

The Crystal Structure of $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$

INGER HJERTÉN and BIRGIT NYBERG

Institute of Inorganic and Physical Chemistry, University of Stockholm, S-113 86 Stockholm, and Division of Inorganic Chemistry 2, Chemical Center, Box 740, S-220 07 Lund 7, Sweden

The crystal structure of thallium(I) copper(II) disulfite has been determined and refined from three dimensional X-ray film and diffractometer data. The structure is triclinic with the space group $P\bar{1}$. The unit cell, which contains one formula unit, has the dimensions

$$a = 5.4738(3) \text{ \AA}, b = 7.3290(4) \text{ \AA}, c = 5.4717(5) \text{ \AA}, \alpha = 111.638(7)^\circ, \beta = 123.570(4)^\circ, \gamma = 88.019(7)^\circ.$$

The structure consists of trigonal pyramids of SO_3^{2-} and somewhat distorted CuO_6 octahedra. The six oxygen atoms around Cu belong to six different SO_3^{2-} groups. The CuO_6 octahedra and the SO_3^{2-} pyramids form $\text{Cu}(\text{SO}_3)_2^{2-}$ layers extending almost parallel to the *ac* plane. These layers are held together by thallium atoms. The average bond distances in the sulfite group are $\text{S}-\text{O} = 1.54 \text{ \AA}$ and $\text{O}-\text{O} = 2.43 \text{ \AA}$. The average value of the angle $\text{O}-\text{S}-\text{O}$ is 104.5° .

During the last years the crystal structures of a series of different metal sulfites have been studied. Reports on the structures of Cu_2SO_3 , $\text{CuSO}_3 \cdot 2\text{H}_2\text{O}$,¹ NH_4CuSO_3 ,² and Ag_2SO_3 ,³ as well as a report on a structural refinement of Na_2SO_3 ,⁴ have been published. In connection with the crystal structure studies of the copper sulfites the compound thallium(I) copper(II) sulfite was investigated.

EXPERIMENTAL

Preparation of the crystals. When synthesizing $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$ a method according to Canneri⁵ was used. To a saturated aqueous solution of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ an equivalent amount of Tl_2CO_3 was added, the latter also as a saturated aqueous solution. SO_2 was passed through the solution, and after a few minutes a yellow crystalline precipitate was obtained. After washing with water the crystals were dried in a nitrogen atmosphere. Microscopic investigation revealed thin yellow transparent plates.

Analysis. A small sample of $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$ was ignited, and the SO_2 formed was converted to H_2SO_4 in an H_2O_2 -solution, whereupon the amount of sulfur was determined by titration with alkali. The amount of copper was determined by atomic absorption spectroscopy. (Found: Cu 10.22 ± 0.5 ; S 8.93 ± 0.25 . Calc. for $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$: Cu 10.05; S 10.14.)

Infrared absorption spectrum. The infrared spectrum of a sample of $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$ was recorded with a Perkin-Elmer 180 spectrophotometer, using the KBr-pellet technique.

The maxima of absorption were observed at the following frequencies (cm^{-1}) and intensities: 980 (st), 895 (st), 860 (st), 670 (m), 590 (w), 500 (st) and 455 (m). The frequencies are in good agreement with the values reported in the literature.⁶

X-Ray diffraction data and computing methods. The unit cell parameters were calculated by least squares refinement from a powder photograph taken with strictly monochromatized $\text{CuK}\alpha_1$ radiation ($\lambda = 1.54050 \text{ \AA}$) in a Guinier-Hägg focusing camera. Potassium chloride ($a = 6.29228 \text{ \AA}$)⁷ was used as an internal standard. The powder pattern was completely indexed (Table 1) on the basis of the following triclinic cell (25°C).

$$\begin{array}{ll} a = 5.4738(3) \text{ \AA} & \alpha = 111.638(7)^\circ \\ b = 7.3290(4) \text{ \AA} & \beta = 123.570(4)^\circ \\ c = 5.4717(5) \text{ \AA} & \gamma = 88.019(7)^\circ \\ V = 165.895 \text{ \AA}^3 & \end{array}$$

Table 1. X-Ray powder pattern for $\text{Ti}_2[\text{Cu}(\text{SO}_3)_2]$. $\text{CuK}\alpha_1$ -radiation ($\lambda = 1.54050 \text{ \AA}$).

