FScopp Database for FactSage 8.3

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

Cu Alloys
Ag, **Al**, As, Au, **Be**, **Bi**, **C**, **Ca**, Cd, **Co**, **Cr**, **Cu**, **Fe**, **Ga**, **Ge**, **H**, Hg, **In**, **Li**, **Mg**, **Mn**, **Mo**, **Na**, **Nb**, **Ni**, **O**, **P**, **Pb**, Pd, **Pt**, **S**, **Sb**, **Se**, **Si**, **Sn**, Te, **Ti**, Tl, **V**, W, **Zn**, **Zr**
Color codes
Red : Cu **Blue** : Major alloying elements (full optimisations of binary systems with **Cu** and with several minor alloying elements, **Cu-Xx-Yy** ternary systems evaluated (good for the Cu-rich), several quaternary systems included); **Green** : Minor alloying elements (full optimisations of binary systems with Cu); **Purple** : Impurity elements (full optimisations of binary systems with Cu and several Cu-M-X systems); Black : Optimized for the **Cu-Zz** system and few **Xx-Zz** and **Cu-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 Cu-rich composition ranges. Please note that the FScopp 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, Al_2O_3, etc.) can be computed with the FScopp 8.3 database. See FactSage (EQUILIB) documentation on physical properties, and the list of phases at the end of the present document.

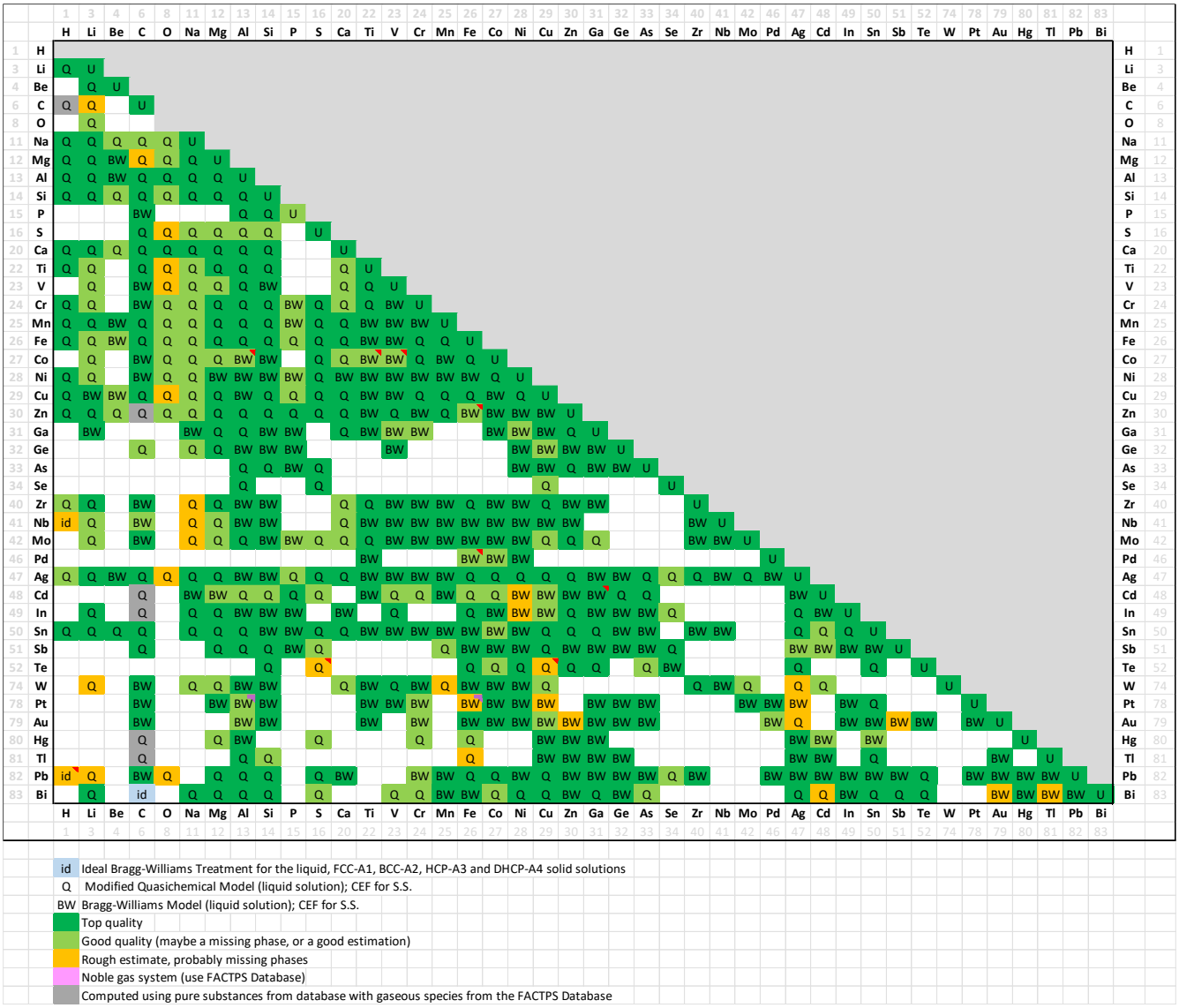

Figure 1: Optimized binary systems in the FScopp 8.3 Database (see also Table 4)

In FScopp 8.3 a total of **603 binary systems** (515 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 Cu-alloys.

Several dozens of ternary systems have been assessed, and important quaternary systems have also been evaluated.

The FScopp 8.3 database contains **269 solution phases** (238 in 8.2) and **1077 pure compounds** (906 in 8.2) with **1442 stoichiometric phases** (1232 in 8.2) counting allotropic forms. **Table 1** lists the important solutions for calculations involving Cu 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 FScopp is simple: simply follow these instructions:

- For pure solid compounds:
  - Right-click on "pure solids"
  - Then click "Select/Clear" > "Add all species from database" > "FScopp"
- 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" > "FScopp";
  - Apply the recommendations related to the CBCC-A12, D82 and D85 solutions, as described in the warning text box in the following page.
- There is no need to select pure liquid phases (the FScopp-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 150 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.

Within the solution database are hard coded default selections such as "+", "I" or "J" (for single phase, 2-phase immiscibility and 3-phase immiscibility). However, when the system has more than 5 elements, a few specific solution phases will see their default selection changed to "!", "!I" or "!J", meaning they become "dormant" (metastable). If in the calculation(s) that will follow one of these phases has a calculated activity higher than 1.0, you should overwrite the "!" (dormant) selection.

CBCC-A12

It is recommended to select the CBCC-A12 solid solution with the "!I" option (metastable + 2-phase immiscibility) in calculations in the EQUILIB module for Al alloys when more than 6 elements are present in the system. This is due to the very numerous potential end-members (1512) in that solution, which increases substantially the computation time. If after a calculation the activity of the CBCC-A12 solution is greater than 1.0, then redo the calculation with the standard "I" option.

D82 Prototype Cu_5Zn_8

Similarly it is recommended to select the D82 solid solution (Cu_5Zn_8, Al_8M_5 with M = Fe, Cr, V) with the "!I" option (metastable + 2-phase immiscibility) in calculations in the EQUILIB module for Al alloys when more than 6 elements are present in the system. This is due to the very numerous potential end-members (8712) in that solution, which increases substantially the computation time. If after a calculation the activity of the D82 solution is greater than 1.0, then redo the calculation with the standard "I" option.

μ-phase Fe_7W_6 D85

Similarly it is recommended to select the D85 solid solution with the "!I" option (metastable + 2-phase immiscibility) in calculations in the EQUILIB module for Al alloys when more than 6 elements are present in the system. This is due to the very numerous potential end-members (6561) in that solution, which increases substantially the computation time. If after a calculation the activity of the D88 solution is greater than 1.0, then redo the calculation with the standard "I" option.

Updates in 8.3 from 8.2

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

1) Al – Pt
2) As – Cd
3) As – Pt
4) As – Zn (replaced)
5) Au – Ga
6) Bi – Mn
7) C – Pt
8) Ca – Cu (replaced)
9) Ca – Ga
10) Ca – Ge
11) Cd - P
12) Co – Ga
13) Co – Pt (replaced)
14) Cr – Ga
15) Cu – Pt (replaced)
16) Fe – In (replaced)
17) Fe – Pt
18) Ga – Li
19) Ga – Mo
20) Ga – Ni
21) Ga – Pt
22) Ga – V
23) Ga – Zr
24) Ge – Na
25) Ge – Ni
26) Ge – Pt
27) Ge – V
28) H – Sn
29) In – Pt
30) In – Se
31) Li – Sb
32) Li – W
33) Mg – Pt
34) Mn – Sb
35) Mo – Pt
36) Ni – Pt

37) P – Sn
38) Pb – Pt
39) Pt – Si
40) Pt – Sn (replaced)
41) Pt – V

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 and V
- CBCC-A12 addition of Sb
- CUB-A13 addition of Sb
- A15 addition of Ga and Ge for Cr_3Ga, Mo_3Ga, V_3Ga, Cr_3Ge, Pt_3Ge, V_3Ge
- B2 AlPt, CoPt, CoTi, CoZr, MnNi
- B2b Au, Pt for PtTi, NiPt, AuTi
- B2e CoGa
- B8x (B81/B82) addition of Ge; updated CuSn, Au-Co, Ni_2Ge, Mn_2Sb
- B11 addition of Au for AuTi
- B20 addition of Pt, Ga, Ni, Mg
- B27 addition of Cr, Mo, Ni, Mn, V
- B31 addition of Pt Ga and Ge for PtGe, PtSi, NiGe
- B32 addition of Ga for LiGa
- B33 addition of Fe, Ge, Mo
- C1a addition of Ga, Mn, Pt for Ga_2Au, Ga_2Pt
- C2 addition of Ag, Pt, As, Se for $PtSb_2$, $CoSe_2$, $CuSe_2$, $FeSe_2$, $NiSe_2$
- C12 addition of Ge for $CaGe_2$
- C15 improvements to the Gibbs energy of metastable end-members
- C15a addition of Au and Bi
- C16 addition of Ga, Mg, Cr, Mo, V for Zr_2Ga, Mg_2Pt
- C23a addition of Ge and Pt for $SnPt_2$, $SiPt_2$, $GeNi_2$, $GeCa_2$, $AlPt_2$
- C36 addition of Mn
- C38 addition of Mn, Bi, S for Mn_2Sb
- C40 addition of Ge
- Ca addition of Mn
- Cb addition of Fe and Mo
- D03 improvements to the Gibbs energy of metastable end-members
- D011 addition of Ge, Mo, V
- D019 addition of Pt for $MoPt_2$;
  improvements to the Gibbs energy of metastable end-members
- D022 addition of Pt for Pt_3V;
  improvements to the Gibbs energy of metastable end-members
- D023 addition of Ga
- D024 addition of Au and Ga for Au_3Ga
- D13 addition of Ga

- D59 modified structure for Zn_3As_2, Zn_3P_3, Cd_3As_2, Cd_3P_2
- D510 addition of Ni
- D513 addition of Ga and Pt for Al_3Pt_2 and Ga_3Pt_2
- D5a addition of Ga, Cr, Mo, Fe, V and Nb
- D85 many changes with Mo, W
- D83 addition of Ga, Ge, Cr, Fe, Mo
- L10 addition of Mn, Zr, Co, Pt, Ni
- L12 addition of Ga
- L12c addition of Ge and Pt for Ni_3Ge, Pt_3Al, Co_3Ti, Pt_3Co, Pt_3In
- L'2b addition of Pt for $SiPt_2$
- hP18 addition of Zr and Al for Zr_5Ga_4, Zr_5Al_4
- mC18 addition of Nb
- mC22 addition of Ga
- mP24 re-organization of the structure for $ZnAs_2$, ZnP_2, $CsAs_2$ and CdP_2
- mS20 addition of Pt
- mS44 addition of Pt and Ga
- oI6 addition of Pt for $MoPt_2$
- oP4 addition of Ti, Pt, Pd
- oP24 addition of P for SiP_2 and GeP_2
- tP20 addition of Ti

Moreover, the following new solid solution phases were created:

1) A3' Prototype La
addition of Au(Sn)
2) BCC-B2e Prototype CsCl
CoGa with vacancies
3) B19 Prototype Beta' AuCd
Au-Ti, (Mo,V,Ti)Pt
4) Bg Prototype-MoB
ZrGa
5) C1c Prototype CaF2
Beta-Cd_3As_2 and betas-Zn_3As_2
6) D0c Prototype SiU3
$SiPt_3$ is stable with Zr solubility
7) oD59 ordered ternary D59
8) D82a D82 prototype Cu5Zn8
V_6Ga_7
9) L11 L11 Prototype CuPt
CuPt
10) L12e L12 Prototype-AuCu3
Pt_3Ga, Pt_3Ge, Ni_3Ga
11) h22P hP22 Prototype-Ti6Sn5
Ti_6Sn_5 and V_6Ga_5
12) h15R hR15 Prototype Al2Li3
$(Al,Ga,In)_2Li_3$
13) mS16 Prototype-Pt3Ge
$Pt_3(Ge,Si)$
14) oF40 Prototype Al3Zr2
$(Al,Ga)_3Zr_2$
15) oS8 oS8 Prototype TlI
GaCa, GeCa, NiZr
16) oS12 oS12 Prototype ZrGa2
$ZrGa_2$
17) o16S oS16 Prototype Pt5Ga3
Ni_5Ga_3, Pt_5Ga_3
18) oS32 oS32 Prototype-Pu3Pd5
Zr_3Ga_5
19) t12I Prototype CdAs2
$CdAs_2$

20) i160	tI160 Prototype Cd3As2
	$(Cd,Zn)_3As_2$
21) tP16	Prototype Pt3Ga
	$Pt_3(Al,Ga)$
22) p160	tP160 Prototype Zn3As2
	$(Cd,Zn)_3As_2$
23) P	oP56 Frank-Kasper phase
	Ternary solution CrMoNi
24) P1	M3Ca2
	$(Cu,Mg)_3Ca_2$
25) P2	MCu3
	$(Ca,Mg)Cu_3$

Table 1: Important phases in Cu alloys present in the FScopp 8.3 Database

Common names	FScopp		Struktur-bericht	Pearson	Space Group (index)
	Soln-Nickname or CMPD*	Solution Full name or compound stoichiometry			
Liquid metal	Liqu	Liquid	-	-	
Cu, α, FCC, (Cu), Ag, Co(lt), γ-Fe, Ni, Pb, Pt, Tl(ht)	A1	FCC-A1	A1	cF4	Fm-3m (225)
Cr, α-Fe, Li, Mo, Na, Nb, Ni, V, W, CuZn(ht), Cu_3Al(ht), Cu_3Be(ht), Cu_3In(ht), Cu_3Sn(ht)	A2	BCC-A2	A2	cI2	Im-3m (229)
Co, Tl(lt), Cu_6Si	A3	HCP-A3	A3	hP2	$P6_3/mmc$ (194)
Si also Ge, α-Sn	A4	Diamond-A4	A4	cF8	Fd-3m (227)
Bi	A7	Rhombehedral-A7	A7	hR2	R-3m (166)
C	-	$C_{(s)}$	A9	hP4	$P6_3/mmc$ (194)
Mn	A12	CBCC-A12	A12	cI58	$I\text{-}4_3m$ (217)
γ-$Cu_{33}Si_7$ ('Cu_5Si')	-	$Cu_{33}Si_{7(s)}$	A13	cP20	$P4_13_2$ (213)
β-NiZn, β'-CuZn, CuBe	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)
CuH	-	$CuH_{(s)}$	B4	hP4	$P6_3mc$ (186)
NiBi, NiAs, MnBi, 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, $InNi_2$, $(Fe,Mn,Ni,Ti)_2Sn$, ε-FeSb, θ-$SiNi_2$, $Sn(Fe,Ti)_2$			$B8_2$	hP6	
MnSi, (Co,Cr,Fe,Mn)Si	B20	B20 Prototype-FeSi	B20	cP8	$P2_13$ (198)
Cu_2O	C3	C3 Prototype-Cu2O	C3	cP6	Pn-3m (224)
$Cu(Ti,Zr)_2$	C11b	C11b Prototype-MoSi2	$C11_b$	tI6	I4/mmm (139)
Cu_2Mg	C14	C14 Prototype-MgZn2	C14	hP12	$P6_3/mmc$ (194)
$CdCu_2$	-	$CdCu_{2(s)}$	C14	hP12	$P6_3/mmc$ (194)
Cu_2Mg, Cu_2Zr	C15	C15 Prototype-MgCu2	C15	cF24	Fd-3m (227)

Cu_9Zr_2 ('Cu_5Zr')	-	$Cu_9Zr_{2(s)}$	$C15_b$	cF24	F-43m (216)
Cu_2Te(s4), η-Cu_2Sb	C38	C38 Prototype-Cu2Sb	C38	tP6	P4/nmm (129)
Cu_2Te(s5)	Ch	Ch Prototype-Cu2Te	C_h	hP6	P6/mmm (191)
Cu_3P	D021	D021 Prototype-Cu3P	$D0_{21}$	hP24	$P6_3cm$ (185)
Cu_3Sn(ht), Cu_3Sb, Mn_3Si	D03	D03 Prototype-BiF3	$D0_3$	cF16	Fm-3m (225)
Fe_3Si	D03a	D03 Prototype-BiF3	$D0_3$	cF16	Fm-3m (225)
$CaCu_5$	D2d	D2d Prototype-CaCu5	$D2_d$	hP6	P6/mmm (191)
Mn_9Si_2	-	$Mn_9Si_{2(s)}$	$D5_9$	tP10	P4/mbm (127)
Cu_2Al(lt)	D83	D83 Prototype-Cu9Al4	$D8_3$	cP52	$P-4_3m$ (215)
Mn_5Si_3	D88	D88 Prototype-Mn5Si3	$D8_8$	hP16	$P6_3/mcm$ (193)
δ-Cu_7In_3	aP40	aP40 Prototype-Cu7In3	-	aP40	P-1 (2)
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)
β'-Cu_4Ti	oP20	oP20 Prototype-ZrAu4	-	oP20	Pnma (62)
$Cu_2Te_{(s6)}$	-	$Cu_2Te_{(s6)}$	-	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)
$Cu_{51}Zr_{14}$	-	$Cu_{51}Zr_{14(s)}$	-	hP68	P6/m (175)
Hg_6Cu_7	-	$Hg_6Cu_{7(s)}$	-	hR*	R3m
Cu_2Se(lt)	-	$Cu_2Se_{(s)}$	-	mS144	C2/c (15)
Cu_3Sn	-	$Cu_3Sn_{(s)}$	-	oS80	Cmcm (63)
$Cu_2Te_{(s1)}$ (rt)	-	$Cu_2Te_{(s1)}$	-	o*	?
$Cu_2Te_{(s2)}$	-	$Cu_2Te_{(s2)}$	-	o*	?
$Cu_2Te_{(s3)}$	-	$Cu_2Te_{(s3)}$	-	?	?
δ-Cu_4Sb	-	$Cu_4Sb_{(s)}$	-	?	?
γ-Cu_6Sb	-	$Cu_6Sb_{(s)}$	-	?	?

