TCCU3: TCS Cu-based Alloys Database

Database name:	TCS Cu-based Alloys Database	*Database acronym:*	TCCU
Database owner:	Thermo-Calc Software AB	*Database version:*	3.1

TCCU3 is a thermodynamic database for Cu-based alloys for use with the Thermo-Calc, Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA). TCCU3 is based on the critical evaluation of binary and ternary systems which enables predictions to be made for multi-component systems and alloys of industrial importance. A hybrid approach of experiments, first-principles calculations and CALPHAD modeling has been used to obtain thermodynamic descriptions of the constituent binary and ternary systems over the whole composition and temperature ranges.

Included Elements (30)

Ag	Al	Au	As	B	Be	Bi	C	Ca	Cd
Co	Cr	Cu	Fe	Ge	Mg	Mn	Mo	Nb	Ni
O	P	Pb	Pt	Se	Si	Sn	Ti	Zn	Zr

A total of 133 of the binary systems have been assessed, mostly to their full range of composition. TCCU3 also contains assessments of 50 assessed ternaries.

The critically thermodynamically assessed binary and ternary systems can be calculated in Thermo-Calc using the Binary and Ternary Calculators (in Graphical Mode) or the BINARY or TERNARY modules (in Console Mode).

- TCCU3 Assessed Binary Systems
- TCCU3 Assessed Ternary Systems

TCCU3 contains 257 solution and intermetallic phases in total. The GAS phase is rejected by default when retrieving the data from the database. One has to manually restore it when it is required for a calculation. See Models for the Phases Included in TCCU3 for details the models, e.g. number of sublattices and constituents on each sublattice.

TCCU3 includes nearly all stable phases in the assessed systems that may form in as-cast and aged Cu-based alloys. The database can be used to calculate various phase diagrams and property diagrams in the assessed systems or even extrapolated higher-order systems. The extrapolation to higher-order systems

helps to understand the phase equilibria in multi-component industrial copper alloys, so as to predict the phase formation, phase fractions and phase compositions or to calculate the driving force of forming a phase. The database can also be used for predicting solidification behaviour of Cu-alloys in Thermo-Calc using the Scheil Calculator (in Graphical Mode) or the SCHEIL GULLIVER module (in Console Mode). You can also simulate multi-particle precipitation during aging treatment with the Precipitation Module (TC-PRISMA).

In Console Mode, you can list phases and constituents in the Database (TDB) module and the Gibbs (GES) module. For some phases, supplementary information is included in the definitions. In order to show the information, it is recommended to use the command LIST_SYSTEM with the option of `Constituents` in the Database (TDB) module.

The database is validated where possible against commercial Cu-based alloys and available experimental information.

TCCU3 Calculation Examples

Limits

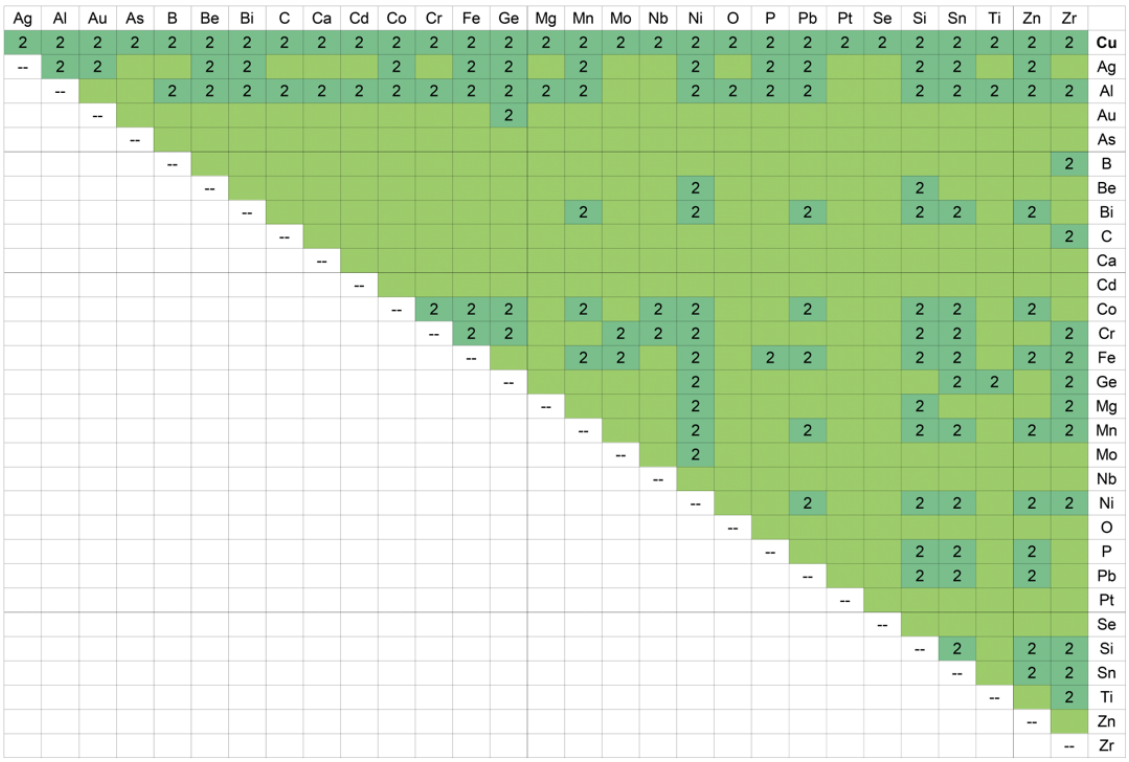
As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.

Database Revision History

If you are interested in the revision history for this or other databases, the information is available in the online help (from Thermo-Calc go to **Help>Online Help**) or in the release notes on our website. For the TCFE (TCS Steel and Fe-alloys) database there is a dedicated page with the history of its development.

TCCU3 Assessed Binary Systems

Low temperature ordered phases are not fully included in Au-Cu and Cu-Pt systems.



TCCU3 Assessed Ternary Systems

These are the assessed ternary systems, which are mostly in the full compositional ranges.

Low temperature ordered phases are not included in Ag-Au-Cu and Au-Cu-Ge.

Ag-Au-Cu
Ag-Cu-Ge
Ag-Cu-Ni
Ag-Cu-P
Ag-Cu-Sn
Al-Cu-Fe
Al-Cu-Mn
Al-Cu-Ni
Al-Cu-O
Al-Cu-Si
Al-Cu-Sn
Al-Cu-Zn
Al-Fe-Ni
Au-Cu-Ge
Be-Cu-Ni
Co-Cr-Cu
Co-Cu-Fe
Co-Cu-Mn
Co-Cu-Nb
Co-Cu-Ni
Cr-Cu-Fe
Cr-Cu-Mo
Cr-Cu-Nb
Cr-Cu-Ni

Cr-Cu-Si
Cr-Cu-Sn
Cr-Cu-Zr
Cu-Fe-Mn
Cu-Fe-Mo
Cu-Fe-Ni
Cu-Fe-Si
Cu-Fe-Sn
Cu-Fe-Zn
Cu-Mg-Ni
Cu-Mg-Si
Cu-Mn-Ni
Cu-Mn-Si
Cu-Mn-Sn
Cu-Mn-Zn
Cu-Mo-Ni
Cu-Ni-Pb
Cu-Ni-Si
Cu-Ni-Sn
Cu-Ni-Zn
Cu-P-Sn
Cu-Pb-Sn
Cu-Pb-Zn
Cu-Si-Zn