$h k l$	$10^5 \sin^2\theta$ obs	$10^5 \sin^2\theta$ calc	I_{obs}
0 1 0	1341	1342	m
-1 0 1	2713	2713	m
1 0 0	2997	2995	st
0 -1 1		2996	
-1 -1 1	3121	3121	st
-1 1 0	3464	3451	v st
0 0 1		3465	
-1 1 1	4985	4990	m
0 -2 1	5213	5212	m
1 1 0		5214	
-1 -2 1	6210	6215	v st
-1 2 0	6613	6611	v v st
0 1 1		6618	
-1 -1 2	7960	7959	v v st
1 -1 1	8859	8862	v v st
-2 -1 1	9231	9237	m
-2 1 1	9354	9352	m
-1 2 1	9951	9952	m
0 -3 1	10112	10114	m
1 2 0		10118	
1 -2 1	10199	10201	m
-2 -1 2	10323	10328	m
-2 0 2	10845	10845	st
-2 1 0	11577	11570	v w
0 -1 2		11581	
2 0 0	11982	11981	st
0 -2 2		11986	
-1 -3 1		11993	
-2 -2 2	12481	12487	w
-2 -2 1	13207	13207	w
-1 -3 2		13208	
-2 2 1	13440	13437	v v w (d)
-1 1 2		13450	
-2 2 0	13850	13844	m
0 0 2		13860	
-2 1 2	14067	14065	m
1 -3 1	14223	14226	v w
0 -3 2	15074	15076	st
2 1 0		15077	

Table 1. Continued.

-2-3 2	17333	17331	w	(d)
-1 3 1	17603	17599	v v w	(d)
0-4 1	17698	17700	w	(d)
1 3 0				
-3 0 2	18340	18337	v w	
-2-1 3				
-3-1 2	18679	18688	w	
-2 3 0	18805	18802	w	
-3 0 1	19182	19182	w	
-3 1 1	19710	19705	m	
-1-4 2	19869	19860	v w	(d)
-2-3 1				
-2 3 1	20213	20207	w	(d)
-1 2 2				
-3 1 2	20681	20223	w	(d)
-2 0 3				
1-4 1	20944	20671	w	(d)
1 2 1				
2-2 1	21178	20935	w	(d)
0 4 0	21479	20953	w	(d)
-3-2 2	21725	21180	v v w	(d)
-2-3 3				
1-3 2	22935	21479	m	
2 0 1				
-1 0 3	24189	21723	st	
-3-2 3				
2-3 1	24339	21730	v w	(d)
1 0 2	24859	24328	m	
-2-4 2	24859	24350	m	
-3 1 0	25672	24860	v w	(d)
-3-2 1	26191	25670	st	
-1-4 3				
		26191	m	
		26195		

The powder photograph was measured and interpreted to $\sin^2 \theta = 0.47$.

A powder photograph without any internal standard showed that no reaction had occurred between $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$ and KCl.

The unit cell is not reduced according to Buerger⁸ or to Delaunay⁹ on account of similarities in cell dimensions and structure with the earlier investigated structure of NH_4CuSO_3 .⁸ The unit cell reduced according to Buerger⁸ as well as to Delaunay⁹ should have the following dimensions

$$\begin{array}{ll}
 a = 5.4717 \text{ \AA} & \alpha = 110.660^\circ \\
 b = 7.3275 \text{ \AA} & \beta = 118.195^\circ \\
 c = 5.1748 \text{ \AA} & \gamma = 92.014^\circ
 \end{array}$$

The observed density of $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$, determined from the apparent loss of weight in chloroform, is $5.98 \pm 0.10 \text{ g/cm}^3$. Assuming one formula unit in the unit cell gives the calculated density = 6.33 g/cm^3 . The rather big difference between the values could depend on the fact that the determination was made in an early stage when the preparation was not quite pure.

