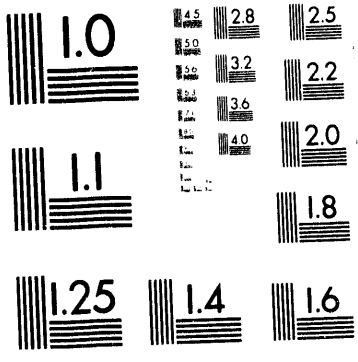
1.0
1.1
1.25
1.4
1.6
1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
4.5
5.0
5.6

1 of 1

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THE NEW METALS AND ALLOYS INDEXES — SEARCH MANUAL A PHASE DIAGRAM RESEARCH TOOL†

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THE NEW METALS AND ALLOYS INDEXES — SEARCH MANUAL

A PHASE DIAGRAM RESEARCH TOOL†

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Abstract

A new **Metals and Alloys (M&A) Indexes** to the Powder Diffraction File (PDF) has been developed. These indexes will be immediately useful to material scientists because the indexes share many features with references such as Hansen, Elliot, Shunk, Pearson, and Villars and Calvert. These indexes, as contained in the *Search Manual*, may be used independently or in conjunction with the Powder Diffraction File. The book contains four indexes: two contain data for all materials in the M&A PDF, and two contain supporting data. The permuted-sort **Alphabetical Formula Index** brings together all entries containing a given element in alphabetical formula order. It has *n* entries for an *n*-component material and a straight-line format for the element being sorted to simplify reading the index. Thus, chemical knowledge can make identifications easier. Further, within binary and ternary phase diagrams, phases are listed in compositional order to facilitate direct use in phase diagram research. The **Pearson Symbol Code Index** has entries arranged in order of the Pearson Symbol Code, hence one can find all the materials with a given structure, and if desired, compare their atomic contents and lattice parameters. The latter are in the standard Crystal Data setting to aid in structural comparisons. The **Common Names Index** cross-references common metallurgical names, such as austenite or cementite, to the appropriate PDF data. The **Strukturbericht Symbol Index** cross-references Strukturbericht Symbols and the equivalent Pearson Symbols and Structure Prototypes. Examples of the uses of this index in phase diagram research are given.

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Introduction

A book entitled, *Metals and Alloys Indexes — Search Manual*,[1] has recently been made available by the International Centre for Diffraction Data (ICDD) — formerly known as the Joint Committee for Powder Diffraction Standards (JCPDS). This *Search Manual*[1] is a result of a group effort of the Metals and Alloy subcommittee of the ICDD. The organization of this book is based on the format used by Hansen, Elliott, Shunk, and Pearson in the 1950's and 60's and later by Villars and Calvert in the 1980's and 90's. Thus, this *Search Manual* is a combination of a metals and alloys index of powder diffraction data and structural data in an easy to use format.

A large part of the contents of this *Search Manual* came from and is related to the x-ray Powder Diffraction File (PDF) and may be used with this file or independently. Most of you will remember the PDF as a set of "cards" issued annually (~2,000 cards each year) with accompanying index books to aid in search for known materials or in matching one's unknown pattern. Over a period of years, some 60,000 cards have been made available on tapes, micro-fiche and, more recently, on CD-ROM with annual updates of ~2,000 materials covering a full range of materials; metals, inorganic, organics, clays, minerals, ceramics, etc. Considerable software is also available for searching and matching. This new *Metals and Alloys Indexes — Search Manual*[1] involves the metallic phases including carbides, oxides, nitrides, hydrides and borides taken from the larger set. There are more than 10,000 entries in this *Search Manual*, which are multi-listed depending on if they are single element, binary, or ternary intermetallics.

