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

by

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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.

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Cu		a=3.61		Parameter at room temperature; measurements were made using a high temperature vacuum camera.	240
Cu_3Au	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	tetragonal	a=3.964 c=3.671 (50 a/o Au)	L10	Superlattice: ordered f.c. lattice below 424°C; from ~37-70 a/o Au.	1,2,3
Cu_2Be	cubic	a=2.80 (750°C)	A2	Exists above 575°C; disordered atomic arrangement.	235
CuBe	cubic	a=2.703 ±0.007	B2	X-ray powder data, with comparison of observed and calculated intensities; some disordering noted; after annealing at 830°C. for two hours completely ordered.	7, 236, 237,238
CuBe	tetragonal	a=2.79 c=2.54		Intermediate phases during precipitation; single crystal x-ray data.	236
CuBe	monoclinic	a=2.54 b=2.54 c=3.24 α=85°25'		"	236
$CuBe_3$	cubic	a=5.952 (at $CuBe_2$)	C15	Maximum solubility range $CuBe_2$ → $CuBe_4$ at 933°C; at room temperature ranges from $CuBe_2$ → $CuBe_4$; maximum in liquidus occurs at $CuBe_3$; structure determined at Cu:Be of 1:2.354; x-ray powder data, with comparison of observed and calculated intensities.	2.35 4, 5,6,7
Cu_2Mg	cubic	a=7.04	C15	Thermal analysis, x-ray powder and microscopic data; congruent m.p. 819°C.	9,213

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
$CuMg_2$	orthorhombic	a=5.284 b=9.07 c=18.25	D_{2h}^{24} — Fddd	Thermal analysis, x-ray powder and microscopic data; congruent m.p. 588°C.	10,218
Cu_5Ca	hexagonal	a=5.092 c=4.086	D_{6h}^{1} — C6/mmm	Originally reported as Cu_4Ca; 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_5Zn_8	cubic	a=8.879 (64.7 a/o Zn)	$D8_2$	Decomposes peritectically at ~ 830°C; thermal analysis, x-ray powder and microscopic data by many investigators.	56
$CuZn_3$	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
$CuZn_5$	hexagonal	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_2Cd		a=4.96 c=7.99		X-ray powder data; line compound; decomposes peritectically at 549°C.	15
Cu_4Cd_3				Decomposes peritectically at 547°C; phase diagram.	15
Cu_5Cd_8	cubic	a=9.654	$D8_2$	X-ray powder data.	
$CuCd_3$				Decomposes peritectically at 397°C; phase diagram.	62
Cu_4Hg_3				Decomposes peritectically at 115°C.	17
~ Cu_3Hg				"X" phase, ~ Cu_3Hg; decomposes peritectically at 150°C.	68

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (A)	STRUCTURE	REMARKS	REFERENCES
CuHg	cubic	a=9.425	$D8_2$	X-ray single crystal data.	18
Cu_4La	hexagonal	a=5.179 c=4.124	$[D^1_{6h}$ -- C6/mmm]	Actually $La(Cu_{4.8}La_{0.2})$ by structural work; line compound; congruent m.p. 902°C	12
Cu_3La				Line compound; decomposes peritectically at 793°C.	70
Cu_2La				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_6Ce	orthorhombic	a=8.08 b=5.09 c=10.17	$[D^{16}_{2h}$ -- 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_4Ce	hexagonal	a=5.151 c=4.140	$[D^1_{6h}$ -- C6/mmm]	$Ce(Cu_{4.8}Ce_{0.2})$; line compound; decomposes peritectically at 780°C; phase diagram; x-ray powder data.	57,58
Cu_2Ce				Line compound; congruent m.p. 820°C; phase diagram.	66
CuCe				Line compound; decomposes peritectically at 515°C; phase diagram.	66
Cu_6Pr				Phase diagram; line compound; congruent m.p. 962°C.	64
Cu_4Pr				Phase diagram; decomposes peritectically at 824°C.	64
Cu_2Pr				Phase diagram; congruent m.p. 841°C.	64

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
CuPr				Phase diagram; decomposes peritectically at 563°C.	64
CuB_{22}				Thermal analysis and microscopic data; complex structure.	20
β-Cu_3Al	cubic	a=2.95	A2	X-ray powder data; disordered structure.	68, 230, 231
β_1-Cu_3Al	cubic	a=5.82		X-ray powder data; ordered structure; on further cooling of alloys < 13.1 w/o Al, β_1 structure transforms to a β' structure which is a distorted γ' structure(Cu_2Al); β' can be converted to γ' by mechanical deformation.	68, 230, 231, 232, 233
γ'-Cu_3Al	orthorhombic	a=4.52 b=5.21 c=4.23	C_{2v}^1 -- 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_2Al	cubic	a=8.7		Decomposes peritectically at 873°C.	68
Cu_9Al_4	cubic	a=8.7040	$D8_3$	Stable > 963° to ~1030°C.	21, 22
$Cu_{32}Al_{19}$	cubic	a=8.703-8.722 (for pseudocubic cell)	$D8_{1-3}$	Structure can be described as a deformed γ-brass type; decomposes peritectically at 690°C.	68, 71
Cu_4Al_3	hexagonal	a=8.10 c=10.00	$D8_3$	Decomposes peritectically at 590°C; x-ray powder data; phase diagram.	23
CuAl	orthorhombic	a=4.10 b=12.0 c=8.65	$D8_3$	Thermal analysis, powder x-ray and microscopic data; decomposes peritectically at 626°C.	23
$CuAl_2$	tetragonal	a=6.05 c=4.87	C16	Congruent m.p. 595°C; thermal analysis, x-ray powder and microscopic data.	9