554 independent reflections were recorded, using Weissenberg multiple film technique, with Ni-filtered CuK radiation. Two crystals were investigated, and the relative intensities were visually estimated by comparison with an intensity scale obtained by photographing one reflection with different exposure times. In spite of the great tendency of twinning, the crystals did not show any such effect. The space group was assumed to be $P\bar{1}$.

The accuracy of the structure determination based upon the film data, especially in the case of the S—O distances, was not as good as wanted, so a new set of three dimensional intensity data was collected. A crystal [an irregular triangular plate, volume = 1.2×10^{-4} mm³, thickness = 0.011 mm (*b** direction)], without satellites or any twinning tendency was selected by means of Weissenberg technique. A Siemens automatic X-ray diffractometer equipped with a scintillation counter with pulse height discrimination was used. The 5-values measuring technique was applied and 1048 independent reflections up to $\theta = 34^\circ$ were measured, using Nb-filtered MoK radiation. The value of $\sigma(I_0)/I_0$ was then ≤ 0.3 . Three standard reflections were measured with a period of 40 reflections.

Corrections were made for Lorentz, polarization and absorption effects, with the linear absorption coefficient value,¹⁰ $\mu = 526.6$ cm⁻¹. The calculations were performed on the electronic computers CD 3600, IBM 1800, and IBM 360/75. A list of the programs used in the calculations is given in Table 2.

Table 2. Computer programs used for the crystallographic calculations. All the programs are written in FORTRAN IV.

Program name and function	Authors
ABS. Absorption, extinction and Lp-factors.	P. E. Werner and M. Leijonmarck, Stockholm, Sweden.
DATA. Reflection data handling including storing on disk, correction of erroneous reflections or inclusions of new ones in a data set stored on disk; index transformation.	B. G. Brandt, Stockholm, Sweden.
DRF. Fourier summations and structure factor calculations.	A. Zalkin, Berkeley, USA. Modified by R. Liminga and J.-O. Lundgren, Uppsala, Sweden. Further modified by O. Lindgren, Göteborg and by A. G. Nord and B. G. Brandt, Stockholm, Sweden.
LALS. Full matrix least-squares refinement of positional and thermal parameters and of scale factors.	P. K. Gantzel, R. A. Sparks and K. N. Trueblood, Los Angeles, USA. Modified by A. Zalkin, Berkeley, USA, and by J.-O. Lundgren, R. Liminga and C.-I. Brändén, Uppsala, Sweden. Further modified by O. Lindgren, Göteborg and by B. G. Brandt and A. G. Nord, Stockholm, Sweden.
DISTAN. Calculation of interatomic distances and bond angles with estimated standard deviations.	A. Zalkin, Berkeley, USA. Modified by A. G. Nord and B. G. Brandt, Stockholm, Sweden.
LAZY. Calculation of $\sin^2 \theta$ and <i>d</i> -values from the measured reflection sites of a Guinier powder photograph after internal standard correction.	A. G. Nord, Stockholm, Sweden.
PIRUM, PURUM. Indexing of powder photographs and determination or refinement of unit cell parameters from powder or diffraction data by the method of least squares.	P.-E. Werner, Stockholm, Sweden.

Table 2. Continued.

TRICL. Calculation of direct and reciprocal cell parameters, the constants in the quadratic formula and tests for reducibility according to Delaunay and Buerger.	L. Kihlberg, Stockholm, Sweden.
VIP. Angle settings for three circle diffractometers.	R. Norrestam, Stockholm, Sweden.
SIP. Generation of steering paper tape for Siemens AED.	R. Norrestam, Stockholm, Sweden.
SIMSA. Interpretation of output on paper tape from Siemens AED and evaluation of intensities.	R. Norrestam, Stockholm, Sweden.
EXTDATA. Calculation of the factor C in Zachariasen's 1963-formula for extinction correction. Application of the correction.	B. G. Brandt, Stockholm, Sweden.
ORTEP. Thermal ellipsoid plot. For crystal structure illustration.	C. K. Johnson, Oak Ridge, USA. Modified by I. Carlbon, Stockholm, Sweden.

