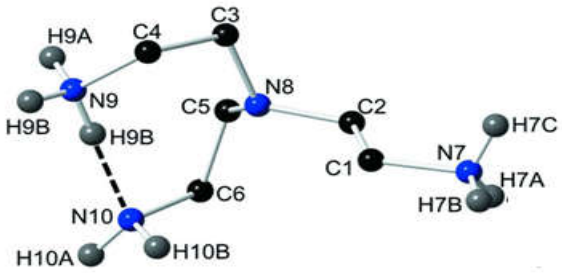
STUDIES ON BIS 1,5′-(3-AMINOETHYLIMINO) ETHYLAMMONIUM TRI-A-SULFIDO-DISULFIDOSTANNATE

*Suganya V, **Buvaneshwari.A, ***S.Arunarani
Assistant professor, Department of Physics,
Prince Shri Venkateshwara Padmavathy Engineering College,Chennai
**Prince Dr.K.Vasudevan College of Engineering & Technology, Chennai.*
***Faculty, Prince Shri Venkateshwara Arts and Science College, Gowriwakkam.*

ABSTRACT

Since an assortment of anionic thiocyanate building blocks has been generated in solvothermal syntheses, the[Sn2S6]4- moiety has been one of the most common. We have now shown that when the reaction is undertaken in anhydrous conditions and without any transition metal present, the anhydrous version of this compound (I) can be accessed. The terminal Sn-S bonds, at 2.3307 (4) and 2.3447 (5) Å, are shorter in the title compound, (H2tren)2[Sn2S6], (Fig. 1) than the Sn-S bond of 2.4565 (6) Å formed with the bridging arsenic. The location of the NH2 pedant amine is the most distinct structural variation between the anhydrous structure and the clinically defined hydrated model (Näther et al., 2003). It is aligned in the hydrated structure to facilitate an H-bonding interaction (H···N-H of 2.08 Å) on an opposing cation with an NH3 + amine.



BIS 1,5′-(3-AMINOETHYLIMINO) ETHYLAMMONIUM TRI-*A*-SULFIDO-DISULFIDOSTANNATE

Crystal data

$(C_6H_{20}N_4)_2[Sn_2S_6]$
M_r = 363.13

Monoclinic, $P2_1/c$ Hall symbol: -P 2ybc
a = 8.911 (2) Å
b = 10.8845 (3) Å
c = 12.2498 (2) Å
β = 105.758 (1)°
V = 1264.15 (5) Å^3
Z = 2

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.01082 (1)	0.468130 (7)	0.66292 (1)	0.02312 (4)
S1	0.18598 (5)	0.52916 (3)	0.87984 (5)	0.03186 (9)
S2	−0.15015 (5)	0.35310 (3)	0.66377 (5)	0.03259 (9)
S3	0.13815 (5)	0.41901 (3)	0.51649 (5)	0.03229 (9)
C1	0.1339 (2)	0.3225 (1)	0.0717 (2)	0.0349 (3)
H1A	0.1600	0.3833	0.0573	0.042*
H1B	0.1715	0.2818	0.0213	0.042*
C2	0.2059 (2)	0.3005 (1)	0.2327 (2)	0.0380 (4)
H2A	0.1620	0.3379	0.2817	0.046*
H2B	0.1862	0.2382	0.2463	0.046*
C3	0.4166 (3)	0.4070 (2)	0.3308 (4)	0.0552 (6)
H3A	0.4711	0.4130	0.4351	0.066*
H3B	0.3308	0.4468	0.2984	0.066*
C4	0.5166 (3)	0.4348 (2)	0.2610 (3)	0.0528 (6)
H4A	0.4596	0.4337	0.1565	0.063*
H4B	0.5507	0.4959	0.2895	0.063*
C5	0.4481 (3)	0.2526 (2)	0.4178 (2)	0.0466 (5)
H5A	0.5397	0.2814	0.4852	0.056*
H5B	0.3875	0.2407	0.4689	0.056*
C6	0.4856 (3)	0.1665 (2)	0.3699 (3)	0.0510 (5)
H6A	0.5435	0.1297	0.4538	0.061*
H6B	0.3942	0.1344	0.3106	0.061*
N7	−0.0318 (2)	0.3140 (1)	0.0112 (2)	0.0350 (3)
H7A	−0.0551	0.2610	0.0361	0.053*
H7B	−0.0715	0.3181	−0.0849	0.053*
H7C	−0.0677	0.3577	0.0462	0.053*
N8	0.3655 (2)	0.3154 (1)	0.2955 (2)	0.0340 (3)
N9	0.6473 (2)	0.3752 (1)	0.3030 (2)	0.0393 (4)
H9A	0.7035	0.3791	0.3981	0.059*
H9B	0.7009	0.3916	0.2564	0.059*