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Cu_3Ga	hexagonal	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_3Ga	cubic		A2		
Cu_9Ga_4	cubic	a=8.729	~$D8_2$	Decomposes peritectically at 836°C; orders on cooling at ~490°C; thermal analysis, x-ray powder and microscopic data.	25,27
$CuGa_2$	tetragonal	a=2.836 c=5.843	C38 (disordered)	Single crystal x-ray data; phase diagram.	25
Cu_4In	cubic		A2	Stable at > 574°C; decomposes peritectically at 715°C; thermal analysis, x-ray powder and microscopic data.	26
Cu_7In_3	cubic		$D8_2$	Maximum temperature at which stable is 682°C; goes to tetragonal form at 630°C. on cooling.	29
Cu_7In_3	tetragonal	a=8.99 c=9.16	~B8	Structure below 630°C; x-ray powder data; phase diagram.	26,29
Cu_2In	hexagonal	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_3Ti	orthorhombic	a=5.06 b=4.36 c=4.53	D_{2h}^{13} — Pmmn	Structure below 600°C; thermal analysis, x-ray powder and microscopic data.	31,32
Cu_3Ti	orthorhombic	a=2.60 b=4.54 c=4.36	D_{2h}^{17} — Cmcm	Structure above 600°C; congruent m.p.905°C.	31,32
CuTi	tetragonal	a=3.15 c=2.87	L10	Low temperature structure; thermal analysis, x-ray powder data.	34, 31,32

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
CuTi	tetragonal	a=3.12 c=5.90	B11	High temperature structure; congruent m.p. 982°C.	31,32,34
$CuTi_2$	cubic	a=11.24	$E9_3$	(33) says there is no oxygen needed to stabilize this compound in the $E9_3$ type structure; congruent m.p. 1014°C; thermal analysis; x-ray powder and microscopic data.	31,33
Cu_2Ti				Phase diagram; decomposes peritectically at 892°C.	31
Cu_3Ti_2				Phase diagram; decomposes peritectically at 935°C.	31,32
Cu_3Zr				Phase diagram; congruent m.p. 1100°C.	35
Cu_5Zr_2				Phase diagram; decomposes peritectically at 1070°C.	35
Cu_3Zr_2				Phase diagram; congruent m.p. 895°C.	35,36
CuZr				Phase diagram; congruent m.p. 935°C.	35
$CuZr_2$	tetragonal	a=3.3 c=11.3	$/D_{4h}^{17}$-- I4/mmm/	Phase diagram; congruent m.p. 1065°C; x-ray powdor data.	35,36
Cu_4Th				At least three compounds in Cu-Th system; formula of this compound not well established; also reported as Cu_6Th.	24,65
Cu_2Th	hexagonal	a=4.36 c=3.48	C32	Phase diagram; x-ray powder data.	65, 24,28
$CuTh_2$	tetragonal	a=7.29 c=5.75	C16	Compound previously reported as Cu_3Th_5 on basis of phase diagram studies is probably this compound; x-ray powder data.	65, 24,28

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Cu_7Si	hexagonal	a=2.58 c=4.19	A3	X-ray powder data.	59
Cu_5Si	cubic	a=6.22	A13	"	59
$Cu_{15}Si_4$	cubic	a=9.71	$D8_6$	Single crystal x-ray data.	8
$Cu_{15}Si_4$	cubic		$D8_{1-3}$	Related to γ-brass structure; x-ray powder data.	59
Cu_5Ge	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
Cu_3Ge	monoclinic	a=2.631 b=4.200 c=4.568 β=89°41'	C_2^2-- $P2_17$ or C_{2h}^2-- $P2_1/m$	Low temperature form; transforms to hexagonal form at 570-635°C; single crystal x-ray data.	38,39
Cu_3Ge	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
Cu_3Ge	cubic		A2	Defect lattice; stable 612°C to 700°C at ~ 27 a/o Ge; thermal analysis, x-ray powder and microscopic data.	38
Cu_5Sn	cubic	a=2.978	A2	Stable at > 700°C; phase diagram, and high temperature x-ray data.	40
$Cu_{31}Sn_8$	cubic	a=17.91	$D8_{2-3}$	Phase diagram, powder and single crystal x-ray data; stable ~350-640°C.	40
$Cu_{20}Sn_6$	hexagonal	a=7.331 c=7.870	D_{3d}^1-- $H\bar{3}m$	Possibly related to the $D8_{2-3}$ structures; thermal analysis and microscopic data; stable 580-640°C.	41