STRUCTURE DETERMINATION

In the space group $P\bar{1}$ eight special point positions and the general position $2(i)$: $\pm(x, y, z)$ exist. By placing the only copper atom in the position $1(h)$: $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ the origin was fixed. The two thallium atoms could be situated either in two special positions or in the general twofold position $2(i)$. From the absence of any high peak in the Patterson projections $P(p\ v\ w)$ and $P(u\ p\ w)$ at u, v or $w = \frac{1}{2}$ it was concluded that the position $2(i)$ was the only one available for thallium. The parameters could be derived, and the electron density projections $\rho(p\ y\ z)$ and $\rho(x\ p\ z)$ were calculated using the signs of $F(0kl)$ and $F(h0l)$ obtained from the thallium and copper contributions. The positions of the two sulfur atoms and the six oxygens atoms, all in position $2(i)$, could then be obtained.

A refinement of the coordinates was performed by means of the least-squares method. Anisotropic temperature factors were used for all the atoms, and it was evident that using the atomic scattering curves for neutral atoms given by Cromer and Waber,¹¹ with the real part of the anomalous dispersion correction¹² applied, gave the best results. When a correction for secondary extinction was made according to Zachariasen,¹³ the R -value from the refinement including all the reflections was down to 3.12%. The weighting function used was that of Cruickshank, $w = (A + |F_{\text{obs}}| + C|F_{\text{obs}}|^2 + D|F_{\text{obs}}|^3)^{-1}$, with the following final values for the parameters: $A = +60$, $C = +0.007$, $D = +0.001$. No unobserved reflections were introduced, and a three dimensional difference synthesis showed no peak heights above 15% of the oxygen peak height. The results thus obtained are good enough to leave the possibility of the lower symmetry out of consideration.

The final values of the atomic parameters, the anisotropic temperature factors of all the atoms and their standard deviations are given in Table 3. A list of observed and calculated structure factors is presented in Table 4. A weight analysis obtained in the last cycle is given in Table 5.

Table 3. The structure of $\text{Ti}_2[\text{Cu}(\text{SO}_3)_2]$.

Space group: $P\bar{1}$.

Unit cell dimensions: $a = 5.4738$ (3) Å
 $b = 7.3290$ (4) Å
 $c = 5.4717$ (5) Å
 $\alpha = 111.638$ (7)°
 $\beta = 123.570$ (4)°
 $\gamma = 88.019$ (7)°

Cell content: 1 $[\text{Ti}_2[\text{Cu}(\text{SO}_3)_2]]$

Arrangement of atoms: 1 Cu in 1(*h*): ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)
 2 Ti, 2 S, 6 O(1)–(3) in 2(*i*): $\pm(x, y, z)$

Fractional atomic coordinates with e.s.d.'s. as calculated from the least-squares refinement, in parentheses.

Atom	<i>x</i>	<i>y</i>	<i>z</i>
Ti	0.70128(7)	0.12150(4)	0.92013(8)
Cu	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
S	0.87579(34)	0.60292(20)	0.22741(38)
O(1)	0.7750(13)	0.7152(8)	0.4390(14)
O(2)	0.2191(11)	0.6866(7)	0.4386(13)
O(3)	0.2506(11)	0.3124(7)	0.0316(13)

Anisotropic thermal parameters, β_{ij} with e.s.d.'s.

The β values refer to the temperature factor

$$\exp(-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)).$$

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ti	0.0217 (2)	0.0079 (1)	0.0227 (2)	0.0060 (1)	0.0206 (3)	0.0097 (1)
Cu	0.0095 (4)	0.0059 (2)	0.0082 (5)	0.0055 (4)	0.0070 (8)	0.0059 (5)
S	0.0096 (6)	0.0047 (2)	0.0092 (7)	0.0020 (5)	0.0073 (11)	0.0059 (6)
O(1)	0.018 (2)	0.011 (1)	0.016 (3)	0.012 (2)	0.025 (4)	0.013 (2)
O(2)	0.007 (2)	0.007 (1)	0.016 (3)	0.006 (2)	0.009 (4)	0.008 (2)
O(3)	0.012 (2)	0.007 (1)	0.012 (2)	0.005 (2)	0.007 (4)	0.009 (2)

R.m.s. components of thermal displacement (in Å) along the principal axes of the ellipsoid of thermal vibration.

