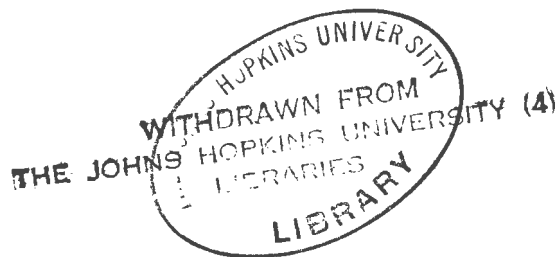


Iowa  
SC  
AL  
ISC-  
906

U N C L A S S I F I E D

ISC-906



UNITED STATES ATOMIC ENERGY COMMISSION

Tabulation, Bibliography, and Structure of Binary  
Intermetallic Compounds. III. Compounds of  
Copper, Silver and Gold

by

H. H. Klepfer, H. E. Shoemaker, J. D. Greiner,  
M. L. Moller and J. F. Smith

September 9, 1957

Ames Laboratory  
at  
Iowa State College  
F. H. Spedding, Director  
Contract W-7405 eng-82

U N C L A S S I F I E D

This report is distributed according to the category Metallurgy and Ceramics, as listed in TID-4500, January 15, 1957.

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

- A. Makes any warranty or representation, express or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or
- B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission to the extent that such employee or contractor prepares, handles or distributes, or provides access to, any information pursuant to his employment or contract with the Commission.

Printed in the U.S.A. Price 30 cents. Available from the

Office of Technical Services  
U. S. Department of Commerce  
Washington 25, D. C.

## TABLE OF CONTENTS

	<u>Page</u>
Part I: Tabulation of Compounds . . . . .	5
Part II: References . . . . .	27
Part III: Structure Details . . . . .	37

This report is the third in a series. ISC-795, the first in this series, listed the compounds of lithium, sodium, potassium, and rubidium; ISC-812, the second in the series, listed the compounds of beryllium, magnesium, and calcium.

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Cu		$a=3.61$		Parameter at room tempera- ture; measurements were made using a high temperature vacuum camera.	240
Cu <sub>3</sub> Au	cubic	$a=3.751$ (25 a/o Au)	L12	Superlattice: ordered f.c.c. lattice below 396°C; from 18- ~37 a/o Au at 25°C.	1,2
CuAu	tetrag- onal	$a=3.964$ $c=3.671$ (50 a/o Au)	L10	Superlattice: ordered f.c.c. lattice below 424°C; from ~37-70 a/o Au.	1,2,3
Cu <sub>2</sub> Be	cubic	$a=2.80$ (750°C)	A2	Exists above 575°C; dis- ordered atomic arrangement.	235
CuBe	cubic	$a=2.703$ $\pm 0.007$	B2	X-ray powder data, with com- parison of observed and cal- culated intensities; some dis- ordering noted; after anneal- ing at 830°C. for two hours completely ordered.	7, 236, 237,238
CuBe	tetrag- onal	$a=2.79$ $c=2.54$		Intermediate phases during precipitation; single crystal x-ray data.	236
CuBe	mono- clinic	$a=2.54$ $b=2.54$ $c=3.24$ $\alpha=85^{\circ}25'$		"	236
CuBe <sub>3</sub>	cubic	$a=5.952$ (at CuBe <sub>2</sub> )	C15	Maximum solubility range CuBe <sub>2</sub> → CuBe <sub>4</sub> at 933°C; at room temperature ranges from CuBe <sub>2</sub> . <sup>35</sup> → CuBe <sub>4</sub> ; maximum in liquidus occurs at CuBe <sub>3</sub> ; structure deter- mined at Cu:Be of 1:2.354; x-ray powder data, with comparison of observed and calculated in- tensities.	4, 5,6,7
Cu <sub>2</sub> Mg	cubic	$a=7.04$	C15	Thermal analysis, x-ray powder and microscopic data; congruent m.p. 819°C.	9,213

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
CuMg <sub>2</sub>	ortho- rhom- bic	a=5.284 b=9.07 c=18.25	$\sqrt{D}_{2h}^{24}$ -- Fddd $\overline{7}$	Thermal analysis, x-ray powder and microscopic data; congruent m.p. 588°C.	10,218
Cu <sub>5</sub> Ca	hexag- onal	a=5.092 c=4.086	$\sqrt{D}_{6h}^1$ -- C6/mmm $\overline{7}$	Originally reported as Cu <sub>4</sub> Ca; thermal analysis, x-ray powder and microscopic data.	11,12
CuZn	cubic	a=2.951 (46.2 a/o Zn)	B2	Structure below 450°C; thermal analysis, x-ray powder and microscopic data.	13
CuZn	cubic	a=2.96	A2	Structure above 450°C.	37
Cu <sub>5</sub> Zn <sub>8</sub>	cubic	a=8.879 (64.7 a/o Zn)	D8 <sub>2</sub>	Decomposes peritectically at ~ 830°C; thermal analysis, x-ray powder and microscopic data by many investigators.	56
CuZn <sub>3</sub>	cubic	a=3.016 (74.8 a/o Zn, 595°C)	A2	Stable above 560°C; decomposes peritectically at 700°C; thermal analysis, x-ray powder, microscopic and other data by many investigators.	13,14
CuZn <sub>5</sub>	hexag- onal	a=2.75 c=4.30 (80 a/o Zn)	A3	Decomposes peritectically at 600°C; thermal analysis, x-ray powder, microscopic and other data by many investigators.	13
Cu <sub>2</sub> Cd		a=4.96 c=7.99		X-ray powder data; line compound; decomposes peritectically at 549°C.	15
Cu <sub>4</sub> Cd <sub>3</sub>				Decomposes peritectically at 547°C; phase diagram.	15
Cu <sub>5</sub> Cd <sub>8</sub>	cubic	a=9.654	D8 <sub>2</sub>	X-ray powder data.	
CuCd <sub>3</sub>				Decomposes peritectically at 397°C; phase diagram.	62
Cu <sub>4</sub> Hg <sub>3</sub>				Decomposes peritectically at 115°C.	17
~ Cu <sub>3</sub> Hg				"X" phase, ~ Cu <sub>3</sub> Hg; decomposes peritectically at 150°C.	68

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (A)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
CuHg	cubic	a=9.425	D <sub>8</sub> <sub>2</sub>	X-ray single crystal data.	18
Cu <sub>4</sub> La	hexagonal	a=5.179 c=4.124	$\sqrt{D}_{6h}^1$ -- C6/mmm	Actually La(Cu <sub>4.8</sub> La <sub>0.2</sub> ) by structural work; line compound; congruent m.p. 902°C	12
Cu <sub>3</sub> La				Line compound; decomposes peritectically at 793°C.	70
Cu <sub>2</sub> La				Line compound; congruent m.p. 834°C; thermal analysis and microscopic data.	70
CuLa				Line compound; decomposes peritectically at 551°C; thermal analysis and microscopic data.	70
Cu <sub>6</sub> Ce	orthorhombic	a=8.08 b=5.09 c=10.17	$\sqrt{D}_{2h}^{16}$ -- Pnma	This space group is correct if structure is centrosymmetric; line compound; congruent m.p. 940°C; phase diagram; x-ray powder data.	57
Cu <sub>4</sub> Ce	hexagonal	a=5.151 c=4.140	$\sqrt{D}_{6h}^1$ -- C6/mmm	Ce(Cu <sub>4.8</sub> Ce <sub>0.2</sub> ); line compound; decomposes peritectically at 780°C; phase diagram; x-ray powder data.	57,58
Cu <sub>2</sub> Ce				Line compound; congruent m.p. 820°C; phase diagram.	66
CuCe				Line compound; decomposes peritectically at 515°C; phase diagram.	66
Cu <sub>6</sub> Pr				Phase diagram; line compound; congruent m.p. 962°C.	64
Cu <sub>4</sub> Pr				Phase diagram; decomposes peritectically at 824°C.	64
Cu <sub>2</sub> Pr				Phase diagram; congruent m.p. 841°C.	64

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
CuPr				Phase diagram; decomposes peritectically at 563°C.	64
CuB <sub>22</sub>				Thermal analysis and microscopic data; complex structure.	20
$\beta$ -Cu <sub>3</sub> Al	cubic	a=2.95	A2	X-ray powder data; disordered structure.	68, 230, 231
$\beta$ '-Cu <sub>3</sub> Al	cubic	a=5.82		X-ray powder data; ordered structure; on further cooling of alloys < 13.1 w/o Al, $\beta$ structure transforms to a $\beta'$ structure which is a distorted $\gamma'$ structure (Cu <sub>2</sub> Al); $\beta'$ can be converted to $\gamma'$ by mechanical deformation.	68, 230, 231, 232, 233
$\gamma$ -Cu <sub>3</sub> Al	orthorhombic	a=4.52 b=5.21 c=4.23	$\sqrt{C}^1_{2v}$ P2mm	X-ray powder and single crystal data; samples quenched from 850-890°C; pseudohexagonal cell with a=2.60, c=4.23.	68, 232, 233
Cu <sub>2</sub> Al	cubic	a=8.7		Decomposes peritectically at 873°C.	68
Cu <sub>9</sub> Al <sub>4</sub>	cubic	a=8.7040	D8 <sub>3</sub>	Stable > 963° to ~1030°C.	21, 22
Cu <sub>32</sub> Al <sub>19</sub>	cubic	a=8.703-8.722 (for pseudocubic cell)	D8 <sub>1-3</sub>	Structure can be described as a deformed $\gamma$ -brass type; decomposes peritectically at 690°C.	68, 71
Cu <sub>4</sub> Al <sub>3</sub>	hexagonal	a=8.10 c=10.00	D8 <sub>3</sub>	Decomposes peritectically at 590°C; x-ray powder data; phase diagram.	23
CuAl	orthorhombic	a=4.10 b=12.0 c=8.65	D8 <sub>3</sub>	Thermal analysis, powder x-ray and microscopic data; decomposes peritectically at 626°C.	23
CuAl <sub>2</sub>	tetragonal	a=6.05 c=4.87	C16	Congruent m.p. 595°C; thermal analysis, x-ray powder and microscopic data.	9



<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Cu <sub>3</sub> Ga	hexag- onal	a=2.599 c=4.238	A3	Three modifications above 420°C; thermal analysis, x-ray powder and microscopic data; no structure data on third modification.	25, 26,27
Cu <sub>3</sub> Ga	cubic		A2		
Cu <sub>9</sub> Ga <sub>4</sub>	cubic	a=8.729	~D8 <sub>2</sub>	Decomposes peritectically at 836°C; orders on cooling at ~490°C; thermal analysis, x-ray powder and microscopic data.	25,27
CuGa <sub>2</sub>	tetrag- onal	a=2.836 c=5.843	C38 (disordered)	Single crystal x-ray data; phase diagram.	25
Cu <sub>4</sub> In	cubic		A2	Stable at > 574°C; decomposes peritectically at 715°C; thermal analysis, x-ray powder and microscopic data.	26
Cu <sub>7</sub> In <sub>3</sub>	cubic		D8 <sub>2</sub>	Maximum temperature at which stable is 682°C; goes to tetragonal form at 630°C. on cooling.	29
Cu <sub>7</sub> In <sub>3</sub>	tetrag- onal	a=8.99 c=9.16	~B8	Structure below 630°C; x-ray powder data; phase diagram.	26,29
Cu <sub>2</sub> In	hexag- onal	a=4.29 c=5.26	B8	Decomposes peritectically at 675°C; x-ray powder data; phase diagram.	30, 26,29
CuIn			~B8	Decomposes peritectically at 310°C; x-ray powder data; phase diagram.	26
Cu <sub>3</sub> Ti	ortho- rhombic	a=5.06 b=4.36 c=4.53	$\sqrt{D}_{2h}^{13}$ -- Pmm $\overline{2}$	Structure below 600°C; thermal analysis, x-ray powder and microscopic data.	31,32
Cu <sub>3</sub> Ti	ortho- rhombic	a=2.60 b=4.54 c=4.36	$\sqrt{D}_{2h}^{17}$ -- Cmcm $\overline{2}$	Structure above 600°C; congruent m.p. 905°C.	31,32
CuTi	tetrag- onal	a=3.15 c=2.87	L10	Low temperature structure; thermal analysis, x-ray powder data.	34, 31,32

