

Database name	Common name	System	Prototype	Space group	No of subl.	Stoichiometry				Constituents			
AGIN2	AgIn ₂	Ag-In	CuAl ₂	I4/mcm	2	.33	.67			Ag	In		
AGSB_ORTHO	ε	Ag-Sb	βTiCu ₃	Pmmn	2	.75	.25			Ag,Au,Sb	Ag,Au,Bi, Sb,Sn		
	ε'		Ag ₃ Sb	Pmm2									
	ε	Ag-Sn	βTiCu ₃	Pmmn									
AGZN_BRASS	γ	Ag-Zn	Cu ₅ Zn ₈	I43m	4	2	2	3	6	Ag,Zn	Ag,Zn	Ag	Zn
AGZN_ZETA	ζ	Ag-Zn	AgZn(LT)	P3	2	1	2			Zn	Ag,Zn		
AU2BI_C15	Au ₂ Bi	Au-Bi	Cu ₂ Mg	Fd3m	2	2	1			Ag,Au	Bi		
AUIN	AuIn	Au-In	-	-	2	.5	.5			Au	In,Sb,Sn		
AUIN_BETA	β	Au-In	Cu ₁₁ Sb ₃	Amm2	2	.785	.215			Au	In		
AUIN_BETAP	β ₁	Au-In	Cu ₁₀ Sb ₃	P3	2	.77778	.22222			Au	In		
AUIN_GAMMA	γ	Au-In	Cu ₉ Al ₄	P43m	3	.69231	.23077	.07692		Au	Au,In	In	
AUIN_PSI	ψ	Au-In	Ni ₂ Al ₃	P3m1	3	.5	.33333	.16667		Au	Au,In	In	
AUIN2	AuIn ₂	Au-In	CaF ₂	Fm3m	2	.333333	.666667			Au	In,Sb,Sn		
AU3IN	ε'	Au-In	βTiCu ₃	Pmmn	2	.75	.25			Au	In		
	ε		-	-									
AU7IN3	γ'	Au-In	Au ₇ In ₃	P3	2	.7	.3			Au	In		
AU4IN3SN3	Au ₄ In ₃ Sn ₃	Au-In-Sn	Pt ₂ Sn ₃	P6 ₃ /mmc	3	.4	.3	.3		Au	In,Sn	In,Sn	
AUNIZSN4	AuNi ₂ Sn ₄	Au-Ni-Sn	-	-	3	.143	.286	.571		Au	Ni	Sn	
AUPB2	AuPb ₂	Au-Pb	CuAl ₂	I4/mcm	2	.333333	.666667			Au	Pb		
AUPB3	AuPb ₃	Au-Pb	αV ₃ S	I42m	2	.25	.75			Au	Pb		
AU2PB_C15	Au ₂ Pb	Au-Pb	Cu ₂ Mg	Fd3m	2	2	1			Au	Pb		
AUSB2	AuSb ₂	Au-Sb	FeS ₂	Pa3	2	.333333	.666667			Ag,Au	Bi,In,Sb		
AUSN2	ε/AuSn ₂	Au-Sn	AuSn ₂	Pbca	2	.333333	.666667			Au	Sn		

