TCS Permanent Magnetic Materials Database (TCPMAG2)

Technical Information

Available Starting with Thermo-Calc Version 2023b

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Contents

About the TCS Permanent Magnetic Materials Database (TCPMAG)

The TCS Permanent Magnetic Materials Database (TCPMAG) is a thermodynamic and properties database for rare-earth permanent magnetic materials. It can be used for a wide range of compositions from pure $Nd_2Fe_{14}B$ to very complex NdFeB-based commercial permanent magnetic materials. It can be used for calculating phase diagrams and thermodynamic properties of assessed systems, but also for predicting phase equilibria, curie temperatures and simulating solidification processes for a wide range of composition.

TCS Permanent Magnetic Materials Database (TCPMAG) is developed to be used with our entire suite of products: Thermo-Calc, the Add-on Modules, and all available SDKs.

In addition to thermodynamic data, it has thermophysical properties data available for:

- Molar volume of liquid and all solid phases
- Viscosity of liquid
- Surface tension of liquid

TCPMAG: TCS Permanent Magnetic Database Revision History. The current version of the database is TCPMAG2. See the link for any subversion release details.

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 area.

The TCS Permanent Magnetic Materials Database (TCPMAG) enables predictions (such as multicomponent phase equilibria calculations, equilibrium solidification simulations, and Scheil solidification simulations) to be made for multicomponent systems and alloys of industrial importance. This means it can be used to extrapolate to higher-order systems by combining several critically assessed systems.

Use the TCS Permanent Magnetic Materials Database (TCPMAG) to calculate the following, based on your actual alloy chemistry:

- Thermophysical properties, such as:
    - Specific heat, enthalpy, latent heat, and molar volume (for all phases), and the viscosity and surface tension (of liquid only)
- Phase-based properties, such as:
    - Critical transformation temperatures such as solvus temperatures of precipitates, amounts and compositions of phases, solubility limits, activities, phase diagrams, and more
- Equilibrium and non-equilibrium solidification, such as:
    - Liquidus, solidus, incipient melt temperatures, freezing range, fraction solid curves, solidification path, fraction eutectic, microsegregation, partition coefficients, latent heat, shrinkage, and more
- Curie temperature

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 Permanent Magnetic Materials Database (TCPMAG) 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 Permanent Magnetic Materials Database (TCPMAG) 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, and summaries of the database revision history by version.
- The *TCS Permanent Magnetic Materials Database (TCPMAG) 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 Permanent Magnetic Materials 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 Permanent Magnets including links to resources such as examples, publications, and more.

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

TCPMAG2 Elements, Systems, Phases and Properties

Included Elements

There are nine (9) elements included in the database.

B	Ce	Co	Dy	Fe	La
Nd	Pr	Tb			

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. Note that in most cases phases having the same crystal structure had been merged as the same phase.

The database contains:

- 36 assessed binary systems
- 29 assessed ternary systems (21 critically assessed; 8 tentatively assessed)
- 54 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

A variety of properties data is included with the TCS Permanent Magnetic Materials Database (TCPMAG).

- Molar volume of liquid and all solid phases
- Viscosity of liquid
- Surface tension of liquid

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.

Properties Data

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*
Surface tension	SIGM	`SURF(LIQUID)`
Dynamic viscosity	VISC	`DVIS(LIQUID)`
Kinematic viscosity		`KVIS(LIQUID)`
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

TCPMAG2 Systems

In this section:

TCPMAG2 Assessed Binary Systems

Thirty-six (36) binary systems are assessed.

	B	Ce	Co	Dy	Fe	La	Nd	Pr
Ce	x							
Co	x	x						
Dy	x	x	x					
Fe	x	x	x	x				
La	x	x	x	x	x			
Nd	x	x	x	x	x	x		
Pr	x	x	x	x	x	x	x	
Tb	x	x	x	x	x	x	x	x

TCPMAG2 Assessed Ternary Systems

Twenty-one (21) critically assessed ternary systems

Critically Assessed Ternary Systems			
B-Ce-Fe	B-Co-Fe	B-Co-La	B-Co-Pr
B-Co-Tb	B-Dy-Fe	B-Fe-La	B-Fe-Nd
B-Fe-Pr	B-Fe-Tb	Ce-Co-Fe	Ce-Fe-La
Ce-Fe-Nd	Ce-Fe-Pr	Co-Fe-La	Co-Fe-Nd
Co-Fe-Tb	Dy-Fe-Tb	Fe-La-Nd	Fe-La-Pr
Fe-Nd-Pr			

Eight (8) tentatively assessed ternary systems

Tentatively Assessed Ternary Systems			
B-Ce-Co	B-Ce-Nd	B-Co-Dy	B-Co-Nd
Ce-Co-La	Co-Fe-Pr	Co-Nd-Pr	Dy-Fe-Nd

TCPMAG2 Phases

In this section:

