Definition of a format for interchange of experimental data in thermochemistry and metallurgy

SGTE database project 1987

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Content

- 1 Introduction
- 1.1 Assessments
- 1.2 Scope
- 1.3 Context dependent quantities
- 1.4 Composition variables
- $1.5~\mathrm{Phase}$ names

2 Block structure

- 2.1 Skeleton block
- 3 Description of the syntax
- 3.1 Defining the system
- 3.2 The state of a system
- 3.3 Experimental data
- 3.4 Reference states
- 3.5 Chemical reactions
- 3.6 Auxilliary quantities

4 Description of the semantics4.1 Global keyword sentences4.2 The EQUILIBRIUM and REACTION keywords

5 Examples 5.1 Fe-Cr

 $5.2~{\rm Fe-C}$

Appendices

- 1. State variables
- 2. Summary of keywords
- 3. Special characters

1 Introduction

A large project for assessments of thermochemical and phase diagram properties for alloys, aqueous solutions, molten salts etc., sponsored by DGXIII of the CEC, has been undertaken by SGTE (Scientific Group Thermodata Europe). An important part of this project was to develop a standard format for interchange of the experimental information that must be collected at the various centers participating in the assessment work. The format proposed in this paper is the result of this part of the project.

The standard format should be self documenting and easily interpreted by unsophisticated computer software. It should also be understandable to a person. Data exchanged according to the format should be easy to process by a computer assisted assessment procedure.

It would be most advantageous if the use of a standard format for experimental data could be introduced already when the data are first made available by the experimentalist. To collect experimental information from literature or lab reports is a very tedious and costly effort. Today it is also difficult to publish large tables with original experimental information and there is a risk that such data are lost. If the experimentalist or the publisher could distribute the original experimental results in a standard format, the value of the experiments will be greatly increased as they will be easier to access, to understand and to use.

1.1 Assessments

Assessments of experimental thermochemical and phase diagram data in order to provide reliable and useful information for scientific and industrial use have always been a very important scientific activity. In the last decade computers have made this work both simpler and more challenging as a computer operated procedure makes it possible to combine scattered and contradictory experimental data by applying thermodynamic relations and models based on physical principles. A number of computer programs for assessments are now available and it has become important that the large effort in collecting the raw experimental data for such programs can be exchanged in a way that makes it possible to use the already collected data in future assessments when perhaps new experimental data become available, a new model has been developed or a better computer program for assessments has been developed.

1.2 Scope

The format for storing raw (experimental) data has to fulfil these conditions:

- It must be self documenting and readable for a person (other than the original assessor).
- It must be capable of being processed by a computer in order to generate a data input file to a program for assessment of thermochemical and phase diagram data.
- It must be independent of the choice of thermochemical model.

The raw data format described in this paper should be used for storage of the data in a machine readable way on a computer. A file with data according to the format is called a raw data file. The format is not intended for use in a database but only for interchange of data.

1.3 Context dependent quantities

One important difficulty that becomes obvious during the design of this raw data format is to separate the thermochemical information from the thermodynamic models used to interpret the data. In many cases experimental results are presented after interpretation in terms of a model e.g. EMF measurements are presented as activity coefficients. However, the model used by the experimentalist may not suit everyone who wants to use the experimental results. An equally difficult problem is that nature is much too complicated to be incorporated to its full extent in an experiment. There are for example no phases with fixed composition but it is obviously no reason to bother about solubilities which are too small to be of significance to the application one has in mind.

There is also a considerable problem with quantities the meaning of which may depend on the context of the experiment. A simple example of such a quantity is an equilibrium constant for the reaction

S(c)+O2(g)=SO2(g)

Actually many more species will be present in the gas e.g. SO3, S1, S2, S3 etc. but their amount may be negligable or their influence can be accounted for by defining an "apparent" equilibrium constant. The "appearent" equilibrium constant may be useful in simple cases but when one deals with a multicomponent system with many more gaseous species it is the properties of the actual gaseous species that are important for calculating the equilibrium by making a Gibbs energy minimization.

The SGTE format for raw data allows context dependent quantities to be defined by using fundamental thermodynamic functions and relations.

1.4 Composition variables

Many different ways of describing the composition of a system are used e.g. mass (weight) fraction, mole fraction, molality, molarity, volume fraction, partial pressures etc. In some cases one can convert from one to the other without problem but often one must consider how the volume depends on temperature or pressure to make a correct conversion. It must be strongly recommended to use composition variables that are independent of the intensive variables like temperature and pressure.

