FSlead Database for FactSage 8.3

The FSlead Database is designed for thermodynamic and phase equilibrium calculations involving **Pb** alloys using the FactSage 8.0 Thermochemical Software Package (and later versions).

Pb Alloys
Ag, As, Au, Ba, **Bi**, **C**, **Ca**, Cd, **Cu**, **Fe**, **Ga**, **Ge**, **H**, Hg, **In**, **Ni**, **O**, **Pb**, **S**, **Sb**, **Se**, **Si**, **Sn**, Sr, Te, Tl, **Zn**
Color codes
Red : Pb **Blue** : Major alloying elements (full optimisations of binary systems with **Pb** and with several minor alloying elements, **Pb-Xx-Yy** ternary systems evaluated (good for the Pb-rich), several quaternary systems included); **Green** : Minor alloying elements (full optimisations of binary systems with Pb); **Purple** : Impurity elements (full optimisations of binary systems with Pb and several Pb-M-X systems); Black : Optimized for the **Pb-Zz** system and few **Xx-Zz** and **Pb-Xx-Zz** systems.

Composition Ranges

The database is intended to allow calculations over all ranges of composition, although the assessed data are often most reliable for Pb-rich composition ranges. Please note that the FSlead database is a self-consistently evaluated database designed to be used independently of any other. Considerable caution must be exercised if it is used in conjunction with other FactSage alloy databases. However, calculations involving the gas phase can be performed with the FACTPS Database.

Temperature Ranges

The database is generally valid for the temperature range of approximately room temperature to 2200°C (please remember that kinetics effects can strongly affect phase relationships in alloys in general and in particular at low temperature), although for some alloys containing high melting point metals the data are reliable to still higher temperatures.

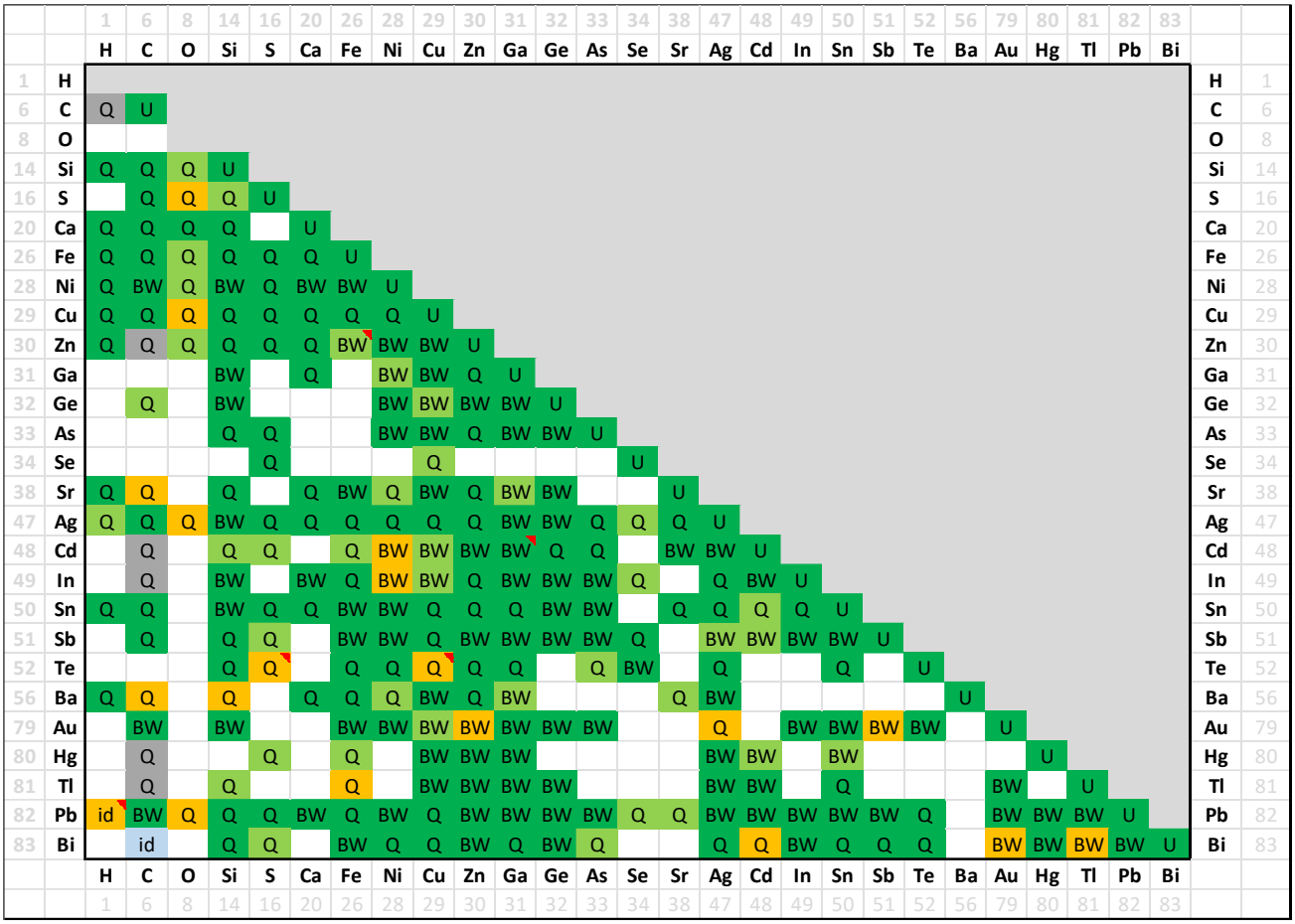
In **Table 4**, comments appearing in red can be found for some binary systems which have spurious stable phases at high temperatures, such as inverted liquid-liquid miscibility gaps, or the presence of an inverted solid solutions. The temperature above which the problem occurs is given in **Table 4** as an indication. These inverted stability regions can cause problems in the computation of liquidus

projection of ternary or higher order systems in the PHASE DIAGRAM Module and affect the computation of precipitation or formation targets in the EQUILIB Module.

Physical Properties

The density and viscosity of the liquid phase can be computed for most important elements present in the database.

The thermal conductivity of most non-metallic stoichiometric solids (ex.: SiC, etc.) can be computed with the FSlead 8.3 database. See FactSage (EQUILIB) documentation on physical properties, and the list of phases at the end of the present document.



id	Ideal Bragg-Williams Treatment for the liquid, FCC-A1, BCC-A2, HCP-A3 and DHCP-A4 solid solutions
Q	Modified Quasichemical Model (liquid solution); CEF for S.S.
BW	Bragg-Williams Model (liquid solution); CEF for S.S.
	Top quality
	Good quality (maybe a missing phase, or a good estimation)
	Rough estimate, probably missing phases
	Noble gas system (use FACTPS Database)
	Computed using pure substances from database with gaseous species from the FACTPS Database

Figure 1: Optimized binary systems in the FSlead 8.3 Database (see also Table 4)

In FSlead 8.3, a total of **235 binary systems** (223 in 8.2) have been evaluated, for most of them over the entire range of composition and for all stable phases. A matrix of assessed binary systems is given in **Figure 1**, for the major and minor alloying elements of Pb-alloys. Several dozens of ternary systems have been assessed, and important quaternary systems have also been evaluated.

The FSlead 8.3 database contains **125 solution phases** (100 in 8.2) and **415 pure compounds** (359 in 8.2) with **618 stoichiometric phases** (548 in 8.2) counting allotropic forms. **Table 1** lists the important solutions for calculations involving Pb alloys. **Table 2** is a detailed list of all solutions. **Table 3** is a generic list of the pure compounds and their associated phases. **Table 4** gives the references for the binary data assessments.

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Use of the Database

The phase diagrams of all the binary systems listed above have been checked using FactSage 8.3.

Phase selection in the EQUILIB or PHASE DIAGRAM modules using FSlead is simple: simply follow these instructions:

- For pure solid compounds:
  - Right-click on “pure solids”
  - Then click “Select/Clear” > “Add all species from database” > “FSlead”
- For solutions:
  - In “Data Search | Options – search for product species”, select “minimum solution components = 2 cpts” (which is the default value);
  - Click on the “Select” button below the “Solution species” list box;
  - Then click “Add all phases from database” > “FSlead”;
- There is no need to select pure liquid phases (the FSlead-Liqu solution contains the liquid species). They may be selected as dormant (metastable, option “!”) for purposes of computing their chemical activity.
- Click “Use V & phys. property data” in the EQUILIB Module if you intend to have density, viscosity, thermal conductivity and surface tension to be calculated for phases, when available. We recommend not to click this option in the PHASE DIAGRAM Module.

There might be cases when a chemical system with many elements results in more than 99 possible solutions to be selected. In these cases, it is recommended to change the selection of some solutions where the “I-option” (“possible 2-phase immiscibility”) or the “J-option” (“possible 3-phase immiscibility”) has been automatically selected, to either “+” (for “I”) or “I-option” (for “J-option”). The solutions where this change must be done should then be selected at the user`s discretion based on his/her knowledge of which solutions might exhibit immiscibility in the composition range the user is interested in.