Common Phases for Permanent Magnetic Alloys

TCPMAG2 Models for the Included Phases

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

LIQUID	*Liquid phase, which covers the melt of permanent magnetic materials*
T1	Re2Fe14B based phase, which covers (Nd, La, Ce, Pr)0.1176471(Fe)0.8235294 (B)0.0588235 compositions
T2	ReFe4B4 based phase, which covers (Nd, La, Ce, Pr)0.121844(Fe)0.439078 (B)0.439078 compositions
Fe2Re	Fe2Re Laves phase, which covers (Ce, Nd, Pr)2Fe compositions
DHCP	Rare-earth rich phase, which covers (Ce, La, Nd, Pr)

TCPMAG2 Models for the Included Phases

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Formula_unit*
B4RE	UB4		tP20	P4/mbm	127		2	(B)0.8(CE,DY,LA,ND,PR,TB)0.2
B5RE2	Pr2B5		mS56	C2/c	15		2	(B)0.714286(CE,ND,PR)0.285714
B66RE	YB66		cF1936	Fm-3c	226		2	(B)0.985075(DY,ND,TB)0.014925
B6RE	CaB6 (D21)	D21	cP7	Pm-3m	221		2	(B)0.857143(B,CE,DY,LA,ND,PR,TB)0.142857
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229		2	(B,CE,CO,DY,FE,LA,ND,PR,TB)1(VA)3
BCC_B2	CsCl (B2)	B2	cP2	Pm-3m	221		3	(B,CE,CO,DY,FE,LA,ND,PR,TB)0.5 (B,CE,CO,DY,FE,LA,ND,PR,TB)0.5(VA)3
BETA_RHOMBO_ B	beta-B (R-105)		hR105	R-3m	166		1	(B)1
CE24CO11	Ce24Co11		hP70	P6_3mc	186		2	(CE)24(CO,FE)11
CECO4B4	CeCo4B4		tP18	P4_2/nmc	137		3	(CO)0.439078(CE,DY,ND,PR,TB)0.121844 (B)0.439078
CEMENTITE_ D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	(CO,FE)3(B)1
CO7DY12	Co7Ho12		mP38	P2_1/c	14		2	(CO)7(DY,TB)12
CO13LA_D23	NaZn13 (D23)	D23	cF112	Fm-3c	226		2	(CO,FE)13(LA)1
CO3LA2	La2Ni3		oS20	Cmce	64		2	(CO)3(LA,ND)2
CO23LA27	LaCo0.85		mS8	C2/m	12		2	(CO)23(LA)27
CO3ND2_HT	Unknown Structure						2	(CO)3(ND)2

Phase	Prototype	Strukturbericht	Pearson_ Symbol	Space_Group_ Symbol	SG#	Info	Sublattices	Formula_unit
CO3ND4	Co3Ho4		hP22	P6_3/m	176		2	(CO,FE)3(ND,PR,TB)4
CO2ND5	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	(CO)2(ND,PR)5
CORE3_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	(CO)1(DY,LA,ND,PR,TB)3
DELTA	alpha-Sm (C19)	C19	hR3	R-3m	166		2	(DY,ND)1(ND)1
DHCP	alpha-La (A3')	A3'	hP4	P6_3/mmc	194		1	(CE,DY,LA,ND,PR,TB)1
DYB2	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	(DY,TB)0.3333(B)0.6667
DYB12	UB12 (D2f)	D2f	cF52	Fm-3m	225		2	(DY,TB)0.0769(B)0.9231
CECO3B2	CeCo3B2		hP6	P6/mmm	191		3	(CE,DY,TB)1(CO)3(B)2
DY3FEB7	Er3CrB7		oS44	Cmcm	63		3	(DY,TB)3(FE)1(B)7
DYFEB4	YCrB4		oP24	Pbam	55		3	(DY,TB)1(CO,FE)1(B)4
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225		2	(B,CE,CO,DY,FE,LA,ND,PR,TB)1(VA)1
FE17DY2	Ni17Th2		hP38	P6_3/mmc	194		2	(FE)17(DY,TB)2
FE17RE2	Zn17Th2		hR57	R-3m	166		2	(CO,FE)0.894737(CE,DY,LA,ND,PR,TB)0.105263
FE17RE5	Nd5Fe17		hP264	P6_3/mmc	194		2	(FE)0.772727(CE,LA,ND,PR)0.227273
FE2B	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	(CO,FE)0.666667(B)0.333333
FE23DY6	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		2	(CO,FE)23(DY,TB)6
FE2RE	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	(CO,FE)0.666667(CE,DY,ND,PR,TB)0.333333
FE3RE	Ni3Pu		hR12	R-3m	166		2	(CE,DY,ND,PR,TB)1(CO,FE)3