Cu-Sn-Zn
Cu-Ti-Zr

TCCU3 Calculation Examples

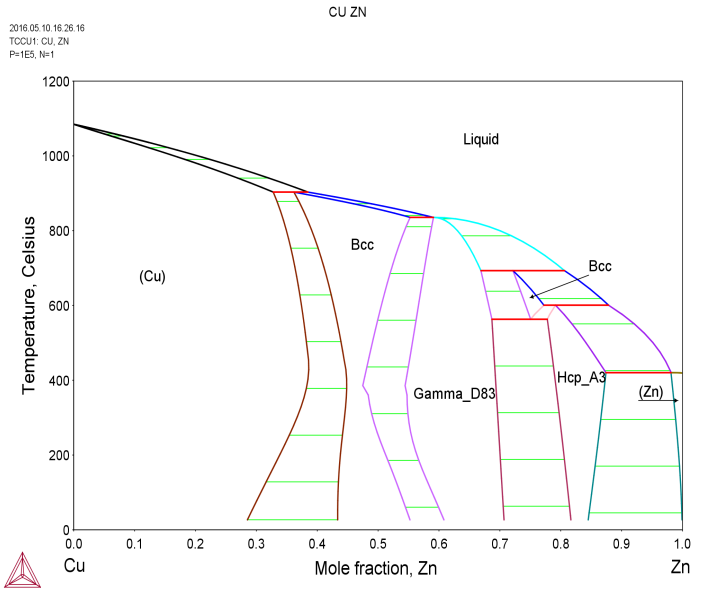


Figure 1: Calculated Cu-Zn phase diagram [2011, Wang].

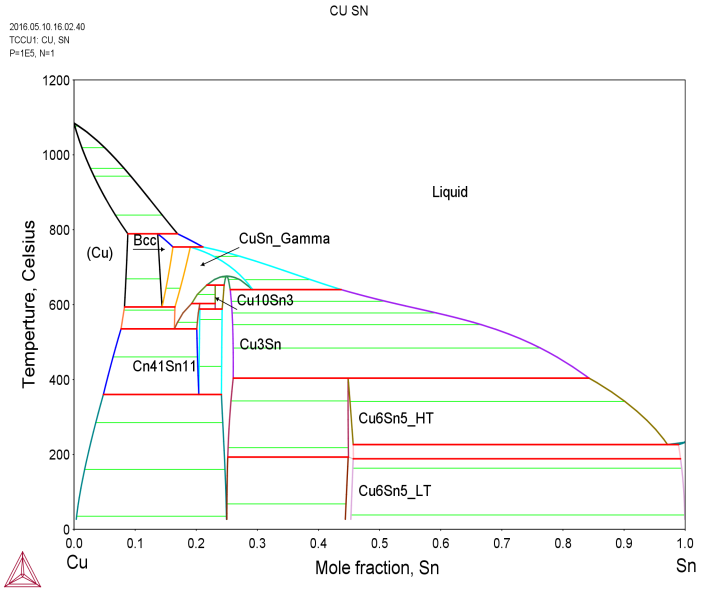


Figure 2: Calculated Cu-Sn phase diagram [2009, Li].

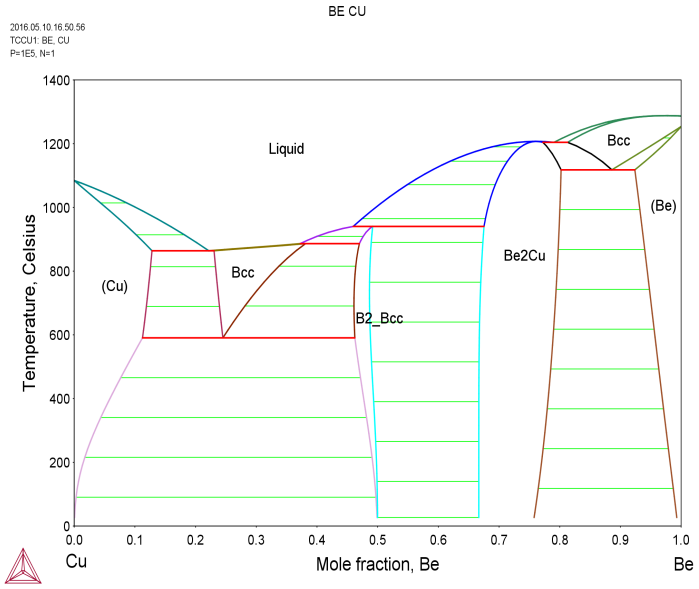


Figure 3: Calculated Cu-Be phase diagram.

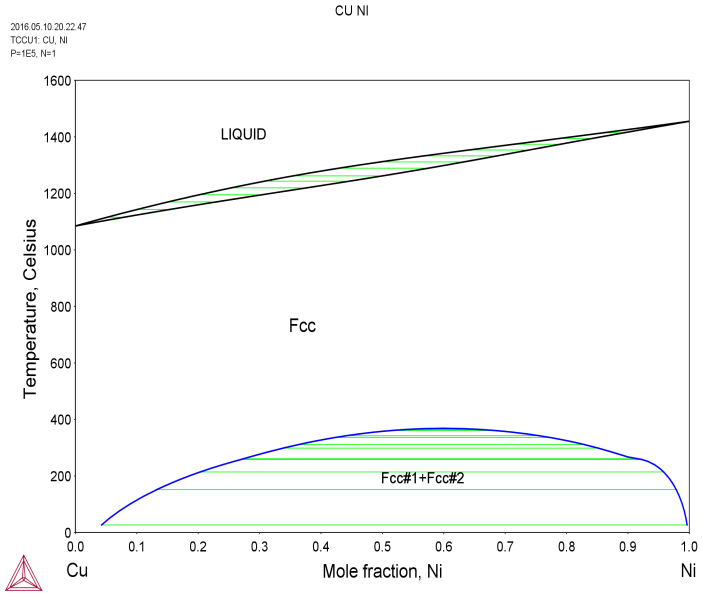


Figure 4: Calculated Cu-Ni phase diagram [1992, an Mey].

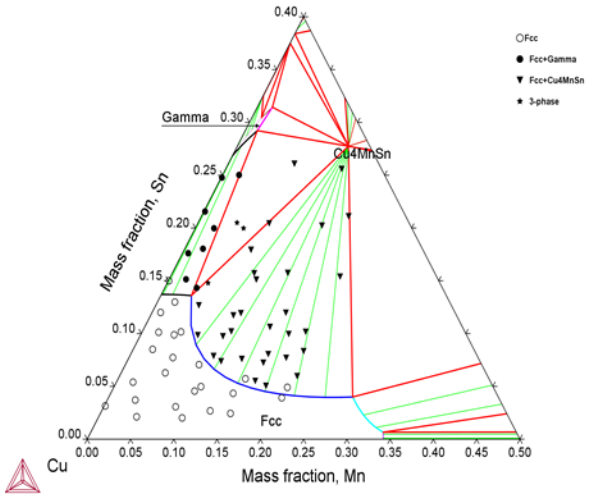


Figure 5: Calculated isothermal section of Cu-Mn-Sn [2004, Miettinen] at 550°C along with experimental data [1953, Blade; 1953, Funk; 1987, Leonova].

