TCS Steel and Fe-alloys Database (TCFE13)

Technical Information

Available Starting with Thermo-Calc Version 2023b

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Contents

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

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.

TCFE: TCS Steels/Fe-Alloys Database Revision History. The current version of the database is TCFE13. See the link for any subversion release details.

The database is compatible with the TCS Steels/Fe-Alloys Mobility Database (MOBFE). The current version is MOBFE8.

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 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
- Use thermophysical property data to predict the viscosity of metallic liquids, the surface tension of metallic liquids, electrical resistivity, and thermal conductivity.
- 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 details about the properties data (e.g. viscosity, surface tension, etc.), 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 an examples collection and the technical information plus 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.

TCFE13 Elements, Systems, Phases and Properties

Included Elements

There are 30 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	Sn	Ta	Ti	V	W	Y	Zn	Zr

Assessed Systems

Also see information about TCFE13 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:

- 371 assessed binary systems
- 316 assessed ternary systems
- 80 assessed quaternary systems
- Several assessed quinary systems

Included Phases

Common Phases for Steel and Fe-alloys and TCFE13 Models for the Included Phases

The TCS Steel and Fe-alloys Database (TCFE) includes 435 phases. It contains an extensive GAS mixture phase for the main purpose of considering oxygen/nitrogen-gas controls in steel-making processes, and different gas atmospheres under e.g. heat treatments.

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 or investigating various steelmaking metallurgical processes, an `IONIC_LIQ` solution phase can be appended from the TCS Metal Oxide Solutions Database (TCOX).

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).

The properties data was gradually added to the database versions as follows. Molar volume with thermal expansion coefficients available starting with TCFE4, the viscosity of metallic liquids starting with TCFE10, surface tension of liquids starting with TCFE11, and electrical resistivity and thermal conductivity starting with TCFE12.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

For more information about the various thermophysical models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

Below is a summary of the available parameters and variables for the databases 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*	*Variables to Show or Plot in Console Mode and TC-Python*
Electrical resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Electrical conductivity		ELCD for a system `ELCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI
Surface tension	SIGM, XI*	`SURF(LIQUID)` `SURF(ION)` **
Dynamic viscosity	VISC	`DVIS(LIQUID)` `DVIS(ION)` **
Kinematic viscosity		`KVIS(LIQUID)` `KVIS(ION)` **
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

* XI is not used in the TCOX database (all versions). As of 2023b it is also not used starting with the following versions of these databases: TCFE13, TCNI12.1, TCTI5.1, TCNOBL3, TCPMAG2, and TCCU6.

** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

TCFE13 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.

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

Element	*Max*	*Element*	*Max*
Al	10	Ni	20
B	Trace	O	Trace
C	7	P	Trace
Ca	Trace	Ru	15
Ce	Trace	S	Trace
Co	20	Si	5

Element	*Max*	*Element*	*Max*
Cr	30	Sn	5
Cu	5	Ta	10
H	Trace	Ti	3
Mg	Trace	V	15
Mn	30	W	15
Mo	10	Y	*
N	5	Zn	**
Nb	5	Zr	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.

TCFE13 Systems

In this section:

TCFE13 Assessed Binary Systems

371 binary systems are assessed.

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

TCFE13 Assessed Ternary Systems

316 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-C-Sn	Al-Cu-Fe	Al-Cu-Mn	Al-Cu-Ni	Al-Fe-H
Al-Fe-Mg	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-Ca-Fe
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	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-Sn	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

Assessed Ternary Systems					
C-Mo-Zr	C-Nb-Ti	C-Nb-V	C-Nb-W	C-Ni-Si	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-Sn	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	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-Sn	Cu-Fe-W	Cu-Fe-Zn	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-Ni
Fe-Mg-O	Fe-Mg-S	Fe-Mg-Si	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-Sn
Fe-Mn-Ti	Fe-Mn-V	Fe-Mn-Zn	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-S	Fe-Nb-Si	Fe-Nb-Sn	Fe-Nb-V	Fe-Nb-Zn	Fe-Nb-Zr

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

TCFE13 Assessed Quaternary Systems

80 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-Ni-Si	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

TCFE13 Phases

In this section:

Common Phases for Steel and Fe-alloys

TCFE13 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

Name in the Database	*Common Name and Description*
R_PHASE	a high temperature Fe-Mo phase
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

TCFE13 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*	*Strukturbericht*	*Pearson Symbol*	*Space Group Symbol*	*SG#*	*Formula Unit*
A_R2O3_D52	La2O3 (D52)	D52	hP5	P-3m1	164	(CE+2, CE+3)2(O-2)2(O-2, VA)1
A_YZN2	Unknown Structure					(Y)0.3333(ZN)0.6667
A1_FCC	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225	(AL, CA, CE, CO, CR, CU, FE, MG, MN, MO, NB, NI, P, RU, S, SI, SN, TA, TI, V, W, Y, ZN, ZR)1(B, C, H, N, O, VA)1
A2_BCC	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229	(AL, CA, CE, CO, CR, CU, FE, MG, MN, MO, NB, NI, P, RU, S, SI, SN, TA, TI, V, W, Y, ZN, ZR)1(B, C, H, N, O, VA)3
AF	FeGaO3		oP40	Pna2_1	33	(AL2O3)1(FE2O3)1
AL11CE3	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194	(AL)0.7857(CE)0.2143
AL12MG17_A12	alpha-Mn (A12)	A12	cI58	I-43m	217	(MG)10(AL, MG, ZN)24(AL, MG, ZN)24
AL13FE4	Al13Fe4		mS102	C2/m	12	(AL)0.6275(FE, MN, ZN)0.235(AL, VA, ZN)0.1375
AL2CR3	MoSi2 (C11b)	C11b	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)0.035

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
AL2S3	alpha-Al2S3		hP30	P6_1	169	(AL2S3)1
AL2TIO5	Pseudobrookite (Fe2TiO5, E41)	E41	oS32	Cmcm	63	(AL+3)2(TI+4)1(O-2)5
AL2Y3	Zr3Al2		tP20	P4_2/mnm	136	(AL, ZN)2(Y, ZR)3
AL3CE_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194	(AL)0.75(CE, Y)0.25
AL3CE_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	(AL)0.75(CE)0.25
AL3NB_D022	Al3Ti (D022)	D022	tI8	I4/mmm	139	(AL)3(NB)1
AL3Y_HT	BaPb3		hR12	R-3m	166	(AL)0.75(Y)0.25
AL4C3_D71	Al4C3 (D71)	D71	hR7	R-3m	166	(AL, SI)4(C)3
AL4CE_D13	Al4Ba (D13)	D13	tI10	I4/mmm	139	(AL)0.8(CE)0.2
AL5FE2	Al2.8Fe		oS24	Cmcm	63	(AL)5(FE, MN)2(VA, ZN)3
AL5FE4	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217	(AL, FE)1
AL6FE6ZR_D2B	Mn12Th (D2b)	D2b	tI26	I4/mmm	139	(AL, FE)12(ZR)1
AL7CR	Al45V7		mS104	C2/m	12	(AL)6(CR)1(AL, ZN)1
AL8MN5_D810	Cr5Al8 (D810)	D810	hR26	R3m	160	(AL)12(MN)5(AL, FE, MN)9
ALCE1	AlCe		oS16	Cmcm	63	(AL)0.5(CE)0.5
ALCE3_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194	(AL)0.25(CE)0.75
ALCE3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	(AL)0.25(CE)0.75
ALCRZN_TAU4	Unknown Structure			R-3m	166	(AL, ZN)0.48(CR)0.1207(ZN)0.3993

