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Acta Cryst. (1991). **B47**, 433–439

Inorganic Structure Types with Revised Space Groups. I*

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(Received 5 September 1990; accepted 15 January 1991)

Abstract

Standardized data sets in space groups which consider all symmetry elements in the structure are given for the following structure types, originally reported in space groups with lower symmetry or with larger unit cells (numbers of original and new space group are indicated within parentheses): Ag_3TlTe_2 (53→65), Au_3Cd (107→139), Ca_3Hg (217→221, $\frac{1}{4}$ volume of primitive cell), CeZn_3 (62→63), CoGe_2 (41→64), CuAu phase I (123→123, $\frac{1}{2}$ cell volume), $\text{Cu}_{10}\text{Sb}_3$ (147→176), GaSe $2H$ ϵ (174→187), InSe II (10→12), LaB_2C_2 (112→131), $\alpha\text{-Li}_3\text{BN}_2$ (94→136), $\text{Li}_{6.45}\text{Mn}_3\text{As}_4$ (16→49 or 67), Li_7Pb_2 (150→164), LiPd_2 (10→10, $\frac{1}{2}$ cell volume), LiRh (174→187), MgAu_{3-x} (38→63), Mg_3In (146→166), Mn_2AlB_2 (21→65), Mn_3As (59→63), MnBi QHT (17→51), $\text{Mn}(\text{Bi}_{0.85}\text{Sb}_{0.15})$ (17→51), Na_2HgO_2 (97→139), $\text{Na}_{1-x}\text{TiS}_2$ (146→160), $\text{NbD}_{0.95}$ (48→66), $\theta\text{-Ni}_2\text{Si}$ (176 or 182→194), Pd_{4-x}Te (216→227), PtSn_4 (41→68), SrFe_2S_4 (117→125), $\text{Tb}_2(\text{Fe}_{0.832}\text{Al}_{0.168})_{17}$ (177→191), $\text{Ti}_3\text{Al}_2\text{N}_2$ (159→186), VAu_2 (38→63), V_6C_5 (144→151), VCo_3 LT (187→194), $\gamma\text{-V}_4\text{D}_3$ (27→49), WAl_5 (173→182), $\delta\text{-Yb}_2\text{S}_3$ (4→11), Zr_4Al_3 (174→191). For all these structures, data conversion is possible without modi-

fying the numerical values of the positional parameters. Reported triclinic NaSbS_2 is shown to be identical with NaSbS_2 previously refined in space group $C2/c$ and crystallizing with a KSbS_2 -type structure.

Introduction

One of the problems in comparative crystal chemical studies arises from the number of possible data sets describing the same crystal structure. To make it easier to recognize identical atom arrangements a standardization procedure was developed (Parthé & Gelato, 1984, 1985; Gelato & Parthé, 1987), which selects one single data set within the reported space group. However, for some structures found in the literature, the space group chosen by the authors is incorrect as far as it does not consider all symmetry elements contained in the structure. Since symmetry properties such as polar axes and noncentrosymmetry are requisites for special physical properties, reporting centrosymmetric structures in noncentrosymmetric space groups for instance, leads the physicist who is looking for materials likely to exhibit particular properties, into error.

In the course of the preparation of a book on inorganic structure types (Parthé, Gelato, Chabot, Penzo & Cenzual, 1991), standardized data sets for some 2000 structure types reported for inorganic compounds (oxides and halides not included) have

* Part II, a complementary list of inorganic structure types with revised space groups, will be submitted to this journal as a Short Communication.

up to now been tested for the presence of additional symmetry elements with the program *MISSYM* (Le Page, 1988). It was found that nearly 2% of the tested structure types can be described in a space group with higher symmetry than that reported, without modification of the published numerical values of the positional parameters. In a previous paper (Cenzual, Gelato, Penzo & Parthé, 1990), the particular case of trigonal structures with *hR* Bravais lattices, originally reported with monoclinic side-face-centred cells, was discussed.

Discussion

Table 1 contains a list of structure types for which the originally reported space group does not consider all symmetry elements actually present in the proposed structure. In the vast majority of cases the authors made no comments on the possibility of describing the structure in another space group, and only for CeZn_3 , Au_3Cd , CuAu phase I and $\theta\text{-Ni}_2\text{Si}$ was the correct space group, or unit cell, mentioned as 'alternative' in the publication, in *Strukturbericht* (SB; 1913–1939) or in *Structure Reports* (SR; 1940–1988). For structure types like Mn_2AlB_2 , Na_2HgO_2 , $\text{Na}_{1-x}\text{TiS}_2$ or VCo_3 LT, structures recognized as being isotypic were refined in the correct space group. However, since such statements have generally not been considered in more recent references or data files, it also seemed worthwhile including these structure types here. In a few cases the authors of the refinement explicitly exclude a space group which perfectly applies to the structure they propose (CoGe_2 , $\delta\text{-Yb}_2\text{S}_3$).

