TCS Steel and Fe-alloys Database (TCFE11)

Technical Information

Available Starting with Thermo-Calc Version 2021a

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Contents

About the TCS Steel and Fe-alloys Database (TCFE)

Current Database Version

TCS Steel and Fe-alloys Database (TCFE) is a thermodynamic and properties database with applications to a variety of steels and Fe-based alloys, such as stainless steels, high-speed steels, tool steels, high-strength low alloy (HSLA) steels, cast irons, corrosion-resistant high strength steels, low-density steels, and also cemented carbides. The databases can be used for alloy compositions, but also their interaction with atmospheres containing oxygen, nitrogen, carbon, hydrogen, or mixtures thereof.

TCS Steel and Fe-alloys Database (TCFE) is developed to be used with our entire suite of products: Thermo-Calc, the Add-on Modules, and all available SDKs. In addition, it is integral to the Steel Model Library, which includes martensite, pearlite, and bainite models designed to help experts working in the steel industry to quickly and easily set up calculations using the Property Model Calculator.

The CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of binary, ternary, and for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

Use Case Examples

There are examples available to both demonstrate the *validation* of the database and to showcase the types of *calculations* that can be used for different materials or application areas such as process metallurgy, heat treatment, and more depending on the database. Sometimes an example is both a validation and a calculation example.

Some use case examples of how this database can be used include the following:

- Calculate various phase diagrams in the assessed systems as well as to extrapolate higher-order systems
- Simulate the solidification process
- Predict the relative stability of matrix phases (austenite and ferrite)
- Predict the precipitation of secondary phases such as sulfides, borides, oxides, phosphides, carbides, nitrides, carbonitrides, and also intermetallic phases such as the sigma and laves phases

- Predict the density, molar volume and thermal expansion coefficients
- Predict the viscosity of metallic liquids
- Predict the surface tension of metallic liquids
- Predict the lath and plate martensite start temperature
- Describe the thermodynamics of bainite and pearlite formation
- Predict oxide scale formation on various steels
- Integrate with a compatible atomic mobility database and use it to simulate diffusion controlled phase transformations with the Add-on Diffusion Module (DICTRA) and multi-particle precipitation kinetics with the Add-on Precipitation Module (TC-PRISMA)

Combining Databases

It is possible to combine several databases to make calculations using Thermo-Calc. For more information related to a specific type of problem, contact one of our support specialists at info@thermocalc.com. The experts are available to make recommendations on the most suitable database to use for your needs.

TCS Steel and Fe-alloys Database (TCFE) Resources

Information about the database is available on our website and in the Thermo-Calc software online Help.

- **Website**: On our website the information is both searchable and the database specific PDFs are available to download.
- **Online Help**: Technical database information is included with the Thermo-Calc software online Help. When in Thermo-Calc, press F1 to search for the same information as is contained in the PDF documents described. Depending on the database, there are additional examples available on the website.

Database Specific Documentation

- The *TCS Steel and Fe-alloys Database (TCFE) Technical Information* PDF document contains version specific information such as the binary, ternary and higher-order assessed systems, phases and models. It also includes a list of the included elements, and summaries of the database revision history by version.
- The *TCS Steel and Fe-alloys Database (TCFE) Examples Collection* PDF document contains a series of validation examples using experimental data, and a set of calculation examples showing some of the ways the database can be used.

Go to the Steels and Fe-Alloys Databases page on our website where you can access the technical information and learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to iron and steels including links to resources such as publications, webinars, videos, and more.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

TCFE11 Elements, Systems, Phases and Properties

Included Elements

There are 29 elements included in the most recent version of the database.

Ar	Al	B	C	Ca	Ce	Co	Cr	Cu	Fe
H	Mg	Mn	Mo	N	Nb	Ni	O	P	Ru
S	Si	Ta	Ti	V	W	Y	Zn	Zr	

Assessed Systems

Also see information about TCFE11 Composition Limits

The database is developed on the basis of complete assessments of binary, ternary, and some higher order systems. However, many intermediate compounds that usually do not occur in steels/Fe-alloys are ignored in the database. Therefore, the database may not be suitable to calculate complete binary and ternary systems, but only rather in the Fe-rich corner.

Sometimes, for some special steels/Fe-alloys, you may prefer to append some other stoichiometric or solution phases (usually intermediate compound phases that have been ignored in the *TCFE Database*) from another compatible database (e.g. *SSOL: SGTE Solutions Database* and/or *SSUB: SGTE Substances Database*). But you must be careful about appropriately appending such data in the combination.

The most recent version of the database contains the following:

- 345 assessed binary systems
- 290 assessed ternary systems
- 79 assessed quaternary systems
- Several assessed quinary systems

Included Phases

Common Phases for Steel and Fe-alloys and TCFE11 Models for the Included Phases

The *TCFE* database contains an extensive GAS mixture phase (Ar and different species in the C-H-N-O-S system) for the main purpose of considering oxygen/nitrogen-gas controls in steel-making processes and different gas atmospheres under, for example, heat treatments. However, it can be replaced by an even more comprehensive description of the GAS phase appended from a compatible database e.g. *SSUB: SGTE Substances Database*.

Similarly, an IONIC_LIQ solution phase can be appended from the *TCOX: TCS Metal Oxide Solutions Database*, when it is really necessary to consider a more comprehensive ionic liquid phase for calculations of e.g. formations of complex oxides on steel surfaces. You can also use the TCOX database and the Process Metallurgy Module to investigate various steelmaking metallurgical processes.

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. To show the information, it is recommended in the Database (TDB) module to use the command LIST_SYSTEM with the option `Constituents`.

Properties Data

A variety of properties data are included with the TCS Steel and Fe-alloys Database (TCFE).

Below is a summary of the available parameters and variables for this database when working in Thermo-Calc. There are differences when you are working in Console Mode versus Graphical Mode as well as if you use the TC-Python SDK. More details are described in the online help.

Property	Model Parameters in TDB File	Variables to Show or Plot in Console Mode and TC-Python
Kinematic viscosity		`KVIS(LIQUID)`
Dynamic viscosity	VISC	`DVIS(LIQUID)`
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI
Surface tension	SIGM, XI	`SURF(LIQUID)`

TCFE11 Composition Limits

The TCS Steel and Fe-alloys Database (TCFE) is applicable for various types of steels/Fe-alloys with an Fe-minimum of 50 wt.%.

The critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations.

A sensible calculation cannot be expected if all alloying elements are at their highest limits. Some combinations of elements at high values do not give reasonable results. However, some alloying elements can exceed their limits considerably and the calculations still give good results.

If you discover any significant deviations and want to help us improve future versions of the database, please contact Thermo-Calc Software at one of our offices or send us an email at info@thermocalc.com.

For alloying elements, the recommended composition limits are given in the table below.

Element	Max	Element	Max	Element	Max	Element	Max
Al	10	Cu	5	Ni	20	Ti	3
B	Trace	H	Trace	O	Trace	V	15
C	7	Mg	Trace	P	Trace	W	15
Ca	Trace	Mn	30	Ru	15	Y	*
Ce	Trace	Mo	10	S	Trace	Zn	**
Co	20	N	5	Si	5	Zr	10
Cr	30	Nb	5	Ta	10		

*Y systems are included mainly for the purpose of oxide dispersion strengthened (ODS) steels with many assessed oxygen containing binary and ternary systems within the Al-Cr-Cu-Fe-Mn-Ni-O-Si-Y-Zr frame of elements.

** The element Zn has been further treated with the focus on the Zn corner of Al-Cr-Fe-Zn system for galvanization process, but several other binaries and ternaries are also included.

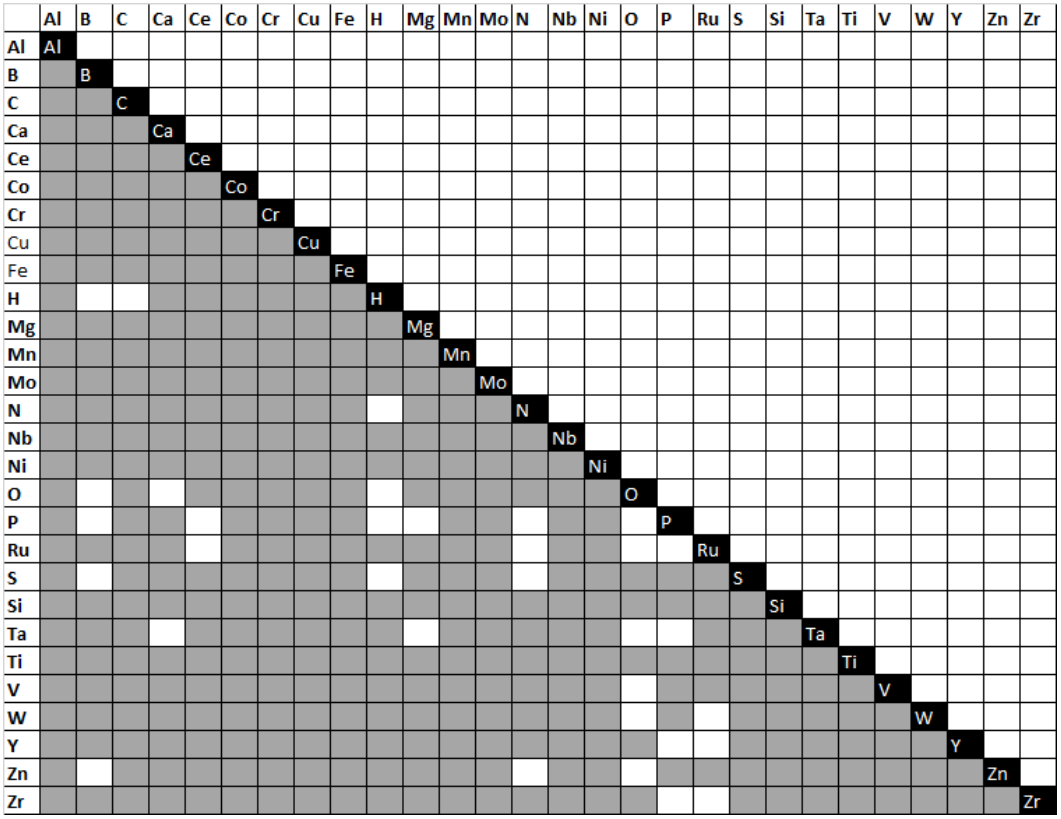
Ar is only considered in the gas phase and no modeling of solubility in the solid solution phases or liquid is taken into account.

TCFE11 Systems

In this section:

TCFE11 Assessed Binary Systems

345 binary systems are assessed.



TCFE11 Assessed Ternary Systems

290 ternary systems are assessed.

