Hathaway, B. J. (1984). *Struct. Bonding (Berlin)*, **57**, 55–118.
Hathaway, B. J. & Tomlinson, A. A. G. (1970). *Coord. Chem. Rev.* **5**, 1–43.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
Klobb, M. T. (1890). *Bull. Soc. Chim. Fr.* **3**, 508–510.
Lautié, A., Fromen, F. & Novak, A. (1976). *Spectrosc. Lett.* **9**, 289–299.
Morosin, B. (1969). *Acta Cryst.* B**25**, 19–30.
Müller, A., Böschen, I., Baran, E. J. & Aymonino, P. J. (1973). *Monatsh. Chem.* **104**, 836–847.
Pajunen, A. & Lehtonen, M. (1972). *Suom. Kemistil. B*, **45**, 43–46.
Pitzer, K. S. (1935). *Z. Kristallogr. A*, **92**, 131–135.
Sheldrick, G. M. (1983). *SHELXTL. An Integrated System for Solving, Refining and Displaying Crystal Structures from Diffraction Data*, Version 4.1. Univ. of Göttingen.

Acta Cryst. (1986). C**42**, 945–949

$Lu_5Co_4Si_{14}$, a New Monoclinic Structure Type* Related to $Sc_5Co_4Si_{10}$ and $La_3Co_2Sn_7$

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(*Received* 18 *December* 1985; *accepted* 8 *May* 1986)

Abstract. $Lu_5Co_4Si_{14}$, $M_r = 1503{\cdot}8$, monoclinic, $mP46$, $P2_1/c$, $a = 12{\cdot}245\,(10)$, $b = 7{\cdot}756\,(3)$, $c = 7{\cdot}684\,(4)$ Å, $\beta = 98{\cdot}87\,(3)°$, $V = 721{\cdot}04\,(8)$ Å^3, $Z = 2$, $D_x = 6{\cdot}927$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 413$ cm^{-1}, $F(000) = 1318$, $T = 293$ K, $R = 0{\cdot}048$ for 2108 contributing independent reflections. The structure can be considered as an intergrowth of three different types of slabs. One slab is built up of close-packed Si-centered trigonal rare-earth prisms arranged as in the AlB_2 type. The second slab corresponds to a segment of a ternary $BaAl_4$-derivative structure, constructed of Lu_4Si_4 square antiprisms, but with only one of every two of the available prism centers occupied by Co atoms. The third slab is made up of rare-earth-centered Si cuboctahedra, connected by vertices, and with extra Co atoms positioned in between the polyhedra.

Introduction. In his thesis Yarovets (1978) reported on the new orthorhombic crystal structure of $Ho_3Co_2Si_7$ and 11 isotypic rare-earth–iron(cobalt)–silicon ($R_3T_2Si_7$) compounds. Our attention was retained by the proposed structure model which contains unexpected coordination polyhedra, in the form of very deformed Si cuboctahedra, around part of the rare-earth atoms. Such deformed polyhedra are unexpected and doubtful if one refers to the rare-earth coordination polyhedra observed in closely related structures, such as $La_3Co_2Sn_7$ (Dörrscheidt & Schäfer, 1980). Since the structure was refined to the very poor reliability R-factor value of 0·212, the proposed structure model is not necessarily fully correct.

In view of these unsatisfactory aspects of the original structure determination it appeared of interest to us to study anew this crystal structure. In connection with another study on non-stoichiometric $CeNiSi_2$-type phases in the Lu–Co–Si system (Chabot, Steinmetz & Parthé, 1986) we decided to investigate the crystal structure of '$Lu_3Co_2Si_7$', for which Yarovets reported an orthorhombic A-centered unit cell with $a = 3{\cdot}826$, $b = 24{\cdot}315$ and $c = 3{\cdot}872$ Å. Our experiments demonstrate the existence of a new phase related to Yarovets' results but yet different.