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Cu_3Sn	ortho-rhombic	a=4.33 b=5.25 c=38.1		Single crystal x-ray data; superlattice based on A3 structure.	60
Cu_6Sn_5	hexag-onal	a=4.20 c=5.10	B8	Powder, Laue, and rotation x-ray data.	40
Cu_3N	cubic	a=3.82	DO_9	X-ray powder data.	61
Cu_3P	hexag-onal	a=7.08 c=7.149	DO_{21}	"	42,224
Cu_3As	cubic	a=9.612	T_d^6-- I$\bar{4}$3d	X-ray powder data; natural domeykite.	42
Cu_3As	hexag-onal	a=7.103 c=7.247	DO_{21}	X-ray powder data; obtained by heating natural domeykite at 225°C.	42,43
Cu_3As	hexag-onal	a=2.586 c=4.229		X-ray powder data; stable below 250°C; 2 atoms per unit cell; algodonite mineral.	42
$Cu_{11}Sb_2$	ortho-rhombic	a=9.30 b=8.20 c=8.64		Stable 400-~488°C; deformed A3 structure; phase diagram; x-ray powder data.	44,45
Cu_9Sb_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
$Cu_{11}Sb_4$	hexag-onal	a=5.505 c=8.704		Decomposes at 375°C; related to A3 structure; phase diagram; x-ray powder data.	44,45
Cu_3Sb	cubic	a=6.00	DO_3	X-ray powder and back-reflection data; samples quenched from 550°C.	221,222 223
Cu_5Sb_2	tetrag-onal	a=9.03 c=8.59		Stable 440-685°C; samples at 56.71 a/o Cu.	44
Cu_2Sb	tetrag-onal	a=4.000 c=6.103	C38	Decomposes peritectically at 585°C; x-ray powder data.	44,46

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Cu_5U	cubic	a=7.03	C15	Thermal analysis, microscopic and single crystal x-ray data.	47, 48
CuS	hexagonal	a=3.76 c=16.2	B18	Covellite mineral.	62
Cu_2S	cubic	a=5.59	C1	X-ray powder data.	49
Cu_2Se	cubic	a=5.75	C1	"	49,219, 220
CuSe	hexagonal	a=3.95 c=17.29	B18	Klockmannite mineral.	19
Cu_2Te	hexagonal	a=4.237 c=7.274	D_{6h}^1 -- C6/mmm	Structure below 640°C; congruent m.p. 890°C.	50,51, 215
Cu_2Te	cubic	a=6.10		High temperature phase, stable above 640°C; 12 atoms per unit cell.	50,51, 215
Cu_4Te_3	tetragonal	a=3.98 c=6.12	C38	Line compound; decomposes peritectically at 623°C; vacant sites in structure.	51,63, 215
CuTe	orthorhombic	a=3.15 b=4.08 c=6.93	D_{2h}^{13} -- Pmmn	Decomposes peritectically at 365°C; thermal analysis, x-ray powder, microscopic, and dilatometric data.	51
Cu_3Rh CuRh $CuRh_3$				Hardness, microscopic, and x-ray powder data indicate these superlattices in quenched solid solution alloys.	52
Cu_4Pd	tetragonal		C_{4h}^2 -- $P4_2/m$	Stable below 478°C; x-ray powder data; phase diagram.	53
Cu_3Pd	cubic		L12	Ordered f.c.c. below 525°C.	54
CuPd	cubic	a=3.00	B2	X-ray powder data; phase diagram.	54

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Cu_3Pt			L12	Electrical conductivity measurements and x-ray diffraction diagrams.	54,55, 69,225
CuPt	rhombohedral	a=7.57 α=90°54'	L11	Stable for composition 40-55 a/o Pt below 810°C.	54
Cu_3Pt_5				Powder diagrams.	69,225
$CuPt_3$	cubic		~L13	Stable for composition 60-75 a/o Pt; powder diagrams.	69
$CuPt_7$	cubic		~L13	Stable ~45 a/o Pt at ~700°C; lattice constants twice those of $CuPt_3$.	54,69
AgLi	cubic	a=3.17	B2	X-ray powder data.	105,108, 117
$AgLi_3$	cubic	a=9.96	$D8_{1-3}$	Composition varies from Li_3Ag to Li_4Ag; thermal analysis and x-ray powder data; formulae Li_9Ag_4, $Li_{10}Ag_3$ and $Li_{12}Ag$ 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_3Au, Ag_3Au_7, Ag_3Au_2, Ag_2Au_3, AgAu, $AgAu_3$: 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
$AgBe_2$	cubic	a=6.300	C15	X-ray powder data, thermal, magnetic and micrographic analysis.	84,85
Ag_3Mg	cubic	a=4.111 (disordered) a=4X4.108 (ordered)		Powder and Weissenberg x-ray data.	107

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
AgMg	cubic	a=3.29	B2		106,108, 109,135
$AgMg_3$				Previously reported as hexagonal with a=4.93 and c=7.81; complicated structure of lower symmetry.	108,110, 109, 135,136
Ag_4Ca				Thermal analysis.	86
Ag_3Ca	tetragonal	a=11.3 c=9.96		Thermal analysis and x-ray powder data.	86,87
Ag_2Ca	hexagonal	a=5.72 c=9.35	C14	"	86,87
AgCa	cubic	a=9.071		"	86,87
$AgCa_2$				"	86
Ag_5Sr	hexagonal	a=5.664 c=4.610	$[D^1_{6h}$ -- C6/mmm]	"	83
Ag_4Sr				Thermal analysis.	118
Ag_5Sr_3				"	118
AgSr				"	118
Ag_2Sr_3				"	118
Ag_5Ba	hexagonal	a=5.708 c=4.636	$[D^1_{6h}$ -- C6/mmm]	Thermal analysis and x-ray powder data.	83
Ag_4Ba				Thermal analysis.	82
Ag_5Ba_3				"	82
Ag_3Ba_2				"	82
AgZn	hexagonal	a=7.6360 c=2.8197	$[C^1_{3i}$ -- P$\bar{3}$]	Stable below 260°C.	134
AgZn	cubic	a=3.156	A2	High temperature phase.	133,134