Assessed Ternary Systems			
Al-Ca-Fe	Al-Ca-O	Al-Ca-Si	Al-C-Fe
Al-C-Mn	Al-Co-Fe	Al-Co-Ni	Al-Co-Zr
Al-Cr-Fe	Al-Cr-Nb	Al-Cr-Ni	Al-Cr-O
Al-Cr-Zn	Al-Cu-Fe	Al-Cu-Mn	Al-Cu-Ni
Al-Fe-H	Al-Fe-Mn	Al-Fe-N	Al-Fe-Nb
Al-Fe-Ni	Al-Fe-O	Al-Fe-P	Al-Fe-S
Al-Fe-Si	Al-Fe-Ti	Al-Fe-Zn	Al-Fe-Zr
Al-H-Ti	Al-Mg-O	Al-Mg-Si	Al-Mg-Zn
Al-Mn-Ni	Al-Mn-O	Al-Nb-Ni	Al-Nb-Ti
Al-Ni-O	Al-Ni-Ti	Al-Ni-Zr	Al-O-Si
Al-O-Ti	Al-O-Y	Al-Ti-V	Al-Y-Zn
B-C-Fe	B-Co-Fe	B-Cr-Fe	B-Cr-Mn
B-Cr-Mo	B-Cr-Ni	B-Fe-Mn	B-Fe-Mo
B-Fe-Nb	B-Fe-Ni	B-Fe-Si	B-Fe-Ti
B-Fe-V	B-Fe-W	B-Fe-Zr	B-Mo-Ni
B-Mo-Ti	B-Ni-Si	B-Ni-Ti	B-Ni-Zr
B-Ti-Zr	Ca-Cr-O	Ca-Cr-S	Ca-Fe-O
Ca-Fe-S	Ca-Mg-O	Ca-Mg-S	Ca-Mn-O
Ca-Mn-S	Ca-Ni-O	Ca-O-Si	C-Co-Cr
C-Co-Fe	C-Co-Nb	C-Co-Ni	C-Co-Ti
C-Co-W	C-Co-Zn	C-Cr-Fe	C-Cr-Mn

Assessed Ternary Systems			
C-Cr-Mo	C-Cr-N	C-Cr-Nb	C-Cr-Ni
C-Cr-Si	C-Cr-Ta	C-Cr-V	C-Cr-W
C-Cr-Zr	C-Cu-Fe	Ce-O-S	C-Fe-H
C-Fe-Mn	C-Fe-Mo	C-Fe-N	C-Fe-Nb
C-Fe-Ni	C-Fe-O	C-Fe-P	C-Fe-S
C-Fe-Si	C-Fe-Ti	C-Fe-V	C-Fe-W
C-Mn-Si	C-Mn-V	C-Mo-N	C-Mo-Nb
C-Mo-Ta	C-Mo-Ti	C-Mo-V	C-Mo-W
C-Mo-Zr	C-Nb-Ti	C-Nb-V	C-Nb-W
C-Ni-W	C-N-Nb	C-N-Ti	C-N-Zr
Co-Cr-Fe	Co-Cr-Ni	Co-Cr-W	Co-Cu-Fe
Co-Fe-Mo	Co-Fe-N	Co-Fe-Nb	Co-Fe-P
Co-Fe-S	Co-Fe-Si	Co-Fe-W	Co-Nb-Si
Co-Ni-W	Co-P-W	Co-Si-Ti	Co-Si-W
Co-Ti-Zr	Co-W-Zr	Cr-Cu-Fe	Cr-Cu-Mo
Cr-Cu-Ni	Cr-Cu-W	Cr-Fe-H	Cr-Fe-Mn
Cr-Fe-Mo	Cr-Fe-N	Cr-Fe-Nb	Cr-Fe-Ni
Cr-Fe-O	Cr-Fe-P	Cr-Fe-Ru	Cr-Fe-S
Cr-Fe-Si	Cr-Fe-V	Cr-Fe-W	Cr-Fe-Zn
Cr-Fe-Zr	Cr-Mg-O	Cr-Mn-Mo	Cr-Mn-N
Cr-Mn-Ni	Cr-Mn-O	Cr-Mn-S	Cr-Mn-Si
Cr-Mo-N	Cr-Mo-Ni	Cr-Mo-Si	Cr-Nb-Ni
Cr-Nb-Si	Cr-Ni-O	Cr-Ni-Ru	Cr-Ni-Si

Assessed Ternary Systems			
Cr-Ni-W	Cr-Ni-Zr	Cr-N-Nb	Cr-N-Ni
Cr-N-Si	Cr-N-Ti	Cr-N-V	Cr-N-W
Cr-O-Ti	Cr-O-Y	Cr-Si-Ti	Cr-Si-W
C-Si-Ti	C-Ta-W	C-Ti-V	C-Ti-W
C-Ti-Zr	Cu-Fe-Mn	Cu-Fe-Mo	Cu-Fe-N
Cu-Fe-Ni	Cu-Fe-P	Cu-Fe-S	Cu-Fe-Si
Cu-Fe-W	Cu-Fe-Zr	Cu-Mn-Ni	Cu-Mn-S
Cu-O-Y	C-V-W	C-V-Zr	C-W-Zr
Fe-H-Mo	Fe-H-Ni	Fe-H-Si	Fe-H-V
Fe-H-W	Fe-Mg-O	Fe-Mg-S	Fe-Mn-Mo
Fe-Mn-N	Fe-Mn-Nb	Fe-Mn-Ni	Fe-Mn-O
Fe-Mn-P	Fe-Mn-S	Fe-Mn-Si	Fe-Mn-V
Fe-Mo-N	Fe-Mo-Ni	Fe-Mo-P	Fe-Mo-Si
Fe-Mo-V	Fe-Mo-W	Fe-Nb-Ni	Fe-Nb-O
Fe-Nb-P	Fe-Nb-Si	Fe-Nb-V	Fe-Nb-Zn
Fe-Nb-Zr	Fe-Ni-O	Fe-Ni-P	Fe-Ni-Si
Fe-Ni-Ti	Fe-Ni-W	Fe-N-Nb	Fe-N-Ni
Fe-N-Ti	Fe-N-V	Fe-N-W	Fe-O-S
Fe-O-Si	Fe-O-Y	Fe-P-Si	Fe-P-Ti
Fe-P-V	Fe-P-W	Fe-Si-Ti	Fe-Si-W
Fe-Si-Zr	Fe-S-Ti	Fe-S-W	Fe-Ti-Zr
H-Ni-Ti	Mg-Mn-O	Mg-Mn-S	Mg-Ni-O
Mg-O-Si	Mn-Mo-Ni	Mn-Mo-Si	Mn-Ni-O

Assessed Ternary Systems			
Mn-Ni-Si	Mn-O-S	Mn-O-Si	Mn-O-Y
Mn-Si-Zn	Mo-Ni-Si	Mo-N-Ni	Mo-N-V
Ni-O-Si	Ni-O-Ti	Ni-O-Y	Ni-P-W
Ni-Si-Ti	Ni-Si-W	Ni-Si-Zr	N-Nb-Ti
N-Nb-V	N-Ti-V	N-Ti-Zr	N-V-W
O-Si-Y	O-Y-Zr		

TCFE11 Assessed Quaternary Systems

79 quaternary systems are assessed.

Assessed Quaternary Systems			
Al-Ca-Mg-O	Al-Ca-O-Si	Al-C-Fe-Mn	Al-Cr-Fe-Ni
Al-Cr-Fe-O	Al-Cr-Fe-Zn	Al-Cr-Mg-O	Al-Cr-Mn-O
Al-Cr-Ni-O	Al-Cr-O-Y	Al-Fe-Mg-O	Al-Fe-Mn-O
Al-Fe-Ni-O	Al-Fe-O-Y	Al-Mg-Mn-O	Al-Mg-Ni-O
Al-Mg-O-Si	Al-Mn-Ni-O	Al-Mn-O-S	Al-O-Si-Y
B-Cr-Fe-Mo	Ca-Fe-Mg-S	Ca-Fe-Mn-S	Ca-Fe-O-Si
Ca-Mg-O-Si	C-Co-Cr-W	C-Co-Fe-Mo	C-Co-Fe-Ni
C-Co-Fe-W	C-Co-Nb-W	C-Co-Ni-W	C-Co-V-W
C-Cr-Fe-Mn	C-Cr-Fe-Mo	C-Cr-Fe-N	C-Cr-Fe-Ni
C-Cr-Fe-V	C-Cr-Fe-W	C-Cr-Mn-V	C-Cr-Mn-W
C-Cr-Mo-V	C-Cr-V-W	C-Fe-Mn-H	C-Fe-Mn-Nb
C-Fe-Mn-Si	C-Fe-Mo-Nb	C-Fe-Mo-Si	C-Fe-Mo-V
C-Fe-Mo-W	C-Fe-Nb-W	C-Fe-Ni-W	C-Fe-N-Ni
C-Fe-Si-W	C-Fe-V-W	C-Mo-N-Ni	C-N-Nb-Ti
C-N-Nb-V	C-N-Ti-V	Cr-Fe-H-Ni	Cr-Fe-Mg-O
Cr-Fe-Mn-N	Cr-Fe-Mn-O	Cr-Fe-Mo-N	Cr-Fe-Ni-O
Cr-Fe-N-Nb	Cr-Fe-N-V	Cr-Fe-O-Y	Cr-Mg-Mn-O
Cr-Mg-Ni-O	Cr-Mn-Ni-O	Cr-Mo-N-Nb	Cr-N-Ni-Si
Fe-Mg-Mn-O	Fe-Mg-Ni-O	Fe-Mg-O-Si	Fe-Mn-Nb-N
Fe-Mn-Ni-O	Mg-Mn-Ni-O	Mn-O-Y-Zr	

TCFE11 Phases

In this section:

Common Phases for Steel and Fe-alloys

TCFE11 Models for the Included Phases

The following lists common phase names and the corresponding Thermo-Calc database phase names for some key steel and Fe-alloys.

Name in the Database	Common Name and Description
FCC_A1	Austenite (γ) as well as cubic carbonitrides (MeX) such as MoC, TiC, WC and ZrC
BCC_A2	Ferrite (α)
HCP_A3	Hcp metals as well as Me2X carbonitrides (ε) such as Cr2N, Mo2C, Ta2C, V2C, and W2C
CEMENTITE_D011	Cementite (θ), Fe3C, Mn3C, Ni3B, and Co3B
C14_LAVES	This phase includes all MgZn2-type phases such as Fe2Mo, Fe2Nb, Fe2Ta, Fe2Ti, and Fe2W
CHI_A12	(χ), an intermetallic compound containing primarily Fe, Cr, and Mo
GRAPHITE	Graphite
M6C_E93	M6C carbides such as W3Fe3C
M7C3_D101	M7C3 carbides such as Mn7C3 and Cr7C3
M23C6_D84	M23C6 carbides such as Cr23C6 and Mn23C6
SIGMA_D8B	Sigma phase (σ), a chromium/molybdenum-rich intermetallic compound which is hard, brittle and non-magnetic.
MU_D85	μ phase, such as W6Fe7
MS_B1	Rocksalt (B1) structure sulfides such as Alabandite (MnS) and Niningerite (MgS)
PI_A13	a Cr-Ni nitride (π)
M5C2	Mn5C2, also metastable Fe5C2 (χ)
M3C2_D510	Cr3C2 (β)
MC_ETA	MoC1-x (η)
MC_SHP	MoC, WC
R_PHASE	a high temperature Fe-Mo phase

Name in the Database	Common Name and Description
CORUNDUM	M2O3 oxides such as Al2O3 (Corundum), Cr2O3 (Eskolaite), and Fe2O3 (Hematite)
HALITE	MO oxides such as FeO (Wustite), MnO, NiO
SPINEL	M3O4 oxides such as Fe3O4 (Magnetite) and Cr3O4
M2P_C22	Phosphides such as Fe2P, Cr2P, Ni2P
M3P_D0E	Phosphide such as Fe3P, Cr3P, Ni3P

TCFE11 Models for the Included Phases

The crystal structure information for all included phases in the database is listed here. Similar information is also available when working in the Console Mode by using the DATABASE_RETRIEVAL module. You can display the information using the LIST_SYSTEM CONSTITUENTS and after the system is defined.