This present new *Search Manual* can best be used in conjunction with, and as a supplement to, the ASM three-volume set of *Binary Alloy Phase Diagrams*[2] and to the ASM four-volume set of Villars and Calvert's *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*.[3] The first section of Villars and Calvert's and the present *Search Manual* are somewhat similar in that both give an alphabetical listing of the intermetallics and space group. Villars and Calvert list the Pearson Symbol Code as a whole number, however, in the *Search Manual*[1] it is the ACTUAL number of atoms in the observed structure. In addition, the PSC section gives the diffraction data (see description in the Alphabetical Formula Index Section and Figures 1 and 2, see next page). The list of intermetallics is indeed more extensive in the four volume set of Villars and Calvert than in the present one volume *Search Manual* since diffraction data is not available for all of the intermetallics as listed by Villars and Calvert. However, as will be shown later, diffraction data available in an organized form can assist in suggesting and possibly identifying structures of intermetallics not previously reported.

The objectives of this compilation of *Metals and Alloys Indexes — Search Manual*[1] are:

- to make characterization of samples easier by providing a new formula index that allows systematic searches for chemical analogs and greater use of partial chemical knowledge, which may add structural information to partial phase diagrams;

- to make characterization of new materials easier and more accurate by providing new structural indexes;

- to aid in using and editing the Metals & Alloys subfile of the Powder Diffraction File (PDF), so that new structural data and existing data may be included in the PDF using information derived from within these indexes.

This book is designed to be used in conjunction with or independently of the Powder Diffraction File (PDF) and contains the following four indexes:

- Alphabetical Formula Index (AFI);
- Pearson Symbol Code Index (PSCI);
- Common Names Index (CNI);
- Strukturbericht Symbol Index (SSI).

Alphabetical Formula Index (AFI)

The AFI contains:

- all of the phases in the Powder Diffraction File (PDF) of the Metals and Alloys subfile (~ 10,000 plus phases);
- a chemically-based alphabetical index consistent with *Binary Alloy Phase Diagrams*[2] and *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*[3] (see Figures 1 and 2 for alphabetical arrangement);
- *n* entries for *n*-component material, which allows for entry using incomplete chemical analysis;
- the Formula, the Pearson Symbol Code, Space Group, Cell Parameters, Three Strongest Lines, PDF #, and Quality Mark for the data, as discussed on the next page, (the last three items concerning the diffraction data are unique to this *Search Manual* and are not given in Villars and Calvert[3]);
- the space group, which conforms to the lattice setting in *Crystal Data*,[4] insures that all examples of a given type have their unit cell parameters directly comparable.

In some cases, some of the data may be incomplete in the AFI Section, as shown in Figure 1. If a portion of a Pearson Symbol Code (PSC) or Space Group is missing, it may be designated by an asterisk. In limited cases "d" spacings may be given with no indication of its crystal structure.

Formula	PSC	Space Group		Cell Parameters			Three Strongest d-Values and Intensities			PDF #	QM
		Symbol	(#)	[a α]	[b β]	[c γ]					
$CCr_{2.4}Pt_{1.7}$	cP5	Pm3m	(221)	3.820			2.20_x	2.70_6	1.91_6	18-391	
$CCr_{4.5}Si_{2.5}$	hP16	$P6_3/mcm$	(193)	6.993		4.725	2.06_x	1.95_9	2.01_8	9-242	
Al_2CCrTe_5	cF112	Fd3m	(227)	11.580			2.23_x	2.36_8	2.66_6	18-11	
C_4Cr_4U	tI18	I4/m	(87)	7.936		3.075	2.51_x	2.33_x	5.62_8	40-1029	i
C_2CrU	oP16	Pnam	(62)	5.433	10.816	3.231	2.46_x	2.20_5	1.72_5	12-464	
$C_{12}Cr_2V$	oC20	Amam	(63)	6.990	9.300	2.870	2.08_x	2.55_8	2.16_8	19-334	
$C_{20}Cr_{23}V_{33}$	oP12.5	P***		5.012	5.736	4.530	2.18_x	2.50_5	2.49_5	18-401	
$C_{16}Cs$	h**			4.950		18.550	3.09_x	3.52_6	2.02_6	4-611	
C_8Cs	h**			4.950		23.810	2.97_x	2.01_8	4.21_6	4-662	
C_8Cs	hP27	$P6_322$	(180)	4.945		17.760	3.47_x	4.28_9	2.44_5	33-348	c
B_1C_4Cs							2.87_x	5.75_4	2.29_5	40-1197	o
$Bi_{0.50}C_4Cs$							2.66_x	2.14_7	1.78_4	40-1196	o
CCs_2S_3							3.34_x	3.48_9	3.13_8	21-226	
CCs_2S_3							3.50_x	3.15_5	2.67_5	21-227	
$CCs_{0.54}S_2Te_2$	h**			3.297		22.440	11.2_x	2.42_8	1.65_8	32-265	
$Al_{11}C_6Cu_3Mo_{12}$	hP32	$P6_3/mmc$	(194)	7.952		7.865	2.21_x	2.17_8	2.45_6	19-12	
$CCuRbS_3$	o*24			9.730	10.130	6.070	3.03_x	3.21_8	9.78_5	27-520	
$CCu_{0.60}S_2Te_2$	hP7	$P\bar{3}m1$	(164)	3.292		8.939	8.89_x	2.40_8	1.65_7	26-560	i