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
ALH3	AlH3		oP24	Pnnm	58	(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	Bergman [Mg32(Al,Zn)49, D8e]	D8e	cI162	Im-3	204	(MG)26(AL, MG)6(AL, MG, ZN)48(AL)1
ALMGZN_T2	Mg46Zn37Al17		cP640	Pa-3	205	(AL)0.15(MG)0.43(ZN)0.42
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	P6_3mc	186	(AL)1(N)1
ALPHA_SPINEL	Hausmannite (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 (B33)	B33	oS8	Cmcm	63	(AL)1(Y)1
ALY2_C37	Co2Si (C37)	C37	oP12	Pnma	62	(AL)1(Y)2
ANDALUSITE	Andalusite (Al2SiO5, S02)	S02	oP32	Pnnm	58	(AL+3)1(AL+3)1(SI+4)1(O-2)5
ANORTHITE	Ca(Al0.5Si0.5)4O8		aP104	P-1	2	(CA+2)1(AL+3)2(SI+4)2(O-2)8
B_YZN2	Unknown Structure					(Y)0.3333(ZN)0.6667
B3SI_D1G	B13C2 B4C (D1g)	D1g	hR15	R-3m	166	(B)6(SI)2(B, SI)6
B4C_D1G	B13C2 B4C (D1g)	D1g	hR15	R-3m	166	(B11C, B12)1(B2, C2B, CB2)1
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229	(AL, CA, CE, CO, CR, CU, FE, MG, MN, MO, NB, NI, P, RU, S, SI, SN, TA, TI, V, W, Y, ZN, ZR)1(B, C, H, N, O, VA)3
BCC_B2	CsCl (B2)	B2	cP2	Pm-3m	221	(AL, CA, CE, CO, CR, CU, FE, MG, MN, MO, NB, NI, P, RU, S, SI, SN, 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, SN, TA, TI, V, W, Y, ZN, ZR)0.5(B, C, H, N, O,

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
						VA)3
BCT_A5	beta-Sn (A5)	A5	tI4	I4_1/amd	141	(AL, CA, CU, S, SN, TI, ZN)1
BETA_PHASE	V2H		mS6	C2/m	12	(H, VA)0.25(H, VA)0.25(V)0.5
BETA_RHOMBO_B	beta-B (R-105)		hR105	R-3m	166	(B)93(B, C, SI)12
BN_BK	BN (Bk)	Bk	hP4	P6_3/mmc	194	(B)1(N)1
C12A7	Mayenite (12CaO.7Al2O3, K74, C12A7)	K74	cI152	I-43d	220	(CA+2)6(AL+3)6(AL+3, FE+3)1(O-2)16.5
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	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
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227	(AL, CA, CE, CO, CR, CU, FE, MG, NB, NI, SI, SN, Y, ZN, ZR)2(AL, CA, CE, CO, CR, CU, FE, MG, NB, NI, SI, SN, Y, ZN, ZR)1
C1A1	Al2CaO4		mP84	P2_1/c	14	(CA+2)1(AL+3)2(O-2)4
C1A2	Al4CaO7		mS48	C2/c	15	(CA+2)1(AL+3)4(O-2)7
C1A6	Magnetoplumbite (PbFe12O19)		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	Unknown Structure					(CAO)2(AL2O3)14(MGO)2
C2F	Ca2Fe2O5		oP36	Pnma	62	(CA+2)2(FE+3)2(O-2)5
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	P6_3/mmc	194	(FE, MG, NI, ZN)2(MG, NB, NI)1
C3A1	Ca3Al2O6		cP264	Pa-3	205	(CA+2)3(AL+3)2(O-2)6
C3A2M1	3CaO.2Al2O3.MgO		oP72	Pbcm	57	(CAO)3(AL2O3)2(MGO)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
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)1
CA2SIO4_ALPHA	Ca2SiO4		hP24	P6_3/mmc	194	(CA+2, MG+2)2(SI+4)1(O-2)4
CA2SIO4_AP	K2CoCl4		oP84	Pna2_1	33	(CA+2, FE+2, MG+2)2(SI+4)1(O-2)4
CA2SN_C37	Co2Si (C37)	C37	oP12	Pnma	62	(CA)2(SN)1
CA31SN20	Pu31Rh20		tI204	I4/mcm	140	(CA)31(SN)20
CA36SN23	Sn23Yb36		tP118	P4/mbm	127	(CA)36(SN)23
CA3ZN_E1A	Re3B		oS16	Cmcm	63	(CA)3(ZN)1
CA5ZN3_D8L	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140	(CA)5(SN, ZN)3
CA7SN6	Ca7Sn6		oP52	Pnma	62	(CA)7(SN)6
CAH2_BETA	Unknown Structure					(CA)1(H)2
CAH2_C37	Co2Si (C37)	C37	oP12	Pnma	62	(CA)1(H)2
CAMN2O4	CaMn2O4		oP28	Pbcm	57	(CA+2)1(MN+3)2(O-2)4
CAMNO3	CaTiO3 Pnma Perovskite		oP20	Pnma	62	(CA+2)1(MN+4)1(O-2)3
CANI3	Ni3Pu		hR12	R-3m	166	(CA)0.25(NI)0.75
CANI5_D2D	CaCu5 (D2d)	D2d	hP6	P6/mmm	191	(CA)1(NI, ZN)5
CASN3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	(CA)1(SN)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
CAV2O4	CaV2O4		oP28	Pnma	62	(CA+2)1(CR+3, FE+3)2(O-2)4
CAZN_B33	CrB (B33)	B33	oS8	Cmcm	63	(SN, ZN)1(CA)1
CAZN11	BaCd11		tI48	I4_1/amd	141	(CA, CE)1(ZN)11
CAZN13_D23	NaZn13 (D23)	D23	cF112	Fm-3c	226	(CA)1(ZN)13
CAZN2	KHg2		oI12	Imma	74	(CU, ZN)2(CA, CE, Y)1
CAZN3	CaZn3		hP32	P6_3/mmc	194	(CA)1(ZN)3
CBCC_A12	alpha-Mn (A12)	A12	cI58	I-43m	217	(AL, CO, CR, CU, FE, MG, MN, MO, NB, NI, P, RU, SI, SN, TA, TI, V, ZN, ZR)1(B, C, N, VA)1
CE13ZN58	Gd13Zn58		hP142	P6_3/mmc	194	(CE)0.183(ZN)0.817
CE1S2	Ce10Se19		tP58	P4_2/n	86	(CE)1(S)2
CE24CO11	Ce24Co11		hP70	P6_3mc	186	(CO)11(CE)24
CE2C3_D5C	Pu2C3 (D5c)	D5c	cI40	I-43d	220	(CE)0.4(C)0.6
CE2CO7	Co7Gd2		hR18	R-3m	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)0.22222(NI)0.77778
CE2O12S3	Unknown Structure					(CE)2(O)12(S)3
CE2O2S1	Ce2O2S		hP5	P-3m1	164	(CE)2(O)2(S)1
CE2S3	Th3P4 (D73)	D73	cI28	I-43d	220	(CE)2(S)3
CE3S4_D73	Th3P4 (D73)	D73	cI28	I-43d	220	(CE)3(S)4