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER - ENCES</u>
CuTi	tetrag- onal	a=3.12 c=5.90	B11	High temperature structure; congruent m.p. 982°C.	31,32,34
CuTi <sub>2</sub>	cubic	a=11.24	E9 <sub>3</sub>	(33) says there is no oxygen needed to stabilize this compound in the E9 <sub>3</sub> type structure; congruent m.p. 1014 C; thermal analysis; x-ray powder and micros- copic data.	31,33
Cu <sub>2</sub> Ti				Phase diagram; decomposes peritectically at 892°C.	31
Cu <sub>3</sub> Ti <sub>2</sub>				Phase diagram; decomposes peritectically at 935°C.	31,32
Cu <sub>3</sub> Zr				Phase diagram; congruent m.p. 1100°C.	35
Cu <sub>5</sub> Zr <sub>2</sub>				Phase diagram; decomposes peritectically at 1070°C.	35
Cu <sub>3</sub> Zr <sub>2</sub>				Phase diagram; congruent m.p. 895°C.	35,36
CuZr				Phase diagram; congruent m.p. 935°C.	35
CuZr <sub>2</sub>	tetrag- onal	a=3.3 c=11.3	$\sqrt{D}_{4h}^{17}$ I4/mmm	Phase diagram; congruent m.p. 1065°C; x-ray powder data.	35,36
Cu <sub>4</sub> Th				At least three compounds in Cu-Th system; formula of this compound not well established; also reported as Cu <sub>6</sub> Th.	24,65
Cu <sub>2</sub> Th	hexag- onal	a=4.36 c=3.48	C32	Phase diagram; x-ray powder data.	65, 24,28
CuTh <sub>2</sub>	tetrag- onal	a=7.29 c=5.75	C16	Compound previously reported as Cu <sub>3</sub> Th <sub>5</sub> on basis of phase diagram studies is probably this compound; x-ray powder data.	65, 24,28

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFERENCES</u>
$\text{Cu}_7\text{Si}$	hexagonal	$a=2.58$ $c=4.19$	A3	X-ray powder data.	59
$\text{Cu}_5\text{Si}$	cubic	$a=6.22$	A13	"	59
$\text{Cu}_{15}\text{Si}_4$	cubic	$a=9.71$	D8 <sub>6</sub>	Single crystal x-ray data.	8
$\text{Cu}_{15}\text{Si}_4$	cubic		D8 <sub>1-3</sub>	Related to $\delta$ -brass structure; x-ray powder data.	59
$\text{Cu}_5\text{Ge}$	hexagonal	$a=2.655$ $c=4.294$ (19.4 a/o Ge)	A3	X-ray powder data; phase diagram; decomposes peritectically at 828°C.	38
$\text{Cu}_3\text{Ge}$	monoclinic	$a=2.631$ $b=4.200$ $c=4.568$ $\beta=89^\circ 41'$	$\sqrt{C}_2^{--}$ P2 <sub>1</sub> /7 or $\sqrt{C}_{2h}^{--}$ P2 <sub>1</sub> /m7	Low temperature form; transforms to hexagonal form at 570-635°C; single crystal x-ray data.	38,39
$\text{Cu}_3\text{Ge}$	hexagonal	$a=4.20$ $c=5.04$		Stable from 570-635°C. to ~800°C. for < 25 a/o Ge; x-ray powder data; distorted A2 structure.	38
$\text{Cu}_3\text{Ge}$	cubic		A2	Defect lattice; stable 612°C to 700°C at ~ 27 a/o Ge; thermal analysis, x-ray powder and microscopic data.	38
$\text{Cu}_5\text{Sn}$	cubic	$a=2.978$	A2	Stable at > 700°C; phase diagram, and high temperature x-ray data.	40
$\text{Cu}_{31}\text{Sn}_8$	cubic	$a=17.91$	D8 <sub>2-3</sub>	Phase diagram, powder and single crystal x-ray data; stable ~ 350-640°C.	40
$\text{Cu}_{20}\text{Sn}_6$	hexagonal	$a=7.331$ $c=7.870$	$\sqrt{D}_{3d}^1$ H3m7	Possibly related to the D8 <sub>2-3</sub> structures; thermal analysis and microscopic data; stable 580-640°C.	41

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
$\text{Cu}_3\text{Sn}$	ortho- rhom- bic	$a=4.33$ $b=5.25$ $c=38.1$		Single crystal x-ray data; superlattice based on A3 structure.	60
$\text{Cu}_6\text{Sn}_5$	hexag- onal	$a=4.20$ $c=5.10$	B8	Powder, Laue, and rotation x-ray data.	40
$\text{Cu}_3\text{N}$	cubic	$a=3.82$	$\text{DO}_9$	X-ray powder data.	61
$\text{Cu}_3\text{P}$	hexag- onal	$a=7.08$ $c=7.149$	$\text{DO}_{21}$	"	42, 224
$\text{Cu}_3\text{As}$	cubic	$a=9.612$	$\sqrt[6]{T_d}$ $\text{I}\bar{4}3d$	X-ray powder data; natural domeykite.	42
$\text{Cu}_3\text{As}$	hexag- onal	$a=7.103$ $c=7.247$	$\text{DO}_{21}$	X-ray powder data; obtained by heating natural domeykite at 225°C.	42, 43
$\text{Cu}_3\text{As}$	hexag- onal	$a=2.586$ $c=4.229$		X-ray powder data; stable below 250°C; 2 atoms per unit cell; algodonite min- eral.	42
$\text{Cu}_{11}\text{Sb}_2$	ortho- rhom- bic	$a=9.30$ $b=8.20$ $c=8.64$		Stable 400-~488°C; deform- ed A3 structure; phase diag- ram; x-ray powder data.	44, 45
$\text{Cu}_9\text{Sb}_2$	hexag- onal	$a=10.858$ $c=8.629$ (70.14 a/o Cu)		Decomposes peritectically at 462°C; related to A3 structure; phase diagram; x-ray powder data.	44, 45
$\text{Cu}_{11}\text{Sb}_4$	hexag- onal	$a=5.505$ $c=8.704$		Decomposes at 375°C; related to A3 structure; phase diagram; x-ray powder data.	44, 45
$\text{Cu}_3\text{Sb}$	cubic	$a=6.00$	$\text{DO}_3$	X-ray powder and back- reflection data; samples quenched from 550°C.	221, 222 223
$\text{Cu}_5\text{Sb}_2$	tetrag- onal	$a=9.03$ $c=8.59$		Stable 440-685°C; samples at 56.71 a/o Cu.	44
$\text{Cu}_2\text{Sb}$	tetrag- onal	$a=4.000$ $c=6.103$	C38	Decomposes peritectically at 585°C; x-ray powder data.	44, 46

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Cu <sub>5</sub> U	cubic	a=7.03	C15	Thermal analysis, microscopic	47, 48
CuS	hexag- onal	a=3.76 c=16.2	B18	Covellite mineral.	62
Cu <sub>2</sub> S	cubic	a=5.59	C1	X-ray powder data.	49
Cu <sub>2</sub> Se	cubic	a=5.75	C1	"	49, 219, 220
CuSe	hexag- onal	a=3.95 c=17.29	B18	Klockmannite mineral.	19
Cu <sub>2</sub> Te	hexag- onal	a=4.237 c=7.274	$\sqrt{D}_{6h}^1$ -- C6/mmm $\overline{7}$	Structure below 640°C; congruent m.p. 890°C.	50, 51, 215
Cu <sub>2</sub> Te	cubic	a=6.10		High temperature phase, stable above 640°C; 12 atoms per unit cell.	50, 51, 215
Cu <sub>4</sub> Te <sub>3</sub>	tetrag- onal	a=3.98 c=6.12	C38	Line compound; decomposes peritectically at 623°C;	51, 63, 215
CuTe	ortho- rhombic	a=3.15 b=4.08 c=6.93	$\sqrt{D}_{2h}^{13}$ -- Pmmn $\overline{7}$	Decomposes peritectically at 365°C; thermal analysis, x-ray powder, microscopic, and dilatometric data.	51
Cu <sub>3</sub> Rh				Hardness, microscopic, and x-ray powder data indicate these superlattices in quenched solid solution alloys.	52
CuRh					
CuRh <sub>3</sub>					
Cu <sub>4</sub> Pd	tetrag- onal		$\sqrt{C}_{4h}^2$ -- P4 <sub>2</sub> /m $\overline{7}$	Stable below 478°C; x-ray powder data; phase diagram.	53
Cu <sub>3</sub> Pd	cubic		L12	Ordered f.c.c. below 525°C.	54
CuPd	cubic	a=3.00	B2	X-ray powder data; phase diagram.	54

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Cu <sub>3</sub> Pt			L12	Electrical conductivity measurements and x-ray diffraction diagrams.	54,55, 69,225
CuPt	rhomboidal	a=7.57 α=90°54'	L11	Stable for composition 40-55 a/o Pt below 810°C.	54
Cu <sub>3</sub> Pt <sub>5</sub>				Powder diagrams.	69,225
CuPt <sub>3</sub>	cubic		~L13	Stable for composition 60-75 a/o Pt; powder diagrams.	69
CuPt <sub>7</sub>	cubic		~L13	Stable ~45 a/o Pt at ~700°C; lattice constants twice those of CuPt <sub>3</sub> .	54,69
AgLi	cubic	a=3.17	B2	X-ray powder data.	105,108, 117
AgLi <sub>3</sub>	cubic	a=9.96	D8 <sub>1-3</sub>	Composition varies from Li <sub>3</sub> Ag to Li <sub>4</sub> Ag; thermal analysis and x-ray powder data; formulae Li <sub>9</sub> Ag <sub>4</sub> , Li <sub>10</sub> Ag <sub>3</sub> and Li <sub>12</sub> Ag also reported and are probably indicative of a region of solid solubility.	105,108, 116
Ag	cubic	a=4.0778		X-ray powder data.	228,229
Ag-Au				Ag <sub>3</sub> Au, Ag <sub>3</sub> Au <sub>7</sub> , Ag <sub>3</sub> Au <sub>2</sub> , Ag <sub>2</sub> Au <sub>3</sub> , AgAu, AgAu <sub>3</sub> : these compounds were reported on the basis of variations in the lattice constants; Norman and Warren have found that no compounds should exist in the system above 160°K.	80,81
AgBe <sub>2</sub>	cubic	a=6.300	C15	X-ray powder data, thermal, magnetic and micrographic analysis.	84,85
Ag <sub>3</sub> Mg	cubic	a=4.111 (disordered) a=4X4.108 (ordered)		Powder and Weissenberg x-ray data.	107

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	
AgMg	cubic	a=3.29	B2		106,108, 109,135
AgMg <sub>3</sub>				Previously reported as hexagonal with a=4.93 and c=7.81; complicated structure of lower symmetry.	108,110, 109, 135,136
Ag <sub>4</sub> Ca				Thermal analysis.	86
Ag <sub>3</sub> Ca	tetragonal	a=11.3 c=9.96		Thermal analysis and x-ray powder data.	86,87
Ag <sub>2</sub> Ca	hexagonal	a=5.72 c=9.35	C114	"	86,87
AgCa	cubic	a=9.071		"	86,87
AgCa <sub>2</sub>				"	86
Ag <sub>5</sub> Sr	hexagonal	a=5.664 c=4.610	$\sqrt{D}_{6h}^1$ -- C6/mmm	"	83
Ag <sub>4</sub> Sr				Thermal analysis.	118
Ag <sub>5</sub> Sr <sub>3</sub>				"	118
AgSr				"	118
Ag <sub>2</sub> Sr <sub>3</sub>				"	118
Ag <sub>5</sub> Ba	hexagonal	a=5.708 c=4.636	$\sqrt{D}_{6h}^1$ -- C6/mmm	Thermal analysis and x-ray powder data.	83
Ag <sub>4</sub> Ba				Thermal analysis.	82
Ag <sub>5</sub> Ba <sub>3</sub>				"	82
Ag <sub>3</sub> Ba <sub>2</sub>				"	82
AgZn	hexagonal	a=7.6360 c=2.8197	$\sqrt{C}_{3i}^1$ -- P3 <sub>1</sub>	Stable below 260°C.	134
AgZn	cubic	a=3.156	A2	High temperature phase.	133,134