Atom	R(1)	R(2)	R(3)
Ti	0.1322	0.1391	0.1670
Cu	0.0794	0.1019	0.1277
S	0.0858	0.1025	0.1145
O(1)	0.0939	0.1251	0.1636
O(2)	0.0762	0.1211	0.1472
O(3)	0.0884	0.1205	0.1390

Table 5. Weight analysis obtained in the final cycle of the least-squares refinement of $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$. w = weighting factor. $\Delta = |F_o| - |F_c|$.

Interval $\sin \theta$	Number of independ- ent reflections	$\overline{w\Delta^2}$	Interval F_o	Number of independ- ent reflections	$\overline{w\Delta^2}$
0.0 - 0.269	134	2.44	0.0 - 11.9	104	1.62
0.269 - 0.339	122	0.95	11.9 - 15.7	105	1.34
0.339 - 0.388	114	0.93	15.7 - 19.7	105	0.71
0.388 - 0.427	110	0.68	19.7 - 23.5	105	0.69
0.427 - 0.460	117	0.41	23.5 - 28.7	105	0.56
0.460 - 0.489	99	0.98	28.7 - 34.3	104	0.51
0.489 - 0.515	99	0.91	34.3 - 42.1	105	0.52
0.515 - 0.538	107	0.65	42.1 - 52.0	105	1.30
0.538 - 0.560	105	0.72	52.0 - 67.8	105	0.89
0.560 - 0.580	41	1.14	67.8 - 189.2	105	1.86

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

The structure of $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$ may be described as consisting of layers of trigonal pyramids of SO_3^{2-} and somewhat distorted CuO_6 octahedra linked together by corner sharing. A projection of the structure is given in Fig. 1, and a stereoscopic view of a part of the structure is shown in Fig. 2.

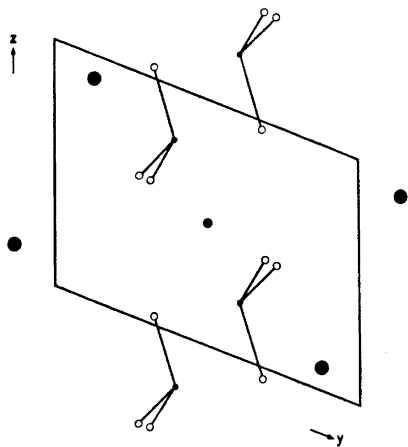


Fig. 1. Projection along the a axis on to the bc plane of the crystal structure of $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$. The sulfite groups are indicated by full lines. Open circles denote oxygen atoms, small filled circles sulfur, medium filled circles copper, and large filled circles denote thallium atoms.

The composition of a layer can be represented by the formula $[\text{Cu}(\text{SO}_3)_2^{2-}]_n$. The layers are almost parallel to the ac plane and are held together by thallium atoms. The function of the thallium atoms is similar to that of the ammonium ions in $\text{NH}_4\text{CuSO}_3 \cdot 2$

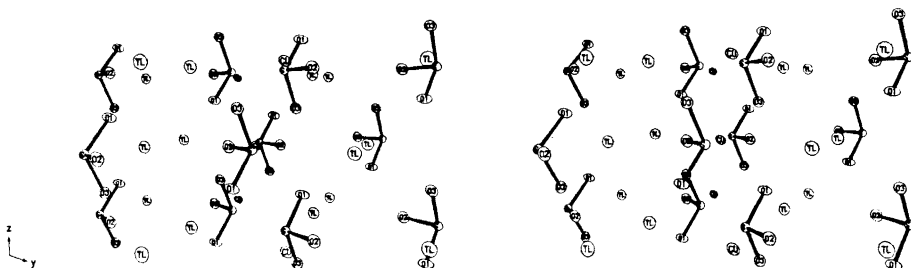


Fig. 2. A stereoscopic view of the structure of $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$ showing the linking in the b^* direction of the $[\text{Cu}(\text{SO}_3)_2]_n$ layers and the thallium atoms. The ac plane is vertical and perpendicular to the paper plane. The atoms are represented by the boundary "thermal ellipsoid" scaled to include 50% of the probability distribution.