The DICTRA_FCC_A1 phases are always rejected by default. It can be restored in the TDB Module (in Console Mode) if it is necessary for your system.

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
A_R2O3_D52	A-La2O3	hP5	P-3m1	D52	164	(CE+3 CE+2)2(O-2)2(O-2 VA)1
A_YZN2	*	structure unknown				(Y)0.33(ZN)0.67
A1_FCC	Cu	cF4	Fm-3m	A1	225	(AL CA CE CO CR CU FE MG MN MO NB NI P RU S SI TA TI V W Y ZN ZR)1(B C H N O VA)1
A2_BCC	W	cI2	Im-3m	A2	229	(AL CA CE CO CR CU FE MG MN MO NB NI P RU S SI TA TI V W Y ZN ZR)1(B C H N O VA)3
AF	FeGaO3	oP40	Pna21		33	(AL2O3)1(FE2O3)1
AL11CE3	CdMg3	hP8	P6_3/mmc			(AL)0.79(CE)0.21
AL12MG17_A12	Mg17Al12	cI58	I-43m	A12	217	(MG)10(AL MG ZN)24(AL MG ZN)24

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
AL13FE4	Al13Fe4	mC102	C2/m		12	(AL)0.63(FE MN ZN)0.23(AL VA ZN)0.14
AL2CR3	MoSi2	tI6	I4/mmm		139	(AL)0.4(CR)0.5(CR ZN)0.1
AL2FE	Al2Fe	aP18	P1		1	(AL)2(FE MN)1(VA ZN)0.04
AL2S3	Al2S3	hP30	P61		169	(AL2S3)
AL2TIO5	Al2TiO5	oC32	Cmcm		63	(AL+3)2(TI+4)1(O-2)5
AL2Y3	Al2Zr3	tP20	P4_2/mnm		136	(AL)2(Y)3
AL3CE_D019	CdMg3	hP8	P6_3/mmc	D019	194	(AL)0.75(CE)0.25
AL3CE_L12	AuCu3	cP4	Pm-3m	L12	221	(AL)0.75(CE)0.25
AL3NB_D022	Al3Ti	tI8	I4/mmm	D022	139	(AL)3(NB)1
AL3Y_HT	BaY3	hR36	R-3m		166	(AL)0.75(Y)0.25
AL3Y_LT	Mg3Cd	hP8	P6_3/mmc		194	(AL)0.75(Y)0.25
AL4C3_D71	Al4C3	hR21	R-3m	D71	166	(AL SI)4(C)3
AL4CE_D13	BaAl4	tI10	I4/mmm	D13	139	(AL)0.8(CE)0.2
AL5FE2	Al2.8Fe	oS24	Cmcm		63	(AL)5(FE MN)2(VA ZN)3
AL5FE4	Cu5Zn8	cI52	I-43m		217	(AL FE)
AL6FE6ZR_D2B						(AL FE)12(ZR)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
AL7CR	Al45V7	mC104	C2/m		12	(AL)6(CR)1(AL ZN)1
AL8MN5_D810	Al8Cr5	hR26	R3m	D810	160	(AL)12(MN)5(AL FE MN)9
ALCE1	AlCe	oC16	Cmcm		63	(AL)0.5(CE)0.5
ALCE3_D019	CdMg3	hP8	P6_3/mmc	D019	194	(AL)0.25(CE)0.75
ALCE3_L12	AuCu3	cP4	Pm-3m	L12	221	(AL)0.25(CE)0.75
ALCRZN_TAU4	*	*	R-3m		166	(AL ZN)0.48(CR)0.12(ZN)0.4
ALH3						(AL)1(H)3
ALMG_BETA	Al45Mg28	cF1832	Fd-3m		227	(AL ZN)140(MG)89
ALMG_EPS	Al30Mg23	hR53	R-3		148	(AL ZN)30(MG)23
ALMGZN_PHI	Mg21(Al,Zn)17	oP152	Pbcm		57	(MG)21(AL ZN)17
ALMGZN_Q	*	Quasicrystal				(AL)0.15(MG)0.44(ZN)0.41
ALMGZN_T1	Mg32(Al,Zn)48	cI160	Im-3		204	(MG)26(MG AL)6(AL MG ZN)48(AL)1
ALMGZN_T2	(itself)	cP640?	Pa-3		205	(AL)0.15(MG)0.43(ZN)0.42
ALN_B4	ZnO	hP4	P6_3mc	B4	186	(AL)1(N)1
ALPHA_SPINEL	Mn3O4	tI28	I4_1/amd		141	(MG+2 MN+2 MN+3 NI+2)1(AL+3 CR+3 FE+3 MN+2 MN+3 VA)2(MN+2 VA)2(O-2)4
ALY_B33	CrB	oC8	Cmcm	B33	63	(AL)1(Y)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
ALY2_C37	Co2Si	oP12	Pnma	C37	62	(AL)1(Y)2
ANDALUSITE	Al2(SiO4)O	oP32	Pnnm		58	(AL+3)1(AL+3)1(SI+4)1(O-2)5
ANORTHITE	Ca(Al0..5Si0.5)4O8	aP52/aP104	P-1		2	(CA+2)1(AL+3)2(SI+4)2(O-2)8
B_YZN2	*	structure unknown				(Y)0.33(ZN)0.67
B3SI_D1G	B4C	hR15	R-3m	D1G	166	(B)6(SI)2(B SI)6
B4C_D1G	B13C2	hR15	R-3m	D1G	166	(B11C B12)1(B2 C2B CB2)1
BCC_A2	W	cI2	Im-3m	A2	229	(AL CA CE CO CR CU FE MG MN MO NB NI P RU S SI TA TI V W Y ZN ZR)1(B C H N O VA)3
BCC_B2	CsCl	cP2	Pm-3m	B2	221	(AL CA CE CO CR CU FE MG MN MO NB NI P RU S SI TA TI V W Y ZN ZR)0.5(AL CA CE CO CR CU FE MG MN MO NB NI P RU S SI TA TI V W Y ZN ZR)0.5(B C H N O VA)3
BETA_PHASE						(H VA)0.25(H VA)0.25(V)0.5
BETA_RHOMBO_B	beta-B	hR105	R-3m		166	(B)93(B C SI)12
BN_B4	BN	hP4	P6_3/mmc		194	(B1N1)
C12A7	Al14Ca12O33	cI152	I-43d		220	(CA+2)6(AL+3)6(AL+3 FE+3)1(O-2)16.5
C14_LAVES	MgZn2	hP12	P63/mmc	C14	194	(AL CO CR CU FE MG MN MO NB NI SI TA TI V W Y ZN ZR)2 (AL CO CR CU FE MG MN MO NB NI SI TA TI V W Y ZN ZR)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
C15_LAVES	Cu2Mg	cF24	Fd-3m	C15	227	(AL CA CE CO CR CU FE MG NB NI SI Y ZN ZR)2(AL CA CE CO CR CU FE MG NB NI SI Y ZN ZR)1
C1A1	Al2CaO4	mP84	P2_1/c		14	(CA+2)1(AL+3)2(O-2)4
C1A2	Al4CaO7	mC48	C2/c		15	(CA+2)1(AL+3)4(O-2)7
C1A6	Fe12PbO19	hP64	P6_3/mmc		194	(CA+2)1(AL+3)12(O-2)19
C1A8M2	CaMg2Al16O27	hP94	P-6m2		187	(CAO)1(AL2O3)8(MGO)2
C2A14M2	*	hR114	R-3m:h		166	(CAO)2(AL2O3)14(MGO)2
C2F	Ca2Fe2O5	oP36	Pnma		62	(CA+2)2(FE+3)2(O-2)5
C3A1	Ca3Al2O6	cP264	Pa-3		205	(CA+2)3(AL+3)2(O-2)6
C3A2M1	*	o??	Pbcm		57	(CAO)3(AL2O3)2(MGO)1
C4WF4	Ca4Fe9O17	mS60	C2		5	(CA+2)4(FE+2)1(FE+3)8(O-2)17
C4WF8	Sr2Fe2O5	oI44	Imma		74	(CA+2)4(FE+2)1(FE+3)16(O-2)29
CA1CR2O4_A	SrCr2O4	oP28	Pmmn		59	(CA1CR2O4)
CA1CR2O4_B	CaV2O4	oP28	Pnma		62	(CA1CR2O4)
CA2NI7	Co7Gd2	hR18	R-3m		166	(CA)2(NI)7
CA2SIO4_ALPHA	Ca2SiO4	hP24	P6_3/mmc		194	(CA+2 MG+2)2(SI+4)1(O-2)4