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
AgZn	cubic	a=3.16	B2	Metastable phase obtained through quenching.	137
Ag <sub>5</sub> Zn <sub>8</sub>	cubic	a=9.33	D8 <sub>2</sub>		132,134
AgZn <sub>3</sub>	hexagonal	a=2.81 c=4.42	A3		134
AgCd	cubic	a=3.32	A2	High temperature phase, exists above 450°C.	89,90
AgCd	hexagonal	a=2.98 c=4.81	A3	Exists between 200° and 450°C.	89,90
AgCd	cubic	a=3.33	B2	Exists below 200°C; from x-ray powder and electrical resistivity versus temperature.	89,90
Ag <sub>5</sub> Cd <sub>8</sub>	cubic	a=9.93- 9.98	D8 <sub>2</sub>	γ-brass structure; range of composition variation; microscopy, thermal and x-ray powder data.	88,90, 91,92
AgCd <sub>3</sub>	hexagonal	a=3.06 c=4.84	A3	Extensive composition variation.	88,90, 92
Ag <sub>10</sub> Hg <sub>13</sub>	cubic	a=10.033	D8 <sub>1-3</sub>	γ-brass structure; thermal analysis and x-ray powder data.	95,96
Ag <sub>5.5</sub> Hg <sub>4.5</sub>	hexagonal	a=2.970 c=4.841 (44.8 a/o Hg)	A3		96
Ag-Hg				Vapor pressure measurements have indicated existence of AgHg and Ag <sub>3</sub> Hg <sub>4</sub> (99); electrochemical potentials indicate existence of Ag <sub>3</sub> Hg, Ag <sub>3</sub> Hg <sub>2</sub> and Ag <sub>3</sub> Hg <sub>4</sub> (138); electron diffraction has indicated existence of a cubic phase and two tetragonal phases (140).	97, 98,99, 138,140



<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Ag <sub>3</sub> La				Thermal analysis; congruent melting.	103,104
Ag <sub>2</sub> La				Thermal analysis; incongruent melting.	103,104
AgLa	cubic	a=3.77	B2	Thermal analysis; congruent melting.	103,104
Ag <sub>3</sub> Ce				Thermal analysis and metallography.	128
Ag <sub>2</sub> Ce				"	128
AgCe	cubic	a=3.74	B2	"	128,104
Ag <sub>3</sub> Pr				"	128,111
Ag <sub>2</sub> Pr				"	128,111
AgPr	cubic	a=3.73	B2	"	128,111
Ag <sub>3</sub> Al	cubic	a=3.24	A2	Thermal analysis, microscopic and x-ray powder data.	72,73,75,76,77
Ag <sub>3</sub> Al	cubic	a=6.920	$\sqrt{T}^{14}$ -- P2 <sub>1</sub> 3 <sup>7</sup>	X-ray powder data.	234
Ag <sub>3</sub> Al <sub>2</sub>	hexagonal	a=2.86 c=4.57-4.65		Thermal analysis and x-ray powder data; also reported as Ag <sub>2</sub> Al.	72,73,75,76,78
Ag <sub>3</sub> Ga	hexagonal	a=2.93 c=4.75	A3	Stable from 378-611°C.	1141
Ag <sub>5</sub> Ga <sub>2</sub>	hexagonal			Thermal analysis, microscopy, powder x-ray data; low-temperature ( $\delta$ ) phase structurally related to $\delta$ -phase of Ag-In system; transforms $\sim$ 380°C to high temperature ( $\beta$ ) phase which is hexagonal closest-packed; both high and low temperature phases exist over a region of composition.	94,1141

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Ag <sub>3</sub> In	hexag- onal	a=2.95-2.98 c=4.77-4.79	A3 or D0 <sub>19</sub>	The former structure exists > 300°C, the latter < 200°C; variable composition; third 100, phase reported > 660°C.	101,102
Ag <sub>2</sub> In	cubic	a=9.885	D8 <sub>1-3</sub>	γ-brass structure, exists < 200°C; thermal analysis, powder x-ray data; some com- position variation.	100
AgIn <sub>2</sub>	tetrag- onal	a=6.869 c=5.604	C16	Thermal analysis, powder x-ray data; some composition variation.	100,102
AgTi	tetrag- onal	a=4.104 c=4.077	L10	Isomorphous with CuAu; x-ray powder data with comparison of observed and calculated intensities.	130,131
AgZr	tetrag- onal	a=3.468 c=6.603	B11	X-ray powder data.	115
AgZr <sub>3</sub>	tetrag- onal	a=4.566 c=3.986	$\sqrt{D}_{4h}^1$ -- P4/mmm <sup>7</sup>	"	115
Ag <sub>5</sub> Th <sub>3</sub>				Thermal analysis, micro- scopic and x-ray investi- gations.	129
Ag <sub>3</sub> Th				"	129
Ag <sub>6</sub> Sn	hexag- onal	a=2.931-2.959 c=4.784-4.781		Lattice parameters are indi- cated for composition extremes; composition varies from 13.3- 142, 19.7 a/o Sn at 400°C; thermal, 143 dilatometric, electrical resist- ivity and x-ray powder data.	
Ag <sub>3</sub> Sn	ortho- rhombic	a=2.991-3.000 b=5.155-5.165 c=4.781-4.781		Lattice parameters are indi- cated for composition extremes; diffraction patterns indicate that this structure is closely related to the above hexagonal one; composition varies from 124, 24-25.5 a/o Sn at 400°C.	142,143

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	
Ag <sub>9</sub> As	hexagonal	a=2.89 c=4.722	A3	X-ray powder data.	79
Ag <sub>3</sub> Sb	hexagonal	a=3.044 c=4.913	A3	"	121,143
Ag <sub>3</sub> Sb	orthorhombic	a=2.990 b=5.225 c=4.820		Single crystal and x-ray powder data.	226,227
Ag <sub>2</sub> Sb	orthorhombic	a=7.77 b=12.35 c=8.44		X-ray powder data.	119, 120, 227
Ag <sub>2</sub> Se	cubic	a=4.993	C1	"	114
Ag <sub>2</sub> Te	cubic	a=5.87	C1	X-ray powder data; stable at > 155°C.	127, 50,114
Ag <sub>2</sub> Te	orthorhombic			High temperature form.	127
Ag <sub>2</sub> Te	orthorhombic	a=16.27 b=26.68 c=7.55	Immm	X-ray powder data; low temperature form; also reported as monoclinic by (214).	125, 127,214
Ag <sub>12</sub> Te <sub>7</sub>	hexagonal	a=13.43 c=8.451	$\sqrt{D6h}$ C6/mmm	Also reported as AgTe, Ag <sub>7</sub> Te <sub>5</sub> , Ag <sub>5</sub> Te <sub>3</sub> , and Ag <sub>2-x</sub> Te, evidently indicating an extended composition range for a homogeneous phase; investigations were made on synthetic and natural occurring samples.	125, 126
Ag <sub>3</sub> Pt	cubic	a=3.895 =0.004	A1	Close-packed structure below 800°C; x-ray powder data and conductivity measurements.	112
AgPt	cubic	a=3.93	L13	X-ray powder data.	112,113
AgPt	cubic	a=4.04	L13	"	112,113
AgPt <sub>3</sub>	cubic	a=3.88	L12	"	112,113

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Au <sub>2</sub> Na	cubic	a=7.7872 ±0.0023	C15	X-ray powder data	144,145, 146,147
AuNa <sub>2</sub>	tetrag- onal	a=7.402 c=5.511	C16	Rotation, Weissenberg, and x-ray powder data.	146
Au <sub>4</sub> K Au <sub>2</sub> K				Au <sub>4</sub> K and Au <sub>2</sub> K were post- ulated on grounds of their x-ray powder spectra, which were distinctly different from pure K and Au; No structures or parameters were determined.	148
Au	cubic	a=4.0781	A1	Gold leaf electron diffraction.	149
Au <sub>3</sub> Be				X-ray powder and back- reflection data; para- meters not reported	150
Au <sub>2</sub> Be				"	150
AuBe	cubic	a=4.668 ±0.001	B20	X-ray powder data with comparison of calculated and observed intensities.	150,151
AuBe <sub>3</sub>				X-ray data indicates this compound exists; structure not determined.	150,152
AuBe <sub>5</sub>	cubic	a=6.083	C15	X-ray powder data with com- parison of calculated and observed intensities; para- meter also reported as a=6.699 by 152.	150,152, 153
AuMg	cubic	a=3.265	B2		154
AuMg <sub>3</sub>	hexag- onal	a=4.64 c=8.46	DO <sub>18</sub>	powder and single crystal x-ray data; Mg <sub>2</sub> Au reported by (156,158) and Mg <sub>5</sub> Au <sub>2</sub> re- ported by(157), both on basis of thermal analysis, are probably this compound.	10,156, 157,158

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Au <sub>6</sub> Ba	hexagonal	a=5.67 c=4.58	$\sqrt{D}_{6h}^1$ -- C6/mmm	X-ray powder data; exists as (Ba <sub>0.86</sub> Au <sub>0.14</sub> )Au <sub>6</sub> in CaCu <sub>5</sub> type structure.	83
Au <sub>3</sub> Zn(α)	cubic	a=4.039	A1	X-ray data and thermal analysis; stable above 420°C.; disordered phase; parameters from sample quenched from 160,161, 500°C.	162
Au <sub>3</sub> Zn(α')	tetragonal	a=4.034 c=4.115		Possibly weakly ordered; parameters at 300°C.; stable 270-420°C; conflicting evidence about this compound.	160,161, 162
Au <sub>3</sub> Zn(α'')	tetragonal	a=3.956 ±0.003 c=8.323 ±0.0012		Stable below 260° C.; ordered structure; approximately doubled c axis; x-ray powder data.	160,161, 162
Au <sub>5</sub> Zn <sub>8</sub>	cubic	a=9.242	D8 <sub>1</sub>	X-ray powder data.	155,165, 56
AuZn	cubic	a=3.152	B2	X-ray powder data; superlattice present in samples quenched from 400-577°C.	163,165, 155,106
~AuZn <sub>2</sub>	cubic	a=11.17		X-ray study of superlattice; ~90 atoms per unit cell.	155,164
AuZn <sub>3</sub>	cubic	a=7.88		X-ray powder data; 32 atoms per unit cell.	155,164, 165
AuZn <sub>6</sub>	hexagonal	a=2.82 c=4.38	A3	X-ray powder data; exact composition and structure open to question; reported as differently as AuZn <sub>9</sub> .	155, 164,165
Au <sub>3</sub> Cd	tetragonal	a=4.107- 4.1177 c=4.138- 4.1298	$\sqrt{D}_{4h}^1$ -- P4/mmm	Deformed Cu <sub>3</sub> Au structure; x-ray powder and back reflection data; parameters from samples quenched at 350°C. and 22.8-25.5 atomic percent Cd.	166,167, 168

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Au <sub>2</sub> Cd	hexagonal	a=2.9085- 2.9224 c=4.7719- 4.8377	A3	X-ray powder and back-reflection data; stacking faults at less than 30% Cd; parameters from samples of 25.30-35.51 atomic percent Cd.	166, 167,168
Au <sub>55</sub> Cd <sub>45</sub>	rhomboidal	a=5.484 c=12.618		Conflicting evidence about the existence of this compound.	166,167, 168
β AuCd	cubic	a=3.3224- 3.3181	B2	X-ray powder and back-reflection data; parameters from samples of 50.8-55.0 atomic percent Cd.	167,169; 170,166, 168,171
β' AuCd	orthorhombic	a=3.141- 3.164 b=4.879- 4.855 c=4.767- 4.768	B19	At 64 ± 6° C., the β' form goes to the β form; possibly another transition at 280-300° C. with no structure change; fiber camera used for structure and self-focusing camera for parameters; range: 46.3-48.1 atomic percent Cd.	166,167, 168, 169,170
AuCd <sub>2</sub>	hexagonal		A3		212
AuCd <sub>3</sub>	cubic	a=4.11	L12		212,172, 173,174, 175
Au <sub>5</sub> Hg	cubic	a=4.122	A3	Parameters measured at 175° C.	176,177, 178
Au <sub>3</sub> Hg	hexagonal	a=2.906- 2.921 c=4.780- 4.812	A3	Formula approximates Au <sub>3</sub> Hg; parameters from samples of 19.1-32.7 weight percent Hg.	176,177, 178
Au <sub>2</sub> Hg <sub>3</sub>					177
AuHg <sub>2</sub>					177

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Au <sub>3</sub> La				Thermal analysis and metallography; Ce-Au, La-Au and Pr-Au systems reported to be analogous.	128, 144
Au <sub>2</sub> La				"	128
AuLa				"	128, 144
AuLa <sub>2</sub>				"	128
Au <sub>3</sub> Ce				"	128
Au <sub>2</sub> Ce				"	128
AuCe				"	128
AuCe <sub>2</sub>				"	128
Au <sub>3</sub> Pr				Reported as Au <sub>4</sub> Pr by (189).	128, 189
Au <sub>2</sub> Pr				Same as Au <sub>3</sub> La.	128
AuPr				"	128
AuPr <sub>2</sub>				"	128
Au <sub>4</sub> Al	cubic	a=6.916	$\sqrt{T}^{4--}$ P2 <sub>1</sub> 37	X-ray powder data.	179, 180, 181
Au <sub>5</sub> Al <sub>2</sub>				Thermal analysis and metallography; compound may be Au <sub>8</sub> Al <sub>3</sub> .	179, 159, 180, 181
Au <sub>2</sub> Al				Thermal analysis and metallography.	159, 179, 180, 182
AuAl	cubic	a=6.05	B3		159, 179, 180, 182
AuAl <sub>2</sub>	cubic	a=6.00	C1	Formed by reaction of elements in liquid phase with evolution of heat; solidifies at 1060°C. to a purple solid.	159, 179, 180, 182, 183, 184