Updates in 8.3 from 8.2

Here is a list of new assessments or new assessments integrated from publications in 8.3:

1) As – Cd
2) As – Zn (replaced)
3) Au – Ga
4) Ba – Ga
5) Ca – Ga
6) Ca – Ge
7) Fe – In (replaced)
8) Ga – Ni
9) Ga – Sr
10) Ga – V
11) Ge – Ni
12) Ge – Sr
13) H – Sn
14) In – Se

Many existing solutions were modified to introduce the new systems (*i.e.* Liquid metal, FCC-A1, BCC-A2, HCP-A3, etc.). Those are not necessarily listed below. Also, many existing solutions were modified to introduce new end-members:

- Diamond-A4 addition of In
- CUB-A13 addition of Sb
- B8x (B81/B82) addition of Ge; updated CuSn, Au-Co, Ni_2Ge
- B11 addition of Au
- B33 addition of Ge and Fe
- C1a addition of Ga
- C2 addition of Ag, As, Te
- C15a addition of Au and Bi for Au_2Bi
- C16 addition of Ga
- C23a addition of Ge
- C38 addition of Bi and S
- D011 addition of Ge
- D59 reconstructed sublattice structure for Zn_3As_2
- D513 addition of Ga
- D81 addition of Ga, Ge and Fe
- L12c addition of Ge
- mS44 addition of Ga
- oP20 addition of Au

Moreover, the following new solid solution phases were created:

1) A3’ Prototype La
addition of Au(Sn)
2) B20 Prototype FeSi
(Fe,Ni)Si
3) B31 Prototype
Ni(Ge,Si)
4) C1c Prototype-Cd3As2
$(Cd,Zn)_3As_2$
5) C12 Prototype-CaSi2
$Ca(Ge,Si,Sn)_2$
6) C14 Prototype-MgZn2
Many compounds
7) C32 Prototype-AlB2
$(Ba,Ca,Sr)Ga_2$
8) D024 Prototype-Ni3Ti
Au_3Ga
9) D13 Prototype-Al4Ba
$(Ga,Si,Zn)_4(Ba,Ca,Sr)$
10) oD59 ordered ternary D59 solid solution (Zn_3As_2-Cd_3As_2)
11) D510 Prototype-Cr3C2
$(Fe,Ni)_3C_2$
12) L12e L12 Prototype-AuCu3
Ni_3Ga
13) cP60 Prototype-Ba8Ga7
$(Ba,Ca,Sr)_8Ga_7$
14) mP24 Prototype-ZnAs2
$(Cd,Zn)As_2$
15) oP4a Prototype Ag3Sb
Ag_3Sb
16) o24P oP24 Prototype-BaSi2
$(Ba,Sr)(Ge,Si)_2$
17) oP52 Prototype Ca7Sn6
$Ca_7(Ge,Si,Sn)_6$
18) oS8 Prototype-TlI
GaCa, GeSr, PbSr
19) o16S oS16 Prototype Pt5Ga3
Ni_5Ga_3

20)	t12I	tI12 Prototype CdAs2 $(Cd,Zn)As_2$
21)	i160	tI160 Prototype Cd3As2 $(Cd,Zn)_3As_2$
22)	p160	tP160 Prototype Zn3As2 $(Cd,Zn)_3As_2$

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Table 1: Important phases in Pb alloys present in the FSlead 8.3 Database

Common names	FSlead		Struktur-bericht	Pearson	Space Group (index)
	Soln-Nickname or CMPD*	Solution Full name or compound stoichiometry			
Liquid metal	Liqu	Liquid	-	-	
Pb, α, FCC, (Pb), Ag, Co(lt), Cu, γ-Fe, Ni, Tl(ht)	A1	FCC-A1	A1	cF4	Fm-3m (225)
α-Fe, Ni, CuZn(ht), Cu_3In(ht), Cu_3Sn(ht)	A2	BCC-A2	A2	cI2	Im-3m (229)
Bi, Cd, Tl(lt), Cu_6Si	A3	HCP-A3	A3	hP2	$P6_3/mmc$ (194)
Zn	A3"	HCP-A3	A3	hP2	$P6_3/mmc$ (194)
Si, Ge, α-Sn	A4	Diamond-A4	A4	cF8	Fd-3m (227)
Sn	A5	BCT-A5	A5	tI4	$I4_1/amd$ (141)
InPb	A6	TET-A6o	A6	tI2	I4/mmm (139)
Bi	A7	Rhombehedral-A7	A7	hR2	R-3m (166)
C	-	$C_{(s)}$	A9	hP4	$P6_3/mmc$ (194)
Ga	A11	ORTH-A11	A11	oC8	Cmca (64)
PbS, PbSe, PbTe	B1	B1 Prototype-NaCl	B1	cF8	Fm-3m (225)
β-NiZn, β'-CuZn	B2	BCC-B2!BCC-A2	B2	cP2	Pm-3m (221)
ZnS-sphalerite	B3	B3 Prototype-ZnS	B3	cF8	F-43m (216)
ZnS-wurtzite	B4	B4 Prototype-ZnS	B4	hP4	$P6_3mc$ (186)
NiBi, NiAs, AuSn, CoS, CrS, FeS, NiS, ε-FeSb, NiSb, (Fe,Ni)Te	B8x	B81/B82 NiAs/InNi2	$B8_1$	hP4	$P6_3/mmc$ (194)
Co_2Sb, $InNi_2$, $(Fe,Ni,Ti)_2Sn$, ε-FeSb, θ-$SiNi_2$, $Sn(Fe,Ti)_2$			$B8_2$	hP6	
Cu_2O	C3	C3 Prototype-Cu2O	C3	cP6	Pn-3m (224)
Cu_3Sn(ht), Cu_3Sb	D03	D03 Prototype-BiF3	$D0_3$	cF16	Fm-3m (225)
Pb_2Hg	-	$Pb_2Hg_{(s)}$	$L1_0$	tP2	P4/mmm (123)
Pb_3Ca	-	$Pb_3Ca_{(s)}$	$L1_2$	cP4	Pm-3m (221)
Cu_2S(ht)-digenite, Cu_2Se(ht)- berzelianite, $(Cu_{2-x}Fe_x)S$-bornite	cF44	cF44 Prototype-Cu2Se	-	cF44	Fm-3m (225)

Cu_2S(mt)-high-chalcocite	hP16	hP16 (high-chalcocite)	-	hP16	$P6_3/mmc$ (194)
Cu_2S(lt)-chalcocite	Chal	Chalcocite	-	mP144	$P2_1/c$ (14)
$Cu_2Te_{(s6)}$	-	$Cu_2Te_{(s6)}$	-	cF12	Fd-3m (227)
ε-$AsCu_8$	-	$AsCu_{8(s)}$	-	h*	$P6_3/mmc$ (194)
Cu_3As-beta-Domeykite	-	$Cu_3As_{(s)}$	-	hP24	P-3c1 (165)
Hg_6Cu_7	-	$Hg_6Cu_{7(s)}$	-	hR*	R3m
Cu_2Se(lt)	-	$Cu_2Se_{(s)}$	-	mS144	C2/c (15)
PbO-massicot (yellow)	-	$PbO_{(s2)}$	-	oP8	Pbcm (57)
Cu_3Sn	-	$Cu_3Sn_{(s)}$	-	oS80	Cmcm (63)
Pb_3Au	-	$AuPb_{3(s)}$	-	tI32	$I\text{-}4_2m$ (121)
Pb_3Sr	-	$Pb_3Sr_{(s)}$	-	tP4	P4/mmm (123)
PbO-litharge (red)	-	$PbO_{(s)}$	-	tP4	P4/nmm (129)

Table 2: Solution names with their major components (not including minor solutes)

■ **Important solutions in Pb alloys**

Common names	FSlead		Major phase components
	Nickname	Full name	
Liquid metal	Liqu	Liquid	most elements
Pb, (Pb), FCC, Ag γ-$Fe_{austenite}$, Ni, Au	A1	FCC-A1	Ag, Cu, γ-$Fe_{austenite}$, Ni, Pb, ... with C, H, O interstitials (→B1)
α-$Fe_{ferrite}$, BCC	A2	BCC-A2	α-$Fe_{ferrite}$, Ba, Sr… ... with C, H, O interstitials
Bi, Cd, HCP	A3	HCP-A3	Bi, Cd, Tl
Au(Sn)	A3'	DHCP-A3'	Au-rich solution with Sn
Zn	A3"	HCP-Zn	Zn
Si, α-Sn	A4	Diamond-A4	$C_{diamond}$, Ge, Si, α-Sn
Sn	A5	BCT-A5	β-Sn
In	A6	TET-A6	α-In
InSn, InPb	A6o	TET-A6o	β-InSn, InPb
As, **Bi**, Sb	A7	RHOM-A7	α-As, Bi, Sb
γ-Se, Te	A8	A8	γ-Se, Te
Hg	A10	RHOM-A10	α-Hg
Ga	A11	ORTH-A11	α-Ga
Ag_3X	A13	CUB-A13	Ag_3X
α-S	A16	A16	S
γ-InSn	Af	HEX-Af	γ-InSn
β-S	Ak	Ak	β-S
Se	Al	Al	Se
PbS, PbSe, PbTe, SnAs, SnS, CaS	B1	FCC-B1	CaS, PbS, PbSe, PbTe, SnAs, SnS, SnTe
β-NiZn, **β'-CuZn**	**B2**	BCC_B2!BCC_A2	CaIn, β-NiZn, β'-CuZn with order/disorder transf.; AlFe, AlMn, FeSi
ZnS, ZnTe, β-SiC-3C	B3	B3 (sphalerite)	GaAs, GaSb, InAs, InSb, β-SiC-3C
ZnS, α-SiC-2H	B4	B4 (wurtzite)	ZnS, α-SiC-2H
(Fe,Ni)S, $B8_1$	**B8x**	B81/B82 NiAs/InNi2	**$B8_1$** : NiBi, NiAs, AuSn, FeS, NiS, ε-FeSb, NiSb, (Fe,Ni)Te
			$B8_2$: $InNi_2$, $(Fe,Ni)_2Sn$, ε-FeSb, θ-$SiNi_2$
HgS	B9	B9 Prototype-HgS	HgS
β1-NiZn	B11	B11 Prototype-CuTi	β1-NiZn
NiS millerite	B13	B13 Prototype-NiS	NiS
SnS, α-SnSe	B16	B16 Prototype-GeS	SnS, α-SnSe
CuS covellite	B18	B18 Prototype-CuS	CuS
FeSi naquite	B20	B20 Prototype-FeSi	FeSi with Ni and Ga solubility
NiSi	B31	B31 Prototype-FeAs	NiSi, NiGe
CaSi, CaSn	B33	B33 Prototype-CrB	CaSi, CaSn