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
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 (D102)	D102	hP20	P6_3mc	186	(CE)0.7(NI)0.3
CE7O12	Pr7O12		hR19	R-3	148	(CE)7(O)12
CEC2_BETA	CaC2		cF36	Fm-3m	225	(CA, CE)1(C)2
CEC2_C11A	CaC2-I (C11a)	C11a	tI6	I4/mmm	139	(CA, CE, Y)1(C)2
CECO3	Ni3Pu		hR12	R-3m	166	(CO)3(CE)1
CECO5_D2D	CaCu5 (D2d)	D2d	hP6	P6/mmm	191	(CE)1(CO, CU, NI, ZN)5
CECU_B27	FeB (B27)	B27	oP8	Pnma	62	(CU)0.5(CE)0.5
CECU4	CeCu4		oP20	Pnnm	58	(CU)0.8(CE)0.2
CECU6	CeCu6		oP28	Pnma	62	(CU)0.857(CE)0.143
CEH3_EPSLON	CeH3		cF44	Fm-3m	225	(CE)1(H, VA)3
CEMENTITE_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62	(AL, CO, CR, FE, MN, MO, NB, NI, SI, V, W)3(B, C, N)1
CENI_B33	CrB (B33)	B33	oS8	Cmcm	63	(CE)0.5(NI)0.5
CENI3	CeNi3		hP24	P6_3/mmc	194	(CE)0.25(NI)0.75
CEZN3	CeZn3		oS16	Cmcm	63	(CE)0.25(ZN)0.75
CF2	Ca3.5Fe14O24.5		mS172	C2	5	(CA+2)1(FE+3)4(O-2)7
CHI_A12	alpha-Mn (A12)	A12	cI58	I-43m	217	(CR, FE, NI)24(CR, MO, W, ZR)10(CR, FE, MO, NI, W)24

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
CLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	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 (C37)	C37	oP12	Pnma	62	(CO, FE, NI, RU)2(SI)1
CO2ZN15	Co2Zn15		mS28	C2/m	12	(CO)2(ZN)15
CO3MO_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194	(CO)3(MO)1
CO3V	Al3Pu		hP24	P6_3/mmc	194	(CO, V)3(CO, V)1
CO3Y2	Unknown Structure		cP*			(CO)3(Y)2
CO3Y4	Co3Ho4		hP22	P6_3/m	176	(CO)3(Y)4
CO5Y_D2D	CaCu5 (D2d)	D2d	hP6	P6/mmm	191	(CO2, Y)1(CO)4(CO, VA)1
CO5Y8	Co5Y8		mP52	P2_1/c	14	(CO)5(Y)8
CO7Y6	Unknown Structure					(CO)7(Y)6
CO9S8	Co9S8 (D89)	D89	cF68	Fm-3m	225	(CO, FE)9(S)8
COP3	Skutterudite (CoAs3, D02)	D02	cI32	Im-3	204	(CO)1(P)3
CORDIERITE	Na0.04 (Mg0.5Fe0.5)2Al4Si5O18		oS120	Cccm	66	(AL4MG2O18SI5)1
CORUNDUM	Corundum (Al2O3, D51)	D51	hR10	R-3c	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 (B33)	B33	oS8	Cmcm	63	(CO)1(Y)1
COZN_A13	beta-Mn (A13)	A13	cP20	P4_132	213	(CO, ZN)1
COZN7	CoZn7		hP60	P6_2	171	(CO)1(ZN)7
CR3RU_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223	(CR)0.685(RU)0.315

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
CR3SI_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223	(CO, CR, FE, MO, NB, SI, V)3(AL, CO, CR, NB, SI, V)1
CR5B3_D8L	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140	(CR, MO)0.625(B)0.375
CR5SI3_D8M	W5Si3 (D8m)	D8m	tI32	I4/mcm	140	(CR, FE)4(CR, FE)1(SI)3
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	Fd-3m	227	(SIO2)1
CRNBSI	ZrNiAl		hP9	P-62m	189	(CR)1(NB)1(SI)1
CRZN17	Unknown Structure		hP*			(AL, CR)1(FE, ZN)17
CU10SN3	Cu10Sn3		hP26	P6_3	173	(CU)0.769(SN)0.231
CU2S_ALPHA	Cu2S-alpha		mP144	P2_1/c	14	(CU)2(S)1
CU2S_BETA	Cu2S-beta		hP16	P6_3/mmc	194	(CU)2(S)1
CU2S_GAMMA	Cu2Se		cF44	Fm-3m	225	(CU, FE, VA)2(CU, VA)1(S)1
CU2Y_H	Unknown Structure		hP*			(CU)2(Y)1
CU31S16	Cu31S16		mP376	P2_1/c	14	(CU)1.93(S)1
CU3P_D021	Cu3P (D021)	D021	hP24	P-3c1	165	(CU, FE)3(P)1
CU3SN_L	Cu3Sn		oS80	Cmcm	63	(CU)0.75(SN)0.25
CU41SN11	Cu41Sn11		cF416	F-43m	216	(CU)0.788(SN)0.212
CU4Y	Cu5Y1.25		mP16	P2_1/m	11	(CU)4(Y)1
CU6SN5_B81	NiAs (B81)	B81	hP4	P6_3/mmc	194	(CU)0.545(SN)0.455
CU6SN5_L	Cu6Sn5		mS44	C2/c	15	(CU)0.545(SN)0.455

