TCS Mo-based Alloys Database (TCMO1)

Technical Information

Available Starting with Thermo-Calc Version 2024b

Document created 5/29/2024

Contents

TCMO1: TCS Mo-based Alloys Database

Molybdenum-based alloys are used in various applications due to their excellent mechanical, thermal, and corrosion-resistant properties. They are commonly used in aerospace components, electrical contacts, industrial machinery, and high-temperature furnace parts. Additionally, they are used in the production of high-strength steel alloys, which are crucial in construction and automotive industries for their durability and resistance to corrosion and heat.

The thermodynamic TCS Mo-based Alloys Database (TCMO) is available for refractory (e.g. Mo-based) superalloys that function at higher temperatures than the Ni-base superalloys.

The database is compatible with the TCS Mo-based Alloys Mobility Database (MOBMO). The current version is MOBMO1.

The Mo-based thermodynamic and kinetic databases include the silicide and borosilicide phases to form SiO_2-based scales, which is to overcome the challenge of poor oxidation resistance that happens with these alloys that contain MoO_3.

In addition to thermodynamic data, TCMO1 has properties data available for:

- Molar volume with thermal expansion coefficients
- Electrical resistivity
- Thermal conductivity
- Viscosity of metallic liquids
- Surface tension of metallic liquids

When combined with the kinetic database you can also use the Add-on Modules — Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA). The thermodynamic database is also compatible with the Additive Manufacturing (AM) Module. Both the thermodynamic and kinetic databases can be used together with the Thermo-Calc Software Development Kits (SDKs).

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.

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 Mo-based Alloys Database (TCMO) 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 Mo-based Alloys Database (TCMO) Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, and the phases and models. It also includes details about the properties data (e.g. viscosity, surface tension, etc.), and a list of the included elements.
- The *TCS Mo-based Alloys Database (TCMO) 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 Molybdenum-based Alloys page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database.

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

TCMO1 Elements, Systems, Phases and Properties

Included Elements

There are 12 elements included in the database.

Al	B	C	Cr	Fe	Hf
Mn	Mo	Re	Si	Ti	Zr

Assessed Systems and Phases

A hybrid approach of experiments, first-principles calculations and CALPHAD modeling have been used to obtain thermodynamic descriptions of the constituent binary and ternary systems over the whole composition and temperature ranges.

All the stable solution phases and intermetallic compounds that exist in each assessed system are included.

The database contains:

- 66 assessed binary systems
- 46 assessed ternary systems
- 3 assessed quaternary systems
- 167 phases

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

For more information about the various thermophysical, thermomechanical, and properties 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.

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 an SDK such as TC-Python or TC-Toolbox for MATLAB®.

Property (and Graphical Mode Variable Name)	*Model Parameters*	*Variables to Show or Plot in Console Mode or the SDKs (TC-Python, or TC-Toolbox for MATLAB®)****
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI
Electrical conductivity	ELQ**	ELCD for a system `ELCD(PHI)` for phase PHI
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
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)` **

* 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. As of 2024a, TCMG7, TCAL9, and TCHEA7. As of 2024b, TCSLD5.

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

*** The examples listed for the SDKs are using Console Mode syntax. The quantities can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity` classes. See the various model descriptions or the SDK help for details.

TCMO1 Systems

In this section:

TCMO1 Assessed Binary Systems

66 binary systems are assessed.

	Al	B	C	Cr	Fe	Hf	Mn	Mo	Re	Si	Ti	Zr
Al	Al											
B	x	B										
C	x	x	C									
Cr	x	x	x	Cr								
Fe	x	x	x	x	Fe							
Hf	x	x	x	x	x	Hf						
Mn	x	x	x	x	x	x	Mn					
Mo	x	x	x	x	x	x	x	Mo				
Re	x	x	x	x	x	x	x	x	Re			
Si	x	x	x	x	x	x	x	x	x	Si		
Ti	x	x	x	x	x	x	x	x	x	x	Ti	
Zr	x	x	x	x	x	x	x	x	x	x	x	Zr

TCMO1 Assessed Ternary Systems

46 ternary systems are assessed.