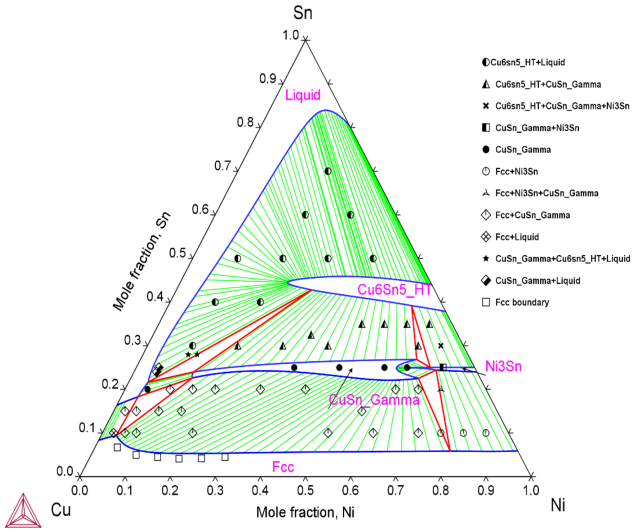


Figure 6: Calculated isothermal section of Cu-Ni-Sn at 800°C along with experimental data [2003, Wang].

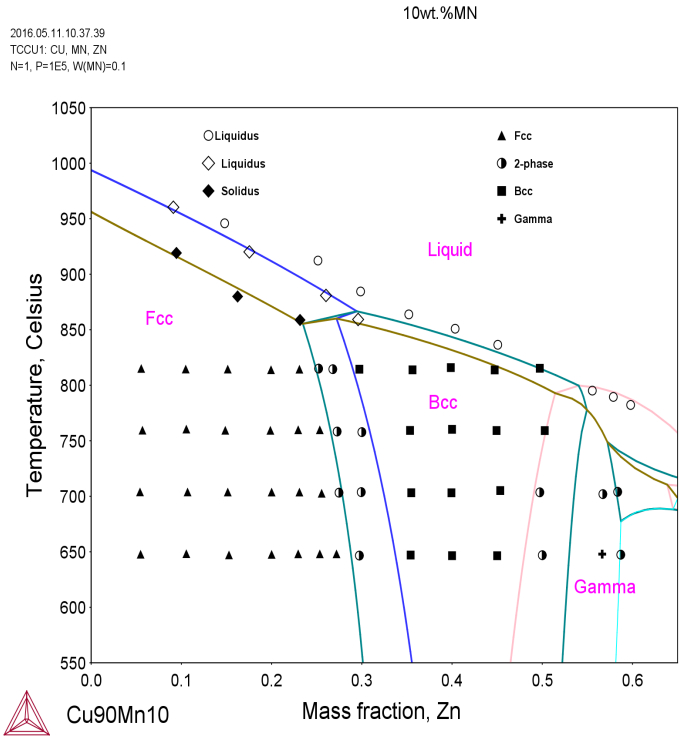


Figure 7: Calculated vertical section 10wt.% Mn in the Cu-Mn-Zn system [2010, Chang] along with the experimental data [1926, Heusler; 1949, Graham; 1972, Watanabe].

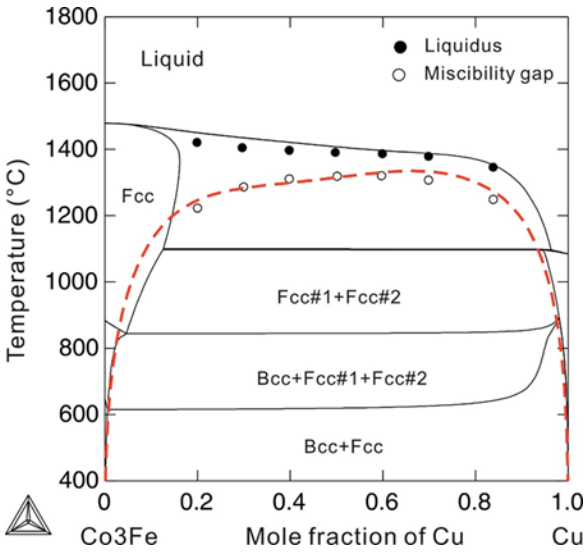


Figure 8: Calculated vertical section Fe:Co = 1:3 (at.%) in the Cu-Co-Fe system [2006, Palumbo] along with the experimental data [2005, Cao]. The red dashed line is the metastable liquid miscibility gap.

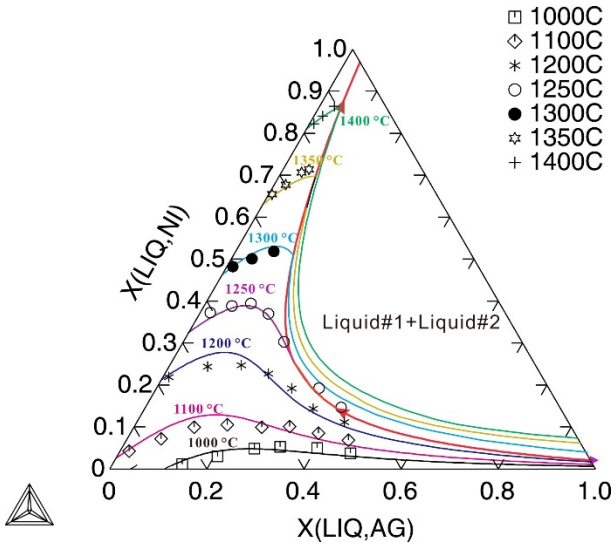


Figure 9: Calculated liquidus projection along with experimental data [1998, Kubaschewski] in the Cu-Ag-Ni system [2008, Liu].

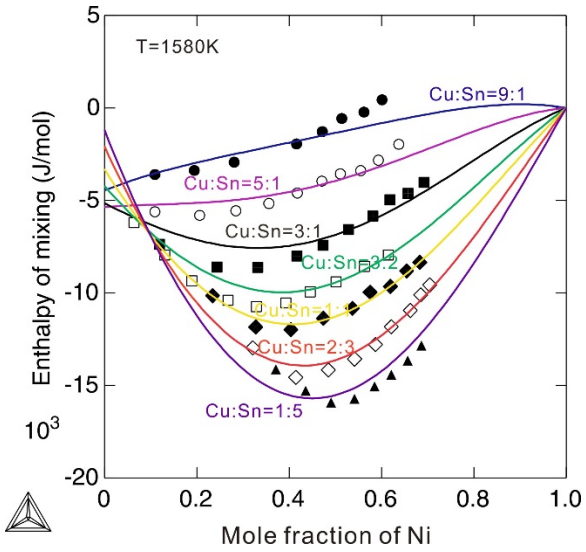


Figure 10: Mixing enthalpies of liquid phase in the Cu-Ni-Sn system at 1583K compared with experimental data [1979, Pool].