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
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 (A13)	A13	cP20	P4_132	213	(AL, CE, CO, CR, CU, FE, MG, MN, MO, NB, NI, P, RU, SI, SN, TA, TI, V, Y, ZN, ZR)1(B, C, N, VA)1
CUO_B26	Tenorite (CuO, B26)	B26	mS8	C2/c	15	(CU+2)1(O-2)1
CUPRITE_C3	Cuprite (Cu2O, C3)	C3	cP6	Pn-3m	224	(CU+1)2(O-2)1
CUS_B18	Covellite (CuS, B18)	B18	hP12	P6_3/mmc	194	(CU)1(S)1
CUZN_EPSILON	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194	(CU, MN, ZN)1(VA)0.5
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	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	(NB, TI, V, Y, ZR)1(H, VA)2
DIAMOND_A4	Diamond (A4)	A4	cF8	Fd-3m	227	(AL, B, C, MN, O, P, SI, SN, ZN)1
DICTRA_FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225	(AL, CA, CE, CO, CR, CU, FE, MG, MN, MO, NB, NI, P, RU, S, SI, SN, TA, TI, V, W, Y, ZN, ZR)1(B, C, H, N, O, VA)1
DIS_BETA	V2H1.1		tI56	I4_1/amd	141	(H, VA)0.5(V)0.5
ETA_M5SIN	Fe3W3C (E93)	E93	cF112	Fd-3m	227	(CR, MO)3(FE, NI)2(SI)1(N)1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225	(AL, CA, CE, CO, CR, CU, FE, MG, MN, MO, NB, NI, P, RU, S, SI, SN, TA, TI, V, W, Y, ZN, ZR)1(B, C, H, N, O, VA)1
FCC_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	(AL, CA, CE, CO, CR, CU, FE, MG, MN, MO, NB, NI, P, RU, S, SI, SN, 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, SN, TA, TI, V, W, Y, ZN, ZR)0.25(B, C, H, N, O, VA)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
FE10SI2B3	Unknown Structure					(FE)2(SI)0.4(B)0.6
FE17Y2	Fe17Lu2		hP80	P6_3/mmc	194	(CO, FE, NI, ZN)17(Y)2
FE1NB1B1_C22	Revised Fe2P (C22)	C22(II)	hP9	P-62m	189	(FE)0.333(NB)0.333(B)0.333
FE29SI42ZR29	Unknown Structure					(FE)29(SI)42(ZR)29
FE2S3O12	Unknown Structure					(FE)2(S)3(O)12
FE2SI2ZR_D13	Al4Ba (D13)	D13	tI10	I4/mmm	139	(FE)2(SI)2(ZR)1
FE2SI3ZR3	Hf3Ni2Si3		oS32	Cmcm	63	(FE)2(SI)3(ZR)3
FE2SITI_L21	Heusler (L21)	L21	cF16	Fm-3m	225	(FE)0.5(SI)0.25(TI)0.25
FE3NB3B4	Unknown Structure					(FE)0.3(NB)0.3(B)0.4
FE3NB4SI5	Fe3Nb4Si5		oP72	Pmn2_1	31	(FE)3(NB)4(SI)5
FE3SIZR2	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194	(FE)3(SI)1(ZR)2
FE3SN2	Fe3Sn2		hR10	R-3m	166	(CR, FE)3(SN)2
FE3SN9ZR10	Unknown Structure					(FE)3(SN)9(ZR)20
FE3ZN7_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217	(CO, CU, FE, MN, NI, ZN)0.154(CU, FE, MN, ZN)0.154(AL, CO, CU, FE, MN, NI, SI, ZN)0.231(ZN)0.461
FE4N_LP1	gama-Fe4N (L'10)	L'10	cP5	Pm-3m	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	Co4Ge7Zr4		tI60	I4/mmm	139	(FE)4(NB, ZR)4(SI)7
FE4SI2ZR1	ZrFe4Si2		tP14	P4_2/mnm	136	(FE)4(SI)2(ZR)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
FE5SI12ZR3	Unknown Structure					(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
FE5SN3_B82	Ni2In (B82)	B82	hP6	P6_3/mmc	194	(CO, CR, FE, MN)5(SN)3
FE6SN6ZR	MgFe6Ge6		hP13	P6/mmm	191	(FE)6(SN)6(ZR)1
FE8SI2C	Mn8Si2C		aP*	P1	1	(FE, MN)8(SI)2(C)1
FEAL2S4	ZnIn2S4		hR7	R3m	160	(FE)1(AL)2(S)4
FEMP_C37	Co2Si (C37)	C37	oP12	Pnma	62	(CO, CR, FE, NB, NI, TI, V, W)1(CO, CR, FE, NB, NI, TI, V, W)1(P)1
FENB2P	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	(FE)1(NB)2(P)1
FENB2SI2	FeNb2Si2		tP198	P4_2/mcm	132	(FE)1(NB)2(SI)2
FENB4P	Nb4CoSi		tP12	P4/mcc	124	(FE)1(NB)4(P, SI)1
FENBSI_C37	MnCuP		oP12	Pnma	62	(FE)1(NB, ZR)1(SI)1
FENBSI2	CrSi2Zr		oP48	Pbam	55	(FE)1(NB)1(SI)2
FENIZN_T	Zn89(Fe0.5Ni0.5)13.8		cF432	F-43m	216	(FE, NI, ZN)1(ZN)5
FESI2_H	FeSi2-h		tP3	P4/mmm	123	(FE)0.3(MG, SI)0.7
FESI2_L	FeSi2-l		oS48	Cmce	64	(FE)0.333333(SI)0.666667
FESI4P4	FeSi4P4		aP9	P1	1	(FE)1(SI)4(P)4
FESN_B35	CoSn (B35)	B35	hP6	P6/mmm	191	(CO, CR, FE, MN, ZN)1(SN)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
FESN2_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140	(CO, FE, MN)1(SN)2
FESNZR_N	Unknown Structure					(FE)16(SN)16(ZR)12
FESNZR_Y	Unknown Structure					(FE)18(SN)9(ZR)5
FESO4	Chalcocyanite (CuSO4)		oP24	Pnma	62	(FE)1(S)1(O)4
FEWB_C37	MnCuP		oP12	Pnma	62	(FE)1(W)1(B)1
FEZN10	FeZn10		hP632	P6_3/mmc	194	(CR, FE)0.058(AL, FE, MN, NI, SI, SN, ZN)0.18(ZN)0.525(ZN)0.237
FEZN13	CoZn13		mS28	C2/m	12	(CO, CR, FE, MN, NI, VA)0.072(AL, SI, VA, ZN)0.072(AL, ZN)0.856
FEZN4	Fe11Zn40		cF408	F-43m	216	(FE)0.137(AL, FE, NI, SI, SN, ZN)0.118(MN, ZN)0.745
FLUORITE_C1	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	(CE+3, CE+4, MN+2, MN+3, NI+2, Y+3, ZR, ZR+4)2(O-2, VA)4
G_PHASE	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225	(AL, CO, CU, FE, NI, TI)16(MN, NB, TI, Y, ZR)6(CO, CU, FE, NI, SI)7
GAMMA2_ALFEZN	Unknown Structure					(AL, FE, ZN)0.255(ZN)0.745
GAS	Gas					(AL, AL1B1O2, AL1B3H12, AL1C1, AL1C2, AL1CU1, AL1CU1S1, AL1CU1S2, AL1H1, AL1H1O1_ALOH, AL1H1O1_HALO, AL1H1O2, AL1H2, AL1H2O2, AL1H3, AL1H3O3, AL1N1, AL1O1, AL1O2, AL1P1, AL1P2, AL1S1, AL1S2, AL2, AL2C2, AL2C6H18, AL2O1, AL2O2, AL2O3, AL2S1, AL2S2, AR, B, B10H14, B1C1, B1C1H3O1, B1C2, B1C2H7O2, B1C3H9, B1C3H9O3, B1C6H15, B1H1, B1H1O1_BOH, B1H1O1_HBO, B1H1O2, B1H1S1, B1H2, B1H2O1, B1H2O2, B1H3, B1H3O1, B1H3O2, B1H3O3, B1H6N1, B1N1, B1O1, B1O2, B1S1, B1S2, B2, B2C1, B2H4O4, B2H6, B2O1, B2O2, B2O3, B2S1, B2S2, B2S3, B3H3O3, B3H3O6, B3H6N3, B4S6, B5H9, C, C1H1, C1H1N1_HCN, C1H1N1_HNC, C1H1N1O1, C1H1N1S1, C1H1O1, C1H1O2, C1H1P1, C1H2, C1H2N4, C1H2O1, C1H2O2_CIS, C1H2O2_DIOXIRANE, C1H2O2_TRANS, C1H3, C1H3O1_CH2OH, C1H3O1_CH3O, C1H3P1, C1H4, C1H4N2O1, C1H4O1, C1H4S1, C1H5N1, C1H5O1P1, C1H5O3P1, C1H5P1, C1H5P1S1, C1H6N1P1_N, C1H6N1P1_P, C1H6P2, C1N1, C1N1O1, C1N1O1_NCO, C1N2_CNN, C1N2_NCN, C1O1, C1O1S1, C1O2, C1P1, C1P1SI1, C1P1SI2, C1P2, C1S1, C1S2, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2H1, C2H1N1, C2H2, C2H2O1, C2H3, C2H4, C2H4O1_ACETALDEHYDE, C2H4O1_OXIRANE, C2H4O2_ACETICACID, C2H4O2_DIOXETANE, C2H4O3_123TRIOXOLANE, C2H4O3_124TRIOXOLANE, C2H5, C2H6, C2H6O1_1, C2H6O1_2, C2H6O1SI1, C2H6O2, C2H7O1P1, C2H7O3P1, C2H7P1_1, C2H7P1_2, C2H7P1S1, C2H8N1P1_N, C2H8N1P1_P, C2H8SI1, C2N1_CCN, C2N1_CNC, C2N2, C2O1, C2P1, C2P2, C2SI1, C2SI2, C2SI3, C3, C3H1, C3H1N1, C3H4_1, C3H4_2, C3H6_1, C3H6_2, C3H6O1_1, C3H6O1_2, C3H8, C3N1, C3O2, C4, C4H1, C4H10_1, C4H10_2, C4H12SI1, C4H2_1, C4H2_2, C4H4_