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Au <sub>3</sub> Ga				Thermal analysis and metallography.	26,185
Au <sub>7</sub> Ga <sub>3</sub>				"	26,185
AuGa	ortho- rhombic	a=6.397 b=6.267 c=3.421	B31	Thermal analysis, metallography and x-ray powder data.	26,185
AuGa <sub>2</sub>	cubic	a=6.086	C1	"	184,185
Au <sub>9</sub> In	hexag- onal	a=2.91 c=4.75		Schubert et. al. have made additional structure studies on the Au-In-Cd system; refer to abstract #5.19, 4th International Congress, International Union of Crystallography, Montreal 10-19, July 1957,	186
Au <sub>8</sub> In <sub>2</sub>	hexag- onal		A3		26
Au <sub>5</sub> In					186
Au <sub>7</sub> In <sub>3</sub>	cubic	a=9.80		Related to $\gamma$ -brass structure.	26,186
AuIn	triclinic	a=4.30 b=10.59 c=3.56 $\alpha=90.54^\circ$ $\beta=90.00^\circ$ $\gamma=90.17^\circ$		Pseudo-orthorhombic	186, 187
AuIn <sub>2</sub>	cubic	a=6.502	C1		186,187, 188
$\sim$ Au <sub>6</sub> Ti	tetrag- onal	a=4.07 c=3.94		Compound may be as high as 96 a/o Au.	131,190, 191
Au <sub>3</sub> Ti	hexag- onal			Reported by (191) to be isomorphous with TiCu <sub>3</sub> ; not observed by (131).	131,190, 191
Au <sub>2</sub> Ti	hexag- onal	a=2.79 c=4.77	A3	X-ray data and thermal analysis; invariant composition.	131,190, 191



<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	
AuTi <sub>3</sub>	cubic	a=5.096	A15	X-ray powder data.	131,190, 191,192
Au <sub>3</sub> Zr					193
Au <sub>3</sub> Th				No crystallography work done; phase diagrams.	24
Au <sub>5</sub> Th <sub>3</sub>				"	24
Au <sub>6</sub> Sn	hexagonal	a=2.93 c=4.78	A3		194
Au <sub>5.13</sub> Sn				X-ray data.	195
Au <sub>2.4</sub> Sn	hexagonal			X-ray data; close-packed crystal.	195
AuSn	hexagonal	a=4.314 c=5.512	B8	Electron diffraction and x-ray data.	195,196
AuSn <sub>2</sub>	orthorhombic	a=6.85 b=7.00 c=11.78		Electron diffraction data.	196,187
AuSn <sub>4</sub>	orthorhombic	a=6.446 b=6.487 c=11.599	$\sqrt{C_{2v}^{17}}$ Aba27	Structure related to C16 type; x-ray powder data.	196,216, 217
Au <sub>2</sub> Pb	cubic	a=7.98 =0.01	C15	X-ray diffraction data.	197,198, 200
AuPb <sub>2</sub>	tetragonal	a=7.310 ±0.003 c=5.644 ±0.003	C16	"	197,198, 199,200
AuNb <sub>3</sub>	cubic	a=5.21 ±0.01	A15		201
AuV <sub>3</sub>	cubic	a=4.88 ±0.01	A15		201
AuSb <sub>2</sub>	cubic	a=6.63	C2	Electron diffraction data.	196,202
Au <sub>2</sub> Bi	cubic	a=7.958	C15		200,203

<u>COMPOUND</u>	<u>CRYSTAL CLASS</u>	<u>LATTICE PARAMETERS (Å)</u>	<u>STRUCTURE</u>	<u>REMARKS</u>	<u>REFER- ENCES</u>
Au <sub>3</sub> U				Thermal analysis and metallography and x-ray diffraction.	206
Au <sub>3</sub> U <sub>2</sub>				Thermal analysis and metallography and x-ray diffraction; forms from peritectic at 216°C.	206
Au <sub>2</sub> Te <sub>3</sub>	triclinic	a=12.10 b=13.46 c=10.80 α=104°30.5' β=97°34.5' γ=107°53.5'		Pseudocubic; x-ray powder data.	204,205
AuTe <sub>2</sub>	ortho- rhom- bic	a=16.51 b=8.80 c=4.45	C46	X-ray powder data.	239
Au <sub>3</sub> Mn				Structure not known; apparently nearly tetragonal with complicated superstructure.	207
Au <sub>2</sub> Mn				Major lines on x-ray patterns belong to body-centered tetragonal structure; a great number of weak interference lines make the indexing questionable. a=3.36, c/a=0.87	207
AuMn	cubic	a=3.249	B2	β phase decomposes into β' or β'' which do not coexist. (below 615°C)	207
AuMn <sub>3</sub>				Same as Au <sub>2</sub> Mn except a=3.310, c/a=0.85	207
AuFe <sub>3</sub>				Compound reported by (208), denied by (209,210).	208,209, 210

## PART II: REFERENCES

1. Harker, D., *Trans. Am. Soc. Metals* 32, 210 (1944).
2. Borelius, Johansson, and Linde, *Ann. phys.* 86, 291-318 (1928).
3. Ohshima and Sachs, *Z. Physik* 63, 210-223 (1930).
4. Losana and Venturello, *Alluminio* 11, 8-16 (1942).
5. Iwasé and Okamoto, *Nippon Kinzoku Gakkai-Shi* 5, 82 (1941).
6. Dahl, Holm, and Masing, *Wiss. Veröffentl. Siemens-Konzern* 8, 154-186 (1929).
7. Misch, L., *Z. physik. Chem.* B29, 42-58 (1935).
8. Morral and Westgren, *Arkiv Kemi, Mineral. Geol.* 11B, No. 37 (1934).
9. Friauf, J., *J. Am. Chem. Soc.* 49, 3017 (1927).
10. Schubert and Anderko, *Z. Metallkunde* 42, 321 (1951).
11. Haucke, W., *Z. anorg. Chem.* 244, 17-22 (1940).
12. Nowotny, H., *Z. Metallkunde* 34, 247-253 (1942).
13. Owen and Preston, *Proc. Roy. Soc. (London)* 36, 49-66 (1923).
14. Schubert and Wall, *Z. Metallkunde* 40, 383-385 (1949).
15. Kripyakevich, Gladyshevskii, and Cherkashin, *Doklady Akad. Nauk S. S. S. R.* 82, 253-256 (1952).
16. Bradley and Gregory, *Phil. Mag.* 12, 143-162 (1931).
17. Lihl, F., *Z. Metallkunde* 44, 160-166 (1953).
18. Schoszberger, F., *Z. physik. Chem.* B29, 65-78 (1935).
19. Early, J., *Am. Mineralogist* 33, 194 (1948).
20. Lihl and Feischl, *Metall* 8, 11 (1954).
21. Nelson and Riley, *Proc. Roy. Soc. (London)* 57, 160-177 (1945).
22. Bradley, A., *Phil. Mag.* 6, 878-888 (1928).
23. Preston, G., *Phil. Mag.* 12, 980-995 (1931).

24. Raub and Engle, Z. Elektrochem. 49, 487-493 (1943).
25. Zintl and Treush, Z. physik. Chem. B34, 225-237 (1936).
26. Hellner and Laves, Z. Naturforsch. 2A, 177-183 (1947)...
27. Betterton and Hume-Rothery, J. Inst. Metals 80, 459-468 (1951-1952).
28. Baenziger, Rundle, and Snow, Acta Cryst. 9, 93 (1956).
29. Reynolds, Wiseman, and Hume-Rothery, J. Inst. Metals 80, 637-640 (1951-1952).
30. Makarov, E., Izvest. Akad. Nauk S. S. S. R., Otdel. Khim. Nauk 1943 269-270 (1943).
31. Trzebiatowski, Berak, and Romotowski, Roczniki Chem. 27, 426 (1953).
32. Joukainen, Grant, and Floe, Trans. Am. Inst. Mining Met. Engrs. 194, 766 (1952).
33. Rostoker, W., J. Metals 4, 209-210 (1952).
34. Karlsson, N., J. Inst. Metals 79, 391-405 (1951).
35. Lundin, McPherson, and Hansen, J. Metals 5, 273-278 (1953).
36. Augustson, R., U. S. Atomic Energy Comm. Report No. AECD - 3456 (1950).
37. Raynor, G., Inst. Metals (London), Annotated Equil. Diagram, No. 3 (1944).
38. Schubert and Brandauer, Z. Metallkunde 43, 262-268 (1952).
39. Nowotny and Bachmayer, Monatsh. Chem. 81, 669-678 (1950).
40. Westgren and Phragmen, Z. anorg. Chem. 175, 80 (1928).
41. Carlsson and Hägg, Z. Krist. 83, 308-317 (1932).
42. Steenberg, B., Arkiv Kemi, Mineral. Geol. 12A, No. 26 (1938).
43. Owen and Rowlands, J. Inst. Metals, 66, 367 (1940).
44. Osawa and Shibata, Science Repts. Tôhoku Imp. Univ. 28, 1-19 (1939).
45. Schubert and Ilchner, Z. Metallkunde 45, 366-370 (1954).
46. Elander, Hägg, and Westgren, Arkiv Kemi, Mineral. Geol. 12B, No. 1, 65, (1935).

47. Wilhelm and Carlson, Trans. Am. Soc. Metals 42, 1311-1325 (1950).
48. Baenziger, Rundle, Snow, and Wilson, Acta Cryst. 3, 34-40 (1950).
49. Hartwig, W., Z. Krist. 64, 503-504 (1926).
50. Nowotny, H., Metallforschung 1, 40-42 (1946).
51. Anderko and Schubert, Z. Metallkunde 45, 371-378 (1954).
52. Zviagintev and Brunoskiy, Izvest. Inst. Izucheniyyu Platiny i Drug. Bladorod. Metal. 12, 37-66 (1935).
53. Geisler and Newkirk, J. Metals 6, 1076-1082 (1954).
54. Johansson and Linde, Ann. phys. 82, 449-473 (1927).
55. You-Chi Tang, Acta Cryst. 4, 377-378 (1951).
56. Bradley and Thewlis, Proc. Roy. Soc. (London) A112, 678-692 (1926).
57. Byström, Kierkegaard, and Knop, Acta Chem. Scand. 6, 709-719 (1952).
58. Heumann, T., Nachr. Ges. Wiss. Göttingen 1, 21-25 (1943).
59. Sautner, K., Forschungsarb. Metallkunde u. Röntgenmetalloge. 9, 31 pp. (1931).
60. Bernal, J., Nature 122, 54 (1928).
61. Fitzgerald, F., J. Am. Chem. Soc. 29, 656 (1907).
62. Orstedal, I., Z. Krist. 83, 9-25 (1932).
63. Chikashige, M., Z. anorg. u. allgem. Chem. 54, 50-57 (1907).
64. Canneri, G., Metallurgia ital. 26, 869-871 (1934).
65. Grube and Botzenhardt, Z. Elektrochem. 48, 418-425 (1942).
66. Hanaman, F., Intern. Z. Metallog. 7, 174-212 (1915).
67. Tammann and Stassfurth, Z. anorg. u. allgem. Chem. 143, 357-369 (1925).
68. Bradley and Jones, J. Inst. Metals 51, 131-161 (1933).
69. Schneider and Esch, Z. Elektrochem. 50, 290-301 (1944).
70. Canneri, G., Metallurgia ital. 23, 813-815 (1931).
71. Bradley, J., Nature 158, 661 (1951).

