Four monazite type structures: comparison of $SrCrO_4$, $SrSeO_4$, $PbCrO_4$ (crocoite), and $PbSeO_4$

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Abstract. For a crystal chemical comparison within the monazite type structure the crystal structures of $SrCrO_4$, $SrSeO_4$, $PbCrO_4$ (crocoite), and $PbSeO_4$ were refined [space group $P2_1/n$, $Z = 4$; $a = 7.065(4)$, $7.101(2)$, $7.127(2)$, $7.154(4)$ Å, $b = 7.375(4)$, $7.340(2)$, $7.438(2)$, $7.407(4)$ Å; $c = 6.741(4), 6.874(2), 6.799(2), 6.954(4)$ Å; $\beta = 103.08(4), 103.48(2), 102.43(2), 103.14(4)°$]. As expected, in the MeO_{10} polyhedra the average $Sr-O$ bonds are slightly shorter than the $Pb-O$ bonds; further the average $Me-O$ bonds are shorter in the chromates than in the two selenates. In $SrSeO_4$ and in $PbSeO_4$ the average $Se-O$ bonds are equal within limits of error (1.640 and 1.642 Å). On the contrary in $SrCrO_4$ the average $Cr-O$ bond is 1.626 Å, in $PbCrO_4$ however 1.663 Å. The largest bond length distortions within the XO_4 tetrahedra were found in $SrCrO_4$ and $PbSeO_4$; the largest bond angle distortion occurs in $PbCrO_4$.

Introduction

A number of compounds with the formula $MeXO_4$ and a tetrahedral anion group XO_4 (X = P, As, Se, Cr, Si, . . .) were found to crystallize in the monazite type structure. So do e.g. the minerals monazite, $CePO_4$ (Ghose, 1968, Beall et al., 1981), huttonite, $ThSiO_4$, cheralite, (REE, Th, Ca, U) (P, Si)O_4 (Finney and Rao, 1967, Bowles et al., 1980), rooseveltite, $BiAsO_4$ (Bedlivy et al., 1969), or tombarthite, $REE_4(Si,H_4)_4O_{12-x}(OH)_{4+2x}$, $O \leq x \leq 4$ (Neumann and Nilssen, 1968).

Crocoite ("Rotbleierz") is a rare mineral found in the oxidation zones of lead deposits. Crystallographic data were determined by Gossner and Mussgnug (1930) and Brill (1931). Gliszczynski (1939) gave a comparison with monazite. The atomic coordinates of the Pb and Cr atoms in crocoite were derived by Brody (1942). The crystal structures of crocoite resp. $SrSeO_4$ were determined by Náray-Szabó and Argay (1964) and Quareni and De Pieri (1964, 1965) resp. by Prévost-Czeskleba and Endres (1984). Pistorius and Pistorius (1962) gave for the four compounds $MeXO_4$ (Me = Sr, Pb; X = Cr, Se) the X-ray powder patterns, lattice parameters as well as linear coefficients of thermal expansion and indicated temperature dependent phase transitions.

An orthorhombic modification of $PbCrO_4$ was described by Quittner et al. (1932) and Collotti et al. (1959) to crystallize in the baryte type structure.

Experimental

For the refinement of the crystal structure of crocoite natural material from Dundas, Tasmania, was used. Crystals of $SrCrO_4$, $SrSeO_4$, and $PbSeO_4$ were prepared by hydrothermal reactions in a steel vessel lined with "teflon" (~ 6 ml capacity). The following reagent grade chemicals were inserted:

(a) for $SrCrO_4$ (bright yellow crystals): 2 g of an equimolar mixture of Cr_2O_3 and $Sr(NO_3)_2$,
(b) for $SrSeO_4$ (colourless crystals): 2 g $Sr(NO_3)_2$ and 2 ml H_2SeO_4, and
(c) for $PbSeO_4$ (colourless to light brown crystals): 2 g of an equimolar mixture of SeO_2 and Pb_3O_4, 2 ml H_2O_2 ("perhydrol") were added.

For all charges the vessel was filled up with H_2O to about 80 vol%. The heating period was 48 h at 493(10) K. All the crystals of the title compounds are elongated parallel to [001]. The crystallographic forms {110} and {111} were observed. The crystals are up to 0.3 mm in length and have an approximate diameter of 0.1 mm.