NiIn, FeSn	B35	B35 Prototype-CoSn	FeSn, NiIn
η-AgZn	Bb	Bb Prototype-AgZn	η-AgZn (also called β')
ω-CdSb, β-ZnSb	Be	Be Prototype-CdSb	ω-CdSb, β-ZnSb
$NiSi_2$	C1a	aC1 Prototype-CaF2	$NiSi_2$, $CoSi_2$, Al_2Au, Ga_2Au
Ni_2S-β1	C1b	C1b Prototype-MgAgAs	Ni_2S-β1
β-Cd_3As_2, β-Zn_3As_2	C1c	C1 Prototype-CaF2	$(Cd,Zn)_3As_2$
$(Fe,Ni)S_2$, $(Cu,Ni)Se_2$, $AuSb_2$	C2	C2 Prototype-FeS2	$(Fe,Ni,Co)S_2$, $AuSb_2$, $(Co,Cu,Ni)Se_2$,
Cu_2O	C3	C3 Prototype-Cu2O	$(Cu,Ag)_2O$
MTe_2, SnS_2	C6	C6 Prototype-CdI2	$(Fe,Ni)Te_{2-x}$, $SiTe_2$, SnS_2 and $SnSe_2$
$Ca(Ge,Si,Sn)_2$	C12	C12 Prototype-CaSi2	$Ca(Ge,Si,Sn)_2$
Laves-C14	C14	C14 Prototype-MgZn2	-
$CaNi_2$, Laves-C15	C15	C15 Prototype-$MgCu_2$ (Laves)	Ni_2Ca
Ag_2Na, Au_2Bi	C15a	C15 Prototype-$MgCu_2$	Ag_2Na, Au_2Bi
Pb_2Au	C16	C16 Prototype-Al2Cu	Pb_2Au, Sn_2Fe
$CuSe_2$, $(Fe,Ni)(As,S,Sb)_2$	C18	C18 Prototype-FeS_2	$CuSe_2$, $(Fe,Ni)(As,S,Sb,Te)_2$
BaH_2, CaH_2, SrH_2	C23	C23 Prototype-PbCl2	α-BaH_2, CaH_2, α-SrH_2
$PbCa_2$	C23a	C23 Prototype-Co2Si	Ca_2Sn, Sr_2Sn, Ca_2Si, Sr_2Si, θ-Ni_2Si, Ni_2Ge, Ca_2Cu, $PbCa_2$
$(Ba,Sr)Ga_2$	C32	C32 Prototype-AlB2	$(Ba,Ca,Sr)Ga_2$
Bi_2Te_3	C33	C33 Prototype-Bi2Te3	Bi_2Te_3, Bi_2Se_3, Sb_2Te_3
$AuTe_2$	C34	C34 Prototype-AuTe2	$AuTe_2$
η-Cu_2Sb	C38	C38 Prototype-Cu2Sb	η-Cu_2Sb, Cu_2As, Cu_2Te, Fe_2Te
$CaZn_2$	C42	C42 Prototype-CeCu2	$CaZn_2$
Cu_2Te	Ch	Ch Prototype-Cu2Te	Cu_2Te
β-Ni_3Sn, γ-Cu_3Sn	D03	D03 Prototype-BiF3	γ-Cu_3Sn, Sn_3Cu, β-Ni_3Sn, Ni_3Sb, Cu_3Sb
Fe_3Si	D03a	D03 Prototype-BiF3	Fe_3Si
θ-Fe_3C	D011	D011 Prototype-Fe3C	θ-Fe_3C, Ni_3Si, Ni_3Ge
Ni_3In, Ni_3Sn(lt)	D019	D019 Prototype-Ni3Sn	Ni_3In, Ni_3Sn(lt)
Au_3Ga	D024	D023 Prototype-Ni3Ti	Au_3Ga
Ag_3Sn, Cu_3Sb $D0_a$	D0a	D0a Prototype-Cu3Ti	Ag_3Sn, Cu_3Sb, Ni_3Sb
$Ga_4(Ba,Ca,Sr)$	D13	D13 Prototype-Al4Ba	$Ga_4(Ba,Ca,Sr)$
$(Ba,Ca,Sr)Zn_{13}$	D23	D23 Prototype-NaZn13	$(Ba,Ca,Sr)Zn_{13}$
$Ca(Cu,Ni,Zn)_5$	D2d	D2d Prototype-CaCu5	$(Ba,Ca,Sr)(Ag,Cu,Ni,Zn)_5$
$(Bi,Sn)_2S_3$	D58	D58 Prototype-Sb2S3	Bi_2S_3, Sb_2S_3
Cd_3As_2, Zn_3As_2	D59	D59 Prototype-Zn3P2	Cd_3As_2, Zn_3As_2
Cd_2ZnAs_2	oD59	D59 Prototype-Zn3P2	ternary ordered D59
$(Fe,Ni)_3C_2$	D510	D510 Prototype-Cr3C2	$(Fe,Ni)_3C_2$
In_3Ni_2	D513	D513 Prototype-Al3Ni2	In_3Ni_2
$(Ag,Cu)_5Zn_8$	D82	D82 Prototype-Cu5Zn8	$(Ag,Cu,Fe)_5Zn_8$, γ-NiZn, $(Ag,Cu)_5Cd_8$
"$InAg_2$"	D83	D83 Prototype-Cu9Al4	In_5Ag_8
ε-$Cu_{15}Si_4$	D86	D86 Prototype-Cu15Si4	ε-$Cu_{15}Si_4$

Fe_5Si_3	D88	D88 Prototype-Mn5Si3	Fe_5Si_3
(Fe-Ni) pentlandite	D89	D89 Prototype-Co9S8	(Fe-Ni) pentlandite
$Ca_5(Ag,Zn,Si,Sn,Ga)_3$ $Sr_5(Pb,Sn)_3$	D8l	D8l Prototype-Cr5B3	Ca_5Si_3, Ca_5Sn_3, Ca_5Zn_3, Ca_5Ag_3, Ca_5Ga_3, Sr_5Pb_3, Sr_5Sn_3
Ni_3S_4, $NiFe_2S_4$	H11	H11 Prototype-Fe3O4	Ni_3S_4(polydymite), $NiFe_2S_4$(violarite)
$Ni_3(Fe,Ge,Si)$ $L1_2$	L12c	L12-FCC!FCC-A1	Ni_3Fe, Ni_3Si, Ni_3Ge, Si_3Ni
$InAg_3$ $L1_2$	L12d	L12d Prototype-AuCu3	$InAg_3$
Ni_3Ga	L12e	L12e Prototype-AuCu3	Ni_3Ga
Cu_7In_3	aP40	aP40 Prototype-Cu7In3	Cu_7In_3
Cu_2S, Cu_2Se	cF44	cF44 Prototype-Cu2Se	Cu_2S(digenite/bornite), Cu_2Se(berzelianite), gamma-Ag_2S, beta1-Ni_2Te(ht)
Argentite-Ag_2S	cI20	cI20 Prototype-Ag2S	Ag_2S, Ag_2Se
$Ga_7(Ba,Sr)_8$	cP60	cP60 Prototype-Ba8Ga7	$Ga_7(Ba,Sr)_8$
Ni_2S-β_2	cP_	beta2	Ni_2S-beta2
δ-CuZn	hP3	CuZn_delta	δ-CuZn, ζ-AgCd, ε-$AgCd_3$
Fe_2Si	hP6	hP6 Prototype-Ni2Al	Fe_2Si
BaCu	hP8	hP8 Prototype-BaCu	BaCu, SrCu
β-Bi_2Te	hP9	hP9 Prototype-Sb2Te	β-Bi_2Te
Cu_2S chalcocite(ht)	hP16	hP16 Prototype-Cu2S	Cu_2S chalcocite(ht)
SbSn	hR3	hR3 Prototype-"SbSn"	SbSn
Bi_2Te_3	hR15	hR15 Prototype-Bi2Te3	Bi_2Te_3
ζ-$Zn_{13}Fe$	mC28	mC28 Prototype-Zn13Co	ζ-$Zn_{13}Fe$
Ni_5Sb_2	m28C	mS28 Prototype-Ni5Sb2	Ni_5Sb_2
Acanthite-Ag_2S	m12P	m12P Prototype-Ag2S	Acanthite-Ag_2S
Ni_3Sn_4	mC14	mS14 Prototype-Ni3Sn4	Ni_3Sn_4
$ZnAs_2$	mP24	mP24 Prototype-ZnAs2	$ZnAs_2$
η_2-AlCu, θ-InCu	mS20	eta2 Prototype-AlCu	η_2-AlCu, θ-InCu
GeAs, SiAs	mS24	mS24 Prototype-SiAs	(Ge,Si)(As,P)
ζ'-$Ni_{13}In_9$, $Ni_{13}Ga_9$	mS44	mS44 Prototype-Ni13Ga9	ζ'-$Ni_{13}In_9$, $Ni_{13}Ga_9$
Ag_3Sb	oP4a	oP4 Prototype-Ag3Sb	Ag_3Sb
naumannite-Ag_2Se	o12P	oP12 Prototype-Ag2Se	naumannite-Ag_2Se
Ni_3Sn_2	o20P	oP20 Prototype-Ni3Sn2	Ni_3Sn_2
$SiAs_2$, $GeAs_2$	oP24	oP24 Prototype-GeAs2	(Ge,Si)As_2
$BaSi_2$, $SrGe_2$	o24P	oP24 Prototype-BaSi2	$BaSi_2$, $SrGe_2$
$BaSi_2$, $SrGe_2$	oP52	oP52 Prototype-Ca7Sn6	$Ca_7(Ge,Sn)_6$
PbSr	oS8	oS8 Prototype-Tl	GaCa, GaSr, PbSr
AgCuS stromayerite	o12S	oS12	AgCuS
Ni_5Ga_3	o16S	oS16 Prototype-Pt5Ga3	Ni_5Ga_3
α-Ni_7S_6	oS56	oS56 Prototype-Ni7S6	Ni_7S_6
Godlevskite Ni_9S_8	oC68	oC68 Prototype-Ni9S8	Ni_9S_8
$CdAs_2$	t12l	tI12 Prototype-CdAs2	$CdAs_2$