Figure 1 Section from the *Search Manual*[1] (p. 76) showing arrangement of data in the Alphabetical Formula Index (AFI) Section.

It should be noted in Figure 1 that the letter **C** is in bold face type and does not necessarily appear at the beginning of the Formula; i.e., Al_2CCrTa_3 — the third line in the figure. The section shown in Figure 1 is in the **C** section of the alphabetical index. This means that this particular intermetallic, Al_2CCrTa_3, will also appear in three other locations of the alphabetical index; namely, in the Al, Cr and Ta sections as $\mathbf{Al}_2CCrTa_3$, $Al_2\mathbf{C}CrTa_3$, and $Al_2CCr\mathbf{Ta}_3$. Thus, the Alphabetical Formula Index (AFI) has entries for an *n*-component material in *n* different locations. In Figure 1, last column, there are Quality Marks (QM) assigned by the editor of PDF to the x-ray patterns and may have one of the following: an "*" mark — good complete patterns; "i" mark — reasonable but may have a maximum of two unindexed diffraction lines; "o" mark — low precision; "c" mark — calculated pattern.

Figure 2 is included to show the ease of relating the ASM phase diagrams[2] to the ASM crystallographic data[3] to the order of the intermetallic listing in the present *Search Manual*. For example, in the Pb-Pu system, there are six low-temperature phases (shown in both Refs. 2 and 3). These same phases are listed in the *Search Manual* in order from phases rich in Pb to those rich in Pu, thus the order is $\mathbf{Pb}_3Pu$ to $\mathbf{Pb}Pu_3$ (see Figure 2). Indeed, in some cases, more than one listing is shown for a given intermetallic, which can be evaluated based on the quality of data (QM).