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

■ **Important solutions in Cu alloys**

Common names	FScopp		Major phase components
	Nickname	Full name	
Liquid metal	Liqu	Liquid	most elements
Cu, (Cu), FCC	A1	FCC-A1	Ag, Al, Cu, γ-$Fe_{austenite}$, Ni, Pb, ... with C, H, O interstitials ($\rightarrow$B1)
BCC	A2	BCC-A2	α-$Fe_{ferrite}$, Cr, Li, Na, β-Ti, β-Zr, Mo, Nb, V, W... ... with C, H, O interstitials
Co, HCP, α-Ti	A3	HCP-A3	Co, Mg, α-Ti, α-Zr ... with C, H, O interstitials
Au(Sn)	A3'	DHCP-A3'	Au-rich solution with Sn
Zn	A3"	HCP-Zn	Zn
Si	A4	Diamond-A4	$C_{diamond}$, Ge, Si, α-Sn
Sn	A5	BCT-A5	β-Sn
In	A6	TET-A6	α-In
InSn	A6o	TET-A6o	β-InSn
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
α-Mn, χ-$(Mo,W)_5Fe_{12}Cr_{12}$, (γ- or β-) $Al_{12}Mg_{17}$	A12	CBCC-A12	α-Mn, β/γ-$Al_{12}Mg_{17}$, χ-FeCr(Mo,W)
β-Mn	A13	CUB-A13	β-Mn, Ag_3Al
Cr_3Si	A15	CUB-A15	Cr_3Si, Nb_3Al, Nb_3Sn, V_3Co, V_3Ni, V_3Si, V_3Sn, Mo_3Al
α-S	A16	A16	S
γ-InSn	Af	HEX-Af	γ-InSn
β-S	Ak	Ak	β-S
Se	Al	Al	Se
P(red)	RedP	Red-Phosphorus	P(red)
CaS, MgS, MnS, PbS	B1	FCC-B1	CaS, MgS, MnS, PbS, PbSe, PbTe, SnAs, SnS, SnTe
β-NiZn, **β'-CuZn**	**B2**	BCC_B2!BCC_A2	AgLi, AgMg, CaIn, β-NiZn, β'-CuZn with order/disorder transf.
TiNi, TiAu, TiPt	B2_b	BCC-B2b	non-stoichiometric TiNi
AlNi	B2_c	BCC-B2c	non-stoichiometric AlNi with vacancies
AlMo	B2_d	BCC-B2d	non-stoichiometric AlMo
CoGa	B2_e	BCC-B2e	non-stoichiometric CoGa
ZnS, ZnTe, AlP, β-SiC-3C	B3	B3 (sphalerite)	AlAs, AlP, AlSb, GaAs, GaP, GaSb, InAs, InP, InSb, β-SiC-3C

ZnS, α-SiC-2H	B4	B4 (wurtzite)	ZnS, α-SiC-2H
(Co,Fe,Cr,Ni)S, $B8_1$	**B8x**	B81/B82 NiAs/InNi2	**$B8_1$** : ε-AlCu, NiBi, NiAs, MnBi, AuSn, CoS, CrS, FeS, NiS, ε-FeSb, NiSb, (Fe,Ni)Te
			$B8_2$: Co_2Sb, β-BiMn, $InNi_2$, $(Fe,Mn,Ni,Ti)_2Sn$, ε-FeSb, θ-$SiNi_2$, $GaTi_2$, $Sn(Fe,Ti)_2$
HgS	B9	B9 Prototype-HgS	HgS
γ-CuTi	B11	B11 Prototype-CuTi	γ-CuTi, Ag(Ti,Zr), β1-NiZn, CdTi
NiS millerite	B13	B13 Prototype-NiS	NiS
SnS, α-SnSe	B16	B16 Prototype-GeS	SnS, α-SnSe
CuS covellite	B18	B18 Prototype-CuS	CuS
(Au,Pt)Ti	B19	B19 Prototype-Beta'AuCd	AuTi, PtTi, MoPt
FeSi	B20	B20 Prototype-FeSi	(Fe,Co,Cr,Mn)Si monosilicide
TiSi, ZrSi	B27	B27 Prototype-FeB	TiSi, ZrSi
FeP, MnP, CoP, NiSi	B31	B31 Prototype-FeAs	(Co,Fe,Mn)P, NiSi
ZnLi, InLi, AlLi	B32	B32 Prototype-NaTl	AlLi, InLi, InNa, ZnLi
CaSi, CaSn	B33	B33 Prototype-CrB	CaSi, CaSn
CoSn, NiIn, FeSn	B35	B35 Prototype-CoSn	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
ZrGa	Bg	Bg Prototype-MoB	ZrGa
γ-MoC, δ-WC	Bh	Bh Prototype-MoC	γ-MoC, δ-WC
TiH_2	C1	C1 Prototype-CaF2	TiH_2, δ-ZrH_2
Mg_2Si	C1a	aC1 Prototype -CaF2	Mg_2Si, Mg_2Sn, Mg_2Ge, Mg_2Pb, Al_2Au, Si_2Co, Si_2Ni
Ni_2S-β1	C1b	C1b Prototype-MgAgAs	Ni_2S-β1
$(Cd,Zn)_3As_{2(ht)}$	C1c	C1c Prototype-CaF2	$(Cd,Zn)_3As_{2(ht)}$
$(Co,Fe,Mn,Ni)S_2$, $(Co,Cu,Mn,Ni)Se_2$, $AuSb_2$	C2	C2 Prototype-FeS2	$(Co,Fe,Mn,Ni)S_2$, $AuSb_2$, $(Co,Cu,Mn,Ni)Se_2$,
Cu_2O	C3	C3 Prototype-Cu2O	$(Cu,Ag)_2O$
MTe_2, SnS_2	C6	C6 Prototype-CdI2	$(Fe,Ni,Co)Te_{2-x}$, $SiTe_2$, SnS_2, ZrS_2 and $SnSe_2$
MoS2	C7	C7 Prototype-MoS2	MoS_2, $MoSe_2$, $MoTe_2$
$CuTi_2$	C11b	C11b Prototype-MoSi2	$MoSi_2$, $AgTi_2$, $AgZr_2$, $AlCr_2$, $CuTi_2$, $CuZr_2$, $ZnTi_2$, $TiAu_2$, $TiPd_2$
$CaSi_2$	C12	C12 Prototype-CaSi2	$CaSi_2$
$MgZn_2$, Laves-C14, Hexagonal Laves	C14	C14 Prototype-$MgZn_2$ (Laves)	Al_2Zr, Co_2Mg, Cr_2Nb, Cr_2Ti, Cr_2Zr, Cu_2Mg, Fe_2Mo, Fe_2Nb, Fe_2Ti, Fe_2W, Li_2Ca, Mg_2Ca, Mn_2Nb, Mn_2Ti, Mn_2Zr, Ti_2Al, Zn_2Mg, Zn_2Ti

$MgCu_2$, Laves-C15, Cubic Laves	C15	C15 Prototype-$MgCu_2$ (Laves)	Al_2Ca, Co_2Ti, Co_2Zr, Co_2Nb, Cr_2Ti, Cr_2Zr, Cr_2Nb, Cu_2Mg, Cu_2Zr, Fe_2Ti, Fe_2Zr, Ni_2Ca, V_2Zr, Zn_2Zr
Laves-Ag_2Na	C15a	C15a Prototype-$MgCu_2$ (Laves)	Ag_2Na
Laves-Ni_5Zr	C15b	C15b Prototype-$MgSnCu_4$ (Laves)	Ni_5Zr
θ-Al_2Cu	C16	C16 Prototype-Al2Cu	θ-Al_2Cu, Pb_2Au, $Sn_2(Co,Fe,Mn)$, Zr_2Si, $(Ti,Zr)_2Ni$, $Zr_2(Co,Fe,Ni,Si)$
$CuSe_2$, $(Co,Fe,Ni)(As,S,Sb)_2$	C18	C18 Prototype-FeS_2	$CuSe_2$, $(Co,Fe,Ni)(As,S,Sb,Te)_2$
Fe_2P	C22	C22 Prototype-Fe2P	Cu_2P, Fe_2P, Mn_2P, Ni_2P, FeNiP
Co_2Si	C23a	C23 Prototype-Co2Si	Ca_2Sn, Sr_2Sn, Ca_2Si, Sr_2Si, θ-Ni_2Si, Ca_2Cu, Co_2Si, $PbCa_2$
Bi_2Te_3	C33	C33 Prototype-Bi2Te3	Bi_2Te_3, Bi_2Se_3, Sb_2Te_3
$AuTe_2$	C34	C34 Prototype-AuTe2	$AuTe_2$
Laves-$MgNi_2$	C36	C36 Prototype-MgNi2 (Laves)	$MgNi_2$, $Cr_2(Ti,Zr)$, Cu_2Mg, ternary phases in Mg-Al-Ca, Co_2Ti
η-Cu_2Sb	C38	C38 Prototype-Cu2Sb	η-Cu_2Sb, Cu_2As, Cu_2Te, Fe_2Te
$CrSi_2$	C40	C40 Prototype-CrSi2	$CrSi_2$, $NbSi_2$, VSi_2, WAl_2, WSi_2
$CaZn_2$	C42	C42 Prototype-CeCu2	$CaZn_2$
Si_2Zr	C49	C49 Prototype-Si2Zr	Si_2Zr, Si_2Ti
$TiSi_2$	C54	C54 Prototype-TiSi2	$TiSi_2$, $ZrSn_2$
$NiMg_2$ C_a	Ca	Ca Prototype-NiMg2	$NiMg_2$
$CuMg_2$	Cb	Cb Prototype-$CuMg_2$	$CuMg_2$, $NbSn_2$, VSn_2
Cu_2Te	Ch	Ch Prototype-Cu2Te	Cu_2Te
$SiPt_3$	D0c	D0c Prototype-SiU3	$SiPt_3$
M_3P (M=Co,Cr,Fe, Mn,Ni,V)	D0e	D0e Prototype-Ni3P	
Kieftite Sb_3Co	D02	D02 Prototype-As3Co	Sb_3Co
β-Ni_3Sn, γ-Cu_3Sn $D0_3$	D03	D03 Prototype-BiF3	γ-Cu_3Sn, Sn_3Cu, β-Ni_3Sn, Ni_3Sb, Cu_3Sb, Mn_3Si, Li_3Bi
Fe_3Si	D03a	D03 Prototype-BiF3	Fe_3Si
Li_2MgSn	D03b	D03b Prototype-BiF3	Li_2MgSn
θ-Fe_3C, Al_3Ni	D011	D011 Prototype-Fe3C	θ-Fe_3C, Mn_3C, Al_3Ni, Ni_3Si
Na_3As, Na_3P	D018	D018 Prototype-Na3As	Na_3As, Na_3Bi, Na_3P, Na_3Sb
α_2-Ti_3Al $D0_{19}$	D019	D019 Prototype-Ni3Sn	Nb_3Al, Ti_3Al, Ti_3Ga, Zr_3Al, Ti_3Sn, Ni_3Zr, Ni_3In, Ni_3Sn(lt), Co_3W, Mo_3Al, Mn_3Sn
Cu_3P	D021	D021 Prototype-Cu3P	Cu_3P
Al_3X $D0_{22}$	D022	D022 Prototype-TiAl3	Al_3Cr, Al_3Mo, Al_3Nb, ε-Al_3Ti, Al_3V, Al_3Zr, Ga_3Ti, Ni_3V
Al_3Zr $D0_{23}$	D023	D023 Prototype-ZrAl3	Al_3Zr
Ni_3Ti $D0_{24}$	D024	D024 Prototype-Ni3Ti	Ni_3Ti
Ag_3Sn, Cu_3Sb $D0_a$	D0a	D0a Prototype-Cu3Ti	Ag_3Sn, Cu_3Sb, γ-Ni_3Mo, Ni_3Nb, Ni_3Sb

$Cr_7C_{3(hT)}$, Mn_7C_3 $D10_1$	D101	D101 Prototype-Mn7C3	Cr_7C_3, Mn_7C_3
$Cr_7C_{3(lT)}$	D102	D102 Prototype-Th7Fe3	Cr_7C_3
$Al_4(Ca,Sr,Ba)$	D13	D13 Prototype-Al4Ba	Al_4Ca
Al_2CaZn_2	D13a	D13a Al2CaZn2	Al_2CaZn_2, Al_2REZn_2 (with *RE* = La,Ce,Pr,Nd)
$TiAu_4$, $MoNi_4$, WNi_4	D1a	D1a Prototype-MoNi4	$TiAu_4$, $MoNi_4$, WNi_4
Mg_2Zn_{11}, $Mg_2Cu_6Al_5$	D22	D22 Prototype-Mg2Zn11	Mg_2Zn_{11}, $Mg_2Cu_6Al_5$
$NaZn_{13}$	D23	D23 Prototype-NaZn13	$NaZn_{13}$, $CaZn_{13}$
$Ca(Cu,Ni,Zn)_5$	D2d	D2d Prototype-CaCu5	$CaZn_5$, $CaCu_5$, $CaNi_5$
Al_6Mn, $Al_6(Fe,Mn)$	D2h	D2h Prototype-Al6Mn	Al_6Mn $(Al_6Fe)_{metastable}$
α-$Mg_3(Bi,Sb)_2$	D52	D52 Prototype-La2O3	$Mg_3(Bi,Sb)_2$
β-$Mg_3(Bi,Sb)_2$	D53	D53 Prototype-Mn2O3	$Mg_3(Bi,Sb)_2$
$(Bi,Sn)_2S_3$	D58	D58 Prototype-Sb2S3	Bi_2S_3, Sb_2S_3
Zn_3P_2	D59	D59 Prototype-Zn3P2	Cd_3As_2, Zn_3As_2, Zn_3P_2
Ordered ternary s.s.	oD59	D59 Prototype-Zn3P2	Ordered ternary s.s.
Cr_3C_2	D510	D510 Prototype-Cr3C2	Cr_3C_2
Al_3Ni_2	D513	D513 Prototype-Al3Ni2	Al_3Ni_2
Si_2Zr_3	D5a	D5a Prototype-Si2U3	Si_2Zr_3
Al_4C_3	D71	D71 Prototype-Al4C3	Al_4C_3
$(Ag,Cu)_5Zn_8$, γ-AlCu	D82	D82 Prototype-Cu5Zn8	$(Ag,Cu,Fe)_5Zn_8$, γ-AlCu, γ-NiZn, $(Ag,Cu)_5Cd_8$, ε-$Al_8(Cr,Fe,V)_5$
$V_6Ga_{7(ht)}$	D82a	D82 Prototype-Cu5Zn8	$V_6Ga_{7(ht)}$
Cu_9Al_4, $InAg_2$	D83	D83 Prototype-Cu9Al4	γ-Cu_9Al_4, γ-Co_9Zn_4, In_5Ag_8
$Cr_{23}C_6$	D84	D84 Prototype-Cr23C6	$Cr_{23}C_6$, $Mn_{23}C_6$
μ-Fe_7W_6	D85	D85 Prototype-Fe7W6 (Frank-Kasper)	$(Co,Fe)_7(Mo,Nb,W)_6$
ε-$Cu_{15}Si_4$	D86	D86 Prototype-Cu15Si4	ε-$Cu_{15}Si_4$
Mn_5Si_3, Ti_5Si_3, Ti_5Sn_3	D88	D88 Prototype-Mn5Si3	Cr_5Si_3, Fe_5Si_3, Mn_5Si_3, Nb_5Si_3, Ti_5Si_3, V_5Si_3, W_5Si_3, Zr_5Si_3, Ti_5Sn_3, Zr_5Sn_3
(Fe-Ni) pentlandite, Co_9S_8	D89	D89 Prototype-Co9S8	(Fe-Ni) pentlandite, Co_9S_8
Al_8Mn_5 Al_8Cr_5	D810	D810 Prototype-Al8Cr5	Al_8Mn_5, Al_8Cr_5
$Co_{23}Zr_6$	D8a	D8a Prototype-Mn23Th6	$Co_{23}Zr_6$
σ-FeCr, σ-AlNb, σ-MnV, σ-NiV, σ-FeMo	D8b	D8b Prototype-FeCr	σ-FeCr, intermetallic phases in Al-Mo-Nb and Mn-Ni-V-W
Al_9Co_2	D8d	D8d Prototype-Al9Co2	Al_9Co_2
T-phase, Tau $Mg_{32}(Al,Zn)_{49}$	D8e	Tau Prototype-Mg32(Al,Zn)49	Ternary phases in Mg-Al-Cu-Zn-(Ag)
$Mg_5(Ga,In)_2$	D8g	D8g Prototype-Ga2Mg5	$Mg_5(Ga,In)_2$

