1·72 and 2·33 Å; the lower limit is typical of those occurring in MoO_4 tetrahedra but it has been reported for MoO_6 octahedra in the structure of sodium dimolybdate (Lindquist, 1950*a*).

Inter-cation distances (Table 4, Fig. 3*a*) also show wide variation, particularly for the edge-sharing octahedra. Distances between cations in octahedra which share corners either within a chain, *e.g.* Co(1)–Mo(1), Mo(2)–Co(2) or between chains, *e.g.* Mo(1)–Co(2) and Co(1)–Mo(2), are close to those found in the complex molybdenum oxides, Mo_8O_{23} and Mo_9O_{26} (Magnéli, 1948), though less than those reported in the complex ions $(Mo_7O_{24})^{6-}$ and $(Mo_8O_{26})^{4-}$ (Lindquist, 1950*b*). On the other hand, the cation distances for the edge-sharing octahedra show a very wide range of distances. Extreme values arise between like cations: *e.g.* Mo(2)–Mo(2) = 3·80 Å compared with Co(1)–Co(2) = 3·07 Å. Other intercation distances compare favorably with those in the complex para- and tetra-molybdate ions.

Why these displacements of the cations from the centers of their octahedra occur is not known, but a study of the magnetic and electrical properties of $CoMoO_4$ might possibly provide pertinent information. There are very few well-refined complex oxide structures reported in the literature, and we believe that the displacements found here are probably more common than one would suspect on the basis of the classic oxide structures, many of which are sorely in need of redetermination or refinement.

It has been reported (Smith, 1962) that nickel molybdate is isomorphous with cobalt molybdate and simple attempts have been made to synthesize the other molybdates of small cations such as Fe, Mg, Mn, and Zn. The X-ray powder photographs of these molybdates all gave exceedingly complex patterns all differing from each other. As the valency state of the iron and manganese in the starting materials was uncertain, the composition of the iron and manganese compounds is in doubt.

However, Young (1964) reports that at ambient pressures $MnMoO_4$ and $MgMoO_4$ give similar diffraction patterns but that $ZnMoO_4$ and $FeMoO_4$ each give unique patterns. It is also reported (Young & Schwartz, 1963) that when the small-cation molybdates are synthesized at high pressures and temperatures the stable structure is of the wolframite type with cell parameters, in each case, very close to those of the tungstate analogues; but after prolonged heating at 600°C reversion takes place to their respective structures at ordinary pressures.

The early calculations were made on a DEUCE computer, using programs written by Dr Rollett, and on an Elliott 803. Thanks are due to Mr D. J. Smith, who made the calculations, for his structure-factor program for the Elliott machine.

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Short Communications

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Stannides and plumbides of Sc, Y, La and Ce with $D8_8$ structure. By W. JEITSCHKO and E. PARTHÉ, *Metallurgy Department, Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, Pa., U.S.A.*

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Introduction

In the past not much attention has been paid to the alloy formation between scandium, yttrium or rare earth elements and tin or lead as second components. AB_3 compounds with Cu_3Au structure type were the only compounds reported which have been analyzed structurally. Partial phase diagrams have been reported for La–Pb (Canneri, 1931) and Ce–Pb (Vogel & Heumann, 1943) based mostly on metallo-

graphic and thermal analysis studies. These two diagrams show compounds with the composition $(RE)_2Pb$ (RE = rare earth element) as the only compound between 50 and 100 at. % RE. However, X-ray studies in related systems demonstrated that phases with composition $(RE)_2X_3$ occur with silicides and germanides of scandium, yttrium and rare earth elements (Parthé, 1960; Arbuckle & Parthé, 1962; Baenziger & Hegenbarth, 1964) and the formation of homolog stannides and plumbides appeared likely. In view of this disagreement between structural studies on silicides and germanides and the result of the phase diagram studies of lead systems, an X-ray investigation of alloys with composition (Sc, Y, La, Ce)$_5$(Sn, Pb)$_3$ seemed to be of interest.