Experimental. Sample of nominal composition $Lu_3Co_2Si_7$ was prepared by arc melting under argon from Lu and Co (99·99%) and Si (99·999%). The sample was then remelted and allowed to cool slowly using a levitation technique. Single crystal of irregular shape with 48 μm mean diameter was obtained from crushed ingots. Automatic four-circle diffractometer (Philips PW 1100), Laue symmetry $2/m$, lattice parameters given in *Abstract* from averaged θ values of 32 reflections and antireflections ($21 < 2\theta < 32°$, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å). Data collection: $\sin\theta/\lambda < 0{\cdot}71$ Å^{-1}, spherical absorption correction $3{\cdot}8 <$ s.a.c. $< 4{\cdot}11$, 2108 unique reflections measured, $-17 \le h \le 17$, $0 \le k \le 10$, $-10 \le l \le 10$; 2 standard reflections (241, $\bar{2}\bar{4}\bar{1}$), ±2·7% variation; ω–2θ scan, ω-scan angle $(1{\cdot}2 + 0{\cdot}1\tan\theta)°$; 2108 observed reflections, 1617 with $|F| > 3\sigma(F)$; systematic absences $h0l$: $l \ne 2n$, $0k0$: $k \ne 2n$ leading to unique space group $P2_1/c$. The structure, however, was initially partially solved in space group $A2/m$ (using Patterson functions) because the weakness of the hkl reflections when $k+l \ne 2n$ led us to assume, erroneously, that the unit cell is A-centered

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instead of primitive. Only a partially ordered structure model could be obtained with the incorrect space group. After testing several of the maximal non-isomorphic subgroups of *A*2/*m*, a satisfactory fully ordered structure was found in $P2_1/c$ which was confirmed by a special least-squares technique (Flack, 1986). It was refined using full-matrix least squares on $|F|^2$ values including all reflections. 47 parameters refined: one scale factor, one secondary isotropic extinction parameter, 45 atomic positional and isotropic displacement parameters.[*] $R = 0{\cdot}048$, $wR = 0{\cdot}064$, $S = 1{\cdot}82$, $w = 1/\sigma^2(F^2_{\rm rel})$, final max. shift/e.s.d. $\leq 2\times10^{-3}$, final residual electron density $(-3{\cdot}4 < \text{r.e.d.} < 4{\cdot}7)$ e Å^{-3}, secondary extinction of type 1 with a Gaussian distribution (Becker & Coppens, 1974) of 22·8 (6) × 10^{-6}. Atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974), all programs used for structure refinement from *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976).

Discussion. Atomic and displacement parameters are given in Table 1, interatomic distances in Table 2.

$Lu_5Co_4Si_{14}$ *related to* $La_3Co_2Sn_7$ *and* $Sc_5Co_4Si_{10}$

A projection of the $Lu_5Co_4Si_{14}$ structure along the *b* axis is shown in Fig. 1. The structure can be considered as an intergrowth of three kinds of structural slabs. Slab type I is built up of close-packed Si[Si(6) and Si(7)]-centered trigonal rare-earth [Lu(1) and Lu(2)] prisms arranged as in the AlB_2 type. Slab type II – there are two slabs per translation period – corresponds to a thin segment of a ternary derivative of the $BaAl_4$ type with the square antiprisms formed by four Si [Si(2,3,4,5)] and four Lu atoms [Lu(1) and Lu(2)]. Only half of the centers of the antiprisms are occupied by transition elements [Co(2)]. The third slab, of type III, is composed of rare-earth [Lu(3)]-centered, corner-connected, deformed cuboctahedra of Si atoms [Si(1,2,3,4,5)] plus extra Co(1) atoms positioned in between the polyhedra. The third slab alone is shown in Fig. 2, in a projection perpendicular to the slab interface. This projection allows not only the cuboctahedra, but also the arrangement of the extra transition-metal atoms [Co(1)] in between these cuboctahedra, to be recognized.

The monoclinic $Lu_5Co_4Si_{14}$ structure is closely related to the orthorhombic $La_3Co_2Sn_7$ structure type (Dörrscheidt & Schäfer, 1980), also found independently for $U_3Fe_2Si_7$ and $U_3Co_2Si_7$ (Akselrud, Yarmolyuk, Rozhdestvenskaya & Gladyshevskii, 1981), and to the

Table 1. *Atom positions for* $Lu_5Co_4Si_{14}$

The isotropic atomic displacement factors are expressed as $T = \exp[-2\pi^2U(2\sin\theta/\lambda)^2]$. E.s.d.'s are given in parentheses.