It is also important to have a method of specifying the constitution of a phase in addition to the composition. By constitution one means the amount of all individual species that make up a phase, e.g. in an ideal gas the partial pressures of all species. In a crystalline phase it can be important to know the fraction of the species on various different crystalline sites e.g. in a sigma phase. At present different quantities are used to give the constitution depending on the type of phase. In a standard one would like to avoid redundant quantities and it is thus proposed that a new variable, the constituent fraction, denoted by Y, shall be used to specify the constitution of any phase. The constituent fraction for a gas species in an ideal gas is thus equal to the partial pressure of the species divided with the total pressure. For a crystalline phase with sublattices the constituent fraction of a species is equal to the fraction of sites of a certain sublattice type occupied by the species.

1.5 Phase names

For species and compounds there exists an established standard how these can be identified e.g. Chemical Abstract numbers. The same is not true for solution phases and each researcher uses the simplest method he can think of. This is very unsatisfactory as it is important to have the same name for the same phase when experimental results from various sources are combined.

As solution phases can exist over a wide range of compositions one must use a name which is independent of any terminal composition. For pure Fe the fcc phase is usually denoted with the Greek letter gamma whereas for pure Ni the fcc phase is often denoted with the Greek letter alpha. Calling it fcc is not sufficiently unique as the NaCl structure is also an fcc phase but with a special atomic arrangement.

Another example is the clino-pyroxene phase which exists in the composition range CaMgSi2O6 to Mg2Si2O6. Pure CaMgSi2O6 is also called diopside and pure Mg2Si2O6 is called clino-enstatite. There are thus three accepted names for the same phase depending on its composition. Although one should not discourage the use of the traditional names for a phase one should look for a neutral "generic" name just denoting the structure independent of the composition.

A neutral concept that could be used for phase names is the Strukturbericht. In some cases those are not sufficient and one may have to use the space group also. As a part of the standard for interchange of thermochemical data it is thus important to establish unique names for all crystalline phases.

The gas phase is generally accepted to be a solution phase with small or no interactions between its constituents (gas species). The liquid phase on the other hand may behave like a solution phase but sometimes the components are strongly demixing. For some applications it is also interesting to know the critical point where one can have a continuous change from a gas to a liquid phase. The property of demixing, also known from the crystalline state and resulting in miscibility gaps, is important in many cases. One may thus wish to describe two phases with the same structure (liquid or crystalline) that can coexist with different compositions. These phases should not be assigned different names. Below a method is described by which the two phases could be distinguished according to the standard format.

2 Block structure

The structure of the raw data file must be as simple as possible but in order to make it possible to process the file by a computer program it must have a defined structure. Such a structure is also of help for the assessor while he is collecting his raw data because he will be reminded of what relevant information that must be stored. The raw data file will be a normal text file which can be created, edited and printed by a normal text editor. The raw data will be stored as one or more independent blocks on this file.

Each block of raw data must be complete and contain all definitions that are needed to interpret the data. Usually an assessment of a binary or ternary system will be one block but in some cases it may be advantageous to divide raw data even for a single system into several blocks, e.g. one containing thermochemical data and another with phase diagram data. The important feature of the block structure is that one must not reference information in another block and blocks must not be nested inside each other. In this way it will always be possible to extract a self-consistent block from the file when the information is needed at a later time.

2.1 Skeleton block

The raw data block will consist of the following parts

- Global data that are valid in the whole or most parts of the block. This could be the names of the components, the value of the pressure or temperature (if they have been the same in most experiments), definitions of auxilliary functions, units used for the values and reference states.
- Local data that are valid for a single measurement or a set of similar measurements. This could be the stable phases, the composition, the temperature and other measured quantities. The local data can override any global data but only within the local set of measurements.
- References for the data. This could be an article or any other source of data if not published. Note that a block may contain data from more than one report.

3 Description of the syntax

In order to make information in a block of raw data readable both to a person and a computer it is necessary to define a kind of language which should be as similar to ordinary English as possible but still strict enough to be readable to a computer program. It would take too much effort to design a computer program which could interpret raw data stored as free text. The program which reads the raw data file may generate as output an input file to an assessment program or store the data in a database or produce a printed report.

It is important that the raw data stored on the file is as close as possible to the data actually measured, and if the measured value is the mass fraction (weight fraction) one should thus store that value and not the mole fraction. The same is true if an activity has been measured. It should not be converted to a chemical potential. The main reason for this is that if the data is going to be processed by statistical methods by an assessment program one will usually assume that the error or uncertainity in each measurement is random i.e. has a gaussian distribution. If that is true for the measured activity it will not be true after conversion to a potential. The currently available assessment programs may not be capable of using all different kinds of experimental data. The conversion may then be made by the assessor using his own judgement. In the future a more general program may be developed that can utilize more general types of thermochemical data.