Formula	PSC	Space Group		Cell Parameters			Three Strongest d-Values and Intensities			PDF #	QM
		Symbol	(#)	[a α]	[b β]	[c γ]					
Pb_3Pu	cP4	Pm3m	(221)	4.806			1.45_x	2.39_7	2.75_6	23-456	
Pb_3Pu	cP4	Pm3m	(221)	4.808			2.78_x	2.40_3	1.45_3	41-1189	c
Pb_2Pu	tI24	$I4_1/amd$	(141)	4.621		31.290	2.77_x	2.59_3	2.31_3	22-392	o
Pb_2Pu	tI24	$I4_1/amd$	(141)	4.621		31.290	2.77_x	2.31_3	1.41_2	41-1190	c
Pb_3Pu_4	hP54	$P6_322$	(182)	16.520		6.440	2.73_x	2.65_x	2.78_3	22-393	o
Pb_4Pu_5	hP18	$P6_3/mcm$	(193)	9.523		6.482	2.74_x	2.80_9	2.66_9	22-670	
Pb_4Pu_5	hP18	$P6_3/mcm$	(193)	9.523		6.482	2.68_x	2.75_9	2.81_4	41-1191	c
Pb_3Pu_5	tI32	I4/mcm	(140)	12.310		6.084	2.73_x	2.66_x	1.48_1	22-395	
Pb_3Pu_5	tI32	I4/mcm	(140)	12.310		6.084	2.68_x	2.75_3	2.73_4	41-1192	c
$PbPu_3$	cP4	Pm3m	(221)	4.737			2.73_x	1.68_4	1.43_3	22-394	
$PbPu_3$	cP4	Pm3m	(221)	4.737			2.74_x	2.37_3	1.43_3	41-1193	c
Pb_2Rh	tI12	I4/mcm	(140)	6.674		5.831	2.66_x	2.20_4	2.11_4	25-454	i
Pb_3Rh_4	oF72	Fmmm	(69)	9.840	26.510	5.711	2.16_x	2.83_9	2.15_8	26-1153	i
$Pb_{12}Rh_{13}$	hP6	P6/mmm	(191)	5.678		4.428	2.15_x	3.29_8	2.84_8	26-1152	
Pb_2Rh_3	hP4	$P6_3/mmc$	(194)	4.330		5.639	2.26_x	2.17_x	3.14_8	26-1154	

Figure 2 Section from the *Search Manual*[1] (p. 269) showing the order of the intermetallics in the Pb-Pu and Pb-Rh systems, as compiled in the AFI Section.

Pearson Symbol Code Index (PSCI)

A sample from the Pearson Symbol Code Index (PSCI) Section of the *Search Manual* is shown in Figure 3. You will note that all entries with the same Pearson Symbol Code (PSC) are grouped together (all being tP10 in this table). Each entry contains the PSC: prototype structure (note Pu_3Si_2 does not have one), example formula, space group and its number, lattice parameters, according to *Crystal Data*[4] setting, axial ratios, and PDF number with quality mark (QM). Under each PSC the entries are sorted first by space group number, then alphabetically by prototype structure formula. This index (PSCI) contains entries for all materials in the Powder Diffraction File (PDF) in the Metals and Alloys subfile, including

those that have either partial PSC or none at all. Alloys without symbols are located at the end of the index and are sorted in alphabetical formula order.

PSC	Prototype Structure	Example Formula	Space Group		Tetragonal Cell Parameters		Tetragonal Axial Ratio	PDF #	QM
			Symbol	(#)	a	c	c/a		
tP10	Pd_4Se	Pd_4S	$P\bar{4}2_1c$	(114)	5.115	5.590	1.09	10-335	
tP10	Pd_4Se	Pd_4Se	$P\bar{4}2_1c$	(114)	5.232	5.647	1.08	11-498	
tP10	Be_2CaGe_2	$LaPd_2Sb_2$	P4/mmm	(123)	4.627	10.422	2.25	37-1300	i
tP10	Pb_4Pt	Pb_4Pt	P4/nbm	(125)	6.640	5.970	0.90	6-463	
tP10		Pu_3Si_2	P4/mbm	(127)	7.483	4.048	0.54	41-1208	c
tP10	Si_2U_3	AlBCrFeMoNiTi	P4/mbm	(127)	5.783	3.134	0.54	26-10	
tP10	Si_2U_3	$AlCo_2U_2$	P4/mbm	(127)	7.091	3.461	0.49	20-762	i
tP10	Si_2U_3	$AlCu_2Re_2$	P4/mbm	(127)	5.716	3.176	0.56	41-1321	c
tP10	Si_2U_3	Al_2Th_3	P4/mbm	(127)	8.130	4.220	0.52	7-308	i
tP10	Si_2U_3	B_2CrNb_2	P4/mbm	(127)	5.925	3.240	0.55	26-434	
tP10	Si_2U_3	$B_2Cr_{1.5}Ta_{1.5}$	P4/mbm	(127)	9.905	3.231	0.55	27-866	i
tP10	Si_2U_3	B_2FeMo_2	P4/mbm	(127)	5.775	3.145	0.54	18-839	
tP10	Si_2U_3	B_2FeMo_2	P4/mbm	(127)	5.807	3.142	0.54	20-525	
tP10	Si_2U_3	B_2FeW_2	P4/mbm	(127)	5.690	3.162	0.56	21-437	
tP10	Si_2U_3	$B_2Fe_{1.25}W_{1.75}$	P4/mbm	(127)	5.753	3.161	0.55	23-306	