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
AgZn	cubic	a=3.16	B2	Metastable phase obtained through quenching.	137
Ag_5Zn_8	cubic	a=9.33	$D8_2$		132,134
$AgZn_3$	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_5Cd_8	cubic	a=9.93-9.98	$D8_2$	γ-brass structure; range of composition variation; microscopy, thermal and x-ray powder data.	88,90, 91,92
$AgCd_3$	hexagonal	a=3.06 c=4.84	A3	Extensive composition variation.	88,90, 92
$Ag_{10}Hg_{13}$	cubic	a=10.033	$D8_{1-3}$	γ-brass structure; thermal analysis and x-ray powder data.	95,96
$Ag_{5.5}Hg_{4.5}$	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_3Hg_4 (99); electrochemical potentials indicate existence of Ag_3Hg, Ag_3Hg_2 and Ag_3Hg_4 (138); electron diffraction has indicated existence of a cubic phase and two tetragonal phases (140).	97, 98,99, 138,140

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Ag_3La				Thermal analysis; congruent melting.	103,104
Ag_2La				Thermal analysis; incongruent melting.	103,104
AgLa	cubic	a=3.77	B2	Thermal analysis; congruent melting.	103,104
Ag_3Ce				Thermal analysis and metallography.	128
Ag_2Ce				"	128
AgCe	cubic	a=3.74	B2	"	128,104
Ag_3Pr				"	128,111
Ag_2Pr				"	128,111
AgPr	cubic	a=3.73	B2	"	128,111
Ag_3Al	cubic	a=3.24	A2	Thermal analysis, microscopic and x-ray powder data.	72,73, 75,76, 77
Ag_3Al	cubic	a=6.920	T^4-- $P2_13$	X-ray powder data.	234
Ag_3Al_2	hexagonal	a=2.86 c=4.57-4.65		Thermal analysis and x-ray powder data; also reported as Ag_2Al.	72, 73,75, 76,78
Ag_3Ga	hexagonal	a=2.93 c=4.75	A3	Stable from 378-611°C.	141
Ag_5Ga_2	hexagonal			Thermal analysis, microscopy, powder x-ray data; low-temperature (γ) phase structurally related to δ-phase of Ag-In system; transforms ~380°C to high temperature (β) phase which is hexagonal closest-packed; both high and low temperature phases exist over a region of composition.	94,141

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Ag_3In	hexagonal	a=2.95-2.98 c=4.77-4.79	A3 or $D0_{19}$	The former structure exists > 300°C, the latter < 200°C; variable composition; third phase reported > 660°C.	100, 101,102
Ag_2In	cubic	a=9.885	$D8_{1-3}$	γ-brass structure, exists < 200°C; thermal analysis, powder x-ray data; some composition variation.	100
$AgIn_2$	tetragonal	a=6.869 c=5.604	C16	Thermal analysis, powder x-ray data; some composition variation.	100,102
AgTi	tetragonal	a=4.104 c=4.077	L10	Isomorphous with CuAu; x-ray powder data with comparison of observed and calculated intensities.	130,131
AgZr	tetragonal	a=3.468 c=6.603	B11	X-ray powder data.	115
$AgZr_3$	tetragonal	a=4.566 c=3.986	D^1_{4h} -- P4/mmm	"	115
Ag_5Th_3				Thermal analysis, microscopic and x-ray investigations.	129
Ag_3Th				"	129
Ag_6Sn	hexagonal	a=2.931-2.959 c=4.784-4.781		Lattice parameters are indicated for composition extremes; composition varies from 13.3-14.2, 19.7 a/o Sn at 400°C; thermal, dilatometric, electrical resistivity and x-ray powder data.	143
Ag_3Sn	orthorhombic	a=2.991-3.000 b=5.155-5.165 c=4.781-4.781		Lattice parameters are indicated for composition extremes; diffraction patterns indicate that this structure is closely related to the above hexagonal one; composition varies from 12.4, 24-25.5 a/o Sn at 400°C.	142,143

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Ag_9As	hexagonal	a=2.89 c=4.722	A3	X-ray powder data.	79
Ag_3Sb	hexagonal	a=3.044 c=4.913	A3	"	121,143
Ag_3Sb	orthorhombic	a=2.990 b=5.225 c=4.820		Single crystal and x-ray powder data.	226,227
Ag_2Sb	orthorhombic	a=7.77 b=12.35 c=8.44		X-ray powder data.	119, 120, 227
Ag_2Se	cubic	a=4.993	C1	"	114
Ag_2Te	cubic	a=5.87	C1	X-ray powder data; stable at > 155°C.	127, 50,114
Ag_2Te	orthorhombic			High temperature form.	127
Ag_2Te	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
$Ag_{12}Te_7$	hexagonal	a=13.43 c=8.451	D_{6h}^{1} — C6/mmm	Also reported as AgTe, Ag_7Te_5, Ag_5Te_3, and $Ag_{2-x}Te$, evidently indicating an extended composition range for a homogeneous phase; investigations were made on synthetic and natural occurring samples.	125, 126
Ag_3Pt	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
$AgPt_3$	cubic	a=3.88	L12	"	112,113