	Position	*x*	*y*	*z*	*U*(Å^2 × 100)
Co(1)	4(*e*)	0·0000 (2)	0·1261 (2)	0·1275 (2)	0·56 (3)
Si(1)	4(*e*)	0·0006 (4)	0·3335 (4)	0·3351 (4)	0·77 (7)
Si(2)	4(*e*)	0·1792 (5)	0·2256 (6)	0·0512 (5)	0·67 (8)
Si(3)	4(*e*)	0·1791 (5)	0·7751 (6)	0·0382 (5)	0·66 (8)
Si(4)	4(*e*)	0·1795 (3)	0·0060 (6)	0·2686 (4)	0·77 (6)
Si(5)	4(*e*)	0·1798 (3)	0·5068 (7)	0·3191 (3)	0·70 (6)
Co(2)	4(*e*)	0·2506 (1)	0·5004 (4)	0·0611 (2)	0·54 (3)
Lu(1)	4(*e*)	0·36551 (8)	0·25154 (7)	0·34236 (8)	0·47 (2)
Si(6)	4(*e*)	0·4393 (3)	0·0004 (7)	0·1105 (4)	0·76 (6)
Si(7)	4(*e*)	0·4410 (3)	0·4988 (6)	0·1098 (4)	0·68 (6)
Lu(2)	4(*e*)	0·63427 (8)	0·25089 (7)	0·15988 (8)	0·53 (1)
Lu(3)	2(*c*)	0	0	$\frac{1}{2}$	0·50 (2)

Table 2. *Interatomic distances* (Å) *up to* 3·4 Å *for* $Lu_5Co_4Si_{14}$

For the Si atoms all redundant distances have been omitted with the exception of Si(6)–Lu and Si(7)–Lu. E.s.d.'s are given in parentheses.

Lu(1)–Si(6)[a]	2·862 (4)	
Si(7)[a]	2·870 (5)	
Si(7)[a]	2·874 (4)	
Si(6)[a]	2·878 (4)	
Si(2)	2·946 (5)	
Si(4)	2·957 (5)	
Si(2)	2·990 (6)	
Si(5)	2·999 (4)	
Si(6)[a]	3·050 (4)	
Si(7)[a]	3·053 (4)	
Co(2)	3·058 (2)	
Co(2)	3·072 (3)	
Lu(2)–Si(6)[a]	2·856 (4)	
Si(7)[a]	2·882 (4)	
Si(7)[a]	2·885 (4)	
Si(6)[a]	2·889 (4)	
Si(3)	2·941 (6)	
Si(5)	2·946 (4)	
Si(3)	3·000 (5)	
Si(4)	3·005 (4)	
Si(7)[a]	3·027 (4)	
Co(2)	3·055 (3)	
Si(6)[a]	3·056 (4)	
Co(2)	3·070 (2)	
Lu(3)–2Si(1)[b]	2·880 (4)	
2Si(1)[b]	2·881 (4)	
2Co(1)[c]	3·024 (2)	
2Si(4)[b]	3·033 (4)	
2Co(2)[c]	3·032 (3)	
2Si(5)[b]	3·033 (3)	
2Si(2)[b]	3·039 (6)	
2Si(3)[b]	3·041 (5)	
2Co(1)[c]	3·061 (2)	
Co(1)–Si(1)	2·265 (4)	
Si(1)	2·270 (4)	
Si(1)	2·287 (4)	
Si(4)	2·478 (5)	
Si(5)	2·480 (5)	
Si(2)	2·481 (7)	
Si(3)	2·482 (6)	
Co(1)	2·769 (3)	
Lu(3)	3·024 (2)	
Lu(3)	3·061 (2)	
Co(2)–Si(4)[d]	2·283 (3)	[f]
Si(5)[d]	2·283 (4)	
Si(3)[d]	2·300 (5)	
Si(2)[d]	2·301 (5)	
Si(7)[d]	2·303 (4)	
Lu(3)[e]	3·032 (3)	
Lu(2)[e]	3·055 (3)	[f]
Lu(1)[e]	3·058 (3)	
Lu(2)[e]	3·070 (2)	
Lu(1)[e]	3·072 (3)	
Si(1)–Si(2)	2·575 (7)	
Si(3)	2·580 (7)	
Si(5)	2·592 (6)	
Si(4)	2·597 (6)	
Si(2)–Si(4)	2·385 (6)	
Si(5)	2·536 (6)	
Si(5)	2·998 (6)	
Si(4)	3·009 (6)	
Si(3)–Si(5)	2·388 (6)	
Si(4)	2·517 (6)	
Si(5)	2·997 (6)	
Si(4)	3·008 (6)	
Si(6)–Si(7)	2·408 (4)	
Si(6)	2·424 (5)	
Lu(2)[g]	2·856 (4)	
Lu(1)[g]	2·862 (4)	
Lu(1)[g]	2·878 (4)	
Lu(2)[g]	2·889 (4)	
Lu(1)[g]	3·050 (4)	
Lu(2)[g]	3·056 (4)	
Si(7)–Si(7)	2·385 (5)	
Lu(1)[g]	2·870 (5)	
Lu(1)[g]	2·874 (4)	
Lu(2)[g]	2·882 (4)	
Lu(2)[g]	2·885 (4)	
Lu(2)[g]	3·027 (4)	
Lu(1)[g]	3·053 (4)	

