SGTE Substances Database (SSUB7)

Technical Information

Available Starting with Thermo-Calc Version 2023b

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About the SGTE Substances Database SSUB7

The SSUB7 SGTE Substances Database is a large thermochemical database containing 5985 pure condensed compounds or gaseous species. This database is used in applications such as alloy design and engineering, inorganic materials, gas phase chemistry, and solid-melts-aqueous-gas interactions.

The SSUB7 database by itself is particularly useful for:

- Tabulations of thermochemical data.
- Computations and tabulations of reactions and equilibrium constants.
- Computations of solid-gas equilibria in multicomponent systems (with no solid solutions), such as CVD calculations, potential diagram calculations, high-temperature corrosion calculations, and so forth.

This database is also extremely useful whenever it is necessary to append additional data for some compound phases and gaseous phase to a multicomponent heterogeneous interaction system that has been defined with uses of some other specific solid/liquid solution and/or compound databases for e.g. steels/Fe-alloys, Ni-based superalloys, Ti-/TiAl-/Al-/Mg-/Cu-/Zr-/...-based alloys, complex oxides/sulfides/nitrides/... solutions, slag, molten salts, Au-/Ag-/Cu-/Sn-based solders, noble metal alloys, semi-/super-conductors, ceramics, nuclear materials, minerals, aqueous solutions, and organic substances/solutions, among others, in various advanced applications of material systems and material processes.

Go to the General Alloys and Pure Substances page on our website where you can access PDFs of the SGTE technical information documents and learn about the compatible kinetic database.

Included Elements (101)

Ac	Ag	Al	Am	Ar	As	At	Au	B	Ba	Be
Bi	Br	C	Ca	Cd	Ce	Cf	Cl	Cm	Co	Cr
Cs	Cu	Dy	Er	Es	Eu	F	Fe	Fm	Fr	Ga
Gd	Ge	H	He	Hf	Hg	Ho	I	In	Ir	K
Kr	La	Li	Lu	Mg	Mn	Mo	N	Na	Nb	Nd
Ne	Ni	Np	O	Os	P	Pa	Pb	Pd	Pm	Po

Pr	Pt	Pu	Ra	Rb	Re	Rh	Rn	Ru	S	Sb
Sc	Se	Si	Sm	Sn	Sr	Ta	Tb	Tc	Te	Th
Ti	Tl	Tm	U	V	W	Xe	Y	Yb	Zn	Zr
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Included Phases

3388 condensed stoichiometric compound phases and one huge gaseous mixture phase are available in the SSUB7 database. The gaseous mixture phase (containing 2597 gaseous species) is the only solution phase in the database, and it is treated as ideal (in both EOS and mixing behaviors) at all temperatures, pressures, and compositions.

Assessed Systems

The SSUB7 database contains assessed thermochemical data for 5985 substances (3388 condensed compounds and 2597 gaseous species) within a chemical framework of 99 elements (and 2 hydrogen isotopes).

The assessed thermochemical data for each compound or species consist of:

- The enthalpy of formation at 298.15 K (relative to pure elements).
- The entropy at 298.15 K (from third thermodynamic law integrations or estimations).
- The temperature dependence of the heat capacity at constant pressure from 298.15 K up to the gaseous state.

SSUB: SGTE Substances Database Revision History

Current Database Version

Database name (acronym):	**SGTE Substances Database (SSUB)**
Database owner:	**Scientific Group Thermodata Europe (SGTE)**
Database version:	**7.0**
First release:	**SSUB1 was released in 1992.**

Changes in the Most Recent Database Release

SSUB6 to SSUB7

Software release version: 2023b (June 2023)

There are now 3388 condensed stoichiometric compound phases and one huge gaseous mixture phase. The database contains assessed thermochemical data for 5985 substances (3388 condensed compounds and 2597 gaseous species). This is an increase of 200 condensed compounds and 39 gaseous species for this version.