The syntax of the storage of the raw data in each block is that each piece of data must be preceded by a keyword. Examples of such keywords can be COMPONENTS, PHASES, CONDITIONS etc. The information after the keyword will vary depending on the keyword but there must be rather strict rules in order not to make it too complicated for a computer program to interpret the information. The whole piece of information including the keyword will be called a "keyword sentence" or simply "sentence" in the following text.

Any amount of comments can also be incorporated into the block in order to make it more readable to a person. The comments are ignored by the program which will extract the data. The comment character is the dollar sign *andanythingaftera* and up to the end of the same line must be a comment.

Normally the keyword sentence is terminated by the end of the line but if it is necessary to continue the sentence to the next line the last non-blank character on the line must be the ampersand &.

In some cases the keyword sentence is very short and it may be advantageous to have more than one sentence on the same line. In such cases the keyword sentences can be separated by a semicolon ;.

Space and tab characters are used as separators between the keywords and the data that follow. They are also used as separators between data items. It is allowed to use a comma "," immediately after an item to make the separation more clear.

3.1 Defining the system

The thermochemical system for which the block contains data must be completely defined within each block. The following keywords are sufficient to define a system:

COMPONENTS PHASES

After COMPONENTS the components of the system must be given. Note that the number of components in a system is usually well defined by the Gibbs phase rule but it may be possible to select the set of components in many ways. It may in some cases be more convenient to use e.g. H2O and O2 as components rather than H and O.

The names of the phases in the system must be specified after the PHASES keyword. The phase names GAS and LIQUID should be used for their normal purpose. There is no international standard way of specifying the phase names for solid or glassy phases but the assessor is recommended to use a Strukturbericht if possible and otherwise give as a comment a fuller description of such phases.

In some cases it is essential to give the constituents of a phase in order to make it possible to interpret the experimental information. This may be true for example in the case of a pure carbon gas where the abundance of the species C1, C2, C3 etc. has been measured. Thus there is a keyword CONSTITUENTS and an example of its use is

CONSTITUENTS GAS C1,C2,C3,C4,C5,C6,C7

Note that the above keywords can be used in their singular form also, e.g. PHASE.

3.2 The state of a system

The state of a system is defined if the degrees of freedom according to Gibbs phase rule is zero. The state of a system is normally defined by specifying values of state variables. In many cases the state is also partly defined by prescribing the set of stable phases.

The phase status is by default FIXED which means that the phase should be stable at the given equilibrium. It is possible to give the amount of a fixed phase after a colon. This is especially useful if one wants to specify that a phase is just stable. One can then set it as fixed with zero amount. In some cases the set of stable phased is not known and then the status ENTERED can be used for those phases that might or might not be stable. An example of a case when this is useful is if the solidus temperature has been measured but the solid phase that becomes stable is not reported. Then all possible solid phases that could be stable can be ENTERED. If the data are used for an assessment procedure this procedure will select the most stable one. It is also possible to exclude a phase from taking part in an equilibrium by giving its status as SUSPENDED or DORMANT. The former means that no data are given for the phase, the latter that some data have been measured or estimated e.g. the driving force for precipitation.

Conditions of other types are set by the keyword CONDITION. Here a large flexibility is required as the various types of conditions are large. Normally a condition is a value of a state variable but other conditions can be used also e.g. the condition that the mole fraction of a component should be equal in two different phases (to describe a congruent transformation). Examples of conditions are:

CONDITION T=1273, P=101325, X(CR)=.12, AC(C)=.023

The identifiers that can be used for the state variables are listed in Appendix 1. The conditions can be much more complicated than in the simple sentence above. Note also that most conditions are measured quantities but the error in the measurement may be so small that it can be considered as a strict condition in comparison to the uncertainty in the quantities regarded as the ones measured in the experiment.

3.3 Experimental data

So far we have only described how the equilibrium state of the system is defined. The important thing is now that at the defined equilibrium a number of experimental values have been measured for other quantities.