(*a*) Si atom in AlB_2-type slab; (*b*) cuboctahedron; (*c*) octahedron; (*d*) small square pyramid; (*e*) large square pyramid; (*f*) square antiprism; (*g*) trigonal prism.

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[*] A list of structure factors, arranged in a standard crystallographic data file (Brown, 1985), has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42925 (39 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

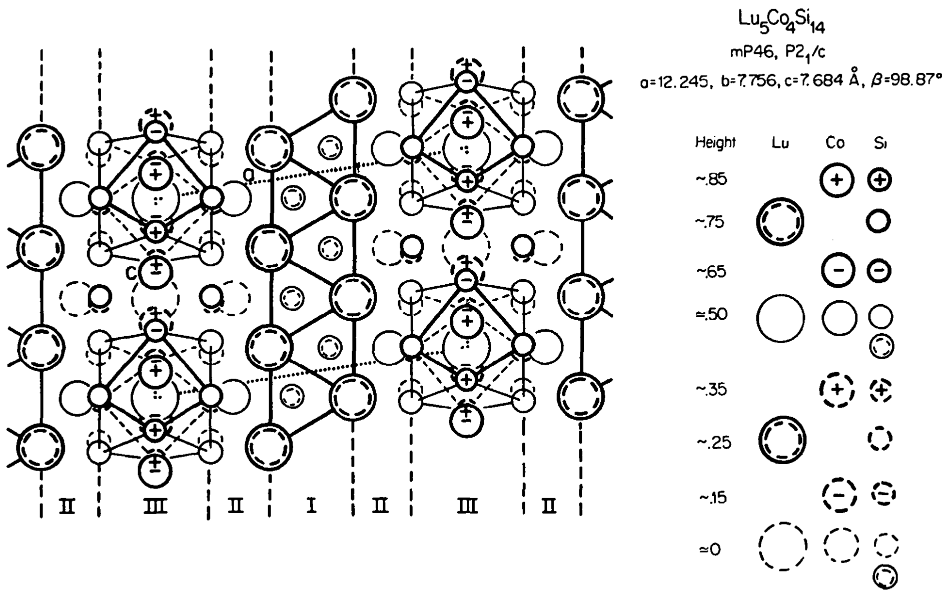

Fig. 1. Projection of the $Lu_5Co_4Si_{14}$ structure along [010]. Roman numerals refer to the structural slabs discussed in the text.