Previous Releases

SSUB5 to SSUB6

Software release version: 2017b (October 2017)

As an upgrade of SSUB5, the SSUB6 SGTE Substances Database is a large thermochemical database that an additional 90 substances included, bringing the total to 5746 pure condensed compounds or gaseous species.

- 3188 condensed stoichiometric compound phases.
- One huge gaseous mixture phase, which contains 2558 gaseous species, is the only solution phase in the database, and it is treated as ideal (in both equation of state (EOS) and mixing behaviors) at all temperatures, pressures and compositions.

New Substances in SSUB6

Name	*Temperature max (K)*
AG1BR1C1H5N1<S>	310
AG1BR1H3N1<S>	310

Name	*Temperature max (K)*
AG1BR1H9N3<S>	310
AG1C1CL1H5N1<S>	310
AG1C1N1O1<S>	310
AG1C1N1S1<S>	300
AG1C2H3O2<S>	310
AG1CL1H3N1<S>	310
AG1CL1H9N3<S>	310
AG1F1H4O2<S>	300
AG1F1H8O4<S>	300
AG1I1O3<S>	300
AG1N3<S>	310
AG2O3<S>	310
AG2S1O3<S>	310
AG2SE1O3<S>	310
AG2SE1O4<S>	310
AG2TE1<S>	900
AL1B3H12<G>	1000
AL1B3H12<L>	300
AL1C1H2NA1O5<S>	500
AL1C3H9<L>	300
AL1CL6FE1<G>	1500
AL1H12N3O15<S>	300

Name	*Temperature max (K)*
AL2C6H18<G>	1000
AL2H12O18S3<S>	300
AL2SR1<S>	9600
AL4SR1<S>	9600
AL7SR8<S>	9600
AM1CL2<L>	1500
AM1CL2<S>	1500
AM1CL3<L>	1500
AM1CL3<S>	1147
AM1O1<G>	3000
AM1O2<G>	3000
AM1O2<S>	2000
AS1O6SB3<G>	1100
AS1SE1<G>	1800
AS1SE1<S>	673
AS2O6SB2<G>	1100
AS3O6SB1<G>	1100
AS4SE3<G>	1000
AS4SE3<S>	440
AU1O4RE1<S>	673
B1C1H3O1<G>	300
B1C2H7O2<G>	300

Name	*Temperature max (K)*
B1C2H7O2<L>	310
B1C3H9<G>	300
B1C3H9<L>	310
B1C3H9O3<G>	1000
B1C3H9O3<L>	300
B1C4H14N1<S>	310
B1C6H15<G>	1000
B1C6H15<L>	300
B1CL3H3P1<S>	310
B4S6<G>	1000
BA1BR2H2O7<S>	300
BA1BR2H4O2<S>	310
BA1BR2O6<S>	310
BA1CL2H2O1<S>	310
BA1CL2H4O2<S>	300
BA1CL2H6O11<S>	310
BA1CL2O4<S>	310
BA1F6SI1<S>	310
BA1H18O10<S>	310
BA1H2I2O7<S>	310
BA1H2N6O1<S>	310
BA1H8O12RE2<S>	310

Name	*Temperature max (K)*
BA1I2O6<S>	310
BA1O3SE1<S>	310
BA1O4SE1<S>	310
BA1O4SR1TI1<S>	300
BA1SE1<S>	310
BE1H4O6S1<S>	500
BE1SE1<S>	310
BE1TE1<S>	310
BI1NA3O4<S>	700
BI2TE1<S>	310
BR2CA1H12O6<S>	310
C2CA1H2O5<S>	300
CA10F2O24P6<S>	300
CA1CL2H12O6<S>	330
CA1CL2H8O8<S>	310
CA1FE1O6SI2<S>	3000
CA1H12I2O12<S>	310
CA1H4O5S1<S>	300
CA1H4O6SE1<S>	310
CA1H6O9P2<S>	300
CA1I2O6<S>	310
CA1O6P2<C>	2000