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Table Crystallographic Data

	5(NO_3)	**5(Cl)**	**5(CH_3COO)**
formula	$C_4H_{10}O_5S_2BiN.H_2O$	$C_4H_{10}O_2S_2BiCl$	$C_6H_{13}O_4BiS_2$
FW	443.24	398.68	422.26
crystal description	yellow, needle	yellow, trigonal-bipyramid	yellow, needle
crystal size (mm)	0.04 x 0.05 x 0.30	0.03 x 0.12 x 0.23	0.30 x 0.10 x 0.05
space group	$I4_1/a$	$P2_1/n$	$P2_1/c$
a/Å	20.337(6)	8.653(2)	8.089(2)
b/Å	20.337(6)	10.618(3)	16.313(3)
c/Å	11.303(7)	10.564(2)	8.708(2)
α/deg	90	90	90
β/deg	90	100.51(2)	98.37(3)
γ/deg	90	90	90
V/Å^3	4674(3)	954.4(4)	1136.8(4)
Z	16	4	4
D_o/(Mg m^{-3})	2.519	2.774	2.467
μ(cm^{-1})	331.91	426.74	337.79
Total reflections	1966	1622	1816
Unique reflections	1847	1514	1687
R-internal	0.067	0.083	0.050#
Oserved reflections	1227 (I > 3.00σ(I))	1262 (I > 3.00σ(I))	1415 (I > 2.00σ(I))
Parameters refined	128	92	118
R	0.048	0.036	0.082
R_w	0.062	0.045	0.204
GOF	2.43	3.94	3.43
Max/min peaks in final diff.map	+1.39/-2.38	+2.31/-2.70	+3.39/-5.32

R = 0.93and wR2 = 0.205 for all 1687 data

R-internal = $\Sigma^n_i\Sigma^m_j|\langle Fi^2\rangle - Fij^2|/\Sigma^n_i m\langle Fi^2\rangle$

n = number of unnique reflections that were observed more than once
m = number of times a given reflection is observed
$\langle Fi^2\rangle$ = the average value for unique reflections

Positional parameters and B(eq) for $[Bi(S(CH_2)_2OH)_2]\ NO_3$

atom	x	y	z	B(eq)
Bi(1)	0.23114(4)	0.60320(4)	0.11023(7)	3.59(4)
S(1)	0.3342(2)	0.5244(2)	0.1161(5)	3.9(2)
S(2)	0.1749(2)	0.4854(2)	0.1145(5)	4.1(2)
O(1)	0.3358(7)	0.6776(6)	0.135(1)	4.7(7)
O(2)	0.1045(6)	0.6177(7)	0.072(1)	5.5(8)
O(3)	0.131(1)	0.8091(9)	0.092(2)	8(1)
O(4)	0.1903(8)	0.7398(8)	0.182(1)	5.8(9)
O(5)	0.1883(8)	0.7398(10)	-0.001(2)	7(1)
O(6)	0.0645(8)	0.6762(8)	-0.125(1)	6.1(9)
N(1)	0.1712(9)	0.7643(9)	0.089(2)	5(1)
C(1)	0.3954(9)	0.575(1)	0.189(2)	4(1)
C(2)	0.399(1)	0.646(1)	0.133(2)	5(1)
C(3)	0.099(1)	0.503(1)	0.040(2)	5(1)
C(4)	0.064(1)	0.562(1)	0.079(2)	5(1)
H(1)	0.3846	0.5790	0.2701	5.4
H(2)	0.4373	0.5549	0.1808	5.4
H(3)	0.4131	0.6430	0.0531	5.5
H(4)	0.4289	0.6722	0.1766	5.5
H(5)	0.1084	0.5074	-0.0418	5.1
H(6)	0.0706	0.4664	0.0519	5.1
H(7)	0.0504	0.5565	0.1584	5.8
H(8)	0.0270	0.5687	0.0296	5.8