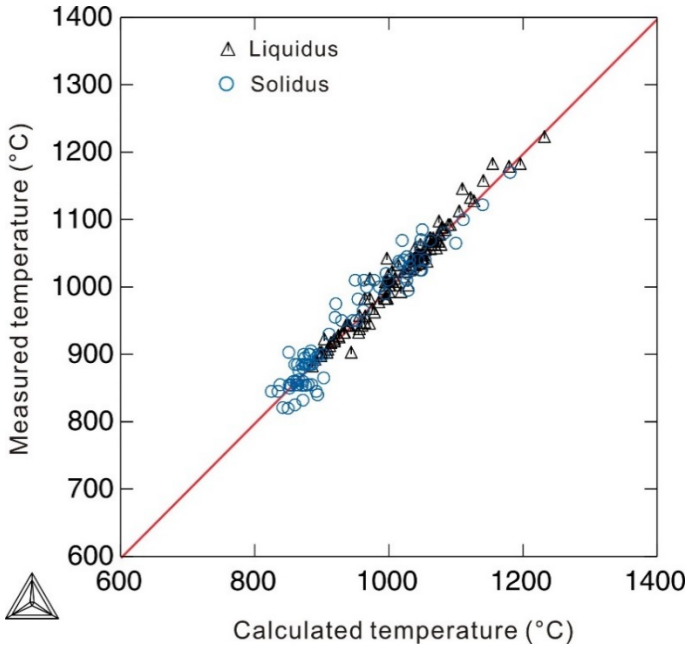


Figure 11: Comparison of calculated and experimental [2001, Davis] liquidus and solidus temperatures for various industry copper alloys.

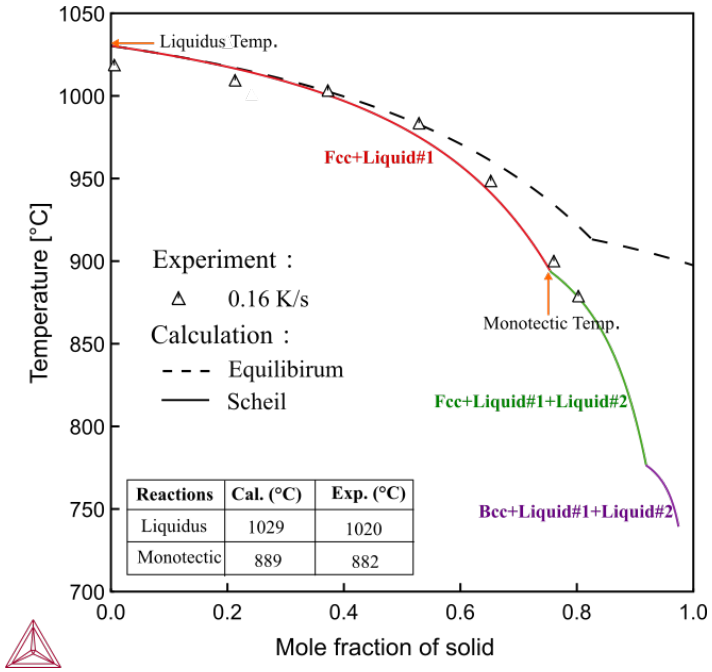


Figure 12: Equilibrium solidification and Scheil solidification simulations of Cu-5.2Sn-4.7Pb alloy, compared with experimental result [2009, Korojy]. The calculated Scheil solidification path, including the solidified phases and the phase transformation temperatures, agrees well with the experimental data.

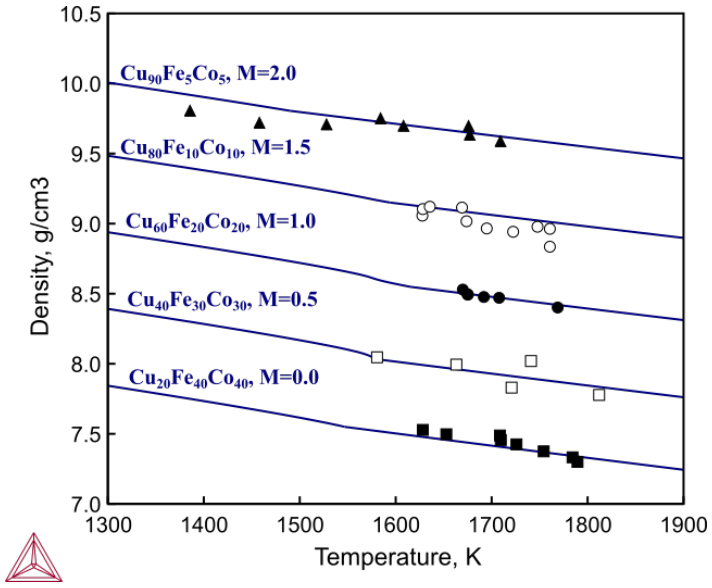


Figure 13: Calculated density of liquid Cu-Co-Fe alloys. Symbols are the experimental values from Brillo [2006]. A constant, M, is added in order to separate the data.

TCCU3 References

[1927, Heusler] O. Heusler, Über das ternäre System Kupfer-Zink-Mangan. Zeitschrift fur Anorg. und Allg. Chemie. 159, 37–54 (1927).

[1949, Graham] T. R. Graham, J. R. Long, C. E. Armantrout, A. H. Roberson, The ternary system, copper-manganese-zinc. Trans. Am. Inst. Min. Met. Pet. Eng. 185, 675–682 (1949).

[1953, Funk] C. W. Funk, J. A. Rowland, Alpha Solid-Solution Area of the Cu-Mn-Sn System. Trans. Am. Soc. Met. AIME. 197, 723–725 (1953).

[1953, Blade] J. C. Blade, J. W. Cuthbertson, The structure and mechanical properties of copper-manganese. J. Inst. Met. 82, 17–24 (1953).

[1972, Watanabe] H. Watanabe, N. Kono, M. Gonda, A Study of the Phase Diagram of the Ternary Cu-Zn-Mn System (in Japanese). J. Japan Inst. Met. 36, 297–305 (1972).

[1979, Pool] M. J. Pool, I. Arpshofen, B. Predel, E. Schultheiss, Ermittlung von Mischungsenthalpien fluessiger Legierungen des Systems Cu-Ni-Sn mit einem SETARAM-Hochtemperatur-Kalorimeter. Zeitschrift fur Met. 70, 656–659 (1979).

[1987, Leonova] N. P. Leonova, N. R. Bochvar, E. V Lysova, Phase equilibria in copper-rich Cu-Mn-Sn alloys. Russ. Metall. 4, 204–206 (1987).

[1992, an Mey] S. an Mey, Thermodynamic re-evaluation of the Cu-Ni system. Calphad. 16, 255–260 (1992).

[1998, Kubaschewski] O. Kubaschewski, Silver-Copper-Nickel in Ternary Alloy Phase Diagrams, G. Petzow, G. Effenberg, Eds., pp. 596–604, (1998).

[1998, Davis] J. R. Davis, Copper and Copper Alloys: ASM Specialty Handbook (ASM International, 2001).

[2003, Wang] C.-H. Wang, S.-W. Chen, Isothermal section of the ternary Sn-Cu-Ni system and interfacial reactions in the Sn-Cu/Ni couples at 800 °C. Metall. Mater. Trans. A. 34, 2281–2287 (2003).

[2004, Miettinen] J. Miettinen, Thermodynamic description of the Cu–Mn–Sn system in the copper-rich corner. Calphad. 28, 71–77 (2004).

[2005, Cao] C.-D. Cao, G. P. Görler, Direct Measurement of the Metastable Liquid Miscibility Gap in Fe–Co–Cu Ternary Alloy System. Chinese Phys. Lett. 22, 482–484 (2005).