For the cell data and for the details concerning the measurements of the X-ray intensities as well as for the final R values cf. Table 1[1]. The lattice parameters for all the four compounds were calculated from accurate 2θ angles measured on the four-circle diffractometer and were refined by least-squares techniques. An absorption correction was applied for the measured intensities (according to empirical ψ scans for $SrCrO_4$, $SrSeO_4$, and $PbSeO_4$, and according to the crystal shape for $PbCrO_4$). The atomic coordinates given by Náray-Szabó and Argay (1964) were used in the

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[1] Additional material to this paper can be ordered from the Fachinformationszentrum Energie-Physik-Mathematik, D-7514 Eggenstein-Leopoldshafen 2, FRG. Please quote CSD 52037, the names of the authors and the title of the paper

Table 1. Lattice parameters, details concerning the X-ray data collection as well as final obtained R values for the four monazite type structures $MeXO_4$ ($Me = Sr, Pb$; $X = Cr, Se$)

		$SrCrO_4$	$SrSeO_4$	$PbCrO_4$	$PbSeO_4$
Space group $P2_1/n$:	a [Å]	7.065(4)	7.101(2)	7.127(2)	7.154(4)
	b [Å]	7.375(4)	7.340(2)	7.438(2)	7.407(4)
	c [Å]	6.741(4)	6.874(2)	6.799(2)	6.9544(4)
	β [°]	103.08(4)	103.48(2)	102.43(2)	103.14(4)
	V [Å^3]	342.1	348.4	352.0	358.8
$Z = 4\{MeXO_4\}$		3.95	4.40	6.10	6.48
ϱ_{calc} [g cm^{-3}]					
$\mu(MoK\alpha)$ [cm^{-1}]		183	253	488	550
Crystal dimensions [mm^3]		$0.09 \times 0.10 \times 0.16$	$0.10 \times 0.10 \times 0.24$	$0.09 \times 0.09 \times 0.30$	$0.06 \times 0.08 \times 0.14$
Diffractometer; program; computer		AED2 four-circle diffractometer; STRUCSY (Stoe and Cie, Darmstadt, FRG), KRISTALLCHEMIE (Nowotny and Zobetz, 1982); ECLIPSE S140 (Data General)			
Radiation		$MoK\alpha$-radiation; graphite monochromator			
Measuring of reflections		$2\theta/\omega$ scan; step width 0.03°; 0.5 to 1.5 s pro step			
Number of steps per reflection		45	40	45	60
2θ maximum		75	85	70	70
Reflections measured		5279	5445	4113	4080
Symmetry independent		1801	2499	1545	1582
With $F_o > 3\,\sigma(F_o)$ (for refinement)		1487	1994	1418	1262
Extinction coefficient g^a		$4.4(5) \cdot 10^{-5}$	$5.3(5) \cdot 10^{-6}$	$2.02(6) \cdot 10^{-5}$	$2.2(2) \cdot 10^{-6}$
R (56 variables)		0.038	0.033	0.039	0.039
R_w; $w = 1/\sigma[(F_o)]^2$		0.034	0.027	0.034	0.029

[a] Zachariasen (1967)

Table 2. Structural parameters for SrCrO$_4$ (upper row), SrSeO$_4$ (second row), PbCrO$_4$ (third row), and PbSeO$_4$ (last row). E.s.d.'s are given in parentheses. ATF = $\exp\left[-2\pi^2 \sum\limits_{i=1}^{3} \sum\limits_{j=1}^{3} U_{ij} h_i h_j a_i^* a_j^* \right]$