Sample preparation

The starting materials used were 99·9 % cerium, 99·9 % lanthanum, 99 % scandium, 99·99 % lead and 99·9 % tin. The alloy specimens were prepared by arc melting stoichiometric mixtures of the metals. On first sight this method might not seem appropriate since the melting points, for example, of scandium (1539 °C) and lead (327 °C) are more than 1000° apart; however, the boiling point of the lower melting metal (lead 1725 °C, tin 2270 °C) was always above the melting point of scandium, yttrium or cerium and lanthanum. Purgon (purified argon) was used as inert atmosphere during the melting process, and a titanium button was melted prior to each melt. After remelting every sample twice, some specimens were annealed for homogenizing in evacuated quarts tubes for 400 hours at 600 °C. However, it was found that the last step was not really necessary as the samples were found to be homogeneous, even with the arc melting alone.

All samples investigated were rapidly attacked by the water vapor of the air. Therefore, it was necessary to keep the samples in a desiccator. The specimens were ground under ligroin which had been dried with metallic sodium. For the X-ray diffraction experiments, the ground material was put into capillaries and X-rayed while still under dried ligroin. When exposed to moist air, the alloy powder reacts rapidly with the formation of hydrogen. The hydrolysis reaction in the case of La_5Pb_3 is probably as follows:

$$La_5Pb_3 + 15H_2O \rightarrow 5La(OH)_3 + 3Pb + \tfrac{15}{2} H_2$$

Only diffraction lines of hexagonal $La(OH)_3$ (Roy & McKinstry, 1953) and elementary Pb were observed in the reaction product of La_5Pb_3. In the case of Y_5Sn_3 and Y_5Pb_3, only Sn and Pb lines were observed and the hydroxide of Y was present in an amorphous form. Interestingly enough, no oxide lines of lead or tin could be observed in any of these films.

Structure of Sc_5Pb_3

A powder diffraction pattern of Sc_5Pb_3 could be indexed with a hexagonal unit cell of:

$$a = 8{\cdot}467 \pm 0{\cdot}004\,, \quad c = 6{\cdot}158 \pm 0{\cdot}003 \text{ Å}.$$

The extinctions for $h0\bar{h}l$ with $l = 2n+1$ lead to possible space groups $P6_3/mcm$ (D^3_{6h}), $P\bar{6}c2$ (D^2_{3h}), $P6_3cm$ (C^3_{6v}), $P\bar{3}c1$ (D^4_{3d}) and $P3c1$ (C^3_{3v}). The pattern of Sc_5Pb_3 resembles the pattern for (Ti, Zr)$_5$Pb$_3$ which has been reported to crystallize with the $D8_8$ structure (Nowotny, Auer-Welsbach, Bruss & Kohl, 1959). Therefore, in the first trial space group $P6_3/mcm$ (D^3_{6h}) was chosen and 4Sc atoms were placed in position 4(*d*), 6Sc in 6(*g*)$_I$ with $x_I = 0{\cdot}25$ and 6 Pb in 6(*g*)$_{II}$ with $x_{II} = 0{\cdot}61$. The calculated intensities agreed rather well with the observed intensities which showed that the structure of Sc_5Pb_3 is of the $D8_8$ structure type. However, efforts were made to change the adjustable parameters in order to improve the agreement. The intensities of a powder film were measured and corrected for absorption (Bradley, 1935). An absorption correction was necessary here, since – as described above – capillaries had to be used for the powder photograph. The best fit between observed and calculated values was obtained for an x_I value of $0{\cdot}24 \pm 0{\cdot}01$ for the Sc atoms in position 6(*g*)$_I$ and an x_{II} value of $0{\cdot}606 \pm 0{\cdot}002$ for the Pb atoms in postisions 6(*g*)$_{II}$. Owing to the larger scattering power of lead, the parameter value of the latter could be determined more accurately than that for scandium. Table 1 shows the intensity calculation for Sc_5Pb_3 with these parameters.