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
CA2SIO4_AP	K2CoCl4	oP84	Pna21		33	(CA+2 FE+2 MG+2)2(SI+4)1(O-2)4
CA3ZN_E1A	Re3B	oC16	Cmcm	E1A	63	(CA)3(ZN)1
CA5ZN3_D8L	Cr5B3	tI32	I4/mcm	D8L	140	(CA)5(ZN)3
CAH2_BETA						(CA)1(H)2
CAH2_C37						(CA)1(H)2
CAMN2O4	CaMn2O4	oP28	Pbcm		57	(CA+2)1(MN+3)2(O-2)4
CAMNO3	GdFeO3/CaTiO3	oP20/cP5	Pnma / Pm-3m		62/221	(CA+2)1(MN+4)1(O-2)3
CANI3	Ni3Pu	hR36	R-3m		166	(CA)0.25(NI)0.75
CANI5_D2D	CaCu5	hP6	p6/mmm	D2D	191	(CA)1(NI ZN)5
CAZN_B33	CrB	oC8	Cmcm	B33	63	(ZN)1(CA)1
CAZN11	BaCd11	tI48	I4_1/amd		141	(CA)1(ZN)11
CAZN13_D23	NaZn13	cF112	Fm-3c	D23	226	(CA)1(ZN)13
CAZN2	Hg2K	oI12	Imma		74	(ZN)2(CA)1
CAZN3	CaZn3	hP32	P6_3/mmc		194	(CA)1(ZN)3
CBCC_A12	alpha-Mn	cI58	I-43m	A12	217	(AL CO CR CU FE MG MN MO NB NI P RU SI TA TI V ZN ZR)1 (B C N VA)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
CE13ZN58	Gd13Zn58	hP142	P6_3/mmc		194	(CE)0.18(ZN)0.82
CE1S2	Ce10Se19	tP58	P42/n		86	(CE)1(S)2
CE24CO11	Ce24Co11	hP70	P6_3mc		186	(CO)11(CE)24
CE2C3_D5C	Pu2C3	cI40	I-43d	D5C	220	(CE)0.4(C)0.6
CE2CO7	Ce2Ni7/Co7Gd2	hP36/hR18	P6_3/mmc / R-3m		194/166	(CO)7(CE)2
CE2FE17	Ni17Th2	hP38	P6_3/mmc		194	(CE)2(FE ZN)17
CE2NI7	Ce2Ni7	hP36	P6_3/mmc		194	(CE)0.22(NI)0.78
CE2O12S3	*	m**	P2_1/c / P6_3/m		14/176	(CE)2(O)12(S)3
CE2O2S1	Ce2SO2	hP5	P-3m1		164	(CE)2(O)2(S)1
CE2S3	Th3P4/Cr3C2-b	cI28/oP20	I-43d/Pnma	D73/D510	220/62	(CE)2(S)3
CE3S4_D73	Th3P4	cI28	I-43d	D73	220	(CE)3(S)4
CE3ZN11	Al11La3	oI28	Immm		71	(CE)0.21(ZN)0.79
CE3ZN22	Ce3Zn22	tI100	I4_1/amd		141	(CE)0.12(ZN)0.88
CE5CO19	Ce5Co19	hR24	R-3m		166	(CO)19(CE)5
CE7NI3_D102	Fe3Th7	hP20	P6_3mc	D102	186	(CE)0.7(NI)0.3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
CE7O12	Pr7O12	hR19	R-3		148	(CE)7(O)12
CEB4_D1E	UB4	tP20	P4/mbm	D1E	127	(B)0.8(CE)0.2
CEB6_D21	CaB6	cP7	Pm-3m	D21	221	(B)0.86(CE)0.14
CEC2_BETA	CaC2	cF36	Fm-3m		225	(CE)0.33(C)0.67
CEC2_C11A	CaC2	tI6	I4/mmm	C11A	139	(CE)0.33(C)0.67
CECO3	Ni3Pu	hR36	R-3m		166	(CO)3(CE)1
CECO5_D2D	CaCu5	hP6	P6/mmm	D2D	191	(CE)1(CO CU NI ZN)5
CECU_B27	FeB	oP8	Pnma	B27	62	(CU)0.5(CE)0.5
CECU2	Hg2K	oI12	Imma		74	(CU)0.67(CE)0.33
CECU4	CeCu4	oP20	Pnnm		58	(CU)0.8(CE)0.2
CECU6	CeCu6	oP28	Pnma		62	(CU)0.86(CE)0.14
CEH3_EPSLON						(CE)1(H VA)3
CEMENTITE_D011	Fe3C	oP16	Pnma	D011	62	(AL CO CR FE MN MO NB NI SI V W)3(B C N)1
CENI_B33	CrB	oC8	Cmcm	B33	63	(CE)0.5(NI)0.5
CENI3	CeNi3	hP24	P6_3/mmc		194	(CE)0.25(NI)0.75
CESI2_CC	Si2Th	tI12	I4_1/amd	CC	141	(CE)0.33(SI)0.67

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
CEZN11	BaCd11	tI48	I4_1/amd		141	(CE)0.08(ZN)0.92
CEZN2	Hg2K	oI12	Imma		74	(CE)0.33(ZN)0.67
CEZN3	CeZn3	oC16	Cmcm		63	(CE)0.25(ZN)0.75
CF1	CaV2O4	oP28	Pnma		62	(CA+2)1(FE+3)2(O-2)4
CF2	Ca3.5Fe14O24.5	mS172	C2		5	(CA+2)1(FE+3)4(O-2)7
CHI_A12	a-Mn	cI58	I-43m	A12	217	(CR FE NI)24(CR MO W ZR)10(CR FE MO NI W)24
CLINO_PYROXENE	CaMgSi2O6	MS40	C2/c		15	(CA+2 FE+2 MG+2)1(FE+2 MG+2)1(SI+4)2(O-2)6
CO2SI_C37	Co2Si	oP12	Pnma	C37	62	(CO FE NI RU)2(SI)1
CO2ZN15_ GAMMA1	Zn7.8Co	mS28	C2m:b1		12	(CO)0.12(ZN)0.88
CO3MO_D019	CdMg3	hP8	P6_3/mmc	D019	194	(CO)3(MO)1
CO3V	Al3Pu	hP24	P6_3/mmc		194	(CO V)3(CO V)1
CO3Y2	*	cP*	*			(CO)3(Y)2
CO3Y4	Co3Ho4	hP22	P6_3/m		176	(CO)3(Y)4
CO5Y_D2D	CaCu5	hP6	P6/mmm	D2D	191	(CO2 Y)1(CO)4(CO VA)1
CO5Y8	Co5Y8	mP52	P2_1/c		14	(CO)5(Y)8
CO7Y6	*	structure				(CO)7(Y)6

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
		unknown				
CO9S8	Co9S8	cF68	Fm-3m		225	(CO FE)9(S)8
COP1	FeAs	oP8	Pnma		62	(CO)1(P)1
COP3	cI32	cI32	Im-3		204	(CO)1(P)3
CORDIERITE	Na0.04 (Mg0.5Fe0.5)2Al4Si5O18	oS120	Cccm		66	(AL4MG2O18SI5)
CORUNDUM	Al2O3	hR30	R-3c	D51	167	(AL+3 CR+2 CR+3 FE+2 FE+3 MN+3 TI+3)2(CR+3 FE+3 NI+2 VA)1(O-2)3
COY_B33	CrB	oC8	Cmcm	B33	63	(CO)1(Y)1
COZN_A13	beta-Mn	cP20	P4_132	A13	213	(CO ZN)1(CO ZN)1
COZN13	Zn13Co	mS28	C2m:b1		12	(CO)0.07(ZN)0.93
COZN4_D83	Zn9(Zn0.5Fe0.5)2Fe2	cI52	I-43m	D83	217	(CO ZN)4(CO ZN)1
CR3RU_A15	Cr3Si	cP8	Pm-3n	A15	223	(CR)0.69(RU)0.32
CR3SI_A15	Cr3Si	cP8	Pm-3n	A15	223	(CO CR FE MO NB SI V)3(AL CO CR NB SI V)1
CR5B3_D8L	CR5B3	tI32	I4/mcm	D8L	140	(CR MO)0.62(B)0.38
CR5SI3_D8M	W5Si3	tI32	I4/mcm	D8m	140	(FE CR)4(FE CR)1(SI)3
CRISTOBALITE	SiO2	tP12/cF24	P4_12_12 / Fd-3m	*/C9	92/227	(SIO2)

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
CRNBSI	ZrNiAl	hP9	P-62m		189	(CR)1(NB)1(SI)1
CRZN17	*	hP*	*			(AL CR)1(FE ZN)17
CU2S_ALPHA	Cu2S	mP144	P121/c1		14	(CU)2(S)1
CU2S_BETA	Cu2S	hP16	P63/mmc		194	(CU)2(S)1
CU2S_GAMMA	Cu2Se	cF44	Fm-3m		225	(CU FE VA)2(CU VA)1(S)1
CU2Y_H	*	hP*	*			(CU)2(Y)1
CU2Y_L	Hg2K	oI12	Imma		74	(CU)2(Y)1
CU31S16	Cu31S16	mP376	P2_1/c:a3		14	(CU)1.93(S)1
CU3P_D021	Cu3P	P3c1	hp24	D021	185	(CU FE)3(P)1
CU4Y	Cu5Y1.25	mP16	P21/m:a		11	(CU)4(Y)1
CU6Y	Cu7Tb	hP8	P6/mmm		191	(CU2 Y)1(CU)5
CU7S4	Cu7S4	oP44	Pnma		62	(CU)1.75(S)1
CU7Y2	Ag51Gd14	hP68	P6/m		175	(CU)7(Y)2
CUB_A13	beta-Mn	cP20	P4_132	A13	213	(AL CE CO CR CU FE MG MN MO NB NI P RU SI TA TI V Y ZN ZR)1(B C N VA)1
CUO_B26	CuO	mS8	C2/c	B26	15	(CU+2)1(O-2)1
CUPRITE_C3	Cu2O	cP6	Pn-3m	C3	224	(CU+1)2(O-2)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
CUS_B18	CuS-b	hP12	P63/mmc	B18	194	(CU)1(S)1
CUZN_EPSILON	Mg	hP2	P6_3/mmc	A3	194	(CU MN ZN)1(VA)0.5
CUZR_B2	CsCl	cP2	Pm-3m	B2	221	(CU)1(Y)1
CW3F	CaFe5O7	oS52	Cmcm		63	(CA+2)1(FE+2)3(FE+3)2(O-2)7
CWF	CaFe3O5	oS36	Cmcm		63	(CA+2)1(FE+2)1(FE+3)2(O-2)5
DELTA_TIH2						(NB TI V ZR Y)1(H VA)2
DIAMOND_A4	C	cF8	Fd-3m	A4	227	(AL B C MN O P SI ZN)
DIS_BETA						(H VA)0.5(V)0.5
ETA_M5SIN	Cr3Ni2SiN	cF112	Fd-3m		227	(CR MO)3(NI FE)2(SI)1(N)1
F_CEO2	CaF2	cF12	Fm-3m	C1	225	(CE+3 CE+4)2(O-2 VA)4
FCC_A1	Cu	cF4	Fm-3m	A1	225	(AL CA CE CO CR CU FE MG MN MO NB NI P RU S SI TA TI V W Y ZN ZR)1(B C H N O VA)1
FCC_L12	AuCu3	cP4	Pm-3m	L12	221	(AL CA CE CO CR CU FE MG MN MO NB NI P RU S SI TA TI V W Y ZN ZR)0.75(AL CA CE CO CR CU FE MG MN MO NB NI P RU S SI TA TI V W Y ZN ZR)0.25(B C H N O VA)1
FE10SI2B3	*	structure unknown				(FE)2(SI)0.4(B)0.6