72. Hansen, M., "Aufbau der Zweistofflegierungen," p. 1 (Edwards Brothers, Inc., Ann Arbor, Michigan, 1943).
73. Hume-Rothery, Mabbott, and Evans, Trans. Roy. Soc. (London) A233, 1-97 (1934).
74. Gautier, H., C. R. Acad. Sci., Paris 123, 109 (1896).
75. Petrenko, G., Z. anorg. u. allgen. Chem. 46, 49-59 (1905).
76. Kokubo, S., Science Repts. Tôhoku Imp. Univ. 33, 45-51 (1934).
77. Faberberg and Westgren, Metallwirtschaft 14, 265-267 (1935).
78. Westgren and Bradley, Phil. Mag. 6, 280-288 (1928).
79. Broderick and Ehret, J. Phys. Chem. 35, 3322-3329 (1931).
80. Phragmen, G., Fysisk Tids. 24, 40-41 (1926).
81. Norman and Warren, J. Appl. Phys. 22, 483 (1951).
82. Hansen, M., op. cit., p. 10.
83. Heumann, T., Nachr. Ges. Wiss. Göttingen 2A(1), 1-6 (1950).
84. Winkler, O., Z. Metallkunde 30, 162 (1938).
85. Misch, L., Metallwirtschaft 15, 163-166 (1936).
86. Hansen, M., op. cit., p. 16.
87. Degard, C., Z. Krist. 90, 399 (1935).
88. Hansen, M., op. cit., p. 17.
89. Muldwer, Amsterdam, and Rothwarf, J. Metals 11, 1458-1459 (1953).
90. Owen, Rogers, and Guthrie, J. Inst. Metals 55, 457 (1939).
91. Perlitz and Aavakivi, Acta Comment. Univ. Tartuensis (Dorpatensis) A35-2, 1-13 (1939).
92. Bain, E., Chem. & Met. Eng. 28, 21-24 (1923).
93. Owens and Morris, J. Inst. Metals 76, 160 (1949-1950).
94. Weibke, Meisel, and Wiegels, Z. anorg. u. allgem. Chem. 226, 201-208 (1936).

95. Weryha, A., Z. Krist. 86, 335-339 (1933).
96. Murphy, A., J. Inst. Metals 46, 507 (1931).
97. Myers, H., Proc. Phys. Soc. (London) 66, 495-499 (1953).
98. Swamy and Shammana, Current Sci. (India) 21, 7-8 (1952).
99. Ogg, A., Z. physik. Chem. 27, 290 (1898).
100. Hellner, E., Z. Metallkunde 42, 17-19 (1951).
101. Goldschmidt, V., Z. physik. Chem. 133, 397-419 (1928).
102. Frevel and Ott, J. Am. Chem. Soc, 57, 228 (1935).
103. Hansen, M., op. cit., p. 36.
104. Vogel and Klose, Z. Metallkunde 45, 670 (1954).
105. Pastorello, S., Gazz. chim. ital. 60, 493-501 (1930).
106. Owen and Preston, Phil. Mag. 2, 1266 (1926).
107. Clarebrough and Nicholas, Anst. J. Sci. Res. 3A, 284-289 (1950).
108. Freeth and Raynor, J. Inst. Metals 82, 575-580 (1954).
109. Stanislas, Goldstamb, and Michel, Compt. rend. 232, 1843-1845 (1951).
110. Dow Chemical Co., private communications.
111. Canneri, G., Met. ital. 26, 794 (1934).
112. Schneider and Esch, Z. Elektrochem. 49, 72 (1943).
113. Johansson and Linde, Ann. Physik. 6, 458-486 (1930).
114. Rahlfs, P., Z. physik Chem. 31, 157-159 (1935-1936).
115. Karlsson, N., Acta. Chem. Scand. 6, 1424-1430 (1952).
116. Perlitz, H., Z. Krist. 86, 155 (1933).
117. Zintl and Brauer, Z. physik Chem. 20, 245-271 (1933).
118. Hansen, M., op. cit., p. 64.

119. Peacock, M., *Am. Mineralogist*, 23, 176 (1938).
120. Peacock, M., *Am. Mineralogist*, 24, 227-241 (1939).
121. Machatski, L., *Z. Krist.*, 67, 171 (1928).
122. Broderick and Ehret, J. *Phys. Chem.*, 35, 2635 (1931).
123. Homer and Plummer, J. *Inst. Metals*, 64, 191 (1939).
124. Michel, P., *Compt. rend.*, 235, 377-379 (1952).
125. Koern, V., *Naturwissenschaften*, 27, 432 (1939).
126. Thompson, R., et. al., *Am. Mineralogist*, 36, 468 (1951).
127. Rowland and Berry, *Am. Mineralogist*, 36, 478 (1951).
128. Rolla, Jendelli, Canneri and Vogel, *Z. Metallkunde*, 35, 24-42 (1943).
129. Raub and Engel, *Z. Metallkunde*, 40, 431 (1949).
130. Van Thyne, Rostoker, and Kessler, J. *Metals*, 5, 670-671 (1953).
131. Raub, Walter, and Engel, *Z. Metallkunde*, 43, 112-118 (1952).
132. Owen and Pickup, *Proc. Roy. Soc. (London)*, A137, 397-417 (1932).
133. Edmunds and Zurashi, *Acta Cryst.*, 4, 417-425 (1951).
134. Andrews, Davis, Hume-Rothery, and Oswin, *Proc. Roy. Soc. (London)*, A177, 149 (1941).
135. Letner and Sidhu, *J. Appl. Phys.*, 18, 833 (1947).
136. Ageew and Kuznezow, *Bull. Acad. Sci. U. R. S. S., Classe sci. math. nat., Ser. chem.*, 289-309 (1937).
137. Shavlo and Alaverdov, *J. Exp. Theoret. Phys. (U.S.S.R.)*, 9, 59 (1939).
138. Reinders, W., *Z. physik. Chem.* 54, 609 (1906).
139. Aylmer, Finch, and Fordham, *Trans. Faraday Soc.* 32, 864-71 (1936).
140. Pinsker and Talarinova, *Acta. Physicochim. U.R.S.S.* 14, 193-200 (1941).
141. Hume-Rothery and Andens, *J. Inst. Metals*, 68, 133 (1942).
142. Nial, Alni, and Westgren, *Z. physik. Chem.* B14, 85 (1937).



143. John and Evans, Phil. Mag. 23, 1033 (1937).
144. Blitz and Weibke, Z. anorg. u. allgem. Chem. 236, 12-23 (1938).
145. Perlitz and Aruja, Z. Krist. A100, 157-166 (1938).
146. Haucke, W., Z. Elektrochem. 43, 712-719 (1937).
147. Ethyl Corporation circular (1953).
148. Blitz and Weibke, Z. anorg. Chem. 232, 297 (1937).
149. Rymer and Buller, Proc. Phys. Soc. (London), A59, 541-554 (1947).
150. Chatterjee and Sidhu, Phys. Rev. 76, 175 (1949).
151. Cullity, B., Trans. Am. Inst. Mining Met. Engrs. 171, 396-400 (1947).
152. Misch, L., Metallwirtschaft 14, 897-899 (1935).
153. Sidhu and Henry, J. Appl. Phys. 21, 1037 (1950).
154. Brauer and Haucke, Z. physik. Chem. 33, 304-310 (1936).
155. Hansen, M., op. cit., pp. 266-269.
156. Urazov, G., Z. Metallkunde 42, 375-396 (1909).
157. Urazov and Vogel, Z. anorg. u. allgem. Chem. 67, 442-447 (1910).
158. Vogel, r., Z. anorg. u. allgem. Chem. 63, 169-183 (1909).
159. Coffinberry and Hultgren, Trans. Am. Inst. Mining Met. Engrs. 128, 249 (1938).
160. Raub, Walter and Engel, Z. Metallkunde 40, 401-405 (1949).
161. Soldau, P., J. Inst. Metals 30, 351 (1923).
162. Koster, W., Z. Metallkunde 32, 152 (1941).
163. Ageew and Shoykhet, Izvest. Sektor Fiz-Khim. Anal. 13, 165-170 (1940).
164. Owen and Edmunds, Proc. Phys. Soc. (London), A50, 389-397 (1938).
165. Westgren and Phragmen, Phil. Mag. 50, 311-341 (1925).
166. Owen and Roberts, J. Inst. Metals 66, 380-400 (1940).

167. Owen and Rees, J. Inst. Metals 67, 141-151 (1941).
168. Bystrom, Anders and Almin, Acta. Chem. Scand. 1, 76-89 (1948).
169. Chang and Read, USAEC U-1552-(1951).
170. Chang, L., Acta. Cryst. 4, 320-324 (1951).
171. Olander, A., Z. Krist. 83, 145 (1932).
172. Vogel, R., Z. anorg. Chem. 48, 333 (1906).
173. Durrant, P., J. Inst. Metals 41, 139 (1929).
174. Koster and Schneider, Z. Metallkunde 32, 156 (1940).
175. Hansen, M., op. cit., pp 209-212.
176. Stenbeck, S., Z. anorg. u. allgem. Chem. 214, 16-24 (1933).
177. Pabst, A., Z. physik. Chem. 3B, 443-455 (1933).
178. Plaksin, I., Izvest. Sektora Fiz. Khim. Anal. 10, 129-159 (1938).
179. Heycock and Neville, Phil. Trans. Roy. Soc. (London) 194A, 201 (1900).
180. Heycock and Neville, Phil. Trans. Roy. Soc. (London) 214A, 267 (1914).
181. Ullner, O., Arkiv Kemi Mineral. Geol. 14A, 20 (1940).
182. Eisenhut and Kaupp, Z. Elektrochem. 37, 466-473 (1931).
183. West and Peterson, Z. Krist. 88, 93 (1934).
184. Zintl, Haseler and Haucke, Z. physik. Chem. 35B, 354 (1937).
185. Pfisterer and Schubert, Z. Metallkunde 41, 358-367 (1950).
186. Kubaschewski and Weibke, Z. Elektrochem. 44, 870-877 (1938).
187. Schubert, Rosler, Kluge, Anderko and Harle, Naturwiss. 40, 437 (1953).
188. Pfisterer and Schubert, Naturwiss. 37, 112-113 (1950).
189. Rossi, A., Gazz. chim. ital. 64, 748 (1934).
190. McQuillan and McQuillan, "Titanium," pp 209-211 (Academic Press, New York, 1956).
191. Wallbaum, H., Naturwiss. 31, 91-92 (1943).

192. Duwez and Jordan, Acta. Cryst. 5, 213-214 (1952).
193. Raub and Engel, Z. Metallkunde 39, 172-177 (1948).
194. Stenback and Westgren, Z. physik. Chem. 114, 91 (1931).
195. Hendus, H., Z. Naturforschung 2A, 505-521 (1947).
196. Boettcher, Haase and Thun, Z. Metallkunde 46, 386-400 (1955).
197. Kleppa and Clifton, Acta. Cryst. 4, 74 (1951).
198. Mets and Torgren, Tallinna Tehnikaulikooli Toinetused 11A, 20 (1940).
199. Wallbaum, H., Z. Metallkunde 35, 218 (1943).
200. Owen and Roberts, J. Inst. Metals 71, 213 (1945).
201. Wood and Mathias, Acta. Cryst. 9, 534 (1956).
202. Graham and Kaiman, Am. Mineralogist 37, 461-469 (1952).
203. Juriase, T., Z. Krist. 90, 323 (1935).
204. Peacock and Thompson, Bull. Geol. Soc. Amer. 56, 1189 (1945).
205. Peacock and Thompson, Am. Mineralogist 31, 204, 515 (1946).
206. Buzzard and Park, AEC Bulletin NBS-D-127
207. Raub, Zwicker and Baur, Z. Metallkunde 44, 312-320 (1953).
208. Hansen, M., op. cit., p.224.
209. Jette, Foote and Bruner, Trans. Am. Inst. Mining Met. Engrs. 111, 354 (1934).
210. Pan, Kaufmann and Bitter, J. Chem. Phys. 10, 318 (1942).
211. Darling, Mintern and Chaston, J. Inst. Metals 81, 125 (1952-53).
212. Smithells, C., "Metals Reference Book" 1, 194-211 (1955), Interscience Publishers Inc., New York.
213. Runquist, Arnfelt and Westgren, Z. anorg. Chem. 175, 43-48 (1928).
214. Tokody, L., Z. Krist. 89, 416 (1934).
215. Forman and Peacock, Am. Mineralogist 34, 441-451 (1949).