For each structure type listed in Table 1 the original description is characterized by its Pearson code, space group and a literature reference.* The transformations indicated in the central part of the table convert the published data into the standardized description based on the correct space group [for criteria for a standardized data set see Parthé & Gelato (1984, 1985)]. With regard to the conversion of data for compounds reported with one of these structure types, different situations occur. In some structure types all atoms occupy special positions with high point symmetry which exist in several space groups [site $3(a)00z$ in space group *R3*, for instance, is also present in *R3m*]. A transformation of the data into the space group with higher symmetry can be applied, without restriction, to any

compound reported as isotypic. Examples of such structure types are LaB_2C_2 and Na_2HgO_2 for which several isotypic compounds are known. For other structures special values ($\frac{1}{4}$, $\frac{1}{6}$ etc.) were reported for parameters which in the low-symmetry space group are refinable, for yet others the data conversion requires mathematical relationships between refinable atom coordinates of the same or different atom sites in the original space group. For CoGe_2 $z(\text{Co}1) + z(\text{Co}2) = -\frac{1}{4}$, whereas for isotypic PdSn_2 the corresponding sum is equal to -0.248 , which however must be considered to be within the limits of experimental error. For $\text{NbD}_{0.95}$ (or $\delta\text{-VD}_{1-x}$) a description in *Cccm* is possible only if the vacancies are equally distributed on both deuterium sites reported in *Pnmm*. For these last categories, compounds reported as isotypic must be examined one by one.

Pearson codes, space groups and Wyckoff sequences corresponding to the corrected standardized description are listed on the right-hand side of Table 1, whereas complete data sets (cell parameters, positional atom coordinates and population parameters when different from 1) can be found in Tables 2–39. Digits or letters in the last column of these tables, denoted as 'old', refer to the site notation (or order in atom coordinate list) in the original description. It is evident that the 'corrected' data sets given here are only valid as far as the reported atom arrangements themselves are correct. Only idealized coordinates were proposed for several structures and intensities calculated from the model were visually compared with X-ray films. Accurate refinements may confirm the space group with lower symmetry. It can however be noted that for all structures where diffraction data are listed in the publication, except for Ca_3Hg discussed below, conditions for additional extinctions in the space group of higher symmetry are respected. Misprints were detected in the data published for Li_7Pb_2 (see SR 20 137) and $\text{Cu}_{10}\text{Sb}_3$ (correction based on interatomic distances and confirmed by comparison with data for $\text{Au}_{10}\text{In}_3$). Site occupations in $\text{Li}_{6.45}\text{Mn}_3\text{As}_4$ are not clearly indicated in the original publication and two data sets are also proposed here. Depending on whether the arrangement of Mn atoms occupying the tetrahedral interstices in the layers at $z = 0$ in the original description is partially ordered or completely disordered, different space groups are found. The interatomic distances calculated from some of the data sets are relatively short [$\text{Mn}(\text{Bi}_{0.85}\text{Sb}_{0.15})$, $\text{GaSe } 2H \epsilon$]; however, the most suspect structure in Table 1 is that proposed for Ca_3Hg . Drawing and atom coordinates correspond to the well known Cu_3Au type, but the intensities of the powder diagram calculated from these coordinates do not agree with the published diagram, where reflections which should be absent are reported with strong intensities.

* A list containing complete references for papers referred to by five-character codes from *Chemical Abstracts Service Source Index* (1989) has been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53892 (4 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Structure types originally reported in space groups that do not consider all symmetry elements

For each structure type the following data are given. Published data: Pearson code; space-group number in *International Tables for X-ray Crystallography*; Hermann-Mauguin symbol of setting used in the original description; literature reference. Transformation: new unit-cell vectors expressed as a combination of the published ones; coordinates of transition to the new axes (to subtract); existence of special conditions to be respected for compounds reported as isotopic. Corrected data: Pearson code; space-group number and Hermann-Mauguin symbol; Wyckoff sequence of standardized data set; reference to the table containing the positional coordinates. Related structure: isotopic and other closely related structures reported in the correct space group; corresponding literature reference.

