8—F3	107.72 (11)
O2^{i}—S1—O2	114.24 (7)	F4^{i}—C8—F3	107.72 (11)
O1—S1—C4	103.51 (7)	F4—C8—S2	111.60 (10)
O2^{i}—S1—C4	102.98 (5)	F4^{i}—C8—S2	111.60 (10)
O2—S1—C4	102.98 (5)	F3—C8—S2	111.27 (13)
F2^{i}—C4—S1—O1	−60.35 (10)	O3—S2—C8—F4	−59.64 (11)
F2—C4—S1—O1	60.35 (10)	O4^{i}—S2—C8—F4	61.06 (13)
F1—C4—S1—O1	180.000 (1)	O4—S2—C8—F4	179.65 (11)
F2^{i}—C4—S1—O2^{i}	179.18 (9)	O3—S2—C8—F4^{i}	59.64 (11)
F2—C4—S1—O2^{i}	−60.13 (11)	O4^{i}—S2—C8—F4^{i}	−179.65 (11)
F1—C4—S1—O2^{i}	59.52 (4)	O4—S2—C8—F4^{i}	−61.06 (13)

F2^{i}—C4—S1—O2	60.13 (12)	O3—S2—C8—F3	180.0
F2—C4—S1—O2	−179.18 (9)	O4^{i}—S2—C8—F3	−59.29 (5)
F1—C4—S1—O2	−59.52 (4)	O4—S2—C8—F3	59.29 (5)

Symmetry code: (i) x, $-y+3/2$, z.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···O4^{ii}	0.98	2.53	3.4075 (16)	149
C1—H1*C*···O3^{iii}	0.98	2.52	3.4038 (18)	150
C3—H3*A*···O4^{ii}	0.98	2.48	3.3536 (13)	149
C3—H3*C*···O4^{iv}	0.98	2.45	3.3536 (13)	152
C5—H5*A*···O2^{ii}	0.98	2.50	3.3734 (12)	148
C5—H5*C*···O2^{iv}	0.98	2.52	3.3734 (12)	145
C6—H6*A*···O4^{v}	0.98	2.56	3.4594 (17)	153
C6—H6*B*···O2^{ii}	0.98	2.47	3.3463 (15)	149

Symmetry codes: (ii) $-x+1$, $y-1/2$, $-z+1$; (iii) $x-1$, y, z; (iv) $-x+1$, $-y+2$, $-z+1$; (v) $x-1$, $-y+3/2$, z.