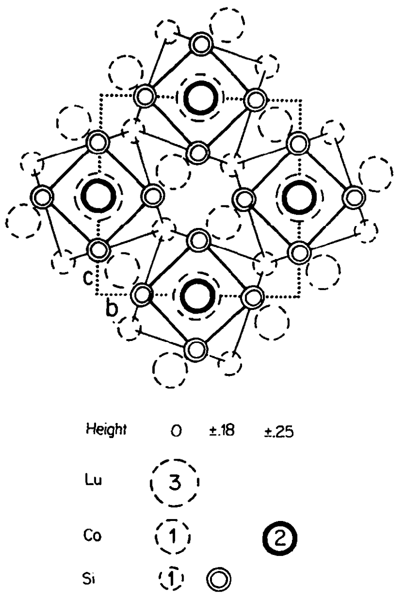

Fig. 2. Projection perpendicular to the slab interface of the cuboctahedron slab. The slab interface is, referred to the $Lu_5Co_4Si_{14}$ cell, parallel to the (100) plane and the height values correspond to the x coordinates of the atoms. The Co atoms drawn with heavy lines [Co(2)] at height ±0·25 already belong to the two neighboring $BaAl_4$-type slabs (type II).

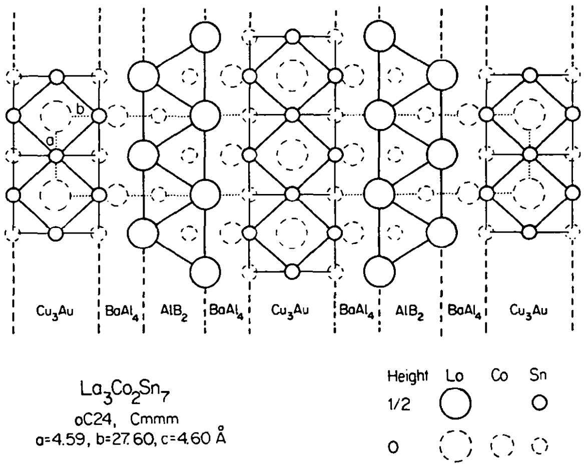

Fig. 3. The orthorhombic $La_3Co_2Sn_7$ structure, interpreted as an intergrowth of AlB_2-, $BaAl_4$- and Cu_3Au-type slabs.

tetragonal $Sc_5Co_4Si_{10}$ structure (Braun, Yvon & Braun, 1980). A comparison of Figs. 1 and 3 shows that $La_3Co_2Sn_7$, as well as $Lu_5Co_4Si_{14}$, consists of three types of intergrown two-dimensional slabs: an AlB_2-type slab, a $BaAl_4$-type slab (occurring twice) and a cuboctahedron slab. One difference with $Lu_5Co_4Si_{14}$ is to be found in the slab containing the rare-earth-centered cuboctahedra which are now face-joined (as in the Cu_3Au type), instead of corner-joined. Further, there are no extra transition-metal atoms in the structure segment. The second difference concerns the $BaAl_4$-type slab. In $La_3Co_2Sn_7$ all the square antiprisms are centered by Co atoms whereas in $Lu_5Co_4Si_{14}$ only half of the the central sites are occupied by a Co atom. Interestingly, the empty sites (vacancies) are arranged in an orderly fashion in this new structure type. In other compounds, on the other hand, as for example in $LuCo_{0.64}Si_2$ with the $CeNiSi_2$ type (an intergrowth of $BaAl_4$- and AlB_2-type slabs), the transition-metal vacancies in the $BaAl_4$-type slab are not ordered (Chabot *et al.*, 1986).

Replacing the two-dimensional AlB_2-, $BaAl_4$- and Cu_3Au-type slabs by their one-dimensional analogs, *i.e.* columns, one can derive the tetragonal $Sc_5Co_4Si_{10}$ structure (Braun *et al.*, 1980), shown in Fig. 4.

One can note from the three drawings of the three related structures that the unshared square faces of the cuboctahedra are always capped by transition elements: in $Lu_5Co_4Si_{14}$ all six square faces are capped (this results in a corner-connected two-dimensional octahedral array of transition elements, as can be deduced from Fig. 2), in $Sc_5Co_4Si_{10}$ only four faces are capped (Co atoms are arranged in the form of a square) while in $La_3Co_2Sn_7$ there are only two capped cuboctahedron faces, which are opposite to each other.