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Au_2Na	cubic	a=7.7872 ±0.0023	C15	X-ray powder data	144,145, 146,147
$AuNa_2$	tetragonal	a=7.402 c=5.511	C16	Rotation, Weissenberg, and x-ray powder data.	146
Au_4K				Au_4K and Au_2K were postulated 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_2K					
Au	cubic	a=4.0781	A1	Gold leaf electron diffraction.	149
Au_3Be				X-ray powder and back-reflection data; parameters not reported	150.
Au_2Be				"	150
AuBe	cubic	a=4.668 ±0.001	B20	X-ray powder data with comparison of calculated and observed intensities.	150,151
$AuBe_3$				X-ray data indicates this compound exists; structure not determined.	150,152
$AuBe_5$	cubic	a=6.083	C15	X-ray powder data with comparison of calculated and observed intensities; parameter also reported as a=6.699 by 152.	150,152, 153
AuMg	cubic	a=3.265	B2		154
$AuMg_3$	hexagonal	a=4.64 c=8.46	DO_{18}	powder and single crystal x-ray data; Mg_2Au reported by (156,158) and Mg_5Au_2 reported by(157), both on basis of thermal analysis, are probably this compound.	10,156, 157,158

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Au_6Ba	hexagonal	a=5.67 c=4.58	D^1_{6h} -- C6/mmm	X-ray powder data; exists as $(Ba_{0.86}Au_{0.14})Au_5$ in $CaCu_5$ type structure.	83
$Au_3Zn(\alpha)$	cubic	a=4.039	A1	X-ray data and thermal analysis; stable above 420°C.; disordered phase; parameters from sample quenched from 500°C.	160,161, 162
$Au_3Zn(\alpha')$	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
$Au_3Zn(\alpha'')$	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_5Zn_8	cubic	a=9.242	$D8_1$	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
~$AuZn_2$	cubic	a=11.17		X-ray study of superlattice; ~90 atoms per unit cell.	155,164
$AuZn_3$	cubic	a=7.88		X-ray powder data; 32 atoms per unit cell.	155,164, 165
$AuZn_6$	hexagonal	a=2.82 c=4.38	A3	X-ray powder data; exact composition and structure open to question; reported as differently as $AuZn_9$.	155, 164,165
Au_3Cd	tetragonal	a=4.107-4.1177 c=4.138-4.1298	D^1_{4h} -- P4/mmm	Deformed Cu_3Au 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

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Au_2Cd	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
$Au_{55}Cd_{45}$	rhombohedral	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
$AuCd_2$	hexagonal		A3		212
$AuCd_3$	cubic	a=4.11	L12		212, 172, 173, 174, 175
Au_5Hg	cubic	a=4.122	A3	Parameters measured at 175° C.	176, 177, 178
Au_3Hg	hexagonal	a=2.906-2.921 c=4.780-4.812	A3	Formula approximates Au_3Hg; parameters from samples of 19.1-32.7 weight percent Hg.	176, 177, 178
Au_2Hg_3					177
$AuHg_2$					177

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Au_3La				Thermal analysis and metallography; Ce-Au, La-Au and Pr-Au systems reported to be analogous.	128, 144
Au_2La				"	128
AuLa				"	128,144
$AuLa_2$				"	128
Au_3Ce				"	128
Au_2Ce				"	128
AuCe				"	128
$AuCe_2$				"	128
Au_3Pr				Reported as Au_4Pr by (189).	128,189
Au_2Pr				Same as Au_3La.	128
AuPr				"	128
$AuPr_2$				"	128
Au_4Al	cubic	a=6.916	T^4-- $P2_13$	X-ray powder data.	179,180, 181
Au_5Al_2				Thermal analysis and metallography; compound may be Au_8Al_3.	179, 159, 180,181
Au_2Al				Thermal analysis and metallography.	159,179, 180,182
AuAl	cubic	a=6.05	B3		159,179, 180,182
$AuAl_2$	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

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Au_3Ga				Thermal analysis and metallography.	26,185
Au_7Ga_3				"	26,185
AuGa	orthorhombic	a=6.397 b=6.267 c=3.421	B31	Thermal analysis, metallography and x-ray powder data.	26,185
$AuGa_2$	cubic	a=6.086	C1	"	184,185
Au_9In	hexagonal	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_8In_2	hexagonal		A3		26
Au_5In					186
Au_7In_3	cubic	a=9.80		Related to γ-brass structure.	26,186
AuIn	triclinic	a=4.30 b=10.59 c=3.56 α=90.54° β=90.00° γ=90.17°		Pseudo-orthorhombic	186, 187
$AuIn_2$	cubic	a=6.502	C1		186,187, 188
~ Au_6Ti	tetragonal	a=4.07 c=3.94		Compound may be as high as 96 a/o Au.	131,190, 191
Au_3Ti	hexagonal			Reported by (191) to be isomorphous with $TiCu_3$; not observed by (131).	131,190, 191
Au_2Ti	hexagonal	a=2.79 c=4.77	A3	X-ray data and thermal analysis; invariant composition.	131,190, 191

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
$AuTi_3$	cubic	a=5.096	A15	X-ray powder data.	131,190, 191,192
Au_3Zr					193
Au_3Th				No crystallography work done;; phase diagrams.	24
Au_5Th_3				"	24
Au_6Sn	hexagonal	a=2.93 c=4.78	A3		194
$Au_{5.13}Sn$				X-ray data.	195
$Au_{2.4}Sn$	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
$AuSn_2$	orthorhombic	a=6.85 b=7.00 c=11.78		Electron diffraction data.	196,187
$AuSn_4$	orthorhombic	a=6.446 b=6.487 c=11.599	C_{2v}^{17} -- Aba2	Structure related to C16 type;; x-ray powder data.	196,216, 217
Au_2Pb	cubic	a=7.98 ±0.01	C15	X-ray diffraction data.	197,198, 200
$AuPb_2$	tetragonal	a=7.310 ±0.003 c=5.644 ±0.003	C16	"	197,198, 199,200
$AuNb_3$	cubic	a=5.21 ±0.01	A15		201
AuV_3	cubic	a=4.88 ±0.01	A15		201
$AuSb_2$	cubic	a=6.63	C2	Electron diffraction data.	196,202
Au_2Bi	cubic	a=7.958	C15		200,203