[2006, Brillo] J. Brillo, I. Egry, T. Matsushita, Density and excess volumes of liquid copper, cobalt, iron and their binary and ternary alloys. Int. J. Mater. Res. 97, 1526–1532 (2006).

[2006, Palumbo] M. Palumbo, S. Curiotto, L. Battezzati, Thermodynamic analysis of the stable and metastable Co–Cu and Co–Cu–Fe phase diagrams. Calphad. 30, 171–178 (2006).

[2008, Liu] X. J. Liu, F. Gao, C. P. Wang, K. Ishida, Thermodynamic Assessments of the Ag-Ni Binary and Ag-Cu-Ni Ternary Systems. J. Electron. Mater. 37, 210–217 (2008).

[2009, Korojy] B. Korojy, L. Ekbom, H. Fredriksson, Microsegregation and Solidification Shrinkage of Copper-Lead Base Alloys. Adv. Mater. Sci. Eng. 2009, 1–9 (2009).

[2009, Li] M. Li, Z. Du, C. Guo, C. Li, Thermodynamic optimization of the Cu–Sn and Cu–Nb–Sn systems. J. Alloys Compd. 477, 104–117 (2009).

[2010, Chang] K. Chang et al., Experimental investigation and thermodynamic modeling of the Cu–Mn–Zn system. Int. J. Mater. Res. 101, 1376–1391 (2010).

[2011, Wang] J. Wang et al., Experimental investigation and thermodynamic modeling of the Cu–Si–Zn system with the refined description for the Cu–Zn system. Calphad. 35, 191–203 (2011).

Scientific Bibliography

See the Thermo-Calc Software scientific bibliography at: https://www.thermocalc.com/support/resources/.

Phases Included in TCCU3

The elements in phase names are rearranged in alphabetical order except for carbides and borides, where B and C are at the end. In order to designate the high- and low-temperature modifications of a phase, respectively, the suffixes "_HT" and "_LT" are used instead of "alpha-", "beta-" or "gamma".

LIQUID
FCC_L10
CBCC_A12
HCP_ZN
RED_P
DIAMOND_A4
C14_LAVES
GAMMA_D82
GAS:G
AGZN3
ALB2_C32
AL4M_D13
AL45CR7
AL4CR
AL13CO4
AL9CO2
ALCU_ETA
GAMMA_H
AL5FE2
ALMG_BETA
AL12MN
AL4MN_U
AL8MN5
AL3NI5

AL18TI7
AL2ZR
CRB_B33
AL3ZR2_OF40
ZRB12
BI3NI
CACU
CD3CU4
CO5GE7
COGE2
COGE
CO5GE3
CO5GE3_ALPHA
CO3GE
CO5GE2
CO2SI_HT
AL2AU_C1_CAF2
COZN_LT
COZN_DELTA
CR3GE
CR5GE3
LCR5GE3
CR11GE8
CR11GE19

CU3GE_EPSILON
CU3GE_THETA
CU3GE_ETA
CUMG2
CUSI_ETA
CU10SN3
CU6SN5_LT
CU4TI1
CUTI3
CU51ZR14
FE2P
FEP4
FESI2_L
FE5SN3_D82
FEZN_GAMMA1
GENI
GE2NI5_HT
GENI2
GENI3_HT
GE3NI5_C2
MNNI2
MN6SI
NI3SN_D019
NI2SI_HT

NI3SI_MT
NI3SN4
NI10ZR7
NI7ZR2
P2ZN
SIZR3_TP32
SI2TI_C54
ALMGZN_PHI
CU7AS3
SIGMA
CRSI2_C40
CU2SE_HT
CUSE_LT
FEZR3
NI19SI6
AL23CUFE4
AL10CU10FE
ALCU3MN2
AL9FENI
CU16MG6SI7
CU4MNSN
FCC_A1
BCC_A2
CUB_A13
RHOMBO_A7
BETA_RHOMBO_B
BCT_A5
C15_LAVES
GAMMA_D83
AG3BE8

AGZN
ALB12
AL14CA13
CUZR2_C11B
ALCR_GAMMA1
AL3CO
ALCU_DEL
ALCU_PRIME
AL2CU_C16
AL5FE4
ALMG_EPS
AL6MN
AL11MN4_LT
AL3NI_D011
ALP
AL3TI_D022
L12_FCC
ALZR2_B82
AL2ZR3_TP20
BIMN_LT
CU6SN5_HT
CACU5_D2D
CD8CU5
COSI_B20
COSN3_OS32
COZN_HT
COZN_GAMMA1
CU33SI7_DELTA
CU15SI4_EPSILON
CU3SN

CU2TI
CU4TI3
CU10ZR7
CU8ZR3
FEP
FE2SI
FESI_B20
FE3SN2
FEZN_DELTA
MN11SI19
MN9SI2
MN2SN
NI3SI2
NISI_B31
NIZN_LT
NI21ZR8
PSI
SI2ZR_C49
SI2ZR3_D5A
SN3ZR5
CU3AS
BE2CU
CRNI2_OP6
CU3P
CU3SE2
CUSE_RT
MG2NI
NI5SI2
AL62CU25FE13
AL28CU4MN7

AL7CU4NI
AL10FE3NI
CU3MG2SI
CUMNZN
FCC_L12
BCC_B2
HCP_A3
WHITE_P
GRAPHITE
B2_BCC
C36_LAVES
CO2SI_C23
AG3SN_L60
AG5ZN8
AL4C3
AL3CA8
AL5CR
GAMMA_D810
AL5CO2
ALCU_EPS
ALCU_ZETA
AL2FE1
AL13FE4
ALMG_GAMMA
AL4MN_R
AL11MN4_HT
AL3NI2
AL2TI
ALTI3_DO19
AL3ZR5_D8M

AL4ZR5
AL3ZR_D023
BIMN_HT
CA2CU
CDCU2
CD10CU3
CO3SI_HT
COSN_HP6
COZN_GAMMA
COZN_GAMMA2
CU56SI11_GAMMA
CUSN_GAMMA
CU41SN11
CU3TI2
CUTI_B11
ZRM5_C15B
FE3P
FEP2
FESI2_H
MN5SI3_D88
FEM_B35
FEZN_ZETA
MN3SI
MN3SN2
MNZN9
NI3SI_HT
NISI2
NIZN8
NI11ZR9
P2ZN3

SI4ZR5_TP36
FEB_B27
SNZR3_A15
CU7AS
NIBE7
CR3SI
CU2SE_LT
CUSE2
CUSE_HT
MG2SI_C1
SN4P3
AL7CU2FE
AL11CU5MN3
AL5CU4ZN
AL71FE5NI24
CU5MN4SI
CU2TIZR
MONI_DELTA
MONI4_BETA
NI3MO_D0A
R_PHASE
CUO
CUPRITE_C3
CORUNDUM
CO7NB2
AGP2
AG3P11
CU2P7
CUP2
CUALO2

