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Tin(II) Oxalate Structures

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The structures of tin(II) oxalate, SnC_2O_4, and (di)potassium(bis)oxalatostannate(II) monohydrate, $K_2Sn(C_2O_4)_2 \cdot H_2O$ have been refined from single crystal X-ray intensity data to R = 3.8 and 7% respectively.

Crystal Data

Tin(II) oxalate, SnC_2O_4 – I, is monoclinic, space group C2/c, a = 10.342(7), b = 5.497(4), c = 8.776(9) Å, β = 129.81(5)°, V = 383.3 (Å)^3, Z = 4, M = 206.7, D_{calc} = 3.56, D_{obs} 3.58 g cm^{-3}.

(Di)potassium(bis)oxalatostannate(II) monohydrate,* $K_2Sn(C_2O_4)_2 \cdot H_2O$ – II, is triclinic, space group $P\bar{1}$, a = 6.457, b = 6.629, c = 11.778 Å, α = 95.531, β = 93.502, γ = 102.628°, V = 487.9 (Å)^3, Z = 2, M = 390.9, D_{calc} = 2.67, D_{obs} = 2.62 g cm^{-3}.

Discussion

The structures were solved by standard methods, using the NRC programs of Ahmed [2], to yield the parameters given in Table I.

The principal feature of the structure of I is infinite chains in which Sn atoms and oxalato (OX) groups alternate (Fig. 1a). Each OX chelates two Sn, forming 5-membered chelate rings in each case, and the Sn–OX–Sn fragment is essentially planar. Each Sn in I, in turn, is chelated by two OX so that its coordination is akin to that of Sn in tetragonal blue/black SnO [3] (Table II). As a result, the infinite Sn[-OX–Sn-]$_\infty$ chains are puckered with the folds occurring at the Sn atoms. Weak Sn–O bonds of length 2.87(1) Å interconnect neighbouring chains and complete the coordination of Sn.

In the structure of II the primary coordination of Sn is similar to that found in I, although the site symmetries differ in the two structures. Infinite chains are also a feature of the structure of II, but in this case the chains contain discrete (bis)oxalatostannate(II) anions linked by hydrogen bonds to water molecules (O–O distances 2.77 and 2.85 Å,

*Identical results have been obtained for this structure quite independently by Donaldson *et al.* [1].

TABLE I. Atomic Parameters. Values in parentheses are e.s.d. s applicable to the least significant digits of each entry.

a) *Tin(II) Oxalate – I*

	Fractional coordinates (×10^3)			Biso (Å)^2
	x	y	z	
Sn	0	129.9(2)	250	1.42(0)
C	417(1)	47(2)	970(1)	1.50(13)
O1	349(1)	223(1)	853(1)	2.18(11)
O2	358(1)	61(1)	540(1)	1.94(10)

b) *(Di)potassium(bis)oxalatostannate(II)monohydrate –II*

	Fractional coordinates (×10^3)			Biso (Å)^2
	x	y	z	
Sn	247.0(2)	161.2(2)	229.7(1)	2.66(2)
K1	514.4(7)	732.5(7)	114.6(4)	3.45(8)
K2	243.0(6)	939.7(6)	583.5(3)	2.60(7)
C1	330(2)	582(2)	367(1)	2.1(3)
C2	246(2)	436(3)	455(1)	2.4(3)
C3	−158(3)	224(3)	115(1)	2.7(3)
C4	−2(2)	256(2)	22(1)	1.9(3)
O1	388(2)	771(2)	392(1)	2.8(2)
O2	331(2)	493(2)	256(1)	2.7(2)
O3	246(2)	521(2)	555(1)	3.0(2)
O4	185(2)	246(2)	422(1)	2.2(2)
O5	−341(2)	241(2)	98(1)	5.5(2)
O6	−78(2)	183(2)	209(1)	3.5(2)
O7	−75(2)	276(2)	−74(1)	2.7(2)
O8	186(2)	252(2)	49(1)	3.0(2)
O9 (Water)	142(2)	258(2)	722(1)	3.9(3)

TABLE II. Bond Lengths and Angles.

a) *Tin Coordination*

	I	II	SnO [3]
Sn–O	2.23(1)×2 2.39(1)×2	2.14(1), 2.13(1) 2.36(1), 2.31(1)	2.21×4
O–$\widehat{Sn}$–O	71.0(3)×2 79.2(3)×2	72.4(4), 72.4(4) 79.5(4), 80.2(4)	75.0×4

b) *Oxalate Groups*

	I	II
C–C	1.53(1)	1.54(2), 1.53(2)
C–O	1.25(1) 1.26(1)	1.22(2), 1.25(2), 1.25(2), 1.29(2) 1.22(2), 1.23(2), 1.23(2), 1.27(2)
O–$\widehat{C}$–O	124.8(9)	123.1(14), 126.4(15) 124.3(16), 125.5(14)
O–$\widehat{C}$–C	117.4(9)	121.8(14), 115.1(13), 115.9(13), 117.7(14)
	117.8(9)	121.5(15), 114.2(14), 117.1(13), 117.4(13)

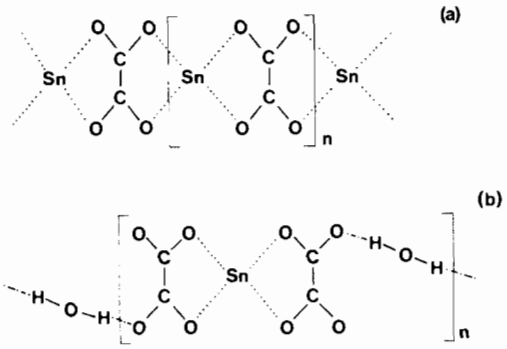

Fig. 1. Schematic representation of the infinite chains in a) tin(II) oxalate, and b) (di)potassium(bis)oxalostannate(II) monohydrate.

Fig. 1b). The chains in II are related to those found in I by the replacement of every second Sn in I by a water molecule. In II the chains are related in position through their contribution to the coordination of potassium.

In both structures the oxalate groups are planar within experimental error, with acceptable bond lengths and angles. Nevertheless, close examination of the two structures reveals subtle, but significant, differences in this area.

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