	x/a	y/b	z/c	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sr/Pb	0.22813(4)	0.15869(5)	0.39806(5)	0.0120(1)	0.0123(1)	0.0131(1)	−0.0001(1)	0.0014(1)	−0.0015(1)
	0.22082(3)	0.15773(3)	0.39876(3)	0.0126(1)	0.0105(1)	0.0133(1)	−0.0002(1)	0.0019(1)	−0.0010(1)
	0.22130(4)	0.14545(4)	0.39692(5)	0.0184(2)	0.0163(2)	0.0152(2)	−0.0016(1)	0.0052(1)	−0.0011(1)
	0.21598(5)	0.14932(3)	0.40191(4)	0.0217(2)	0.0204(1)	0.0178(1)	−0.0009(1)	0.0041(1)	−0.0001(1)
Cr/Se	0.19769(7)	0.16487(8)	0.88691(8)	0.0109(2)	0.0117(2)	0.0126(2)	−0.0003(2)	0.0018(2)	0.0002(2)
	0.19364(3)	0.16510(3)	0.88588(3)	0.0111(1)	0.0093(1)	0.0110(1)	−0.0003(1)	0.0019(1)	0.0000(1)
	0.20107(16)	0.16364(16)	0.88184(19)	0.0093(4)	0.0092(5)	0.0088(5)	−0.0007(3)	0.0027(4)	−0.0014(3)
	0.19595(11)	0.16362(8)	0.88195(10)	0.0171(4)	0.0162(3)	0.0122(3)	−0.0001(2)	0.0015(3)	−0.0003(2)
O(1)	0.2584(4)	0.0055(4)	0.0562(4)	0.023(1)	0.014(1)	0.018(1)	0.002(1)	0.004(1)	0.000(1)
	0.2484(3)	0.0052(3)	0.0552(3)	0.027(1)	0.012(1)	0.016(1)	0.002(1)	0.003(1)	0.003(1)
	0.2538(11)	0.0042(10)	0.0574(12)	0.031(3)	0.018(3)	0.019(3)	0.003(3)	0.006(3)	0.004(3)
	0.2397(12)	0.0057(7)	0.0490(9)	0.048(5)	0.018(2)	0.019(3)	0.006(2)	0.006(3)	0.004(2)
O(2)	0.1201(4)	0.3373(4)	0.0024(5)	0.015(1)	0.018(1)	0.026(1)	0.001(1)	0.006(1)	−0.003(1)
	0.1154(3)	0.3375(3)	−0.0004(3)	0.017(1)	0.014(1)	0.023(1)	0.001(1)	0.006(1)	−0.006(1)
	0.1245(9)	0.3425(8)	−0.0110(12)	0.017(2)	0.017(3)	0.024(3)	0.001(2)	0.009(2)	−0.006(2)
	0.1196(10)	0.3396(7)	−0.0142(9)	0.028(4)	0.021(2)	0.031(3)	0.005(2)	0.011(3)	−0.009(2)
O(3)	0.0256(4)	0.1012(4)	0.6981(5)	0.015(1)	0.023(1)	0.021(1)	−0.006(1)	−0.004(1)	0.001(1)
	0.0192(3)	0.1094(3)	0.6935(3)	0.017(1)	0.021(1)	0.016(1)	−0.006(1)	−0.002(1)	0.000(1)
	0.0295(10)	0.0999(9)	0.6858(12)	0.018(2)	0.020(3)	0.022(4)	−0.005(2)	−0.003(2)	−0.001(2)
	0.0252(9)	0.1102(7)	0.6851(9)	0.016(3)	0.027(2)	0.022(3)	−0.004(2)	−0.003(2)	−0.001(2)
O(4)	0.3776(4)	0.2179(5)	0.7881(5)	0.015(1)	0.025(1)	0.019(1)	−0.002(1)	0.003(1)	−0.004(1)
	0.3752(3)	0.2167(3)	0.7872(3)	0.014(1)	0.024(1)	0.017(1)	−0.003(1)	0.005(1)	−0.001(1)
	0.3859(8)	0.2141(11)	0.7819(11)	0.010(2)	0.029(3)	0.019(3)	−0.001(2)	0.006(2)	−0.002(3)
	0.3806(9)	0.2083(8)	0.7881(9)	0.018(3)	0.034(2)	0.020(3)	−0.005(2)	0.003(2)	−0.007(2)

Table 3. The coordination of the Sr and Pb atoms in the monazite type structures. All distances (in Å) up to 3.50 Å are given. E.s.d.'s in parentheses. Symmetry operators: $^i xyz, ^{ii}\bar{x}\bar{y}1-z, ^{iii}\frac{1}{2}-x\frac{1}{2}+y\frac{1}{2}-z, ^{iv}\frac{1}{2}-x-\frac{1}{2}+y\frac{1}{2}-z, ^{v}\frac{1}{2}+x\frac{1}{2}-y\frac{1}{2}+z, ^{vi}-\frac{1}{2}+x\frac{1}{2}-y-\frac{1}{2}+z$. Average Me$-$O distances are given considering (a) 8-fold and (b) 10-fold coordination for the Me atoms