U values for $[Bi(S(CH_2)_2OH)_2]\ NO_3$

atom	U11	U22	U33	U12	U13	U23
Bi(1)	0.0382(5)	0.0391(5)	0.0589(5)	-0.0006(3)	0.0013(3)	-0.0009(3)
S(1)	0.039(3)	0.044(3)	0.065(3)	0.007(2)	0.001(2)	0.003(3)
S(2)	0.051(3)	0.044(3)	0.062(3)	-0.012(2)	-0.002(2)	-0.003(2)
O(1)	0.057(9)	0.045(8)	0.08(1)	0.002(7)	0.008(7)	-0.011(7)
O(2)	0.032(8)	0.07(1)	0.10(1)	-0.003(7)	-0.014(8)	0.015(9)
O(3)	0.11(2)	0.08(1)	0.11(1)	0.03(1)	-0.02(1)	-0.03(1)
O(4)	0.08(1)	0.08(1)	0.06(1)	0.01(1)	-0.015(9)	-0.006(9)
O(5)	0.07(1)	0.12(2)	0.08(1)	0.01(1)	0.01(1)	-0.02(1)
O(6)	0.07(1)	0.08(1)	0.08(1)	0.002(9)	-0.014(9)	-0.008(9)
N(1)	0.05(1)	0.07(1)	0.06(1)	0.00(1)	0.01(1)	-0.01(1)
C(1)	0.02(1)	0.07(1)	0.08(2)	0.02(1)	-0.01(1)	-0.01(1)
C(2)	0.03(1)	0.06(1)	0.09(2)	-0.01(1)	0.01(1)	0.00(1)
C(3)	0.06(1)	0.06(1)	0.06(1)	-0.03(1)	0.00(1)	-0.02(1)
C(4)	0.03(1)	0.10(2)	0.07(1)	-0.02(1)	-0.01(1)	0.00(1)

H(1)	0.0689
H(2)	0.0689
H(3)	0.0691
H(4)	0.0691
H(5)	0.0648
H(6)	0.0648
H(7)	0.0730
H(8)	0.0730

Intramolecular Distances Involving the Nonhydrogen Atoms for $[Bi(S(CH_2)_2OH)_2]\ NO_3$

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
BI1	S1	2.639(5)	1	O1	C2	1.43(2)	1
BI1	S1	2.920(6)	3	O2	C4	1.40(3)	1
BI1	S2	2.655(5)	1	O3	N1	1.22(2)	1
BI1	S2	2.837(6)	45412	O4	N1	1.23(2)	1
BI1	O1	2.63(1)	1	O5	N1	1.18(2)	1
BI1	O2	2.63(1)	1	C1	C2	1.58(3)	1
S1	C1	1.82(2)	1	C3	C4	1.47(3)	1
S2	C3	1.79(2)	1				

Intramolecular Distances Involving the Hydrogen Atoms for $[Bi(S(CH_2)_2OH)_2]\ NO_3$

atom	atom	distance	atom	atom	distance
C1	H1	0.950	C3	H5	0.950
C1	H2	0.950	C3	H6	0.950
C2	H3	0.950	C4	H7	0.950
C2	H4	0.950	C4	H8	0.950

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Selected Intermolecular Distances Involving the Nonhydrogen Atoms for $[Bi(S(CH_2)_2OH)_2]\ NO_3$

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
Bi1	Bi1	4.134(2)	3	O2	O5	3.12(2)	1
Bi1	Bi1	4.134(2)	45412	O2	O4	3.28(2)	1
BI1	S1	2.920(6)	3	O2	N1	3.28(2)	1
BI1	S2	2.837(6)	45412	O3	O6	2.72(2)	55416
BI1	O4	3.01(2)	1	O4	O4	2.90(3)	56513
BI1	O5	3.17(2)	1	O5	O6	3.12(2)	55416
BI1	N1	3.50(2)	1	O5	O6	3.16(2)	1
O1	O4	2.72(2)	56513	O6	O6	2.82(2)	35415
O1	O3	3.18(2)	56513	O6	O6	2.82(2)	55416
O1	O4	3.26(2)	1	O6	N1	3.29(3)	35415
O1	N1	3.34(2)	56513				
O2	O6	2.65(2)	1				

Estimated standard deviations in the least significant figure are given in parentheses.

(*)footnote

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one digit numbers and one two digit number: TA(1st digit) + TB(2nd digit) + TC(3rd digit) + SN(4th and 5th digit). TA, TB, & TC are the crystal lattice translation digits along cell edges a, b, and c. A translation digit of 5 indicates the origin unit cell. If TA=4, this indicates a translation of one unit cell length along the a axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus (+/-)4 lattice translations from the origin (TA=5,TB=5,TC=5) can be represented.