Isotypic stannides and plumbides

The powder patterns of Sc_5Sn_3, Y_5Sn_3, Y_5Pb_3, La_5Pb_3, and Ce_5Pb_3 could be indexed with similar hexagonal unit cells. The lattice constants, axial ratios and calculated densities are given in Table 2. The intensities of the diffraction lines of Y_5Sn_3, La_5Pb_3 and Ce_5Pb_3 agreed very well with those

Table 1. *Intensity calculation for* Sc_5Pb_3 *with* $D8_8$ *structure* (Cr $K\alpha$ *radiation*)

hkil	d_c(Å)	$10^3 \cdot \sin^2\theta_o$	$10^3 \cdot \sin^2\theta_c$	I_c	I_o
$10\bar{1}0$	7.333	24.4	*)	2.66	*)
$11\bar{2}0$	4.233	73.2	73.8	2.95	2.5
$20\bar{2}0$	3.667	97.6	97.9	1.81	2
$11\bar{2}1$	3.488	107.8	107.8	10.00	10
0002	3.079	138.4	138.1	3.94	4
$10\bar{1}2$	2.839	162.8	-	0.16	-
$21\bar{3}0$	2.771	170.8	171.2	0.63	0.5
$21\bar{3}1$	2.528	205.4	205.6	7.77	8
$11\bar{2}2$	2.490	211.6	211.4	4.82	4
$30\bar{3}0$	2.444	219.6	219.3	3.41	3.5
$20\bar{2}2$	2.358	236.0	236.6	2.32	2.5
$22\bar{4}0$	2.117	292.8	-	0.02	-
$21\bar{3}2$	2.060	309.2	-	0.04	-
$31\bar{4}0$	2.034	317.2	317.5	1.14	1
$22\bar{4}1$	2.002	327.4	327.4	1.65	1.5
$31\bar{4}1$	1.931	351.8	351.5	4.39	4.5
$30\bar{3}2$	1.914	358.0	358.4	1.36	1
$11\bar{2}3$	1.847	384.6	384.4	1.76	2
$40\bar{4}0$	1.833	390.4	-	0.04	-
$22\bar{4}2$	1.780	431.2	431.9	0.48	0.5
$31\bar{4}2$	1.697	455.6	455.8	0.66	0.6
$32\bar{5}0$	1.682	463.6	463.4	0.65	0.6
$21\bar{3}3$	1.650	482.2	482.8	2.29	2.5
$32\bar{5}1$	1.623	498.2	497.8	0.19	0.2
$41\bar{5}0$	1.600	512.4	-	0.00	-
$40\bar{4}2$	1.575	528.8	-	0.00	-
$41\bar{5}1$	1.549	547.0	547.2	0.11	0.2
0004	1.539	553.6	553.6	0.95	0.8
$10\bar{1}4$	1.507	578.0	578.3	0.11	0.2
$32\bar{5}2$	1.476	602.0	603.1	1.91	2.5
$22\bar{4}3$	1.474	604.2		0.87	
$50\bar{5}0$	1.467	610.0	610.4	1.65	1.5
$11\bar{2}4$	1.447	626.8	628.1	0.43	3.5
$31\bar{4}3$	1.445	628.6		2.59	
$41\bar{5}2$	1.420	650.8	651.4	0.47	1
$20\bar{2}4$	1.419	651.2		0.41	
$33\bar{6}0$	1.411	658.8	-	0.02	-
$42\bar{6}0$	1.386	683.2	683.4	1.01	1
$33\bar{6}1$	1.376	693.4	693.4	0.83	0.9
$42\bar{6}1$	1.352	717.8	717.2	3.20	3
$21\bar{3}4$	1.346	724.4	725.0	0.22	0.2
$50\bar{5}2$	1.324	748.4	748.1	4.61	4.5
$51\bar{6}0$	1.317	756.4	756.3	0.23	0.2
$30\bar{3}4$	1.303	773.2	773.6	2.18	2.5
$32\bar{5}3$	1.301	775.0		0.18	
$51\bar{6}1$	1.288	791.0	790.8	0.33	0.4
$33\bar{6}2$	1.283	797.2	-	0.09	-
$42\bar{6}2$	1.264	821.6	822.1	1.52	1.5
$41\bar{5}3$	1.262	823.8		0.13	
$22\bar{4}4$	1.245	846.4	-	0.03	-
$31\bar{4}4$	1.227	870.8	870.8	1.77	2
$60\bar{6}0$	1.222	878.4	-	0.00	-
$51\bar{6}2$	1.211	894.8	-	0.17	-
$43\bar{7}0$	1.206	902.8	-	0.18	-
$43\bar{7}1$	1.183	937.4	937.9	3.56	8
$11\bar{2}5$	1.183	938.2		2.70	
$40\bar{4}4$	1.179	944.0	-	0.14	-
$52\bar{7}0$	1.174	951.6	951.6	1.84	2
$33\bar{6}3$	1.163	970.2	970.1	2.58	4