Phase	Prototype	Strukturbericht	Pearson_ Symbol	Space_Group_ Symbol	SG#	Info	Sublattices	Formula_unit
FEB	FeB (B27)	B27	oP8	Pnma	62		2	(CO,FE)0.5(B)0.5
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194		2	(CE,CO,DY,FE,LA,ND,PR,TB)1(VA)0.5
LA1B9	Unknown Structure						2	(LA)0.1(B)0.9
LACO2B3	Unknown Structure						3	(LA)1(CO)2(B)3
LIQUID	Liquid						1	(B,CE,CO,DY,FE,LA,ND,PR,TB)1
ND3CO13B2	Nd3Ni13B2		hP18	P6/mmm	191		3	(ND)3(CO)13(B)2
ND2CO5B2	Ce2Co5B2		hP36	P63/mmc			3	(ND,PR,TB)2(CO)5(B)2
ND2CO5B3	*		oS*	Ccce	68		3	(ND,PR)2(CO)5(B)3
RE2CO7	Co7Gd2		hR18	R-3m	166	Ce2Ni7 (hP36, P6_3/mmc) and Co7Gd2 (hR54, R-3m)	2	(CE,DY,LA,ND,PR,TB)2(CO,FE)7
CE2CO7B3	Ce2Co7B3		hP24	P6/mmm	191		3	(CE,DY,ND,PR,TB)2(CO)7(B)3
RE5CO19	Ce5Co19		hR24	R-3m	166		2	(CE,LA,ND,PR)5(CO,FE)19
RECO5_D2D	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	(CE,DY,LA,ND,PR,TB)1(CO,FE)5
RE3CO11B4	Ce3Co11B4		hP19	P6/mmm	191		3	(CE,DY,ND,PR,TB)3(CO,FE)11(B)4
RECO2B2	ThCr2Si2		tI10	I4/mmm	139		3	(DY,LA,PR,TB)1(CO,FE)2(B)2
RECO4B	CeCo4B		hP12	P6/mmm	191		3	(CE,DY,LA,ND,PR,TB)1(CO,FE)4(B)1
RECO12B6	SrNi12B6		hR19	R-3m	166		3	(CE,DY,LA,ND,PR,TB)1(CO,FE)12(B)6
T1	Nd2Fe14B		tP68	P4_2/mnm	136		3	(CO,FE)0.823529(CE,DY,LA,ND,PR,TB)0.117647 (B)0.0588235
T2	Nd19Fe68B68		tP310	P4_2/n	86		3	(FE)0.439078(CE,DY,LA,ND,PR,TB)0.121844

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Formula_unit*
								(B)0.439078
T3	Pr5Co2B6		hR39	R-3m	166		3	(CO,FE)0.153846(CE,DY,LA,ND,PR,TB)0.384615 (B)0.461539
TB4COB13	Er4NiB13		tP36	P4/mnc	128		3	(TB)4(CO)1(B)13
GAS	Gas						1	(B,B2,CE,CO,CO2,DY,FE,FE2,LA,ND,PR,TB)1

TCPMAG2 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 Permanent Magnetic Materials 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 Permanent Magnets including links to resources such as examples, publications, and more.

TCPMAG: TCS Permanent Magnetic Database Revision History

Current Database Version

Database name (acronym):	**TCS Permanent Magnetic Materials Database (TCPMAG)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**2.0**
First release	**TCPMAG1 was released with 2022a**

Changes in the Most Recent Database Release

TCPMAG1 to TCPMAG2

Software release version: 2023b (June 2023)

New Elements and Phases

- Three new elements: Co, Dy, and Tb; now a 9 elements framework
- 35 new phases (total of 54)
- The gas description is included

New Binary and Ternary Systems

- 21 new assessed binary systems (for a total of 36); 18 new assessed ternary systems (for a total of 29):
    - Added Co: Assessed or tentatively assessed 8 binary systems(B-Co, Ce-Co, Co-Fe, Co-Dy, Co-La, Co-Nd, Co-Pr, Co-Tb) and 14 ternary systems (B-Ce-Co, B-Co-Fe, B-Co-La, Ce-Co-Fe, Ce-Co-La, B-Co-Dy, B-Co-Nd, B-Co-Pr, B-Co-Tb, Co-Fe-La, Co-Fe-Nd, Co-Fe-Pr, Co-Fe-Tb, Co-Nd-Pr).
    - Added Dy: Assessed or tentatively assessed 6 binary systems (B-Dy, Ce-Dy, Dy-Fe, Dy-Nd, Dy-La, Dy-Pr) and 2 ternary systems (B-Dy-Fe, Dy-Fe-Nd).
    - Added Tb: Assessed or tentatively assessed 7 binary systems(B-Tb, Ce-Tb, Dy-Tb, Fe-Tb, La-Tb, Nd-Tb, Pr-Tb) and 2 ternary systems (B-Fe-Tb, Dy-Fe-Tb).

Surface Tension Re-assessed

- The surface tension was re-assessed based on the Redlich-Kister-Muggianu (R-K-M) sub-regular solution model.