All quantities needed for defining the state must of course be measured and it is a choice which ones to put as conditions and which ones as experimental quantities. The general idea is that quantities that are most accurately known should be given as conditions. In many cases one may not give any condition and instead give only experimental data. However, it is important that the data given as conditions and experiments can uniquely describe the equilibrium. An example of an experiment sentence is

\$ Measured activity and mass fraction of carbon and the temperature.

```
$ The estimated error is given after the colon. The error for
$ the mass fraction is given in percent of measured value.
EXPERIMENT ACT(C)=0.28:0.02, W(C)=0.0155:2%, T=1273:5
```

In some cases the experimental conditions are such that a quantity has been kept constant but at an unknown or very inaccurately measured value. For instance the carbon activity in a sealed capsule with several specimens of various alloy content is fixed but might not be known. In such cases an identifier (see section 3.5) should be used instead of a value. In an assessment procedure one should then try to find the optimal value of the activity.

In an assessment procedure the measured values will be compared with the same values calculated from the models selected to describe the system. The difference between the experimental values and the calculated ones are then used to guide the assessment program in estimating the best set of model parameters.

3.4 Reference state

The thermochemical data are usually measured relative to a reference state. The activity and the enthalpy in particular are often measured with respect to a reference state which may vary depending on the context. In the raw data file the reference state is by default the SER (Selected Element Reference) state, i.e. a (mechanical) mixture of the elements in their stable states at 298.15 K and 1 bar. This is usually convenient for measurements of the integral enthalpy but is not suitable for activities or excess quantities. It is thus possible to define the reference state for a component by the following keyword sentence

```
$ Set the reference state of Cr to BCC at 1273 K and
$ the reference state of Fe to FCC at 1273 K
$ (Note that the units for temperature is interpreted according to the
$ currently active UNITS keyword. SI units are the default)
REFERENCE_STATE Cr<BCC,T=1273>, Fe<FCC,T=1273>
```

The part inside the <> brackets should give a phase name and optionally a temperature. If the temperature is omitted the reference state is the pure phase at the equilibrium temperature. There is no provision for using a reference state at another pressure than 1 bar.

A reference-state sentence will change the reference state in the whole block. In some cases it may be convenient to define the reference state in a specific condition or experiment sentence. This can be done by including the component with a $\langle \rangle$ bracket in the state variable. Some examples

```
$ Use the condition that the activity of carbon is unity with respect to
$ graphite. This is equivalent to state that graphite is stable
$ at the current termperature.
CONDITION AC(C<GRAPHITE>)=1
```

\$ A measurement of the enthalpy of mixing in the bcc phase refered

```
$ to pure Fe as FCC and Cr as bcc at the current temperature.
EXPERIMENT HM(BCC,FE<FCC>,CR<BCC>)=34000:3000
$ The same as above but using the default reference states (or those
$ set by a REFERENCE_STATE keyword)
EXPERIMENT HM(BCC)=127000:3000
$ A value for the entropy using pure Fe as BCC at zero kelvin as
$ reference state.
```

```
EXPERIMENT SM(FE<BCC,T=0>)=45.56:2
```

Sometimes a measurement may concern the difference for a quantity at two equilibrium states, neither of which is a reference state, e.g. the difference in enthalpy for an alloy at two different temperatures. This can be described in the raw data file by specifying both states independently and to refer the experimental value to both states. For example:

```
$ The first equilibrium (the initial state):
CONDITION T=1000,....;
ASSIGN H1000=HM;
```

```
$ The second equilibrium (the final state):
CONDITION T=1200,....;
EXPERIMENT HM-H1000=5600:200;
```

3.5 Chemical reactions

A large number of thermochemical measurements are related to chemical reactions, for instance heat of reactions or equilibrium constants. Such information can always be described using the method outlined in the previous sections. However, in order to provide a shorthand notation for data that are most easily described by referring to a reaction it is possible to give the reaction after the keyword REACTION. In the reaction both phases and constituents are defined. It should be remembered that chemical reactions are most useful when the context gives most of the conditions. Thus reactions in an aqueous solution and between solid compounds can be written in the same way but require quite different interpretation.