Assessed Ternary Systems				
Al-B-Mo	Al-C-Mo	Al-Fe-Mn	Al-Fe-Si	Al-Mn-Si
Al-Mo-Si	B-C-Hf	B-C-Mo	B-C-Si	B-C-Ti
B-C-Zr	B-Cr-Mo	B-Cr-Si	B-Fe-Mo	B-Hf-Mo
B-Hf-Si	B-Hf-Zr	B-Mn-Mo	B-Mn-Si	B-Mo-Re
B-Mo-Si	B-Mo-Ti	B-Mo-Zr	B-Si-Ti	B-Si-Zr
C-Cr-Mo	C-Fe-Mo	C-Hf-Mo	C-Hf-Si	C-Hf-Zr
C-Mn-Mo	C-Mo-Re	C-Mo-Si	C-Mo-Ti	C-Mo-Zr
C-Si-Ti	Cr-Fe-Ti	Cr-Mo-Si	Cr-Mo-Ti	Cr-Mo-Zr
Fe-Mo-Si	Hf-Mo-Si	Mo-Re-Si	Mo-Si-Ti	Mo-Si-Zr
Mo-Ti-Zr				

TCMO1 Assessed Quaternary Systems

3 quaternary systems are assessed.

Assessed Quaternary Systems		
B-Hf-Mo-Si	B-Mo-Si-Ti	B-Mo-Si-Zr

TCMO1 Phases

In this section:

Common Phases for Molybdenum Materials

TCMO1 Models for the Included Phases

The following lists common phase names and the corresponding Thermo-Calc database phase names for some key molybdenum materials.

Name in the Database	*Common Name and Description*
BCC_A2	Disordered Mo-based BCC solution phase
FCC_A1#1	Disordered FCC solution phase
FCC_A1#2	MC carbide
GAS	Gas
HCP_A3#1	Disordered HCP solution phase
HCP_A3#2	M2C carbide
LIQUID	Liquid
MOSIZR	MoSiHf and MoSiZr
MO3SI_A15	Mo_3Si
MO5SIB2	T2
MO5SI3_D8M	Mo_5Si_3, T1
TI5SI3_D88	Ti_5Si_3

TCMO1 Models for the Included Phases

The table lists all phases and the thermodynamic model used to describe the phase.

Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
LIQUID	Liquid				LIQUID mixture.	1	(AL, B, C, CR, FE, HF, MN, MO, RE, SI, TI, ZR)1.0
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)		2	(AL, CR, FE, HF, MN, MO, RE, SI, TI, ZR)1.0(B, C, VA)1.0
FCC_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		2	(AL, ZR)0.75(AL, ZR)0.25
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)		2	(AL, CR, FE, HF, MN, MO, RE, SI, TI, VA, ZR)1.0(B, C, VA)3.0
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)		3	(AL, CR, FE, HF, MN, MO, RE, SI, TI, VA, ZR)0.5(AL, CR, FE, HF, MN, MO, RE, SI, TI, VA, ZR)0.5(B, C, VA)3.0
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)		2	(AL, CR, FE, HF, MN, MO, RE, SI, TI, ZR)1.0(B, C, VA)0.5
CBCC_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		2	(AL, CR, FE, MN, MO, RE, SI, TI, ZR)1.0(B, C, VA)1.0
CUB_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)		2	(AL, CR, FE, HF, MN, MO, RE, SI, TI, ZR)1.0(B, C, VA)1.0
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)		1	(AL, B, C, SI)1.0
BETA_RHOMBO_ B	beta-B (R-105)		hR105	(166, R-3m)		2	(B)93.0(B, C, SI, TI)12.0
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	(194, P6_ 3/mmc)		1	(B, C)1.0
BCT_D022	Al3Ti (D022)	D022	tI8	(139, I4/mmm)		2	(AL, TI)3.0(TI)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)		2	(AL, CR, FE, HF, MN, MO, RE, SI, TI, ZR)2.0(AL, CR, FE, HF, MN, MO, RE, SI, TI, ZR)1.0
DIS_MU	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)		1	(FE, MN, MO, SI)1.0
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)		4	(FE, MN, MO, SI)1.0(FE, MN, MO, SI)2.0(FE, MN, MO, SI)6.0(FE, MN, MO, SI)4.0
DIS_SIG	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		1	(CR, FE, MN, MO, RE, SI)1.0
SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		3	(CR, FE, MN, MO, RE, SI)10.0(CR, FE, MN, MO, RE, SI)4.0(CR, FE, MN, MO, RE, SI)16.0
R_PHASE	R-(Co,Cr,Mo)		hR53	(148, R-3)		3	(FE, RE)27.0(MO)14.0(FE, MO, RE)12.0
CHI_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		3	(RE)24.0(HF, MO, TI, ZR)10.0(MO, RE)24.0
MC_ETA	CMo		hP12	(194, P6_ 3/mmc)		2	(HF, MO, ZR)1.0(C, VA)1.0
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	(187, P-6m2)		2	(MO)1.0(C)1.0
M23C6	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)		3	(CR, FE, MN)20.0(CR, FE, MN, MO)3.0(C)6.0
CEMENTITE	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(CR, FE, MN, MO)3.0(C)1.0
M3C2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(CR, MO)3.0(C)2.0
M7C3	C3Cr7 (D101)	D101	oP40	(62, Pnma)		2	(CR, FE, MN, MO)7.0(C)3.0
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(MN)5.0(C)2.0
AL4C3	Al4C3 (D71)	D71	hR7	(166, R-3m)		2	(AL)4.0(C)3.0
MB_B33	CrB (B33)	B33	oS8	(63, Cmcm)		2	(CR, FE, HF, MO, TI)1.0(B)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MB2_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)		2	(B, VA)2.0(AL, CR, HF, MN, MO, TI, ZR)1.0
M3B2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)		3	(CR, FE, MO)0.4(CR, FE)0.2(B)0.4
M2B_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(CR, FE, MN, MO, RE, TI)2.0(B)1.0
MOB1	MoB (Bg)	Bg	tI16	(141, I4_ 1/amd)		2	(MO)1.0(B)1.0
B12ZR	UB12 (D2f)	D2f	cF52	(225, Fm-3m)		2	(B)12.0(ZR)1.0
MB_B27	FeB (B27)	B27	oP8	(62, Pnma)		2	(B)1.0(CR, FE, HF, MN, MO, TI, ZR)1.0
M2B_CB	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)		2	(CR, MO)2.0(B)1.0
MN2B_D1F	Mn2B (D1f)	D1f	oF48	(70, Fddd)		2	(MN)0.6707(B)0.3293
MNB4	MnB4		mS10	(12, C2/m)		2	(MN)0.2(B)0.8
RE3B	Re3B		oS16	(63, Cmcm)		2	(MO, RE)3.0(B)1.0
M3B4_D7B	Ta3B4 (D7b)	D7b	oI14	(71, Immm)		2	(B)4.0(CR, HF, MN, MO, TI)3.0
RE7B3	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)		3	(MO, RE)7.0(B)3.0(B, VA)3.0
CR5B3_D8L	CR5B3_D8L (D8l)	D8l	tI32	(140, I4/mcm)		2	(CR, MO)0.625(B)0.375
B4C	B13C2 B4C (D1g)	D1g	hR15	(166, R-3m)		2	(B11C, B12)1.0(B2, C2B, CB2, SI2)1.0
ALB12_ALPHA	alpha-AlB12		tP216	(92, P4_12_ 12)		2	(AL)1.0(B)12.0
CRB4	CrB4		oI10	(71, Immm)		2	(CR)0.2(B)0.8
MOB4	MoB4		hP16	(194, P6_ 3/mmc)		2	(MO)0.2(B)0.8