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AUSN4	η /AuSn ₄	Au-Sn	PtSn ₄	<i>Aba</i> 2	2	.2	.8		Au,Ni	In,Sn		
AU1SN	δ /AuSn	Au-Sn	NiAs	<i>P</i> ₆₃ / <i>mmc</i>	2	.5	.5		Au,Ni	In,Sn		
AU5SN	ζ /Au ₅ Sn	Au-Sn	Au ₅ Sn	<i>R</i> $\bar{3}$	2	.84	.16		Au	Sn		
AUZN_A1	α ₁	Au-Zn	Ag ₃ Mg	-	3	.6	.2	.2	Au	Au,Zn	Zn	
AUZN_A2	α ₂	Au-Zn	-	<i>Abam</i> (<i>Cmca</i>)	2	.75	.25		Au	Zn		
AUZN_A3	α ₃	Au-Zn	PdCu ₃	<i>P</i> 4 <i>mm</i>	3	.64286	.25	.10714	Au	Au,Zn	Zn	
AUZN_BETA	β'	Au-Zn	CsCl	<i>Pm</i> $\bar{3}$ <i>m</i>	2	.5	.5		Au,Zn	Au,Zn		
AUZN_BRASS	γ / γ -brass	Au-Zn	Cu ₅ Zn ₈	<i>I</i> $\bar{4}$ 3 <i>m</i>	4	2	2	3	6	Au,Zn	Au	Au,Zn
AUZN_DELTA	δ	Au-Zn	2	.44	.56		Au	Zn		
AUZN_E1	ϵ'	Au-Zn	2	.15	.85		Au	Zn		
AUZN_G2	γ ₂	Au-Zn	UH ₃	<i>Pm</i> $\bar{3}$ <i>n</i>	2	.25	.75		Au	Zn		
AUZN_G3	γ ₃	Au-Zn	...	<i>P</i> 6/ <i>mmm</i>	3	.12	.16	.72	Au	Au,Zn	Zn	
AU5ZN3	Au ₅ Zn ₃	Au-Zn	Au ₅ Zn ₃	<i>Pmc</i> 21	2	.625	.375		Au	Zn		
BCC_A2	β	Ag-In	W	<i>Im</i> $\bar{3}$ <i>m</i>	2	1	3		Ag,Au,Bi, Cu,In,Ni, Pb,Pd,Sb, Sn,Zn	Va		
		Cu-In										
		Cu-Sb ^(a)										
	γ	Cu-Sn ^(a)	<i>Fm</i> $\bar{3}$ <i>m</i>									
	β	Cu-Sn		<i>Im</i> $\bar{3}$ <i>m</i>								
		Cu-Zn										
	δ	Cu-Zn	<i>Fm</i> $\bar{3}$ <i>m</i>									
	Ni ₃ Sn_HT	Ni-Sn ^(a)		<i>Fm</i> $\bar{3}$ <i>m</i>								
	β	Ni-Zn ^(a)	<i>Pm</i> $\bar{3}$ <i>m</i>	<i>CsCl</i>								

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BCC_B2	InPd	In-Pd	CsCl	$Pm\bar{3}m$	2	.5	.5		Ag, In, Pd	Pd, Va	
B2_BCC	β'	Cu-Zn	CsCl	$Pm\bar{3}m$	3	.5	.5	3	Cu, Zn	Cu, Zn	Va
BCT_A5	(βSn)	Ag-Sn	βSn	$I4_1/amd$	1				Ag, Bi, In, Ni, Pb, Sb, Sn, Zn		
		Au-Sn									
		Bi-Sn									
		Cu-Sn									
		In-Sn									
		Ni-Sn									
		Pb-Sn									
		Pd-Sn									
		Sb-Sn									
Sn-Zn											
BIIN	BiIn	Bi-In	PbO	$P4/nmm$	2	.5	.5		Bi	In	
BIIN_BRASS	BiIn ₂	Bi-In	Ni ₂ In	$P6_3/mmc$	2	.333333	.666667		Bi	In	
BI3IN5	Bi ₃ In ₅	Bi-In	Cr ₅ B ₃	$I4/mcm$	2	.375	.625		Bi	In	
BINI	NiBi	Bi-Ni	NiAs	$P6_3/mmc$	2	.5	.5		Bi	Ni, Va	
BI3NI	NiBi ₃	Bi-Ni	LiCaSi ₂	$Pnma$	2	.75	.25		Bi	Ni	
BIPD	$\alpha\text{BiPd(LT)}$	Bi-Pd	-	$P2_1$	2	.5	.5		Bi	Pd	
	$\beta\text{BiPd(HT)}$		PdBi	$Cmc2_1$							
BIPD3	αBiPd_3	Bi-Pd	Pd _{1.5} PbBi ₄	$Pmma$	2	.25	.75		Bi	Pd	
	βBiPd_3		-	-							
BI2PD	$\alpha\text{Bi}_2\text{Pd}$	Bi-Pd	PdBi ₂	$C2/m$	2	.666	.334		Bi	Pd	
	$\beta\text{Bi}_2\text{Pd}$		MoSi ₂	$I4/mmm$							