An example of a reaction is

```
$ Formation of ammonia from N2 and H2 gas
REACTION 1 N2<G>+3H2<G>=2NH3<G>
$ The measured values for this reaction is the temperature, pressure
$ and enthalpy difference between product and reactants.
EXPERIMENT T=1000:10, P=2E6:5%, H=-25000:1000
```

3.6 Auxilliary quantities

In order to make the raw data format easy to use it is possible to define different auxiliary quantities. One such quantity is the constant. Rather than giving the same numeric value

several times one can define an identifier and assign the value to that identifier. An example is

CONSTANT P0=101325

Another useful quantity is the table. In a table a large number of numeric values can be stored and then later referred to in condition and experiment sentences. A table is started by a table sentence. After this any number of lines with numeric values can be given. These lines must be terminated by an END_TABLE keyword. An example of a table is

TABLE	TAB1						
\$ T	X1	err	X2	err	ACT	err	Reference
1000	.02	.01	.025	.01	.04	.02	73TUR
1020	.04	н	.06	н	.1	.02	н
1040	.10	н	.15	н	.2	.05	н
1060	.20	.03	.32	.05	.5	.10	н
END_TA	BLE						

The name of the table must follow directly after the keyword TABLE. In this case the name is TAB1. The following line is a comment line and gives a heading to the columns for the convenience of the reader. Then a number of lines with values follow. Note that the number of values on each line should be the same. A double quote " can be used to denote the same value as on the line above. Some columns may contain non-numeric information, e.g. the name of the reference. Note that a table does not describe an equilibrium state but the numbers in the table can be used in condition and experimental sentences in the following way:

```
$ This experiment sentence refers to the table above.
$ Instead of values one give references to the table. Such references
$ consist of the table name followed by an index giving the column
$ where the value should be found.
EXPERIMENT X(FCC,CR)=TAB1(2):TAB1(3), T=TAB1(1):10, &
X(BCC,CR)=TAB1(4):TAB1(5),ACT(CR<BCC>)=TAB1(6):TAB1(7)^fo17
```

Except for the temperature the estimated inaccuracy is also taken from the table where it is called "err" and given after the colon. Each line in the table represent a studied equilibrium.

It is also possible to define functions in terms of state variables. Such functions are useful to introduce quantities that are practical but depend on the context as e.g. excess energies or activity coefficients. Examples of function definitions are

```
$ Here GAMMA is defined as an activity coefficient
FUNCTION GAMMA=ACT(CR)/X(BCC,CR)
$ PART is defined as a partition coefficient
FUNCTION PART(CMP)=X(FCC,CMP)/X(LIQ,CMP)
$ PH is defined as the negative logarithm of the constituent fraction
$ of H+ in water. Note that a postive charge is denoted /+. A negative
```

```
$ charge is denoted /-. A valence value may follow but can be omitted
$ if unity.
FUNCTION PH=-LOG10(Y(AQ,H/+))
$ Defining the compressibility
$ Note that all the thermodynamic functions (listed in Appendex 1) can
$ be used when defining functions. A period "." is used to denote a
$ partial derivative.
FUNCTION KAPPA=V.P/V
```

Note that a partial derivative like V.P can only be calculated if V has been set constant i.e. a condition. The other variables kept constant during the partial derivation are the other variables selected as conditions.

\$ The following experiment sentence uses the functions PART and \$ GAMMA defined above. The measurements are the partition coefficients \$ for Mn and Cr between liquid and fcc and the activity coefficient of Cr. EXPERIMENT PART(MN)=3.15:0.2, PART(CR)=0.5:0.04, GAMMA=2.1:0.1

In some cases experimental information involves two equilibrium states, an initial and a final state. In such cases there may be a need to transfer a value from one equilibrium to another. In section 3.4 it was described how to achieve this.

4 Description of the semantics

A summary of valid keywords is found in Appendix 2. Lines that are empty can be inserted anywhere and also comment lines which start with the comment character \$. All other lines should start with a keyword except those lines that follow a line ending with the continuation character &. The continuation lines are textually appended to the previous line. Any other line should generate a warning when processed by the computer program. The keyword dependent data for some keywords will not be described here.

Each data block must start with the keyword sentence

BLOCK <label> <assessor> <date>

The label is any text e.g. "Fe-S system", "Ca-CaCl2 system", "Al-Ti activities" etc. It should be descriptive of the type of data in the block as it may be used for searching the raw data file for information. The assessor is simply the name of the person who has collected the data in the block and the date is the date the block was created.

A block is terminated by the keyword END_BLOCK. All other keywords must only appear between a BLOCK and an END_BLOCK sentence.

4.1 Global keyword sentences

As has been stated several times the keyword sentences inside a block are only valid inside the block. Some of these sentences are global to the block while others only apply to a specific equilibrium state. A block may contain any number of specifications of equilibrium states with associated experimental data. Examples of sentences which can apply to the whole block are

COMPONENTS <chemical formula>, ... PHASES <phase name>, ...