α-Cd_3As_2, α-Zn_3As_2	i160	tI160 Prototype-Cd3As2	α-Cd_3As_2, α-Zn_3As_2
α-$FeSi_2$(high-T)	tP3	Ferdisilicite Prototype-FeSi2	α-$FeSi_2$(high-T)
α'-Cd_3As_2	p160	tP160 Prototype-Zn3As2	α'-Cd_3As_2
γ_1-FeZn	Gam1	FeZn-Gamma-1	$Fe_7(Fe,Zn)_6Zn_{38}$
δ_1-FeZn	FeZ2	FeZn-delta-1	$Fe(Al,Fe,Zn)_3Zn_{13}$
$CuNi_2S_6$	Vill	Villamaninite	$(Cu,Ni)S_2$
Heazlewoodite-Ni_3S_2	Heaz	Heaz Prototype-Ni3S2	Ni_3S_2
Chalcocite-Cu_2S(lt)	Chal	Chalcocite	Cu_2S(lt)
$Cu_{1.95}S$(djurleite)	Djur	Djurleite	$Cu_{1.95}S$
Iss-$CuMeS_{2-x}$	CuMS	iss_CuMeS2-x	non-stoichiometric solid solution $[Cu,Ni,Fe]_2S$
$(Fe,Ni)_3Te_2$	M3T2	M3T2	$(Fe,Ni)_3Te_2$

Table 3: Pure compounds and their phases in the FSlead 8.3 Database

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FSlead 8.3 database
415 compounds,  618 phases

Ag                          PB83   S1   S2   S3   S4   S5   L
Ag11Hg15                    PB83   S
Ag11Hg9                     PB83   S
Ag2Ba                       PB83   S
Ag2Ba3                      PB83   S
Ag2Ca                       PB83   S
Ag2Ga                       PB83   S
Ag2O                        PB83   S
Ag2S                        PB83   S1   S2   S3
Ag2Se                       PB83   S1   S2
Ag2Sr                       PB83   S
Ag2Sr3                      PB83   S
Ag2Te                       PB83   S1   S2   S3
Ag3Ca5                      PB83   S
Ag3CuS2                     PB83   S
Ag3Ga2                      PB83   S
Ag3Sb                       PB83   S
Ag4Sr                       PB83   S
Ag5Ba                       PB83   S
Ag5Cu3S4                    PB83   S
Ag5Sr                       PB83   S
Ag5Sr3                      PB83   S
Ag5Te3                      PB83   S1   S2
Ag7Ca2                      PB83   S
Ag8SnS6                     PB83   S1   S2
Ag9Ca2                      PB83   S
AgBa                        PB83   S
AgCa                        PB83   S
AgCa3                       PB83   S
AgCd                        PB83   S
AgCuS                       PB83   S
AgSr                        PB83   S
As                          PB83   S1   S2   S3   S4   S5   L
'As2Cu5'                    PB83   S                              (As)2.058(Cu)4.942
As2S3                       PB83   S
As2S5                       PB83   S
As2Te3                      PB83   S
As4S3                       PB83   S1   S2
As4S4                       PB83   S1   S2
AsCu8                       PB83   S
AsIn                        PB83   S
Au                          PB83   S1   S2   S3   L
Au2Bi                       PB83   S
Au2Pb                       PB83   S
Au3In                       PB83   S
'Au4Zn5'                    PB83   S                                (Au)3.96(Zn)5.04
Au5Zn3                      PB83   S
Au7Ga2                      PB83   S
Au7Ga3                      PB83   S
Au7In3                      PB83   S
'Au8Ga2'                    PB83   S                          (Au)7.89476(Ga)2.10526
AuGa                        PB83   S
AuGa2                       PB83   S
AuIn                        PB83   S
AuIn2                       PB83   S
AuSb2                       PB83   S
AuSn                        PB83   S
AuSn2                       PB83   S
AuSn4                       PB83   S
AuTe2                       PB83   S
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AuZn3	PB83	S				
Ba	PB83	S1	S2	S3	L	
Ba10Ga	PB83	S				
Ba2Si	PB83	S				
Ba2Zn	PB83	S				
Ba3Si4	PB83	S				
Ba5Ga6	PB83	S				
Ba5Si3	PB83	S				
Ba8Ga7	PB83	S				
BaC2	PB83	S1	S2			
BaCu	PB83	S				
BaCu13	PB83	S				
BaGa2	PB83	S				
BaGa4	PB83	S				
BaGe2	PB83	S				
BaH2	PB83	S1	S2			
BaSi	PB83	S				
BaSi2	PB83	S				
BaZn	PB83	S				
BaZn13	PB83	S				
BaZn2	PB83	S				
BaZn5	PB83	S				
Bi	PB83	S1	S2	S3	S4	L
Bi2S3	PB83	S				
Bi2Te	PB83	S				
Bi3In5	PB83	S				
Bi3Ni	PB83	S				
Bi4Te3	PB83	S				
BiIn	PB83	S				
BiIn2	PB83	S				
C	PB83	S1	S2	L		
Ca	PB83	S1	S2	S3	L	
Ca11Ga7	PB83	S				
Ca14Si19	PB83	S				
Ca25Ga59	PB83	S				
Ca28Ga11	PB83	S				
Ca2Cu	PB83	S				
Ca2Ge	PB83	S				
Ca2Ni7	PB83	S				
Ca2Pb	PB83	S				
Ca2Si	PB83	S				
Ca2Sn	PB83	S				
Ca3Ga5	PB83	S				
Ca3Ga8	PB83	S				
Ca3Si4	PB83	S				
Ca3Zn	PB83	S				
Ca5Ga3	PB83	S				
Ca5Ge3	PB83	S				
Ca5Pb3	PB83	S				
Ca5Si3	PB83	S				
Ca5Zn3	PB83	S				
Ca7Ge6	PB83	S				
Ca7Sn6	PB83	S				
CaC2	PB83	S1	S2	S3	S4	L
CaCu	PB83	S				
CaCu5	PB83	S				
CaGa	PB83	S				
CaGa2	PB83	S1	S2			
CaGa4	PB83	S1	S2			
CaGe2	PB83	S				
CaH2	PB83	S				
CaNi2	PB83	S				
CaNi3	PB83	S				
CaNi5	PB83	S				
CaO	PB83	S				

CaPb	PB83	S						
CaPb3	PB83	S						
CaS	PB83	S						
CaSi	PB83	S						
CaSi2	PB83	S						
CaZn	PB83	S						
CaZn11	PB83	S						
CaZn13	PB83	S						
CaZn2	PB83	S						
CaZn3	PB83	S						
CaZn5	PB83	S						
Cd	PB83	S1	S2	S3	S4	L		
Cd10Cu3	PB83	S						
Cd3As2	PB83	S1	S2	S3	S4			
Cd3Cu4	PB83	S						
Cd3In	PB83	S						
Cd5Ni	PB83	S						
Cd8Cu5	PB83	S						
CdAs2	PB83	S						
CdCu2	PB83	S						
CdNi	PB83	S						
CdS	PB83	S						
CdSb	PB83	S						
Cu	PB83	S1	S2	S3	S4	L		
'Cu10Sn3'	PB83	S						(Cu)9.997(Sn)3.003
Cu11Fe2S13	PB83	S						
Cu15Si4	PB83	S						
Cu19Si6	PB83	S						
Cu2O	PB83	S						
Cu2S	PB83	S1	S2	S3	S4			
Cu2Sb	PB83	S						
Cu2Se	PB83	S1	S2					
Cu2SiS3	PB83	S1	S2					
Cu2Te	PB83	S1	S2	S3	S4	S5	S6	
Cu33Si7	PB83	S						
'Cu3As'	PB83	S						(Cu)2.94(As)1.06
Cu3FeS4	PB83	S						
Cu3FeS8	PB83	S						
Cu3Ge	PB83	S						
Cu3Sb	PB83	S1	S2					
Cu3Se2	PB83	S						
Cu3Sn	PB83	S1	S2					
Cu4Fe5S8	PB83	S						
Cu4In	PB83	S						
Cu4Sb	PB83	S						
'Cu4Sn'	PB83	S						(Cu)3.94(Sn)1.06
Cu5Sr	PB83	S						
'Cu6Sb'	PB83	S						(Cu)5.95(Sb)1.05
'Cu6Sn5'	PB83	S						(Cu)5.995(Sn)5.005
Cu7Ga2	PB83	S						
Cu7In3	PB83	S						
'Cu7In4'	PB83	S						(Cu)7.04(In)3.96
Cu7S4	PB83	S						
'Cu7Sb2'	PB83	S						(Cu)6.93(Sb)2.07
Cu8SiS6	PB83	S						
Cu9Fe8S16	PB83	S						
Cu9Fe9S16	PB83	S						
Cu9S8	PB83	S						
Cu9Si2	PB83	S						
CuAsS	PB83	S						
CuFe2S3	PB83	S						
CuFeS2	PB83	S						
CuH	PB83	S						
CuNi2S6	PB83	S						
CuO	PB83	S						