Structure type	Published data		Transformation		Corrected data		Related structure	Reference ^b	
	Pearson code ^a	Space group	New unit-cell vectors	Shift	Cond ^c	Pearson code ^a			Space group - Wyckoff sequence ^d
Ag ₂ TlTe ₂	oP12 (53)	<i>Pnma</i>	a, -c, b	0	*	oS12 (65)	<i>Cmnm - jica</i>	2	ZrAl ₃
Au ₃ Cd	rI16 (107)	<i>I4mm</i>	a, -c, b	0	*	rI16 (139)	<i>I4/mmm - e²dc</i>	3	Cu ₃ Au
Cu ₃ Hg	rI32 (217)	<i>I43m</i>	a/2, b/2, c/2	0	*	rI32 (221)	<i>P63m - ca</i>	4	Pu ₃ Bi ₃
CeZn ₃	oP16 (62)	<i>Pnma</i>	b, c, a	0	*	oP16 (63)	<i>Cmcm - f²</i>	5 ^e	ACCRA 1 265
CoGe ₂	oP16 (62)	<i>Bha2</i>	a, b, c	0	*	oS24-1 (64)	<i>Cmca - fed</i>	6	JUPSA 17 1313
CuAu phase I	rP4 (123)	<i>P4/mmm</i>	a/2 + b/2, -a/2 + b/2, c	0	*	rP2 (123)	<i>P4/mmm - da</i>	7	MnHg ₂ LT
Cu ₂ Sb ₂	rP4 (123)	<i>P3</i>	a, b, c	0	*	rP26 (176)	<i>P6₃/m - h²c</i>	8	Au ₂ Al ₃
GeSe ZH ε	rP8 (174)	<i>P6</i>	b - c, a, -b	0	*	rP8 (187)	<i>P6m2 - h²g²</i>	9	
InSe II	rP8 (10)	<i>P2/m11</i>	b, c, a	0	*	mS8 (12)	<i>C2/m - i²</i>	10	
LaB ₂ C ₂	rI12 (112)	<i>P42c</i>	b, c, a	0	*	rP10 (131)	<i>P4₂/mnc - mke</i>	11	
α-Li ₂ BN ₃	rP12 (94)	<i>P4₂2₁2</i>	b, c, a	0	*	rP12 (136)	<i>P4₂/mnm - fdha</i>	12	
Li _{2-x} Mn _{2-x} As ₂	oP16-2,55 (16)	<i>P222</i>	a, -b, c	0	*	rP12 (136)	<i>Pccm - q²hg²c</i>	13	
Li ₂ Pb ₂	rP9 (150)	<i>P321</i>	a/2 + c/2, -b, a/2 - c/2	0	*	oP16-2,55 (49)	<i>Cmca - g²ba²</i>	14	
LiPb ₂	rP8 (10)	<i>P2/m1</i>	a, -b, c	0	*	hP9 (164)	<i>P3m1 - d²ca</i>	15	
LiRh	rP2 (174)	<i>P6</i>	a/2 + c/2, -b, a/2 - c/2	0	*	hP2 (187)	<i>P6m2 - da</i>	16	
MgAl _{2-x}	rP2 (38)	<i>Cm2m</i>	-b, a + b, c	0	*	mP4 (10)	<i>P2/m - g²fea</i>	17	MOCMB 93 263
Mg ₂ In	rP2 (146)	<i>R3</i>	a, b, c	0	*	oS160 (63)	<i>Cmcm - h²g²fe²a</i>	18	ACCRA 18 294
Mn _{2-x} AlB ₂	oS10 (21)	<i>C222</i>	a, -b, c	0	*	hR48 (166)	<i>R3m - h²c²</i>	19	PuGa ₃ HT
Mn ₂ As	oP16 (59)	<i>Pnmm</i>	a, -c, b	0	*	oS10 (65)	<i>Cmnm - jia</i>	20	Fe ₂ AlB ₂
MnBi quenched	oP10-1,78 (17)	<i>P222₁</i>	a, c, b	0	*	oS16 (63)	<i>Cmcm - e²</i>	21	ACCRA 25 163
Mn ₂ HgO ₂	oP10-1,96 (17)	<i>P222₁</i>	a, b, c	0	*	oP10-1,78 (51)	<i>Pnma - f²da</i>	22	INOMA 5 321
α-Na ₂ Si ₂ S ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	oP10-1,96 (51)	<i>Pnma - f²da</i>	23	
Nb ₂ O ₇	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	25	
Nb ₂ Si ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	26	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	27	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	28	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	29	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	30	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	31	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	32	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	33	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	34	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	35	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	36	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	37	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	38	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	39	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	40	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	41	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	42	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	43	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	44	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	45	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	46	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	47	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	48	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	49	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	50	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	51	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	52	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	53	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	54	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	55	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	56	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	57	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	58	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	59	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	60	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	61	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	62	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	63	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	64	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	65	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	66	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	67	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	68	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	69	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	70	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	71	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	72	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	73	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	74	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	75	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	76	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	77	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	78	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	79	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	80	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	81	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	82	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	83	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	84	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	85	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	86	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	87	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	88	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	89	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	90	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	91	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²a</i>	92	
Nb ₂ Te ₂	rI10 (97)	<i>I422</i>	a, -b, -a + b, -c	0	*	rI10 (139)	<i>I4/mmm - e²</i>		

Table 2. Corrected structure data for Ag_3TlTe_2 (original data from SPHCA 17 237)(65) $Cm\bar{m}m$, $a = 4.60$, $b = 15.45$, $c = 4.76$ Å.

		x	y	z	PP	Old
Te	4(f)	0	0.127	$\frac{1}{2}$		
Ag(1)	4(i)	0	0.315	0		1
Ag(2)	2(c)	$\frac{1}{2}$	0	$\frac{1}{2}$		2
Tl	2(a)	0	0	0		

Table 3. Corrected structure data for Au_3Cd (original data from JUPSA 20 89)(139) $I4/m\bar{m}m$, $a = 4.109$, $c = 16.552$ Å, $X = \text{Cd}_{0.96}\text{Au}_{0.04}$.

		x	y	z	PP	Old
Au(1)	4(e)	0	0	0.1241		3,3
X	4(e)	0	0	0.3733		1,2
Au(2)	4(d)	0	$\frac{1}{2}$	$\frac{1}{2}$		2
Au(3)	4(c)	0	$\frac{1}{2}$	0		1