Examples of chemical formulae are e.g. Fe, H2O, MnO. Examples of phase names are Gas, Liquid, Wustite_B1, FCC_A1, Sigma_D8B

The source of data can either be given as a comment or after a SOURCE keyword. An example:

SOURCE 73TUR Turkdogan et al., Met. Trans. 11A, 1973, p 11-14

Directly after the keyword there is an identifier which should be used in tables or individual equilibrium descriptions.

Most of the auxiliary keyword sentences are global, for example CONSTANT, TABLE, FUNCTION. It is also possible to use most other keywords as global e.g. CONDITION. However, in the description of an equilibrium state the global sentences can be overridden by sentences local to the equilibrium. See the next section.

The units that are used for the numbers can be defined by a keyword UNITS. Example UNITS ENERGY=CALORIE, TEMPERATURE=CELSIUS, PRESSURE=BAR

It is not possible to mix different units for the same quantity in one block. It is possible to define the units of a function together with the function. For example

FUNCTION KAPPA=G.P.P/V UNITS INCH**2/LB

Use of units like LB and INCH may not be recognized by the computer software and it should then give a warning. The assessor may then change the units descriptor to give the correct interpretation of the units, usually the factor for conversion to SI units.

4.2 The EQUILIBRIUM and REACTION sentences

Inside the block several equilibrium states with experimental data will usually be described. Each such state must start by an equilibrium sentence. There is no keyword for terminating the description of an equilibrium or reaction. It is terminated either by a new equilibrium sentence, a reaction sentence, a TABLE sentence or an END_BLOCK sentence.

EQUILIBRIUM <number> <comment>

```
REACTION <number> <chemical reaction>
```

The number must be unique inside the block and is used to identify the equilibrium or reaction. The comment can be any text describing the kind of equilibrium, e.g. "activity measurements in the liquid". The chemical reaction must be a valid chemical reaction. After an equilibrium or reaction sentence all keyword sentences are local for that equilibrium or reaction. It is possible to override global keyword sentences inside an equilibrium/reaction, e.g. to define a new phase status or new conditions. Most keywords can be used both for the whole block and inside an equilibrium/reaction description. Some keywords are by their nature global for the whole block and must be used before the first EQUILIBRIUM keyword. Those are e.g. FUNCTION, TABLE and CONSTANT which are used to define auxillary quantities. Most keywords can appear both outside and inside an EQUILIBRIUM. If e.g. a CONDITION T=1273 is first used globally, then inside an equilibrium one may define CONDITION T=1473 which will apply for that specific equilibrium only. For the following equilibria the global condition for the temperature will apply again unless there is again a local sentence to override it.

5 Examples

Definitions of standards are usually difficult to understand and misinterpretations are very common. Now a few examples of applications will be given, hopefully to make it a little more understandable.

5.1 Experimental data block for Fe-Cr

```
BLOCK Cr_Fe Assar_Assarsson 84-07-12
CONSTANT PO=101325, TERR=10
SOURCE X_Periment Internal report TRM-AX 00043B (1923)
SOURCE A_Currate My own results (1983)
SOURCE A_Proximate personal communication (1985)
TABLE TAB1 $activities
$ X(Cr)
          ACT(Cr)
                   ERROR
                            Т
                                       Reference
                    .01
  .12
        .17
                            1273
                                       X_Periment
. . .
END_TABLE
TABLE TAB2 $Solubility lines
$ T
      X(bcc,Cr)
                     ERR
                            X(Fcc,Cr)
                                           ERR
                                                  Reference
1273
     0.12
                     5%
                            0.13
                                            5%
                                                   A_Currate
. . .
END_TABLE
TABLE TAB3 $Heats
                H(mix)-HFe<Fcc>-HCR<bcc> Err
$ W(Cr)
                                                    Reference
.01
                 2275
                                           500
                                                    A_Proximate
```