Ca_5X_3 $D8_l$	D8l	D8l Prototype-Cr5B3	Ca_5Si_3, Ca_5Sn_3, Ca_5Zn_3, Ca_5Ag_3
Cr_5Si_3	D8m	D8m Prototype-W5Si3	$(Cr,Mo,Nb,V,W)_5Si_3$
CuFeS2	E11	E11 Prototype-CuFeS2	chalcopyrite
$FeZr_3$, $CoZr_3$	E1a	E1a Prototype-FeZr3	$(Co,Fe)Zr_3$
$(Fe,Mn,Ti)_3AlC$	E21	E21 Prototype-CaTiO3	$(Fe,Mn,Ti)_3AlC$
Al_7Cu_2Fe, Al_7CuMn_2	E9a	E9a Prototype-Al7Cu2Fe	Al_7Cu_2Fe, Al_7CuMn_2, τ_9-Al_7Cu_2Zr
$(Co,Fe,Ni)_3W_3C$	E93	E93 Prototype-Fe3W3C	$(Co,Fe,Ni)_3W_3C$
$(Co,Ni)_3S_4$, $NiFe_2S_4$	H11	H11 Prototype-Fe3O4	Ni_3S_4(polydymite), $NiFe_2S_4$(violarite), Co_3S_4(linnaeite)
γ-AlTi, MgIn, $L1_0$	L10	L10 Prototype-AuCu	AlTi, MgIn, GaTi
CuTi $L1_1$	L11	L11 Prototype-CuTi	CuTi
Al_3M $L1_2$	L12	L12 Prototype-AuCu3	Pt_3Ti
$Ni_3(Al,Fe,Si)$ $L1_2$	L12c	L12-FCC!FCC-A1	Ag_3Mg, Ni_3Al, Ni_3Fe, Ni_3Si, Si_3Ni
$MgIn_3$, $InMg_3$ $L1_2$	L12d	L12d Prototype-AuCu3	$MgIn_3$, $InMg_3$, $InAg_3$
Pt_3Ga, Pt_3Ge, Ni_3Ga	L12e	L12e Prototype-AuCu3	Pt_3Ga, Pt_3Ge, Ni_3Ga
$AlCu_2Mn$, $AlNi_2Ti$	L21	Heusler Prototype-AlCu2Mn	$AlCu_2Mn$, $AlNi_2Ti$
TiH_2(low-T), ZrH_2	L'2	L'2 Prototype-TiH2	TiH_2(low-T), ZrH_2, $SiPt_2$
$AgMg_3$	AMg3	cF264 Prototype-AgMg3	$AgMg_3$
$Al_{11}Mn_4$(low-T)	aP15	aP15 Prototype-Al11Mn4	$Al_{11}Mn_4$(low-T), $Al_{11}Cr_4$
ξ-Al_2Fe	aP18	aP18 Prototype-Al2Fe	ξ-Al_2Fe
$(Al,In)_3Ca_8$	aP22	aP22 Prototype-Ca8In3	$(Al,In)_3Ca_8$
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)
Ti_2Co, Ti_2Ni	cF96	cF96 Prototype-Ti2Ni	Ti_2Co, Ti_2Ni
Argentite-Ag_2S	cI20	cI20 Prototype-Ag2S	Ag_2S, Ag_2Se
$Al_{12}Mn$, $Al_{12}W$	cI26	cI26 Prototype-Al12W	Al_{12}(Mn,Mo,W) ($Al_{12}Fe$-metastable)
Ni_2S-β_2	cP_	beta2	Ni_2S-beta2
CaAlSi, SrAlSi	hP3_	hP3 Prototype-AlB2	CaAlSi, SrAlSi
δ-CuZn	hP3	CuZn_delta	δ-CuZn, ζ-AgCd, ε-$AgCd_3$
Fe_2Si	hP6	hP6 Prototype-Ni2Al	Ni_2Al, Fe_2Si
M_2AlC	hP8c	MAX Prototype-Cr2AlC	M_2AlC (M = Cr, Ti, Nb, V)
Bi_2Te_3	hP9	hP9 Prototype-Sb2Te	Bi_2Te_3
δ-WC, η-MoC	hP12	eta-MoC	δ-WC, η-MoC
Cu_2S chalcocite(ht)	hP16	hP16 Prototype-Cu2S	Cu_2S chalcocite(ht)
Ti_5Ga_4	hP18	hP18 Prototype-Ti5Ga4	Ti_5Ga_4
β-Ti_6Sn_5, V_6Ga_5	h22P	hP22 Prototype Ti6Sn5	β-Ti_6Sn_5, V_6Ga_5

β-AlMnSi	hP26	AlMnSi_beta	β-AlMnSi
SbSn	hR3	hR3 Prototype-“SbSn”	SbSn
Bi_2Te_3	hR15	hR15 Prototype-Bi2Te3	Bi_2Te_3
$(Al,Ga,In)_2Li_3$	h15R	hR15 Prototype-Al2Li3	$(Al,Ga,In)_2Li_3$
V_4C_3	hR21	hR21 Prototype-Sn4P3	V_4C_3
Cr_2S_3	hR30	hR30 Prototype-Cr2S3	Cr_2S_3
Al_5Mo	h36R	h36R Prototype-MoAl5	Al_5Mo
Mg_3In	hR48	hR48 Prototype-Mg3In	Mg_3In
Ni_7Zr_2, Co_7Nb_2	mC18	mC18 Prototype-Ni7Zr2	Ni_7Zr_2, Co_7Nb_2
Mo_3Al_8	mC22	mC22 Prototype-Mo3Al8	Mo_3Al_8
ζ-$Zn_{13}Fe$, γ_2-$Zn_{13}Co$	mC28	mC28 Prototype-Zn13Co	ζ-$Zn_{13}Fe$, γ_2-$Zn_{13}Co$
Ni_5Sb_2	m28C	mS28 Prototype-Ni5Sb2	Ni_5Sb_2
Al_4Mo, Al_4W	mC30	mC30 Prototype-Al4W	Al_4Mo, Al_4W
β-AlFeSi (τ_6)	mC52	AlFeSi_beta	β-AlFeSi (τ_6)
$(Ag,Cu)P_2$	mP12	mP12 Prototype-CuP2	$(Ag,Cu)P_2$
Acanthite-Ag_2S	m12P	m12P Prototype-Ag2S	Acanthite-Ag_2S
$ZnAs_2$	mP24	mP24 Prototype-ZnAs2	$ZnAs_2$, β-ZnP_2
‘Al_3Fe’	m102	mC102 Prototype-Al13Fe4	$Al_{13}Fe_4$, $Al_{13}Co_4$
Mg_2Zn_3	m110	Mg2Zn3	Mg_2Zn_3
CrS	mS8	mS8 Prototype-CrS	CrS
Ni_3Sn_4	mC14	mS14 Prototype-Ni3Sn4	Ni_3Sn_4
Cr_3S_4	mS14	mS14 Prototype-Cr3S4	Cr_3S_4
Pt_3Ge, $Pt_3Si_{(lt)}$	mS16	mS16 Prototype-Pt3Ge	$Pt_3(Ge,Si)$
η_2-AlCu, θ-InCu	mS20	eta2 Prototype-AlCu	η_2-AlCu, θ-InCu
GeAs, SiAs	mS24	mS24 Prototype-SiAs	(Ge,Si)(As,P)
Hägg χ-Fe_5C_2	mS28	Haegg Prototype-Mn5C2	χ-Fe_5C_2, Mn_5C_2
$MoAl_3$	mS32	mS32 Prototype-MoAl3	$MoAl_3$
ζ’-$Ni_{13}In_9$	mS44	mS44 Prototype-Ni13Ga9	ζ’-$Ni_{13}In_9$
$Al_{14}Ca_{13}$	mS54	mS54 Prototype-Al14Ca13	$Al_{14}Ca_{13}$
Al_3Hf_2, Al_3Zr_2, Ga_3Zr_2	oF40	oF40 Prototype-Al_3Zr_2	Al_3Hf_2, Al_3Zr_2, Ga_3Zr_2
$(Cr,Mo,V)Ni_2$	oI6	oI6 Prototype-MoPt2	$(Cr,Mo,V)Ni_2$
$(Nb,Ti)_6Sn_5$	oI44	oI44 Prototype-Ti6Sn5	$(Nb,Ti)_6Sn_5$
α-(Pd,Pt)Ti	oP4	oP4 Prototype-AuCd	α-(Pd,Pt)Ti
Ag_3Sb	oP4a	oP4a Prototype-Ag3Sb	Ag_3Sb
CaMgSi	oP12	oP12 Prototype-TiNiSi	CaMgSi
naumannite-Ag_2Se	o12P	oP12 Prototype-Ag2Se	naumannite-Ag_2Se
Cu_4Ti	oP20	oP20 Prototype-ZrAu4	β’-Cu_4Ti
$(Co,Mn,Ni)_3Sn_2$	o20P	oP20 Prototype-Ni3Sn2	$(Co,Mn,Ni)_3Sn_2$
$SiAs_2$, $GeAs_2$	oP24	oP24 Prototype-GeAs2	$(Ge,Si)As_2$

Ca_7Ge_6, Ca_7Sn_6	oP52	oP52 Prototype-Ca7Sn6	$Ca_7(Ge,Sn)_6$
δ-NiMo	oP56	NiMo-delta	δ-NiMo
GaCa, GeCa, NiZr	oS8	oS8 Prototype-TlI	GaCa, GeCa, NiZr
$ZrGa_2$	oS12	oS12 Prototype-ZrGa2	$ZrGa_2$
AgCuS stromayerite	o12S	oS12	AgCuS
$(Pt,Ni)_5Ga_3$	o16S	oS16 Prototype-Pt5Ga3	$(Pt,Ni)_5Ga_3$
$Zr_3(Ga,Ge,Si)_5$	oS32	oS32 Prototype-Pu3Pd5	$Zr_3(Ga,Ge,Si)_5$
Li_7Sn_2	oS36	oS36 Prototype-Li7Ge2	Li_7Sn_2
β-$FeSi_2$	oS48	Luobusaite Prototype-FeSi2	β-$FeSi_2$
α-Ni_7S_6	oS56	oS56 Prototype-Ni7S6	Ni_7S_6
'$Ni_{10}Zr_7$'	oS68	oS68 Prototype-Zr7Ni10	'$Ni_{10}Zr_7$'
Godlevskite Ni_9S_8	oC68	oC68 Prototype-Ni9S8	Ni_9S_8
$(Cd,Zn)As_2$	t12I	tI12 Prototype-CdAs2	$(Cd,Zn)As_2$
η-Al_2Ti	tI24	tI24 Prototype-HfGa2	η-Al_2Ti, Ga_2Ti, Al_2Mg-metastable
ε-Al_3Ti(lt)	tI32	tI32 Prototype-$TiAl_3$	ε-Al_3Ti(lt)
$CaZn_{11}$	tI48	tI48 Prototype-BaCd11	$CaZn_{11}$
$(Cd,Zn)_3(As)_2$	i160	tI160 Prototype-Cd3As2	$(Cd,Zn)_3(As)_2$
α-$FeSi_{2(ht)}$	tP3	Ferdisilicite Prototype-FeSi2	α-$FeSi_2$(high-T)
$Pt_3Ga_{(ht)}$, Pt_3Al	tP16	tP16 Prototype-Pt3Ga	$Pt_3Ga_{(ht)}$, Pt_3Al
Al_2Zr_3	tP20	tP20 Prototype-Al2Zr3	Al_2Zr_3, Zn_2Zr_3
$(Cd,Zn)P_2$	tP24	tP24 Prototype-ZnP2	$(Cd,Zn)P_2$
ζ-Al_5Ti_2	tP28	tP28 Prototype Al_5Ti_2	ζ-Al_5Ti_2
Ti_3P, Ti_3Si	tP32	tP32 Prototype-Ti3P	M_3P (with M = Ti,V,Zr) X_3Si (with X = Nb, Ti,Zr)
$(Ti,Zr)_5Si_4$	tP36	tP36 Prototype-Zr5Si4	$(Ti,Zr)_5Si_4$
$(Cd,Zn)_3(As)_2$	p160	tP160 Prototype-Zn3As2	$(Cd,Zn)_3(As)_2$
β-Al_3Mg_2	Beta	Beta Prototype-Mg28Al45	β-Al_3Mg_2
η-Al_5Fe_2	Eta	Eta Prototype-Al5Fe2	η-Al_5Fe_2
ϕ-$Mg_6(Al,Zn)_5$	Phi	Phi AlMgZn	ϕ-$Mg_6(Al,Zn,Cu)_5$
ζ-AlCu or ζ-Al_9Cu_{11}	Zeta	Zeta Prototype-AlCu	ζ-Al_9Cu_{11}
E-phase $Al_{18}Cr_2Mg_3$ $Zn_{22}Zr$, $CaCr_2Al_{20}$	E	E Prototype-CeCr2Al20	$Al_{18}Cr_2Mg_3$, $Al_{18}Mn_2Mg_3$, $Al_{18}Mo_2Mg_3$, $Al_{18}Ti_2Mg_3$, $Al_{18}V_2Mg_3$, $Al_{18}W_2Mg_3$ $CaCr_2Al_{20}$, $Zn_{22}Zr$
Q-$Al_3Cu_2Mg_9Si_7$	Q	Q Prototype-Th7S12	$Al_3Cu_2Mg_9Si_7$
P phase	P	P phase	CrMoNi ternary solution
P1	P1	M3Ca2	$(Mg,Cu)_3Ca_2$

P2	P2	MCu3	$(Mg,Ca)Cu_3$
R phase	R	R phase	$(Co,Fe,Ni)_{27}W_{14}(Co,Cr,Fe,Ni,W)_{12}$
S-Al_2CuMg	S	S Prototype-Al2CuMg	*S*-Al_2CuMg (ordered E1a)
μ-Al_4Mn, Al_4Cr	Al4M	Al4Mn	Al_4Mn, Al_4Cr (metastable Al_4Fe)
'Al_3Mn(ht)'	A3M_	oP156 Prototype-Al11Mn4	$Al_{29}Mn_{10}$(high-T)
$Al_{11}Cr_2$	AlCr	Al11Cr2	$Al_{11}Cr_2$
α-AlFeSi, τ_5	Tau5	AlFeSi_alpha	stoichiometry ~Al_7Fe_2Si (chinese script/rods)
γ-AlFeSi, τ_2	Tau2	AlFeSi_gamma	stoichiometry τ_2~Al_3FeSi
α-AlMnSi	AlM1	AlMnSi_alpha	stoichiometry τ_9~Al_9Mn_2Si
α-AlFeMnSi	AFMS	AlFeMnSi_alpha	stoichiometry ~$Al_{18}(Fe,Mn)_4Si_3$
'MgZn' or $Mg_{12}Zn_{13}$	MgZn	Mg12Zn13	$Mg_{12}Zn_{13}$
δ-AlCu or δ-Al_2Cu_3	Dlta	AlCu_delta	δ-Al_2Cu_3
η_1-AlCu	EtaH	Eta1 Prototype-AlCu	η_1-AlCu
γ-AlCu(high-T)	Gam5	gamma Prototype-AlCu	γ-Al_4Cu_9(high-T)
τ-AlCuZn	Tau_	AlCuZn_Tau	τ-$Al_9Cu_9Zn_2$ (approx.)
β-Zn_3Li_2	Li2Z	Zn3Li2	β-Li_2Zn_3
σ-CrMn	HSig	High_Sigma	~Cr_2Mn_7
$Ca(Mg,Zn)_5$	IM1	IM1-CaMgZn	$CaMg_4Zn$, $CaMgZn_4$
$(Li,Mg)_{17}Sn_4$	L17X	cF420 Prototype-Li17Pb4	$Li_{17}Sn_4$
γ-$AgMg_4$	hP_G	AgMg4 gamma_hp	γ-$AgMg_4$
$Ag_{17}Mg_{54}$	A17M	oP142 Prototype-Hf54Os17	$Ag_{17}Mg_{54}$
Li_2Ag	L2A	Prototype-Li2Ag	~Li_2Ag
Li_3Ag	L3A	Prototype-Li3Ag	~Li_3Ag
Li_6Ag	L6A	Prototype-Li6Ag	~Li_6Ag
$(Co,Fe)_6W_6C$	M12C	cF104 Prototype-Fe6W6C	$(Co,Fe)_6W_6C$
$Mn_{11}Si_{19}$	NCL1	tP20 Prototype-Mn11Si19	$Mn_{11}(Si,Al)_{19}$ Nowotny Chimney Ladder Phase
$Al_{63}Mo_{37}$	AM8	AM8 Al63Mo37	$Al_{63}Mo_{37}$
"As_3P_2" or "AsP"	AsP	AsP-orthorhombic	~"As_3P_2"
γ_1-FeZn	Gam1	FeZn-Gamma-1	$Fe_7(Fe,Zn)_6Zn_{38}$
δ_1-FeZn	FeZ2	FeZn-delta-1	$Fe(Al,Fe,Zn)_3Zn_{13}$
$(Cu,Ni)S_2$	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	$(Fe,Ni)_3Te_2$
M_4AlC_3	MAX2	MAX2 Prototype-CsYb3Se4	$(Cr,Nb,Ti,V)AlC_3$