The SN or symmetry operator number refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of

the symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell (TA=5,TB=5,TC=5) and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always ADC=55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of that atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (i.e.cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	+X	, +Y	, +Z	(2)	-X	,1/2-Y	, +Z
(3)	3/4-Y	,1/4+X	,1/4+Z	(4)	1/4+Y	,1/4-X	,1/4+Z
(5)	-X	, -Y	, -Z	(6)	+X	,1/2+Y	, -Z
(7)	3/4+Y	,1/4-X	,1/4-Z	(8)	1/4-Y	,1/4+X	,1/4-Z
(9)	1/2+X	,1/2+Y	,1/2+Z	(10)	1/2-X	, -Y	,1/2+Z
(11)	1/2-Y	,3/4+X	,3/4+Z	(12)	3/4+Y	,3/4-X	,3/4+Z
(13)	1/2-X	,1/2-Y	,1/2-Z	(14)	1/2+X	, +Y	,1/2-Z
(15)	1/2+Y	,3/4-X	,3/4-Z	(16)	3/4-Y	,3/4+X	,3/4-Z

Intramolecular Bond Angles Involving the Nonhydrogen Atoms for $[Bi(S(CH_2)_2OH)_2]\ NO_3$

atom	atom	atom	angle	atom	atom	atom	angle
S1	BI1	S1	85.7(2)	BI1	S1	BI1	96.0(2)
S1	BI1	S2	78.1(2)	BI1	S1	C1	102.1(6)
S1	BI1	S2	83.0(1)	BI1	S1	C1	112.2(7)
S1	BI1	O1	72.8(3)	BI1	S2	BI1	97.6(2)
S1	BI1	O2	148.3(4)	BI1	S2	C3	100.6(7)
S1	BI1	S2	81.1(1)	BI1	S2	C3	107.0(7)
S1	BI1	S2	160.8(1)	BI1	O1	C2	118(1)
S1	BI1	O1	90.2(3)	BI1	O2	C4	118(1)
S1	BI1	O2	98.0(4)	O3	N1	O4	119(2)
S2	BI1	S2	81.3(2)	O3	N1	O5	122(2)
S2	BI1	O1	150.1(3)	O4	N1	O5	118(2)
S2	BI1	O2	71.4(3)	S1	C1	C2	112(1)
S2	BI1	O1	101.2(3)	O1	C2	C1	111(1)
S2	BI1	O2	83.8(4)	S2	C3	C4	116(1)
O1	BI1	O2	138.3(4)	O2	C4	C3	112(2)

Intramolecular Bond Angles Involving the Hydrogen Atoms for $[Bi(S(CH_2)_2OH)_2]\ NO_3$

atom	atom	atom	angle	atom	atom	atom	angle
S1	C1	H1	108.92	S2	C3	H5	107.82
S1	C1	H2	108.92	S2	C3	H6	107.82
C2	C1	H1	108.92	C4	C3	H5	107.83
C2	C1	H2	108.92	C4	C3	H6	107.84
H1	C1	H2	109.46	H5	C3	H6	109.46
O1	C2	H3	109.01	O2	C4	H7	108.97
O1	C2	H4	109.01	O2	C4	H8	108.97
C1	C2	H3	108.99	C3	C4	H7	108.94
C1	C2	H4	109.00	C3	C4	H8	108.94
H3	C2	H4	109.46	H7	C4	H8	109.46

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Positional parameters and B(eq) for $[Bi(S(CH_2)_2OH)_2]$ Cl

atom	x	y	z	B(eq)
Bi(1)	0.22308(6)	0.48441(5)	0.43624(5)	0.52(3)
Cl(1)	0.4528(4)	0.3262(3)	0.4473(4)	1.4(1)
S(1)	0.0477(4)	0.3288(3)	0.5363(3)	1.1(1)
S(2)	0.0856(4)	0.3880(3)	0.2234(4)	1.2(1)
O(1)	0.355(1)	0.588(1)	0.230(1)	1.7(5)
O(2)	0.326(1)	0.476(1)	0.703(1)	2.5(5)
C(1)	0.181(2)	0.281(2)	0.682(2)	2.1(7)
C(2)	0.244(2)	0.387(2)	0.768(2)	3.1(9)
C(3)	0.240(2)	0.408(2)	0.127(2)	3.3(9)
C(4)	0.289(2)	0.535(2)	0.108(2)	2.9(9)
H(1)	0.1268	0.2251	0.7285	1.7
H(2)	0.2675	0.2377	0.6570	1.7
H(3)	0.3149	0.3548	0.8403	2.2
H(4)	0.1596	0.4286	0.7965	2.2
H(5)	0.3293	0.3624	0.1686	3.0
H(6)	0.2022	0.3722	0.0448	3.0
H(7)	0.2004	0.5836	0.0689	3.5
H(8)	0.3648	0.5346	0.0535	3.5