Table 4. Corrected structure data for Ca_3Hg (original data from CCACA 51 75)(221) $Pm\bar{3}m$, $a = 4.92$ Å, structure does not correspond to published diffraction diagram.

		x	y	z	PP	Old
Ca	3(c)	0	$\frac{1}{2}$	$\frac{1}{2}$		1,2
Hg	1(a)	0	0	0		

Table 5. Corrected structure data for CeZn_3 (original data from JCOMA 22 253)(63) $Cmcm$, $a = 4.627$, $b = 10.437$, $c = 6.644$ Å.

		x	y	z	PP	Old
Zn(1)	8(f)	0	0.120	0.055		2,3
Ce	4(c)	0	0.400	$\frac{1}{2}$		
Zn(2)	4(c)	0	0.690	$\frac{1}{2}$		1

Table 6. Corrected structure data for CoGe_2 (original data from ZEMTA 41 433)(64) $Cmca$, $a = 10.818$, $b = 5.681$, $c = 5.681$ Å, cell parameters converted from kX units (see SR 11 96).

		x	y	z	PP	Old
Ge(1)	8(f)	0	0.158	0.342		1
Ge(2)	8(e)	$\frac{1}{2}$	0.25	$\frac{1}{2}$		2
Co	8(d)	0.113	0	0	0.875	1,2

Table 7. Corrected structure data for CuAu phase I (original data from SB 1 484)(123) $P4/m\bar{m}m$, $a = 2.81$, $c = 3.72$ Å.

		x	y	z	PP	Old
Au	1(d)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Cu	1(a)	0	0	0		1,2

Table 8. Corrected structure data for $\text{Cu}_{10}\text{Sb}_3$ (original data from ZEMTA 49 124)(176) $P6_3/m$, $a = 9.920$, $c = 4.319$ Å.

		x	y	z	PP	Old
Cu(1)	6(h)	0.029	0.444	$\frac{1}{2}$		2
Cu(2)	6(h)	0.169	0.056	$\frac{1}{2}$		1
Sb	6(h)	0.259	0.363	$\frac{1}{2}$		
Cu(3)	6(h)	0.505	0.294	$\frac{1}{2}$		3
Cu(4)	2(c)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		4*

* z coordinate is misprinted as $\frac{1}{2}$ instead of $\frac{1}{4}$ in paper.Table 9. Corrected structure data for GaSe 2H ϵ (original data from ZEMTA 46 216)(187) $P\bar{6}m2$, $a = 3.743$, $c = 15.919$ Å.

		x	y	z	PP	Old
Se(1)	2(i)	$\frac{1}{2}$	$\frac{1}{2}$	0.150		2
Ga(1)	2(h)	$\frac{1}{2}$	$\frac{1}{2}$	0.425		1
Ga(2)	2(g)	0	0	0.075		2
Se(2)	2(g)	0	0	0.350		1

Table 10. Corrected structure data for InSe II (original data from JSSCB 43 140)(12) $C2/m$, $a = 11.74$, $b = 4.11$, $c = 4.61$ Å, $\beta = 110.3^\circ$.

		x	y	z	PP	Old
Se	4(i)	0.160	0	0.142		1,2
In	4(i)	0.384	0	0.505		1,2

Table 11. Corrected structure data for LaB_2C_2 (original data from ACBCA 36 1540)(131) $P4_2/m\bar{m}c$, $a = 3.8218$, $c = 7.9237$ Å.

		x	y	z	PP	Old
C	4(m)	0.173	$\frac{1}{2}$	0		
B	4(k)	0.226	$\frac{1}{2}$	$\frac{1}{2}$		
La	2(e)	0	0	$\frac{1}{2}$		

Table 12. Corrected structure data for $\alpha\text{-Li}_3\text{BN}_2$ (original data from JSSCB 71 1)(136) $P4_2/m\bar{m}m$, $a = 4.6435$, $c = 5.2592$ Å.

		x	y	z	PP	Old
N	4(f)	0.2038	x	0		
Li(1)	4(d)	0	$\frac{1}{2}$	$\frac{1}{2}$		2
Li(2)	2(b)	0	0	$\frac{1}{2}$		1
B	2(a)	0	0	0		

Table 13. Corrected structure data for $\text{Li}_{6.45}\text{Mn}_3\text{As}_4$ (original data from ZAACA 356 253)

(a) Partially ordered arrangement of Mn in tetrahedral voids

(49) $Pccm$, $a = 6.129$, $b = 6.200$, $c = 5.928$ Å, $X = \text{Li}_{0.3}\text{Mn}_{0.5}$.

		x	y	z	PP	Old
Li(1)	4(g)	0.25	0.25	0	0.3625	u
As	4(g)	0.25	0.75	0		
Li(2)	2(h)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		g,h
Li(3)	2(g)	0	$\frac{1}{2}$	$\frac{1}{2}$		d,f
Mn	2(f)	$\frac{1}{2}$	0	$\frac{1}{2}$		c,e
X	2(e)	0	0	$\frac{1}{2}$		a,b