*) not observed

Table 2. *Lattice constants and theoretical densities of $D8_8$ phases*

Compound	*a*	*c*	*c/a*	*ϱ*
Sc_5Sn_3	8·408 ± 0·004 Å	6·081 ± 0·003 Å	0·7232 ± 0·0005	4·65 g.cm^{-3}
Sc_5Pb_3	8·467 ± 0·004	6·158 ± 0·003	0·7273 ± 0·0005	6·45
Y_5Sn_3	8·878 ± 0·005	6·516 ± 0·004	0·7339 ± 0·0005	5·53
Y_5Pb_3	8·971 ± 0·004	6·614 ± 0·003	0·7373 ± 0·0003	6·93
La_5Pb_3	9·528 ± 0·005	6·993 ± 0·003	0·7339 ± 0·0006	7·32
Ce_5Pb_3	9·473 ± 0·004	6·825 ± 0·002	0·7204 ± 0·0004	7·63

for Sc_5Ga_3 (Schob & Parthé, 1964) and the intensities of Sc_5Sn_3 and Y_5Pb_3 were similar to those of Zr_5Pb_3 (Nowotny & Schachner, 1953). All five compounds, therefore, crystallize with the $D8_8$ structure type. The *d* values and the intensities observed with chromium $K\alpha$ radiation for the five compounds are listed in Table 3*.

Conclusion

The X-ray study has demonstrated that the published phase diagrams for La–Pb and Ce–Pb are not complete, since the phases La_5Pb_3 and Ce_5Pb_3 do not appear in the diagrams. An additional correction is necessary for the diagram Ce–Pb, since it was shown recently that a compound Ce_3Pb exists which crystallizes with a Cu_3Au structure (Jeitschko, Nowotny & Benesovsky, 1964). Therefore, in the system Ce–Pb there occur two compounds with the Cu_3Au structure, one having composition Ce_3Pb, the second $CePb_3$. (Zintl & Neumayr, 1933).

The six new compounds reported here increase the number of known $D8_8$ phases to more than fifty. The available results indicate that the $D8_8$ structure occurs with transition metals of the third to the eighth group as one partner and B elements of the third, fourth and fifth group as the second component. The structure can accommodate a very wide range of size differences of the participating atoms. The size ratio varies from 0·83 for Ti_5Pb_3 to 1·35 for Y_5Si_3. A more detailed study on the characteristics of the $D8_8$ structure type and its variations will appear in the near future.

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* *Note added in proof.* – The compound Y_5Sn_3 has been found recently also by Holmen (1964), who reports the same structure type but slightly larger unit-cell constants.