Figure 3 A short section of the Pearson Symbol Code Index (PSCI) taken from the Tetragonal Section of the *Search Manual*[1] (p. 529).

Two other rather short but important Sections of the *Search Manual* are:

Common Names Index (CNI)

This section permits cross-referencing to common metallurgical and mineral names. It includes some mixtures with reference to their component phases (i.e., pearlite referenced to αFe and CFe_3, provides reference to phase groups such as sigma and Laves phases). This index includes Common Name, Formula, Pearson Symbol Code (PSC), as given in Ref. 3, Powder Diffraction File (PDF) Number, and Quality Mark (QM), as shown in Figure 4.

Common Name	Formula	PSC	PDF #
Austenite	$C_{0.35}Fe_{10}$	cF4	31-619
Austenitic Steel	$Cr_{0.19}Fe_{0.70}Ni_{0.11}$	cF4	33-397
Austenitic Steel	$Co_{0.70}Fe_{0.36}Ni_{2.90}$	cF4	33-945
Baddeleyite	O_2Zr	mP12	37-1484
Bainite (lower) (a mixture of iron and iron carbide formed when austenite is decomposed)	C,Fe	cI2	
Bainite (upper)	ϵ-CFe_3 or ϵ-Fe	hP8	

Figure 4 A short section of the Common Names Index (CNI) taken from the *Search Manual*[1] (p. 654).

Strukturbericht Symbol Index (SSI)

As shown in Figure 5, this file provides cross-reference between the old *Strukturbericht Symbols*,[5] the prototype structures, and the Pearson Symbol. In some cases subsequent work has resulted in changes of prototype, as required, or that different symbols correspond to the same structure. For convenience, all equivalent symbols are fully cross-referenced.

Strukturbericht Symbol [A]	Prototype Structure	Pearson Symbol
A1	Cu	cF4
A2	W	cI2
A3	Mg	hP2
A4	C, diamond	cF8
A5	β-Sn, white	tI4
A6	In	tI2
A7	As	hR2
A8	Se	hP3
A9	C, graphite	hP4
A10 [B]	Hg	hR1
A11 [C]	Ga	oC8
A12	α-Mn	cI58
A13	β-Mn	cP20
A15	Cr_3Si (B-W)	cP8

[A] It should be noted that the format used here is that used in Vols. II-VII of Strukturbericht (SB) e.g. Vol. I used D_2 for $D0_2$ and D51 for $D5_1$.
[B] SB I,31 gives an incorrect description; SB I,737 is correct.
[C] SB I,738 gives an incorrect description; SBIII,3 is correct.

Figure 5 Small section from the *Search Manual*[1] (p. 671) showing typical Strukturbericht listing.