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DIAMOND_A4	(αSn)	Ag-Sn	C-diam	$Fd\bar{3}m$	1				Sn,Zn		
		Au-Sn									
		Bi-Sn									
		Cu-Sn									
		In-Sn									
		Ni-Sn									
		Pb-Sn									
		Pd-Sn									
		Sb-Sn									
		Sn-Zn									
		FCC_A1									
Ag-Bi											
Ag-Cu											
Ag-In											
Ag-Ni											
Ag-Pb											
Ag-Pd											
Ag-Sb											
Ag-Sn											
Ag-Zn											
Au-Bi											
Au-Cu											
Au-In											
Au-Ni											
Au-Pb											
Au-Pd											

Database name	Common name	System	Prototype	Space group	No of subl.	Stoichiometry			Constituents		
FCC_A1	(Au)	Au-Sb	Cu	$Fm\bar{3}m$	2	1	1	Va	Ag,Au,Bi, Cu,In,Ni, Pb,Pd,Sb, Sn,Zn		
	(Cu)	Au-Sn									
	(Ni)	Au-Zn									
	(Pb)	Bi-Cu									
	(Pd)	Bi-Ni									
	(Cu)	Bi-Pb									
	(Cu,Ni)	Bi-Pd									
	(Cu),(Pb)	Cu-In									
	(Cu,Pd)	Cu-Ni									
	(Cu)	Cu-Pb									
	(Ni)	Cu-Pd									
	(Pb)	Cu-Sb									
	(Pd)	Cu-Sn									
	(Ni),(Pb)	Cu-Zn									
	(Ni,Pd)	In-Ni									
	(Ni)	In-Pb									
	(Pb),(Pd)	In-Pd									
	(Pb)	Ni-Pb									
	(Pd)	Ni-Pd									
	(Ni)	Ni-Sn									
(Pb),(Pd)	Ni-Zn										
(Pb)	Pb-Pd										
(Pd)	Pb-Sb										
	Pb-Sn										
	Pb-Zn										
	Pd-Sn										
	Pd-Zn										

Database name	Common name	System	Prototype	Space group	No of subl.	Stoichiometry			Constituents		
HCP_A3	ζ	Ag-In	Mg	$P6_3/mmc$	2	1	.5	Va	Ag,Au,Bi, Cu,In,Ni, Pb,Pd,Sb, Sn,Zn		
		Ag-Sb									
	Ag-Sn										
	Ag-Zn										
	Au-In										
	Au-Sn										
	Au-Zn										
ε	Bi-Pb	Bi-Zn									
		Cu-Zn									
	ε	Cu-Zn									
HCP_ZN	(Zn)	Ag-Zn	Mg	$P6_3/mmc$	2	1	.5	Va	Ag,Au,Bi, Cu,In,Pb, Pd,Sn,Zn		
		Au-Zn									
		Bi-Zn									
		Cu-Zn									
		In-Zn									
		Ni-Zn									
		Pb-Zn									
		Pd-Zn									
		Sb-Zn									
		Sn-Zn									
		INNI_DELTA									
INNI_CHI	ζ	In-Ni	3	1	1	1	Ni,Va	Ni	In,Ni
INNI_CHI_PRIME	ζ' (Ni ₁₃ In ₉)	In-Ni	Pt ₁₃ In ₉	$C2/m$	3	1	1	1	Ni,Va	Ni	In
INPD2_ALPHA	αInPd ₂	In-Pd	Co ₂ Si	$Pnma$	2	.333	.667		In	Pd	
INPD3_ALPHA	αInPd ₃	In-Pd	In	$I4/mmm$	2	.25	.75		In	Pd	