216. Schubert and Rosler, Z. Metallkunde 41, 298-300 (1950).
217. Schubert and Rosler, Z. Naturforsch. 5A, 127 (1950).
218. Ekwall and Westgren, Arkiv. Kemi, Mineral. Geol. 14B, 8 (1940).
219. Eborall, R., J. Inst. Metals 70, 435-436 (1944).
220. Gorla, C., Gazz. chim. ital. 70, 461-471 (1940).
221. Ageev and Makarov, Izvest. Sektora Fiz. Khim. Anal. 13, 171-176 (1940).
222. Hofmann, W., Z. Metallkunde 33, 61-62 & 373 (1941).
223. Schrader and Hanemann, Z. Metallkunde 33, 49-60 (1941).
224. Nowotny and Henglein, Monatsh. Chem. 69, 385-393 (1948).
225. Linde, I., Ann. Physik 30, 151 (1937).
226. Peacock, M., Univ. Toronto Studies, Geol. Ser. 44, 31-46 (1940).
227. Weibke and Efinger, Z. Elektrochem. 46, 53-60 (1940).
228. Kuznecov, V., Izvest. Sektora Fiz. Khim. Anal. 20, 5-20 (1946).
229. Hultgren, I., Private communication in: The System of Mineralogy, Vol. I, 7th ed., p. 96, New York, (1944).
230. Ellwood and Bagley, J. Inst. Metals 76, 631-642 (1950).
231. Zakharova, M., Doklady Akad. Nauk S.S.S.R. 70, 55-56 (1950).
232. Kurdjumov, Mireckij and Stelleckaja, Z. Tekh. Fiz. S.S.S.R. 8, 1959 (1938).
233. Knappwost and Nowotny, Z. Metallkunde 33, 153-157 (1941).
234. Roberts, B., Bull. Amer. Phys. Soc. 24, no. 3, 12 (1949).
235. Kossolapow and Trapesnikow, Metallwirtschaft 14, 45-46 (1935).
236. Geisler, Mallery and Steigert, J. Metals 4, 307-316 (1952).
237. Guiner and Jacquet, Rev. met. 41, 1-16 (1944); Compt. rend. 217, 22-24 (1943).
238. Bowles and Tegort, Acta. Met. 3, 590 (1955).
239. Tunell and Ksanda, J. Wash. Acad. Sci. 26, 507-509 (1936).
240. Eppelsheimer and Penman, Physica 16, 792-794 (1950).

## PART III: STRUCTURE DETAILS

- A 1:  $O_h^5 \rightarrow Fm\bar{3}m$   
 A<sub>2</sub>: Cu structure  
 with 4 Cu ( $O_h$ ):  $000; \frac{1}{2}0\frac{1}{2}; \frac{1}{2}\frac{1}{2}0; 0\frac{1}{2}\frac{1}{2}$   
 Reported compounds:  $Ag_3Pt$ , Au,  $\alpha$ - $Au_3Zn$   
 Remarks: Implied in this structure is a random distribution of the atomic species on the lattice sites. This possibly is not true at low temperatures.
- A 2:  $O_h^9 \rightarrow Im\bar{3}m$   
 A<sub>2</sub>: W structure  
 with 2 W ( $O_h$ ):  $000; \frac{1}{2}\frac{1}{2}\frac{1}{2}$   
 Reported compounds:  $Cu_3Ge$ ,  $CuZn$ ,  $CuZn_3$ ,  $\beta$ - $Cu_3Al$ ,  $Cu_3Ga$ ,  $Cu_4In$ ,  $Cu_5Sn$ ,  $Cu_2Be$ ,  $AgZn$ ,  $AgCd$ ,  $Ag_3Al$   
 Remarks: See remarks under A 1 structure.
- A 3:  $D_{6h}^4 \rightarrow P6_3/mmc$   
 A<sub>2</sub>: Mg structure  
 with 2 Mg ( $D_{3h}$ ):  $2/3, 1/3, 0; 1/3, 2/3, 1/2$   
 Reported compounds:  $Cu_7Si$ ,  $Cu_7Ge$ ,  $CuZn_5$ ,  $Cu_3Ga$ ,  $Ag_5As$ ,  $Ag_3Sb$ ,  $Ag_{5.5}Hg_{4.5}$ ,  $Ag_3Ga$ ,  $AgZn_3$ ,  $AgCd$ ,  $AgCd_3$ ,  $\sim Ag_3In$ ,  $Au_2Cd$ ,  $AuCd_2$ ,  $Au_3Hg$ ,  $Au_8In_2$ ,  $Au_2Ti$ ,  $Au_6Sn$ ,  $AuZn_6$ ,  $Au_5Hg$   
 Remarks: See remarks under A 1 structure.
- A 13:  $O^6 \rightarrow P4_33$  and  $O^7 \rightarrow P4_13$   
 A<sub>20</sub>:  $\beta$ -Mn structure  
 with 8 Mn ( $C_3$ ):  $xxx; (1/2 + x)(1/2 - x) x; \varnothing; (3/4 - x)$   
 $(3/4 - x)(3/4 - x); (1/4 - x)(3/4 + x)$   
 $(1/4 + x); \varnothing : x=0.061$   
 12 Mn ( $C_2$ ):  $3/8, \bar{x}, (3/4 + x); \varnothing; 7/8, (1/2 + x)$   
 $(1/4 - x); \varnothing; 1/8, x, (1/4 + x); \varnothing;$   
 $5/8, (1/2 - x)(3/4 - x); \varnothing : x=0.206$   
 Reported compounds with related structure:  $Cu_5Si$

A 15:  $O_h^3$ ---Pm3n

A=8: Cr<sub>3</sub>Si structure

with 2 Si ( $T_h$ ): 000;  $\frac{111}{222}$   
 6 Cr ( $D_{2d}$ ): 1/2,0,1/4;  $\bar{2}$ ; 1/2,0,3/4;  $\bar{2}$

Reported compounds: AuTi<sub>3</sub>, AuNb<sub>3</sub>, AuV<sub>3</sub>

B 2:  $O_h^1$ ---Pm3m

A=1: ordered  $\beta$ -brass or CsCl structure

with Cs ( $O_h$ ): 000  
 Cl ( $O_h$ ):  $\frac{111}{222}$

Reported compounds: CuBe, CuZn, CuPd, AgZn, AgCd, AgLa, AgCe,  
 AgPr, AgLi, AgMg, AuMg, AuZn,  $\beta$ -AuCd, AuMn

B 3:  $T_d^2$ --- $\bar{F}43m$

A=8: Sphalerite structure, ZnS

with 4 Zn ( $T_d$ ): 000 + F.C.  
 4 S ( $T_d$ ):  $\frac{111}{444}$  + F.C.

Reported compounds: AuAl

B 8:  $D_{6h}^4$ ---P6<sub>3</sub>/mmc

A=4:  $\alpha$ -NiAs structure

with 2 Ni ( $D_{3d}$ ): 000;  $00\frac{1}{2}$   
 2 As ( $D_{3h}$ ): 1/3,2/3,1/4; 2/3,1/3,3/4

$D_{6h}^4$ ---P6<sub>3</sub>/mmc

A=6:  $\beta$ -Ni<sub>2</sub>In structure

with 2 Ni ( $D_{3d}$ ): 000;  $00\frac{1}{2}$   
 2 Ni ( $D_{3h}$ ): 1/3,2/3,3/4; 2/3,1/3,1/4  
 2 In ( $D_{3h}$ ): 1/3,2/3,3/4; 2/3,1/3,3/4

Reported compounds: Cu<sub>2</sub>In, Cu<sub>6</sub>Sn<sub>5</sub>, Cu<sub>7</sub>In<sub>3</sub>, CuIn, AuSn

Remarks: The compounds listed have structures based on the  $\alpha$ -NiAs and  $\beta$ -Ni<sub>2</sub>In structures. Intermediate arrangement of the atoms allows deviations in stoichiometry. There exists a close relationship to the C6 structure. Cu<sub>6</sub>Sn<sub>5</sub>, Cu<sub>7</sub>In<sub>3</sub> and CuIn have approximately the B8 structure.

B 11:  $D_{4h}^7$  -- $P4/nmm$

$A_{2d}$ : PbO structure

with 2 Pb ( $C_{4v}$ ):  $0\frac{1}{2}z; \frac{1}{2}0\bar{z}$ :  $z=0.24$   
 2 O ( $C_{4v}$ ): the same with  $z=0.74$

Reported compounds: CuTi with  $z(\text{Ti})=0.65, z(\text{Cu})=0.10$ ; AgZr with  
 $z(\text{Ag})=0.105, z(\text{Zr})=0.645$

B 18:  $D_{6h}^4$  -- $P6_3/mmc$

$A_{12}$ : Covellite structure, CuS

with 2 Cu ( $D_{3h}$ ):  $\pm(2/3, 1/3, 1/4)$   
 4 Cu ( $C_{3v}$ ):  $\pm(1/3, 2/3, z)$ ;  $\pm(1/3, 2/3, 1/2 - z)$ :  $z=0.107$   
 2 S ( $D_{3h}$ ):  $\pm(1/3, 2/3, 1/4)$   
 4 S ( $C_{3v}$ ):  $\pm(00z)$ ;  $\pm(00\ 1/2 - z)$ :  $z=0.063$

Reported compounds: CuS, CuSe

Remarks: For CuSe, reflections (hk $l$ ) were present only for  
 $l=2n$  and reflections (hk5) were all absent due to a "structural  
 peculiarity."

B 19:  $D_{2h}^5$  -- $Pmcm$

$A_{2d}$ : AuCd structure

with 2 Au ( $C_{2v}$ ):  $\pm(0y\frac{1}{4})$ :  $y=0.805$   
 2 Cd ( $C_{2v}$ ):  $\pm(\frac{1}{2}y\frac{1}{4})$ :  $y=0.315$

Reported compounds:  $\beta'$ -AuCd

B 20:  $T^4$  -- $P2_13$

$A_{28}$ : FeSi structure

with 4 Fe ( $C_3$ ):  $xxx; (\frac{1}{2} + x)(\frac{1}{2} - x)\bar{x}$ ;  $\bar{0}$ :  $x=0.137$   
 4 Si ( $C_3$ ): the same with  $x=0.158$

Reported compounds: AuBe with  $x(\text{Au})=0.150, x(\text{Be})=0.844$

B 31:  $D_{2h}^{16}$  -- $Pcmn$

$A_{28}$ : MnP structure

with 4 Mn ( $C_s$ ):  $\pm(x\frac{1}{4}z)$ ;  $\pm(\frac{1}{2} - x, \frac{1}{4}, \frac{1}{2} + z)$ :  $x=0.20, z=0.005$   
 4 P ( $C_s$ ): the same with  $x=0.57, z=0.19$

Reported compounds: AuGa with  $x(\text{Au})=0.184, z(\text{Au})=0.010,$   
 $x(\text{Ga})=0.590, z(\text{Ga})=0.195$

C 1:  $O_h^5 \rightarrow Fm3m$

A<sub>2</sub>12: fluorite structure, CaF<sub>2</sub>  
with 4 Ca (O<sub>h</sub>): 000 + F.C.  
8 F (T<sub>d</sub>):  $\pm(\frac{111}{444})$  + F.C.

Reported compounds: Cu<sub>2</sub>S, Cu<sub>2</sub>Se, Ag<sub>2</sub>Se, AuAl<sub>2</sub>, AuGa<sub>2</sub>, AuIn<sub>2</sub>

C 2:  $T_h^6 \rightarrow Pa3$

A<sub>2</sub>12: FeS<sub>2</sub> structure  
with 4 Fe (S<sub>3i</sub>): 000;  $\frac{11}{2}0$ ;  $\bar{2}$   
8 S (C<sub>3j</sub>):  $\pm(xxx; \frac{1}{2} + x, \frac{1}{2} - x, \bar{x}; \bar{2})$ :  $x=0.386$

Reported compounds: AuSb<sub>2</sub>

C 11:  $D_{4h}^{17} \rightarrow I4/mmm$

A<sub>2</sub>6: CaC<sub>2</sub> structure  
with 2 Ca (D<sub>4h</sub>): 000 + B.C.  
4 C (C<sub>4v</sub>):  $\pm(00z)$ :  $z=0.38$  + B.C.

Reported compounds: CuZr<sub>2</sub> with  $z=0.342$

C 14:  $D_{6h}^4 \rightarrow P6_3/mmc$

A<sub>2</sub>12: MgZn<sub>2</sub> structure--Laves phase  
with 4 Mg (C<sub>3v</sub>):  $\pm(1/3, 2/3, z; 1/3, 2/3, 1/2 - z)$ :  $z \approx 0.062$   
2 Zn (D<sub>3d</sub>): 000;  $00\frac{1}{2}$   
6 Zn (C<sub>2v</sub>):  $\pm(x, 2x, \frac{1}{4}; \bar{2}x, \bar{x}, \frac{1}{4}; x, \bar{x}, \frac{1}{4})$ :  $x \approx -0.017$

Reported compounds: Ag<sub>2</sub>Ca

C 15:  $O_h^7 \rightarrow Fd3m$

A<sub>2</sub>24: MgCu<sub>2</sub> structure--Laves phase  
with 8 Mg (T<sub>d</sub>): 000;  $\frac{111}{444}$  + F.C.  
16 Cu (D<sub>3d</sub>):  $5/8, 5/8, 5/8; 7/8, 7/8, 5/8; 7/8, 5/8, 7/8;$   
 $5/8, 7/8, 7/8$  + F.C.