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

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FScopp83 database
1077 compounds,  1442 phases

Ag                          FScopp83   S1   S2   S3   S4   S5   L
Ag11Hg15                    FScopp83   S
Ag11Hg9                     FScopp83   S
Ag2Ca                       FScopp83   S
Ag2Ga                       FScopp83   S
Ag2O                        FScopp83   S
Ag2S                        FScopp83   S1   S2   S3
Ag2Se                       FScopp83   S1   S2
Ag2Te                       FScopp83   S1   S2   S3
'Ag3Be8'                    FScopp83   S                                (Ag)2.97(Be)8.03
Ag3Ca5                      FScopp83   S
Ag3CuS2                     FScopp83   S
Ag3Ga2                      FScopp83   S
Ag3P11                      FScopp83   S
Ag3Sb                       FScopp83   S
Ag5Cu3S4                    FScopp83   S
Ag5Te3                      FScopp83   S1   S2
Ag7Ca2                      FScopp83   S
Ag8SnS6                     FScopp83   S1   S2
Ag9Ca2                      FScopp83   S
AgCa                        FScopp83   S
AgCa3                       FScopp83   S
AgCd                        FScopp83   S
AgCu4Zr                     FScopp83   S
AgCuS                       FScopp83   S
AgMg4                       FScopp83   S
AgP2                        FScopp83   S
AgTi2                       FScopp83   S
AgZr                        FScopp83   S
AgZr2                       FScopp83   S
Al                          FScopp83   S1   S2   S3   S4   S5   S6   S7   ...  L1   L
Al10V                       FScopp83   S
Al116Cr63Si21               FScopp83   S
Al11Cr2                     FScopp83   S
Al11Cu5Mn3                  FScopp83   S
Al11Fe3Si6                  FScopp83   S
Al11Mn3Zn2                  FScopp83   S
Al11Mn4                     FScopp83   S
Al12Mn                      FScopp83   S
Al12Mo                      FScopp83   S
Al12W                       FScopp83   S
Al13Co4                     FScopp83   S
Al13Cr4Si4                  FScopp83   S
Al14Ca13                    FScopp83   S
Al14Fe3Si3                  FScopp83   S
Al15Cu8Li2                  FScopp83   S
Al17Mo4                     FScopp83   S
Al18Cr2Mg3                  FScopp83   S
Al18Mg3Mn2                  FScopp83   S
Al18Mg3Mo2                  FScopp83   S
Al18Mg3Ti2                  FScopp83   S
Al18Mg3V2                   FScopp83   S
Al18Mg3W2                   FScopp83   S
Al21Pt5                     FScopp83   S
Al21Pt8                     FScopp83   S
Al22Mo5                     FScopp83   S
Al23CuFe4                   FScopp83   S
Al23V4                      FScopp83   S
Al2Au                       FScopp83   S
Al2Ca                       FScopp83   S1   S2
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Al2CaZn2	FScopp83	S				
Al2Cu	FScopp83	S1	S2	S3		
Al2Cu3	FScopp83	S				
Al2CuLi	FScopp83	S				
Al2CuMg	FScopp83	S				
Al2Fe	FScopp83	S				
Al2Li	FScopp83	S1	S2			
Al2Li18Si6	FScopp83	S				
Al2Li3	FScopp83	S				
Al2Mn2Si3	FScopp83	S				
Al2O3	FScopp83	S1	S2	S3	S4	
Al2Pt	FScopp83	S				
Al2S3	FScopp83	S				
Al2Se3	FScopp83	S				
Al2Ti	FScopp83	S1	S2			
Al2W	FScopp83	S				
Al2Zr	FScopp83	S				
Al2Zr3	FScopp83	S				
Al30Mg23	FScopp83	S				
Al39Cu33Zr6	FScopp83	S				
Al3Ca8	FScopp83	S				
Al3Co	FScopp83	S				
Al3Cr	FScopp83	S1	S2			
Al3Cu	FScopp83	S				
Al3Cu2	FScopp83	S				
Al3Li	FScopp83	S1	S2	S3		
Al3Li15Si6	FScopp83	S				
Al3Li7Si4	FScopp83	S				
Al3Mg	FScopp83	S				
Al3MnSi2	FScopp83	S				
Al3Mo	FScopp83	S				
Al3Nb	FScopp83	S				
Al3Ni	FScopp83	S				
Al3Ni5	FScopp83	S				
Al3Pt2	FScopp83	S				
Al3Pt5	FScopp83	S				
Al3Ti	FScopp83	S1	S2	S3	S4	
Al3V	FScopp83	S1	S2	S3		
Al3Zr	FScopp83	S1	S2	S3		
Al3Zr2	FScopp83	S				
Al3Zr5	FScopp83	S				
Al4C3	FScopp83	S				
Al4C4Si	FScopp83	S				
Al4Ca	FScopp83	S				
Al4Cr	FScopp83	S				
Al4Fe	FScopp83	S				
Al4Li9	FScopp83	S				
Al4Mn	FScopp83	S				
Al4Mo	FScopp83	S				
Al4W	FScopp83	S				
Al4Zr5	FScopp83	S				
Al53Mg14Li33	FScopp83	S				
Al57Cu11Li32	FScopp83	S				
Al5Co2	FScopp83	S				
Al5Cu2Mg8Si6	FScopp83	S				
Al5Cu6Mg2	FScopp83	S				
'Al5CuLi3'	FScopp83	S				(Al)4.95(Cu)1.053(Li)2.997
Al5Li	FScopp83	S				
Al5Mo	FScopp83	S				
Al5W	FScopp83	S				
Al63Mo37	FScopp83	S				
Al6Fe	FScopp83	S				
Al6Mn	FScopp83	S				
Al6Ni3Si	FScopp83	S				
Al77W23	FScopp83	S				

Al7Cr	FScopp83	S						
Al7Cu2Fe	FScopp83	S						
Al7Cu2Zr	FScopp83	S						
Al7Cu3Mg6	FScopp83	S						
Al7CuFe2	FScopp83	S						
Al7CuMn2	FScopp83	S						
Al7CuZr2	FScopp83	S						
Al7W3	FScopp83	S						
Al8C7Si	FScopp83	S						
Al8Cr5	FScopp83	S1	S2					
Al8CrTi3	FScopp83	S						
Al8FeMg3Si6	FScopp83	S						
Al8Mo3	FScopp83	S						
Al8V5	FScopp83	S						
Al99Mn23	FScopp83	S						
Al9Co2	FScopp83	S						
Al9Cr3Si	FScopp83	S						
Al9Cr4	FScopp83	S1	S2					
Al9Cu11	FScopp83	S						
AlAs	FScopp83	S						
AlAu	FScopp83	S						
AlAu2	FScopp83	S						
AlAu4	FScopp83	S						
AlCa5Zn2	FScopp83	S						
AlCo	FScopp83	S						
AlCr2	FScopp83	S						
AlCu	FScopp83	S1	S2					
AlCu2	FScopp83	S						
AlCu3Mn2	FScopp83	S						
AlH3	FScopp83	S						
AlLi	FScopp83	S1	S2					
AlLiSi	FScopp83	S						
AlMg	FScopp83	S						
AlMgAg	FScopp83	S						
AlMo3	FScopp83	S						
AlNaSi	FScopp83	S						
AlP	FScopp83	S						
AlPt	FScopp83	S						
AlPt2	FScopp83	S1	S2					
AlPt3	FScopp83	S						
AlSb	FScopp83	S						
AlSn2Zr5	FScopp83	S						
AlTi	FScopp83	S						
AlZr	FScopp83	S1	S2					
AlZr2	FScopp83	S						
AlZr3	FScopp83	S1	S2					
As	FScopp83	S1	S2	S3	S4	S5	L	
'As2Cu5'	FScopp83	S						(As)2.058(Cu)4.942
As2S3	FScopp83	S						
As2S5	FScopp83	S						
As2Te3	FScopp83	S						
As4S3	FScopp83	S1	S2					
As4S4	FScopp83	S1	S2					
AsCu8	FScopp83	S						
AsIn	FScopp83	S						
Au	FScopp83	S1	S2	S3	L			
Au2Bi	FScopp83	S						
Au2Pb	FScopp83	S						
Au2Ti	FScopp83	S						
Au3In	FScopp83	S						
Au3Sn12Co5	FScopp83	S						
'Au4Zn5'	FScopp83	S						(Au)3.96(Zn)5.04
Au5Zn3	FScopp83	S						
Au7Ga2	FScopp83	S						
Au7Ga3	FScopp83	S						

Au7In3	FScopp83	S					
Au8Al3	FScopp83	S					
'Au8Ga2'	FScopp83	S					(Au)7.89476(Ga)2.10526
AuGa	FScopp83	S					
AuGa2	FScopp83	S					
AuIn	FScopp83	S					
AuIn2	FScopp83	S					
AuSb2	FScopp83	S					
AuSn	FScopp83	S					
AuSn2	FScopp83	S					
AuSn4	FScopp83	S					
AuTe2	FScopp83	S					
AuTi	FScopp83	S1	S2				
AuTi3	FScopp83	S					
AuZn3	FScopp83	S					
Be	FScopp83	S1	S2	S3	L		
Bi	FScopp83	S1	S2	S3	S4	L	
Bi2S3	FScopp83	S					
Bi2Te	FScopp83	S					
Bi3In5	FScopp83	S					
Bi3Ni	FScopp83	S					
Bi4Te3	FScopp83	S					
BiIn	FScopp83	S					
BiIn2	FScopp83	S					
BiLi	FScopp83	S					
BiNa	FScopp83	S					
C	FScopp83	S1	S2	L			
Ca	FScopp83	S1	S2	S3	L		
Ca11Ga7	FScopp83	S					
Ca14Si19	FScopp83	S					
Ca25Ga59	FScopp83	S					
Ca28Ga11	FScopp83	S					
Ca2Cu	FScopp83	S					
Ca2Ge	FScopp83	S					
Ca2Mg55Zn43	FScopp83	S					
Ca2Mg5Zn13	FScopp83	S					
Ca2Ni7	FScopp83	S					
Ca2Pb	FScopp83	S					
Ca2Si	FScopp83	S					
Ca2Sn	FScopp83	S					
Ca3Ga5	FScopp83	S					
Ca3Ga8	FScopp83	S					
Ca3Mg3Zn14	FScopp83	S					
Ca3P2	FScopp83	S					
Ca3Si4	FScopp83	S					
Ca3Zn	FScopp83	S					
Ca4Al3Mg	FScopp83	S					
Ca5Ga3	FScopp83	S					
Ca5Ge3	FScopp83	S					
Ca5Pb3	FScopp83	S					
Ca5Si3	FScopp83	S					
Ca5Zn3	FScopp83	S					
Ca7Ge6	FScopp83	S					
Ca7Mg6Si14	FScopp83	S					
Ca7Sn6	FScopp83	S					
CaAl2Si2	FScopp83	S					
CaAlH5	FScopp83	S					
CaBe13	FScopp83	S					
CaC2	FScopp83	S1	S2	S3	S4	L	
CaCr2Al20	FScopp83	S					
CaCu	FScopp83	S					
CaCu5	FScopp83	S					
CaGa	FScopp83	S					
CaGa2	FScopp83	S1	S2				
CaGa4	FScopp83	S1	S2				

CaGe2	FScopp83	S					
CaH2	FScopp83	S					
CaLi2	FScopp83	S					
CaMgSi	FScopp83	S					
CaNi2	FScopp83	S					
CaNi3	FScopp83	S					
CaNi5	FScopp83	S					
CaO	FScopp83	S					
CaPb	FScopp83	S					
CaPb3	FScopp83	S					
CaS	FScopp83	S					
CaSi	FScopp83	S					
CaSi2	FScopp83	S					
CaTi2Al20	FScopp83	S					
CaZn	FScopp83	S					
CaZn11	FScopp83	S					
CaZn13	FScopp83	S					
CaZn2	FScopp83	S					
CaZn3	FScopp83	S					
CaZn5	FScopp83	S					
Cd	FScopp83	S1	S2	S3	S4	L	
Cd10Cu3	FScopp83	S					
Cd11Na2	FScopp83	S					
Cd2Na	FScopp83	S					
Cd3As2	FScopp83	S1	S2	S3	S4		
Cd3Cu4	FScopp83	S					
Cd3In	FScopp83	S					
Cd3P2	FScopp83	S1	S2	S3			
Cd5Ni	FScopp83	S					
Cd6P7	FScopp83	S					
Cd7P10	FScopp83	S					
Cd8Cu5	FScopp83	S					
CdAs2	FScopp83	S					
CdCu2	FScopp83	S					
CdNi	FScopp83	S					
CdP2	FScopp83	S1	S2				
CdP4	FScopp83	S					
CdS	FScopp83	S					
CdSb	FScopp83	S					
CdTi	FScopp83	S					
CdTi2	FScopp83	S					
Co	FScopp83	S1	S2	S3	S4	S5	L
Co11Zr2	FScopp83	S					
Co16Nb9	FScopp83	S					
Co23C6	FScopp83	S					
Co23Zr6	FScopp83	S					
Co2Nb	FScopp83	S					
Co2P	FScopp83	S					
Co2Si	FScopp83	S					
Co2Ti	FScopp83	S1	S2	S3			
Co2Zr	FScopp83	S					
Co3C2	FScopp83	S					
Co3Mo	FScopp83	S					
Co3Nb	FScopp83	S					
Co3S4	FScopp83	S					
Co3Si	FScopp83	S					
Co3Sn2	FScopp83	S1	S2				
Co3V	FScopp83	S					
Co3W	FScopp83	S					
Co4Zn9	FScopp83	S					
Co6W6C	FScopp83	S					
Co7C3	FScopp83	S					
Co7Nb2	FScopp83	S					
Co9S8	FScopp83	S					
CoGa3	FScopp83	S					

CoIn2	FScopp83	S							
CoIn3	FScopp83	S							
CoO	FScopp83	S							
CoP	FScopp83	S							
CoS	FScopp83	S							
CoS2	FScopp83	S							
CoSb	FScopp83	S							
CoSb2	FScopp83	S							
CoSb3	FScopp83	S							
CoSe2	FScopp83	S							
CoSi	FScopp83	S							
CoSi2	FScopp83	S							
CoSn	FScopp83	S							
CoSn2	FScopp83	S							
CoTe	FScopp83	S							
CoTe2	FScopp83	S							
CoTi2	FScopp83	S							
CoV3	FScopp83	S							
CoZn7	FScopp83	S							
CoZr2	FScopp83	S							
CoZr3	FScopp83	S							
Cr	FScopp83	S1	S2	S3	S4	S5	S6	L	
Cr23C6	FScopp83	S							
Cr2AlC	FScopp83	S							
Cr2C	FScopp83	S							
Cr2O3	FScopp83	S							
Cr2P	FScopp83	S							
Cr2S3	FScopp83	S							
Cr2Ti	FScopp83	S1	S2						
Cr2Zr	FScopp83	S1	S2	S3					
Cr3C	FScopp83	S							
Cr3C2	FScopp83	S							
Cr3Ga	FScopp83	S1	S2						
Cr3Mn5	FScopp83	S							
Cr3P	FScopp83	S							
Cr3S4	FScopp83	S1	S2						
Cr3Si	FScopp83	S							
'Cr4S6'	FScopp83	S							(Cr)4.1(S)5.9
Cr5S6	FScopp83	S							
Cr5Si3	FScopp83	S1	S2	S3					
Cr7C3	FScopp83	S							
Cr7S8	FScopp83	S							
CrGa4	FScopp83	S							
CrS	FScopp83	S1	S2						
CrSi	FScopp83	S							
CrSi2	FScopp83	S							
CrZn13	FScopp83	S							
CrZn17	FScopp83	S							
Cu	FScopp83	S1	S2	S3	S4	L			
'Cu10Sn3'	FScopp83	S							(Cu)9.997(Sn)3.003
Cu10Zr7	FScopp83	S							
Cu11Fe2S13	FScopp83	S							
Cu15Si4	FScopp83	S							
Cu16Mg6Si7	FScopp83	S							
Cu19Si6	FScopp83	S							
Cu2Mg	FScopp83	S1	S2	S3					
Cu2O	FScopp83	S							
Cu2P	FScopp83	S							
Cu2S	FScopp83	S1	S2	S3	S4				
Cu2Sb	FScopp83	S							
Cu2Se	FScopp83	S1	S2						
Cu2SiS3	FScopp83	S1	S2						
Cu2Te	FScopp83	S1	S2	S3	S4	S5	S6		
Cu2Ti	FScopp83	S							
Cu2TiZr	FScopp83	S							