A bounded straight projection (along b^*) of a part of a layer together with the nearest thallium atoms is given in Fig. 3.

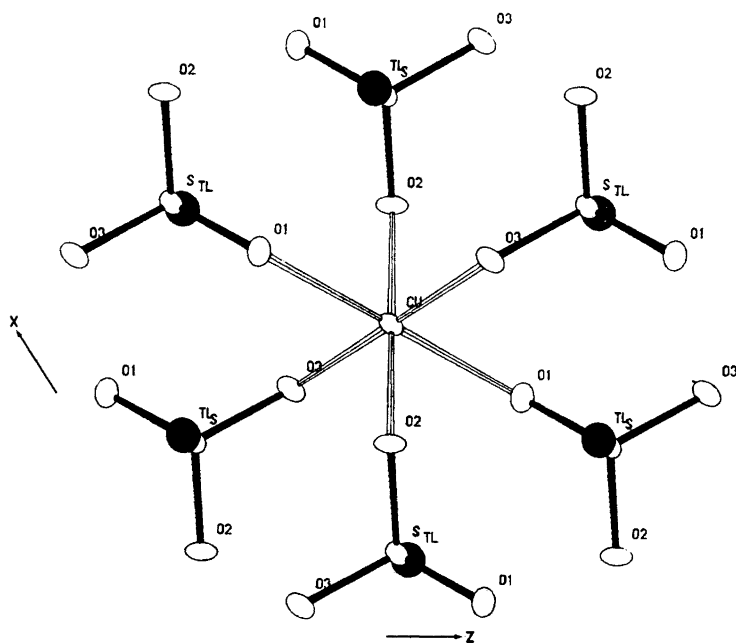


Fig. 3. A bounded straight projection on the ac plane of the environment of the copper atom.

Thallium is coordinated to one sulfur atom and to six oxygen atoms from three different sulfite groups in one layer and to three oxygen atoms from three different sulfite groups in the next layer (Fig. 4, Fig. 5b).

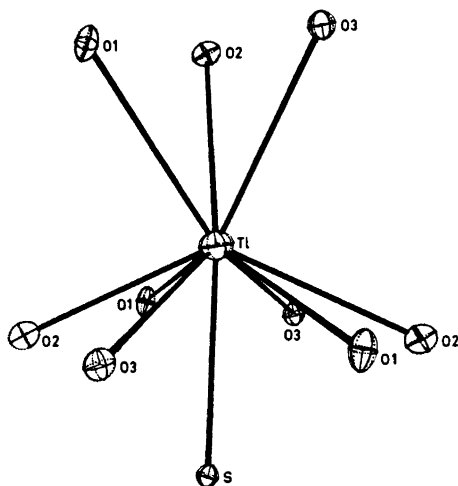


Fig. 4. A view of the environment of the thallium atom in $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$. The atoms are represented by "thermal ellipsoids" scaled to include 50 % of the probability distribution.

The interatomic distances and angles with standard deviations are given in Table 6.

The mean value of the S–O distances in the sulfite ion is 1.538 Å, well corresponding to the theoretical value of 1.54 Å suggested by Gillespie and Robinson.¹⁴ The dimensions of the SO_3^{2-} group are also consistent with the values found in $(\text{NH}_4)_2\text{SO}_3 \cdot \text{H}_2\text{O}$,¹⁵ $\text{NiSO}_3 \cdot 6\text{H}_2\text{O}$,¹⁶ and $\text{ZnSO}_3 \cdot 2\frac{1}{2}\text{H}_2\text{O}$.¹⁷ In these com-

Table 6. Interatomic distances (Å) and angles (°) and their e.s.d.'s in $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$. The distances are uncorrected for thermal motion.