Reported compounds: Cu<sub>7</sub>Mg; CuBe<sub>3</sub>: (7.15 Cu + 0.85 Be  
in 000;  $\frac{111}{444}$ ; and 16 Be in  $5/8, 5/8, 5/8; 3/8, 3/8, 5/8; \bar{2}$ ) + F.C.;  
Cu<sub>7</sub>U: (4 U in 000, 4 Cu in  $\frac{111}{444}$ , 16 Cu in  $5/8, 5/8, 5/8; 3/8,$   
 $3/8, 5/8; \bar{2}$ ) + F.C.; AgBe<sub>2</sub>, AuBe<sub>5</sub>, Au<sub>2</sub>Na, Au<sub>2</sub>Pb, Au<sub>2</sub>Bi.

Remarks: Those compounds which deviate from the AB<sub>2</sub> formula evidently have some atomic sites which are occupied either statistically by both atomic species or there are some sites in which one type of atom preferentially replaces the other.



C 16:  $D_{4h}^{18} \rightarrow I4/mcm$

A=12:  $CuAl_2$  structure

with 4 Cu ( $D_{4h}$ ):  $\pm(00\frac{1}{4}) + B.C.$   
 8 Al ( $C_{2v}$ ):  $\pm(x, \frac{1}{2} + x, 0; \frac{1}{2} + x, \bar{x}, 0) + B.C. x=0.158$

Reported compounds:  $CuTh_2$ ,  $CuAl_2$  with  $x=0.167$ ,  $AgIn_2$ ,  $AuNa_2$ ,  
 $AuPb_2$  with  $x=0.159$ .

C 32:  $D_{6h}^1 \rightarrow P6/mmm$

A=3:  $AlB_2$  structure

with 1 Al ( $D_{6h}$ ): 000  
 2 B ( $D_{3h}$ ):  $1/3, 2/3, 1/2; 2/3, 1/3, 1/2$

Reported compounds:  $Cu_2Th$

C 38:  $D_{4h}^7 \rightarrow P4/nmm$

A=6:  $Cu_2Sb$  structure

with 2 Cu ( $D_{2d}$ ):  $000; \frac{1}{2}\frac{1}{2}0$   
 2 Cu ( $C_{4v}$ ):  $0\frac{1}{2}z; \frac{1}{2}0\bar{z}; z=0.27$   
 2 Sb ( $C_{4v}$ ): the same with  $z=0.70$

Reported compounds:  $Cu_2Sb$ ,  $CuGa_2$ ,  $Cu_4Te_3$

Remarks:  $CuGa_2$  has a disordered structure; Some Cu sites are  
 vacant in  $Cu_4Te_3$ .

C 46:  $C_{2v}^4 \rightarrow Pma$

A=24:  $AuTe_2$  structure

with 2 Au ( $C_2$ ):  $00z; \frac{1}{2}0z; z=0$   
 2 Au ( $C_3$ ):  $\frac{1}{2}yz; 3/4, \bar{y}, z; y=0.319, z=0.014$   
 4 Au ( $C_1$ ):  $xyz; \bar{x}\bar{y}z; (\frac{1}{2} - x), y, z; (\frac{1}{2} + x), \bar{y}, z; x=0.124,$   
 $y=0.666, z=0.500$   
 2 Te ( $C_3$ ):  $\frac{1}{2}yz; 3/4, \bar{y}, z; y=0.018, z=0.042$   
 2 Te ( $C_1$ ): the same with  $y=0.617, z=0.042$   
 4 Te ( $C_1$ ): as 4 Au ( $C_1$ ), with  $x=0.003, y=0.699, z=0.042$   
 4 Te ( $C_1$ ): the same with  $x=0.132, y=0.364, z=0.500$   
 4 Te ( $C_1$ ): the same with  $x=0.119, y=0.964, z=0.500$

Reported compounds:  $AuTe_2$

D  $O_3$ :  $O_h^5$ ---Fm3m

A=16: BiLi<sub>3</sub> structure

with 4 Bi ( $O_h$ ): 000 + F.C.  
 4 Li ( $O_h$ ):  $\frac{1}{2}\frac{1}{2}\frac{1}{2}$  + F.C.  
 8 Li ( $T_d$ ):  $=(\frac{1}{4}\frac{1}{4}\frac{1}{4})$  + F.C.

Reported compounds: Cu<sub>3</sub>Sb

D  $O_9$ :  $O_h^1$ ---Pm3m

A=4: Cu<sub>3</sub>N structure

with 1 N ( $O_h$ ): 000  
 3 Cu ( $D_{4h}$ ):  $\frac{1}{2}00$ ;  $\curvearrowright$

Reported compounds: Cu<sub>3</sub>N

D  $O_{18}$ :  $D_{6h}^4$ ---P6<sub>3</sub>/mmc

A=8: Na<sub>3</sub>As structure

with 2 As ( $D_{3h}$ ):  $\pm(1/3, 2/3, 1/4)$   
 2 Na ( $D_{3h}$ ):  $\pm(00\frac{1}{4})$   
 4 Na ( $C_{3v}$ ):  $\pm(1/3, 2/3, z; 2/3, 1/3, 1/2 + z)$ :  $z=0.583$

Reported compounds: AuMg<sub>3</sub>

D  $O_{19}$ :  $D_{6h}^4$ ---P6<sub>3</sub>/mmc

A=8: Mg<sub>3</sub>Cd structure

with 2 Cd ( $D_{3h}$ ):  $\pm(1/3, 2/3, 1/4)$   
 6 Mg ( $C_{2v}$ ):  $\pm(2x, x, \frac{1}{4}; \bar{x}, x, \frac{1}{4}; \bar{x}, 2x, \frac{1}{4})$ :  $x \approx 0.167$

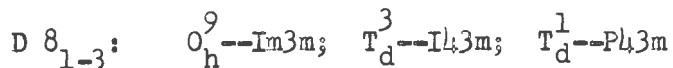
Reported compounds:  $\sim$ Ag<sub>3</sub>In

D  $O_{21}$ :  $D_{3d}^4$ ---P3ci

A=24: Cu<sub>3</sub>P structure

with 6 P ( $C_2$ ):  $\pm(x0\frac{1}{4}; 0x\frac{1}{4}; \bar{x}\bar{x}\frac{1}{4})$ :  $x=0.38$   
 2 Cu ( $C_{3i}$ ): 000;  $00\frac{1}{2}$   
 4 Cu ( $C_3$ ):  $\pm(1/3, 2/3, z; 1/3, 2/3, 1/2 + z)$ :  $z=0.17$   
 12 Cu ( $C_1$ ):  $=\sqrt{xyz}; \bar{y}(x-y)z; (y-x)\bar{x}z; \bar{y}\bar{x}(\frac{1}{2} + z); x(x-y)$   
 $(\frac{1}{2} + z); (x-y)y(\frac{1}{2} + x)$ :  $x=0.69, y=0.07,$   
 $z=0.08$

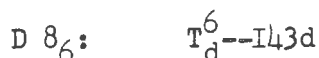
Reported compounds: Cu<sub>3</sub>P; Cu<sub>3</sub>As with  $x(\text{As})=0.33$ ,  $z(\text{Cu}_{\text{II}})=0.15$   
 $x(\text{Cu}_{\text{III}})=0.68$ ,  $y(\text{Cu}_{\text{III}})=0.075$ ,  $z(\text{Cu}_{\text{III}})=0.08$



**A=52:**  $\gamma$ -brass structures. The basic structure consists of a cubic unit cell whose edge is three times the edge of a simple body-centered cubic cell. From this large cell of 54 atomic sites is abstracted 2 atomic sites with small attendant shifts in parameters of some of the 52 occupied sites. The space group depends upon the formula of the compound and the atomic species occupying the various atomic sites.

Reported compounds:  $Cu_{32}Al_{19}$ ,  $Cu_9Al_{11}$ ,  $Cu_4Al_3$ ,  $Cu_9Ga_{11}$ ,  $Cu_7In_3$ ,  $Cu_5Zn_8$ ,  $Cu_5Cd_8$ ,  $CuHg$ ,  $Cu_{31}Sn_8$ ,  $Cu_{15}Si_4$ ,  $Ag_{10}Hg_{13}$ ,  $Ag_2In$ ,  $AgLi_3$ ,  $Ag_5Zn_8$ ,  $Au_5Zn_8$ .

Remarks:  $\gamma$ -brass structures usually exhibit extensive composition variation. Those formulae indicating more than 52 atoms/formula may be due to disorder or possibly they crystallize in closely related structures. Composition variation in  $Cu_9Ga_{11}$  evidently occurs by defect structure reducing the number of Ga atoms per cell in such a way as to maintain a constant valence electron concentration.



**A=76:**  $Cu_{15}Si_4$  structure

with 12 Cu ( $S_{11}$ ):  $0, 1/4, 3/8; \rho; 0, 3/4, 1/8; \rho$  + B.C.  
 48 Cu ( $C_1$ ):  $xyz; \rho; x, \bar{y}, \frac{1}{2} - z; \rho; \frac{1}{2} - x, y, \bar{z}; \rho;$   
 $\bar{x}, \frac{1}{2} - y, z; \rho; \frac{1}{4} + y, \frac{1}{4} + x, \frac{1}{4} + z;$   
 $\rho; \frac{1}{4} - y, \frac{1}{4} + x, 3/4 - z; \rho; \frac{1}{4} + y,$   
 $3/4 - x, \frac{1}{4} - z; \rho; 3/4 - y, \frac{1}{4} - x,$   
 $\frac{1}{4} + z; \rho; x=0.12, y=0.16, z=0.04$  + B.C.  
 16 Si ( $C_3$ ):  $xxx; x, \bar{x}, \frac{1}{2} - x; \rho; \frac{1}{4} + x, \frac{1}{4} + x, \frac{1}{4} + x;$   
 $\frac{1}{4} - x, \frac{1}{4} + x, 3/4 - x; \rho; x=0.208$  + B.C.

Reported compounds:  $Cu_{15}Si_4$



**A=112:**  $Fe_2W_3C$  structure

with 16 Fe ( $D_{3d}$ ):  $5/8, 5/8, 5/8; 5/8, 7/8, 7/8;$  + F.C.  
 32 Fe ( $C_{3v}$ ):  $xxx; xxx; \rho; \frac{1}{4} - x, \frac{1}{4} - x, \frac{1}{4} - x;$   
 $\frac{1}{4} - x, \frac{1}{4} + x, \frac{1}{4} + x; \rho; x=0.175$  + F.C.  
 48 W ( $C_{2v}$ ):  $(x00; \rho); \frac{1}{4} + x, \frac{1}{4}, \frac{1}{4}; \rho; \frac{1}{4} - x, \frac{1}{4}, \frac{1}{4}; \rho;$   
 $x=0.195$  + F.C.  
 16 C ( $D_{3d}$ ):  $1/8, 1/8, 1/8; 1/8, 3/8, 3/8; \rho$  + F.C.

Reported compounds:  $CuTi_2$

Remarks: There is some question as to whether or not it is necessary to have oxygen atoms present in order to stabilize  $\text{CuTi}_2$  in this structure. Presumably the oxygens if present would occupy the C positions and Ti would occupy the 192 fold and 64 fold sets.

L 10:  $D_{4h}^1 \rightarrow C4/mmm$

$A=4$ : CuAu structure

with 2 Cu ( $D_{4h}$ ): 000 + B.C.  
2 Au ( $D_{4h}$ ):  $\frac{1}{2}0\frac{1}{2}$  + B.C.

Reported compounds: AuCu, AgTi, CuTi

Remarks: Parameters given for CuTi in the tabulation section are for  $A=2$  (1 Ti in 000 and 1 Cu in  $\frac{111}{222}$ ); conversion to the above type structure can be accomplished by a  $45^\circ$  rotation of the a and b axes.

L 11:  $D_{3d}^5 \rightarrow R\bar{3}m$

$A=32$ : CuPt structure

with 16 Cu ( $D_{3d}$ ): 000;  $\frac{111}{442}$ ;  $\bar{2}$  + B.C.  
16 Pt ( $D_{3d}$ ):  $\frac{111}{222}$ ;  $3/4, 3/4, 0$ ;  $\bar{2}$  + B.C.

Reported compounds: CuPt

L 12:  $O_h^1 \rightarrow Pm\bar{3}m$

$A=4$ :  $\text{Cu}_3\text{Au}$  structure

with 3 Cu ( $D_{4h}$ ):  $\frac{11}{22}0$ ;  $\bar{2}$   
1 Au ( $O_h$ ): 000

Reported compounds:  $\text{Cu}_3\text{Au}$ ,  $\text{Cu}_3\text{Pd}$ ,  $\text{AgPt}_3$ ,  $\text{AuCd}_3$ ,  $\text{Cu}_3\text{Pt}$

L 13:  $O_h^7 \rightarrow Fd\bar{3}m$

$A=32$ : 16 Pt ( $D_{3d}$ ): 000;  $\frac{11}{44}0$ ;  $\bar{2}$  + F.C.  
16 Cu ( $D_{3d}$ ):  $\frac{111}{222}$ ;  $3/4, 3/4, 1/2$ ;  $\bar{2}$  + F.C.