SPINEL
MU_PHASE
TIGE2
TI6GE5
TI5GE3

Models for the Phases Included in TCCU3

LIQUID :AG CU FE GE MN MO NI SI ZN SN CO P PB BE AU AL AS B BI C CA CD CR MG NB PT SE TI ZR O CU2SE CU2O CUO AL2/3O1 AL4/3O2:	
FCC_A1 :AG AL AU AS BE BI CA CD CO CR CU FE GE MG MN MO NB NI P PB PT SE SI SN TI ZN ZR:B C O VA :	2 SUBL, 1 1
FCC_L12 :AL CU FE GE MG MN NI SI ZN CR SN TI ZR AG CA CO PB BE BI CD P AU AS NB PT SE:AL CU FE MG MN NI SI ZN CR SN TI ZR AG CA CO GE PB BE BI CD P AU AS NB PT SE:B C VA:	3 SUBL, 0.75 0.25 1
FCC_L10 :AL CU MN NI TI:AL CU MN NI TI:	2 SUBL, 0.5 0.5
BCC_A2 :AG AL AU AS BE BI CA CD CO CR CU FE GE MG MN MO NB NI P PB PT SE SI SN TI ZN ZR VA:B C O VA:	2 SUBL, 1 3
BCC_B2 :AG AL AU AS BE BI CA CD CO CR CU FE GE MG MN MO NB NI P PB PT SE SI SN TI ZN ZR VA:AG AL AU AS BE BI CA CD CO CR CU FE GE MG MN MO NB NI P PB PT SE SI SN TI ZN ZR VA:B C O VA:	3 SUBL, 0.5 0.5 3
CBCC_A12 :AL BI CO CU FE MN NI SI ZN MG CR TI ZR SN:B C O VA:	2 SUBL, 1 1
HCP_A3 :AG AL AU AS BE BI CA CD CO CR CU FE GE MG MN MO NB NI PB PT SI SN TI ZN ZR:B C O VA:	2 SUBL, 1 0.5
HCP_ZN :AG AU BI AL CO CR CU FE GE NI MN PB SI ZN SN PT:VA:	2 SUBL, 1 0.5
RHOMBO_A7 :AS AG BI P PB SN ZN:	
WHITE_P :P:	
RED_P :P:	
BETA_RHOMBO_B :B:CU SI B C:	2 SUBL, 93 12
GRAPHITE	

:B C:	
DIAMOND_A4 :AG B C GE P AL SI ZN SN TI:	
BCT_A5 :AG AL B BI CD CU NI PB ZN SN SI TI:	
B2_BCC :AL CO FE CU ZN BE NI:BE CO MN TI VA ZR:	2 SUBL, 1 1
C14_LAVES :AL CO CU CR FE MG MN NB NI TI ZN ZR:AL CO CU CR FE MG MN NBTI ZN ZR:	2 SUBL, 2 1
C15_LAVES :AL CA CO CU FE MG MN NB NI SI ZN CR TI ZR:AL CA CO CU FE MG MN NB NI SI ZN CR TI ZR:	2 SUBL, 2 1
C36_LAVES :AL CU CO CR FE MG MN NB NI ZN ZR:AL CU CO CR FE MG MN NB NI ZN ZR:	2 SUBL, 2 1
GAMMA_D82 :FE MN ZN:FE MN NI ZN:AL CU FE MN NI SI ZN:AL ZN:	4 SUBL, 2 2 3 6
GAMMA_D83 :AL FE NI SI ZN:AL CU NI SI ZN:CU MN FE NI ZN SN:	3 SUBL, 4 1 8
CO2SI_C23 :AL CO CA CU FE NI SI:AL CO SI SN ZN:	2 SUBL, 2 1
GAS:G :AG,AG2,AL,AL2,AL1O1,AL1O2,AL2O1,AL2O2,AL2O3,AS,AS2,AS3,AS4,AU,AU2, B,B2,BE,BE2,BI,BI2,BI3,BI4,CD,CO,CO2,CU,CU2,FE,FE2,MN,MO,MO2,NB,NI,NI2, O,O2,O3,P,P2,P3,P4,PB,PB2,PT,SE,SE2,SE3,SE4,SE5,SE6,SE7,SE8,SI,SI2,SI3,SN,SN2, ZN, ZR, ZR2:	
AG3BE82 SUBL 2.97 8.03 :AG:BE:	
AGZN3 :AG ZN:	
AGZN :ZN:AG ZN:	2 SUBL, 1 2
AG5ZN8 :AG ZN:AG:AG ZN:AG ZN:	4 SUBL, 2 2 3 6
ALB2_C32	2 SUBL, 1 2

:MG AL MN CR ZR TI:B:	
AL4CR :CR:AL SI VA:	2 SUBL, 1 4
ALB12 :AL:B:	2 SUBL, 1 12
AL4C3 :AL SI:C:	2 SUBL, 4 3
AL4M_D13 :AL:CA:	2 SUBL, 4 1
AL3CA8 :AL:CA MG:	2 SUBL, 3 8
AL45CR7 :AL:CR:	2 SUBL, 45 7
CUZR2_C11B :AL CR CU SI ZN:AL CR TI ZR:	2 SUBL, 1 2
AL5CR :AL SI:CR:	2 SUBL, 5 1
ALCU_DEL :AL ZN:CU FE:	2 SUBL, 2 3
ALCU_EPS :AL CU ZN NI:CU FE	2 SUBL, 1 1
ALCU_ETA :AL CU:CU FE ZN NI:	2 SUBL, 1 1
ALCU_PRIME :AL:CU:	2 SUBL, 2 1
ALCU_ZETA :AL:CU FE:	2 SUBL, 9 11
GAMMA_H :AL ZN:AL CU ZN:CU MN FE NI:	3 SUBL, 4 18
AL2CU_C16 :AL FE SN ZR MN NI:AL CU FE NI B MN SI CO:	2 SUBL, 2 1
AL2FE1 :AL CU SI ZN:FE MN NI:	2 SUBL, 2 1

AL5FE2 :AL CU SI ZN:FE MN NI:	2 SUBL, 5 2
AL5FE4 :AL CU FE MN:	
AL13FE4 :AL CU:FE MN NI ZN:AL SI VA ZN:	3 SUBL, 0.63 0.23 0.14
ALMG_BETA :MG:AL ZN:	2 SUBL, 89 140
ALMG_EPS :MG:AL ZN:	2 SUBL, 23 30
AL12MN :AL:MN:	2 SUBL, 12 1
ALMG_GAMMA :MG:AL MG ZN:AL MG ZN:	3 SUBL, 5 12 12
AL6MN :AL ZN:MN FE:	2 SUBL, 6 1
AL4MN_R :AL:MN FE:	2 SUBL, 461 107
AL4MN_U :AL ZN:MN:	2 SUBL, 4 1
AL11MN4_LT :AL ZN:MN FE:	2 SUBL, 11 4
AL11MN4_HT :AL MN:MN:	2 SUBL, 29 10
AL8MN5 :AL ZN:MN:AL MN SI CU:	3 SUBL, 12 5 9
AL3NI_D011 :AL MN NI:FE NI:	2 SUBL, 0.75 0.25
AL3NI2 :AL SI ZN:AL CU FE NI:NI VA:	3 SUBL, 3 1 2
AL3NI5 :AL:NI:	2 SUBL, 0.38 0.62
ALP	2 SUBL, 1 1