CuS	PB83	S							
CuS2	PB83	S1	S2						
CuSe	PB83	S1	S2	S3					
CuSe2	PB83	S1	S2						
CuSr	PB83	S							
CuTe	PB83	S							
Fe	PB83	S1	S2	S3	S4	S5	S6	S7	L
Fe10S11	PB83	S							
Fe11S12	PB83	S							
Fe2O3	PB83	S							
Fe2S	PB83	S1	S2	S3					
Fe2S3	PB83	S							
Fe2Si	PB83	S							
Fe2SiS4	PB83	S							
Fe3C	PB83	S1	S2						
Fe3C2	PB83	S							
Fe3O4	PB83	S1	S2	S3	S4				
Fe3S4	PB83	S1	S2						
Fe3Si	PB83	S							
Fe3Sn2	PB83	S							
Fe5C2	PB83	S1	S2						
Fe5Si3	PB83	S1	S2						
Fe5Sn3	PB83	S1	S2	S3					
Fe60Te71	PB83	S							
Fe7C3	PB83	S							
Fe7S6	PB83	S							
'Fe7S8'	PB83	S							(Fe)7.016(S)8
Fe9S10	PB83	S							
Fe9S8	PB83	S1	S2						
FeS	PB83	S1	S2						
FeS2	PB83	S1	S2						
FeSb	PB83	S							
FeSb2	PB83	S							
FeSe2	PB83	S							
FeSi	PB83	S1	S2	S3					
FeSi2	PB83	S1	S2	S3					
FeSn	PB83	S1	S2						
FeSn2	PB83	S							
FeTe	PB83	S							
FeTe2	PB83	S1	S2						
Ga	PB83	S1	S2	S3	S4	S5	L		
Ga2Cu	PB83	S							
Ga2Te3	PB83	S							
Ga2Te5	PB83	S							
Ga3Te4	PB83	S							
Ga4Cu9	PB83	S							
Ga6SnTe10	PB83	S							
GaAs	PB83	S							
GaSb	PB83	S							
GaTe	PB83	S							
Ge	PB83	S1	S2	S3	L				
GeAs	PB83	S							
GeAs2	PB83	S							
GeCa	PB83	S							
GeTe	PB83	S							
H	PB83	S	L						
Hg	PB83	S1	S2	S3	S4	L			
Hg3Zn	PB83	S							
Hg6Cu7	PB83	S							
HgPb2	PB83	S							
HgS	PB83	S1	S2						
HgSn38	PB83	S							
HgSn4	PB83	S							
HgSn7	PB83	S							
HgZn2	PB83	S							

HgZn3	PB83	S					
In	PB83	S1	S2	S3	L		
In2Ag	PB83	S					
In2Ca	PB83	S					
In2Se3	PB83	S1	S2	S3	S4		
In4Se3	PB83	S					
In5Se7	PB83	S					
In6Se7	PB83	S					
In9Se11	PB83	S					
InAg3	PB83	S					
InCa3	PB83	S					
InSb	PB83	S					
InSe	PB83	S					
Ni	PB83	S1	S2	S3	S4	S5	L
Ni11As8	PB83	S					
Ni13Ga9	PB83	S					
Ni20Te17	PB83	S					
Ni23C6	PB83	S					
Ni2Ga	PB83	S					
Ni2Ga3	PB83	S					
Ni2Ge	PB83	S1	S2				
Ni2In	PB83	S					
Ni2In3	PB83	S					
Ni2S	PB83	S					
Ni2Si	PB83	S1	S2				
Ni2Te	PB83	S					
Ni3Ga	PB83	S					
Ni3Ga4	PB83	S					
Ni3Ga7	PB83	S					
Ni3Ge	PB83	S					
Ni3In	PB83	S					
Ni3In7	PB83	S					
Ni3S2	PB83	S					
Ni3S4	PB83	S					
Ni3Sb	PB83	S1	S2				
Ni3Si	PB83	S1	S2				
Ni3Si2	PB83	S					
Ni3Sn	PB83	S1	S2				
Ni3Sn2	PB83	S					
Ni52Te40	PB83	S					
Ni5As2	PB83	S					
Ni5Ga3	PB83	S					
Ni5Ge2	PB83	S					
Ni5Ge3	PB83	S					
Ni5Sb2	PB83	S					
Ni5Si2	PB83	S					
Ni7S6	PB83	S					
Ni9S8	PB83	S1	S2				
NiAs	PB83	S					
NiAs2	PB83	S1	S2				
NiAsS	PB83	S					
NiFe2S4	PB83	S					
NiGa	PB83	S1	S2				
NiGe	PB83	S1	S2				
NiIn	PB83	S					
NiO	PB83	S					
NiS	PB83	S1	S2				
NiS2	PB83	S					
NiSb	PB83	S					
NiSb2	PB83	S					
NiSe2	PB83	S					
NiSi	PB83	S1	S2				
NiSi2	PB83	S					
NiSn	PB83	S1	S2				
NiSr	PB83	S					

NiTe	PB83	S							
NiTe2	PB83	S							
NiZn8	PB83	S							
Pb	PB83	S1	S2	S3	S4	S5	S6	S7	L
Pb2Au	PB83	S							
Pb3Au	PB83	S							
Pb3O4	PB83	S							
Pb3Sr	PB83	S							
Pb3Sr2	PB83	S							
Pb3Sr5	PB83	S							
Pb4Sr5	PB83	S							
Pb5Sr3	PB83	S							
PbO	PB83	S1	S2						
PbO2	PB83	S							
PbS	PB83	S							
PbSe	PB83	S							
PbSr	PB83	S							
PbSr2	PB83	S							
PbTe	PB83	S							
S	PB83	S1	S2	S3	S4	S5	L		
Sb	PB83	S1	S2	S3	L				
Sb2S3	PB83	S							
Sb2Se3	PB83	S							
Sb2Sn3	PB83	S							
Sb2SnZn	PB83	S							
SbFe2	PB83	S							
SbNi2	PB83	S							
Se	PB83	S1	S2	L					
Si	PB83	S1	S2	S3	S4	S5	S6	S7	L
Si2Te3	PB83	S1	S2						
SiAs	PB83	S							
SiAs2	PB83	S							
SiC	PB83	S1	S2	S3	S4	S5	S6		
SiO2	PB83	S1	S2	S3	S4	S5	S6	S7	S8
SiS	PB83	S							
SiS2	PB83	S							
SiTe2	PB83	S1	S2						
Sn	PB83	S1	S2	S3	S4	S5	L		
Sn20Ca31	PB83	S							
Sn23Ca36	PB83	S							
Sn3Ca	PB83	S							
Sn3Ca5	PB83	S							
Sn3Sr	PB83	S							
Sn3Sr5	PB83	S							
Sn4As3	PB83	S							
Sn4Sr	PB83	S							
Sn5Sr3	PB83	S							
SnAg3	PB83	S							
SnAs	PB83	S							
SnCa	PB83	S							
SnFe2	PB83	S							
SnNi2	PB83	S							
SnS	PB83	S1	S2						
SnS2	PB83	S							
SnSe	PB83	S1	S2						
SnSe2	PB83	S							
SnSr	PB83	S							
SnSr2	PB83	S							
SnTe	PB83	S							
Sr	PB83	S1	S2	S3	L				
Sr13Cd58	PB83	S							
Sr2Ge	PB83	S							
Sr2Si	PB83	S							
Sr5Cd3	PB83	S							
Sr5Ge3	PB83	S							

Sr5Si3	PB83	S									
Sr8Ga7	PB83	S									
SrC2	PB83	S1	S2								
SrCd	PB83	S									
SrCd11	PB83	S									
SrCd2	PB83	S									
SrCd6	PB83	S									
SrGa2	PB83	S									
SrGa4	PB83	S									
SrGe	PB83	S									
SrGe2	PB83	S									
SrH2	PB83	S1	S2								
SrSi	PB83	S									
SrSi2	PB83	S1	S2								
SrZn	PB83	S									
SrZn13	PB83	S									
SrZn2	PB83	S									
SrZn5	PB83	S1	S2								
Te	PB83	S1	S2	L							
Tl	PB83	S	L								
Zn	PB83	S1	S2	S3	S4	S5	S6	S7	...	L1	L
Zn3As2	PB83	S1	S2	S3	S4						
Zn3Sb2	PB83	S									
Zn4Sb3	PB83	S1	S2								
Zn5Sb3	PB83	S									
ZnAs2	PB83	S									
ZnO	PB83	S									
ZnS	PB83	S1	S2								
ZnSb	PB83	S									
ZnTe	PB83	S									

Modeling

In the thermodynamic assessments, the liquid phase has been described using the Modified Quasichemical Model in the Pair Approximation (MQMPA) in order to evaluate short-range order (SRO) between the elements. Within this model, it is possible to force some binary interactions to respect a Bragg-Williams (BW) type of configurational entropy (which neglects SRO for the specific binary interactions). This makes possible the incorporation of several optimized binary systems coming from the CALPHAD community where a Bragg-Williams configurational entropy with a Redlich-Kister-Muggianu (R-K) polynomial expression of the excess Gibbs energy are typically used. For each binary system in the present database, the type of configurational entropy is given in the "List of optimized systems and calculated binary phase diagrams". In many cases, an important part of the experimental information on a given binary system is associated to solid-liquid equilibria. Hence a thermodynamic model for the liquid phase that takes into account SRO can permit a better fit of the thermodynamic and phase equilibrium data for the important solid phases that constitute the alloy.

Most solid solution phases have been described using sublattice models based on the Compound Energy Formalism (long-range order (LRO)) which include interstitials and vacancies where appropriate. The FCC_A1 and BCC_B2 solid solutions have C as an interstitial species. Please note that HCP_A3 does not have C as an interstitial species.