Cu2Zr	FScopp83	S							
Cu33Si7	FScopp83	S							
'Cu3As'	FScopp83	S							(Cu)2.94(As)1.06
Cu3FeS4	FScopp83	S							
Cu3FeS8	FScopp83	S							
Cu3Ge	FScopp83	S							
Cu3Mg2Si	FScopp83	S							
Cu3P	FScopp83	S1	S2						
Cu3Sb	FScopp83	S1	S2						
Cu3Se2	FScopp83	S							
Cu3Sn	FScopp83	S1	S2						
Cu3Ti2	FScopp83	S							
Cu4Fe5S8	FScopp83	S							
Cu4In	FScopp83	S							
Cu4Sb	FScopp83	S							
'Cu4Sn'	FScopp83	S							(Cu)3.94(Sn)1.06
Cu4Ti3	FScopp83	S							
Cu51Zr14	FScopp83	S							
Cu5Zr8	FScopp83	S							
'Cu6Sb'	FScopp83	S							(Cu)5.95(Sb)1.05
'Cu6Sn5'	FScopp83	S							(Cu)5.995(Sn)5.005
Cu7Ga2	FScopp83	S							
Cu7In3	FScopp83	S							
'Cu7In4'	FScopp83	S							(Cu)7.04(In)3.96
Cu7S4	FScopp83	S							
'Cu7Sb2'	FScopp83	S							(Cu)6.93(Sb)2.07
Cu8SiS6	FScopp83	S							
Cu8Zr3	FScopp83	S							
Cu9Fe8S16	FScopp83	S							
Cu9Fe9S16	FScopp83	S							
Cu9S8	FScopp83	S							
Cu9Si2	FScopp83	S							
Cu9Zr2	FScopp83	S							
CuAsS	FScopp83	S							
CuBe2	FScopp83	S							
CuFe2S3	FScopp83	S							
CuFeS2	FScopp83	S							
CuH	FScopp83	S							
CuNi2S6	FScopp83	S							
CuO	FScopp83	S							
CuP2	FScopp83	S							
CuS	FScopp83	S							
CuS2	FScopp83	S1	S2						
CuSe	FScopp83	S1	S2	S3					
CuSe2	FScopp83	S1	S2						
CuTe	FScopp83	S							
CuTi2	FScopp83	S							
CuZr	FScopp83	S							
CuZr2	FScopp83	S							
Fe	FScopp83	S1	S2	S3	S4	S5	S6	S7	L
Fe10S11	FScopp83	S							
Fe11S12	FScopp83	S							
Fe2Mo	FScopp83	S							
Fe2MoC	FScopp83	S							
Fe2Nb	FScopp83	S							
Fe2O3	FScopp83	S							
Fe2P	FScopp83	S							
Fe2S	FScopp83	S1	S2	S3					
Fe2S3	FScopp83	S							
Fe2Si	FScopp83	S							
Fe2SiS4	FScopp83	S							
Fe2Ti	FScopp83	S							
Fe2W	FScopp83	S							
Fe3C	FScopp83	S1	S2						
Fe3C2	FScopp83	S							

Fe3O4	FScopp83	S1	S2	S3	S4			
Fe3P	FScopp83	S						
Fe3S4	FScopp83	S1	S2					
Fe3Si	FScopp83	S						
Fe3Sn2	FScopp83	S						
Fe5C2	FScopp83	S1	S2					
Fe5Si3	FScopp83	S1	S2					
Fe5Sn3	FScopp83	S1	S2	S3				
Fe60Te71	FScopp83	S						
Fe6W6C	FScopp83	S						
Fe7C3	FScopp83	S						
Fe7S6	FScopp83	S						
'Fe7S8'	FScopp83	S						(Fe)7.016(S)8
Fe7W6	FScopp83	S						
Fe9S10	FScopp83	S						
Fe9S8	FScopp83	S1	S2					
FeBe12	FScopp83	S						
FeBe2	FScopp83	S						
FeBe5	FScopp83	S						
FeCr2S4	FScopp83	S						
FeP	FScopp83	S						
FeP2	FScopp83	S						
FeP4	FScopp83	S						
FeS	FScopp83	S1	S2					
FeS2	FScopp83	S1	S2					
FeSb	FScopp83	S						
FeSb2	FScopp83	S						
FeSe2	FScopp83	S						
FeSi	FScopp83	S1	S2	S3				
FeSi2	FScopp83	S1	S2	S3				
FeSn	FScopp83	S1	S2					
FeSn2	FScopp83	S						
FeSn2Zr6	FScopp83	S						
FeTe	FScopp83	S						
FeTe2	FScopp83	S1	S2					
FeTi	FScopp83	S						
Ga	FScopp83	S1	S2	S3	S4	S5	L	
Ga2Cu	FScopp83	S						
Ga2Pt	FScopp83	S1	S2					
Ga2Te3	FScopp83	S						
Ga2Te5	FScopp83	S						
Ga2Ti	FScopp83	S						
Ga2Zr	FScopp83	S						
Ga2Zr3	FScopp83	S						
Ga39Na22	FScopp83	S						
Ga3Pt2	FScopp83	S						
Ga3Pt5	FScopp83	S						
Ga3Te4	FScopp83	S						
Ga3Ti	FScopp83	S						
Ga3Ti2	FScopp83	S						
Ga3Ti5	FScopp83	S						
Ga3Zr	FScopp83	S						
Ga3Zr2	FScopp83	S						
Ga3Zr5	FScopp83	S						
Ga4Cr3	FScopp83	S						
Ga4Cu9	FScopp83	S						
Ga4Na	FScopp83	S						
Ga4Zr5	FScopp83	S						
Ga5Zr3	FScopp83	S						
Ga6Pt	FScopp83	S						
Ga6SnTe10	FScopp83	S						
Ga7Pt3	FScopp83	S						
Ga8Mo3	FScopp83	S						
GaAs	FScopp83	S						
GaCr	FScopp83	S						

GaP	FScopp83	S				
GaPt	FScopp83	S				
GaPt2	FScopp83	S				
GaPt3	FScopp83	S1	S2	S3		
GaSb	FScopp83	S				
GaTe	FScopp83	S				
GaZr	FScopp83	S1	S2			
GaZr2	FScopp83	S				
Ge	FScopp83	S1	S2	S3	L	
GeAs	FScopp83	S				
GeAs2	FScopp83	S				
GeCa	FScopp83	S				
GeP	FScopp83	S				
GeTe	FScopp83	S				
H	FScopp83	S	L			
Hg	FScopp83	S1	S2	S3	S4	L
Hg3Zn	FScopp83	S				
Hg6Cu7	FScopp83	S				
HgMg	FScopp83	S				
HgMg3	FScopp83	S				
HgPb2	FScopp83	S				
HgS	FScopp83	S1	S2			
HgSn38	FScopp83	S				
HgSn4	FScopp83	S				
HgSn7	FScopp83	S				
HgZn2	FScopp83	S				
HgZn3	FScopp83	S				
In	FScopp83	S1	S2	S3	L	
In2Ag	FScopp83	S				
In2Ca	FScopp83	S				
In2Li3	FScopp83	S				
In2Pt	FScopp83	S				
In2Pt3	FScopp83	S1	S2			
In2Se3	FScopp83	S1	S2	S3	S4	
In3Li13	FScopp83	S				
In3Pt2	FScopp83	S				
In4Se3	FScopp83	S				
In5Na3	FScopp83	S				
In5Pt6	FScopp83	S				
In5Se7	FScopp83	S				
In6Se7	FScopp83	S				
In7Pt3	FScopp83	S				
In9Na5	FScopp83	S				
In9Pt13	FScopp83	S				
In9Se11	FScopp83	S				
InAg3	FScopp83	S				
InCa3	FScopp83	S				
InLi2	FScopp83	S				
InLi6	FScopp83	S				
InMg2	FScopp83	S				
InNa	FScopp83	S				
InNa2	FScopp83	S				
InP	FScopp83	S				
InPt	FScopp83	S				
InPt2	FScopp83	S				
InSb	FScopp83	S				
InSe	FScopp83	S				
Li	FScopp83	S1	S2	S3	L	
Li12Si7	FScopp83	S				
Li13Si4	FScopp83	S				
Li22Si5	FScopp83	S				
Li2Ga	FScopp83	S				
Li2Ga7	FScopp83	S				
Li2O	FScopp83	S				
Li2Sb	FScopp83	S				

Li3AlH6	FScopp83	S						
Li3Bi	FScopp83	S						
Li3Ga14	FScopp83	S						
Li3Ga2	FScopp83	S						
Li3Ga8	FScopp83	S						
Li3Sb	FScopp83	S1	S2					
Li5Ga4	FScopp83	S						
Li5Ga9	FScopp83	S						
Li7Si3	FScopp83	S						
LiAlH4	FScopp83	S						
LiGa	FScopp83	S						
LiH	FScopp83	S						
LiPb	FScopp83	S1	S2					
LiZn	FScopp83	S						
LiZn4	FScopp83	S						
Mg	FScopp83	S1	S2	S3	S4	S5	S6	S7	L
Mg11Si7Al3	FScopp83	S						
Mg12Zn13	FScopp83	S						
Mg2Ca	FScopp83	S1	S2					
Mg2Cu	FScopp83	S1	S2					
Mg2Ga	FScopp83	S						
Mg2Ga5	FScopp83	S						
Mg2Ge	FScopp83	S						
Mg2Ni	FScopp83	S						
Mg2Pb	FScopp83	S						
Mg2Pt	FScopp83	S						
Mg2Si	FScopp83	S						
Mg2Si6Al3	FScopp83	S1	S2					
Mg2Sn	FScopp83	S						
Mg2Zn	FScopp83	S						
Mg2Zn11	FScopp83	S						
Mg2Zn3	FScopp83	S						
Mg3Bi2	FScopp83	S1	S2					
Mg3P2	FScopp83	S						
Mg3Pt	FScopp83	S						
Mg3Sb2	FScopp83	S1	S2					
Mg3Si6Al2	FScopp83	S1	S2					
Mg4Si4Al4	FScopp83	S						
Mg4Si6Al	FScopp83	S1	S2					
Mg4Si6Al2	FScopp83	S						
Mg4Si7	FScopp83	S						
Mg4Si8	FScopp83	S						
Mg51Zn20	FScopp83	S						
Mg5Ga2	FScopp83	S						
Mg5In2	FScopp83	S						
Mg5Si6	FScopp83	S1	S2					
Mg6Pt	FScopp83	S						
Mg6Si3	FScopp83	S						
Mg6Si4	FScopp83	S						
Mg9Si5	FScopp83	S						
Mg9Si7Al3	FScopp83	S						
Mg9Si7Al5	FScopp83	S						
Mg9Si9Al3	FScopp83	S						
MgAl2O4	FScopp83	S						
MgBe13	FScopp83	S						
MgCo2	FScopp83	S						
MgGa	FScopp83	S						
MgGa2	FScopp83	S						
MgH2	FScopp83	S						
MgNi2	FScopp83	S						
MgO	FScopp83	S						
MgPt	FScopp83	S						
MgPt3	FScopp83	S						
MgPt7	FScopp83	S						
MgS	FScopp83	S						

MgSi	FScopp83	S							
MgSi2Al2	FScopp83	S							
MgSi6Al4	FScopp83	S1	S2						
MgZn2	FScopp83	S1	S2						
Mn	FScopp83	S1	S2	S3	S4	S5	S6	L	
Mn11Si19	FScopp83	S							
Mn19Sn6	FScopp83	S							
Mn23C6	FScopp83	S							
Mn2Bi	FScopp83	S							
Mn2CaAl10	FScopp83	S							
Mn2P	FScopp83	S							
Mn2Sb	FScopp83	S1	S2						
Mn2Sn	FScopp83	S							
Mn2Ti	FScopp83	S							
Mn2Ti2	FScopp83	S							
Mn2Zr	FScopp83	S							
Mn3AlC	FScopp83	S							
Mn3C	FScopp83	S							
Mn3C2	FScopp83	S							
Mn3Ni	FScopp83	S							
Mn3P	FScopp83	S							
Mn3Si	FScopp83	S							
Mn3Ti	FScopp83	S							
Mn5C2	FScopp83	S							
Mn5Si3	FScopp83	S1	S2						
Mn5SiC	FScopp83	S							
Mn5Sn3	FScopp83	S							
Mn6Si	FScopp83	S							
Mn7C3	FScopp83	S							
Mn7Mo6	FScopp83	S							
Mn8Si2C	FScopp83	S							
Mn9Si2	FScopp83	S							
'Mn9Ti2'	FScopp83	S							(Mn)8.965(Ti)2.035
MnBe12	FScopp83	S							
MnBe2	FScopp83	S							
MnBe5	FScopp83	S							
MnBi	FScopp83	S							
MnCa4Al7	FScopp83	S							
MnNi2	FScopp83	S							
MnNi3	FScopp83	S							
MnO	FScopp83	S							
MnP	FScopp83	S							
MnS	FScopp83	S1	S2						
MnS2	FScopp83	S							
MnSe2	FScopp83	S							
MnSi	FScopp83	S							
MnSn2	FScopp83	S							
'MnTi'	FScopp83	S							(Mn)1.03(Ti)0.97
Mo	FScopp83	S1	S2	S3	L				
Mo23C6	FScopp83	S							
Mo2C	FScopp83	S							
Mo2S3	FScopp83	S1	S2						
Mo2Zr	FScopp83	S							
Mo3Ga	FScopp83	S							
Mo3Ni11	FScopp83	S							
Mo3P	FScopp83	S1	S2						
Mo3Si	FScopp83	S							
Mo4Ni3	FScopp83	S							
Mo5Si3	FScopp83	S							
Mo5Sn3	FScopp83	S							
MoC	FScopp83	S							
MoGa4	FScopp83	S							
MoNi4	FScopp83	S							
MoP	FScopp83	S							
MoPt	FScopp83	S							

MoPt2	FScopp83	S					
MoS2	FScopp83	S					
MoSe2	FScopp83	S					
MoSi2	FScopp83	S1	S2				
MoTe2	FScopp83	S					
MoZn22	FScopp83	S					
MoZn7	FScopp83	S					
Na	FScopp83	S1	S2	S3	L		
Na2C2	FScopp83	S1	S2				
Na2LiAlH6	FScopp83	S					
Na2O	FScopp83	S1	S2	S3			
Na2S	FScopp83	S					
Na2Te	FScopp83	S					
Na3AlH6	FScopp83	S1	S2				
Na3As	FScopp83	S					
Na3Bi	FScopp83	S					
Na3Ge	FScopp83	S					
Na3P	FScopp83	S					
Na3Sb	FScopp83	S					
NaAlH4	FScopp83	S					
NaGe	FScopp83	S					
NaH	FScopp83	S					
NaMgH3	FScopp83	S					
NaSi	FScopp83	S					
NaTe	FScopp83	S					
NaTe3	FScopp83	S					
NaZn13	FScopp83	S					
Nb	FScopp83	S	L				
Nb2AlC	FScopp83	S					
Nb2C	FScopp83	S					
Nb2Zn3	FScopp83	S					
Nb3C2	FScopp83	S					
Nb3P	FScopp83	S					
Nb4FeSi	FScopp83	S					
Nb5Si3	FScopp83	S1	S2				
Nb5Sn3	FScopp83	S					
Nb6Fe7	FScopp83	S					
NbNi8	FScopp83	S					
NbS2	FScopp83	S					
NbSe2	FScopp83	S					
NbSn2	FScopp83	S					
NbZn	FScopp83	S					
NbZn12Fe	FScopp83	S					
NbZn15	FScopp83	S					
NbZn2	FScopp83	S					
NbZn3	FScopp83	S					
NbZn7	FScopp83	S					
Ni	FScopp83	S1	S2	S3	S4	S5	L
Ni10Mn3Si7	FScopp83	S					
Ni11As8	FScopp83	S					
Ni12P5	FScopp83	S					
Ni13Ga9	FScopp83	S					
Ni16Mn6Si7	FScopp83	S					
Ni16Si7Ti6	FScopp83	S					
Ni20Te17	FScopp83	S					
Ni23C6	FScopp83	S					
Ni2Cr	FScopp83	S					
Ni2Ga	FScopp83	S					
Ni2Ga3	FScopp83	S					
Ni2Ge	FScopp83	S1	S2				
Ni2In	FScopp83	S					
Ni2In3	FScopp83	S					
Ni2Mg3Al	FScopp83	S					
Ni2Mn3Si	FScopp83	S					
Ni2MnMg3	FScopp83	S					

Ni2Mo	FScopp83	S		
Ni2P	FScopp83	S		
Ni2S	FScopp83	S		
Ni2Si	FScopp83	S1	S2	
Ni2Te	FScopp83	S		
Ni2V	FScopp83	S		
Ni3Ga	FScopp83	S		
Ni3Ga4	FScopp83	S		
Ni3Ga7	FScopp83	S		
Ni3Ge	FScopp83	S		
Ni3In	FScopp83	S		
Ni3In7	FScopp83	S		
Ni3Mo	FScopp83	S		
Ni3P	FScopp83	S		
Ni3S2	FScopp83	S		
Ni3S4	FScopp83	S		
Ni3Sb	FScopp83	S1	S2	
Ni3Si	FScopp83	S1	S2	
Ni3Si2	FScopp83	S		
Ni3SiTi2	FScopp83	S		
Ni3Sn	FScopp83	S1	S2	
Ni3Sn2	FScopp83	S		
Ni3Ti	FScopp83	S		
Ni3V	FScopp83	S		
Ni49Si37Ti14	FScopp83	S		
Ni4Si7Ti4	FScopp83	S		
Ni4W	FScopp83	S		
Ni52Te40	FScopp83	S		
Ni5As2	FScopp83	S		
Ni5Ga3	FScopp83	S		
Ni5Ge2	FScopp83	S		
Ni5Ge3	FScopp83	S		
Ni5P2	FScopp83	S		
Ni5Sb2	FScopp83	S		
Ni5Si2	FScopp83	S		
'Ni5Zr4'	FScopp83	S		(Ni)4.95(Zr)4.05
Ni6P5	FScopp83	S		
Ni7S6	FScopp83	S		
'Ni7Zr2'	FScopp83	S		(Ni)7.02(Zr)1.98
'Ni8Zr3'	FScopp83	S		(Ni)7.975(Zr)3.025
Ni9Mn3Si8	FScopp83	S		
Ni9S8	FScopp83	S1	S2	
NiAs	FScopp83	S		
NiAs2	FScopp83	S1	S2	
NiAsS	FScopp83	S		
NiFe2S4	FScopp83	S		
NiGa	FScopp83	S1	S2	
NiGe	FScopp83	S1	S2	
NiIn	FScopp83	S		
NiMnSi	FScopp83	S		
NiO	FScopp83	S		
NiP2	FScopp83	S		
NiS	FScopp83	S1	S2	
NiS2	FScopp83	S		
NiSb	FScopp83	S		
NiSb2	FScopp83	S		
NiSe2	FScopp83	S		
NiSi	FScopp83	S1	S2	
NiSi2	FScopp83	S		
NiSi4Ti4	FScopp83	S		
NiSiTi	FScopp83	S		
NiSn	FScopp83	S1	S2	
NiTe	FScopp83	S		
NiTe2	FScopp83	S		
NiTi2	FScopp83	S1	S2	