All transition elements belonging to the $BaAl_4$- (or related) type segments, which means all Co atoms for $Sc_5Co_4Si_{10}$ and $La_3Co_2Sn_7$ and only the Co(2) atoms in $Lu_5Co_4Si_{14}$, have the same atom surrounding. It consists of two interpenetrating pyramids (double pyramidal coordination according to Braun, Engel & Parthé, 1983) one formed (first coordination shell) by five Si (or Sn) atoms and the other one built up by five rare-earth (or Sc) atoms. Such typical atom surrounding of the transition element, first mentioned by Braun (1981) for Co atoms in $Sc_5Co_4Si_{10}$, is characteristic of the $BaNiSn_3$ type (a ternary ordered derivative of the $BaAl_4$ type) and has been discussed in detail by Engel, Braun & Parthé (1983) for isotypic $LaIrSi_3$. The remaining transition elements in $Lu_5Co_4Si_{14}$ are located [see Co(1) atoms in Fig. 2] between the cuboctahedra of the type III slabs. They are also surrounded by ten atoms: seven Si atoms belonging to two square faces of two sharing corner cuboctahedra, two Lu(3) atoms centering these two polyhedra and finally another Co(1) atom ($d_{Co-Co} = 2{\cdot}769$ Å). As is generally the case in ternary silicides the Co—Si as well as the Si—Si distances are short and compatible with covalent bonding (see Table 2).

Problems with the $Ho_3Co_2Si_7$ *or* $Lu_3Co_2Si_7$ *structure*

Since the thesis of Yarovets is not easily accessible we reproduce here the data for the $Ho_3Co_2Si_7$ type by referring, however, to the isotypic $Lu_3Co_2Si_7$ compound for the cell parameters. The Yarovets' data are: $a = 3{\cdot}826$, $b = 24{\cdot}315$, $c = 3{\cdot}872$ Å; space group *Amm*2; Ho(1) in 2(*a*) 00*z*, $z = 0{\cdot}0062$; Ho(2,3) in 2(*b*) $\frac{1}{2}0z$, $z = 0{\cdot}3170$, $0{\cdot}6822$; Co(1,2) in 2(*a*), $z = 0{\cdot}1321$, $0{\cdot}8673$; Si(1,2,3,4) in 2(*a*), $z = 0{\cdot}2200$, $0{\cdot}7762$, $0{\cdot}3934$, $0{\cdot}6123$; Si(5,6,7) in 2(*b*), $z = 0{\cdot}0992$, $0{\cdot}8917$, $0{\cdot}5391$.

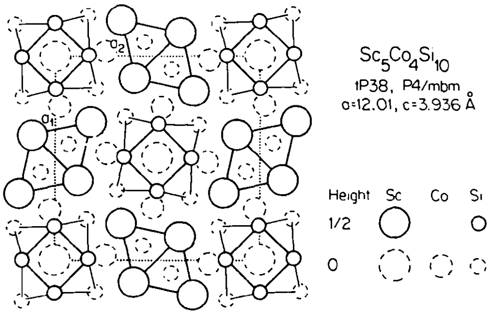

Fig. 4. The tetragonal $Sc_5Co_4Si_{10}$ structure, interpreted as an intergrowth of AlB_2-, $BaAl_4$- and Cu_3Au-type columns.

It is obvious that the given unit cell and the atom coordinates are incompatible. The 24 different *z* parameters for the 24 atoms present in the unit cell must apply to the long translation period. In their structure-data compilation, Gladyshevskii & Bodak (1982) have for this reason described the structure type with the *b* and *c* axes interchanged. This interchange of axes is probably not the correct one since it causes the Si-centered rare-earth prisms present in the structure to be compressed. This compression of the prisms – *i.e.* when the height of the trigonal prism (measured along the trigonal-prism axis) is smaller than the (averaged) side length of its triangular-prism base – is not to be expected with binary and ternary rare-earth silicides (Parthé, 1981; Parthé, Chabot & Hovestreydt, 1983). In contrast, it is known from many examples that the Si-centered trigonal rare-earth prisms are stretched. This is in particular the case in $Lu_5Co_4Si_{14}$, $LuCo_{0.64}Si_2$, $Sc_5Co_4Si_{10}$ and also in the stannide $La_3Co_2Sn_7$. In simple cases one can recognize easily that the trigonal prisms are stretched from the value of the appropriate cell-parameter ratio, *i.e.* for $Lu_5Co_4Si_{14}$ ($P2_1/c$): $b/c > 1$, for $LuCo_{0.64}Si_2$ with the $CeNiSi_2$ type (*Cmcm*): $a/c > 1$ and for $La_3Co_2Sn_7$ (*Cmmm*): $c/a > 1$. The correct interchange of the Yarovets' cell parameters should assure the presence of stretched trigonal prisms. For this reason we believe that a cyclic permutation should be performed which, in the case of $Lu_3Co_2Si_7$,