Table 4: Optimized binary systems of the FSlead 8.3 Database (quality → Figure 1)

System	Liquid Model	Comments	Source
Ag - As	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Ag - Au	MQMPA (Pair Fraction Exp.)	BW liquid converted to MQMPA, no ordered phases	M. Hassam, J. Agren, M.Gaune-Escard, J.P.Bros, Metall. Trans. 21A (1990) 1877-1884.
Ag - Ba	Bragg-Williams R-K Polynomial		SGTE
Ag - Bi	MQMPA (Pair Fraction Exp.)		J. Wang, CRCT, 2015
Ag - C	MQMPA (Pair Fraction Exp.)	graphite saturation	P. Chartrand, CRCT, 2014
Ag - Ca	MQMPA (Pair Fraction Exp.)		J. Wang, I.-H. Jung and P. Chartrand, "Thermodynamic modeling of then Ag-(Ca, Li, Zn) and Ca-(In, Li) binary systems", 2014
Ag - Cd	Bragg-Williams R-K Polynomial		Fisher et al., CALPHAD, 2019, 64, 292-305
Ag - Cu	MQMPA (Pair Fraction Exp.)		J. Wang, CRCT, 2015
Ag - Fe	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2014
Ag - Ga	Bragg-Williams R-K Polynomial	Stoichiometric Ag_2Ga	W. Gierlotka, D. Jendrzejczyk-Handzlik / Journal of Alloys and Compounds 509 (2011) 38–42
Ag - Ge	Bragg-Williams R-K Polynomial		P.Y. Chevalier, Thermochimica Acta 130 (1988) 25-32.
Ag - H	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Ag-rich region	P. Chartrand, CRCT, 2014
Ag - Hg	Bragg-Williams R-K Polynomial		Y. Liu et al. / Thermochimica Acta 547 (2012) 83–88
Ag - In	MQMPA (Pair Fraction Exp.)		J. WANG, P. HUDON, D. KEVORKOV, P. CHARTRAND, I.-H. JUNG and M. MEDRAJ, "Thermodynamic and Experimental Study of the Mg-Sn-Ag-In Quaternary System", *Journal of Phase Equilibria and Diffusion*, Volume 35, Issue 3, (June 2014), pp 284-31.
Ag – Ni	MQMPA (Pair Fraction Exp.)		J. Wang, CRCT, 2015
Ag - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database (or SGPS) Valid for Ag-rich region	P. Chartrand, CRCT, 2021
Ag – Pb	Bragg-Williams R-K Polynomial		Leo Lukas (Unpublished work, 2000) based on original work of Zimmermann (B. Zimmerman, Thesis, University of Stuttgart 1976 "Optimisation by experimental and calculation of the binary and ternary systems of Ag, Bi, Pb and Tl").
Ag - S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2018
Ag - Sb	Bragg-Williams R-K Polynomial	Stoichiometric Ag_3Sb	E. Zoro, C. Servant, B. Legendre, Journal of Phase equilibria and Diffusion, 2007, 28, 250-257
Ag - Se	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Ag - Si	Bragg-Williams R-K Polynomial		P.Y. Chevalier, Thermochimica Acta 113 (1988) 33-41.
Ag - Sn	MQMPA (Pair Fraction Exp.)		J. WANG, P. HUDON, D. KEVORKOV, P. CHARTRAND, I.-H. JUNG and M. MEDRAJ, "Thermodynamic and Experimental Study of the Mg-Sn-Ag-In Quaternary System", *Journal of Phase Equilibria and Diffusion*, Volume 35, Issue 3, (June 2014), pp 284-31
Ag - Sr	MQMPA (Pair Fraction Exp.)		Jian Wang, Ph.D. Thesis, Ecole Polytechnique, Montreal, 2014
Ag - Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
Ag - Tl	Bragg-Williams R-K Polynomial		H. L. Lukas, unpublished reassessment based on data set collected in Zimmermanns thesis 1976 (1994).
Ag - Zn	MQMPA (Pair Fraction Exp.)		J. Wang, I.-H. Jung and P. Chartrand, "Thermodynamic modeling of then Ag-(Ca, Li, Zn) and Ca-(In, Li) binary systems", submitted 2014
As - Au	Bragg-Williams R-K Polynomial		P.J.Spencer, June 1998

As - Bi	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2018
As - Cd	MQMPA (Pair Fraction Exp.)		O. Kidari, M.Sc.Thesis, CRCT, 2023
As - Cu	Bragg-Williams R-K Polynomial	Stoichiometric Cu_3As	M.Hamalainen, private communication
As - Fe	Bragg-Williams R-K Polynomial	Missing stoichiometric compounds	P. J. Spencer, 2008
As - Ga	Bragg-Williams R-K Polynomial		C Chatillon, I. Ansara, A. Watson and B. B. Argent: CALPHAD, 1990, 14(2), 203-14.
As - Ge	Bragg-Williams R-K Polynomial		I. Ansara and D. Dutarte: CALPHAD, 1984, 8(4), 323-342
As - In	Bragg-Williams R-K Polynomial		C.Chatillon, I.Ansara, A.Watson, B.B.Argent, Calphad 14 (1990) 203-214
As - Ni	Bragg-Williams R-K Polynomial		S.Uhland et al., CALPHAD 25[1] (2001) 109-124
As - Pb	Bragg-Williams R-K Polynomial		M.Hamalainen, private communication
As - S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2021; from Prostakova, Shishin, Jak 2021 (change in g0 sulfur)
As - Sb	Bragg-Williams R-K Polynomial		H.Ohtani, Calphad 18 (1994) 196
As - Si	MQMPA (Pair Fraction Exp.)		P.-J. Spencer, 2006
As - Sn	Bragg-Williams R-K Polynomial		L.Wu et al., CALPHAD (74) 2021, 102296
As - Te	MQMPA (Pair Fraction Exp.)	Approx..	P. Chartrand, CRCT, 2018
As - Zn	MQMPA (Pair Fraction Exp.)		P.Chartrand, CRCT, 2022
Au - Bi	Bragg-Williams R-K Polynomial		P.Y.Chevalier, Thermochimica Acta 136 (1988) 15-24
Au - C	Bragg-Williams R-K Polynomial		P.J. Spencer (2007)
Au - Cu	Bragg-Williams R-K Polynomial	No ordered $L1_2$ & $L1_0$ phases	B.Sundman, S.G.Fries, A.Oates, Calphad 22 (1998) 335-354
Au – Fe	Bragg-Williams R-K Polynomial		Y.Liu et al., CALPHAD 476 (2009) 79-83
Au - Ga	Bragg-Williams R-K Polynomial		J. Wang, Y. Liu, L. Liu, H. Zhou, Z. Jin, Calphad 35(2) (2011) 242-248
Au - Ge	Bragg-Williams R-K Polynomial		P. Y. Chevalier: Thermochimica Acta, 1989, 141, 217-22
Au - In	Bragg-Williams R-K Polynomial		I.Ansara, J.P.Nabot, Calphad 16 (1992) 13-18
Au – Ni	Bragg-Williams R-K Polynomial		J. Wang et al., CALPHAD (2005) pp.263-268
Au - Pb	Bragg-Williams R-K Polynomial		J.P.Nabot, Thesis, Grenoble,1986
Au - Sb	Bragg-Williams R-K Polynomial		E.Zoro, C.Servant and B.Legendre, J.Thermal Anal. & Calo., 90[2] (2007) pp.347-353
Au - Si	Bragg-Williams R-K Polynomial		SGTE
Au - Sn	Bragg-Williams R-K Polynomial	dhcp missing in Au-rich region	P.Y.Chevalier, Thermochimica Acta 130 (1988) 1-13
Au – Te	Bragg-Williams R-K Polynomial		Y. Feutelais, D. Mounai, J. R. Didry, B. Legendre: J. Phase Equil., 1994, 15(4), 380-385 (modified by SGTE)
Au - Tl	Bragg-Williams R-K Polynomial		P.Y. Chevalier: Thermochimica Acta, 1989, 155, 211-225
Au - Zn	Bragg-Williams R-K Polynomial	Intermetallic solutions missing – liquid and FCC-A1 only	COST-531
Ba - Ca	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2004
Ba - Cu	Bragg-Williams R-K Polynomial		SGTE
Ba - Fe	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Ba - Ga	Bragg-Williams R-K Polynomial		X.Li et al., CALPHAD 43 (2013) 52-60
Ba - H	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Ba – BaH_2	P. Chartrand, 2016
Ba - Ni	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2016
Ba - Si	MQMPA (Pair Fraction Exp.)		J.P. Harvey 2005

Ba – Sr	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Ba - Zn	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014 modified from J.P. Spencer 2006
Bi – Cd	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Bi – Cu	MQMPA (Pair Fraction Exp.)		J. Wang, CRCT, 2015
Bi – Fe	Bragg-Williams R-K Polynomial		from FSstel
Bi – Ga	MQMPA (Pair Fraction Exp.)		B.Kumar et al., CALPHAD 74 (2021)
Bi – Ge	Bragg-Williams R-K Polynomial		P. Y. Chevalier: Thermochimica Acta, 1988, 132, 111-116
Bi - Hg	Bragg-Williams R-K Polynomial		Unpublished assessment from S. A. Mucklejohn (SGTE)
Bi – In	Bragg-Williams R-K Polynomial		D.Boa, I.Ansara, Thermochimica Acta 314 (1998) 79-86
Bi - Ni	MQMPA (Pair Fraction Exp.)		J. Wang, CRCT, 2015
Bi - Pb	Bragg-Williams R-K Polynomial		D.Boa, I.Ansara, Thermochimica Acta 314 (1998) 79-86
Bi – S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2018
Bi – Sb	MQMPA (Pair Fraction Exp.)		P. Chartrand 2018 modified from P.J. Spencer, 2006
Bi – Si	MQMPA (Pair Fraction Exp.)		P.J. Spencer, 2006
Bi – Sn	MQMPA (Pair Fraction Exp.)		J. Wang, CRCT, 2015
Bi – Te	MQMPA (Pair Fraction Exp.)		B.Kumar et al. (Paliwal) CALPHAD 74 (2021)
Bi – Tl	Bragg-Williams R-K Polynomial		unpublished assessment of H.L. Lukas based on an earlier assessment of Zimmermann B., Henig E. T., Lukas H. L.: Z. Metallkde., 1976, 67(12), 815-820.
Bi – Zn	Bragg-Williams R-K Polynomial		C.Girard, Thesis, Marseille, 1985
C – Ca	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
C – Cu	MQMPA (Pair Fraction Exp.)		S. Shubhank and Y.-B.Kang CALPHAD 45 (2014) 127–137
C – Fe	MQMPA (Pair Fraction Exp.)	Incl. metastable carbides	M-S Kim, Y-B Kang JPE 2015
C – Ge	MQMPA (Pair Fraction Exp.)		P.Chartrand, 2014
C – Ni	Bragg-Williams R-K Polynomial		B. J. Lee: CALPHAD, 1992, 16(2), 121-149
C - Pb	Bragg-Williams R-K Polynomial		unpublished assessment of T. G. Chart, NPL 1987
C - S	Bragg-Williams R-K Polynomial	Gaseous species must be taken from FACTPS Database	Fahmi TAFWIDLI and Youn-Bae KANG, ISIJ, 2017
C - Sb	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
C - Si	MQMPA (Pair Fraction Exp.)		M-K Paek, Y-B Kang CALPHAD 46 (2014) 92–102
C - Sn	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2007
Ca - Cu	MQMPA (Pair Fraction Exp.)		Jian Wang et al., Calphad 75 (2021) 102325
Ca - Fe	MQMPA (Pair Fraction Exp.)		S.Cui, M.Paliwal and I.-H. Jung, MetTrans 2014
Ca - Ga	Bragg-Williams R-K Polynomial		X.Li et al., CALPHAD 43 (2013) 52-60
Ca - Ge	MQMPA (Pair Fraction Exp.)		P.Chartrand, CRCT, 2023
Ca - H	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Ca – CaH_2	J.-P. HARVEY and P. CHARTRAND, "Modeling the Hydrogen Solubility in Liquid Aluminum Alloys", *Metallurgical and Materials Transactions. B, Process Metallurgy and Materials Processing Science*, 41(4), p. 908-924, 2010.
Ca - In	MQMPA (Pair Fraction Exp.) + BW		J. Wang, I.-H. Jung and P. Chartrand, "Thermodynamic modeling of then Ag-(Ca, Li, Zn) and Ca-(In, Li) binary systems", submitted 2014
Ca - Ni	Bragg-Williams R-K Polynomial		M. Medraj, 2006
Ca - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Ca - CaO	P. Chartrand, 2000