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Au_3U				Thermal analysis and metallography and x-ray diffraction.	206
Au_3U_2				Thermal analysis and metallography and x-ray diffraction; forms from peritectic at 216°C.	206
Au_2Te_3	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
$AuTe_2$	orthorhombic	a=16.51 b=8.80 c=4.45	C46	X-ray powder data.	239
Au_3Mn				Structure not known; apparently nearly tetragonal with complicated superstructure.	207
Au_2Mn				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
$AuMn_3$				Same as Au_2Mn except a=3.310, c/a=0.85	207
$AuFe_3$				Compound reported by (208), denied by (209,210).	208,209,210

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PART III: STRUCTURE DETAILS

A 1: O_h^5--Fm3m

A=4: Cu structure
with 4 Cu (O_h): $000;\frac{1}{2}0\frac{1}{2};\frac{11}{22}0;0\frac{11}{22}$

Reported compounds: Ag_3Pt, Au, α-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--Im3m

A=2: W structure
with 2 W (O_h): $000;\frac{111}{222}$

Reported compounds: Cu_3Ge, CuZn, $CuZn_3$, β-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--$P6_3/mmc$

A=2: Mg structure
with 2 Mg (D_{3h}): 2/3,1/3,0;1/3,2/3,1/2

Reported compounds: Cu_7Si, Cu_5Ge, $CuZn_5$, Cu_3Ga, Ag_8As, Ag_3Sb, $Ag_{5.5}Hg_{4.5}$, Ag_3Ga, $AgZn_3$, AgCd, $AgCd_3$, ~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--$P4_32$ and O^7--$P4_12$

A=20: β-Mn structure
with 8 Mn (C_3): xxx;(1/2 + x)(1/2 - x) x; ↻;(3/4 - x) (3/4 - x)(3/4 - x); (1/4 - x)(3/4 + x) (1/4 + x); ↻ : x=0.061
12 Mn (C_2): 3/8,$\bar{x}$,(3/4 + x); ↻ ; 7/8,(1/2 + x) (1/4 - x); ↻ ;1/8,x,(1/4 + x); ↻ ; 5/8,(1/2 - x)(3/4 - x); ↻ : x=0.206

Reported compounds with related structure: Cu_5Si

A 15: O_h^3--Pm3n

A=8: Cr_3Si structure
with 2 Si (T_h): 000;$\frac{111}{222}$
6 Cr (D_{2d}): 1/2,0,1/4; ;1/2,0,3/4;

Reported compounds: $AuTi_3$, $AuNb_3$, AuV_3

B 2: O_h^1--Pm3m

A=1: ordered β-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, β-AuCd, AuMn

B 3: T_d^2--F$\bar{4}$3m

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--$P6_3/mmc$

A=4: α-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--$P6_3/mmc$

A=6: β-Ni_2In 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_2In, Cu_6Sn_5, Cu_7In_3, CuIn, AuSn

Remarks: The compounds listed have structures based on the α-NiAs and β-Ni_2In structures. Intermediate arrangement of the atoms allows deviations in stoichiometry. There exists a close relationship to the C6 structure. Cu_6Sn_5, Cu_7In_3 and CuIn have approximately the B8 structure.

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

A=4: 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(Ti)=0.65, z(Cu)=0.10; AgZr with z(Ag)=0.105, z(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 (hkl) were present only for l=2n and reflections (hk5) were all absent due to a "structural peculiarity."

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

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

Reported compounds: β'-AuCd

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

A=8: FeSi structure
with 4 Fe (C_3): $xxx;(\frac{1}{2}+x)(\frac{1}{2}-x)\bar{x};$ ↻: x=0.137
4 Si (C_3): the same with x=-0.158

Reported compounds: AuBe with x(Au)=0.150, x(Be)=0.844

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

A=8: 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(Au)=0.184, z(Au)=0.010, x(Ga)=0.590, z(Ga)=0.195

C 1: O_h^5--Fm3m

A=12: fluorite structure, CaF_2
with 4 Ca (O_h): 000 + F.C.
8 F (T_d): $\pm(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ + F.C.

Reported compounds: Cu_2S, Cu_2Se, Ag_2Se, $AuAl_2$, $AuGa_2$ $AuIn_2$

C 2: T_h^6--Pa3

A=12: FeS_2 structure
with 4 Fe (S_{3i}): 000; $\frac{1}{2}\frac{1}{2}0$; ↻
8 S (C_3): $\pm(xxx; \frac{1}{2}+x, \frac{1}{2}-x, \bar{x}; ↻)$: x=0.386

Reported compounds: $AuSb_2$

C 11: D_{4h}^{17}--$I4_1/mmm$

A=6: CaC_2 structure
with 2 Ca (D_{4h}): 000 + B.C.
4 C (C_{4v}): $\pm(00z)$: z=0.38 + B.C.