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
REB2	ReB2		hP6	(194, P6_ 3/mmc)		3	(RE)1.0(B)2.0(B, VA)2.0
MO2B5_D8I	Mo2B5 (D8i)	D8i	hR7	(166, R-3m)		2	(MO, TI)0.32(B)0.68
TI5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)		4	(CR, FE, HF, MN, MO, SI, TI, ZR)2.0(AL, SI)3.0(CR, FE, HF, MN, MO, TI, ZR)3.0(B, C, VA)1.0
MO5SI3_D8M	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)		3	(CR, MO, RE, TI, ZR)4.0(CR, MO, RE, SI)1.0(AL, B, SI)3.0
ZR5SI4	Si4Zr5		tP36	(92, P4_12_ 12)		2	(HF, MO, TI, ZR)5.0(SI)4.0
MO3SI_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		3	(AL, CR, FE, HF, MO, RE, SI, TI, ZR)3.0(AL, CR, MO, SI)1.0(VA)3.0
M3SI1	Ti3P		tP32	(86, P4_2/n)		2	(TI, ZR)3.0(SI)1.0
MSI_B27	FeB (B27)	B27	oP8	(62, Pnma)		2	(HF, TI, ZR)1.0(SI)1.0
FESI_B20	FeSi (B20)	B20	cP8	(198, P2_13)		2	(CR, FE, MN, MO, RE)1.0(AL, SI)1.0
CRSI2_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)		2	(CR, HF, MO, SI, TI)1.0(AL, CR, SI)2.0
MOSI2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(CR, MO)1.0(AL, SI)2.0
ZRSI2_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	Also YSi2-orth of SG Imma	2	(HF, ZR)1.0(SI)2.0
TISI2_C54	TiSi2 (C54)	C54	oF24	(70, Fddd)		2	(MO, TI)1.0(AL, SI)2.0
M3SI2_D5A	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)		2	(HF, ZR)3.0(SI)2.0
RE2SI	Re2Si		mP24	(14, P2_1/c)		2	(RE)2.0(SI)1.0
RESI2_C11B	Re4Si7		mS44	(8, Cm)		2	(RE)0.357(SI)0.643