H9C	0.6165	0.3187	0.2799	0.059*
N10	0.5705 (3)	0.1814 (1)	0.2875 (3)	0.0535 (5)
H10A	0.6363	0.1388	0.2887	0.080*
H10B	0.5046	0.1868	0.1857	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.02520 (5)	0.02399 (6)	0.02090 (5)	−0.00209 (3)	0.01070 (4)	−0.00039 (3)
S1	0.0316 (2)	0.0363 (2)	0.0254 (2)	−0.0069 (1)	0.0102 (1)	−0.0050 (1)
S2	0.0325 (2)	0.0375 (2)	0.0268 (2)	−0.0115 (2)	0.0120 (1)	0.0009 (1)
S3	0.0400 (2)	0.0321 (2)	0.0300 (2)	0.0127 (2)	0.0201 (2)	0.0057 (1)
C1	0.0357 (8)	0.0370 (9)	0.0362 (9)	0.0016 (7)	0.0196 (7)	0.0056 (7)
C2	0.0316 (8)	0.049 (1)	0.0347 (9)	−0.0045 (7)	0.0157 (7)	−0.0022 (8)
C3	0.052 (1)	0.036 (1)	0.089 (2)	−0.0123 (9)	0.041 (1)	−0.019 (1)
C4	0.049 (1)	0.037 (1)	0.075 (2)	−0.0066 (8)	0.022 (1)	0.011 (1)
C5	0.042 (1)	0.062 (1)	0.037 (1)	−0.0056 (9)	0.0190 (9)	−0.0023 (9)
C6	0.043 (1)	0.056 (1)	0.053 (1)	0.0121 (9)	0.020 (1)	0.021 (1)
N7	0.0356 (7)	0.0375 (8)	0.0291 (7)	0.0014 (6)	0.0112 (6)	0.0019 (6)
N8	0.0280 (6)	0.0343 (7)	0.0407 (8)	−0.0060 (5)	0.0160 (6)	−0.0056 (6)
N9	0.0330 (7)	0.0461 (9)	0.0379 (8)	−0.0106 (7)	0.0146 (6)	0.0023 (7)
N10	0.055 (1)	0.049 (1)	0.067 (1)	−0.0051 (9)	0.037 (1)	−0.009 (1)

Geometric parameters (Å, º)