Reported compounds: $CuZr_2$ with z=0.342

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

A=12: $MgZn_2$ structure--Laves phase
with 4 Mg (C_{3v}): $\pm(1/3,2/3,z; 1/3,2/3,1/2-z)$: $z \approx 0.062$
2 Zn (D_{3d}): 000; $00\frac{1}{2}$
6 Zn (C_{2v}): $\pm(x,2x,\frac{1}{4}; \bar{2x}, \bar{x}, \frac{1}{4}; x, \bar{x}, \frac{1}{4})$: $x \approx -0.017$

Reported compounds: Ag_2Ca

C 15: O_h^7--Fd3m

A=24: $MgCu_2$ structure--Laves phase
with 8 Mg (T_d): 000; $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ + F.C.
16 Cu (D_{3d}): 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_2Mg; $CuBe_3$: (7.15 Cu + 0.85 Be in 000; $\frac{1}{4}\frac{1}{4}\frac{1}{4}$; and 16 Be in 5/8,5/8,5/8; 3/8,3/8,5/8; ↻) + F.C.; Cu_2U: (4 U in 000, 4 Cu in $\frac{1}{4}\frac{1}{4}\frac{1}{4}$, 16 Cu in 5/8,5/8,5/8;3/8, 3/8,5/8; ↻) + F.C.; $AgBe_2$, $AuBe_5$, Au_2Na, Au_2Pb, Au_2Bi.

Remarks: Those compounds which deviate from the AB_2 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}--I4/mcm

A=12: $CuAl_2$ structure
with 4 Cu (D_4): $\pm(00\frac{1}{4})$ + 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}--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}--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}--Pma

A=24: $AuTe_2$ structure
with 2 Au (C_2): $00z;\frac{1}{2}0z$: z=0
2 Au (C_s): $\frac{1}{4}yz;3/4,\bar{y},z$: 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_s): $\frac{1}{4}yz;3/4,\bar{y},z$: 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: $BiLi_3$ 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_3Sb

D O_9: O_h^1--Pm3m

A=4: Cu_3N structure
with 1 N (O_h): 000
3 Cu (D_{4h}): $\frac{1}{2}$00; ↻

Reported compounds: Cu_3N

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

A=8: Na_3As structure
with 2 As (D_{3h}): ±(1/3,2/3,1/4)
2 Na (D_{3h}): ±(00$\frac{1}{4}$)
4 Na (C_{3v}): ±(1/3,2/3,z; 2/3,1/3,1/2 + z): z=0.583

Reported compounds: $AuMg_3$

D O_{19}: D_{6h}^4--$P6_3/mmc$

A=8: Mg_3Cd structure
with 2 Cd (D_{3h}): ±(1/3,2/3,1/4)
6 Mg (C_{2v}): ±(2x,x,$\frac{1}{4}$; $\bar{x}$,x,$\frac{1}{4}$; $\bar{2}$x,2x,$\frac{1}{4}$): x≈0.167

Reported compounds: ~Ag_3In

D O_{21}: D_{3d}^4--$P\bar{3}ci$

A=24: Cu_3P structure
with 6 P (C_2): ±(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): ±(1/3,2/3,z; 1/3,2/3,1/2 + z): z=0.17
12 Cu (C_1): =[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_3P; Cu_3As with x(As)=0.33, z(Cu_{II})=0.15 x(Cu_{III})=0.68, y(Cu_{III})=0.075, z(Cu_{III})=0.08

D 8_{1-3}: O_h^9--Im3m; T_d^3--I$\bar{4}$3m; T_d^1--P$\bar{4}$3m

A=52: γ-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_4, Cu_4Al_3, Cu_9Ga_4, 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: γ-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_4 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.

D 8_6: T_d^6--I$\bar{4}$3d

A=76: $Cu_{15}Si_4$ structure
with
12 Cu (S_4): 0,1/4, 3/8; ↻ ; 0,3/4,1/8; ↻ + B.C.
48 Cu (C_1): xyz; ↻; x,$\bar{y}$,$\frac{1}{2}$ − z; ↻ ; $\frac{1}{2}$ − x,y,$\bar{z}$; ↻ ; $\bar{x}$,$\frac{1}{2}$ − y, z; ↻ ; $\frac{1}{4}$ + y, $\frac{1}{4}$ + x, $\frac{1}{4}$ + z; ↻ ; $\frac{1}{4}$ − y, $\frac{1}{4}$ + x, 3/4 − z; ↻ ; $\frac{1}{4}$ + y, 3/4 − x, $\frac{1}{4}$ − z; ; 3/4 − y, $\frac{1}{4}$ − x, $\frac{1}{4}$ + z; ↻ ; x≈0.12, y≈0.16, z≈0.04 + B.C.
16 Si (C_3): xxx; x,$\bar{x}$,$\frac{1}{2}$ − x; ↻ ; $\frac{1}{4}$ + x, $\frac{1}{4}$ + x, $\frac{1}{4}$ + x; $\frac{1}{4}$ − x, $\frac{1}{4}$ + x, 3/4 − x; ↻ : x≈0.208 + B.C.