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FCC_L10	CuAu (L10)	L10	tP2	(123, P4/mmm)		2	(AL, CR, MN, MO, TI)0.5(AL, CR, MN, MO, TI)0.5
ALZR1	CrB (B33)	B33	oS8	(63, Cmcm)		2	(AL)1.0(HF, ZR)1.0
ALPHA_B19	beta'-AuCd (B19)	B19	oP4	(51, Pmma)		2	(MO, TI, ZR)1.0(MO, TI, ZR)1.0
HFMN	NiTi2		cF96	(227, Fd-3m)		2	(HF)0.5(MN)0.5
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(AL, CR, FE, HF, MN, MO, RE, SI, TI, ZR)2.0(AL, CR, FE, HF, MO, RE, SI, TI, ZR)1.0
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)		2	(AL, CR, FE, HF, MN, MO, TI, ZR)2.0(AL, CR, FE, HF, MN, MO, TI, ZR)1.0
C16_THETA	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(HF, TI, ZR)2.0(AL, FE, SI)1.0
NITI2	NiTi2		cF96	(227, Fd-3m)		2	(FE)1.0(HF)2.0
REZR2	Zr21Re25		hR92	(167, R-3c)		2	(RE)1.0(ZR)2.0
ALTI3_D019	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)		2	(AL, CR, MO, TI)3.0(AL, CR, MO, TI)1.0
AL3ZR1	Al3Zr (D023)	D023	tI16	(139, I4/mmm)		2	(AL)3.0(HF, ZR)1.0
MZR3_E1A	MgCuAl2 (E1a)		oS16	(63, Cmcm)		2	(FE)1.0(ZR)3.0
AL12MN	Al12W		cI26	(204, Im-3)		2	(AL)12.0(MN)1.0
AL4MN_R	lambda-Al4Mn		hP586	(194, P6_ 3/mmc)		2	(AL)461.0(FE, MN)107.0
AL4MN_U	mu-Al4Mn		hP574	(194, P6_ 3/mmc)		2	(AL)4.0(MN)1.0
AL11MN4_LT	Al11Mn4		aP15	(2, P-1)		2	(AL)11.0(FE, MN)4.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25		oP156	(62, Pnma)		2	(AL, MN)29.0(MN)10.0
AL8MN5	Cr5Al8 (D810)	D810	hR26	(160, R3m)		3	(AL)12.0(MN)5.0(AL, MN, SI)9.0
AL6MN	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)		2	(AL)6.0(FE, MN, RE)1.0
ALZR2	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(AL)1.0(ZR)2.0
AL2ZR3	Zr3Al2		tP20	(136, P4_ 2/mnm)		2	(AL)2.0(HF, ZR)3.0
AL3ZR4	Al3Zr4		hP7	(191, P6/mmm)		2	(AL)3.0(HF, ZR)4.0
AL3ZR2	Zr2Al3		oF40	(43, Fdd2)		2	(AL)3.0(HF, ZR)2.0
AL12W	Al12W		cI26	(204, Im-3)		2	(AL, SI)12.0(MO, RE)1.0
AL4W	Al4W		mS30	(8, Cm)		2	(AL, SI)4.0(MO)1.0
AL5W	Al5W		hP12	(182, P6_322)		2	(AL)5.0(MO)1.0
MN11SI19	Mn11Si19		tP120	(118, P-4n2)		2	(MN)11.0(AL, SI)19.0
MN3SI	BiF3 (D03)	D03	cF16	(225, Fm-3m)		2	(MN)3.0(AL, SI)1.0
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)		2	(AL, MN)17.0(SI)3.0
MN9SI2	Mn9Si2		oI186	(71, Immm)		2	(MN)33.0(SI)7.0
AL13FE4	Al13Fe4		mS102	(12, C2/m)		3	(AL)0.6275(FE, MN)0.235(AL, SI, VA)0.1375
AL2FE	Al2Fe		aP18	(1, P1)		2	(AL)2.0(FE, MN)1.0
AL5FE2	Al2.8Fe		oS24	(63, Cmcm)		2	(AL)5.0(FE, MN)2.0
AL5FE4	gamma-brass (Cu5Zn8,	D82	cI52	(217, I-43m)		1	(AL, FE)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
	D82)						