:AL:P:	
AL2TI :AL:TI:	2 SUBL, 2 1
AL18TI7 :AL:TI:	2 SUBL, 0.72 0.28
AL3TI_D022 :AL MN NI:MN TI ZR:	2 SUBL, 3 1
ALTI3_DO19 :AL TI:AL TI:	2 SUBL, 3 1
AL2ZR :AL:ZR:	2 SUBL, 2 1
L12_FCC :AL NI SI TI:AL FE ZR NI ZN:	2 SUBL, 1 3
AL3ZR5_D8M :AL SI:ZR CR:	2 SUBL, 3 5
CRB_B33 :AL CA CR NI:AG B SI SN ZR:	2 SUBL, 1 1
ALZR2_B82 :AL MN SN VA:ZR MN TI VA:	2 SUBL, 1 2
AL4ZR5 :AL:ZR:	2 SUBL, 4 5
AL3ZR2_OF40 :AL:ZR:	2 SUBL, 3 2
AL2ZR3_TP20 :AL ZN:ZR:	2 SUBL, 2 3
AL3ZR_D023 :AL:TI ZR:	2 SUBL, 3 1
ZRB12 :B:ZR:	2 SUBL, 12 1
CACU :CA:CU:	2 SUBL, 1 1
CACU5_D2D :CA:CU NI ZN:	2 SUBL, 1 5

CDCU2 :CD:CU:	2 SUBL, 1 2
CD3CU4 :CD:CU:	2 SUBL, 0.43 0.57
CD8CU5 :CU:CD CU:CU:CU CD:	4 SUBL, 2 3 2 6
CD10CU3 :CD:CU:	2 SUBL, 0.77 0.23
CO2SI_HT :CO SI:CO SI:	2 SUBL, 0.67 0.33
COSI_B20 :AL CO SI:CO SI:	2 SUBL, SITES 0.5 0.5
CO3SI_HT :CO CU NI SI SN:CO CU NI SN:CO CU NI:	3 SUBL, 0.25 0.25 0.5
AL2AU_C1_CAF2 :AG AL AU CU SI SN:AL AU CO NI PT:	2 SUBL, 0.67 0.33
CO5GE7 :CO:GE:	2 SUBL, 0.417 0.583
COGE2 :CO:GE:	2 SUBL, 0.333 0.667
COGE :CO:GE:	2 SUBL, 0.5 0.5
CO5GE3 :CO VA:CO:CO GE SN:	3 SUBL, 0.125 0.5 0.375
CO5GE3_ALPHA :CO:GE:	2 SUBL, 0.625 0.375
CO5GE2 :CO:GE:	2 SUBL, 0.714 0.286
CO3GE :CO:GE:	2 SUBL, 0.75 0.25
COSN3_OS32 :CO:SN:	2 SUBL, 0.25 0.75

COSN_HP6 :CO:SN:	2 SUBL, 0.5 0.5
COZN_LT :CO ZN:VA:	2 SUBL, 1 1
COZN_HT :CO ZN:VA:	2 SUBL, 1 1
COZN_GAMMA :CO ZN:VA:	2 SUBL, 1 1
COZN_DELTA :CO:ZN:	2 SUBL, 0.12 0.88
COZN_GAMMA2 :CO:ZN:	2 SUBL, 0.07 0.93
COZN_GAMMA1 :CO:ZN:	2 SUBL, 0.12 0.88
LCR5GE3 :CR GE:CR GE:	2 SUBL, 0.625 0.375
CR3GE :CR GE:CR GE:	2 SUBL, 0.75 0.25
CR5GE3 :CR GE:CR GE:	2 SUBL, 0.625 0.375
CR11GE8 :CR:GE:	2 SUBL, 0.579 0.421
CR11GE19 :CR:GE:	2 SUBL, 0.367 0.633
CU10SN3 :CU NI:SN:	2 SUBL, 0.77 0.23
CU10ZR7 :CU:ZR:	2 SUBL, 10 7
CU15SI4_EPSILON :CU MN MG ZN:AL SI:	2 SUBL, 0.79 0.21
CU2TI :CU:TI:	2 SUBL, 2 1

CU3TI2 :CU:TI:	2 SUBL, 3 2
CU33SI7_DELTA :CU ZN:SI:	2 SUBL, 0.82 0.17
CU3GE_EPSILON :AG CU:GE:	2 SUBL, 0.765 0.235
CU3GE_THETA :AG CU:GE:	2 SUBL, 0.735 0.265
CU3GE_ETA :AG CU:GE:	2 SUBL, 0.75 0.25
CU3SN :CU SN NI:CU SN:	2 SUBL, 3 1
CU56SI11_GAMMA :CU MG MN NI SI ZN:SI:	2 SUBL, 0.84 0.16
CU4TI1 :CU TI:CU TI:	2 SUBL, 4 1
CU4TI3 :CU:TI:	2 SUBL, 4 3
CU41SN11 :CU SN ZN:CU SN ZN:	2 SUBL, 41 11
CU51ZR14 :CU:ZR:	2 SUBL, 51 14
CU6SN5_LT :CU:CU SN:SN:	3 SUBL, 1 1 1
CU6SN5_HT :AG CO CU MN NI VA:AG AL BI CU GE NI PB SI SN:CO CU MN NI SN VA:	3 SUBL, 1 1 1
CU8ZR3 :CU:ZR:	2 SUBL, 8 3
CUMG2 :CU NI:MG:	2 SUBL, 1 2
CUSI_ETA :CU MN NI ZN:SI:	2 SUBL, 0.76 0.24

CUSN_GAMMA :CU MN NI SN ZN:	
CUTI_B11 :CU TI:CU TI:	2 SUBL, 1 1
CUTI3 :CU TI:TI:	2 SUBL, 1 3
ZRM5_C15B :CU NI:ZR:	2 SUBL, 5 1
FE3P :FE:P:	2 SUBL, 0.75 0.25
FE2P :FE:P:	2 SUBL, 0.67 0.33
FEP :FE:P:	2 SUBL, 0.5 0.5
FEP2 :FE:P:	2 SUBL, 0.33 0.67
FEP4 :FE:P:	2 SUBL, 0.2 0.8
FE2SI :FE NI:AL SI:	2 SUBL, 2 1
FESI2_H :FE NI:AL SI:	2 SUBL, 3 7
FESI2_L :FE NI:AL SI:	2 SUBL, 1 2
FESI_B20 :FE GE MN NI CR:AL SI:	2 SUBL, 1 1
MN5SI3_D88 :CU FE MN NI CR ZR TI:AL CR SI GE SN:	2 SUBL, 5 3
FE5SN3_D82 :FE:SN:	2 SUBL, 5 3
FE3SN2 :FE:SN:	2 SUBL, 3 2
FEM_B35	2 SUBL, 1 1

:FE:SN:	
FEZN_GAMMA1 :FE:AL CU FE NI SI ZN:MN ZN:	3 SUBL, 0.14 0.12 0.74
FEZN_DELTA :FE:AL CU FE MN NI SI ZN:ZN:ZN:	4 SUBL, 0.06 0.18 0.53 0.24
FEZN_ZETA :FE MN NI VA:AL ZN:AL CU SI VA ZN:	3 SUBL, 0.07 0.86: 0.07
GE2NI5_HT :NI:GE:	2 SUBL, 0.72 0.28
GENI :GE:NI:	2 SUBL, 0.5 0.5
GENI2 :NI:GE:	2 SUBL, 0.665 0.335
GENI3_HT :NI:GE:	2 SUBL, 0.744 0.256
GE3NI5_C2 :NI:GE:	2 SUBL, 0.625 0.375
MNNI2 :MN NI:NI:	2 SUBL, 1 2
MN11SI19 :MN:AL SI:	2 SUBL, 11 19
MN3SI :FE MN NI:AL SI:	2 SUBL, 3 1
MN6SI :AL MN:SI ZN:	2 SUBL, 17 3
MN9SI2 :MN:SI:	2 SUBL, 33 7
MN3SN2 :MN:SN:	2 SUBL, 3 2
NI3SN_D019 :CU NI AL SN VA:CU MN FE NI SN:	2 SUBL, 1 3
MN2SN	2 SUBL, 0.64 0.36