Table 3. *d values and observed intensities* (Cr $K\alpha$ *radiation*) *for new compounds with $D8_8$ structures*

Sc_5Sn_3			Y_5Sn_3			Y_5Pb_3			La_5Pb_3			Ce_5Pb_3		
hkl	d_c(Å)	I_o	hkl	d_c(Å)	I_o	hkl	d_c(Å)	I_o	hkl	d_c(Å)	I_o	hkl	d_c(Å)	I_o
100	7.281	*)	100	7.689	*)	100	7.769	*)	100	8.251	*)	100	8.204	*)
110	4.204	-	110	4.441	vvw	110	4.485	vvw	110	4.766	-	110	4.736	-
200	3.640	vvvw	200	3.845	-	200	3.885	-	200	4.126	-	200	4.101	-
111	3.459	w	111	3.669	vvw	111	3.713	w	111	3.938	vvw	111	3.891	vw
002	3.040	w	002	3.258	w	002	3.307	w	002	3.497	vw	002	3.413	w
102	2.806	-	102	3.000	vvw	102	3.043	-	102	3.219	-	102	3.150	-
210	2.752	vvw	210	2.906	vw	210	2.937	vw	210	3.120	vvw	210	3.100	vw
211	2.507	ms	211	2.654	s	211	2.684	s	211	2.848	s	211	2.824	s
112	2.464	m	112	2.626	s	112	2.662	ms	112	2.819	ms	112	2.769	s
300	2.427	mw	300	2.563	w	300	2.590	m	300	2.751	ms	300	2.735	ms
202	2.333	w	202	2.485	vw	202	2.518	w	202	2.667	mw	202	2.624	w
220	2.102	-	220	2.219	-	220	2.256	-	220	2.382	-	220	2.368	-
212	2.040	-	212	2.169	-	212	2.196	-	212	2.328	-	212	2.295	-
310	2.020	w	310	2.132	vvw	310	2.155	vw	310	2.289	vw	310	2.275	vvw
221	1.986	w	221	2.101	vw	221	2.124	w	221	2.255	w	221	2.237	vw
311	1.916	s	311	2.027	w	311	2.049	ms	311	2.179	ms,d	311	2.158	m
302	1.897	vw	302	2.015	-	302	2.039		302	2.162		302	2.134	-
113	1.826	w	113	1.951	-	113	1.979	vw	113	2.095	vw	400	2.051	vw
400	1.820		400	1.922	-	400	1.942	-	400	2.063	-	113	2.050	
222	1.729	w	222	1.834	w	222	1.856	mw	222	1.968	w	222	1.946	w
312	1.682	-	312	1.784	-	312	1.804	-	312	1.915	-	312	1.893	-
320	1.671	-	320	1.764	-	320	1.782	vvw	320	1.893	-	320	1.882	-
213	1.632	s	213	1.740	s	213	1.763	ms	213	1.869	ms	213	1.834	s
321	1.611	vw	321	1.703	w	321	1.721	vw	321	1.827	vvw	321	1.814	vvw
410	1.589	-	410	1.678	w	410	1.696	-	410	1.801	-	410	1.790	-
402	1.562	-	402	1.655	w	402	1.675	vvw	402	1.777	vvw	402	1.758	vvw
411	1.537	-	004	1.629	m	004	1.654	mw	004	1.748	m	411	1.732	-
004	1.520	w	411	1.625	-	411	1.642	-	411	1.744		004	1.706	w
104	1.488	-	104	1.594	-	104	1.617	-	104	1.710	-	104	1.670	-
322	1.464	m	223	1.552	mw	223	1.572	m	223	1.668	m	322	1.648	
223	1.459	m	322	1.551		322	1.569		322	1.665		500	1.641	m,d
500	1.456		500	1.538	w	500	1.554	mw	500	1.650	w	223	1.641	
313	1.431	m	114	1.529	-	114	1.552		114	1.641	-	313	1.609	w
114	1.430		313	1.522	vw	313	1.541	m	313	1.635	m	114	1.605	-