$SrCrO_4$		$SrSeO_4$		$PbCrO_4$		$PbSeO_4$	
$O(1)^{iii}$	2.575(2)	$O(4)^{vi}$	2.566(1)	$O(3)^{ii}$	2.532(7)	$O(3)^{ii}$	2.562(5)
$O(4)^{vi}$	2.584(2)	$O(1)^{iii}$	2.573(2)	$O(2)^{iv}$	2.553(6)	$O(4)^{vi}$	2.575(6)
$O(3)^{ii}$	2.604(2)	$O(3)^{ii}$	2.579(2)	$O(4)^{vi}$	2.572(6)	$O(2)^{iv}$	2.615(5)
$O(1)^{i}$	2.619(2)	$O(2)^{iv}$	2.643(2)	$O(1)^{i}$	2.592(8)	$O(3)^{i}$	2.654(6)
$O(2)^{iv}$	2.626(3)	$O(1)^{i}$	2.662(2)	$O(3)^{i}$	2.645(7)	$O(1)^{iii}$	2.672(5)
$O(4)^{i}$	2.639(3)	$O(4)^{i}$	2.675(2)	$O(4)^{i}$	2.677(7)	$O(4)^{i}$	2.712(6)
$O(2)^{v}$	2.699(2)	$O(2)^{v}$	2.725(1)	$O(1)^{iii}$	2.687(7)	$O(1)^{i}$	2.715(6)
$O(3)^{i}$	2.762(2)	$O(3)^{i}$	2.763(1)	$O(2)^{v}$	2.808(6)	$O(2)^{v}$	2.814(6)
$O(2)^{i}$	2.917(3)	$O(2)^{i}$	2.978(2)	$O(2)^{i}$	3.081(7)	$O(2)^{i}$	3.151(6)
$O(3)^{v}$	3.264(2)	$O(3)^{v}$	3.286(2)	$O(3)^{v}$	3.440(7)	$O(3)^{v}$	3.443(6)
(a)	2.639	(a)	2.648	(a)	2.633	(a)	2.665
(b)	2.729	(b)	2.745	(b)	2.759	(b)	2.791

starting sets for structure refinements. Their labeling of atoms is maintained. Complex scattering functions for neutral atoms were taken from the International Tables for X-ray Crystallography (1974). The structure parameters are compiled in Table 2.

Discussion

The coordination of the Me atom within the monazite type structure is not clear-cut. Beall et al. (1981) indicate nine coordination for the Me atom in synthetic monazite, $CePO_4$. Nevertheless, in $CePO_4$ as well as in the four isotypic compounds $MeXO_4$ with Me $=$ Sr, Pb and X $=$ Cr, Se (cf. Table 3) ten O atoms have Me$-$O $<$ 3.50 Å. The eight shortest Me$-$O bond lengths within each of the coordination polyhedra differ by $\sim$ 0.20 Å for $CePO_4$ and $SrXO_4$ and by $\sim$ 0.25 Å for $PbXO_4$. Larger gaps are occurring between the eight and the ninth oxygen atom (from 0.14 Å to 0.34 Å) and between the ninth and the tenth neighbouring O atom (from 0.29 Å to 0.40 Å). The coordination numbers of the Me atoms (based on $r_{Me}:r_X:r_O = 1:1:1$) referred to Hoppe (1970) resp. O'Keeffe (1979) are: 7.70/7.76 ($SrCrO_4$), 7.58/7.61 ($SrSeO_3$), 7.60/7.75 ($PbCrO_4$), 7.69/7.94 ($PbSeO_4$) as well as 7.56/7.58 ($CePO_4$). These values are indicators for the similar coordination polyhedra of the Me atoms in all these five members of the monazite type structure.

The geometry of the XO_4 tetrahedra is given in Table 4. It is worth mentioning, that the average Se$-$O bond lengths of 1.640 Å and 1.642 Å in the selenate groups of $SrSeO_4$ and $PbSeO_4$ are equal to each other within

Table 4. The coordination of the Cr and Se atoms for the monazite structure type. Cr—O and Se—O distances (in Å) are underlined. Further O—O distances (in Å) and O—X—O angles (in °) are given. E.s.d.'s in parentheses

SrCrO$_4$	O(1)	O(2)	O(3)	O(4)
O(1)	1.627(3)	106.8(2)	112.0(2)	111.0(2)
O(2)	2.629(4)[a]	1.648(3)	108.9(2)	112.7(2)
O(3)	2.689(4)	2.658(4)[b]	1.618(3)	105.5(2)
O(4)	2.668(4)	2.713(4)	2.571(4)[c]	1.611(2)

SrSeO$_4$	O(1)	O(2)	O(3)	O(4)
O(1)	1.635(2)	105.3(1)	113.9(1)	112.4(1)
O(2)	2.611(3)[a]	1.650(2)	107.4(1)	113.8(1)
O(3)	2.744(3)	2.651(3)[b]	1.639(2)	104.1(1)
O(4)	2.718(3)	2.753(3)	2.582(3)[c]	1.635(1)

PbCrO$_4$	O(1)	O(2)	O(3)	O(4)
O(1)	1.667(7)	107.4(4)	112.5(4)	112.3(4)
O(2)	2.686(10)[a]	1.664(6)	108.9(4)	111.4(4)
O(3)	2.776(11)	2.714(11)[b]	1.672(7)	104.3(4)
O(4)	2.756(11)	2.738(10)	2.624(10)[c]	1.650(6)