Reported compounds: CuPt, AgPt

Remarks:  $\text{CuPt}_3$  and  $\text{CuPt}_7$  are based on this structure.

$\text{CuPt}_3$  has: 8 Cu in 000;  $\frac{11}{44}0$  and 24 Pt in  $\frac{111}{222}$ ;  $3/4, 3/4, 1/2$ ;  
 $1/2, 3/4, 3/4$ ;  $3/4, 1/2, 3/4$ ;  $0\frac{11}{44}$ ;  $3/4, 0, \frac{1}{4}$ ; + F.C.

$\text{CuPt}_7$  has: 4 Cu in 000 and 28 Pt in  $\frac{11}{44}0$ ;  $\frac{111}{222}$ ;  $3/4, 3/4, 1/2$ ;  
 $1/2, 3/4, 3/4$ ;  $3/4, 1/2, 3/4$ ;  $0\frac{11}{44}$ ;  $3/4, 0, 1/2$ ; + F.C.

---  $C_{2v}^{17}$  --Aba2

A<sub>20</sub>: AuSn<sub>4</sub> structure

with 4 Au (C<sub>2</sub>): 00z;  $\frac{1}{2}\frac{1}{2}z$ ; z=0 + A.C.  
 8 Sn (C<sub>1</sub>): xyz;  $\bar{x}\bar{y}z$ ;  $\frac{1}{2} - x, \frac{1}{2} + y, z$ ;  $\frac{1}{2} + x, \frac{1}{2} - y, z$ ;  
 $x=0.173, y=0.327, z=0.125$  + A.C.  
 8 Sn (C<sub>1</sub>): same with  $x=0.327, y=0.173, z=0.875$  + A.C.  
 (A.C. = add  $0\frac{1}{2}\frac{1}{2}$  to all coordinates)

Reported compounds: AuSn<sub>4</sub>

Remarks: Related to the Cl6 structure.

---  $C_{4h}^2$  --Pl<sub>4</sub>2/m

A<sub>8</sub>: Cu<sub>4</sub>Pd structure

with 2 Cu (C<sub>2h</sub>): 000;  $00\frac{1}{2}$   
 2 Cu (S<sub>4</sub>):  $\frac{1}{2}\frac{1}{2}\frac{1}{4}$ ;  $\frac{1}{2}, \frac{1}{2}, 3/4$   
 4 Pd (C<sub>S</sub>): xy0;  $\bar{x}\bar{y}0$ ;  $\bar{y}, x, \frac{1}{2}$ ;  $y, \bar{x}, \frac{1}{2}$ ;  $x=0.1, y=0.3$

Reported compounds: Cu<sub>4</sub>Pd

---  $D_{4h}^{24}$  --Fddd

A<sub>48</sub>: CuMg<sub>2</sub> structure

with 16 Cu (C<sub>2</sub>): 00z;  $00\bar{z}$ ;  $\frac{1}{4}, \frac{1}{4}, \frac{1}{4} + z$ ;  $\frac{1}{4}, \frac{1}{4}, \frac{1}{4} - z$ ;  
 $z=0.128$  + F.C.  
 16 Cu (C<sub>2</sub>): same with  $z=0.411$   
 16 Mg (C<sub>2</sub>): 0y0;  $0\bar{y}0$ ;  $\frac{1}{4}, \frac{1}{4} + y, \frac{1}{4}$ ;  $\frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}$ ;  
 $y=0.161$  + F.C.

Reported compounds: CuMg<sub>2</sub>

---  $T_d^6$  --I $\bar{4}$ 3d

A<sub>64</sub>: Cu<sub>3</sub>As structure

with 16 As (C<sub>3</sub>): xxx;  $\frac{1}{2} + x, \frac{1}{2} - x, \bar{x}$ ;  $\bar{x}, \frac{1}{2} + x, \frac{1}{2} - x$ ;  
 $\frac{1}{2} - x, \bar{x}, \frac{1}{2} + x$ ;  $\frac{1}{4} + x, \frac{1}{4} + x, \frac{1}{4} + x$ ;  
 $3/4 + x, 1/4 - x, 3/4 - x$ ;  $3/4 - x,$   
 $3/4 + x, \frac{1}{4} - x$ ;  $\frac{1}{4} - x, 3/4 - x, 3/4 + x$ ;  
 $x=0.03$  + B.C.  
 48 Cu (C<sub>1</sub>): xyz + full symmetry operations with  
 $x=0.03, y=0.12, z=0.20$  + B.C.

Reported compounds: Cu<sub>3</sub>As

---  $D_{6h}^1$  --C6/mmm

A<sub>6</sub>: Cu<sub>5</sub>Ca structure

with 1 Ca ( $D_{6h}$ ): 000  
 2 Cu ( $D_{3h}$ ):  $1/3, 2/3, 0; 2/3, 1/3, 0$   
 3 Cu ( $D_{2h}$ ):  $\frac{1}{2}0\frac{1}{2}; 0\frac{1}{2}\frac{1}{2}; \frac{1}{2}\frac{1}{2}\frac{1}{2}$

Reported compounds: Cu<sub>5</sub>Ca, Ag<sub>5</sub>Ba, Ag<sub>5</sub>Sr, Au<sub>6</sub>Ba.

---  $D_{6h}^1$  --C6/mmm

A<sub>6</sub>: Cu<sub>4</sub>Ce structure

with 1 Ce ( $D_{6h}$ ): 000  
 2 (Ce<sub>0.04</sub>Cu<sub>0.96</sub>) ( $D_{3h}$ ):  $1/3, 2/3, 0; 2/3, 1/3, 0$   
 3 (Ce<sub>0.04</sub>Cu<sub>0.96</sub>) ( $D_{2h}$ ):  $\frac{1}{2}0\frac{1}{2}; 0\frac{1}{2}\frac{1}{2}; \frac{1}{2}\frac{1}{2}\frac{1}{2}$

Reported compounds: Cu<sub>4</sub>Ce, Cu<sub>4</sub>La

---  $D_{4h}^1$  --P4/mmm

A<sub>4</sub>: AgZr<sub>3</sub> structure

with 1 Ag ( $D_{4h}$ ): 000  
 1 Zr ( $D_{4h}$ ):  $\frac{1}{2}\frac{1}{2}0$   
 2 Zr ( $D_{2h}$ ):  $0\frac{1}{2}\frac{1}{2}; \frac{1}{2}0\frac{1}{2}$

Reported compounds: AgZr<sub>3</sub>,  $\alpha$ -Au<sub>3</sub>Cd

Remarks: Tetragonally deformed L12

---  $D_{6h}^1$  --C6/mmm

A<sub>6</sub>: Cu<sub>2</sub>Te structure

with 2 Te ( $C_{6v}$ ):  $\pm(00z); z=0.306$   
 4 Cu ( $C_{3v}$ ):  $\pm(1/3, 2/3, z; 2/3, 1/3, z); z=0.160$

Reported compounds: Cu<sub>2</sub>Te

---  $D_{2h}^{13}$  --Pmmm

A<sub>4</sub>: CuTe structure

with 2 Cu ( $C_{2v}$ ):  $0\frac{1}{2}z; \frac{1}{2}0z; z=0.46$   
 2 Te ( $C_{2v}$ ):  $00z; \frac{1}{2}\frac{1}{2}z; z=0.22$

Reported compounds: CuTe

---  $D_{2h}^{17}$  ---Cmcm

A=4:  $Cu_3Ti$  structure (high temperature)  
with 4 Ti or Cu ( $C_{2v}$ ):  $0y\frac{1}{4}; 0, \bar{y}, 3/4; y=0.345 \uparrow (000; \frac{1}{2}\frac{1}{2}0)$

Reported compounds:  $Cu_3Ti$

Remarks: Evidently there is a statistical occupancy of the sites.

---  $D_{2h}^{13}$  ---Pmmm

A=8:  $Cu_3Ti$  structure (low temperature)  
with 2 Ti ( $C_{2v}$ ):  $00z; \frac{1}{2}\frac{1}{2}z; z=0.655$   
2 Cu ( $C_{2v}$ ):  $0\frac{1}{2}z; \frac{1}{2}0z; z=0.395$   
4 Cu ( $C_s$ ):  $x0z; \bar{x}0z; \frac{1}{2} + x, \frac{1}{2}, z; \frac{1}{2} - x, \frac{1}{2}, z;$   
 $x=0.25, z=0.155$

Reported compounds:  $Cu_3Ti$

---  $D_{3d}^1$  --- $\bar{H}3m$

A=27:  $Cu_{20}Sn_6$  structure  
with 2 Sn ( $D_3$ ):  $\pm(1/3, 2/3, 0)$   
4 Sn ( $C_2$ ):  $\pm(1/3, 2/3, z; 2/3, 1/3, z); z=1/3$   
2 Cu ( $C_{3v}$ ):  $\pm(00z); z=1/3$   
6 Cu ( $C_s$ ):  $\pm(xxz; 0\bar{x}z; \bar{x}0z); x=1/3, z=1/9$   
6 Cu ( $C_s$ ): same with  $x=1/3, z=4/9$   
6 Cu ( $C_s$ ): same with  $x=1/3, z=7/9$

Reported compounds:  $Cu_{20}Sn_6$

Remarks: Parameters calculated for a statistical distribution of atoms.

---  $C_{2v}^1$  ---P2mm

A=  $\gamma'$ -AlCu<sub>3</sub> structure  
with 1 Al ( $C_{2v}$ ):  $x00; x=0$   
1 Al ( $C_{2v}$ ):  $x\frac{1}{2}\frac{1}{2}; x=1/3$   
1 Cu ( $C_{2v}$ ):  $x\frac{1}{2}0; x=0$   
1 Cu ( $C_{2v}$ ):  $x0\frac{1}{2}; x=1/3$   
2 Cu ( $C_s$ ):  $xy0; x\bar{y}0; x=\frac{1}{2}, y=\frac{1}{4}$   
2 Cu ( $C_s$ ):  $xy\frac{1}{2}; x\bar{y}\frac{1}{2}; x=5/6, y=\frac{1}{4}$

Reported compounds:  $\gamma'$ -AlCu<sub>3</sub>

---  $T^4_{--}P2_13$

A=20:  $Au_4Al$  structure

with  $12 Au (C_1)$ :  $xyz; \bar{0}; \frac{1}{2} + x, \frac{1}{2} - y, \bar{z}; \bar{0}; \bar{x}, \frac{1}{2} + y,$   
 $\frac{1}{2} - z; \bar{0}; \frac{1}{2} - x, \bar{y}, \frac{1}{2} + z; \bar{0}; x=0.785,$   
 $y=0.950, z=0.385$

$4 Au (C_3)$ :  $xxx; \frac{1}{2} + x, \frac{1}{2} - x, \bar{x}; \bar{x}, \frac{1}{2} + x, \frac{1}{2} - x;$   
 $\frac{1}{2} - x, \bar{x}, \frac{1}{2} + x; x=0.690$

$4 Al (C_3)$ : same with  $x=0.054$

Reported compounds:  $Au_4Al, Ag_3Al$

Remarks:  $\beta$ -Mn like phase.  $Ag_3Al$  has a statistical distribution of Ag and Al atoms.

---  $C^1_{3i}--C\bar{3}$

A=9: AgZn structure

with  $1 (C_{3i})$ : 000

$2 (C_3)$ :  $2/3, 1/2, z; 1/3, 2/3, \bar{z}; z=0.250$

$6 (C_1)$ :  $xyz; \bar{y}, x-y, z; y-x, \bar{x}, z; \bar{xy}\bar{z}; y, y-x, \bar{z}; x-y, x, \bar{z};$   
 $x=0.35, y=0.32, z=0.75$

Reported compounds: AgZn

Remarks: 1 and 2 fold positions are almost exclusively Zn; remaining Zn and Ag statistically distributed on 6-fold positions.

---  $C^2_{2h}--P2_1/m$  or  $C^2_{2}--P2_1$

A=4:  $Cu_3Ge$  structure; coordinates for latter space group

with  $2 (Cu, Ge)$ :  $(C_1)$ :  $xyz; \bar{x}, \frac{1}{2} + y, \bar{z}; x=0, y=0, z=1/6$

$2 (Cu, Ge)$ :  $(C_1)$ : same with  $x=1/2, y=0, z=1/3$

Reported compounds:  $Cu_3Ge$