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
FE17Y2	Fe17Lu2	hP80	P6_3/mmc		194	(CO FE NI ZN)17(Y)2
FE1NB1B1_C22	Fe2P	hP9	P26m	C22	189	(FE)0.33(NB)0.33(B)0.33
FE29SI42ZR29						(FE)29(SI)42(ZR)29
FE2S3O12	Fe2(SO4)3	mP68/hR102	P2_1/c / R-3		14/148	(FE)2(S)3(O)12
FE2SI2ZR_DI3						(FE)2(SI)2(ZR)1
FE2SI3ZR3						(FE)2(SI)3(ZR)3
FE2SITI_L21	BiF3	cF16	Fm-3m	D03	225	(FE)0.5(SI)0.25(TI)0.25
FE3NB3B4	*	structure unknown				(FE)0.3(NB)0.3(B)0.4
FE3NB4SI5	Nb12Fe7 (Fe0.5Si0.5)5Si12	oP72	Pmn21		31	(FE)3(NB)4(SI)5
FE3SIZR2						(FE)3(SI)1(ZR)2
FE3ZN7_D82	Cu5Zn8	cI52	I-43m	D82	217	(FE ZN)0.15(FE ZN)0.15(AL FE ZN)0.23(ZN)0.46
FE4N_LP1	Fe4N	cP5	Pm-3m	L'1	221	(CO CR FE MN NI)4(C N VA)1
FE4NB2O9	Nb2Mn4O9	hP30	P-3c1		165	(FE+3)4(NB+2)1(NB+4)1(O-2)9
FE4NB4SI7	Zr4Co4Ge7	tI60	I4/mmm		139	(FE)4(NB)4(SI)7
FE4SI2ZR1						(FE)4(SI)2(ZR)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
FE4SI7ZR4						(FE)4(SI)7(ZR)4
FE5SI12ZR3						(FE)5(SI)12(ZR)3
FE5SI2B	Nb5Sn2Si	tI32	I4/mcm		140	(FE)4.7(SI)2(B)1
FE5SIB2	Mo5SiB2	tI32	I4/mcm		140	(FE)5(SI)1(B)2
FE8SI2C	Mn8Si2C3	aP*	P1			(FE MN)8(SI)2(C)1
FEAL2S4	ZnIn2S4	hR21	R3m		160	(FE)1(AL)2(S)4
FEMP_C23	NiSiTi	oP12	Pnma	C23	62	(CR FE NB NI TI)1(CR FE NB NI TI)1(P)1
FENB2P	Cu3Au	cP4	Pm-3m		221	(FE)1(NB)2(P)1
FENB2SI2	Nb39Fe20Si40	tP198	P42/mcm		132	(FE)1(NB)2(SI)2
FENB4P	Nb4CoSi	tP12	P4/mcc		124	(FE)1(NB)4(P)1
FENB4SI	Nb4CoSi	tP12	P4/mcc		124	(FE)1(NB)4(SI)1
FENBSI_C23	TiNiSi	oP12	Pnma	C23	62	(FE)1(NB ZR)1(SI)1
FENBSI2	ZrCrSi2	oP48	Pbam		55	(FE)1(NB)1(SI)2
FESI2_H	FeSi2-h	oC48	Cmca		64	(FE)0.3(SI)0.7
FESI2_L	FeSi2-l	tP3	P4/mmm		123	(FE)0.33(SI)0.67
FESI4P4	FeSi4P4	aP9	P1		1	(FE)1(SI)4(P)4

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
FESO4	CuSO4	oP24	Pnma		62	(FE)1(S)1(O)4
FEWB_C37	NiSiTi	oP12	Pnma	C23	62	(FE)1(W)1(B)1
FEZN10	FeZn10	hP632	P6_3/mmc		194	(CR FE)0.06(AL FE ZN)0.18(ZN)0.53(ZN)0.24
FEZN13	CoZn13	mC28	C2/m		12	(CR FE VA)0.07(AL ZN VA)0.07(AL ZN)0.86
FEZN4	Fe11Zn40	cF408	F-43m		216	(FE)0.14(AL FE ZN)0.12(ZN)0.74
FLUORITE_C1	CaF2	cF12	Fm-3m	C1	225	(MN+2 MN+3 NI+2 Y+3 ZR ZR+4)2(O-2 VA)4
G_PHASE	Mn23Th6	cF116	Fm-3m	D8A	225	(AL CO CU FE NI TI)16(MN NB TI Y ZR)6(CO CU FE NI SI)7
GAMMA_D82	Cu5Zn8	cI52	I-43m	D82		(ZN)4(CU ZN)1(CU ZN)8
GAMMA2_ALFEZN	*	structure unknown				(AL FE ZN)0.26(ZN)0.74
GAS						(AR C C1H1 C1H1N1O1 C1H1N1_HCN C1H1N1_HNC C1H1O1 C1H1O2 C1H2 C1H2O1 C1H2O2_CIS C1H2O2_DIOXIRANE C1H2O2_TRANS C1H3 C1H3O1_CH2OH C1H3O1_CH3O C1H4 C1H4O1 C1N1 C1N1O1 C1N1O1_NCO C1N2_CNN C1N2_NCN C1O1 C1O1S1 C1O2 C1S1 C1S2 C2 C2H1 C2H1N1 C2H2 C2H2O1 C2H3 C2H4 C2H4O1_ACETALDEHYDE C2H4O1_OXIRANE C2H4O2_ACETICACID C2H4O2_DIOXETANE C2H4O3_123TRIOXOLANE C2H4O3_124TRIOXOLANE C2H5 C2H6 C2H6O1 C2H6O2 C2N1_CCN C2N1_CNC C2N2 C2O1 C3 C3H1 C3H1N1 C3H4_1 C3H4_2 C3H6 C3H6O1 C3H6_2 C3H8 C3N1 C3O2 C4 C4H1 C4H10_1 C4H10_2 C4H2

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
						C4H4 C4H4_1_3 C4H6_1 C4H6_2 C4H6_3 C4H6_4 C4H6_5 C4H8 C4H8_1 C4H8_2 C4H8_3 C4H8_4 C4H8_5 C4N1 C4N2 C5 C5H1N1 C5N1 C60 C6H6 C6H6O1 C6N1 C6N2 C9N1 H H1N1 H1N1O1 H1N1O2_CIS H1N1O2_ TRANS H1N1O3 H1N3 H1O1 H1O1S1_HSO H1O1S1_SOH H1O2 H1S1 H2 H2N1 H2N2O2 H2N2_1_1N2H2 H2N2_ CIS H2N2_TRANS H2O1 H2O1S1_H2SO H2O1S1_HSOH H2O2 H2O4S1 H2S1 H2S2 H3N1 H3N1O1 H4N2 N N1O1 N1O2 N1O3 N1S1 N2 N2O1 N2O3 N2O4 N2O5 N3 O O1S1 O1S2 O1Y1 O1Y2 O2 O2S1 O2Y1 O2Y2 O3 O3S1 S S2 S3 S4 S5 S6 S7 S8 V Y ZN ZR ZR2)
GRAPHITE_A9	C	hP4	P6_3/mmc	A9	194	(B C)
H_R2O3	H-La2O3	hP10	P6_3/mmc		194	(CE+2 CE+3)2(O-2)2(O-2 VA)1
HALITE	NaCl	cF8	Fm-3m	B1	225	(AL+3 CA+2 CR+3 FE+2 FE+3 MG+2 MN+2 MN+3 NI+2 NI+3 SI+4 VA)1(O-2)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
HATRURITE	Ca3(SiO4)O-b	hR81	R3m		160	(CA+2)3(SI+4)1(O-2)5
HCP_A3	Mg	hP2	P6_3/mmc	A3	194	(AL CA CE CO CR CU FE MG MN MO NB NI P RU S SI TA TI V W Y ZN ZR)1(B C H N O VA)0.5
HIGH_SIGMA	CrFe	tP30	P4_2/mnm		136	(MN)8(CR)4(CR MN)18
K_PHASE	CaTiO3	cP5	Pm-3m	E21	221	(C CO ZN)51(ZN)32(C)17
KAPPA_E21	CaTiO3	cP5	Pm-3m	E21	221	(AL)1(FE MN)3(C VA)1
KSI_CARBIDE	Mo6Fe11C5	mS44	C12/m1		12	(CR FE MO W)3(C)1
KYANITE	Al2SiO5	aP32	P-1		2	(AL+3)1(AL+3)1(SI+4)1(O-2)5
LARNITE	CaSiO3	mP60	P2_1/n		14	(CA+2)2(SI+4)1(O-2)4
LIQUID						(AL ALN ALO3/2 AL2/3S B C CA CAS CE CEO2 CEO3/2 CO COS CR CRO3/2 CRS CU CU2O CUO CU2S FE FEO FEO3/2 FES H MG MGS MN MNO MNO3/2 MNS MO MO1/2S N NB NBO NBO2 NBS NI NIO NIS P RU S S2ZR S3ZR2 SI SIO2 SI1/2S SZN TA TI TIO TIO3/2 TIO2 V W Y Y2/3O ZN ZR ZR1/2O)
LOWCLINO_ PYROXENE	CaMgSi2O6	mS40	P2_1/c		15	(CA+2 MG+2)1(MG+2)1(SI+4)2(O-2)6

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
M11SI8	Cr8Nb3Si8	oP76	Pnma		62	(CR NB)11(SI)8
M12C	W6Fe6C	cF104	Fd-3m		227	(CO)6(W)6(C)1
M1B6_D21	CaB6	cP7	Pm3m	D21	221	(CA Y)1(B)6
M23C6_D84	Cr23C6	cF116	Fm-3m	D84	225	(CO CR FE MN NI V)20(CO CR FE MN MO NI V W)3(B C)6
M2B_C16	Al2Cu	tI12	I4/mcm	C16	140	(CO CR FE MN MO NI V W)2(B)1
M2B_CB	Mg2Cu	oF48	Fddd	CB	70	(CR FE MO MN NI)0.67(B)0.33
M2B3	V2B3	oS20	Cmcm		63	(NB V)0.4(B)0.6
M2O3C_D53	(Mn0.5Fe0.5)2O3	cI80	Ia-3	D53	206	(AL+3 CE+3 CE+4 CR+3 FE+3 MN+3 NI+2 Y Y+3 ZR+4)2(O-2 VA)3(O-2 VA)1
M2O3H_D52	La2O3	hP5	P-3m1	D52	164	(MN+3 Y Y+3 ZR+4)2(O-2 VA)3(O-2 VA)1
M2P_C22	Fe2P	hP9	P-62m	C22	189	(AL CO CR FE MN MO NB NI TI V W)2(P SI)1
M2P_C37	Co2P	oP12	Pnma	C37	62	(CO FE NI V W)1(CO FE NI V W)1(P)1
M2SI_TETA	Ga3Ge6Ni13	hP66	P3_121		152	(FE NI)1(FE NI VA)1(SI)1
M3B2_D5A	Mo2FeB2	tP10	P4/mbm	D5A	127	(CR FE MO NI W)0.4(CR FE NI)0.2(B)0.4
M3B4_D7B	Ta3B4	oI14	Immm	D7B	71	(CR FE NB V)0.43(B)0.57
M3C2_D510	Cr3C2	oP20	Pnma	D510	62	(CO CR MO V W)3(C)2