412	1.408	vw	204	1.500	-	204	1.521	-	204	1.609	-	412	1.588	vvw
204	1.403	-	412	1.492	vvw	412	1.509	vw	412	1.601	vw	330	1.579	vvvw
330	1.401	-	330	1.480	-	330	1.495	-	330	1.588	-	204	1.575	
420	1.376	w	420	1.451	w	420	1.468	w	420	1.559	vw	420	1.550	vvw
331	1.365	w	331	1.443	w	331	1.458	w	331	1.549	vw	331	1.538	vvw
421	1.342	s	214	1.421	m,d	214	1.441	vvw	214	1.525	ms	421	1.512	w
214	1.331	vw	421	1.418		421	1.433	m	421	1.522		214	1.495	vw
502	1.311	vs	502	1.391	s	502	1.406	s	502	1.492	s	502	1.479	ms,d
510	1.308	-	510	1.381	-	510	1.395	ms	510	1.482		510	1.474	
323	1.289	s	304	1.375	m,d	304	1.394		304	1.475	ms,d	323	1.450	s
304	1.288		323	1.369		323	1.386	vvw	323	1.472		304	1.447	
511	1.278	vvw	511	1.351	m,d	511	1.369	w	511	1.450	vw,d	511	1.440	vvw
332	1.273	-	332	1.347		332	1.362		332	1.446		332	1.431	-
422	1.256	m	413	1.328	vw	413	1.344	w	413	1.427	-	422	1.412	vw,d
413	1.251	-	422	1.327		422	1.342		422	1.424	w	413	1.407	
224	1.232	-	224	1.313	-	224	1.331	-	224	1.409	-	224	1.384	-
314	1.215	m	314	1.295	w	314	1.312	w	314	1.389	w	600	1.367	-
600	1.214	-	600	1.281	-	600	1.295	-	600	1.375	-	314	1.365	vw
512	1.201	-	512	1.271	-	512	1.286	-	512	1.365	-	512	1.353	-
430	1.197	-	430	1.264	-	430	1.277	-	430	1.357	-	314	1.349	-
431	1.174	s	115	1.250	-	115	1.269	vw	115	1.342	vvw	431	1.323	vvw
115	1.168	w	404	1.243	-	404	1.259	-	404	1.314	-	520	1.314	
404	1.167	-	431	1.241	m	431	1.254	m	431	1.332	w	404	1.312	vw
520	1.166	w	520	1.231	vw	520	1.244	w	520	1.321	vvw	115	1.312	
			333	1.223	m	333	1.237	mw	333	1.315	w	333	1.297	-
			521	1.210	m,d	521	1.225	s	423	1.298	ms	521	1.290	vw,d
			423	1.208		423	1.222		521	1.298		423	1.281	m
			324	1.197	-	324	1.214	vw	324	1.284	-	602	1.269	vvw
			602	1.193	s,d	215	1.206		602	1.280	vw	324	1.264	-
			215	1.189		602	1.206	vs	215	1.276	ms	432	1.254	-
			432	1.178	-	432	1.191	-	432	1.264	-	610	1.251	
						610	1.185		610	1.258		215	1.248	vs
						414	1.184	s	414	1.254	w,d	513	1.237	
						513	1.179	vw	513	1.251		414	1.235	w,d
						611	1.166	s	611	1.238		611	1.231	
									522	1.236	w	522	1.226	vw,d
									225	1.206	vw	440	1.184	
									504	1.200	s	504	1.183	vs
									315	1.191	m	225	1.181	
									440	1.191	-	612	1.178	vw
									612	1.184	w	700	1.172	
									700	1.179	vw	530	1.172	s
									530	1.179		315	1.170	

*) not observed
Intensities were not corrected for absorption