(b) Disordered arrangement of Mn in tetrahedral voids

(67) $Cmma$, $a = 5.928$, $b = 6.129$, $c = 6.200$ Å, $X = \text{Li}_{0.25}\text{Mn}_{0.75}$.

		x	y	z	PP	Old
Li(1)	4(g)	0	$\frac{1}{2}$	0.25	0.3625	
As	4(g)	0	$\frac{1}{2}$	0.75		
Li(2)	4(b)	$\frac{1}{2}$	0	$\frac{1}{2}$		d,f,g,h
X	4(a)	$\frac{1}{2}$	0	0		a,b,c,e

Table 8. Corrected structure data for $\text{Cu}_{10}\text{Sb}_3$ (original data from ZEMTA 49 124)(176) $P6_3/m$, $a = 9.920$, $c = 4.319$ Å.

		x	y	z	PP	Old
Cu(1)	6(h)	0.029	0.444	$\frac{1}{2}$		2
Cu(2)	6(h)	0.169	0.056	$\frac{1}{2}$		1
Sb	6(h)	0.259	0.363	$\frac{1}{2}$		
Cu(3)	6(h)	0.505	0.294	$\frac{1}{2}$		3
Cu(4)	2(c)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		4*

* z coordinate is misprinted as $\frac{1}{2}$ instead of $\frac{1}{4}$ in paper.Table 14. Corrected structure data for Li_7Pb_2 (original data from JPCHA 60 234)(164) $P\bar{3}m1$, $a = 4.751$, $c = 8.589$ Å.

		x	y	z	PP	Old
Li(1)	2(d)	$\frac{1}{2}$	$\frac{1}{2}$	0.08333		1a*
Li(2)	2(d)	$\frac{1}{2}$	$\frac{1}{2}$	0.41667		1b
Pb	2(d)	$\frac{1}{2}$	$\frac{1}{2}$	0.75000		
Li(3)	2(c)	0	0	0.33333		2
Li(4)	1(a)	0	0	0		3

* z coordinate is misprinted as $-\frac{1}{2}$ instead of $-\frac{1}{12}$ in paper.

Table 15. Corrected structure data for LiPd_2 (original data from JCOMA 63 P83)(10) $P2/m$, $a = 4.686$, $b = 2.729$, $c = 4.695$ Å, $\beta = 109.60^\circ$, $X = \text{Li}_{0.12}\text{Pd}_{0.88}$ (in SR 45A 93 site occupation is interpreted as $\text{Li}_{0.24}\text{Pd}_{0.76}$).

		x	y	z	PP	Old
Li	1(g)	$\frac{1}{2}$	0	$\frac{1}{2}$		1.2
Pd(1)	1(f)	0	$\frac{1}{2}$	$\frac{1}{2}$		3
X	1(e)	$\frac{1}{2}$	$\frac{1}{2}$	0		
Pd(2)	1(a)	0	0	0		1.2

Table 16. Corrected structure data for LiRh (original data from ACCRA 18 906)(187) $P\bar{6}m2$, $a = 2.649$, $c = 4.359$ Å.

		x	y	z	PP	Old
Li	1(d)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Rh	1(a)	0	0	0		

Table 17. Corrected structure data for MgAu_{3-x} ($x = 0$) (original data from ZEMTA 56 864)(63) $Cmcm$, $a = 5.740$, $b = 19.83$, $c = 23.59$ Å.

		x	y	z	PP	Old
Au(1)	16(h)	0.25	0.045	0.05		4.6
Au(2)	16(h)	0.25	0.205	0.15		1.7
Au(3)	16(h)	0.25	0.295	0.05		3.5
Au(4)	16(h)	0.25	0.455	0.15		2.8
Au(5)	8(g)	0.25	0.125	$\frac{1}{2}$		9.11
Au(6)	8(g)	0.25	0.375	$\frac{1}{2}$		10.12
Au(7)	8(f)	0	0.085	0.15		14.20
Au(8)	8(f)	0	0.085	0.55		16.17
Mg(1)	8(f)	0	0.165	0.05		4.5
Mg(2)	8(f)	0	0.165	0.65		1.8
Au(9)	8(f)	0	0.335	0.15		13.19
Au(10)	8(f)	0	0.335	0.55		15.18
Mg(3)	8(f)	0	0.415	0.05		3.6
Mg(4)	8(f)	0	0.585	0.15		2.7
Mg(5)	4(c)	0	0.000	$\frac{1}{2}$		9.12
Mg(6)	4(c)	0	0.250	$\frac{1}{2}$		10.11
Au(11)	4(c)	0	0.500	$\frac{1}{2}$		22.23
Au(12)	4(c)	0	0.750	$\frac{1}{2}$		21.24

Table 18. Corrected structure data for Mg_3In (original data from ZEMTA 54 422)(166) $R\bar{3}m$, $a = 6.323$, $c = 31.060$ Å.

		x	y	z	PP	Old
Mg(1)	18(h)	0.5	-x	0.125		1.4
Mg(2)	18(h)	0.5	-x	0.2917		2.3
In(1)	6(c)	0	0	0.125		1.2
In(2)	6(c)	0	0	0.2917		3.4