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
M3P_D0E	Ni3P	tI32	I-4	D0E	82	(AL CO CR CU FE MN MO NI TI)3(B P)1
M3SI	BiF3	cF16	Fm-3m		225	(FE MN)3(SI)1
M4SI1_G3	AlAu4	cP20	P2_13	G3	198	(CR FE NI)3(NI)1(SI)1(C VA)1
M5B6	V5B6	oS22	Cmmm		65	(V NB)0.46(B)0.55
M5C2	Mn5C2	mC28	C2/c		15	(FE MN NB V)5(C N)2
M5SI3_D88	Mn5Si3	hP16	P6_3/mcm	D88	193	(CR FE MN NI Y)5(SI)3(C VA)1
M6C_E93	W3Fe3C	cF112	Fd-3m	E93	227	(CO FE NI)2(MO NB W)2(CO CR FE MO NB NI SI V W)2(C)1
M6SI5	V6Si5	oI44	Ibam		72	(CR NB)6(SI)5
M7C3_D101	Cr7C3	oP40	Pnma	D101	62	(AL CO CR FE MN MO NB NI SI V W)7(B C)3
M7Y2	Co7Gd2	hR18	R-3m		166	(CO NI)7(Y)2
MB_B27	FeB	oP8	Pbnm	B27	62	(B)1(CO CR FE MN MO NI TI V ZR)1
MB_B33	CrB	oC8	Cmcm	B33	63	(CR FE MN MO NB NI TA TI V)1(B)1
MB_BG	MoB	tI16	I4/amd	BG	141	(CR FE MO)0.5(B)0.5
MB2_C32	AlB2	hp3	P6/mmm	C32	166	(B)2(AL CR MG TI Y ZR)1
MC_ETA	MoC	hP12	P63/mmc	B_i	194	(MO TI V W)1(C VA)1
MC_SHP	WC	hP2	P-6m2	B_h	187	(MO W)1(C N)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
MELILITE	Ca2MgSi2O7	tP24	P-42_1m		113	(CA+2)2(AL+3 MG+2)1(AL+3 SI+4)1(SI+4)1(O-2)7
MERWINITE	Ca3Mg(SiO4)2	mP56	P2_1/a		14	(CA+2)3(MG+2)1(SI+4)2(O-2)8
MG12R_D2B	Mn12Th	tI26	I4/mmm	D2B	139	(MG)12(CE)1
MG12ZN13	Re25Zr21	hR92	R-3c		167	(MG)12(AL ZN)13
MG17R2	CeMg10	hP44	P6_3/mmc		194	(MG)17(CE)2
MG2C3	Mg2C3	oP10	Pnnm		58	(MG)2(C)3
MG2NI_CA	Mg2Ni	hP18	P6_222	Ca	180	(MG)2(NI)1
MG2SI_C1	CaF2	cF12	Fm-3m	C1	225	(MG)2(SI)1
MG2ZN11_D8C	Mg2Zn11	cP39	Pm-3	D8C	200	(MG)2(AL ZN)11
MG2ZN3	Mg4Zn7	mC110	C2/m		12	(MG)2(AL ZN)3
MG3M_D03	BiF3	cF16	Fm-3m	D03	225	(MG)3(CE MG)1
MG3N2_D53	Mn2O3	cI180	Ia-3	D53	206	(CA MG)3(N)2
MG41M5	Ce5Mg41	tI92	I4/m		87	(MG)41(CE)5
MG51ZN20	Mg51Zn20	oI158	Immm		71	(MG)51(ZN)20
MGB4	MgB4	oP20	Pnma		62	(MG)1(B)4
MGB7	MgB7	oI64	Imma		74	(MG)1(B)7

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
MGC2	MgC2	tP6	P4_2/mnm		136	(MG)1(C)2
MGH2_C4						(MG)1(H)2
MN11SI19	Mn11Si19	tP120	P-4n2		118	(MN)0.37(SI)0.63
MN2YO5	DyMn2O5	oP32	Pbam		55	(Y+3)1(MN+3)1(MN+4)1(O-2)5
MN3N2	Mn3N2	tI10	I4/mmm		139	(MN)3(N)2
MN5SIC	CoO	tI4	I4/mmm		139	(MN)0.71(SI)0.14(C)0.14
MN6N5	Mn5SiC	oS56	CmC2_1		36	(MN)6(N)5
MN6SI	R-(Co,Cr,Mo)	hR53	R-3		166	(MN)0.86(SI)0.14
MN9SI2	Mn9Si2	oI186	Immm		71	(MN)0.82(SI)0.18
MNO2_C4	TiO2	tP6	P4_2/mnm	C4	136	(MN+4)1(O-2)2
MNP_B31	MnP	oP8	Pnma	B31	62	(CR FE MN W)1(P SI)1
MNTA	*	structure unknown				(MN)1(TA)1
MNYO3_HEX	LuMnO3	hP30	P6_3cm		185	(Y+3)1(MN+3)1(O-2)3
MNZN9	MnZn9?	h**	*			(MN)0.1(ZN)0.9
MO2B5_D8I	MO2B5	hR7	R3m	D8I	166	(MO)0.32(B)0.68
MO2S3	Mo2S3	mP10	P2_1/m		11	(MO)2(S)3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
MO3P_D0E	V3S	tI32	I-42m	D0E	121	(MO)3(P)1
MO5SI3_D8M	Si3W5	tI32	I4/mcm	D8M	140	(MO)5(SI)3
MOB2_C32	AlB2	hp3	P6/mmm	C32	191	(MO)0.38(B)0.62
MOP_BH	WC	hP2	P-6m2	BH	187	(MO)1(P)1
MOS2_C7	MoS2	hP6	P6_3/mmc		194	(MO W)1(S)2
MOSI2_C11B	MoSi2	tI6	I4/mmm	C11B	139	(MO)1(SI)2
MOZN22	Zn93 (Zn0.43Mo0.57)Mo4	cF420	F-43m		216	(MO)1(ZN)22
MOZN7	CuPt7	cF32	Fm-3m		225	(MO)1(ZN)7
MS_B1	NaCl	cF8	Fm-3m	B1	225	(CA CE CO CR CU FE MG MN Y)1(S)1
MS_B81	NiAs	hP4	P63/mmc	B81	194	(AL CO CR CU FE MN NB NI TI V VA)1(S)1
MS2_C2	FeS2	cP12	Pa-3	C2	205	(CO FE MN)1(S)2
MSI_B20	FeSi	cP8	P213	B20	198	(CO CR FE MN NI RU)0.5(AL SI)0.5
MSI2_C40	CrSi2	hP9	P6_222	C40	180	(CR NB)1(SI)2
MU_D85	Fe7W6	hR13	R-3m	D85	166	(AL CO CR FE MN NB NI TA)7(MO NB TA W)2(CO CR FE MO NB NI TA W)4
MULLITE	Al(Al0.7Si0.3)2O4.8	oP24	Pbam		55	(AL+3)1(AL+3)1(AL+3 SI+4)1(O-2 VA)5

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
MY3_D011	Fe3C	oP16	Pnma	D011	62	(CO NI)1(Y)3
NB1ZN1						(NB)1(ZN)1
NB2ZN3_D85						(NB)2(ZN)3
NB3B2_D5A	U3Si2	tP10	P4/mbm	D5A	127	(FE NB V)0.6(B)0.4
NB3RU5	*/CsCl	o**/cP2	?/Pm-3m		?/221	(NB RU)0.38(RU)0.62
NB3SI	Ti3P	tP32	P4_2/n		86	(NB)3(SI)1
NB5SI3_D8L	Cr5B3	tI32	I4/mcm	D8L	140	(CR NB)5(SI)3
NB5SI3_D8M	W5Si3	tI32	I4/mcm	D8M	140	(NB)4(CR NB SI)1(SI)3
NB7P4	Nb7P4	mS44	C12/m1		12	(NB)7(P)4
NBFEZN12						(NB)0.07(FE)0.07(ZN)0.86
NBH_BETA						(NB)1(H VA)1.1
NBNI3_D0A	Cu3Ti	oP8	Pmmn	D0A	59	(FE NB NI)3(FE NB NI)1
NBO	NbO	cP6	Pm-3m		221	(NB+2)1(O-2)1
NBP	NbAs	tI8	I41md		109	(NB)1(P)1
NBZN15						(NB)1(ZN)15
NBZN2_C36						(NB)1(ZN)2

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
NBZN3_L12						(NB)1(ZN)3
NBZN7						(NB)1(ZN)7
NI2Y1	Ni2Tm	cF192	F-43m		216	(NI)2(Y)1
NI2Y3	Ni2Y3	tP80	P4_12_12		92	(NI)2(Y)3
NI2ZN11_D82	Cu5Zn8	cI52	I4-3m	D82	217	(NI ZN)1(VA)1
NI31SI12	Ni31S12	hP42	P321		150	(FE NI)5(SI)2
NI3S2_LT	Ni3S2	hR15	R32		155	(NI)3(S)2
NI3SI2	Ni3Si2	oP80	Cmc2_1		36	(FE NI)3(SI)2
NI3TI_D024	Ni3Ti	hP16	P6_3/mmc	D024	194	(FE NI TI)0.75(NI TI)0.25
NI3Y	Ni3Pu	hR36	R-3m		166	(FE CO NI)3(Y)1
NI4Y	*	hR*	*			(NI)4(Y)1
NI5Y_D2D	CaCu5	hP6	P6/mmm	D2D	191	(NI)5(Y)1
NI6MNO8	NaCl	cF8	Fm-3m	B1?	225	(MG+2 NI+2)6(MN+4)1(O-2)8
NIMNO3	*	hR10	R-3		148	(MN+3 MN+4 NI+2)2(O-2)3
NISI_B31	MnP	oP8	Pnma		62	(FE NI)1(SI)1
NITI2	NiTi2	cF96	Fd-3m		227	(NI)0.33(TI)0.67

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
NIY_B27	FeB	oP8	Pnma	B27	62	(NI)1(Y)1
NIZN_B2	CsCl	cP2	Pm-3m	B2	221	(NI ZN)1(VA)1
NIZN_L10	AuCu	tP4	P4/mmm	L10	123	(NI ZN)1(VA)3
NIZN8	Ni3Zn22	mC50	C2/m		12	(NI)1(ZN)8
OLIVINE	Mg2SiO4	oP28	Pnma		62	(CA+2 FE+2 MG+2 MN+2 NI+2)1(CA+2 FE+2 MG+2 MN+2 NI+2)1(SI+4)1(O-2)4
ORTHO_ PYROXENE	MgSiO3	oP80	Pbca		61	(CA+2 MG+2)1(MG+2)1(SI+4)2(O-2)6
ORTHORHOMBIC_ S	alpha-S	oF128	Fddd	A16	70	(S)
P_PHASE	Cr9Mo21Ni20	oP56	Pnma		62	(CR FE NI)24(CR FE MO NI)20(MO)12
P2S5	P2S5	aP28	P-1		2	(P)2(S)5
PI_A13	Mo3Al2C	cP20	P4_1 32	A13	213	(CR)12.8(FE NI SI)7.2(N)4
PROTO_ PYROXENE	MgSiO3	oP40	Pbcn		60	(CA+2 MG+2)1(SI+4)1(O-2)3
PSEUDO_ WOLLASTONITE	CaSiO3	mS120	C2/c		15	(CA+2)1(SI+4)1(O-2)3
QUARTZ	SiO2	hP9	P3_121 / P6_222	*/C8	152/180	(SIO2)