. . . END_TABLE COMPONENTS Fe, Cr \$ The condition P=PO applies to all equilibria in this block CONDITION P=P0 \$ The BCC phase is stable in all equilibria unless explicitly suspended PHASE BCC=FIX EQUILIBRIUM 1 ACTIVITIES_BCC \$ This describes experimental activities of Cr in a binary bcc phase. \$ Note that BCC is by default the stable phase here CONDITION T=TAB1(4), X(CR<BCC>)=TAB1(1) EXPERIMENT ACT(CR)=TAB1(2):TAB1(3) EQUILIBRIUM 2 FCC_BCC \$ This describes measured compositions for the fcc/bcc equilibrium \$ in binary Fe-Cr PHASE FCC_A1=FIX CONDITION T=TAB2(1) EXPERIMENT X(FCC,CR)=TAB2(2):TAB2(3),X(BCC,CR)=TAB2(4):TAB2(5) EQUILIBRIUM 3 MINIMUM \$ This describes the minimum in the liquidus curve in Fe-Cr PHASE LIQUID=FIX CONDITION X(LIQUID,CR)-X(BCC,CR)=0 EXPERIMENT T=1723: TERR, X(FCC, CR)=.22:0.02REACTION 4 CR<BCC>=CR<LIQUID> \$ This gives the heat of melting for pure Cr \$ Note that the component Fe will be suspendend in this reaction EXPERIMENT T=2190:TERR, H=24000:2000 EQUILIBRIUM 5 Three_phase_equilibrium_BCC_SIGMA_BCC \$ There is a three phase equilibrium with two BCC phases and a \$ sigma phase in Fe-Cr. This describes the three phase equilibrium PHASE BCC#1=FIX, BCC#2=FIX, SIGMA=FIX \$ Note that a phase with a miscibility gap must be given twice \$ and the symbol #<digit> is used to distinguish the two. EXPERIMENT T=700:25,X(BCC#1,CR)=.05:.01 EQUILIBRIUM 6 EXCESS_HEATS

PHASE FCC=FIX, BCC=SUSPENDED CONDITION T=1273, X(CR)=TAB3(1) EXPERIMENT HM(FCC,FE<FCC>,CR<BCC>)=TAB3(2):TAB3(3)

END_BLOCK

Appendix 1	1 State	variables
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Intensive	e properties
Symbol	Property
Т	Temperature
Р	Pressure
AC(i)	Activity of component i
MU(i)	Chemical potential of component i
Extensiv	e properties
Symbol	Property
S	Entropy of the whole system
V	Volume of the whole system
G	Gibbs energy of the whole system
Н	Enthalpy for the whole system
А	Helmholtz energy for the whole system

The values of the extensice properties depend on the size of the system. The same state variables can also be used followed by a phase name, e.g. H(phase) and is then the enthalpy for that phase. It is possible to normalize the properties by adding a second letter. The normalization is for the whole system or for the phase respectively.

Suffix	Meaning	
М	extensive property Z per mole of atoms (in the system or phase)	
W	extensive property Z per mass (gram) of the system or phase	
V	extensive property Z per volume (m3) of the system or phase	
For example		
GM	Gibbs energy per mole of atoms for the whole system	
HW(phase)	HW(phase) Enthalpy per mass for phase	
The total amo	unt	
Symbol Pro	perty	
N Nur	mber of moles of components in the system	
B Mas	ss in the system	

These can also be normalized as above. NV is thus the number of moles per volume in the system and BV is the density of the system.

Amount of components

Symbol	Property
N(component)	Number of moles of component in the system
N(phase,component)	Number of moles of component in a phase
B(component)	Mass of component in the system
B(phase, component)	Mass of component in a phase

Note that these properties can be normalized as above. Thus NM means the mole fraction and MW the mass fraction. However, these are so commonly used that there are special mnemonics X and W for these two properties.

In some cases the fraction of a constituent is needed. If the constituent can go inte several sublattices the constituent can have a suffix character # followed by a number indicates the sublattice. Y(phase,constituent)

Amount of phases

Symbol	Property
NP(phase)	Number of moles formula units of a phase
BP(phase)	Mass of a phase
VP(phase)	Volume of a phase

The normalizing of these are for the whole system. Thus BPV(phase) is the density of a phase. A number of nonsensical combinations can be made, e.g. BW is the mass per mass and thus always equal to unity.

Appendix 2 Summary of keywords

BLOCK END_BLOCK UNITS SOURCE REFERENCE_STATE

COMPONENTS PHASES CONSTITUENTS

TABLE END_TABLE

FUNCTION CONSTANT VARIABLE

EQUILIBRIUM REACTION CONDITION EXPERIMENT ASSIGN

Appendix 3 Special characters

```
! Not used
" used to surround text which should be treated as one entity.
# used to identify phases with a miscibility gap. Also for sublattice
identification of constituents.
$ used to indicate that the following text up to end of line is a comment.
% after a number to indicate that it is a percentage (of a given value).
' can be used in the same way as ".
& indicates that the end of line should be ignored (not in comments).
: separates a value from its estimated uncertainity.
; separates keyword sentences on the same line.
* Multiplication sign
_ Can be used as a letter in phase names
= Equal sign
- Minus sign
+ Plus sign
( for indexing of tables and functions e.g. LOG and also in state variables.
) See (
< in pair with > to give phases of reacting compounds.
Also used for in-line specification of reference states.
> See <
, Separator
. Decimal point. Also used to denote partial derivative.
? Not used
^ Not used
@ Not used
```

Comparison with the COSTAT format

Most of the examples in the COSTAT report have been rewritten according to the SGTE format below. Notably the SGTE format lacks possibility to specify Chemical Abstract Registry number but otherwise there is no problem to convert. The SGTE format is certainly less compact but maybe more readable.