There are also several Appendices:

Pearson Symbol (PS) and Pearson Symbol Code (PSC)

The Pearson Symbol is given as a useful reference for locating phases with the same structure. It may be recalled that Pearson[7] proposed the lower case letters:

a	for	triclinic	t	for	tetragonal
m	for	monoclinic	h	for	hexagonal
o	for	orthorhombic	c	for	cubic

and the second (capital) letter to represent:

P	for a	Primitive Cell	F	for a	Face-Centered Cell
C	for a	Centered Cell	R	for a	Rhombohedral Cell
I	for a	Body-Centered Cell			

Thus, the 14 mnemonic combinations designates the 14 Bravais lattices, as per Pearson,[6] are:

cP cF cI | hR hP | tP tI | oP oC oI oF | mP mC | aP

It is very important to point out that a Pearson Symbol would consist of a combination of the two letters together with the number of atoms in the ideal, completely filled, prototype model

structure, whereas the Pearson Symbol Code (as used in the present *Search Manual*) uses the actual number of atoms in the observed structure (i.e., CTa is cF8 and $C_{0.71}Ta$ is $hR_{6.1}$).

Atomic Volumes

The data shown in Figure 6 are useful for estimating unit cell contents for metallic compounds with close packing of atoms in which some substitution has taken place. The use of this information will be shown under the Application Section.

Atomic Number	Element	Valence Electrons	Volume Å
89	Ac	3	37.3
47	Ag	1	17.0
95	Am	4	29.2
33	As	5	21.5
5	B	3	7.3
4	Be	2	8.1
83	Bi	5	35.3
6	C	4	5.6
20	Ca	2	43.3
48	Cd	2	21.5
58	Ce	3	35.5
58	Ce	4	26.3
27	Co	9	11.1

Figure 6 Taken from the *Search Manual*[1] (p. 12) Appendix C — Atomic Volumes. Useful for estimating unit cell contents for metallic compounds with close packing of atoms.

Application

One application is to use the Alphabetical Formula Index (AFI) and the Pearson Symbol Code Index (PSCI) to assign a prototype structure to an indexed pattern.

For example, the original PDF #2-722 (Figure 7a) was an indexed pattern of CrTe with the Pearson Symbol Code (PSC) and prototype structure unknown. Searching the AFI for binary compounds of Cr with S or Se that have monoclinic cells, one finds the following:

Formula	PSC	S.G.	a	b	c	β	PDF #
CrTe orig.	—	C2/m	6.85	3.82	6.09	91.12	2-722
Cr_3S_4	mC14	I2/m	11.272	3.428	5.964	91.50	11-8
Cr_3S_4	mC14	I2/m	11.270	3.425	5.960	91.53	24-310
Cr_3Se_4	mC7	C2/m	6.310	3.610	5.864	91.50	2-1328
Cr_2Se_3	mC*	I2/m	11.528	3.582	6.227	90.77	23-930
Cr_3Te_4 rev.	mC14	C2/m	6.850(3)	3.917(2)	12.179(4)	91.16(5)	2-722 rev.

CrTe

Chromium Telluride

Rad. CrKα λ 2.2909 Filter d-sp
Cutoff Int. Visual $I/I_{cor.}$
Ref. Haraldsen, Neuber, Z. *Anorg. Chem.*, 234 365 (1937)

Sys. Monoclinic S.G. C2/m (12)
a 6.85 b 3.92 c 6.09 A C
α β 91.12 γ Z mp
Ref.

D_x D_m SS/FOM F_{15} = 1.0(0.1388,112)

β phase. Monoclinic deformation of hexagonal unit cell.
Homogenity range 54.55-58.33% Te.

d Å	Int.	h k l	d Å	Int.	h k l
3.04	90	002			
2.95	100	$\bar{1}11$			
2.27	40	$\bar{1}12$			
2.25	60	202			
1.96	60	020			
1.75	40	$\bar{1}13$			
1.73	80	203			
1.64	40	401			
1.63	40	221			
1.52	90	004			
1.48	10	402			
1.31	40	$\bar{2}23$			
1.30	60	223			
1.26	40	511			
1.25	80	$\bar{4}13$			

Figure 7a The original PDF #2-722.