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
R_PHASE	Co5Cr2Mo3	hR53	R-3h		148	(CO CR FE MN NI)27(MO W)14(CO CR FE MN MO NI W)12
RANKINITE	Ca3O7Si2?	m*4	P121/a1		14	(CA+2)3(SI+4)2(O-2)7
RED_P	*	*	*			(P)
RHODONITE	MgSiO3	mP40	P2_1/c		14	(MN+2)1(SI+4)1(O-2)3
RU1S2	FeS2	cP12	Pa-3		205	(RU)1(S)2
RU2SI3	Ge3Ru2	oP40	Pbcn		60	(RU)2(SI)3
RU4SI3	Ru4Si3	oP28	Pnma		62	(RU)4(SI)3
RUTILE_MO2	TiO2	tP6	P4_2/mnm	C4	136	(MN+4 NB+4 TI+4)1(O-2)2
S2ZR1	CdI2	hP3	P-3m1		164	(TA ZR)1(S)2
SAPPHIRINE	CaMg3Si3O10	aP68	P-1		2	(AL18MG7O40SI3)
SI2Y_C32	AlB2	hP3	P6/mmm	C32	191	(Y)1(SI)2
SI2Y_CC	Si2Th	tI12	I4_1/amd	CC	141	(Y)1(SI)2
SI3N4	Si3N4	hP28/hP14	P31c/P6_3		159/173	(SI)3(N)4
SI4Y5	Gd5Si4	oP36	Pnma		62	(Y)5(SI)4
SI5Y3_C32	AlB2	hP3	P6/mmm	C32	191	(Y)3(SI)5
SI5Y3_CC	Si2Th	tI12	I4_1/amd	CC	141	(Y)3(SI)5

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
SIC_B3	ZnS	cF8	F-43m	B3	227	(SI)1(C)1
SIGMA_D8B	CrFe	tP30	P4_2/mnm	DB8	136	(AL CO CR FE MN NI RU TA V)10(CR MO NB TA TI V W)4(AL CO CR FE MN MO NB NI RU SI TA TI V W)16
SILLIMANITE	Al2(SiO4)O-a	oP32	Pnma		62	(AL+3)1(AL+3)1(SI+4)1(O-2)5
SIP1	SiP	oC48	Cmc2_1		36	(P)1(SI)1
SIP2	GeAs2/FeS2	oP24/cP12	Pbam/Pa-3		55/205	(P)2(SI)1
SIS2_C42	SiS2	oI12	Ibam	C42	72	(SIS2)
SIY_B33	CrB	oC8	Cmcm	B33	63	(Y)1(SI)1
SPINEL	Al2MgO4	cF56	Fd-3m	H11	227	(AL+3 CR+2 CR+3 FE+2 FE+3 MG+2 MN+2 NI+2)1(AL+3 CR+3 FE+2 FE+3 MG +2 MN+2 MN+3 MN+4 NI+2 VA)2(CR+2 FE+2 MG+2 MN+2 VA)2(O-2)4
TA2H_EPSLON						(TA)2(H VA)1
TAN_EPS	TaN	hP6	P-62m		189	(TA)1(N)1
TI2N_C4	TiO2	tP6	P4_2/mnm	C4	136	(TI)2(C N)1
TI2NIH						(TI)2(NI)1(H)1
TI2ZN	CuZr2	tI6	I4/mmm		139	(TI)2(ZN)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
TI3O2	Ti3O2	hP5	P6/mmm		191	(TI+2)2(TI)1(O-2)2
TI3P	Ti3P	tP32	P4_2/n		86	(NB TI)3(P)1
TI4C2S2	Cr2AlC	hP8	P63/mmc		194	(TI)4(C)2(S)2
TIO_ALPHA	alpha-TiO	mS20	C2/m		12	(TI+2)1(O-2)1
TIO_B1	NaCl	cF8	Fm-3m	B1	225	(TI+2 TI+3 VA)1(TI VA)1(O-2)1
TIZN10	Ti3Zn22	tP100	P4_2/mbc		135	(TI)1(ZN)10
TIZN15	TiZn16	oC68	Cmcm		63	(TI)1(ZN)15
TIZN2_C14	MgZn2	hP12	P6_3/mmc	C14	194	(TI)1(ZN)2
TIZN3_L12	AuCu3	cP4	Pm-3m	L12	221	(TI)1(ZN)3
TIZN5	*	structure unknown				(TI)1(ZN)5
TRIDYMITE	SiO2	mS144	Cc		9	(SIO2)
V3H2						(V)0.6(H)0.4
V4ZN5	V4Zn5	tI18	I4/mmm		139	(V)4(ZN)5
WHITE_P	*	*	*			(P)
WOLLASTONITE	CaSiO3	aP30	Å-1		2	(CA+2 FE+2 MG+2)1(SI+4)1(O-2)3
WP2	MoP2	oS12	Cmc21		36	(W)1(P)2

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
VZN3_L12	AuCu3	cP4	Pm-3m	L12	221	(V)0.25(ZN)0.75
X_R2O3	Nd2O3	cI26	Im-3m		229	(CE+3 CE+2)2(O-2 VA)3
Y13ZN58	Y13Zn58	hP146	P6_3/mmc		194	(Y)0.18(ZN)0.82
Y15C19_ALPHA	alpha-Y15C19	oP18	Pbam		55	(C)19(Y)15
Y15C19_BETA			structure unknown			(C)19(Y)15
Y2C3_ALPHA	Sc3C4	tP70	P4/mnc		128	(Y)2(C)2(C VA)1
Y2C3_BETA			structure unknown			(Y)2(C)2(C VA)1
Y2CU2O5	Cu2Ho2O5	oP36	Pna2_1		33	(Y+3)2(CU+2)2(O-2)5
Y2S2A_Y2SI2O7	La4Ge3(GeO4)O10	aP44	P-1		2	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2B_Y2SI2O7	Y2Si2O7	oP44	Pnma		62	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2D_Y2SI2O7	Ce2Si2O7	mP44	P2_1/c		14	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2G_Y2SI2O7	Y2(Si2O7)	mP22	P2_1/c		14	(Y+3)1(Y+3)1(SI2O7-6)1
Y2SIO5	Y2SiO5	mS64	C2/c		15	(Y+3)1(Y+3)1(SIO4-4)1(O-2)1
Y3ZN11	Al11La3	oI28	Immm		71	(Y)0.21(ZN)0.79
YAG	Al2Ca3Si3O12	cI160	Ia-3d		230	(AL+3 CR+3 FE+3)5(Y+3)3(O-2)12

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
YAM	Al2Y4O9	mP60	P2_1/c		14	(AL+3 SI+4)2(Y+3)4(O-2 VA)1(O-2)9
YAP	AlYO3	hP10	P6_3/mmc		194	(AL+3 CR+3 FE+3)1(Y+3)1(O-2)3
YB12_D2F	UB12	cF52	Fm3m	D2F	225	(B)12(Y)1
YB4_D1E	UB4	tP20	P4/mbm	D1E	127	(Y)1(B)4
YB66	YB66	cF1936	Fm-3c		226	(Y)1(B)66
YC_B1	NaCl	cF8	Fm-3m	B1	225	(Y)1(C C2 VA)1
YC2_C11A	CaC2	tI6	I4/mmm	C11A	139	(C2Y1)
YCUO2	AgFeO2	hP8	P6_3/mmc		194	(Y+3)1(CU+1)1(O-2)2
YFE2O4	E(Eu0.5Yb0.5)Fe2O4	hR21	R-3m		166	(FE+2 FE+3)2(Y+3)1(O-2)4
YH3_EPSLON						(Y)1(H VA)3
YZN_B2	CsCl	cP2	Pm-3m	B2	221	(CE TI Y ZR)0.5(ZN)0.5
YZN12_D2B	Mn12Th	tI26	I4/mmm	D2B	139	(Y)0.08(ZN)0.92
YZN3	YZn3	oP16	Pnma		62	(Y)0.25(ZN)0.75
YZN5	ErZn5	hP36	P6_3/mmc		194	(Y)0.17(ZN)0.83
Z_PHASE	CrNbN	tP6	P4/nmm		129	(CR FE)1(MO NB V)1(N VA)1
ZINCBLENDE_B3	ZnS	cF8	F-43m	B3	216	(AL)1(P)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF Formula unit*
ZN22ZR	Zn22Zr	cF184	Fd-3m		227	(ZN)0.96(ZR)0.04
ZN2ZR3	Zr3Al2	tP20	P4_2/mnm		136	(ZN)0.4(ZR)0.6
ZN39ZR5	Zn39Zr5	mC88	C2/m		12	(ZN)0.89(ZR)0.11
ZN3P2	Mn2O3/Zn3P2	cI80/tP40	Ia-3/P4_2/nmc	D5_3/D5_9	206/137	(ZN)3(P)2
ZN3ZR_D023	Al3Zr	tI16	I4/mmm	D023	139	(ZN)0.75(ZR)0.25
ZN3ZR_HT	*	c**	*			(ZN)0.75(ZR)0.25
ZNP2	ZnP2/ZnAs2	tP24/mP24	P4_12_12/P2_1/c		92/14	(ZN)1(P)2
ZNS_B3	ZnS 3C	cF8	F-43m	B3	216	(ZN)1(S)1
ZNS_B4	ZnS 2H	hP4	P6_3mc	B4	186	(ZN)1(S)1
ZNZR2	CuZr2	tI6	I4/mmm		139	(ZN)0.33(ZR)0.67
ZR2S3	Zr0.77S	mS32	C2/m		12	(S3ZR2)
ZR3Y4O12	Y6UO12	hR57	R-3		148	(ZR+4)3(Y+3)4(O-2)12
ZRO2_C43	Zro2-m	mP12	P2_1/c	C43	14	(Y+3 ZR+4)2(O-2 VA)4
ZRO2_TETR	HgI2	tP6	P4_2/nmc		137	(MN+2 MN+3 NI+2 Y+3 ZR+4)2(O-2 VA)4

TCFE11 Properties Data

For more information about the models, and when in Thermo-Calc, press F1 to search the online help.

You can find information on our website about the thermophysical properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources will also be made available on our website in the near future so keep checking back or subscribe to our newsletter.

TCFE: TCS Steels/Fe-Alloys Database Revision History

Current Database Version

Database name (acronym):	**TCS Steel and Fe-alloys Database (TCFE)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**11.0**
First release:	**TCFE1 was released in 1992**

Read more in the TCFE history section on our website.

Changes in the Most Recent Database Release

TCFE10.1 to TCFE11

Software release version: 2021a (December 2020/January 2021)

Thermophysical Properties

- Added surface tension of the metallic liquid.
- Updated molar volume of the liquid.