U values for $[Bi(S(CH_2)_2OH)_2]$ Cl

atom	U11	U22	U33	U12	U13	U23
Bi(1)	0.0064(3)	0.0065(4)	0.0071(3)	-0.0006(2)	0.0014(2)	-0.0022(2)
Cl(1)	0.015(2)	0.018(2)	0.022(2)	0.007(2)	0.004(2)	0.003(2)
S(1)	0.011(2)	0.014(2)	0.018(2)	-0.001(2)	0.004(1)	0.005(1)
S(2)	0.014(2)	0.014(2)	0.015(2)	-0.006(2)	-0.001(2)	-0.005(1)
O(1)	0.033(7)	0.014(6)	0.019(6)	-0.010(5)	0.005(5)	0.002(5)
O(2)	0.048(8)	0.026(7)	0.017(6)	-0.003(6)	-0.001(6)	0.001(5)
C(1)	0.02(1)	0.02(1)	0.04(1)	0.004(7)	0.009(8)	0.018(8)
C(2)	0.04(1)	0.07(2)	0.01(1)	0.01(1)	0.009(8)	0.016(9)
C(3)	0.07(1)	0.03(1)	0.04(1)	-0.03(1)	0.03(1)	-0.011(8)
C(4)	0.04(1)	0.03(1)	0.04(1)	0.00(1)	0.02(1)	0.004(9)

H(1)	0.0220
H(2)	0.0220
H(3)	0.0273
H(4)	0.0273
H(5)	0.0383
H(6)	0.0383
H(7)	0.0339
H(8)	0.0339

Intramolecular Distances and Selected Contacts Involving the Nonhydrogen Atoms for $[Bi(S(CH_2)_2OH)_2]$ Cl

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
BI1	BI1	4.328(1)	56603	BI1	O2	2.80(1)	1
BI1	CL1	2.589(3)	1	S1	C1	1.82(2)	1
BI1	CL1	3.488(4)	66603	S2	C3	1.83(2)	1
BI1	S1	2.595(3)	1	O1	C4	1.43(2)	1
BI1	S1	3.124(4)	56603	O2	C2	1.43(2)	1
BI1	S2	2.558(4)	1	C1	C2	1.49(3)	1
BI1	O1	2.86(1)	1	C3	C4	1.44(2)	1

Intramolecular Distances Involving the Hydrogen Atoms for $[Bi(S(CH_2)_2OH)_2]$ Cl

atom	atom	distance	atom	atom	distance
C1	H1	0.950	C3	H5	0.950
C1	H2	0.950	C3	H6	0.950
C2	H3	0.950	C4	H7	0.950
C2	H4	0.950	C4	H8	0.950

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

(*)footnote

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one digit numbers and one two digit number: TA(1st digit) + TB(2nd digit) + TC(3rd digit) + SN(4th and 5th digit). TA, TB, & TC are the crystal lattice translation digits along cell edges a, b, and c. A translation digit of 5 indicates the origin unit cell. If TA=4, this indicates a translation of one unit cell length along the a axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus (+/-)4 lattice translations from the origin (TA=5,TB=5,TC=5) can be represented.