FESI2_H	FeSi2-h		tP3	(123, P4/mmm)		2	(FE)0.3(SI)0.7
FESI2_L	FeSi2-l		oS48	(64, Cmce)		2	(FE)0.333333(SI)0.666667
FE2SI	AlNi2		hP6	(164, P-3m1)		2	(FE)0.666667(SI)0.333333
HFRE	Zr21Re25		hR92	(167, R-3c)		2	(HF)1.0(RE)1.0
MNTI_LT	Zr21Re25		hR92	(167, R-3c)		2	(MN)1.0(TI)1.0
MNTI_HT	Unknown Structure		t**			2	(MN)0.515(TI)0.485
MN3TI	Unknown Structure					2	(MN)3.0(TI)1.0
MN4TI	R-(Co,Cr,Mo)		hR53	(148, R-3)		2	(MN)0.815(TI)0.185
CR3MN5	alpha-Mn (A12)	A12	cI58	(217, I-43m)		2	(CR)3.0(MN)5.0
HIGH_SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		3	(MN)8.0(CR)4.0(CR, MN)18.0
B3SI	B13C2 B4C (D1g)	D1g	hR15	(166, R-3m)		3	(B)6.0(SI)2.0(B, SI)6.0
B6SI	SiB6		oP280	(58, Pnnm)		3	(B)210.0(SI)23.0(B, SI)48.0
BNSI	alpha-B (hR12)		hR12	(166, R-3m)		3	(B)61.0(SI)1.0(B, SI)8.0
SIC	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(SI)1.0(B, C)1.0
AL4ZR5	Ti5Ga4		hP18	(193, P6_ 3/mcm)		2	(AL)4.0(ZR)5.0
AL3ZR5	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)		2	(AL)3.0(ZR)5.0
AL11TI5	Al3Zr (D023)	D023	tI16	(139,		2	(AL)17.0(TI)8.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				I4/mmm)			
AL2TI	Ga2Hf		tI24	(141, I4_ 1/amd)		2	(AL)2.0(TI)1.0
AL11RE4	Al11Mn4		aP15	(2, P-1)		2	(AL)11.0(RE)4.0
AL4RE	Al4Re		aP71	(2, P-1)		2	(AL)4.0(RE)1.0
ALRE2	CuZr2		tI6	(139, I4/mmm)		2	(AL)1.0(RE)2.0
ALRE1	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)		2	(AL)1.0(RE)1.0
AL17MO4	Al17Mo4		mS84	(5, C2)		2	(AL)17.0(MO)4.0
AL22MO5	Al22Mo5		oF216	(43, Fdd2)		2	(AL)22.0(MO)5.0
AL3MO	MoAl3		mS32	(12, C2/m)		2	(AL)3.0(MO)1.0
AL63MO37	Unknown Structure					2	(AL)63.0(MO)37.0
AL8MO3	Al8Mo3		mS22	(12, C2/m)		2	(AL, SI)8.0(MO)3.0
AL11CR2	Al5Cr		mS732	(15, C2/c)		3	(AL)10.0(AL)1.0(CR)2.0
AL13CR2	Al45V7		mS104	(12, C2/m)		2	(AL)13.0(CR)2.0
AL4CR	mu-Al4Mn		hP574	(194, P6_ 3/mmc)		2	(AL)4.0(CR)1.0
AL8CR5_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		2	(AL)8.0(CR)5.0
AL8CR5_L	Cr5Al8 (D810)	D810	hR26	(160, R3m)		2	(AL)8.0(CR)5.0
AL9CR4_H	Unknown Structure					2	(AL)9.0(CR)4.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL9CR4_L	Unknown Structure					2	(AL)9.0(CR)4.0
AL1CR2	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AL)1.0(CR)2.0
ALBMO	ZrSi2 (C49)	C49	oS12	(63, Cmcm)		3	(AL)1.0(B)1.0(MO)1.0
ALFESI_ALPHA_TAU5	Fe23Al81Si15		hP246	(194, P6_3/mmc)		4	(AL)0.6612(FE)0.19(SI)0.0496(AL, SI)0.0992
ALFESI_BETA_TAU6	Fe2Al9Si2		mS52	(15, C2/c)		3	(AL)14.0(FE)3.0(SI)3.0
ALFESI_GAMMA_TAU2	Unknown Structure		mS*			3	(AL)3.0(FE)1.0(SI)1.0
ALFESI_DELTA_TAU4	FeAl3Si2		oP24	(60, Pbcn)		3	(AL)0.55(FE)0.15(SI)0.3