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
						1, C4H4_2, C4H6_1, C4H6_2, C4H6_3, C4H6_4, C4H6_5, C4H8_1, C4H8_2, C4H8_3, C4H8_4, C4H8_5, C4H8_6, C4N1, C4N2, C4NI1O4, C5, C5FE1O5, C5H1N1, C5N1, C60, C6H6, C6H6O1, C6MO1O6, C6N1, C6N2, C9N1, CA, CA1H1, CA1H1O1, CA1H2O2, CA1O1, CA1S1, CA2, CE, CE1O1, CE1S1, CO, CO1H1, CO1H1O1, CO1H2O2, CO1O1, CO1S1, CO2, CR, CR1H1, CR1H1O1, CR1H1O2, CR1H1O3, CR1H2O2, CR1H2O3, CR1H2O4, CR1H3O3, CR1H3O4, CR1H4O4, CR1H4O5, CR1N1, CR1O1, CR1O2, CR1O3, CR1S1, CR1S2, CR2, CR2O1, CR2O2, CR2O3, CU, CU1H1, CU1H1O1, CU1O1, CU1S1, CU2, CU2S1, FE, FE1H1, FE1H1O1, FE1H1O2, FE1H2O2, FE1O1, FE1O2, FE1S1, FE2, H, H1MG1, H1MG1O1, H1MN1, H1MN1O1, H1MO1O1, H1MO1O2, H1MO3, H1N1, H1N1O1, H1N1O2_CIS, H1N1O2_TRANS, H1N1O3, H1N3, H1NI1, H1NI1O1, H1O1, H1O1P1, H1O1S1_HSO, H1O1S1_SOH, H1O1W1, H1O1ZN1, H1O2, H1O2W1, H1P1, H1S1, H1SI1, H1ZN1, H1ZR1, H2, H2MG1O2, H2MO1O2, H2MO1O3, H2MO1O4, H2N1, H2N2_1_1N2H2, H2N2_CIS, H2N2_TRANS, H2N2O2, H2NI1O2, H2O1, H2O1S1_H2SO, H2O1S1_HSOH, H2O2, H2O2W1, H2O2ZN1, H2O3SI1, H2O3W1, H2O4S1, H2O4W1, H2P1, H2S1, H2S2, H2SI1, H3N1, H3N1O1, H3P1, H3SI1, H4N2, H4O4SI1, H4SI1, H4SN1, H6SI2, MG, MG1N1, MG1O1, MG1S1, MG2, MN, MN1O1, MN1O2, MN1S1, MO, MO1N1, MO1O1, MO1O2, MO1O3, MO1S1, MO1S2, MO2, MO2O6, MO3O9, MO4O12, MO5O15, N, N1NB1, N1O1, N1O2, N1O3, N1P1, N1S1, N1SI1, N1SI2, N1TI1, N1V1, N1ZR1, N2, N2O1, N2O2, N2O3, N2O4, N2O5, N3, NB, NB1O1, NB1O2, NB1S1, NI, NI1O1, NI1S1, NI2, O, O10P4, O10V4, O12W4, O15W5, O1P1, O1RU1, O1S1, O1S2, O1SI1, O1SN1, O1TA1, O1TI1, O1V1, O1W1, O1Y1, O1Y2, O1ZN1, O1ZR1, O2, O2P1, O2RU1, O2S1, O2SI1, O2SI2, O2SN1, O2TA1, O2TI1, O2V1, O2W1, O2Y1, O2Y2, O2ZR1, O3, O3P2, O3RU1, O3S1, O3W1, O4P2, O4RU1, O5P2, O6P3, O6P4, O6W2, O7P4, O8P4, O8W3, O9P4, O9W3, P, P1S1, P1SI1, P1SI2, P2, P2SI2, P3, P4, P4S3, RU, S, S1SI1, S1SN1, S1TA1, S1TI1, S1V1, S1W1, S1Y1, S1ZN1, S1ZR1, S2, S2SI1, S2SN1, S2SN2, S2TI1, S2W1, S2ZR1, S3, S4, S5, S6, S7, S8, SI, SI2, SI3, SN, SN2, TA, TI, TI2, V, W, Y, ZN, ZR, ZR2)1
GRAPHITE_A9	Hexagonal Graphite (A9)	A9	hP4	P6_3/mmc	194	(B, C)1
H_R2O3	H-La2O3		hP10	P6_3/mmc	194	(CE+2, CE+3)2(O-2)2(O-2, VA)1
HALITE	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	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
HATRURITE	Ca3(SiO4)O-b		hR81	R3m	160	(CA+2)3(SI+4)1(O-2)5
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194	(AL, CA, CE, CO, CR, CU, FE, MG, MN, MO, NB, NI, P, RU, S, SI, SN, TA, TI, V, W, Y, ZN, ZR)1(B, C, H, N, O, VA)0.5
K_PHASE	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221	(C, CO, ZN)51(ZN)32(C)17
KAPPA_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221	(AL)1(FE, MN)3(C, VA)1
KSI_CARBIDE	Mo6Fe11C5		mS44	C2/m	12	(CR, FE, MO, W)3(C)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
KYANITE	Kyanite (Al2SiO5, S01)	S01	aP32	P-1	2	(AL+3)1(AL+3)1(SI+4)1(O-2)5
LARNITE	Parawollastonite (CaSiO3, S33(II))	S33(II)	mP60	P2_1/c	14	(CA+2)2(SI+4)1(O-2)4
LIQUID	Liquid					(AL, AL2/3S, ALN, ALO3/2, B, C, CA, CA2SN, CAC2, CAS, CE, CEO2, CEO3/2, CO, COS, CR, CRO3/2, CRS, CU, CU2O, CU2S, CUO, FE, FEO, FEO3/2, FES, H, MG, MG2SN1, MGS, MN, MNO, MNO3/2, MNS, MO, MO1/2S, N, NB, NBO, NBO2, NBS, NI, NIO, NIS, P, RU, S, S1ZR1/2, SI, SI1/2S, SIO2, SN, SN1/2O, SNO, SNS, SZN, TA, TI, TIO, TIO2, TIO3/2, V, W, Y, Y2/3O, ZN, ZR, ZR1/2O)1
LOWCLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	C2/c	15	(CA+2, MG+2)1(MG+2)1(SI+4)2(O-2)6
M11SI8	Cr11Ge8		oP76	Pnma	62	(CR, NB)11(SI)8
M12C	Fe6W6C		cF104	Fd-3m	227	(CO)6(W)6(C)1
M1B6_D21	CaB6 (D21)	D21	cP7	Pm-3m	221	(CA, CE, Y)1(B)6
M23C6_D84	Cr23C6 (D84)	D84	cF116	Fm-3m	225	(CO, CR, FE, MN, NI, V)20(CO, CR, FE, MN, MO, NI, V, W)3(B, C)6
M2B_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140	(CO, CR, FE, MN, MO, NI, V, W)2(B)1
M2B_CB	Mg2Cu (Cb)	Cb	oF48	Fddd	70	(CR, FE, MN, MO, NI)0.667(B)0.333
M2B3	V2B3		oS20	Cmcm	63	(NB, V)0.4(B)0.6
M2O3C_D53	Bixbyite (Mn2O3, D53)	D53	cI80	Ia-3	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 (D52)	D52	hP5	P-3m1	164	(MN+3, Y, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2P_C22	Revised Fe2P (C22)	C22(II)	hP9	P-62m	189	(AL, CO, CR, FE, MN, MO, NB, NI, TI, V, W)2(P, SI)1
M2SI_TETA	AlNi2		hP6	P-3m1	164	(FE, NI)1(FE, NI, VA)1(SI)1
M3B2_D5A	Si2U3 (D5a)	D5a	tP10	P4/mbm	127	(CR, FE, MO, NI, W)0.4(CR, FE, NI)0.2(B)0.4
M3B4_D7B	Ta3B4 (D7b)	D7b	oI14	Immm	71	(CR, FE, NB, V)0.429(B)0.571