NiV3	FScopp83	S							
NiW	FScopp83	S							
NiW2	FScopp83	S							
NiZn8	FScopp83	S							
NiZr	FScopp83	S							
NiZr2	FScopp83	S							
P	FScopp83	S1	S2	S3	S4	L			
Pb	FScopp83	S1	S2	S3	S4	S5	S6	S7	L
Pb2Au	FScopp83	S							
'Pb2Pd'	FScopp83	S							(Pb)2.001(Pd)0.999
'Pb2Pd3'	FScopp83	S							(Pb)2.05(Pd)2.95
Pb2Zr	FScopp83	S							
Pb3Au	FScopp83	S							
Pb3O4	FScopp83	S							
Pb3Pd5	FScopp83	S							
Pb3Zr5	FScopp83	S							
Pb5Li22	FScopp83	S							
PbO	FScopp83	S1	S2						
PbO2	FScopp83	S							
PbPd	FScopp83	S							
PbPd3	FScopp83	S							
PbS	FScopp83	S							
PbSe	FScopp83	S							
PbTe	FScopp83	S							
PbZr4	FScopp83	S							
Pd	FScopp83	S1	S2	L					
Pd2Ti	FScopp83	S							
Pd3Ti	FScopp83	S							
Pd3Ti2	FScopp83	S							
Pd5Ti3	FScopp83	S							
PdTi	FScopp83	S1	S2						
PdTi2	FScopp83	S							
Pt	FScopp83	S1	S2	L					
Pt17Si8	FScopp83	S1	S2						
Pt25Si7	FScopp83	S							
Pt2Ge	FScopp83	S							
Pt2Ge3	FScopp83	S							
Pt2Si	FScopp83	S1	S2						
Pt2Sn3	FScopp83	S							
Pt2V	FScopp83	S							
Pt3Ge	FScopp83	S							
Pt3Ge2	FScopp83	S							
Pt3Pb	FScopp83	S							
Pt3Si	FScopp83	S1	S2						
Pt3Sn	FScopp83	S							
Pt3Ti	FScopp83	S							
Pt3Ti4	FScopp83	S							
Pt5Si2	FScopp83	S							
Pt6Si5	FScopp83	S							
Pt8Ti	FScopp83	S							
PtAs2	FScopp83	S							
PtGe	FScopp83	S							
PtGe2	FScopp83	S							
PtPb	FScopp83	S							
PtPb4	FScopp83	S							
PtS2	FScopp83	S1	S2						
PtSb2	FScopp83	S							
PtSe2	FScopp83	S1	S2						
PtSi	FScopp83	S							
PtSn	FScopp83	S							
PtSn2	FScopp83	S							
PtSn4	FScopp83	S							
PtTe2	FScopp83	S1	S2						
PtTi	FScopp83	S1	S2						
PtTi3	FScopp83	S							

S	FScopp83	S1	S2	S3	S4	S5	L		
Sb	FScopp83	S1	S2	S3	L				
Sb2S3	FScopp83	S							
Sb2Se3	FScopp83	S							
Sb2Sn3	FScopp83	S							
Sb2SnZn	FScopp83	S							
SbFe2	FScopp83	S							
SbNi2	FScopp83	S							
Se	FScopp83	S1	S2	L					
Si	FScopp83	S1	S2	S3	S4	S5	S6	S7	L
Si2Te3	FScopp83	S1	S2						
Si2V	FScopp83	S							
Si2W	FScopp83	S							
Si2Zr3	FScopp83	S							
Si3Ti	FScopp83	S							
Si3Zr5	FScopp83	S1	S2						
Si4Zr5	FScopp83	S							
Si5V6	FScopp83	S							
Si6Al5	FScopp83	S1	S2						
SiAs	FScopp83	S							
SiAs2	FScopp83	S							
SiC	FScopp83	S1	S2	S3	S4	S5	S6		
SiO2	FScopp83	S1	S2	S3	S4	S5	S6	S7	S8
SiP	FScopp83	S1	S2						
SiP2	FScopp83	S							
SiS	FScopp83	S							
SiS2	FScopp83	S							
SiTe2	FScopp83	S1	S2						
SiZr	FScopp83	S							
SiZr2	FScopp83	S							
Sn	FScopp83	S1	S2	S3	S4	S5	L		
Sn14Ca12Mg7	FScopp83	S							
Sn20Ca31	FScopp83	S							
Sn23Ca36	FScopp83	S							
Sn2Li5	FScopp83	S							
Sn2Na	FScopp83	S							
Sn2Zr	FScopp83	S							
Sn3Ca	FScopp83	S							
Sn3Ca5	FScopp83	S							
Sn3Li7	FScopp83	S							
Sn3Li8	FScopp83	S							
Sn3Na	FScopp83	S							
Sn3Na4	FScopp83	S							
Sn4As3	FScopp83	S							
Sn4Li17	FScopp83	S							
Sn4Na	FScopp83	S							
Sn4Na15	FScopp83	S							
Sn4Na9	FScopp83	S							
Sn4P3	FScopp83	S							
Sn5Li13	FScopp83	S							
Sn5Li2	FScopp83	S							
Sn6Na	FScopp83	S							
SnAg3	FScopp83	S							
SnAs	FScopp83	S							
SnCa	FScopp83	S							
SnFe2	FScopp83	S							
SnLi	FScopp83	S							
SnMgLi4	FScopp83	S							
SnNa	FScopp83	S1	S2						
SnNa3	FScopp83	S							
SnNi2	FScopp83	S							
SnS	FScopp83	S1	S2						
SnS2	FScopp83	S							
SnSe	FScopp83	S1	S2						
SnSe2	FScopp83	S							

SnTe	FScopp83	S							
SnTi2	FScopp83	S							
SnZr4	FScopp83	S							
Te	FScopp83	S1	S2	L					
Ti	FScopp83	S1	S2	S3	S4	S5	S6	S7	L
Ti2Al	FScopp83	S							
Ti2AlC	FScopp83	S							
Ti2C	FScopp83	S							
Ti2Cr	FScopp83	S							
Ti2H	FScopp83	S							
Ti2Mn	FScopp83	S							
Ti2O	FScopp83	S							
Ti2O3	FScopp83	S1	S2						
Ti2Zn	FScopp83	S							
Ti3Al	FScopp83	S							
Ti3AlC	FScopp83	S							
Ti3AlC2	FScopp83	S							
Ti3AlSi5	FScopp83	S							
Ti3O2	FScopp83	S							
Ti3P	FScopp83	S							
Ti3Si	FScopp83	S							
Ti3Sn	FScopp83	S							
Ti4AlSi7	FScopp83	S							
Ti5Si3	FScopp83	S1	S2						
Ti5Si4	FScopp83	S							
Ti5Sn3	FScopp83	S1	S2						
Ti6Sn5	FScopp83	S1	S2						
TiC	FScopp83	S							
TiH2	FScopp83	S							
TiO	FScopp83	S							
TiO2	FScopp83	S1	S2						
TiSi	FScopp83	S							
TiSi2	FScopp83	S							
TiZn	FScopp83	S							
TiZn10	FScopp83	S							
TiZn15	FScopp83	S							
TiZn2	FScopp83	S							
TiZn3	FScopp83	S							
TiZn5	FScopp83	S							
Tl	FScopp83	S	L						
V	FScopp83	S1	S2	S3	S4	S5	L		
V11Ge8	FScopp83	S							
V17Ge31	FScopp83	S							
V23C6	FScopp83	S							
V2AlC	FScopp83	S							
V2Ga5	FScopp83	S							
V2Zr	FScopp83	S							
V3C2	FScopp83	S							
V3Ga	FScopp83	S							
V3Ge	FScopp83	S							
V3P	FScopp83	S							
V3Si	FScopp83	S							
V4Zn5	FScopp83	S							
V5C2	FScopp83	S							
V5Ge3	FScopp83	S							
V5Si3	FScopp83	S1	S2						
V6Ga5	FScopp83	S							
V7Al45	FScopp83	S							
V8Ga41	FScopp83	S							
VSn2	FScopp83	S							
VZn16	FScopp83	S							
VZn3	FScopp83	S							
W	FScopp83	S1	S2	S3	L				
W2Zr	FScopp83	S							
W3C2	FScopp83	S							

W5Si3	FScopp83	S1	S2								
WC	FScopp83	S									
WS2	FScopp83	S									
WSe2	FScopp83	S									
Zn	FScopp83	S1	S2	S3	S4	S5	S6	S7	...	L1	L
Zn22Fe2Ti	FScopp83	S									
Zn22Zr	FScopp83	S									
Zn2Li	FScopp83	S									
Zn2Zr	FScopp83	S									
Zn2Zr3	FScopp83	S									
Zn39Zr5	FScopp83	S									
Zn3AlLi	FScopp83	S									
Zn3As2	FScopp83	S1	S2	S3	S4						
Zn3Li2	FScopp83	S									
Zn3P2	FScopp83	S1	S2	S3	S4						
Zn3Sb2	FScopp83	S									
Zn3Zr	FScopp83	S1	S2								
Zn4Sb3	FScopp83	S1	S2								
Zn5Li2	FScopp83	S									
Zn5Sb3	FScopp83	S									
Zn62Ca8Al30	FScopp83	S									
Zn7Li3	FScopp83	S									
Zn9Mn	FScopp83	S									
ZnAlLi	FScopp83	S									
ZnAs2	FScopp83	S									
ZnO	FScopp83	S									
ZnP2	FScopp83	S1	S2								
ZnS	FScopp83	S1	S2								
ZnSb	FScopp83	S									
ZnSiP2	FScopp83	S									
ZnTe	FScopp83	S									
ZnZr	FScopp83	S									
ZnZr2	FScopp83	S									
Zr	FScopp83	S1	S2	S3	S4	S5	S6	S7	S8	L	
Zr2AlC	FScopp83	S									
Zr3P	FScopp83	S									
Zr3Si	FScopp83	S									
Zr5Sn3	FScopp83	S1	S2								
ZrC	FScopp83	S									
ZrH2	FScopp83	S									
ZrS2	FScopp83	S									
ZrSi2	FScopp83	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, BCC-A2 and HCP-A3 solid solutions have C, H and O as interstitial species.

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

System	Liquid Model	Comments	Source
Ag - Al	Bragg-Williams R-K Polynomial		S.S. Lim, P.L. Rossiter, J.W. Tibbals, Calphad 19 (1995) 131-142.
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 - Be	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 - Co	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2014
Ag - Cr	Bragg-Williams R-K Polynomial		SGTE
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 – Li	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
Ag - Mg	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 - Mn	Bragg-Williams R-K Polynomial		I. Karakaya, W. T. Thompson, Bull. Alloy Phase Diagrams, 1990, 11, (5), 80-486
Ag - Mo	MQMPA (Pair Fraction Exp.)		Refitted from unpublished assessment of J.Korb
Ag – Na	MQMPA (Pair Fraction Exp.)		J. WANG, N. MIAO, P. CHARTRAND, I.-H. JUNG, "Thermodynamic evaluation and optimization of the (Na + X) binary systems (X = Ag, Ca, In, Sn, Zn) using combined Calphad and first-principles methods of calculation", Journal of Chemical Thermodynamics, 66 (2013) 22-33
Ag - Nb	Bragg-Williams R-K Polynomial		SGTE
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 - P	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
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 - Pd	Bragg-Williams R-K Polynomial		G. Ghosh, C. Kantner, G. B. Olson, J. Phase Equilib., 1999, 20(3), 295-308
Ag – Pt	Bragg-Williams R-K Polynomial		P.J. Spencer, 1998, based on I. Karakaya and W.T. Thompson, Bull. Alloy Phase Diagrams 8 (1987) 334.
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		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 - Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
Ag - Ti	Bragg-Williams R-K Polynomial		Mei Li, Changrong Li, Fuming Wang, Weijing Zhang, CALPHAD, 2005, 29, 269-275
Ag - Tl	Bragg-Williams R-K Polynomial		H. L. Lukas, unpublished reassessment based on data set collected in Zimmermanns thesis 1976 (1994).
Ag - V	Bragg-Williams R-K Polynomial		SGTE
Ag - W	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
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
Ag - Zr	MQMPA (Pair Fraction Exp.)		Y-B. Kang & I.-H. Jung, Intermetallics 2010
Al - As	MQMPA (Pair Fraction Exp.)		P.J. Spencer, 2006 (VLAB Project)
Al - Au	Bragg-Williams R-K Polynomial		J.Murray, H.Okamoto, T.B.Massalski, Bull.Alloy Phase Diags.8 (1987) 20-30 (Modified by A.T.Dinsdale to give compatibility with SGTE unary data and to prevent high-temp. stability of fcc)
Al - Be	Bragg-Williams R-K Polynomial		M. Piché, M.A.Sc., École Polytechnique, 2002
Al - Bi	MQMPA (Pair Fraction Exp.)		M. Paliwal and In-Ho Jung, "Thermodynamic modeling of Al-Bi, Al-Sb, Mg-Al-Bi and Mg-Al-Sb systems"Calphad, 2010, vol. 34, pp. 51-63.
Al - C	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2004
Al - Ca	MQMPA (Pair Fraction Exp.)		Y-B. Kang, CRCT, 2008
Al - Cd	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2017
Al - Co	Bragg-Williams R-K Polynomial	Stoichiometric AlCo-B2	N. Dupin, I. Ansara, La Revue de Metallurgie-CIT/Sceince et Genie des Materiaux, September 1998, 1121-1129, "Thermodynamic evaluation of the system Al-Co"
Al - Cr	MQMPA (Pair Fraction Exp.)		S.Cui and I.-H.Jung, J. Alloys and Compounds, no.708, 2017 pp.887-902
Al - Cu	Bragg-Williams R-K Polynomial		COST 507, pp.28-33; Vol.Data: C. Robelin, CRCT, 2006 (VLAB Project)
Al - Fe	MQMPA (Pair Fraction Exp.)	Missing Fe_3Al $D0_3$ (lt)	A. T. Phan & Y-B Kang, Acta Materiala 2014
Al - Ga	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2016 modified from A.Watson CALPHAD 1992
Al - Ge	Bragg-Williams R-K Polynomial		I. Ansara, J. P. Bros, M. Gambino, CALPHAD 1979, 3(3), 225
Al - H	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Al – AlH_3	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.
Al - Hg	Bragg-Williams R-K Polynomial		A. J. McAlister, Bull. Alloy Phase Diagrams, 1985, 6, (3), 219-221

Al - In	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
Al - Li	MQMPA (Pair Fraction Exp.)		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.
Al - Mg	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2006; Vol.Data: F.Gemme, CRCT, 2003 (VLAB project); C.Aliravci, 2007 (GM Project).
Al - Mn	MQMPA (Pair Fraction Exp.)		M.-S. Kim and Y-B Kang, JPED 2015
Al - Mo	MQMPA (Pair Fraction Exp.)		Zhijun Zhu, CRCT, 2021
Al - Na	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2000 (FACT Consortium Project)
Al - Nb	Bragg-Williams R-K Polynomial		C Servant and I. Ansara, J. Chim. Phys. 1997, 94, 869-888
Al - Ni	Bragg-Williams R-K Polynomial		COST-507 K. Hack, GTT-Technologies, private communication, 2003
Al - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Al - AlO	P. Chartrand, CRCT, 2021
Al - P	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Al - Pb	MQMPA (Pair Fraction Exp.)		Y.-B. Kang, CRCT, 2009
Al - Pt	Bragg-Williams R-K Polynomial		K.Wu and Z.Jin, Journal of Phase Equilibria, 21(3), 2000, 221-226
Al - S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2007; based on R.C.Sharma and Y.A.Chang BAPD, 8(2) 1987 p.128-131
Al - Sb	MQMPA (Pair Fraction Exp.)		M. Paliwal and In-Ho Jung, "Thermodynamic modeling of Al-Bi, Al-Sb, Mg-Al-Bi and Mg-Al-Sb systems"Calphad, 2010, vol. 34, pp. 51-63.
Al - Se	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Al - Si	MQMPA (Pair Fraction Exp.)		J.-P. Harvey, M.A.Sc. thesis, Ecole Polytechnique, 2006; Vol. Data: F. Gemme, CRCT, 2003 (VLAB project)
Al - Sn	MQMPA (Pair Fraction Exp.)		Y.-B. Kang and A.D. Pelton, CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 34 (2010) 180 188
Al - Ti	MQMPA (Pair Fraction Exp.)		Zhijun Zhu, CRCT, 2021
Al - Tl	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018; from McAlister 1989 BAPD
Al - V	Bragg-Williams R-K Polynomial		COST 507, pp.95-98.
Al - W	Bragg-Williams R-K Polynomial		COST 507, pp.103-108.
Al - Zn	MQMPA (Pair Fraction Exp.)		Liquid: P. Chartrand, CRCT, 2006 (VLAB Project); Vol.Data. F.Gemme, CRCT, 2003 (VLAB Project); solids S. –L. Chen and Y.A. Chang, Calphad, 17 (1993), pp. 113-124.
Al - Zr	Bragg-Williams R-K Polynomial		COST 507, pp.112-116.
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, Master 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 - P	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