The SN or symmetry operator number refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of

the symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell (TA=5,TB=5,TC=5) and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always ADC=55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of that atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (i.e.cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	+X ,	+Y ,	+Z	(2)	1/2-X	,1/2+Y	,1/2-Z
(3)	-X ,	-Y ,	-Z	(4)	1/2+X	,1/2-Y	,1/2+Z

Intramolecular Bond Angles Involving the Nonhydrogen Atoms for $[Bi(S(CH_2)_2OH)_2]$ Cl

atom	atom	atom	angle	atom	atom	atom	angle
BI1	BI1	CL1	139.19(8)	S1	BI1	O1	154.2(2)
BI1	BI1	CL1	123.48(6)	S1	BI1	O2	70.9(3)
BI1	BI1	S1	45.64(8)	S1	BI1	S2	95.7(1)
BI1	BI1	S1	36.44(6)	S1	BI1	O1	103.7(2)
BI1	BI1	S2	90.34(8)	S1	BI1	O2	91.9(3)
BI1	BI1	O1	135.3(2)	S2	BI1	O1	70.8(2)
BI1	BI1	O2	80.1(2)	S2	BI1	O2	152.3(2)
CL1	BI1	CL1	78.3(1)	O1	BI1	O2	132.9(3)
CL1	BI1	S1	94.0(1)	BI1	CL1	BI1	101.7(1)
CL1	BI1	S1	172.2(1)	BI1	S1	BI1	97.9(1)
CL1	BI1	S2	90.6(1)	BI1	S1	C1	101.1(5)
CL1	BI1	O1	82.8(2)	BI1	S1	C1	118.2(6)
CL1	BI1	O2	80.4(3)	BI1	S2	C3	100.0(6)
CL1	BI1	S1	135.7(1)	BI1	O1	C4	112.5(9)
CL1	BI1	S1	99.76(9)	BI1	O2	C2	114(1)
CL1	BI1	S2	139.1(1)	S1	C1	C2	114(1)
CL1	BI1	O1	68.9(2)	O2	C2	C1	111(1)
CL1	BI1	O2	64.8(2)	S2	C3	C4	117(1)
S1	BI1	S1	82.1(1)	O1	C4	C3	109(2)
S1	BI1	S2	83.7(1)				

Intramolecular Bond Angles Involving the Hydrogen Atoms for $[Bi(S(CH_2)_2OH)_2]$ Cl

atom	atom	atom	angle	atom	atom	atom	angle
S1	C1	H1	108.29	S2	C3	H5	107.63
S1	C1	H2	108.29	S2	C3	H6	107.64
C2	C1	H1	108.29	C4	C3	H5	107.64
C2	C1	H2	108.29	C4	C3	H6	107.65
H1	C1	H2	109.46	H5	C3	H6	109.45
O2	C2	H3	109.01	O1	C4	H7	109.61
O2	C2	H4	109.01	O1	C4	H8	109.61
C1	C2	H3	109.03	C3	C4	H7	109.62
C1	C2	H4	109.03	C3	C4	H8	109.62
H3	C2	H4	109.46	H7	C4	H8	109.46

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

$[Bi(SCH_2CH_2OH)_2][CH_3COO]$

	x	y	z	U(eq)
Bi(1)	5456(1)	7938(1)	1211(1)	38(1)
S(1)	7839(9)	7365(5)	3272(9)	51(2)
S(2)	3122(9)	7511(4)	2772(9)	46(2)
O(1)	5430(23)	6395(12)	791(23)	49(5)
O(2)	2949(24)	9065(12)	679(25)	53(5)
O(3)	6177(26)	9005(11)	3004(25)	54(5)
O(4)	7159(33)	9510(13)	940(30)	72(7)
C(1)	8084(39)	6331(20)	2513(38)	60(9)
C(2)	6349(52)	5930(20)	2042(46)	79(12)
C(3)	1886(44)	8453(21)	2819(40)	64(9)
C(4)	1500(38)	8840(22)	1229(34)	55(8)
C(5)	6993(36)	9539(16)	2412(33)	41(7)
C(6)	7902(40)	10209(19)	3424(44)	64(9)

Table 3. Bond lengths [Å] and angles [°] for 1.

$[Bi(SCH_2CH_2OH)_2][CH_3COO]$

Bi(1)-O(3)	2.35(2)	Bi(1)-O(1)	2.54(2)
Bi(1)-S(2)	2.578(7)	Bi(1)-S(1)	2.608(7)
Bi(1)-O(2)	2.73(2)	Bi(1)-S(2)#1	3.379(8)
Bi(1)-S(1)#1	3.457(8)	Bi(1)-Bi(1)#1	4.5825(11)
S(1)-C(1)	1.83(3)	S(2)-C(3)	1.84(3)
O(1)-C(2)	1.44(4)	O(1)-O(3)#1	2.67(3)
O(2)-C(4)	1.38(3)	O(2)-O(4)#2	2.71(3)
O(3)-C(5)	1.25(3)	O(4)-C(5)	1.31(3)
C(1)-C(2)	1.55(5)	C(3)-C(4)	1.51(4)
C(5)-C(6)	1.52(4)		