Table 19. Corrected structure data for Mn_2AlB_2 (original data from ZAACA 344 140)(65) $Cmmm$, $a = 2.92$, $b = 11.08$, $c = 2.89$ Å.

		x	y	z	PP	Old
Mn	4(f)	0	0.355	$\frac{1}{2}$		
B	4(i)	0	0.209	0		
Al	2(a)	0	0	0		

Table 20. Corrected structure data for Mn_3As (original data from MOCMB 82 513)(63) $Cmcm$, $a = 3.788$, $b = 16.29$, $c = 3.788$ Å.

		x	y	z	PP	Old
As	4(c)	0	0.159	$\frac{1}{2}$		1.2
Mn(1)	4(c)	0	0.3155	$\frac{1}{2}$		3.6
Mn(2)	4(c)	0	0.5565	$\frac{1}{2}$		2.5
Mn(3)	4(c)	0	0.9435	$\frac{1}{2}$		1.4

Table 21. Corrected structure data for MnBi quenched (original data from ACSAA 26 175)(51) $Pmma$, $a = 5.959$, $b = 4.334$, $c = 7.505$ Å.

		x	y	z	PP	Old
Bi(1)	2(f)	$\frac{1}{2}$	$\frac{1}{2}$	0.165		1*
Mn(1)	2(e)	$\frac{1}{2}$	0	0.398	0.33	(1)
Bi(2)	2(e)	$\frac{1}{2}$	0	0.699	0.88	2
Mn(2)	2(d)	0	$\frac{1}{2}$	$\frac{1}{2}$		1*
Mn(3)	2(a)	0	0	0	0.90	2

* Sites with $0.96 < PP < 1.02$ are assumed to be fully occupied.Table 22. Corrected structure data for $\text{Mn}(\text{Bi}_{0.85}\text{Sb}_{0.15})$ (original data from PSSAB 34 553)(51) $Pmma$, $a = 5.70$, $b = 4.27$, $c = 7.40$ Å, $X = \text{Bi}_{0.85}\text{Sb}_{0.15}$.

		x	y	z	PP	Old
X(1)	2(f)	$\frac{1}{2}$	$\frac{1}{2}$	0.136		1*
Mn(1)	2(e)	$\frac{1}{2}$	0	0.285	0.63	(1)2
X(2)	2(e)	$\frac{1}{2}$	0	0.709		2*
Mn(2)	2(d)	0	$\frac{1}{2}$	$\frac{1}{2}$		1*
Mn(3)	2(a)	0	0	0	0.39	2

* Sites with $0.96 < PP < 1.04$ are assumed to be fully occupied.Table 23. Corrected structure data for Na_2HgO_2 (original data from ZAACA 329 110)(139) $I4/mmm$, $a = 3.42$, $c = 13.32$ Å.

		x	y	z	PP	Old
O	4(e)	0	0	0.147		
Na	4(e)	0	0	0.325		
Hg	2(a)	0	0	0		

Table 24. Structure data for $\alpha\text{-NaSbS}_2$ refined in space group $C2/c$ (ZAACA 446 159) with, in parentheses, deviations from these values observed for data refined in $P\bar{1}$ (JSTCA 20 122) and transformed according to Table 1(15) $C2/c$, $a = 8.232$ (3), $b = 8.252$ (7), $c = 6.836$ (3) Å, $\alpha = 90.00$ (1), $\beta = 124.28$ (2), $\gamma = 90.00$ (3)°.

		x	y	z	PP	Old
S	8(f)	0.2203 (3)	0.4118 (5)	0.2404 (2)		
Na	4(e)	0.0000 (11)	0.1336 (9)	0.2500 (5)		
Sb	4(e)	0.0000 (0)	0.6027 (1)	0.2500 (0)		

Table 25. Corrected structure data for $\text{Na}_{1-x}\text{TiS}_2$ ($x = 0.45$) (original data from BSCFA 1971 3930)(160) $R3m$, $a = 3.433$, $c = 20.94$ Å.

		x	y	z	PP	Old
Ti	3(a)	0	0	0.00		
Na	3(a)	0	0	0.17	0.55	
S(1)	3(a)	0	0	0.39		2
S(2)	3(a)	0	0	0.60		1

Table 26. Corrected structure data for $\text{NbD}_{0.95}$ (original data from SPSSA 10 1076)(66) $Ccmm$, $a = 3.447$, $b = 4.860$, $c = 4.860$ Å.

		x	y	z	PP	Old
Nb	4(e)	$\frac{1}{2}$	$\frac{1}{2}$	0		
D	4(a)	0	0	$\frac{1}{2}$	0.95	1.2

Table 27. Corrected structure data for θ -Ni₂Si (original data from ACCRA 5 329)

(194) *P6₃/mmc*, *a* = 3.805, *c* = 4.890 Å.

		x	y	z	PP	Old
Si	2(d)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Ni(1)	2(c)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		2
Ni(2)	2(a)	0	0	0		1

Table 33. Corrected structure data for VAu₂ (original data from ZEMTA 53 433)

(63) *Cmcm*, *a* = 8.482, *b* = 4.810, *c* = 4.684 Å.