PbSeO$_4$	O(1)	O(2)	O(3)	O(4)
O(1)	1.628(5)	106.6(3)	113.8(3)	112.9(4)
O(2)	2.622(8)[a]	1.643(5)	107.2(3)	113.2(3)
O(3)	2.756(9)	2.660(8)[b]	1.662(6)	103.2(3)
O(4)	2.719(9)	2.737(9)	2.584(9)[c]	1.635(6)

There are common O—O edges between the coordination polyhedra of the Sr/Pb and Cr/Se atoms: [a]O(1')—O(2'), [b]O(2')—O(3'), [c]O(3')—O(4') (see Table 3)

limits of error, but on the contrary the average Cr−O bond length in SrCrO$_4$ (1.626 Å) is significantly shorter than the average Cr−O bond length in PbCrO$_4$ (1.663 Å). The same relationships are found for the volumes of the space filling polyhedra of the X atoms ($r_{Me}:r_X:r_O = 1:1:1$): 7.43 Å^3 (SrSeO$_4$) and 7.46 Å^3 (PbSeO$_4$), but 7.27 Å^3 (SrCrO$_4$) and 7.75 Å^3 (PbCrO$_4$). In CePO$_4$ this value is only 6.03 Å^3.

It should be mentioned that the volumes of the space filling polyhedra of the X atoms as well as those of the Me atoms increase from SrCrO$_4$ ($V_{Sr} = 14.93$ Å^3) to SrSeO$_4$ ($V_{Sr} = 15.15$ Å^3); for the lead compounds the increase of the volumes of the space filling polyhedra of the Pb atoms from PbCrO$_4$ (15.13 Å^3) to PbSeO$_4$ (15.69 Å^3) do not correlate with the decrease of those of the X atoms. Depending on the effective ionic radii of Cr$^{6+[4]}$ (0.26 Å) and Se$^{6+[4]}$ (0.28 Å) resp. Sr$^{2+[10]}$ (1.36 Å) and Pb$^{2+[10]}$ (1.40 Å) (Shannon, 1976) one would have to presume a larger selenate tetrahedron as compared with the chromate tetrahedron. Definitely for the chromate and selenate tetrahedra in PbXO$_4$ these two values are interchanged.

The distortion of the XO$_4$ tetrahedra can be expressed by the "mean quadratic elongation" (Robinson et al., 1971, Fleet, 1976): The bond length distortion is defined as $\Delta = \frac{1}{4} \sum_{i=1}^{4} [(R_i - \bar{R})/\bar{R}]^2$ (R_i is the individual X−O bond length and $\bar{R}$ is the average X−O bond length). This parameter calculated for the four title compounds is 2.9×10^{-4} (SrCrO$_4$), 0.6×10^{-4} (SrSeO$_4$), 1.0×10^{-4} (PbCrO$_4$), and 2.4×10^{-4} (PbSeO$_4$). The bond angle variance for the tetrahedron is defined as $\sigma^2 = \frac{1}{5} \sum_{i=1}^{6} (\theta_i - 109.47)^2$ (θ_i is the individual O−X−O angle). σ^2 is 8.48 (SrCrO$_4$), 12.42 (SrSeO$_4$), 10.45 (PbCrO$_4$), and 19.43 (PbSeO$_4$). For CePO$_4$ the distortion of the PO$_4$ tetrahedron can be described with the distortion parameters $\Delta = 0.2 \times 10^{-4}$ and $\sigma^2 = 16.31$.

Considering only the eight shortest Me−O bonds, all the four crystallographically different O atoms are coordinated to one X atom and to two Me atoms. The Me−O−Me angles then vary from 107.6° to 123.9°; one of the two kinds of Me−O−X angles around each oxygen atom varies from 96.3° to 111.1°, the other one varies from 129.1° to 143.0°. Very flat pyramids are built around the atoms O(1) and O(4) (sum of the three angles at the O atoms from 356.4° to 360.0°). The atoms O(2) and O(3) in addition build the ninth resp. tenth Me−O bond (the sum of angles at these O atoms for the three nearest cations varies from 344.1° to 356.1°).

The r.m.s. amplitudes for all the individual atom types are quite similar in the four title compounds. The thermal motion of the Me and X atoms is only weakly anisotropic: the ratio longest by shortest r.m.s. amplitude varies for all these atoms from 1.11 to 1.24. For the O atoms these values vary from 1.33 to 1.86.

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