Ca - Pb	Bragg-Williams R-K Polynomial		V.P.Itkin and C.B.Alcock, J. Phase Equilib. 1992, pp.162-169
Ca - Si	MQMPA (Pair Fraction Exp.)		M. HEYRMAN and P. CHARTRAND, "Thermodynamic Evaluation and Optimization of the Ca-Si System", *J. Phase Equilibria and Diffusion*, 27 [3], 220-230, 2006
Ca - Sn	MQMPA (Pair Fraction Exp.)		Jian Wang, Ph.D. Thesis, Ecole Polytechnique, Montreal, 2014
Ca - Sr	MQMPA (Pair Fraction Exp.)		Jian Wang, Ph.D. Thesis, Ecole Polytechnique, Montreal, 2014
Ca - Zn	MQMPA (Pair Fraction Exp.)		P. Spencer, A.D. Pelton., Y.-B. Kang, P. Chartrand, and C. Fuerst, Calphad 32 (2007), pp. 423-431
Cd – Cu	Bragg-Williams R-K Polynomial		X-M Chen, L-B Liu, L-G Zhang, H. Bo and Z-P Jin Trans Nonferrous Met Soc. China, 20 (2010) 649-654
Cd – Fe	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cd - Ga	Bragg-Williams R-K Polynomial		Zakulski W., Moser Z., Rzyman K., Lukas H. L., Fries S. G., Sikiennik M., Kaczmarczyk R., Castanet R.: J. Phase Equil., 1993, 14(2), 184-196.
Cd – Ge	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cd – Hg	Bragg-Williams R-K Polynomial		Jang J., Silk N. J., Watson A., Bryant A. W., Chart T. G., Argent B. B.: CALPHAD, 1995, 19(3), 415-430
Cd - In	Bragg-Williams R-K Polynomial		Zakulski W., Moser Z., Rzyman K., Lukas H. L., Fries S. G., Sikiennik M., Kaczmarczyk R., Castanet R.: J. Phase Equil. 1993,14(2),184-196
Cd - Ni	Bragg-Williams R-K Polynomial		H.Azza, N.Selhaoui, L. Bouirden, Int. J. Adv. Res. in Phys. Sc. 5[5] (2018) pp.17-23
Cd – Pb	Bragg-Williams R-K Polynomial		W. Zakulski, Z. Moser: J. Phase Equilib, 1995, 16(3), 239-242. W. Zakulski, Z. Moser: J. Phase Equilib, 1995, 16(6), 484
Cd – S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2018
Cd – Sb	Bragg-Williams R-K Polynomial		L. A. Zabdyr: CALPHAD 1997, 21(3), 349-358.
Cd - Si	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cd – Sn	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cd - Sr	Bragg-Williams R-K Polynomial		C.Zhang et al., CALPHAD 42 (2013) 6-12
Cd – Tl	Bragg-Williams R-K Polynomial		Y. Liu et al. / Journal of Alloys and Compounds 473 (2009) 60–64
Cd - Zn	Bragg-Williams R-K Polynomial		L. A. Zabdyr: CALPHAD 1997, 21(3), 349-358
Cu - Fe	MQMPA (Pair Fraction Exp.)		Shubhank and Y-B. Kang, CALPHAD 2014
Cu - Ga	Bragg-Williams R-K Polynomial	Missing Cu_9Ga_4 γ_1, γ_2, γ_3 solid solutions	Li et al., CALPHAD 32(2) (2008), 447-453
Cu - Ge	Bragg-Williams R-K Polynomial		Wang et al. J.Alloys Cmpds 2010
Cu - H	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Cu - CuH	J.-P. HARVEY and P. CHARTRAND, "Modeling the Hydrogen Solubility in Liquid Aluminum Alloys", *Metallurgical and Materials Transactions. B, Process Metallurgy and Materials Processing Science*, 41(4), p. 908-924, 2010.
Cu - Hg	Bragg-Williams R-K Polynomial		Y. Liu et al. / Thermochimica Acta 547 (2012) 83–88
Cu - In	Bragg-Williams R-K Polynomial	γ-CuIn, η-CuIn are missing	C.R.Kao, A.Bolcavage et al, J Phase Equilibria 14 (1993) 22-30
Cu - Ni	MQMPA (Pair Fraction Exp.)		J. Wang, CRCT, 2015
Cu - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Cu – Cu_2O	P. Chartrand, CRCT, 2018
Cu - Pb	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cu - S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P.Waldner, Met.Trans.B, 51B (2020) 805-817
Cu - Sb	Bragg-Williams R-K Polynomial		SGTE 2004
Cu – Se	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cu – Si	MQMPA (Pair Fraction Exp.)		S. Cui and I-H. Jung, CALPHAD, 2017

Cu – Sn	MQMPA (Pair Fraction Exp.)		J. Wang, CRCT, 2015
Cu - Sr	Bragg-Williams R-K Polynomial		SGTE
Cu – Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cu - Tl	Bragg-Williams R-K Polynomial		P.Y.Chevalier, Thermochimica Acta 156 (1989) 383-392
Cu – Zn	Bragg-Williams R-K Polynomial		Liang, Hsiao, Schmid-Fezter CALPHAD, 2015
Fe - H	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Fe-rich region	J.-P. HARVEY and P. CHARTRAND, "Modeling the Hydrogen Solubility in Liquid Aluminum Alloys", *Metallurgical and Materials Transactions. B, Process Metallurgy and Materials Processing Science*, 41(4), p. 908-924, 2010.
Fe - Hg	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Fe - In	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2022, Modified from M.Ohno and K.Yoh, Materials Transactions, Vol. 50, No. 5 (2009) pp. 1202 to 1207
Fe – Ni	Bragg-Williams R-K Polynomial		A.Dinsdale, T.Chart, NPL, unpublished work, 1986: I.Ansara - fcc ordering
Fe - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Fe – FeO **Missing non-stoichiometric wustite-FeO** (considered stoichiometric)	P. Chartrand, CRCT, 2021
Fe – Pb	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Fe - S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P.Waldner & A.D.Pelton, JPE, 26(1) 2005
Fe – Sb	Bragg-Williams R-K Polynomial		C.Li et al., CALPHAD 47 (2014) 23-34
Fe – Si	MQMPA (Pair Fraction Exp.)		S. Cui and I-H Jung CALPHAD 2017
Fe - Sn	Bragg-Williams R-K Polynomial		K.C.H.Kumar, P.Wollants, L.Delaey, Calphad 20 (1996) 139-149 (with modifs from P. Chartrand (2018))
Fe - Sr	Bragg-Williams R-K Polynomial		P. Chartrand, CRCT, 2014
Fe - Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
Fe - Tl	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Fe - Zn	MQMPA (Pair Fraction Exp.)		P. Chartrand (2018) MQMPA calibrated on the solids of Xiong, Du Liu CALPHAD 2009 (later modifications by M.Jacobs)
Ga - Ge	Bragg-Williams R-K Polynomial		I Ansara, J P Bros, M Gambino: CAPHAD, 1979, 3, 225-233
Ga - Hg	Bragg-Williams R-K Polynomial		unpublished assessment of I. Ansara, (1991); from SGTE
Ga - In	Bragg-Williams R-K Polynomial		B. C. Rugg, T. G. Chart: CALPHAD, 1990, 14(2), 115-123
Ga - Ni	Bragg-Williams R-K Polynomial		Z.-M.Cao, X.Shi, W.Xie, I.Ohnuma, K.Ishida & Z.-Y.Qiao, Rare Met. (2015) 34(2) 864-872
Ga - Pb	Bragg-Williams R-K Polynomial		I. Ansara, F. Ajersch: J. Phase Equil., 1991, 12(1), 73-77
Ga - Sb	Bragg-Williams R-K Polynomial		I. Ansara, C. Chatillon, H. L. Lukas, T. Nishizawa, H. Ohtani, K. Ishida, M. Hillert, B. Sundman, B. B. Argent, A. Watson, T. G. Chart, T. Anderson: CALPHAD, 1994, 18(4), 177-222
Ga - Si	Bragg-Williams R-K Polynomial		Olesinski BAPD (6) 1985, 362-364
Ga – Sn	MQMPA (Pair Fraction Exp.)		B.Kumar et al., Metals (2021)
Ga - Sr	Bragg-Williams R-K Polynomial		X.Li et al., CALPHAD 43 (2013) 52-60
Ga - Te	MQMPA (Pair Fraction Exp.)		B.Kumar et al. (Paliwal) CALPHAD 74 (2021)
Ga - Tl	Bragg-Williams R-K Polynomial		I. Katayama et al., T. Iida, Z. Metallknd. 94, 2003, p.1296
Ga - Zn	MQMPA (Pair Fraction Exp.)		Dutkiewicz, J., Moser, Z., Zabdyr, L., Gohil ,D. D., Chart, T. G., Ansara I., Girard, C.: Bull. Alloy Phase Diagrams, 1990, 11(1), 77-82; liquid converted to MQMPA [2022Cha]
Ge - In	Bragg-Williams R-K Polynomial		P. Y. Chevalier: 1989, 155, 227-240
Ge - Ni	Bragg-Williams R-K Polynomial		S.Jin et al./CALPHAD 38 (2012) 23–34