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
M3C2_D510	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62	(CO, CR, MO, V, W)3(C)2
M3P_D0E	Ni3P (D0e)	D0e	tI32	I-4	82	(AL, CO, CR, CU, FE, MN, MO, NI, TI)3(B, P)1
M3SI_D03	BiF3 (D03)	D03	cF16	Fm-3m	225	(FE, MN)3(SI)1
M4SI1_G3	AlAu4		cP20	P2_13	198	(CR, FE, NI)3(NI)1(SI)1(C, VA)1
M5B6	V5B6		oS22	Cmmm	65	(NB, V)0.455(B)0.545
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15	(FE, MN, NB, V)5(C, N)2
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193	(CR, FE, MN, NI, Y)5(SI)3(C, VA)1
M6C_E93	Fe3W3C (E93)	E93	cF112	Fd-3m	227	(CO, FE, NI)2(MO, NB, W)2(CO, CR, FE, MO, NB, NI, SI, V, W)2(C)1
M6SI5	Si5V6		oI44	Ibam	72	(CR, NB)6(SI)5
M7C3_D101	C3Cr7 (D101)	D101	oP40	Pnma	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(CA, Y)2
MB_B27	FeB (B27)	B27	oP8	Pnma	62	(B)1(CO, CR, FE, MN, MO, NI, TI, V, ZR)1
MB_B33	CrB (B33)	B33	oS8	Cmcm	63	(CR, FE, MN, MO, NB, NI, TA, TI, V)1(B)1
MB_BG	MoB (Bg)	Bg	tI16	I4_1/amd	141	(CR, FE, MO)0.5(B)0.5
MB2_C32	Hexagonal omega (C32)	C32	hP3	P6/mmm	191	(B)2(AL, CR, MG, TI, Y, ZR)1
MC_ETA	CMo		hP12	P6_3/mmc	194	(MO, TI, V, W)1(C, VA)1
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	P-6m2	187	(MO, W)1(C, N)1
MELILITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	P-42_1m	113	(CA+2)2(AL+3, MG+2)1(AL+3, SI+4)1(SI+4)1(O-2)7

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MERWINITE	Ca3Mg(SiO4)2		mP56	P2_1/c	14	(CA+2)3(MG+2)1(SI+4)2(O-2)8
MG12R_D2B	Mn12Th (D2b)	D2b	tI26	I4/mmm	139	(MG)12(CE)1
MG12ZN13	Zr21Re25		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 (Ca)	Ca	hP18	P6_222	180	(MG)2(NI)1
MG2SI_C1	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	(MG)2(SI, SN)1
MG2ZN11_D8C	Mg2Zn11 (D8c)	D8c	cP39	Pm-3	200	(MG)2(AL, SI, ZN)11
MG2ZN3	Mg4Zn7		mS110	C2/m	12	(MG)2(AL, ZN)3
MG3M_D03	BiF3 (D03)	D03	cF16	Fm-3m	225	(MG)3(CE, MG)1
MG3N2_D53	Bixbyite (Mn2O3, D53)	D53	cI80	Ia-3	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
MGC2	MgC2		tP6	P4_2/mnm	136	(MG)1(C)2
MGH2_C4	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136	(MG)1(H)2
MN11SI19	Mn11Si19		tP120	P-4n2	118	(MN)0.367(SI)0.633

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
MN2YO5	HoMn2O5		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	Mn5SiC		oS56	Cmc2_1	36	(MN)0.714(SI)0.143(C)0.143
MN6N5	CoO		tI4	I4/mmm	139	(MN)6(N)5
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166	(MN)0.85714(SI)0.14286
MN9SI2	Mn9Si2		oI186	Immm	71	(MN)0.81818(SI)0.18182
MNP_B31	MnP (B31)	B31	oP8	Pnma	62	(CO, CR, FE, MN, NI, W)1(P, SI)1
MNTA	Unknown Structure					(MN)1(TA)1
MNYO3_HEX	LuMnO3		hP30	P6_3cm	185	(Y+3)1(MN+3)1(O-2)3
MNZN9	Unknown Structure		h**			(MN)0.1(ZN)0.9
MO2B5_D8I	Mo2B5 (D8i)	D8i	hR7	R-3m	166	(MO)0.32(B)0.68
MO2S3	Mo2S3		mP10	P2_1/m	11	(MO)2(S)3
MO3P	alpha-V3S		tI32	I-42m	121	(MO)3(P)1
MO5SI3_D8M	W5Si3 (D8m)	D8m	tI32	I4/mcm	140	(MO)5(SI)3
MOB2_C32	Hexagonal omega (C32)	C32	hP3	P6/mmm	191	(MO)0.38(B)0.62
MOP_BH	Tungsten Carbide (Bh)	Bh	hP2	P-6m2	187	(MO)1(P)1
MOS2_C7	Molybdenite (MoS2, C7)	C7	hP6	P6_3/mmc	194	(MO, W)1(S)2
MOSI2_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139	(MO)1(SI)2

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
MOZN22	Zn93(Zn0.43Mo0.57)Mo4		cF420	F-43m	216	(MO)1(ZN)22
MOZN7	Ca7Ge		cF32	Fm-3m	225	(MO)1(ZN)7
MS_B1	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225	(CA, CE, CO, CR, CU, FE, MG, MN, Y, ZR)1(S)1
MS_B81	NiAs (B81)	B81	hP4	P6_3/mmc	194	(AL, CO, CR, CU, FE, MN, NB, NI, TI, V, VA, ZR)1(S)1
MS2_C2	Pyrite (FeS2, C2)	C2	cP12	Pa-3	205	(CO, FE, MN, RU)1(S)2
MSI_B20	FeSi (B20)	B20	cP8	P2_13	198	(CO, CR, FE, MN, NI, RU)0.5(AL, MG, SI)0.5
MSI2_C40	CrSi2 (C40)	C40	hP9	P6_222	180	(CR, NB)1(SI)2
MU_D85	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	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
MY3_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62	(CO, NI)1(Y)3
NB1ZN1	Unknown Structure					(NB)1(ZN)1
NB2ZN3_D85	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166	(NB)2(ZN)3
NB3B2_D5A	Si2U3 (D5a)	D5a	tP10	P4/mbm	127	(FE, NB, V)0.6(B)0.4
NB3RU5	Rh5Ge3		oP16	Pbam	55	(NB, RU)0.375(RU)0.625
NB5SI3_D8L	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140	(CR, NB)5(SI)3
NB5SI3_D8M	W5Si3 (D8m)	D8m	tI32	I4/mcm	140	(NB)4(CR, NB, SI)1(SI)3
NB7P4	Nb7P4		mS44	C2/m	12	(NB)7(P)4
NBFEZN12	Unknown Structure					(NB)0.071(FE)0.071(ZN)0.857