New Elements and Systems

- Added binary M-H systems where M=Al, Ca, Ce, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, Ru, Si, Ta, Ti, V, W, Y, Zn, Zr.
- Liquid, FCC, BCC and HCP solutions and important hydrides are included. In addition, ternary C-Fe-H, Fe-H-Si, Cr-Fe-H, Al-Fe-H, Fe-H-Mo, Fe-H-Ni, Fe-H-V, Fe-H-W, Al-H-Ti, H-Ni-Ti, H-Ti-Zr systems and quaternary C-Fe-Mn-H, Cr-Fe-H-Ni systems were verified against the experimental data.
- Al-Fe-Nb, Fe-Nb-Ni, Co-Fe-Nb, Al-Cr-Nb
- Al-Fe-Zr, Cr-Fe-Zr, Cu-Fe-Zr
- Ca-P, Ca-Ti, Ca-V, Ca-W
- Ce-Nb, Ce-Ta, Ce-Ti, Ce-W
- Ca-N, N-Y, Ce-N
- Nb-Zn, Ta-Zn, W-Zn, Fe-Nb-Zn

- P-V, Fe-P-V
- S-Ta

Updated Systems and Phases

- Fe-N and C-Fe-N are updated to a more recent modeling work including the non-stoichiometric composition of Fe_4N nitride.
- Fe-Si and C-Fe-Si are updated to avoid a high temperature miscibility gap in the liquid.
- Cr-Si, Cr-Fe-Si, and C-Cr-Si are updated to a more recent modeling work.
- FeNbP, FeTiP, NbCrP, NbNiP, CrNiP are modeled as FEMP_C23 phase.
- Co-Nb, Cr-Nb, and Cr-Nb-Ni are updated to separate C15 and C14 laves phases.
- Fe-Y is updated to a more recent modeling work.
- Fe-Zr and Fe-Si-Zr are updated to a more recent modeling work.
- Fe-Nb is updated with an updated formation energy of MU_D85 phase.
- Nb-N is updated to a more recent modeling work.
- Ni-S is updated to assess the solubility of S in Fcc nickel.

TCFE8.1 to TCFE8.2 and TCFE9.2 to TCFE9.3

A simulanteous release as part of software release version: 2021a (December 2020/January 2021)

- For users who have TCFE8 and TCFE9 and also use the Steel Model Library, there is an update to correct the volume of liquid Zn.

Previous Releases

TCFE10 to TCFE10.1

Software release version: 2020b (June 2020)

There was a simultaneous update to both TCFE9 and TCFE10 that is bundled with the 2020b software release and needed for the Steel Model Library Martensite Temperature Model.

- Revised parameters of BCC_A2 phase in Fe-Mn-N system to avoid the appearance of a high N composition set at low temperatures.
- Removed a previously added ad-hoc modification to the lattice stability of BCC_A2 Nickel at temperatures below 450K.

TCFE9.1 to TCFE9.2

Software release version: 2020b (June 2020)

There was a simultaneous update to both TCFE9 and TCFE10 that is bundled with the 2020b software release and needed for the Steel Model Library Martensite Temperature Model.

- Removed a previously added ad-hoc modification to the lattice stability of BCC_A2 Nickel at temperatures below 450K.

TCFE9 to TCFE10

Software release version: 2020a (January 2020)

The TCFE10 database is significantly improved compared to TCFE9. Below is a summary of the major updates. Read more detail on the TCFE history section on our website.

- 53 new binary and 13 new ternary systems are included.
- More than 15 binary and 14 ternary systems , and many quaternary, are either completely updated or partially modified to improve the database's robustness and predictability.
- Addition of Ru and 19 Ru-X binary systems (X=Al, B, C, Ca, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, S, Si, Ta, Ti, V, Zn). In addition, the Cr-Fe-Ru is assessed at the Fe corner.
- Better predictive capacity for nitrogen alloyed duplex stainless steels: The systems relevant for nitrogen alloyed duplex stainless steels were systematically reviewed and revised as necessary.
    - The database predictivity is improved in these critical areas: Equilibria at liquidus - solidus; equilibria of matrix phases (α+γ) at high temperature; and equilibria of secondary phases at intermediate temperature.
- TCFE10 contains 31 new phases among which the so called η- silicide is named as ETA_M5SIN; and τ1-silicide (Fe2.5Ni1.5Si) and π-silicide (Cr1.5Ni2.5Si) are modeled as M4SI1_G3.
- The viscosity of metallic liquid alloys is modeled in TCFE10.
- Split description of ordered phases: The ordered phases BCC_B2 and FCC_L12 are described based on the order/disorder partitioning model as described by Lukas et al. [2007].

TCFE9 to TCFE9.1

Software release version: 2019b (June 2019)

The changes include:

- Revision of C-Fe-S system.
- Revision of Cr-Fe-Nb and Fe-Nb-Si system and the addition of 15 new silicide phases.
- Revision of the Laves phase description in Fe-Nb-W and Cr-Mo-Nb systems.
- Updates to the molar volumes of Liquid Mn, CEMENTITE, Fe-Si-B ternary phases, MNS, and several sulfides.
- Correction of the magnetic properties of CBCC_A12 phase.
- Removing the pressure dependent parameters from Fe for compatibility with GES6.

TCFE8 to TCFE9

Software release version: 2017a (March 2017)

Below is a summary of the major updates. Read more detail on the TCFE history section on our website

The database is developed and validated for simulation of the solidification process, the relative stability of matrix phases (austenite and ferrite), precipitation of secondary phases such as sulfides, borides, oxides, phosphides, carbides, nitrides, carbonitrides, and also intermetallic phases such as the sigma and laves phases.

The TCFE9 database is significantly improved compared to the previous TCFE8 version, with 32 new binary and 35 new ternary systems added to the database. In addition, more than 50 binary and 39 ternary, and many quaternary, systems are either completely updated or partially modified to improve the robustness and predictability of the database.

TCFE8 to TCFE8.1

Software release version 2016b (November 2016)

- A bug fix that previously resulted in a faulty estimation of molar volume of borides.
- The change of description of Fe-B and Fe-Ti-B systems due to incompatibility

TCFE7 to TCFE8

Software release version: 2015a (June 2015)

In order to increase the predictive capability of the database, several significant re-assessments have been performed by Thermo-Calc Software AB which are incorporated in the new release.

The elements Zn and Y and relevant phases associated with these elements have been added in the new TCFE8.

The element Zn has been added mainly for the purpose of galvanization process with the focus on the Zn corner of Al-Cr-Fe-Zn system for, but several other binaries and ternaries are also included. The element Y has been added mainly for the purpose of oxide dispersion strengthened (ODS) steels and the Al-Cr-Cu-Fe-Mn-Ni-O-Si-Y-Zr has been included which contains many assessed oxygen containing binary and ternary systems.

The description of Cu containing systems are improved with addition of Co-Cu, Co-Cu-Fe and Cu-Fe-Si data.

The FE2SITI_L21 phase has been added in the database which is important for the Fe-Si-Ti precipitation hardening steels.

The LIQUID, MU_PHASE, LAVES_PHASE_C14, SIGMA and L12_FCC phases have been improved due to the modifications for the LIQUID in the Mn-O-S, Mo-Si, C-Fe-Si and C-Fe-O systems, MU_PHASE in the Co-Nb and Co-Ta systems, LAVES_PHASE_C14 in Co-Mo and Cu-Fe systems, SIGMA phase in the Co-Cr, Al-Nb, Mn-Ta, Mo-V, Nb-V, Ta-Ti and Ta-V systems, and L12_FCC in Co-V system.

The description of C-Co-Cr system has also been added for cemented carbide applications.

All necessary volume data (including molar volume and thermal expansion) has been updated for all phases in this new release. However, the molar volume data incorporated has no pressure dependence.

Some of the major improvements to the TCFE8 database include improved/added thermodynamic descriptions for several binary, ternary and quaternary systems.

TCFE6 to TCFE7

TCFE7 released in 2012.

In order to increase the predictive capability of the database, several significant re-assessments have been performed by Thermo-Calc Software AB which are incorporated in the new release. The elements Ta and Zr and relevant phases associated with these elements have been added. Three more B containing phases and two more Mn nitride phases have been also implemented into the new TCFE7 database. All oxide phases for the Fe-Al-Ca-Cr-Mg-Mn-Ni-Si-O system have been updated or added, which includes the addition of many new oxide phases.Within the latter system all lower-order sub-systems have been evaluated.

In version 4 (TCFE4), all necessary volume data (including molar volume and thermal expansion) for various alloy phases were incorporated; such volume data has been updated for all phases in this new release. However, the molar volume data incorporated has no pressure dependence.

Some of the major improvements to the TCFE7 database include improved/added thermodynamic descriptions for the following binary, ternary and quaternary systems (with many sub-systems also re-assessed).

TCFE5 to TCFE6

TCFE6 released in 2008.

In order to increase the predictive capability of the database, several significant re- assessments have been performed by Thermo-Calc Software AB and incorporated in the new release. The element Ca has been added and the alloying ranges for the elements C, Co, Cu, N, Ti and V have been extended. In version 4 (TCFE4), all necessary volume data (including molar volume and thermal expansion) for various alloy phases were incorporated; such volume data has been updated for all phases in this new release. However, the molar volume data incorporated has no pressure dependence.

Some of the major improvements to the TCFE6 database include improved thermodynamic descriptions for the following ternary and quaternary systems (with many sub-systems also re-assessed).

TCFE4 to TCFE5

TCFE5 released in 2007.

This release builds on to the previous version of the database, i.e. TCFE4, and additionally includes complete reassessments of several binary and ternary systems performed under a three year collaborative program within the framework of the CCT-Applied project for stainless steels. CCT (Centre of Computational Thermodynamics) is a collaborative effort between the Royal Institute of Technology (Stockholm, Sweden), Kimab and Swedish industries.

Some of the major improvements to the TCFE5 database include improved thermodynamic descriptions for the following ternary and quaternary systems:

- C-Cr-Si
- Cr-Ni-N
- Fe-Cr-Cu
- Fe-Cr-Si
- Fe-Ni-N
- Fe-Ni-Si
- Fe-Cr-Mo-C
- Fe-Cr-C-N
- Fe-Cr-Mn-N
- Fe-Cr-Mo-N
- Fe-Cr-Ni-N
- Fe-Cr-Si-N
- Fe-Cr-Ni-Al
- Nb-V-C-N

TCFE3 to TCFE4

TCFE4 released in 2005-6.

This release builds on the previous version of the database, i.e. TCFE3, and additionally includes a complete assessment of molar volume data for all phases typically present in steels.

The benefit from having molar volume data included in the database is the possibility to calculate and plot directly within Thermo-Calc:

- Volume fraction of phases.
- Volume for a phase or for the whole system.
- Density for a phase or for the whole system.
- Lattice parameters (for phases having cubic structures).
- Relative length change and thermal expansion coefficients.

TCFE2 to TCFE3

TCFE3 released in 2002-3.

TCFE3 is the successor of the well-known TCFE2 (i.e., TCFE-2000 or TCFE2K) thermodynamic database for steels and Fe-alloys. A number of improvements have been made in order to increase the predictive capability of the TCFE3 database.

Some of the major improvements are:

- Improved data for the important ♦-phase in stainless steels.
- Addition of data for the binary Nb-Ni system.
- Improved data for the ternary Fe-Cr-Mo system.
- Improved data for the ternary Cr-Mo-Ni system.
- Improved data for the fcc Ti(C,N) carbonitride.