As - Pb	Bragg-Williams R-K Polynomial		M.Hamalainen, private communication
As - Pt	Bragg-Williams R-K Polynomial		M. Li et al. / Journal of Alloys and Compounds 437 (2007) 71–79
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.)		O. Kidari, Master Thesis, CRCT, 2023
Au - Bi	Bragg-Williams R-K Polynomial		C. Servant, E. Zoro and B. Legendre, Calphad, 30 (2006) 443
Au - C	Bragg-Williams R-K Polynomial		P.J. Spencer (2007)
Au - Co	Bragg-Williams R-K Polynomial		H.Q.Dong et al., J. Electronic Mater., 38(10) 2009, p.2158
Au - Cr	Bragg-Williams R-K Polynomial		P.J. Spencer, (1998)
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 - Pd	Bragg-Williams R-K Polynomial		COST-531
Au – Pt	Bragg-Williams R-K Polynomial		P.J. Spencer, 1994
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		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 - Ti	Bragg-Williams R-K Polynomial		W.Luo et al., CALPHAD 25(1) 2001 19-26
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
Be - Ca	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Be - Cu	Bragg-Williams R-K Polynomial		P.J. Spencer, 2003
Be – Fe	Bragg-Williams R-K Polynomial	Stoichiometric BeFe	M. Piché, M.A.Sc., École Polytechnique, 2002
Be – Li	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Be - Mg	Bragg-Williams R-K Polynomial		M. Piché, M.A.Sc., École Polytechnique, 2002
Be - Mn	Bragg-Williams R-K Polynomial		M. Piché, M.A.Sc., École Polytechnique, 2002
Be – Na	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Be – Si	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Be – Sn	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Be – Zn	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Bi – Cd	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Bi - Co	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014

Bi - Cr	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 - Li	MQMPA (Pair Fraction Exp.)		Z.M. CAO, W. XIE, P. CHARTRAND, S.H. WEI, G.W. DU and Z.-Y. QIAO, "Thermodynamic assessment of the Bi-alkali metal (Li, Na, K, Rb) systems using the modified quasichemical model for the liquid phase", *CALPHAD*, 46 (2014), pp.159-167
Bi - Mg	MQMPA (Pair Fraction Exp.)		M. Paliwal and In-Ho Jung, "Thermodynamic modeling of Mg-Bi and Mg-Sb systems and short-range-ordering behavior of the liquid solutions"Calphad, 2009, vol. 33, pp. 744-754.
Bi - Na	MQMPA (Pair Fraction Exp.)		Z.M. CAO, W. XIE, P. CHARTRAND, S.H. WEI, G.W. DU and Z.-Y. QIAO, "Thermodynamic assessment of the Bi-alkali metal (Li, Na, K, Rb) systems using the modified quasichemical model for the liquid phase", *CALPHAD*, 46 (2014), pp.159-167
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 - V	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2014
Bi - Zn	Bragg-Williams R-K Polynomial		C.Girard, Thesis, Marseille, 1985
C - Ca	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
C - Co	Bragg-Williams R-K Polynomial		A. Fernandez Guillermet: Z. Metallkde., 1987, 78, 700-9
C - Cr	Bragg-Williams R-K Polynomial		B. J. Lee: CALPHAD 1992, 16(2), 121-149
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 - Mg	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
C - Mn	MQMPA (Pair Fraction Exp.)		M.K. Paek, Y-B Kang, CALPHAD 46 (2014), 92-102
C – Mo	Bragg-Williams R-K Polynomial		SGTE
C – Na	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2013
C - Nb	Bragg-Williams R-K Polynomial		WM Huang: Mater. Sci. and Techn. 1990, 6(8), 687-694
C - Ni	Bragg-Williams R-K Polynomial		B. J. Lee: CALPHAD, 1992, 16(2), 121-149
C - P	Bragg-Williams R-K Polynomial		P. Gustafson: Inst. Met. Res. (Report IM-2549, 1990))
C - Pb	Bragg-Williams R-K Polynomial		unpublished assessment of T. G. Chart, NPL 1987
C – Pt	Bragg-Williams R-K Polynomial		GTT, 2005
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
C - Ti	MQMPA (Pair Fraction Exp.)	(C solubility in Ti-HCP is neglected)	P.J. Spencer, 2007 (VLAB Project)
C - V	Bragg-Williams R-K Polynomial		WM Huang : Z. Metallkde, 1991, 82, (3), 174-181
C - W	Bragg-Williams R-K Polynomial		P. Gustafson: Report TRITA 0212 (1985), Mat. Sci and Tech. 1986, 2(7), 653-658
C - Zr	Bragg-Williams R-K Polynomial		A. Fernandez Guillermet: J. Alloys Compounds, 1995, 217, 69-89
Ca – Co	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2014
Ca - Cr	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2014
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 - Li	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
Ca - Mg	MQMPA (Pair Fraction Exp.)		J. Wang, Ph.D. Thesis, Ecole Polytechnique, 2014
Ca – Mo	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Ca - Mn	MQMPA (Pair Fraction Exp.)		P.J. Spencer, 2006 (GM project)
Ca - Na	MQMPA (Pair Fraction Exp.)		J. WANG, N. MIAO, P. CHARTRAND, I.-H. JUNG, "Thermodynamic evaluation and optimization of the (Na + X) binary systems (X = Ag, Ca, In, Sn, Zn) using combined Calphad and first-principles methods of calculation", Journal of Chemical Thermodynamics, 66 (2013) 22-33
Ca - Nb	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2016
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 - Ti	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2018
Ca – V	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2018
Ca - W	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2018
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
Ca - Zr	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Cd - Co	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cd – Cr	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018

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 – Mg	Bragg-Williams R-K Polynomial		Ren, Li, Guo, Du, Thermochimica Acta 2012
Cd – Mn	Bragg-Williams R-K Polynomial		Qin et al, CALPHAD 47 (2014) 83-91
Cd – Na	Bragg-Williams R-K Polynomial		Y. Liu et al. / Journal of Alloys and Compounds 473 (2009) 60–64
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 – Ti	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 - V	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cd – W	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cd - Zn	Bragg-Williams R-K Polynomial		L. A. Zabdyr: CALPHAD 1997, 21(3), 349-358
Co - Cr	MQMPA (Pair Fraction Exp.)		A.Kusoffsky, B.Jansson, Calphad 21 (1997) 321-333; liquid converted to MQMPA [2022Cha]
Co - Cu	Bragg-Williams R-K Polynomial		P.J.Spencer - L.Kaufman interaction parameters with SGTE element data
Co - Fe	MQMPA (Pair Fraction Exp.)		A.F.Guillermet, High Temp. High Press. 19 (1988) 477-499; liquid converted to MQMPA [2021Cha]
Co - Ga	Bragg-Williams R-K Polynomial		A. Chari et al. / CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 34 (2010) 189–195
Co – In	Bragg-Williams R-K Polynomial		D. Boa, B. K. Dongui, I. Ansara: CALPHAD 25 (2001) 645-650
Co – Li	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Co – Mg	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2018
Co – Mn	Bragg-Williams R-K Polynomial		W.Huang, Calphad 13 (1989) 231-242
Co - Mo	Bragg-Williams R-K Polynomial		SGTE
Co – Na	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Co – Nb	Bragg-Williams R-K Polynomial		K.C.H.Kumar, I.Ansara, P.Wollants, L.Delaey, J.Alloys and Cpds. 267 (1998) 105-112
Co – Ni	Bragg-Williams R-K Polynomial		A.F.Guillermet, Z.Metallkde. 78 (1987) 639-647; Z.Metallkde. 79 (1988) 524-536
Co - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Co - CoO	P. Chartrand, CRCT, 2021
Co – Pb	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2018
Co - Pd	Bragg-Williams R-K Polynomial		G. Ghosh, C. Kantner, G.B. Olson, J.Phase Equilibria 20 (1999) 295-308

Co - Pt	Bragg-Williams R-K Polynomial		D.E. Kim et al. / CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 35 (2011) 323–330
Co - S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	F. Kongoli, Y. Dessureault and A.D. Pelton, "Thermodynamic Modeling of Liquid Fe-Ni-Co-Cu-S Mattes", Met. Trans.,29B, 591-601 (1998).
Co - Sb	Bragg-Williams R-K Polynomial		Y.Zhang et al., CALPHAD 33 (2009) 405–414
Co – Si	Bragg-Williams R-K Polynomial	Stoichiometric CoSi Inverted L-L miscibility gap above 3000°C	S.D.Choi, Calphad 16 (1992) 151-159
Co – Sn	Bragg-Williams R-K Polynomial		L.Liu et al., J.Electron.Mater.33(9) (2004) 935-939
Co - Te	Bragg-Williams R-K Polynomial		H. Yuan, J. Wang, B. Hu, R. Zhao, Y. Du and S.-Y. Zhang, CALPHAD 68 (2020) 10174
Co – Ti	Bragg-Williams R-K Polynomial		G.Cacciamani, R.Ferro, I.Ansara, N.Dupin, submitted to "Intermetallics", 1999
Co – V	Bragg-Williams R-K Polynomial	Stoichiometric Co_3V	J. Bratberg, B. Sundman: J. Phase Equil., (2003), 24(6), 495-503
Co – W	Bragg-Williams R-K Polynomial		Markstrom, Sundman & Frisk JPE (2005)
Co – Zn	Bragg-Williams R-K Polynomial	Missing $CoZn_7$(ht) and CoZn(ht)	G.P. Vassilev, M. Jiang: J. Phase Equil. and Diffusion 2004, 25, 259-268
Co - Zr	Bragg-Williams R-K Polynomial		Durga & Kumar, CALPHAD 2010
Cr - Cu	MQMPA (Pair Fraction Exp.)		S. Cui and I-H Jung, CALPHAD 2017
Cr - Fe	MQMPA (Pair Fraction Exp.)		S. Cui and I-H Jung, CALPHAD 2017
Cr - Ga	Bragg-Williams R-K Polynomial		P.Chartrand, CRCT, 2022
Cr - H	MQMPA (Pair Fraction Exp.)	estimated from Ti-H; Gaseous species must be taken from FactPS Database Valid for Cr rich region	P. Chartrand 2010
Cr - Hg	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cr - Li	MQMPA (Pair Fraction Exp.)	estimated from Fe-Li	P. Chartrand 2003
Cr - Mg	MQMPA (Pair Fraction Exp.)		S. Cui et al., Journal of Alloys and Compounds, 2017
Cr - Mn	Bragg-Williams R-K Polynomial		COST 507, pp.145-148.
Cr - Mo	Bragg-Williams R-K Polynomial		COST 507
Cr - Na	MQMPA (Pair Fraction Exp.)	estimated from Fe-Na	P. Chartrand, CRCT, 2003
Cr - Nb	Bragg-Williams R-K Polynomial		J.G.Costa Neto, S.G.Fries, H.-L.Lukas, Calphad 17 (1993) 219-228
Cr - Ni	Bragg-Williams R-K Polynomial		B.J. Lee, Calphad 16 1992, pp. 121-149.
Cr - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Cr - CrO	P.Chartrand, CRCT, 2021
Cr - P	Bragg-Williams R-K Polynomial	Valid in the Cr – Cr_2P region only	SGTE
Cr - Pb	Bragg-Williams R-K Polynomial		P. Chartrand, 2003
Cr - Pt	Bragg-Williams R-K Polynomial		Oikawa et al. Journal of Magnetism and Magnetic Materials 236 (2001) 220–233
Cr - S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P.Waldner and W.Sitte, Int. J. Mat. Res. (formerly Z. Metallkd.) 102 (2011) 10, 1216-1225.
Cr - Si	MQMPA (Pair Fraction Exp.)		Senlin Cui & In-Ho Jung, Met.Trans.2017
Cr - Sn	Bragg-Williams R-K Polynomial		R. Jerlerud Perez, B. Sundman: CALPHAD, 25 (2001) 59-66
Cr - Ti	MQMPA (Pair Fraction Exp.)		Zhijun Zhu, CRCT, 2021
Cr - V	Bragg-Williams R-K Polynomial		B.J.Lee, Z.Metallkde 83 (1992) 292-299
Cr - W	Bragg-Williams R-K Polynomial		P. Gustafson, Calphad 12 (1988), pp. 277-292.
Cr - Zn	Bragg-Williams R-K Polynomial		I.Ansara, COST 507 (1998) ISBN 92-828-3902-8, p.158-160

Cr - Zr	Bragg-Williams R-K Polynomial		K.Zeng, M.Hamalainen, I.Ansara, COST 507 (1998) ISBN 92-828-3902-8 p 161-164
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 - Li	Bragg-Williams R-K Polynomial		COST 507, pp.168-169.
Cu - Mg	MQMPA (Pair Fraction Exp.)		S. Cui and I-H. Jung, 2017
Cu - Mn	MQMPA (Pair Fraction Exp.)		S. Cui and I-H. Jung, 2017
Cu – Mo	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cu - Na	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2014
Cu - Nb	Bragg-Williams R-K Polynomial		B.J. Lee database, private comunication to SGTE, 1999.
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 - P	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cu - Pb	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cu – Pd	Bragg-Williams R-K Polynomial	Liquid only (Cu-rich)	G.K.Sigworth, J.F.Elliott, Canad.Met.Quarterly 13 (1974) 455-461.
Cu - Pt	Bragg-Williams R-K Polynomial		T.Abe, B.Sundman, H.Onodera, JPEDAV (2006) 27:5-13
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 – Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cu – Ti	Bragg-Williams R-K Polynomial		K.C.H. Kumar, I. Ansara, P. Wollants, L. Delaey, Z.Metallkde. 87 (1996), pp. 666-672.
Cu - Tl	Bragg-Williams R-K Polynomial		P.Y.Chevalier, Thermochimica Acta 156 (1989) 383-392
Cu – V	Bragg-Williams R-K Polynomial		B.J. Lee database, private comunication to SGTE, 1999.
Cu – W	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Cu – Zn	Bragg-Williams R-K Polynomial		Liang, Hsiao, Schmid-Fezter CALPHAD, 2015
Cu – Zr	MQMPA (Pair Fraction Exp.)		D.H.Kang I.H.Jung Intermetallics 2010
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 - Li	MQMPA (Pair Fraction Exp.)	from Fe in liquid Li	P. Chartrand, 2003
Fe - Mg	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2006

Fe - Mn	MQMPA (Pair Fraction Exp.)		M-S Kim, Y-B Kang, JPE, 2015
Fe - Mo	Bragg-Williams R-K Polynomial		SGTE
Fe - Na	MQMPA (Pair Fraction Exp.)	from Fe in liquid Na	P. Chartrand, CRCT, 2003
Fe - Nb	Bragg-Williams R-K Polynomial		Khvan & Hallstedt CALPHAD 2013
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 – P	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Fe – Pb	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Fe - Pd	Bragg-Williams R-K Polynomial		G. Ghosh, C. Kantner, G.B. Olson, J.Phase Equilibria 20 (1999) 295-308
Fe - Pt	Bragg-Williams R-K Polynomial		P.Fredriksson & B.Sundman, CALPHAD 25(4) 2001, 535-548
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 - Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
Fe - Ti	Bragg-Williams R-K Polynomial		P.J. Spencer, 2001 (FACT Consortium)
Fe - Tl	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Fe - V	Bragg-Williams R-K Polynomial		W.Huang, Z.Metallkde 82 (1991) 391-401
Fe - W	Bragg-Williams R-K Polynomial		J-O Andersson and P Gustafson: CALPHAD, 1983, 7(4), 317-326
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)
Fe - Zr	MQMPA (Pair Fraction Exp.)		J.J. Marin Bejarano, CRCT, 2009
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 - Li	Bragg-Williams R-K Polynomial		H.Azza et al., J. Phase Equilib. Diffus. (2017) 38:788–795
Ga - Mg	MQMPA (Pair Fraction Exp.)		Y-B. Kang, CALPHAD 2014
Ga – Mo	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2023
Ga - Na	Bragg-Williams R-K Polynomial		J. Wang et al. / Journal of Crystal Growth 307 (2007) 59-65
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 - P	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 - Pb	Bragg-Williams R-K Polynomial		I. Ansara, F. Ajersch: J. Phase Equil., 1991, 12(1), 73-77
Ga - Pt	Bragg-Williams R-K Polynomial		M. Li et al. / Intermetallics 14 (2006) 826–831
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 - Te	MQMPA (Pair Fraction Exp.)		B.Kumar et al. (Paliwal) CALPHAD 74 (2021)
Ga – Ti	Bragg-Williams R-K Polynomial		Y.Liu et al., CALPHAD 41 (2013) 140-149
Ga - Tl	Bragg-Williams R-K Polynomial		I. Katayama et al., T. Iida, Z. Metallknd. 94, 2003, p.1296
Ga - V	Bragg-Williams R-K Polynomial		D. Ling et al./CALPHAD 51(2015) 125-132
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]
Ga - Zr	Bragg-Williams R-K Polynomial		W. Luo et al. / Journal of Alloys and Compounds 587 (2014) 497–505
Ge - In	Bragg-Williams R-K Polynomial		P. Y. Chevalier: 1989, 155, 227-240
Ge - Mg	MQMPA (Pair Fraction Exp.)		Dmitri Nassyrov and In-Ho Jung, "Thermodynamic modeling of the Mg-Ge-Pb system"Calphad, 2009, vol. 33, pp. 521-529.
Ge - Na	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2023 using solids from Y. Wang et al. / CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 37 (2012) 72–76
Ge - Ni	Bragg-Williams R-K Polynomial		S.Jin et al./CALPHAD 38 (2012) 23–34
Ge - P	Bragg-Williams R-K Polynomial		H. Dong, X. Tao and M. Paulasto-Krockel, Journal of Electronic Materials (2021) 50:4272-4
Ge - Pb	Bragg-Williams R-K Polynomial		P. Chevalier, Thermochemica Acta, 1989, vol 155, pp. 227-240
Ge - Pt	Bragg-Williams R-K Polynomial		J.S. Wang et al. / CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 33 (2009) 561-569
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 – Tl	Bragg-Williams R-K Polynomial		P. Chevalier, Thermochimica Acta, 1989, vol 155, pp. 227-240
Ge - V	Bragg-Williams R-K Polynomial		C.P. Wang et al. / Intermetallics 16 (2008) 544-549
Ge - Zn	Bragg-Williams R-K Polynomial		P. Chevalier, Thermochimica Acta, 1989, vol 155, pp. 227-240
H - Li	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Li - LiH	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 - Mg	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Mg – MgH_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 - Mn	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Mn-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 - Na	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Na - NaH	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 - 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 Si-rich region	P. Chartrand, CRCT, 2023 using model from M.-C. Heuzey, Master Thesis, CRCT