Searching the above compounds and in view of the cell size reported in 2-722, it would appear that the formula of CrTe (shown in original 2-722) is likely to be Cr_3Te_4. Its unit cell volume can be calculated from the lattice parameters (a = 6.85 Å ; b = 3.92 Å; c = 6.09 Å; and β = 91.7°) giving a volume of 163.5 $Å^3$. From the atomic volumes of 12.0 $Å^3$ and 33.9 $Å^3$ for Cr and Te, respectively (Figure 6 shows part of Appendix C — Atomic Volumes), the volume per formula unit for Cr_3Te_4 is 171.6 $Å^3$ indicating that Z = 163.5/171.6; therefore, Z is approximately 1. The partial PSC can then be m*7 (i.e., either mP7 or mC7). Searching the PSCI, no match is found at mP7, but there is an entry, Cr_3Se_4, at mC7 with the prototype structure Cr_3S_4 and cell dimensions matching PDF original #2-722, CrTe. From crystallographic theory, there should not be 7 atoms in a C-centered cell. However, doubling the number of atoms in the unit cell yields mC14, and in the PSCI there are many entries assigned to the Cr_3S_4 prototype structure at mC14. These structures have a c-axis approximately double that given for PDF #2-722, CrTe. This tentative match can be confirmed by a comparison of the strong lines of CrTe and Cr_3S_4. Thus, it is concluded that CrTe is Cr_3Te_4, and that is has the Cr_3S_4 structure with PSC:mC14; the PSCI has been revised to include Cr_3S_4 at mC14. This also implies that Cr_3Te_4 (PDF #2-722) should be re-indexed with the c-axis value doubled. PDF revised #2-722 (Figure 7b) has been updated to reflect all of the above changes and a doubling of the c-axis. By a similar analysis, it should be possible to confirm a better PSC for Cr_3Se_4, probably in mC14.

Another application of this book is to discover when two prototype structures, which have the same PS, are actually isostructural. For example, consider mC12, for which two prototypes can be found in Villars and Calvert[3] are: $NbSb_2$ (space group C2) and Ge_2Os (space group C2/m). The coordinates reported for $NbSb_2$ in Villars and Calvert,[3] by a suitable transformation, match those given for Ge_2Os; thus, the two structures may be identical in type. A check of *Structure Reports*[7] showed that the lower symmetry space group, C2, was assigned from photographic data, whereas the space group C2/m was obtained from accurate diffractometer data. Thus, there is evidence that C2/m is preferable; and Ge_2Os should be adopted as the type structure instead of $NbSb_2$. Therefore, in the current version of the PSCI, Ge_2Os is used.

2-722

Cr_3Te_4	d Å	Int.	h k l	d Å	Int.	h k l
Chromium Telluride	3.04	90	[004]			
	2.95	100	[112]			
Rad. CrKα λ 2.2909 **Filter** **d-sp**	2.27	40	[$\bar{1}$14]			
Cutoff **Int.** Visual $I/I_{cor.}$	2.25	60	[204]			
Ref. Haraldsen, Neuber, Z. *Anorg. Chem.*, **234** 365 (1937)	1.96	60	[020]			
Sys. Monoclinic **S.G.** [C2/m (12)]	1.75	40	[$\bar{1}$16]			
a 6.850(3) **b** 3.917(2) **c** 12.179(4) Å **C**	1.73	80	[206]			
α β 91.16(5) γ **Z** 2 **mp**	1.64	40	[402]			
Ref. Ibid.	1.63	40	[222]			
	1.52	90	[315]			
D_x 6.769 D_m **SS/FOM** F_{15} = 2(.079,111)	1.48	10	[404]			
β phase. Monoclinic deformation of hexagonal unit cell.	1.31	40	[$\bar{2}$26]			
Homogenity range 54.55-58.33% Te. Cell parameters	1.30	60	[027]			
generated by least squares refinement. Ref reports: CrTe	1.26	40	[512]			
and c = 6.09. Cr_3S_4 type. C.D. Cell: a = 12.179,	1.25	80	[209]			
b = 3.917, c = 6.850, β = 91.16, a/b = 3.1093,						
c/b = 1.7488, S.G. = A2/m (12). PSC: mC14.						