Reported compounds: $Cu_{15}Si_4$

E 9_3: O_h^7--Fd3m

A=112: Fe_3W_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; $\bar{x}\bar{x}\bar{x}$; ↻ ; $\frac{1}{4}$ − x, $\frac{1}{4}$ − x, $\frac{1}{4}$ − x; $\frac{1}{4}$ − x, $\frac{1}{4}$ + x, $\frac{1}{4}$ + x; ↻ : x≈0.175 + F.C.
48 W (C_{2v}): ≈(x00; ↻); $\frac{1}{4}$ + x, $\frac{1}{4}$, $\frac{1}{4}$; ↻ ; $\frac{1}{4}$ − x, $\frac{1}{4}$, $\frac{1}{4}$; ↻ : x≈0.195 + F.C.
16 C (D_{3d}): 1/8,1/8,1/8; 1/8,3/8,3/8; ↻ + 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 $CuTi_2$ in this structure. Presumably the oxygens if present would occupy the C positions anf Ti would occupy the 192 fold and 64 fold sets.

L 10: D_{4h}^1--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° rotation of the a and b axes.

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

A=32: CuPt structure
with 16 Cu (D_{3d}): 000; $\frac{111}{442}$; ↻ + B.C.
16 Pt (D_{3d}): $\frac{111}{222}$; 3/4, 3/4, 0; ↻ + B.C.

Reported compounds: CuPt

L 12: O_h^1--Pm3m

A=4: Cu_3Au structure
with 3 Cu (D_{4h}): $\frac{11}{22}0$; ↻
1 Au (O_h): 000

Reported compounds: Cu_3Au, Cu_3Pd, $AgPt_3$, $AuCd_3$, Cu_3Pt

L 13: O_h^7--Fd3m

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

Reported compounds: CuPt, AgPt

Remarks: $CuPt_3$ and $CuPt_7$ are based on this structure.
$CuPt_3$ 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.
$CuPt_7$ 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=20: $AuSn_4$ structure
with 4 Au (C_2): 00z; $\frac{1}{2}\frac{1}{2}$z; z=0 + A.C.
8 Sn (C_1): 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_1): 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: $AuSn_4$

Remarks: Related to the C16 structure.

--- C_{4h}^{2}--$P4_2/m$

A=8: Cu_4Pd structure
with 2 Cu (C_{2h}): 000; $00\frac{1}{2}$
2 Cu (S_4): $\frac{1}{2}\frac{1}{2}\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},3/4$
4 Pd (C_s): 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_4Pd

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

A=48: $CuMg_2$ structure
with 16 Cu (C_2): 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_2): same with z=0.411
16 Mg (C_2): 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: $CuMg_2$

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

A=64: Cu_3As structure
with 16 As (C_3): xxx; $\frac{1}{2}+x, \frac{1}{2}-x, \bar{x}$; $\bar{x}, \frac{1}{2}+x, \frac{1}{2}-x$;
$\frac{1}{2}-x, \bar{x}, \frac{1}{2}+x$; $\frac{1}{4}+x, \frac{1}{4}+x, \frac{1}{4}+x$;
$3/4+x, 1/4-x, 3/4-x$; $3/4-x, 3/4+x, \frac{1}{4}-x$; $\frac{1}{4}-x, 3/4-x, 3/4+x$:
x=-0.03 + B.C.
48 Cu (C_1): xyz + full symmetry operations with
x=-0.03, y=0.12, z=0.20 + B.C.

Reported compounds: Cu_3As

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

A=6: Cu_5Ca 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_5Ca, Ag_5Ba, Ag_5Sr, Au_6Ba.

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

A=6: Cu_4Ce structure
with 1 Ce (D_{6h}): 000
2 ($Ce_{0.04}Cu_{0.96}$) (D_{3h}): 1/3,2/3,0; 2/3,1/3,0
3 ($Ce_{0.04}Cu_{0.96}$) (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_4Ce, Cu_4La

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

A=4: $AgZr_3$ 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: $AgZr_3$, α-Au_3Cd

Remarks: Tetragonally deformed L12

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

A=6: Cu_2Te structure
with 2 Te (C_{6v}): ±(00z): z=0.306
4 Cu (C_{3v}): ±(1/3,2/3,z; 2/3,1/3,z): z=0.160

Reported compounds: Cu_2Te

--- D_{2h}^{13}--Pmmn

A=4: 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 + (000; $\frac{11}{22}0$)

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; $\frac{11}{22}\bar{z}$: z=0.655
2 Cu (C_{2v}): $0\frac{1}{2}z$; $\frac{1}{2}0\bar{z}$: 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}--$H\bar{3}m$

A=27: $Cu_{20}Sn_6$ structure
with 2 Sn (D_3): ±(1/3,2/3,0)
4 Sn (C_3): ±(1/3,2/3,z; 2/3,1/3,z): z=1/3
2 Cu (C_{3v}): ±(00z): z=1/3
6 Cu (C_s): ±(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= γ'-$AlCu_3$ structure
with 1 Al (C_{2v}): x00: x=0
1 Al (C_{2v}): $x\frac{11}{22}$: 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: γ'-$AlCu_3$

T^4—$P2_13$

A=20: Au_4Al structure
with 12 Au (C_1): xyz; ↻; $\frac{1}{2}+x, \frac{1}{2}-y, \bar{z}$; ↻; $\bar{x}, \frac{1}{2}+y, \frac{1}{2}-z$; ↻; $\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z$; ↻: 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: β-Mn like phase. Ag_3Al has a statistical distribution of Ag and Al atoms.

C_{3i}^1—$C\bar{3}$

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; $\bar{x}\bar{y}\bar{z}$; 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 positioms are almost exclusively Zn; remaining Zn and Ag statistically distributed on 6-fold positions.

C_{2h}^2—$P2_1/m$ 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 $x=\frac{1}{2}$, y=0, z=1/3

Reported compounds: Cu_3Ge