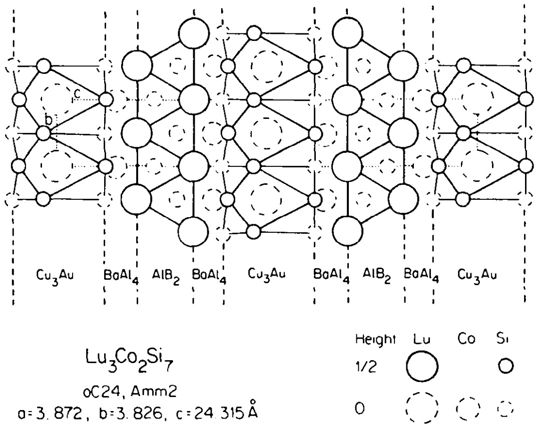

Fig. 5. The orthorhombic structure of $Lu_3Co_2Si_7$ with the $Ho_3Co_2Si_7$ type. The structure drawing refers to Yarovets' data but with an interchange of the original unit-cell parameters to assure that the long axis is the *c* axis and that the Si-centered trigonal Lu prisms are stretched.

results in: $a = 3{\cdot}872$, $b = 3{\cdot}826$ and $c = 24{\cdot}315$ Å. The structure of $\mathrm{Lu_3Co_2Si_7}$, shown in Fig. 5, is described with these permutated unit-cell parameters. The structure consists of $\mathrm{AlB_2}$-type slabs intergrown with double the number of $\mathrm{BaAl_4}$-type slabs and strongly deformed $\mathrm{Cu_3Au}$-type slabs. In rough approximation the structure thus resembles the $\mathrm{La_3Co_2Sn_7}$ structure (Fig. 3).

Whether or not an $\mathrm{Ho_3Co_2Si_7}$-type phase exists in the Lu–Co–Si phase diagram is a difficult question to answer. We can report, however, from microprobe analyses, the existence of a phase with a composition compatible with 5:4:14, but not with 3:2:7, in three samples prepared at nominal compositions: $\mathrm{Lu_3Co_2Si_7}$ (1073 K/7 d), $\mathrm{Lu_3Co_2Si_8}$ (1073 K/7 d) and $\mathrm{Lu_5Co_4Si_{14}}$ (levitated). We cannot exclude the possibility that an $\mathrm{Ho_3Co_2Si_7}$-type phase is stable in a different temperature range. In our opinion, however, the coordination around the rare-earth atoms in the $\mathrm{Cu_3Au}$-type slab is unlikely and the crystal structure of $\mathrm{Ho_3Co_2Si_7}$ should be reinvestigated. We have tried, on the other hand, to correlate the lattice constants reported for '$\mathrm{Lu_3Co_2Si_7}$' with those of $\mathrm{Lu_5Co_4Si_{14}}$ assuming, on a hypothetical basis, that a displacement by $\frac{1}{2}c$ of the triple slab (II–III–II) shown in Fig. 1 is possible. This shift will not change the interaction with the neighboring $\mathrm{AlB_2}$ type slabs but should lead, when randomly repeated in the crystal, to an A-centered pseudotetragonal orthorhombic unit cell with a metric very similar to the unit-cell parameters given by Yarovets. Naming the original orthorhombic cell parameters A, B and C, the corresponding monoclinic cell parameters of $\mathrm{Lu_5Co_4Si_{14}}$ are obtained as follows: $a = \frac{1}{2}(A^2 + B^2)^{1/2}$, $b = 2C$, $c = 2A$, $\beta = 90° + \mathrm{arctg}\,A/B$. Applying these equations to the original orthorhombic data given by Yarovets for the '$\mathrm{Lu_3Co_2Si_7}$' compound leads to the following monoclinic parameters: $a = 12{\cdot}307$, $b = 7{\cdot}744$, $c = 7{\cdot}652$ Å and $\beta = 98{\cdot}94°$. These values are in acceptable agreement with the lattice parameters reported for $\mathrm{Lu_5Co_4Si_{14}}$ in this work.