S–O(1)	1.515 (6)	O(1)–S–O(2)	105.22 (30)
S–O(2)	1.549 (5)	O(1)–S–O(3)	104.89 (29)
S–O(3)	1.551 (5)	O(2)–S–O(3)	103.51 (28)
O(1)–O(2)	2.434 (7)		
O(1)–O(3)	2.431 (8)		
O(2)–O(3)	2.435 (7)		
Cu–2O(1)	2.444 (6)	O(1)–Cu–O(2)	86.45 (19)
Cu–2O(2)	1.992 (5)	O(1)–Cu–O(3)	86.34 (20)
Cu–2O(3)	1.996 (5)	O(2)–Cu–O(3)	86.80 (21)
Tl–O(1)	2.818 (6)	Tl–S	3.205 (1)
Tl–O(1)	2.823 (6)		
Tl–O(2)	3.008 (5)	Tl–O(1)	3.357 (6)
Tl–O(2)	3.032 (5)	Tl–O(2)	3.281 (5)
Tl–O(3)	3.001 (5)	Tl–O(3)	3.277 (5)
Tl–O(3)	3.035 (5)		
		Tl–Tl	3.492 (1)
		Tl–Tl	3.495 (1)
		Tl–Tl	3.513 (1)

pounds the sulfite oxygen atoms are affected by hydrogen bonding or metal bonding, and the S–O distances and angles are slightly different from the values found in Na_2SO_3 .⁴

In $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$ the individual S–O distances in the sulfite group can be correlated to the length of the bond between oxygen and copper. When the oxygen atom is found at a short distance (2.00 Å) from the copper atom its distance to the sulfur atom is long (1.55 Å), while a long Cu–O distance (2.44 Å) corresponds to a short S–O distance (1.52 Å).

As could be seen in the discussion of various sulfites performed by Kierkegaard *et al.*¹⁸ there is a rather regular variation of the O–S–O angle with the S–O distance, which is also consistent with $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$. The distorted octahedron CuO_6 has dimensions very similar to those found for divalent copper in $\text{Cu}_2\text{SO}_3 \cdot \text{CuSO}_3 \cdot 2\text{H}_2\text{O}$.¹

The coordination around thallium can hardly be described in terms of a regular polyhedron, but there are similarities with half a cuboctahedron (Fig. 5a, b).

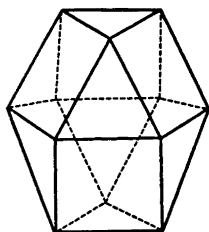


Fig. 5a. An ideal cuboctahedron.

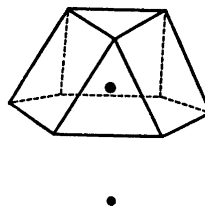


Fig. 5b. An idealization of the environment of Tl (I) in $\text{Tl}_2[\text{Cu}(\text{SO}_3)_2]$. The small full circle denotes the sulfur atom and the large filled circle denotes the thallium atom. The nine oxygen atoms are to be found at the corners of the indicated coordination polyhedron.

The Tl–S distance (3.21 Å) is below the value found in the ionic compound Tl(I)Tl(III)S_2 (Tl(I)–8 S: 3.32 Å).¹⁹ According to Shannon and Prewitt²⁰ the sum of the ionic radii for Tl^+ and S^{2-} with a coordination number of eight is 3.44 Å (1.60 Å + 1.84 Å). The values of the ionic radii are somewhat uncertain, but with regard to the distribution of the atoms around Tl and the relatively short Tl–S distance, a covalent bond may be assumed. The six nearest oxygen atoms, all belonging to the same layer, have a mean distance to the thallium atom of 2.95 Å. The sum of the ionic radii of Tl^+ and O^{2-} is 3.00 Å (1.60 + 1.40 Å).²⁰ Three additional bond distances from the thallium atom to oxygen atoms in another layer have a mean value of 3.30 Å. The shortest distance between two thallium atoms is 3.492 Å, which may be compared to the Tl–Tl metal distance: 3.408 Å.²¹

In this compound the inert pair of electrons in thallium (I) is not very stereochemically active. In the compounds Tl_2SO_4 ²² and $\text{TlNO}_3 \cdot 4\text{TU}$ ²³ (TU = thiourea) thallium(I) is stereochemically inactive.

Further studies of metal sulfites are in progress to gain more information of the sulfite group.

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