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INPD2_BETA	β InPd ₂	In-Pd	2	.34	.66		In	Pd	
INPD3_BETA	β InPd ₃	In-Pd	AuCu	<i>P4/mmm</i>	2	.26	.74		In	Pd	
IN3PD2	In ₃ Pd ₂	In-Pd	Ni ₂ Al ₃	<i>P$\bar{3}$ m1</i>	2	.6	.4		In	Ag,Pd	
IN3PD5	In ₃ Pd ₅	In-Pd	Rh ₅ Ge ₃	<i>Pbam</i>	2	.375	.625		In	Pd	
IN7PD3	In ₃ Pd	In-Pd	Cu ₅ Zn ₈	<i>I$\bar{4}$3m</i>	2	.71	.29		In	Pd	
INSN_GAMMA	γ	In-Sn	InBi	<i>P6/mmm</i>	1	1			In,Sn		
NIIN	NiIn	In-Ni	CoSn	<i>P6/mmm</i>	2	1	1		Ni	In	
NI2IN	Ni ₂ In	In-Ni	Ni ₂ In	<i>P6$\bar{3}$/mmc</i>	2	2	1		Ni	In	
NI2IN3	Ni ₂ In ₃	In-Ni	Ni ₂ Al ₃	<i>P$\bar{3}$ m1</i>	2	2	3		Ni	In	
NI3IN	Ni ₃ In	In-Ni	Ni ₃ Sn	<i>P6$\bar{3}$/mmc</i>	2	3	1		Ni	In	
NI3IN7	Ni ₂₈ In ₇₂	In-Ni	Cu ₅ Zn ₈	<i>I$\bar{4}$3m</i>	2	3	7		Ni	In	
NI3SN_LT	Ni ₃ Sn_LT	Ni-Sn	Ni ₃ Sn	<i>P6$\bar{3}$/mmc</i>	2	.75	.25		Cu,Ni	In,Sn	
NI3SN2	Ni ₃ Sn ₂ _LT	Ni-Sn	Ni ₃ Sn ₂	<i>Phma</i>	3	.5	.25	.25	Ni,Sn	Au,Cu,Ni	Au,Cu,Ni
	Ni ₃ Sn ₂ _HT		<i>P6$\bar{3}$/mmc</i>								
NI3SN4	Ni ₃ Sn ₄	Ni-Sn	Ni ₃ Sn ₄	<i>C2/m</i>	3	.25	.25	.5	Cu,Ni	Ni,Sn	Sn
NIZN_BETA1	β ₁	Ni-Zn	AuCu	<i>I4/mmm</i>	1	1			Ni,Zn		
NIZN_DELTA	δ	Ni-Zn	CoZn ₁₃	<i>C2/m</i>	2	.111	.889		Ni	Zn	
NIZN_GAMMA	γ	Ni-Zn	Cu ₅ Zn ₈	<i>I$\bar{4}$3m</i>	1	1			Ni,Zn		
PDPB	α PbPd	Pb-Pd	-	<i>P$\bar{1}$</i>	2	1	1		Pd	Pb	
	β PbPd		-								
PDPB2	Pb ₂ Pd	Pb-Pd	CuAl ₂	<i>I4/mcm</i>	2	1	2		Pd	Pb	
PD3PB	Pb Pd ₃	Pb-Pd	AuCu ₃	<i>Pm$\bar{3}$ m</i>	2	.75	.25		Pd	Pb,Pd	