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
NBH_BETA	Ta2H		oS8	C222	21	(NB)1(H, VA)1.1
NBNI3_D0A	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59	(FE, NB, NI)3(FE, NB, NI)1
NBO	NbO		cP6	Pm-3m	221	(NB+2)1(O-2)1
NBP	NbAs		tI8	I4_1md	109	(NB)1(P)1
NBZN7	Unknown Structure					(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
NI31SI12	Ni31S12		hP42	P321	150	(FE, NI)5(SI)2
NI3S2_LT	Hazelwoodite (Ni3S2, D5e)	D5e	hR5	R32	155	(NI)3(S)2
NI3SI2	Ni3Si2		oP80	Cmc2_1	36	(FE, NI)3(SI)2
NI3SN_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194	(SN)1(FE, MN, NI)3
NI3SN_D03	BiF3 (D03)	D03	cF16	Fm-3m	225	(NI, SN)1
NI3SN2	Ni3Sn2		oP20	Pnma	62	(CO, FE, MN, NI)3(SN)2
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	C2/m	12	(NI)3(SN)4
NI3TI_D024	Ni3Ti (D024)	D024	hP16	P6_3/mmc	194	(FE, NI, TI)0.75(NI, TI)0.25
NI3Y	Ni3Pu		hR12	R-3m	166	(CO, FE, NI)3(Y)1
NI4Y	Unknown Structure		hR*			(NI)4(Y)1
NI5Y_D2D	CaCu5 (D2d)	D2d	hP6	P6/mmm	191	(NI)5(Y)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
NI6MNO8	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225	(MG+2, NI+2)6(MN+4)1(O-2)8
NIMNO3	Ilmenite (FeTiO3, E22)	E22	hR10	R-3	148	(MN+3, MN+4, NI+2)2(O-2)3
NITI2	NiTi2		cF96	Fd-3m	227	(NI)0.3333(TI)0.6667
NIY_B27	FeB (B27)	B27	oP8	Pnma	62	(NI)1(Y)1
NIZN_L2A	delta-CuTi (L2a)	L2a	tP2	P4/mmm	123	(NI, ZN)1(NI, ZN)1
NIZN8	Ni3Zn22		mS50	C2/m	12	(FE, NI)1(ZN)8
OLIVINE	Forsterite (Mg2SiO4, S12)	S12	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	Enstatite (MgSiO3, S43)	S43	oP80	Pbca	61	(CA+2, MG+2)1(MG+2)1(SI+4)2(O-2)6
ORTHORHOMBIC_S	alpha-S (A16)	A16	oF128	Fddd	70	(S)1
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	beta-Mn (A13)	A13	cP20	P4_132	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	alpha-Quartz (low Quartz)		hP9	P3_121	152	(SIO2)1
R_PHASE	R-(Co,Cr,Mo)		hR53	R-3	166	(CO, CR, FE, MN, NI)27(MO, W)14(CO, CR, FE, MN, MO, NI, W)12
RANKINITE	3CaO.2SiO2		mP48	P2_1/c	14	(CA+2)3(SI+4)2(O-2)7
RED_P	Unknown Structure					(P)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
RHODONITE	Rhodonite (MnSiO3-b)		aP50	P-1	2	(MN+2)1(SI+4)1(O-2)3
RU2SI3	Ge3Ru2		oP40	Pbcn	60	(RU)2(SI)3
RU4SI3	Ru4Si3		oP28	Pnma	62	(RU)4(SI)3
RUTILE_C4	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136	(MN+4, NB+4, SN+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)1
SI2Y_C32	Hexagonal omega (C32)	C32	hP3	P6/mmm	191	(Y)1(SI)2
SI2Y_CC	alpha-ThSi2 (Cc)	Cc	tI12	I4_1/amd	141	(CE, Y)1(SI)2
SI3N4	Nierite (alpha-Si3N4)		hP28	P31c	159	(SI)3(N)4
SI4Y5	Gd5Si4		oP36	Pnma	62	(Y)5(SI, SN)4
SI5Y3_C32	Hexagonal omega (C32)	C32	hP3	P6/mmm	191	(Y)3(SI)5
SI5Y3_CC	alpha-ThSi2 (Cc)	Cc	tI12	I4_1/amd	141	(Y)3(SI)5
SIC_B3	Zincblende (ZnS, B3)	B3	cF8	F-43m	216	(SI)1(C)1
SIGMA_D8B	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	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	Sillimanite (Al2SiO5, S03)	S03	oP32	Pnma	62	(AL+3)1(AL+3)1(SI+4)1(O-2)5
SIP1	(SiP)		oS48	Cmc2_1	36	(P)1(SI)1
SIP2	Pyrite (FeS2, C2)	C2	cP12	Pa-3	205	(P)2(SI)1
SIS2_C42	SiS2 (C42)	C42	oI12	Ibam	72	(SIS2)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
SIY_B33	CrB (B33)	B33	oS8	Cmcm	63	(Y)1(SI)1
SN10Y11	Ge10Ho11		tI84	I4/mmm	139	(SN)10(Y)11
SN2Y_C49	ZrSi2 (C49)	C49	oS12	Cmcm	63	(SN)2(Y)1
SN2ZR_C54	TiSi2 (C54)	C54	oF24	Fddd	70	(SN)2(ZR)1
SN3Y1	GdSn2.75		oS16	Amm2	38	(SN)3(Y)1
SN3Y5_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193	(Y, ZR)5(SN)3(SN, VA)1
SN5Y2	Shcherbinaite (V2O5) (Revised)		oP14	Pmmn	59	(SN)5(Y)2
SNS_B16	GeS (B16)	B16	oP8	Pnma	62	(SN)1(S)1
SNZR4_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223	(SN, ZR)1(SN, ZR)3
SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	Fd-3m	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	Unknown Structure					(TA)2(H, VA)1
TAN_EPS	TaN-eps		hP6	P-62m	189	(TA)1(N)1
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136	(TI)2(C, N)1
TI2NIH	Ti2NiH		cF128	Fd-3m	227	(TI)2(NI)1(H)1
TI2ZN	CuZr2		tI6	I4/mmm	139	(TI, ZR)2(ZN)1
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, SI)1
TI4C2S2	AlCCr2		hP8	P6_3/mmc	194	(TI)4(C)2(S)2