H - Ti	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Ti – TiH_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.
H - Zr	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FactPS Database Valid for Zr-rich region	P. Chartrand, CRCT, 2014 from Ti-H of J.P. Harvey 2006
Hg – Mg	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
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 - Li	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
In - Mg	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 - Na	MQMPA (Pair Fraction Exp.)		J. WANG, N. MIAO, P. CHARTRAND, I.-H. JUNG, "Thermodynamic evaluation and optimization of the (Na + X) binary systems (X = Ag, Ca, In, Sn, Zn) using combined Calphad and first-principles methods of calculation", Journal of Chemical Thermodynamics, 66 (2013) 22-33
In - Ni	Bragg-Williams R-K Polynomial		P.Waldner and H.Ipser, Z.Metallk, 93(8) 2002, 825-832
In - P	Bragg-Williams R-K Polynomial		I.Ansara, C.Chatillon, Calphad 18 (1994) 204
In - Pb	Bragg-Williams R-K Polynomial		D.Boa, I.Ansara, Thermochimica Acta 314 (1998) 79-86
In - Pt	Bragg-Williams R-K Polynomial		Y. Liang et al. / Journal of Alloys and Compounds 475 (2009) 220–226
In - Sb	Bragg-Williams R-K Polynomial		T.J.Anderson, Calphad 18 (1994) 206
In - Se	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2023, refitted liquid 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 - V	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
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
Li - Mg	MQMPA (Pair Fraction Exp.)		P.J. Spencer, 2006
Li - Mn	MQMPA (Pair Fraction Exp.)		Y.-B. Kang, CRCT, 2005
Li – Mo	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2003
Li - Na	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2001
Li – Nb	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2016
Li – Ni	MQMPA (Equivalent Fraction Exp.)		P. Chartrand, 2003
Li – O	MQMPA (Pair Fraction Exp.)	Gaseous species taken from FACTPS Database	P. Chartrand, CRCT, 2021

Li - Pb	MQMPA (Pair Fraction Exp.)	Liquid only	P. Chartrand, 2003
Li - Sb	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
Li – Si	MQMPA (Pair Fraction Exp.)		J.-P. Harvey, CRCT, 2007
Li – Sn	MQMPA (Pair Fraction Exp.)		J. WANG, J. HAN, I.-H. JUNG, D. BAIROS and P. CHARTRAND, "Thermodynamic optimizations on the binary Li-Sn system and ternary Mg-Sn-Li system", *CALPHAD*, accepted, (July 2014).
Li – Ti	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Li – V	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Li – W	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2022
Li – Zn	MQMPA (Pair Fraction Exp.)		P.J. Spencer, 2006
Li – Zr	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Mg - Mn	MQMPA (Pair Fraction Exp.)		Y.-B. Kang, A.D. Pelton. P. Chartrand, P. Spencer and C. Fuerst, J. Phase Equil. Diff. 28 (2007), pp. 342-354
Mg - Mo	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Mg - Na	MQMPA (Equivalent Fraction Exp.)		P. Chartrand, CRCT, 2003 (FACT Consortium)
Mg – Nb	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Mg - Ni	Bragg-Williams R-K Polynomial		M.Jacobs, COST 507 report (1998) ISBN 92-828-3902-8, p.218-220
Mg - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Mg - MgO	P. Chartrand, CRCT, 2021
Mg - Pb	MQMPA (Pair Fraction Exp.)		Dmitri Nassyrov and In-Ho Jung, "Thermodynamic modeling of the Mg-Ge-Pb system"Calphad, 2009, vol. 33, pp. 521-529.
Mg - Pt	Bragg-Williams R-K Polynomial		W.Gierlotka et al., J.Mater.Res.,37(11) 2022,p.1904
Mg – S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2021
Mg - Sb	MQMPA (Pair Fraction Exp.)		M. Paliwal and In-Ho Jung, "Thermodynamic modeling of Mg-Bi and Mg-Sb systems and short-range-ordering behavior of the liquid solutions"Calphad, 2009, vol. 33, pp. 744-754
Mg - Si	MQMPA (Pair Fraction Exp.)		J.-P. Harvey, M.A.Sc. thesis, Ecole Polytechnique, 2006 (VLAB Project); Vol. Data F. Gemme, CRCT, 2003 (VLAB project)
Mg - Sn	MQMPA (Pair Fraction Exp.)		Y.-B. Kang and A.D. Pelton, CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 34 (2010) 180 188
Mg - Ti	MQMPA (Pair Fraction Exp.)		X.-F. Sheng, Projet de fin d'etudes, CRCT, 2008
Mg – V	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Mg – W	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Mg - Zn	MQMPA (Pair Fraction Exp.)		Liquid: P.J. Spencer, 2006; Solids from COST-507; Vol. Data liquid: F. Gemme, CRCT, 2003; Vol. Data solids C.Aliravci, CRCT, 2007
Mg - Zr	MQMPA (Pair Fraction Exp.)		J.J. Marin Bejarano, CRCT, 2009
Mn - Mo	Bragg-Williams R-K Polynomial		COST-507
Mn - Na	MQMPA (Pair Fraction Exp.)	from Fe-Na	P. Chartrand, 2013
Mn - Nb	Bragg-Williams R-K Polynomial		Z.-K. Liu & B. Hallstedt CALPHAD 2012
Mn - Ni	Bragg-Williams R-K Polynomial		NPL (National Physics Laboratory, UK), unpublished work, 1989.
Mn - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Mn - MnO	P. Chartrand, CRCT, 2021
Mn – P	Bragg-Williams R-K Polynomial	Valid for Mn-Mn_3P region	SGTE
Mn - Pb	Bragg-Williams R-K Polynomial		SGTE

Mn – S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	Y-.B. Kang, CRCT, 2009
Mn – Sb	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2023
Mn - Si	MQMPA (Pair Fraction Exp.)	Mn_5Si_2 not present	M.K. Paek, Y-B Kang, CALPHAD 46 (2014), 92-102; A. Shukla, Y.-B. Kang and A.D.
Mn - Sn	Bragg-Williams R-K Polynomial		J. Miettinen: CALPHAD, 2001, 25(1), 43-58
Mn - Ti	Bragg-Williams R-K Polynomial		N.Saunders, COST 507 (1998) ISBN 92-828-3902-8, p.241-244
Mn - V	Bragg-Williams R-K Polynomial		W. Huang, Met. Trans.A 22A (1991) pp. 1911-1920.
Mn - W	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Mn - Zn	MQMPA (Pair Fraction Exp.)		Y.-B. Kang, CRCT, 2005
Mn - Zr	Bragg-Williams R-K Polynomial		H.J. Seifert, J. Groebner, F. Aldinger, F.H. Hayes, G. Effenberg, C. Baetzner, H. Flandorfer, P. Rogl, A. Saccone, R. Ferro, Proc.3rd. International Magnesium Conference, Ed. G. W. Lorimer, Inst.of Materials, London, 1997, pp. 257-270.
Mo - Na	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2003
Mo - Nb	Bragg-Williams R-K Polynomial		COST-507
Mo - Ni	Bragg-Williams R-K Polynomial		COST-507
Mo - P	Bragg-Williams R-K Polynomial		SGTE
Mo - Pt	Bragg-Williams R-K Polynomial		Ph.D. Thesis Tewfik BENLAHARCHE from U. Lorraine (France) 2008
Mo – S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database	P. Chartrand, CRCT, 2021
Mo - Si	Bragg-Williams R-K Polynomial		P.Y. Chevalier, 2003 Report to SGTE
Mo - Ti	MQMPA (Pair Fraction Exp.)		Zhijun Zhu, CRCT, 2021
Mo - V	Bragg-Williams R-K Polynomial		SGTE
Mo - W	MQMPA (Pair Fraction Exp.)	Ideal liquid	SGTE
Mo - Zn	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2014
Mo - Zr	Bragg-Williams R-K Polynomial	Stoichiometric Mo_2Zr C15	Perez, B. Sundman, CALPHAD 27 2003, 253-262
Na - Nb	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2016
Na - Ni	MQMPA (Pair Fraction Exp.)	from Fe-Na	P. Chartrand, 2013
Na - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Na – Na_2O	P. Chartrand, CRCT, 2021
Na – S	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Na-Na2S.	P. Chartrand, CRCT, 2022
Na - Si	MQMPA (Pair Fraction Exp.)		J.-P. Harvey, M.A.Sc. thesis, Ecole Polytechnique, 2006 (VLAB Project)
Na - Sn	MQMPA (Pair Fraction Exp.)		J. WANG, N. MIAO, P. CHARTRAND, I.-H. JUNG, "Thermodynamic evaluation and optimization of the (Na + X) binary systems (X = Ag, Ca, In, Sn, Zn) using combined Calphad and first-principles methods of calculation", Journal of Chemical Thermodynamics, 66 (2013) 22-33
Na - Ti	MQMPA (Pair Fraction Exp.)	from Fe-Na	P. Chartrand, 2013
Na - V	MQMPA (Pair Fraction Exp.)	from Fe-Na	P. Chartrand, 2013
Na - W	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2018
Na - Zn	MQMPA (Pair Fraction Exp.)		J. WANG, N. MIAO, P. CHARTRAND, I.-H. JUNG, "Thermodynamic evaluation and optimization of the (Na + X) binary systems (X = Ag, Ca, In, Sn, Zn) using combined Calphad and first-principles methods of calculation", Journal of Chemical Thermodynamics, 66 (2013) 22-33

Na - Zr	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014
Nb - Nd	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2017
Nb - Ni	Bragg-Williams R-K Polynomial		J.-M. Joubert, N.Dupin, B.Sundman CALPHAD 2004
Nb - Si	Bragg-Williams R-K Polynomial		SGTE
Nb - Sn	Bragg-Williams R-K Polynomial		C. Toffolon, Gachon, B. Sundman, JPE 2002
Nb – Ti	Bragg-Williams R-K Polynomial		COST 507, pp.256-260.
Nb - V	Bragg-Williams R-K Polynomial		K.C.H. Kumar, P. Wollants, L. Delaey, Calphad **18** (1994), pp. 71-79.
Nb - W	Bragg-Williams R-K Polynomial		P. Gustafson, Z. Metallkde **79** (1988), pp. 388-396.
Nb - Zn	Bragg-Williams R-K Polynomial		Z. Long, JPED 2016
Nb - Zr	Bragg-Williams R-K Polynomial		A.F. Guillermet, Z. Metallkde. **82** (1991), pp. 478-487.
Ni - O	MQMPA (Pair Fraction Exp.)	Gaseous species must be taken from FACTPS Database Valid for Ni - NiO	P. Chartrand, CRCT, 2021
Ni - P	Bragg-Williams R-K Polynomial	Ni-Ni_6P_5	NPL, unpublished work, 1989
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 - Pd	Bragg-Williams R-K Polynomial		COST-531
Ni - Pt	Bragg-Williams R-K Polynomial		X.-G. Lu et al. / CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 33 (2009) 450-456
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 – Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
Ni - Ti	Bragg-Williams R-K Polynomial		C.S. Oh, J. Korean Inst.Met.Mater. **33** (1995), pp. 129-136.
Ni - V	Bragg-Williams R-K Polynomial		COST 507, pp. 261-263.
Ni - W	Bragg-Williams R-K Polynomial		SGTE
Ni – Zn	Bragg-Williams R-K Polynomial		SGTE
Ni - Zr	Bragg-Williams R-K Polynomial		G. Ghosh, J.Mater.Res. 9 (1994), pp. 598-616.
O – Pb	MQMPA (Pair Fraction Exp.)	Gaseous species taken from FACTPS Database Valid for Pb - PbO	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 – Ti	MQMPA (Pair Fraction Exp.)	Gaseous species taken from FACTPS Database Valid for Ti – Ti_2O	P. Chartrand, CRCT, 2021
O – V	MQMPA (Pair Fraction Exp.)	Gaseous species taken from FACTPS Database Valid for V – V_2O	P. Chartrand, CRCT, 2021
O - Zn	MQMPA (Pair Fraction Exp.)	Gaseous species taken from FACTPS Database Valid for Zn – ZnO	P. Chartrand, CRCT, 2021
P - Sb	Bragg-Williams R-K Polynomial		I.Ansara, C.Chatillon, Calphad 18 (1994) 208
P - Si	MQMPA (Pair Fraction Exp.)		P.J. Spencer, 2006
P - Sn	Bragg-Williams R-K Polynomial		J..Miettinen, Calphad, Vol. 25, No. 1, pp. 67-78
P - Zn	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
Pb – Pd	Bragg-Williams R-K Polynomial		COST-531

Pb - Pt	Bragg-Williams R-K Polynomial		Z.H.Long et al.,JPEDAV (2009) 30:318–322
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, -TlBull.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 – 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
Pb – Zr	Bragg-Williams R-K Polynomial		Dixon P. R., Argent B. B., Chart T. G.: CALPHAD, 1998, 22(3), 397-416
Pd - Pt	Bragg-Williams R-K Polynomial		K. Hack, GTT-Technologies, 1995
Pd - Sn	Bragg-Williams R-K Polynomial		P. Chartrand, CRCT, 2023 based on solids from J.Hu et al., Mater. Res. Express 9 (2022) 016507
Pd - Ti	Bragg-Williams R-K Polynomial		P. Chartrand 2018 (Liq + BCC + HCP + FCC) K.Hack, GTT-Technologies,1996;
Pt - Si	Bragg-Williams R-K Polynomial		L.L. Xu et al. / Computer Coupling of Phase Diagrams and Thermochemistry 32 (2008) 101–105
Pt – Sn	MQMPA (Pair Fraction Exp.)		COST-531
Pt – Ti	Bragg-Williams R-K Polynomial		K. Hack, GTT-Technologies, 1996
Pt - V	Bragg-Williams R-K Polynomial		C.P. Wang et al. / Intermetallics 16 (2008) 544-549
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 – Te	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2021
Si – Ti	MQMPA (Pair Fraction Exp.)		FSstel
Si - Tl	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Si - V	Bragg-Williams R-K Polynomial		COST 507, pp. 270-273.

Si - W	Bragg-Williams R-K Polynomial		C. Vahlas, P.Y. Chevalier, E. Blanquet, Calphad **13** (1989), pp. 273-292.
Si - Zn	MQMPA (Pair Fraction Exp.)		A. Shukla, Y.-B. Kang and A.D. Pelton, Calphad 32 (2008) pp. 470-477
Si - Zr	Bragg-Williams R-K Polynomial		COST 507, pp. 280-283.
Sn – Te	MQMPA (Pair Fraction Exp.)		M. Paliwal, 2021
Sn – Ti	Bragg-Williams R-K Polynomial		F.Hayes, COST 507 (1998) ISBN 92-828-3902-8, p.284-28
Sn – Tl	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2018
Sn - V	MQMPA (Pair Fraction Exp.)		Chen, Gierlotka, and Chen, Journal of ELECTRONIC MATERIALS, Vol. 37, No. 11, 2008
Sn - Zn	MQMPA (Pair Fraction Exp.)		M. Medraj, Concordia, 2011
Sn - Zr	Bragg-Williams R-K Polynomial	Spurious inverted L-L miscibility gap above 1700°C in the Sn-rich region	J.Korb, K.Hack, COST 507 (1998) ISBN 92-828-3902-8, p.290-292
Te - Zn	MQMPA (Pair Fraction Exp.)		P. Chartrand, CRCT, 2022
Ti - V	MQMPA (Pair Fraction Exp.)		Liquid from Zhijun Zhu, CRCT, 2021; Solids from N.Saunders, COST 507 (1998) ISBN 92-828-3902-8, p.297-298
Ti - W	Bragg-Williams R-K Polynomial		N.Saunders, COST 507 (1998) ISBN 92-828-3902-8, p.297-298
Ti - Zn	Bragg-Williams R-K Polynomial		K. Doi, S. Ono, H. Ohtani, M. Hasebe: J. Phase Equilib. Diff., 2006, 27(1), 63-74
Ti - Zr	MQMPA (Pair Fraction Exp.)		Liquid from P. Chartrand, CRCT, 2022; Solids from K.C.H. Kumar, P. Wollants, L. Delaey, J.Alloys and Compounds, 225 (1994), pp.121-127.
Tl - Zn	Bragg-Williams R-K Polynomial		S. S. Kim, T. H. Sanders, Z. Metallkunde 2003
V - W	MQMPA (Pair Fraction Exp.)		P. Chartrand, 2014 changed to MQMPA from FSstel
V - Zn	MQMPA (Pair Fraction Exp.)	estimated	P. Chartrand, 2018 (L. est. From Fe-Zn)
V - Zr	Bragg-Williams R-K Polynomial		COST 507, pp. 303-304.
W - Zr	MQMPA (Pair Fraction Exp.)		Liquid from P. Chartrand, CRCT, 2022; Solids from SGTE
Zn - Zr	Bragg-Williams R-K Polynomial		SGTE