O(3)-Bi(1)-O(1)	145.4(7)	O(3)-Bi(1)-S(2)	88.9(6)
O(1)-Bi(1)-S(2)	79.5(5)	O(3)-Bi(1)-S(1)	73.8(5)
O(1)-Bi(1)-S(1)	74.6(5)	S(2)-Bi(1)-S(1)	93.7(2)
O(3)-Bi(1)-O(2)	73.8(7)	O(1)-Bi(1)-O(2)	130.7(6)
S(2)-Bi(1)-O(2)	71.9(4)	S(1)-Bi(1)-O(2)	144.6(5)
O(3)-Bi(1)-S(2)#1	143.2(5)	O(1)-Bi(1)-S(2)#1	70.5(4)
S(2)-Bi(1)-S(2)#1	92.9(2)	S(1)-Bi(1)-S(2)#1	142.5(2)
O(2)-Bi(1)-S(2)#1	71.9(5)	O(3)-Bi(1)-S(1)#1	119.1(5)
O(1)-Bi(1)-S(1)#1	75.2(5)	S(2)-Bi(1)-S(1)#1	151.9(2)
S(1)-Bi(1)-S(1)#1	91.3(2)	O(2)-Bi(1)-S(1)#1	116.9(5)
S(2)#1-Bi(1)-S(1)#1	67.2(2)	O(3)-Bi(1)-Bi(1)#1	145.7(5)
O(1)-Bi(1)-Bi(1)#1	63.6(4)	S(2)-Bi(1)-Bi(1)#1	121.2(2)
S(1)-Bi(1)-Bi(1)#1	116.1(2)	O(2)-Bi(1)-Bi(1)#1	98.7(5)
S(2)#1-Bi(1)-Bi(1)#1	33.67(12)	S(1)#1-Bi(1)-Bi(1)#1	34.39(12)
C(1)-S(1)-Bi(1)	100.9(9)	C(3)-S(2)-Bi(1)	103.2(12)
C(2)-O(1)-Bi(1)	115(2)	C(2)-O(1)-O(3)#1	114(2)
Bi(1)-O(1)-O(3)#1	112.1(8)	C(4)-O(2)-O(4)#2	116(2)
C(4)-O(2)-Bi(1)	114(2)	O(4)#2-O(2)-Bi(1)	129.3(9)
C(5)-O(3)-Bi(1)	110(2)	C(2)-C(1)-S(1)	110(2)
O(1)-C(2)-C(1)	109(3)	C(4)-C(3)-S(2)	112(2)
O(2)-C(4)-C(3)	111(3)	O(3)-C(5)-O(4)	121(3)
O(3)-C(5)-C(6)	120(3)	O(4)-C(5)-C(6)	119(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z-1/2 #2 -x+1,-y+2,-z

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$

$[Bi(SCH_2CH_2OH)_2][CH_3COO]$

	U11	U22	U33	U23	U13	U12
Bi(1)	38(1)	35(1)	39(1)	1(1)	7(1)	-1(1)
S(1)	41(4)	60(5)	50(4)	4(4)	-3(3)	0(3)
S(2)	43(4)	39(4)	56(4)	8(3)	7(3)	-3(3)
O(1)	36(11)	50(12)	60(13)	15(10)	3(9)	11(9)
O(2)	37(11)	53(12)	70(14)	12(11)	13(10)	-2(9)
O(3)	61(13)	31(10)	66(14)	-7(10)	0(11)	-11(9)
O(4)	94(19)	46(13)	85(18)	9(12)	39(15)	-17(12)
C(1)	51(19)	73(22)	51(19)	1(17)	-11(15)	36(17)
C(2)	111(33)	42(19)	77(27)	23(18)	-7(23)	18(20)
C(3)	61(22)	68(22)	63(22)	0(18)	13(17)	7(17)
C(4)	50(19)	69(21)	45(18)	6(16)	5(14)	-2(16)
C(5)	47(17)	33(15)	43(17)	2(12)	8(13)	2(13)
C(6)	43(19)	50(19)	100(28)	2(18)	15(18)	-17(15)