Sn1—S1	2.3307 (4)	C4—H4A	0.9700
Sn1—S2	2.3447 (4)	C4—H4B	0.9700
Sn1—S3^{i}	2.4550 (4)	C5—C6	1.477 (4)
Sn1—S3	2.4564 (4)	C5—N8	1.491 (3)
S3—Sn1^{i}	2.4550 (4)	C5—H5A	0.9700
C1—N7	1.490 (2)	C5—H5B	0.9700
C1—C2	1.521 (3)	C6—N10	1.446 (3)
C1—H1A	0.9700	C6—H6A	0.9700
C1—H1B	0.9700	C6—H6B	0.9700
C2—N8	1.445 (2)	N7—H7A	0.8900
C2—H2A	0.9700	N7—H7B	0.8900
C2—H2B	0.9700	N7—H7C	0.8900
C3—N8	1.444 (3)	N9—H9A	0.8900
C3—C4	1.512 (4)	N9—H9B	0.8900
C3—H3A	0.9700	N9—H9C	0.8900
C3—H3B	0.9700	N10—H10A	0.9066
C4—N9	1.474 (3)	N10—H10B	0.9645
S1—Sn1—S2	120.55 (2)	C6—C5—N8	113.0 (2)
S1—Sn1—S3^{i}	113.87 (2)	C6—C5—H5A	109.0
S2—Sn1—S3^{i}	108.22 (2)	N8—C5—H5A	109.0
S1—Sn1—S3	109.28 (2)	C6—C5—H5B	109.0
S2—Sn1—S3	108.51 (2)	N8—C5—H5B	109.0

S3^{i}—Sn1—S3	92.78 (1)	H5A—C5—H5B	107.8
Sn1^{i}—S3—Sn1	87.22 (1)	N10—C6—C5	110.8 (2)
N7—C1—C2	110.3 (1)	N10—C6—H6A	109.5
N7—C1—H1A	109.6	C5—C6—H6A	109.5
C2—C1—H1A	109.6	N10—C6—H6B	109.5
N7—C1—H1B	109.6	C5—C6—H6B	109.5
C2—C1—H1B	109.6	H6A—C6—H6B	108.1
H1A—C1—H1B	108.1	C1—N7—H7A	109.5
N8—C2—C1	110.9 (2)	C1—N7—H7B	109.5
N8—C2—H2A	109.5	H7A—N7—H7B	109.5
C1—C2—H2A	109.5	C1—N7—H7C	109.5
N8—C2—H2B	109.5	H7A—N7—H7C	109.5
C1—C2—H2B	109.5	H7B—N7—H7C	109.5
H2A—C2—H2B	108.0	C2—N8—C3	117.1 (2)
N8—C3—C4	111.8 (2)	C2—N8—C5	112.0 (2)
N8—C3—H3A	109.3	C3—N8—C5	112.1 (2)
C4—C3—H3A	109.3	C4—N9—H9A	109.5
N8—C3—H3B	109.3	C4—N9—H9B	109.5
C4—C3—H3B	109.3	H9A—N9—H9B	109.5
H3A—C3—H3B	107.9	C4—N9—H9C	109.5
N9—C4—C3	111.9 (2)	H9A—N9—H9C	109.5
N9—C4—H4A	109.2	H9B—N9—H9C	109.5
C3—C4—H4A	109.2	C6—N10—H10A	119.0
N9—C4—H4B	109.2	C6—N10—H10B	110.6
C3—C4—H4B	109.2	H10A—N10—H10B	102.6
H4A—C4—H4B	107.9		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N9—H9*C*···N10	0.89	2.10	2.965 (3)	163
N9—H9*B*···S1^{ii}	0.89	2.44	3.314 (2)	167
N9—H9*A*···S2^{iii}	0.89	2.49	3.370 (2)	168
N7—H7*C*···S1^{i}	0.89	2.36	3.243 (2)	174
N7—H7*B*···S2^{iv}	0.89	2.40	3.278 (2)	170
N7—H7*A*···S2^{v}	0.89	2.57	3.411 (2)	159

REFERENCES

Behrens, M., Scherb, S., Na¨ther, C. & Bensch, W. (2003). Z. Anorg. Allg. Chem. 629, 1367–1373. Bruker (1998). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.

Jia, D. X., Dai, J., Zhu, Q. Y., Lu, W. & Guo, W. J. (2005). Chin. J. Struct. Chem. 24, 1157–1163.

Jiang, T., Lough, A. & Ozin, G. A. (1998b). Adv. Mater. 10, 42–46