		x	y	z	PP	Old
Au	8(g)	0.33	0.22	$\frac{1}{2}$		1.2
V	4(c)	0	0.22	$\frac{1}{2}$		1.2

Table 28. Corrected structure data for Pd_{4-x}Te (*x* = 0.5) (original data from SPHCA 14 779)

(227) *Fd $\bar{3}m$* , *a* = 12.69 Å.

		x	y	z	PP	Old
Pd(1)	48(f)	0.375	$\frac{1}{2}$	$\frac{1}{2}$		3.4
Pd(2)	32(e)	0.250	$\frac{1}{2}$	$\frac{1}{2}$		1.2
Te(1)	16(d)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		1
Pd(3)	16(c)	0	0	0	$\frac{1}{2}$	5
Te(2)	8(a)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		2.3

Table 34. Corrected structure data for V₆C₅ (original data from PHMAA 18 177)

(151) *P3₁12*, *a* = 5.09, *c* = 14.40 Å.

		x	y	z	PP	Old
V(1)	6(c)	0.111	0.222	0.417		3.4
V(2)	6(c)	0.111	0.556	0.250		1.6
V(3)	6(c)	0.444	0.222	0.250		2.5
C(1)	3(b)	0.444	-x	$\frac{1}{2}$		5
C(2)	3(b)	0.778	-x	$\frac{1}{2}$		4
C(3)	3(a)	0.111	-x	$\frac{1}{2}$		2
C(4)	3(a)	0.444	-x	$\frac{1}{2}$		1
C(5)	3(a)	0.778	-x	$\frac{1}{2}$		3

Table 29. Corrected structure data for PtSn₄ (original data from ZEMTA 41 298)

(68) *Ccca*, *a* = 6.419, *b* = 11.357, *c* = 6.388 Å.

		x	y	z	PP	Old
Sn	16(f)	0.327	0.125	0.077		1.2
Pt	4(a)	0	$\frac{1}{2}$	$\frac{1}{2}$		

Table 35. Corrected structure data for VCo₃ LT (original data from ACCRA 12 500)

(194) *P6₃/mmc*, *a* = 5.032, *c* = 12.27 Å.

		x	y	z	PP	Old
Co(1)	12(k)	0.1667	2x	0.0833		2.3
Co(2)	6(h)	0.5000	2x	$\frac{1}{2}$		1.4
V(1)	4(f)	$\frac{1}{2}$	$\frac{1}{2}$	0.5833		2.3
V(2)	2(b)	0	0	$\frac{1}{2}$		1.4

Table 30. Corrected structure data for SrFe₂S₄ (original data from MOCMB 109 975)

(125) *P4/nbm*, *a* = 7.917, *c* = 5.505 Å.

		x	y	z	PP	Old
S	8(m)	0.409	-x	0.25		
Fe(1)	2(d)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		2
Fe(2)	2(c)	$\frac{1}{2}$	$\frac{1}{2}$	0		1
Sr(1)	2(b)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.25	2
Sr(2)	2(a)	$\frac{1}{2}$	$\frac{1}{2}$	0	0.75	1

Table 36. Corrected structure data for γ -V₄D₃ (original data from PSSAB 15 267)

(49) *Pccm*, *a* = 4.445, *b* = 6.286, *c* = 4.445 Å.

		x	y	z	PP	Old
V(1)	4(g)	0.250	0.125	0		2
V(2)	4(g)	0.250	0.625	0		1
D(1)	4(f)	$\frac{1}{2}$	0.250	$\frac{1}{2}$	0.96	1
D(2)	2(e)	0	0	$\frac{1}{2}$	0.96	2

Table 31. Corrected structure data for Tb₂(Fe_{0.832}Al_{0.168})₁₇ (original data from JCOMA 45 103)

(191) *P6/mmm*, *a* = 8.532, *c* = 4.175 Å, *X* = Fe_{0.8324}Al_{0.1676}.

		x	y	z	PP	Old
X(1)	6(m)	0.167	2x	$\frac{1}{2}$		1
X(2)	6(j)	0.333	0	0		2
X(3)	4(h)	$\frac{1}{2}$	$\frac{1}{2}$	0.28	0.50	4
X(4)	3(g)	$\frac{1}{2}$	0	$\frac{1}{2}$		3
Tb(1)	2(c)	$\frac{1}{2}$	$\frac{1}{2}$	0	0.50	1
Tb(2)	1(a)	0	0	0		2

Table 37. Corrected structure data for WAl₅ (original data from ACCRA 8 349)

(182) *P6₃22*, *a* = 4.9020, *c* = 8.8570 Å.

		x	y	z	PP	Old
Al(1)	6(g)	0.333	0	0		3
W	2(d)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Al(2)	2(c)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		1
Al(3)	2(b)	0	0	$\frac{1}{2}$		2

Table 32. Corrected structure data for Ti₃Al₂N₂ (original data from JSSCB 53 260)

(186) *P6₃mc*, *a* = 2.9875, *c* = 23.350 Å.