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PD5PB3_ALPHA	α Pb ₃ Pd ₅	Pb-Pd	Ni ₅ Ge ₃	C2	2	5	3				Pd	Pb	
PD5PB3_BETA	β Pb ₃ Pd ₅	Pb-Pd	NiAs	P6 ₃ /mmc	3	1	1	1			Pd	Pb	Pd,Va
PD5PB3_GAMMA	γ Pb ₃ Pd ₅	Pb-Pd	-	-	3	1	1	1			Pd	Pb	Pd,Va
PD13PB9	α Pb ₉ Pd ₁₃	Pb-Pd	α Pd ₁₃ Pb ₉	C2/c	2	.59	.41				Pd	Pb	
	β Pb ₉ Pd ₁₃		P6 ₃ /mmc										
	γ Pb ₉ Pd ₁₃		-										
PDSN	PdSn	Pd-Sn	FeB	Prma	2	.5	.5				Pd,Va	Pd,Sn	
PDSN2	PdSn ₂	Pd-Sn	PdSn ₂	Aba2	2	.333	.667				Pd,Sn	Sn	
PDSN3	PdSn ₃	Pd-Sn	PdSn ₃	Cmca	2	.25	.75				Pb,Pd	Pd,Sn	
PDSN4	PdSn ₄	Pd-Sn	PtSn ₄	Aba2	2	.2	.8				Pd	Pb,Pd,Sn	
PD2SN	Pd ₂ Sn	Pd-Sn	Co ₂ Si	Prma	2	.667	.333				Pd	Sn	
PD2SN_GAMMA	γ	Pd-Sn	NiAs	P6 ₃ /mmc	3	1	1	1			Pd	Sn	Pd,Va
PD3SN	Pd ₃ Sn	Pd-Sn	AuCu ₃	Pm $\bar{3}$ m	2	.75	.25				Pd,Sn	Pd,Sn	
PD3SN2_ALPHA	α Pd ₃ Sn ₂	Pd-Sn	Ni ₂ In	P6 ₃ /mmc	2	.6	.4				Pd	Sn	
PD3SN2_BETA	β Pd ₃ Sn ₂	Pd-Sn	2	.6	.4				Pd	Sn	
PD3SN2_DELTA	δ	Pd-Sn	2	.59	.41				Pd	Sn	
PD20SN13	Pd ₂₀ Sn ₁₃	Pd-Sn	Ni ₄ GaGe ₂	P3 ₁ 21	2	.6	.4				Pd,Sn	Pd,Sn	
PDZN_BETA	β	Pd-Zn	CsCl	Pm $\bar{3}$ m	2	1	1				Pd,Zn	Pd,Zn	
PDZN_1BETA	β_1	Pd-Zn	AuCu	P4/mmm	2	1	1				Pd,Zn	Pd,Zn	
PDZN_GAMMA	γ	Pd-Zn	Cu ₅ Zn ₈	I $\bar{4}$ 3m	2	2	9				Pd,Zn	Pd,Zn	
PDZN2	PdZn ₂	Pd-Zn	PdZn ₂	Cmmm	2	1	2				Pd	Zn	
PD2ZN	δ	Pd-Zn	Co ₂ Si	Prma	2	2	1				Pd	Zn	

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PDZN_ETA	η	Pd-Zn	2	.09	.91			Pd	Zn		
RHOMBO_A7	(Bi)	Ag-Bi	α As	$R\bar{3}m$	1					Bi,In,Pb, Pd,Sb,Sn, Zn			
	(Sb)	Ag-Sb											
	(Bi)	Au-Bi											
	(Sb)	Au-Sb											
	(Bi)	Bi-Cu											
		Bi-In											
		Bi-Ni											
		Bi-Pb											
													Bi-Pd
	(Bi, Sb)	Bi-Sb											
	(Bi)	Bi-Sn											
		Bi-Zn											
	(Sb)	Cu-Sb											
		In-Sb											
Pb-Sb													
Sb-Sn													
Sb-Zn													
Sb-Sn													
SB2SN3	Sn_3Sb_2		2	2	3		Sb	Sn			
SBSN	β	Sb-Sn	NaCl	$Fm\bar{3}m$	2	1	1		Bi,In,Pb, Sb,Sn	Bi,In,Sb, Sn			
SBZN_BETA	β	Sb-Zn	CdSb	$Pbca$	2	.5	.5		Sb	Zn			
SBZN_DELTA	δ	Sb-Zn	Zn_4Sb_3	$R\bar{3}c$	2	.425	.575		Sb	Zn			
SBZN_EPSILON	ϵ	Sb-Zn	Zn_4Sb_3	$R\bar{3}c$	2	.425	.575		Sb	Zn			
SBZN_ETA	η	Sb-Zn	...	$Pmmn$	2	.38	.62		Sb	Zn			

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SBZN_GAMMA	γ	Sb-Zn	2	.45	.55		Sb	Zn	
SBZN_ZETA	ζ	Sb-Zn	2	.4	.6		Sb	Zn	
TET_ALPHA1	ε	Bi-In	In	$I4/mmm$	1	1			Bi,In,Pb, Sn		
	α	In-Pb									
		In-Sn									
TETRAG_A6	(In)	Ag-In	In	$I4/mmm$	1	1			Bi,In,Pb, Sn, Zn		
		Au-In									
		Bi-In									
		Cu-In									
		In-Ni									
		In-Pb									
		In-Pd									
		In-Sb									
		In-Sn									
		In-Zn									
		ZINCBLLENDE_B3									

(a) Real crystallographic structure was modelled as BCC_A2 in the Cu-Sb, Cu-Sn, Ni-Sn and Ni-Zn to retain the consistency in ternary systems (see the text in the relevant binary systems)