ALFESI_TAU1	Unknown Structure					3	(AL)2.0(FE)2.0(SI)1.0
ALFESI_TAU3	Fe(Al0.67Si0.33)3		oS128	(67, Cmme)		3	(AL)2.0(FE)1.0(SI)1.0
AL2MN2SI3	(Al2Mn2Si3)		hP21	(174, P-6)		3	(AL)2.0(MN)2.0(SI)3.0
AL5MN6SI7	CrSi2 (C40)	C40	hP9	(180, P6_222)		3	(AL)5.0(MN)6.0(SI)7.0
AL1MN1SI1	TiSi2 (C54)	C54	oF24	(70, Fddd)		3	(AL)1.0(MN)1.0(SI)1.0
AL3MNSI2	(Al3MnSi2)		tP48	(85, P4/n)		3	(AL)3.0(MN)1.0(SI)2.0
AL3MN4SI2	Unknown Structure					3	(AL)3.0(MN)4.0(SI)2.0
ALMNSI_T6	Unknown Structure					2	(AL, MN)4.0(SI)1.0
ALMNSI_T8	Mn3Al10		hP26	(194, P6_3/mmc)		5	(MN, VA)6.0(MN, VA)2.0(AL)12.0(AL, SI)6.0(AL, SI)2.0
AL2MO3C	beta-Mn (A13)	A13	cP24	(213, P4_132)		3	(AL)2.0(AL, MO)3.0(C)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL15SI2M4	Al15(Mn,Fe)3Si2		cI168	(204, Im-3)		3	(AL)14.0(MN)4.0(AL, SI)5.0
AL2MNSI3	Ga5Pd		tI24	(140, I4/mcm)		3	(AL)2.0(MN)1.0(SI)3.0
AL16FEMN3	mu-Al4Mn		hP574	(194, P6_ 3/mmc)		2	(AL)4.0(FE, MN)1.0
AL13FE2MN2	Al13Fe4		mS102	(12, C2/m)		2	(FE, MN)4.0(AL)13.0
AL10FEMN2	Mn3Al10		hP26	(194, P6_ 3/mmc)		2	(FE, MN)3.0(AL)10.0
B2MNMO2	Mo2FeB2		tP10	(127, P4/mbm)		3	(B)2.0(MN)1.0(MO)2.0
CR7FE17TI5	alpha-Mn (A12)	A12	cI58	(217, I-43m)		2	(CR, FE)24.0(TI)5.0
FE2MOB4	Ta3B4 (D7b)	D7b	oI14	(71, Immm)		3	(FE)2.0(MO)1.0(B)4.0
FEMO3SI	FeMo3Si		tI56	(120, I-4c2)		3	(FE)1.0(MO)3.0(SI)1.0
FE2MOSI2	Unknown Structure					3	(FE)2.0(MO)1.0(SI)2.0
FE3MO5SI2	R-(Co,Cr,Mo)		hR53	(148, R-3)		3	(FE)3.0(MO)5.0(SI)2.0
HF9MO4B	Hf9Mo4B		hP28	(194, P6_ 3/mmc)		3	(HF, ZR)9.0(MO)4.0(B)1.0
M6C	Fe3W3C (E93)	E93	cF112	(227, Fd-3m)		4	(FE, MN)2.0(MO)2.0(FE, MN, MO)2.0(C)1.0
MO2BC	Mo2BC		oS16	(63, Cmcm)		3	(MO)2.0(B)1.0(C)1.0
MO5SIB2	Mo5SiB2		tI32	(140, I4/mcm)		3	(AL, CR, FE, HF, MN, MO, TI, ZR)0.625(B, SI)0.125(B)0.25
MOSIZR	TiNiSi		oP12	(62, Pnma)		3	(MO)1.0(SI)1.0(HF, MO, ZR)1.0
MO3SI5ZR2	Unknown Structure					3	(MO)3.0(SI)5.0(ZR)2.0

Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
MO5SI9ZR6	Unknown Structure					3	(MO)5.0(SI)9.0(ZR)6.0
MO4TI7SI9	Unknown Structure					2	(MO, TI)0.55(SI)0.45
TI6SI2B	K2UF6		hP9	(189, P-62m)		3	(TI)6.0(SI)2.0(B)1.0
TI3SIC2	CMo		hP12	(194, P6_ 3/mmc)	N, Ti3AlC2-x	3	(TI)3.0(SI)1.0(C, VA)2.0
GAS	Gas				Gas mixture	1	(AL, AL1C1, AL1C2, AL2, AL2C2, B, B1C1, B1C2, B2, B2C1, C, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2SI1, C2SI2, C2SI3, C3, C4, C5, C60, CR, CR2, FE, FE2, HF, MN, MO, MO2, RE, SI, SI2, SI3, TI, TI2, ZR, ZR2)1.0

TCMO1 Properties Data

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