		x	y	z	PP	Old
N(1)	2(b)	$\frac{1}{2}$	$\frac{1}{2}$	0.05	0.9	2
Ti(1)	2(b)	$\frac{1}{2}$	$\frac{1}{2}$	0.10	0.1	5
Ti(2)	2(b)	$\frac{1}{2}$	$\frac{1}{2}$	0.20	0.9	2
N(2)	2(b)	$\frac{1}{2}$	$\frac{1}{2}$	0.25	0.1	3
Al(1)	2(b)	$\frac{1}{2}$	$\frac{1}{2}$	0.40		2
N(3)	2(b)	$\frac{1}{2}$	$\frac{1}{2}$	0.55	0.1	4
Ti(3)	2(b)	$\frac{1}{2}$	$\frac{1}{2}$	0.60	0.9	3
Ti(4)	2(b)	$\frac{1}{2}$	$\frac{1}{2}$	0.70	0.1	4
N(4)	2(b)	$\frac{1}{2}$	$\frac{1}{2}$	0.75	0.9	1
Ti(5)	2(a)	0	0	0.00		1
Al(2)	2(a)	0	0	0.30		1

Table 38. Corrected structure data for δ -Yb₂S₃ (original data from RJICA 21 1565)

(11) *P2₁/m*, *a* = 10.37, *b* = 4.06, *c* = 18.15 Å, β = 100°.

		x	y	z	PP	Old
S(1)	2(e)	0.0029	$\frac{1}{2}$	0.0459		4
S(2)	2(e)	0.0537	$\frac{1}{2}$	0.7490		1
Yb(1)	2(e)	0.1202	$\frac{1}{2}$	0.9277		2
Yb(2)	2(e)	0.1865	$\frac{1}{2}$	0.2197		4
Yb(3)	2(e)	0.1865	$\frac{1}{2}$	0.5195		1
S(3)	2(e)	0.2881	$\frac{1}{2}$	0.6943		3
S(4)	2(e)	0.3047	$\frac{1}{2}$	0.3906		5
S(5)	2(e)	0.3604	$\frac{1}{2}$	0.0225		7
Yb(4)	2(e)	0.4824	$\frac{1}{2}$	0.8926		5
Yb(5)	2(e)	0.5400	$\frac{1}{2}$	0.6104		6
S(6)	2(e)	0.6582	$\frac{1}{2}$	0.4893		8
S(7)	2(e)	0.6787	$\frac{1}{2}$	0.8076		6
S(8)	2(e)	0.7275	$\frac{1}{2}$	0.1250		2
Yb(6)	2(e)	0.8301	$\frac{1}{2}$	0.2842		3
S(9)	2(e)	0.9512	$\frac{1}{2}$	0.4365		9

Table 39. Corrected structure data for Zr_4Al_3 (original data from ACCRA 13 56)

(191) $P6/mmm$, $a = 5.433$, $c = 5.390$ Å.						
		x	y	z	PP	Old
Al	3(f)	$\frac{1}{2}$	0	0		
Zr(1)	2(e)	0	0	$\frac{1}{2}$		1
Zr(2)	2(d)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		2,3

Structures reported in the correct space group and which may be considered as isotypic, anti-types ($PuGa_3$ HT, $ZrAl_3$), representatives of structure-type branches ($MnHg$ LT, WC), or site-ordering variants ($CoMnSb$, $PuBr_3$) of the structure types discussed here, are indicated in the last column of Table 1. The coordinates of $NaSbS_2$ refined in space group $P\bar{1}$ become, after transformation, very similar to those of $NaSbS_2$ previously reported with a $KSbS_2$ -type structure. The deviations from the data refined in $C2/c$ (see Table 24) are only slightly outside the e.s.d. ranges indicated for this structure, and the fact that this work was not known to the authors of the refinement in $P\bar{1}$ makes the existence of a triclinic deformation variant under these conditions unlikely. Among the compounds crystallizing with an Na_2HgO_2 -type structure, some were reported in the incorrect space group $I422$, some refined in space group $I4/mmm$ but were identified as isotypic (e.g.

Na_2PdH_2), and some were published in space group $I4/mmm$ without being recognized as isotypic (e.g. U_2IrC_2).

This study was supported by the Swiss National Science Foundation under contract 20-28490.90.

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The Importance of Accurate Crystal Structure Determination of Uranium Minerals. I. Phosphuranylite $KCa(H_3O)_3(UO_2)_7(PO_4)_4O_4 \cdot 8H_2O$

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(Received 28 September 1990; accepted 16 January 1991)

Abstract

On the basis of accurate crystal structure determination, the mineral phosphuranylite corresponds to the chemical formula $KCa(H_3O)_3(UO_2)_7(PO_4)_4O_4 \cdot 8H_2O$.

$Cmcm$, $a = 15.778$ (3)– 15.899 (2), $b = 13.702$ (2)– 13.790 (5), $c = 17.253$ (3)– 17.330 (3) Å, $Z = 4$, $D_x = 4.575$ – 4.631 g cm⁻³, $\mu = 287.6$ – 291.1 cm⁻¹. The presence of potassium (about 1.80 wt% K_2O), overlooked until now, has been confirmed by microprobe