:MN:SN:	
MNZN9 :MN:ZN:	2 SUBL, 0.10 0.90
NI2SI_HT :CU NI:NI VA:AL SI:	3 SUBL, 1 1 1
NI3SI2 :FE NI:SI:	2 SUBL, 3 2
NI3SI_HT :FE NI:AL SI:	2 SUBL, 3 1
NI3SI_MT :SI:NI:	2 SUBL, 1 3
NISI_B31 :FE NI:SI ZN:	2 SUBL, 1 1
NISI2 :AL CU SI ZN:CU FE MN NI:	2 SUBL, 2 1
NI3SN4 :CU NI:NI SN:SN:	3 SUBL, 0.25 0.25 0.25
NIZN_LT :AL FE MN NI SI ZN:AL FE MN NI SI ZN:	2 SUBL, 0.5 0.5
NIZN8 :NI:AL ZN:	2 SUBL, 0.11 0.89
NI10ZR7 :NI:ZR:	2 SUBL, 23 17
NI21ZR8 :ZR:NI:	2 SUBL, 8 21
NI11ZR9 :NI:ZR:	2 SUBL, 11 9
NI7ZR2 :NI:ZR:	2 SUBL, 7 2
PSI :P:SI:	2 SUBL, 1 1
P2ZN3 :P:ZN:	2 SUBL, 2 3

P2ZN :P:ZN:	2 SUBL, 2 1
SI2ZR_C49 :SI GE:ZR:	2 SUBL, 2 1
SI4ZR5_TP36 :SI GE:TI ZR:	2 SUBL, 4 5
SIZR3_TP32 :SI GE:ZR TI:	2 SUBL, 1 3
SI2ZR3_D5A :SI:ZR:	2 SUBL, 2 3
FEB_B27 :FE MN TI ZR:B GE SI ZN:	2 SUBL, 1 1
SI2TI_C54 :SI SN:TI ZR:	2 SUBL, 2 1
SN3ZR5 :ZR:SN:SN VA:	3 SUBL, 5 3 1
SNZR3_A15 :SN ZR:SN ZR:	2 SUBL, 3 1
TI5GE3 :GE:TI:	2 SUBL, 3 5
TI6GE5 :GE:TI:	2 SUBL, 5 6
TIGE2 :GE:TI:	2 SUBL, 2 1
ALMGZN_PHI :MG:AL ZN:	2 SUBL, 6 5
CU3AS :CU:CU AS:	2 SUBL, 3 1.15
CU7AS :CU:AS:	2 SUBL, 7 1
CU7AS3 :CU:AS:	2 SUBL, 7 3
BE2CU	2 SUBL, 2 1

:BE CU:BE CU:	
NIBE7 :NI BE:NI:BE:	3 SUBL, 2 2 9
SIGMA :FE MN NI CO:CR MO:FE CR MN MO NI:	3 SUBL, 8 4 18
CRNI2_OP6 :CR:NI:	2 SUBL, 1 2
CR3SI :CR SI:AL CR SI:	2 SUBL, 3 1
CRSI2_C40 :CR SI CU:AL CR SI CU:	2 SUBL, 1 2
CU3P :CU:P:	2 SUBL, 3 1
CU2SE_LT :CU SE:SE:	2 SUBL, 2 1
CU2SE_HT :CU SE:SE:	2 SUBL, 2 1
CU3SE2 :CU:SE:	2 SUBL, 3 2
CUSE2 :CU:SE:	2 SUBL, 1 2
CUSE_LT :CU:SE:	2 SUBL, 1 1
CUSE_RT :CU:SE:	2 SUBL, 1 1
CUSE_HT :CU:SE:	2 SUBL, 1 1
FEZR3 :FE:ZR:	2 SUBL, 1 3
MG2NI :MG ZN:CU NI ZN:	2 SUBL, 2 1
MG2SI_C1 :MG:SI SN:	2 SUBL, 2 1

NI19SI6 :SI:CU NI:	2 SUBL, 0.24 0.76
NI5SI2 :CU FE NI:AL SI:	2 SUBL, 5 2
SN4P3 :SN:P:	2 SUBL, 4 3
AL23CUFE4 :AL:CU:FE:	3 SUBL, 23 1 4
AL62CU25FE13 :FE:AL CU:AL:	3 SUBL, 0.12 0.26 0.62
AL7CU2FE :FE NI:CU:AL:	3 SUBL, 1 2
AL10CU10FE :FE:AL CU:AL:	3 SUBL, 1 10 10
AL28CU4MN7 :AL:MN:CU:	3 SUBL, 28 7 4
AL11CU5MN3 :AL:MN:CU:	3 SUBL, 11 3 5
ALCU3MN2 :AL:MN:CU:	3 SUBL, 1 2 3
AL7CU4NI :AL:FE CU NI VA:	2 SUBL, 1 1
AL5CU4ZN :AL CU:AL:CU:ZN:	4 SUBL, 1 4 4 1
AL9FENI :AL:FE NI :	2 SUBL, 9 2
AL10FE3NI :AL:FE NI:	2 SUBL, 5 2
AL71FE5NI24 :AL:FE:NI:	3 SUBL, 0.71 0.05 0.24
CU16MG6SI7 :CU:MG:SI:	3 SUBL, 16 6 7

CU3MG2SI :CU:MG:SI:	3 SUBL, 2.74 2 1.26
CU5MN4SI :CU:MN:SI:	3 SUBL, 0.50 0.37 0.13
CU4MNSN :CU:SN:MN:	3 SUBL, 0.67 0.17 0.17
CUMNZN :CU:MN:ZN:	3 SUBL, 0.33 0.33 0.33
CU2TIZR :CU:TI:ZR:	3 SUBL, 0.5 0.25 0.25
MU_PHASE : CU CO NB FE : CU MO NB :CO NB FE MO :	3 SUBL, 7 2 4
MONI_DELTA :NI : MO NI :CU MO:	3 SUBL, 24 20 12
MONI4_BETA :MO: NI :	2 SUBL, 1 4
NI3MO_D0A : NI : MO NI :	2 SUBL, 3 1
R_PHASE :FE : MO : FE MO:	3 SUBL, 27 14 12
CUO :CU+2 : O-2 :	2 SUBL, 1 1
CUPRITE_C3 CUPRITE_C3 :CU+1 : O-2 :	2 SUBL, 2 1
CORUNDUM :AL+3,VA : VA : O-2 :	3 SUBL, 2 1 3
CO7NB2 : CO :NB :	2 SUBL, 7 2
AGP2 :AG :P :	2 SUBL, 1 2
AG3P11 :AG :P :	2 SUBL, 3 11
CU2P7	2 SUBL, 2 7

:CU : P :	
CUP2 :CU : P :	2 SUBL, 1 2
SPINEL :AL+3,CU+2 : AL+3,CU+2,VA : VA : O-2 :	4 SUBL, 1 2 2 4
CUALO2 :CU+1:AL+3: O-2 :	3 SUBL, 1 1 2