We would like to thank Dr J. Steinmetz (Laboratoire de Microanalyse, Université de Nancy I, France) for the electron microprobe analyses. We acknowledge the help of Mrs Birgitta Künzler with the preparation of the drawings and technical assistance from F. Liniger. The study was supported by the Swiss National Science Foundation under contract 2·604–0·85.

References

Akselrud, L. G., Yarmolyuk, Ya. P., Rozhdestvenskaya, I. V. & Gladyshevskii, E. I. (1981). *Sov. Phys.-Crystallogr.* **26**, 103–104.

Becker, P. J. & Coppens, P. (1974). *Acta Cryst.* A**30**, 129–147.

Braun, H. F. (1981). *Ternary Superconductors,* edited by G. K. Shenoy, B. D. Dunlap & F. Y. Fradin, pp. 225–231. New York: Elsevier.

Braun, H. F., Engel, N. & Parthé, E. (1983). *Phys. Rev. B,* **28**, 1389–1395.

Braun, H. F., Yvon, K. & Braun, R. M. (1980). *Acta Cryst.* B**36**, 2397–2399.

Brown, I. D. (1985). *Acta Cryst.* A**41**, 399.

Chabot, B., Steinmetz, J. & Parthé, E. (1986). *J. Less-Common Met.* Submitted.

Dörrscheidt, W. & Schäfer, H. (1980). *J. Less-Common Met.* **70**, P1–P10.

Engel, E., Braun, H. F. & Parthé, E. (1983). *J. Less-Common Met.* **95**, 309–315.

Flack, H. D. (1986). *Acta Cryst.* To be submitted.

Gladyshevskii, E. I. & Bodak, O. I. (1982). In *Crystal Chemistry of Intermetallic Compounds of the Rare Earth Metals* (in Russian). Lvov: Vishcha Shkola Publishing House.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

Parthé, E. (1981). *Structure and Bonding in Crystals,* Vol. 2, ch. 25, edited by M. O'Keeffe & A. Navrotsky, pp. 259–296. New York: Academic Press.

Parthé, E., Chabot, B. & Hovestreydt, E. (1983). *Acta Cryst.* B**39**, 596–603.

Stewart, J. M., Machin, P. A., Dickinson, C. W., Ammon, H. L., Heck, H. & Flack, H. (1976). The *XRAY*76 system. Tech. Rep. TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland.

Yarovets, V. I. (1978). Thesis, Ivan Franko Univ. Lvov, USSR.

Acta Cryst. (1986). C**42**, 949–952

Structure of Hexasodium *trans*-Diaquatetrasulfatozinc(II)

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(*Received* 21 *November* 1985; *accepted* 17 *March* 1986)

Abstract. $\mathrm{Na_6[Zn(SO_4)_4(H_2O)_2]}$, $M_r = 623{\cdot}6$, triclinic, $P\bar{1}$, $a = 6{\cdot}052\ (1)$, $b = 6{\cdot}815\ (1)$, $c = 10{\cdot}141\ (2)$ Å, $\alpha = 70{\cdot}07\ (2)$, $\beta = 77{\cdot}29\ (2)$, $\gamma = 74{\cdot}72\ (2)°$, $V = 375{\cdot}41\ (1)$ Å^3, $Z = 1$, $D_x = 2{\cdot}758$ g cm^{-3}, $\lambda(\mathrm{Mo}\ K\alpha) = 0{\cdot}71069$ Å, $\mu(\mathrm{Mo}\ K\alpha) = 25{\cdot}1$ cm^{-1}, $F(000) = 308$, room temperature, $R = 0{\cdot}029$ for 1272 observed

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0108-2701/86/080949-04$01.50