Figure 7b The revised PDF #2-722.

The Alphabetical Formula Index (AFI) can also be used to search for phases with analogous chemistry and stoichiometry. For example, PDF #5-704 for CCo_2 previously had no unit cell and no structure given. A similar phase, CFe_2 was found and used to define starting lattice parameters for CCo_2, which were then refined. One could then calculate the intensities based on the proposed structure to confirm results. Needed structural details may be obtained from Ref. 3 under oP6.

In a recent investigation of the U-Si phase diagram by Birtcher et al.,[8] it was confirmed that U_3Si_2 was tetragonal, ~7.3 x 7.3 x 3.9 Å and 10 atoms/unit cell, as shown in Figure 8. The most striking feature, as shown in Figure 8, resulting from the Rietveld refinements is the

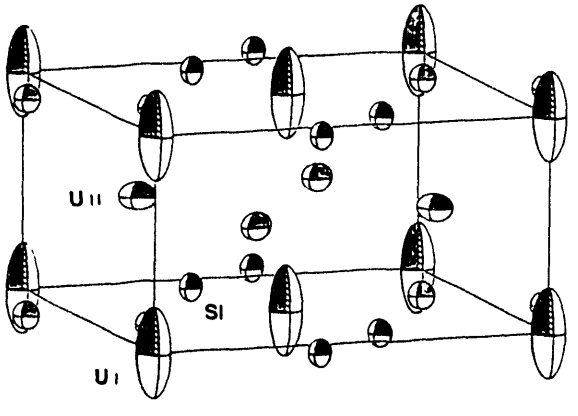

Figure 8 ORTEP drawing of U_3Si_2 structure showing dramatic out-of-plane displacements on U_1 (Ref. 8).

large out-of-plane displacement parameters for U_1 in all forms of U_3Si_2 both unirradiated and irradiated, pure phase and second phase with U_3Si_2. This could be an indication that the space group is not correct; and that the correct structure includes ordering displacements of the U_1

atoms from the origin, either within the plane or between planes. It is conceivable, on the other hand, that the huge thermal displacement parameter represents a random distribution of static displacement along the [001] direction. Since, as noted in Figure 3, Si_2U_3 is regarded as a prototype structure. It would be of interest to look at thermal parameters of some of the other tP10 compounds. In the present Pearson Code Index Section of the *Search Manual*,[1] one can find a number of other compounds which are isostructural such as: La_3Si_2, Si_2Th_3, Si_2Zr_3, etc. Since anisotropic thermal parameters are of concern, one would look for rather recent data for other compounds which might contain this information. As an aid to a detailed structural investigation, it would be prudent to make use of the four-volume set of *Atlas of Crystal Structure Types for Intermetallic Phases*,[9] which shows great detail in coordination of atoms in the various related Pearson Symbol Code intermetallics.

In a recent investigation[10] of intermetallics found in bonding Ni alloys to a U-Zr alloy, a number of Zr-Ni and U-Ni compounds were observed as expected from the binary phase diagrams.[2] However, in the case of an expected $NiZr_2$, which is to have a reported cubic structure, we observed such a structure, but with a somewhat smaller lattice constant. It seemed possible that U might form a ternary and if so, as expected from atomic volume comparisons of U and Zr (see Appendix C of the *Search Manual*), one would expect a smaller cell size for the $(U,Zr)_2Ni$ structure; such was the indeed the case. No NiU_2 line compound is reported.

For other application illustrations, the reader is referred to the Descriptive Information Section of the *Metal & Alloys Indexes — Search Manual.*[1]

Conclusion

We believe that the *Metals and Alloys Indexes — Search Manual* can assist in identifying crystallographic structures of the various intermetallics. It is our hope that new data will be assembled by various investigators so that we can obtain a more updated version of the Alphabetical Formula Index and the Pearson Symbol Code Index.

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