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
TIO_ALPHA	alpha-TiO		mS20	C2/m	12	(TI+2)1(O-2)1
TIO_B1	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	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		oS68	Cmcm	63	(NB, TI)1(ZN)15
TIZN3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	(NB, TI, V)1(ZN)3
TIZN5	Unknown Structure					(TI)1(ZN)5
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	Cc	9	(SIO2)1
V3H2	Unknown Structure					(V)0.6(H)0.4
V4ZN5	V4Zn5		tI18	I4/mmm	139	(V)4(ZN)5
WHITE_P	Unknown Structure					(P)1
WOLLASTONITE	Wollastonite (CaSiO3)		aP30	P-1	2	(CA+2, FE+2, MG+2)1(SI+4)1(O-2)3
WP2	MoP2		oS12	Cmc2_1	36	(W)1(P)2
X_R2O3	Nd2O3		cI26	Im-3m	229	(CE+2, CE+3)2(O-2, VA)3
Y13ZN58	Y13Zn58		hP146	P6_3/mmc	194	(Y)0.1831(ZN)0.8169
Y15C19_ALPHA	alpha-Y15C19		oP18	Pbam	55	(C)19(Y)15
Y15C19_BETA	Unknown Structure					(C)19(Y)15
Y2C3_ALPHA	Sc3C4		tP70	P4/mnc	128	(Y)2(C)2(C, VA)1
Y2C3_BETA	Unknown Structure					(Y)2(C)2(C, VA)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
Y2CU2O5	Cu2Ho2O5		oP36	Pna2_1	33	(Y+3)2(CU+2)2(O-2)5
Y2S2A_Y2SI2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	C2/m	12	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2B_Y2SI2O7	La4Ge3[GeO4]O10		aP44	P-1	2	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2D_Y2SI2O7	Possible delta-Y2Si2O7		oP44	Pnma	62	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2G_Y2SI2O7	Y2Si2O7-b		mP22	P2_1/c	14	(Y+3)1(Y+3)1(SI2O7-6)1
Y2SIO5	Y2SiO5 (RE2SiO5 X2)		mS64	C2/c	15	(Y+3)1(Y+3)1(SIO4-4)1(O-2)1
Y3ZN11	Al11La3		oI28	Immm	71	(CE, Y)0.2143(ZN)0.7857
YAG	Garnet (Co3Al2Si3O12, S14)	S14	cI160	Ia-3d	230	(AL+3, CR+3, FE+3)5(Y+3)3(O-2)12
YAM	Y4Al2O9		mP60	P2_1/c	14	(AL+3, SI+4)2(Y+3)4(O-2, VA)1(O-2)9
YAP	CaTiO3 Pnma Perovskite		oP20	Pnma	62	(AL+3, CR+3, FE+3)1(Y+3)1(O-2)3
YB12_D2F	UB12 (D2f)	D2f	cF52	Fm-3m	225	(B)12(Y)1
YB4_D1E	ThB4 (D1e)	D1e	tP20	P4/mbm	127	(CE, Y)1(B)4
YB66	YB66		cF1936	Fm-3c	226	(Y)1(B)66
YC_B1	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225	(Y)1(C, C2, VA)1
YCUO2	Hexagonal Delafossite (CuAlO2)		hP8	P6_3/mmc	194	(Y+3)1(CU+1)1(O-2)2
YFE2O4	MnBi2Te4		hR7	R-3m	166	(FE+2, FE+3)2(Y+3)1(O-2)4
YH3_EPSLON	H3Ho		hP24	P-3c1	165	(Y)1(H, VA)3
YZN_B2	CsCl (B2)	B2	cP2	Pm-3m	221	(CE, TI, Y, ZR)0.5(ZN)0.5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Formula Unit
YZN12_D2B	Mn12Th (D2b)	D2b	tI26	I4/mmm	139	(Y)0.0769(ZN)0.9231
YZN3	Zn3Y		oP16	Pnma	62	(Y)0.25(ZN)0.75
YZN5	ErZn5		hP36	P6_3/mmc	194	(Y)0.1667(ZN)0.8333
Z_PHASE	CrNbN		tP6	P4/nmm	129	(CR, FE)1(MO, NB, V)1(N, VA)1
ZINCBLENDE_B3	Zincblende (ZnS, B3)	B3	cF8	F-43m	216	(AL)1(P)1
ZN22ZR	Zn22Zr		cF184	Fd-3m	227	(ZN)0.9565(ZR)0.0435
ZN39ZR5	Zn39Zr5		mS88	C2/m	12	(ZN)0.8864(ZR)0.1136
ZN3P2	Zn3P2 (D59)	D59	tP40	P4_2/nmc	137	(ZN)3(P)2
ZN3ZR_D023	Al3Zr (D023)	D023	tI16	I4/mmm	139	(ZN)0.75(ZR)0.25
ZN3ZR_HT	Unknown Structure		c**			(ZN)0.75(ZR)0.25
ZNP2	ZnAs2		mP24	P2_1/c	14	(ZN)1(P)2
ZNS_B3	Zincblende (ZnS, B3)	B3	cF8	F-43m	216	(ZN)1(S)1
ZNS_B4	Wurtzite (ZnS, B4)	B4	hP4	P6_3mc	186	(ZN)1(S)1
ZR3Y4O12	UY6O12		hR19	R-3	148	(ZR+4)3(Y+3)4(O-2)12
ZRO2_C43	Baddeleyite (ZrO2, C43)	C43	mP12	P2_1/c	14	(Y+3, ZR+4)2(O-2, VA)4
ZRO2_TETR	HgI2 (C13)	C13	tP6	P4_2/nmc	137	(MN+2, MN+3, NI+2, Y+3, ZR+4)2(O-2, VA)4

TCFE13 Properties Data

Model Descriptions

For more information about the various thermophysical models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

Examples

Go to the Steels and Fe-Alloys Databases page on our website where you can access an examples collection and the technical information plus 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.

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:	**13.0**
First release:	**TCFE1 was released in 1992**

Changes in the Most Recent Database Release

TCFE12 to TCFE13

Software release 2023b (June 2023)

- The full gas description is included.
- Assessed Fe-Mn-Ti system.
- Revised Cr-Fe-Ni-Si subsystems (Cr-Fe-Si, Cr-Ni-Si) to increase the accuracy of phase equilibria involving the FCC/BCC/LIQUID phases.
- Reassessed THCD of FeTi-B2 and added THCD ELRS of BN_BK.
- Updated the Diamond molar volume and corrected wrong volume parameters.
- Updated Ca-Fe to a more recent description.
- Removed the HIGH_SIGMA phase from the Cr-Mn binary.
- Revised S-Zr and Fe-S-Zr.
- Estimated Fe-Nb-S.
- Revised the liquid in Fe-O-Y and C-Ni-Si.
- The surface tension was re-assessed based on the Redlich-Kister-Muggianu (R-K-M) sub-regular solution model.

Previous Releases

TCFE11 to TCFE12

Software release 2022a (December 2021/January 2022)

Added Tin (Sn)

- 26 Binaries Sn-X (X=Al, B, C, Ca, Ce, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, O, P, Ru, S, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)
- 13 Ternaries: Fe-Sn-X (X=C, Cr, Cu, Mn, Nb, Ni, O, S, Si, W, Zn, Zr), and Al-C-Sn

New Thermophysical Properties

- Electrical resistivity is modeled for crystalline phases and liquid. The descriptions can be used for deriving electrical conductivity.
- Thermal conductivity is modeled for crystalline phases and liquid. The descriptions can be used for deriving thermal resistivity as well as thermal diffusivity (by combining with our density and heat capacity data).

Updated Zinc Corner

As well as systems related for the galvanization process:

- Remodeled and unified all gamma-brass D82 phases stable in Fe-Zn, Cu-Zn, Ni-Zn, Mn-Zn, Co-Zn with a 4SL FE3ZN7_D82.
- Added Al-Fe-Mg, Cu-Fe-Zn, Fe-Ni-Zn, Fe-Si-Zn, Fe-Mg-Si, Fe-Mg-Ni, Fe-Mn-Zn, Mg-Si-Zn

Other Updates

- Unified several phases with the same crystallography
- Corrected the low melting pseudobinary in Fe-O-Si
- Extended a ternary phosphide: FEMP_C37 (CO,CR,FE,NB,NI,TI,V,W)1(CO,CR,FE,NB,NI,TI,V,W)1P1
- Revised C-Ca and estimated C-Ca-Fe

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.

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.