Ge - Pb	Bragg-Williams R-K Polynomial		P. Chevalier, Thermochemica Acta, 1989, vol 155, pp. 227-240
Ge - Sb	Bragg-Williams R-K Polynomial		P. Y. Chevalier, Thermochimica Acta, 1989, 155, 227-240
Ge - Si	Bragg-Williams R-K Polynomial		Z. H. Long, H.S. Liu, Z.P. Jin: J. Alloys Compounds, 479 (2009) 262-267
Ge - Sn	Bragg-Williams R-K Polynomial		Y. Feutelais, B. Legendre, S. G. Fries: CALPHAD, 1996, 20(1), 109-123
Ge - Sr	Bragg-Williams R-K Polynomial		Y. Du et al. / CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 33 (2009) 719–722
Ge – Tl	Bragg-Williams R-K Polynomial		P. Chevalier, Thermochimica Acta, 1989, vol 155, pp. 227-240
Ge - Zn	Bragg-Williams R-K Polynomial		P. Chevalier, Thermochimica Acta, 1989, vol 155, pp. 227-240
H - Ni	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Ni-rich region	J.-P. HARVEY and P. CHARTRAND, "Modeling the Hydrogen Solubility in Liquid Aluminum Alloys", *Metallurgical and Materials Transactions. B, Process Metallurgy and Materials Processing Science*, 41(4), p. 908-924, 2010.
H - Si	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Si-rich region	J.-P. HARVEY and P. CHARTRAND, "Modeling the Hydrogen Solubility in Liquid Aluminum Alloys", *Metallurgical and Materials Transactions. B, Process Metallurgy and Materials Processing Science*, 41(4), p. 908-924, 2010.
H - Sn	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Sn-rich region	P.Chartrand, CRCT, 2023 from M.Sc.Thesis of M.-C.Heuzey, Polytechnique Montreal (in FTmisc)
H - Sr	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Sr – SrH_2	J.-P. HARVEY and P. CHARTRAND, "Modeling the Hydrogen Solubility in Liquid Aluminum Alloys", *Metallurgical and Materials Transactions. B, Process Metallurgy and Materials Processing Science*, 41(4), p. 908-924, 2010.
H - Zn	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Zn-rich region	J.-P. HARVEY and P. CHARTRAND, "Modeling the Hydrogen Solubility in Liquid Aluminum Alloys", *Metallurgical and Materials Transactions. B, Process Metallurgy and Materials Processing Science*, 41(4), p. 908-924, 2010.
Hg - Pb	Bragg-Williams R-K Polynomial		A. Maitre, J. M. Fiorani, M. Vilasi: J. Phase Equilib., 2002, 23(4), 329
Hg – S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2018
Hg – Sn	Bragg-Williams R-K Polynomial		Yee-Wen Yen, Joachim Grobner, Steve C. Hansen, and Rainer Schmid-Fetzer JPE, 24(2), p.151-167, 2003
Hg – Zn	Bragg-Williams R-K Polynomial		S. C. Hansen: CALPHAD, 1998, 22, 359-373.
In - Ni	Bragg-Williams R-K Polynomial		P.Waldner and H.Ipser, Z.Metallk, 93(8) 2002, 825-832
In – Pb	Bragg-Williams R-K Polynomial		D.Boa, I.Ansara, Thermochimica Acta 314 (1998) 79-86
In – Sb	Bragg-Williams R-K Polynomial		T.J.Anderson, Calphad 18 (1994) 206
In – Se	MQMPA (Pair Fraction Exp.)		P.Chartrand, CRCT, 2023 using solids from J.-B.Li, M.-C.Record,J.-C.Tedenac, Z.Metallkd 94 (2003) 4, 381-389
In - Si	Bragg-Williams R-K Polynomial		R.W.Olesinski, N.Kanani, G.J.Abbaschian, Bull.Alloy Phase Diags.6 (1985) 128-130
In – Sn	MQMPA (Pair Fraction Exp.)		J. WANG, P. HUDON, D. KEVORKOV, P. CHARTRAND, I.-H. JUNG, M. MEDRAJ, "Experimental and thermodynamic study of the Mg-Sn-In-Zn quaternary system", *Journal of Alloys and Compounds*, 588 (2014) 75-95
In - Zn;	MQMPA (Pair Fraction Exp.)		J. WANG, P. HUDON, D. KEVORKOV, P. CHARTRAND, I.-H. JUNG, M. MEDRAJ, "Experimental and thermodynamic study of the Mg-Sn-In-Zn quaternary system", *Journal of Alloys and Compounds*, 588 (2014) 75-95
Ni - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Ni - NiO	P. Chartrand, CRCT, 2021
Ni - Pb	Bragg-Williams R-K Polynomial		Cui Ping Wang, Xing Jun Liu, I. Ohnuma, R. Kainuma, K. Ishida: CALPHAD, 2000, 24(2), 149-167
Ni - S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P.Waldner and A.D.Pelton, Z. fur Metallk. 95[8] (2004), 672-681

Ni - Sb	Bragg-Williams R-K Polynomial		Y. Zhang et al., CALPHAD 32 (2008) 378–388
Ni - Si	Bragg-Williams R-K Polynomial	Spurious Ni_3Si $L1_2$ below 120°C	M. Lindholm, B. Sundman, Met.Trans.A 26A (1996), pp. 2897-2903.
Ni - Sn	Bragg-Williams R-K Polynomial	Stoichiometric α-$Ni_3Sn_{2(lt)}$	COST-531
Ni - Sr	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Ni – Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
Ni – Zn	Bragg-Williams R-K Polynomial		SGTE
O – Pb	MQMPA (Pair Fraction Exp.)	Gaseous species taken from FACTPS Database Valid for Pb - PbO	P. Chartrand, CRCT, 2021
O - S	MQMPA (Pair Fraction Exp.)	Gaseous species taken from FACTPS Database Valid for S – SO_3	P. Chartrand, CRCT, 2021
O - Si	MQMPA (Pair Fraction Exp.)	Gaseous species taken from FACTPS Database Valid for Si - SiO	P. Chartrand, CRCT, 2021
O - Zn	MQMPA (Pair Fraction Exp.)	Gaseous species taken from FACTPS Database Valid for Zn – ZnO	P. Chartrand, CRCT, 2021
Pb - S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2018
Pb - Sb	Bragg-Williams R-K Polynomial		H.Ohtani, K.Okuda, K.Ishida, J.Phase Equilibria 16 (1995) 416-429
Pb – Se	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Pb – Si	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2022; based on R.W.Olesinski, G.J.Abbaschian, Bull.Alloy Phase Diags. 5 (1984) 271-273
Pb – Sn	Bragg-Williams R-K Polynomial		Based on H.Ohtani, K.Okuda, K.Ishida, J.Phase Equilib.16 (1995) 416-429
Pb - Sr	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018 using solids from H.Zhang, C.Zhang, W.W.Wang, Y.Du, P.Zhou, B.Hu, Z.Liu, J.C.Wang, J.Wang, J.Min.Metall.Sect.B-Metall. 53(3) B (2017) 179-187
Pb – Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Pb - Tl	Bragg-Williams R-K Polynomial		unpublished assessment by I. Ansara, H.L. Lukas and S. G. Fries (SGTE)
Pb – Zn	Bragg-Williams R-K Polynomial		T.Jantzen, P.J.Spencer, Calphad 22 (1998) 417-434
S – Sb	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2018
S – Se	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2021
S – Si	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2021
S – Sn	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2018
S - Te	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2018
S – Zn	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2018
Sb - Se	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2021
Sb – Si	MQMPA (Pair Fraction Exp.)		P.J. Spencer, 2006
Sb – Sn	Bragg-Williams R-K Polynomial		C.S.Oh, J.H.Shim, B.J.Lee, D.N.Lee, J.Alloys and Cpds. 238 (1996) 155-166
Sb – Zn	Bragg-Williams R-K Polynomial		L.A.Zabdyr, Calphad 21 (1997) 349-358
Se - Te	Bragg-Williams R-K Polynomial		G. Ghosh, R. C. Sharma, D. T. Li, Y. A. Chang: J. Phase Equil., 1994, 15(2), 213-224

Si – Sn	Bragg-Williams R-K Polynomial		M.H.G.Jacobs, P.J.Spencer, Calphad 20 (1996) 89-91
Si – Sr	MQMPA (Pair Fraction Exp.)		J.-P. Harvey, CRCT, 2005
Si – Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2021
Si – Tl	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Si - Zn	MQMPA (Pair Fraction Exp.)		A. Shukla, Y.-B. Kang and A.D. Pelton, Calphad 32 (2008) pp. 470-477
Sn - Sr	MQMPA (Pair Fraction Exp.)		Jian Wang, Ph.D. Thesis, Ecole Polytechnique, Montreal, 2014
Sn – Te	MQMPA (Pair Fraction Exp.)		M. Paliwal, 2021
Sn – Tl	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Sn – Zn	MQMPA (Pair Fraction Exp.)		M. Medraj, Concordia, 2011
Sr - Zn	MQMPA (Pair Fraction Exp.)		P. Spencer, A.D. Pelton., Y.-B. Kang, P. Chartrand, and C. Fuerst, Calphad 32 (2007), pp. 423-431
Te - Zn	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
Tl - Zn	Bragg-Williams R-K Polynomial		S. S. Kim, T. H. Sanders, Z. Metallkunde 2003