Example 1

```
BLOCK "triple point for pure benzoic_acid" COSTAT 86-8-28
EQUILIBRIUM 1 triple_point
$ Note the chemical formula for bensoic_acid should be given also.
COMPONENT BENZOIC_ACID
$ By default the phases below are FIXED i.e. stable.
PHASES LIQUID, GAS, SOLID_UNKNOWN_STRUCTURE
$ Units are default, T/K, P/Pa, HM/(J/MOL)
EXPERIMENT T=391.1:0.05, P=.562:0.01, HM(LIQUID)-HM(SOLID)=25610:150
END_BLOCK
   Example 2
BLOCK "binary liquid/gas equilibrium" COSTAT 86-8-28
UNITS temperature=celsius, pressure=atm, HM=kJ/mol
CONSTANT UNK=0.01
EQUILIBRIUM 1 binary_two-phase_equil
COMPONENTS TOLUENE, PROPANOL
PHASES GAS, LIQUID
$ N=1 which means that the size of the system is 1 mole of components. It is
$ here taken into account by use of the suffix M meaning
$ that the quantity is normalized to hold for one mole of atoms
$ independent of the actual size of the system.
CONDITIONS T=75.23,X(LIQUID,PROP)=0.45,N=1
EXPERIMENT P=0.821:UNK,X(GAS,PROP)=0.52:UNK,HM(GAS)-HM(LIQUID)=35.11:UNK,&
 SM(GAS)-SM(LIQUID)=100.78:UNK
END_BLOCK
   Example 3
BLOCK "Enthalpy of vaporization of a ternary system" COSTAT 86-8-28
UNITS temp=fahr, energy=BTU_IT/LB
COMPONENTS WATER, METHANOL, PROPANONE
CONDITIONS W(WATER)=.75, W(METHANOL)=.11, T=221.3, N=1
EQUILIBRIUM 1 "initial"
$ The amount of the fixed stable phases are given after the colon.
$ At the initial state the gas is just stable (zero moles)
PHASE LIQUID=FIXED:1,GAS=FIXED:0
ASSIGN H1=HM
```

```
EQUILIBRIUM 2 "final"
$ At the final state the liquid is just stable (zero moles)
PHASE LIQUID=FIXED:0,GAS=FIXED:1
EXPERIMENT HM-H1=75.6
END_BLOCK
  Example 4
BLOCK "excess volume and Gibbs energy of mixing" COSTAT 86-8-28
$ Note that the standard does not specify how to write stoichiometries. One
$ can either use all capital letters (preferred here) or always
$ have the second letter (if any) of an element symbol in lower case.
COMPONENTS HEXANE, C1CL4
PHASE LIQUID
CONDITION T=300, P=101325, N=1
TABLE T1
$ MOLE FRACTION OF C1CL4
                                EXCESS VOLUME ENTHALPY OF MIXING
                                -8.5
                                               76.3
        .5
                                -9.2
                                               85.20
        .55
        .58
                                -9.9
                                               92.34
END_TABLE
REFERENCE_STATES C1CL4<LIQUID>, HEXANE<LIQUID>
$ uncertainity not known
CONSTANT UNK=0
$ The reference states are the pure components as liquid. Note that
$ the entropy of mixing is included in GE. It is more common to
$ measure enthalpies of mixing i.e. HM.
FUNCTION GE=GM
$ In order to know the molar volumes of each pure component one must
$ define two additional equilibria
EQUILIBRIUM 1 Pure_C1C14
COMPONENT HEXANE=SUSPENDED
ASSIGN VOC1CL4=VM
EQUILIBRIUM 2 Pure_HEXANE
COMPONENT C1CL4=SUSPENDED
ASSIGN VOHEX=VM
EQUILIBRIUM 3 Excesses
CONDITION X(C1CL4)=T1(1)
EXPERIMENT VM-X(C1CL4)*VOC1CL4-X(HEXANE)*VOHEX=T1(2):UNK,GE=T1(3):UNK
END_BLOCK
```