Thermodynamic Reference Database

JSON formatted generic database structure

THEREDA Technical Paper

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Change Log

Rev. 1.0
(x) First version released, produced from internal version 0.3

Pending changes

(x) Information about the various units associated to the values is missing
(x) Information about p-functions is missing
(x) Remove the export of the audit status
(x) Documentation meta block at the end of exported JSON files

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1 Introduction

JSON (*J*ava*S*cript *O*bject *N*otation) is a lightweight text-based open standard designed for human-readable data interchange. Although JSON is based on a subset of the JavaScript scripting language and is commonly used with that language, it is a language-independent data format. Code for parsing and generating JSON data is readily available for a large variety of scripting languages. The projects webpage http://json.org (accessed 2011-06-27) provides a comprehensive listing of existing and well-tested JSON libraries.

JSON is a generic plain text (ASCII) format with a low overhead. This combined with the above listed properties renders it a suitable tool to both provide long-term archiving of the database and to produce a well-structured yet human readable copy of the database (or parts of it). The latter is important to provide a generic, intermediate format for database content to be further processed, e.g., in various parsers/converters to produce input files specifically formatted for a variety of geochemical speciation codes.

By documenting the JSON structure applied to the THEREDA database external third-parties shall be enabled to write their own parsers/converters to address their specific needs, e.g. other in-house codes.

The database entries in this technical paper are more or less fictitious examples to explain the structure of the database. The values in this paper should not be used for chemical calculations. This technical paper is not a complete description of the structure and functions of the databases. It is primarily intended to describe the exported JSON format.

2 Data structure and format definition

2.1 General data structure and format definition

JSON covers the following data types:

- Object
- Array
- Value
- String
- Number
- Boolean value
- Empty value

These data types can be combined and nested to build complex structures.

An ***object*** is an unordered comma-separated collection of name/value pairs enclosed in curly brackets `{` and `}`. Name and value are separated by a colon (`name:value`). The name of all properties in an object must be a unique string. Values can be of any type, i.e. again an object, but also an array, string, number, Boolean, or `NULL`. The type of values can vary within one object.

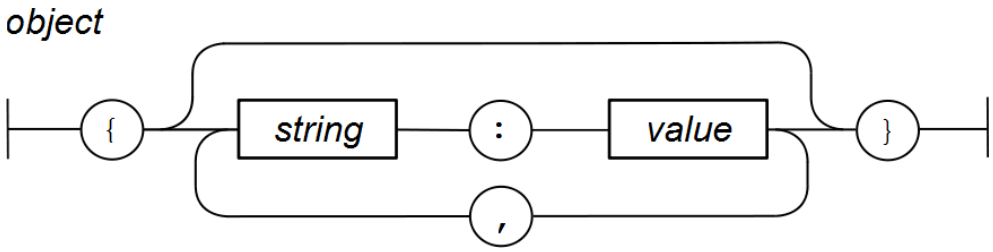

Figure 2-1 Schematic illustration of an object in JSON format (Image from http://json.org (2011-06-27))

An ***array*** is enclosed in square brackets `[` and `]`. It contains a comma-separated, ordered list of values of the same or different type. Empty arrays are allowed.

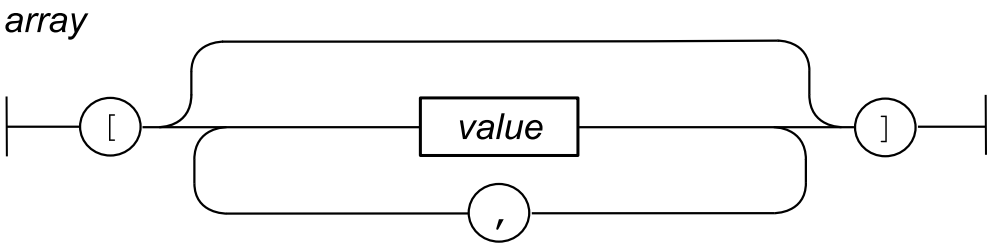

Figure 2-2 Schematic illustration of an array in JSON format (Image from http://json.org (2011-06-27))

A ***value*** can be a string in double quotes ("), or an object, an array, a number, the Boolean values `true` or `false` or the empty value `NULL`. Therefore structures can be nested.

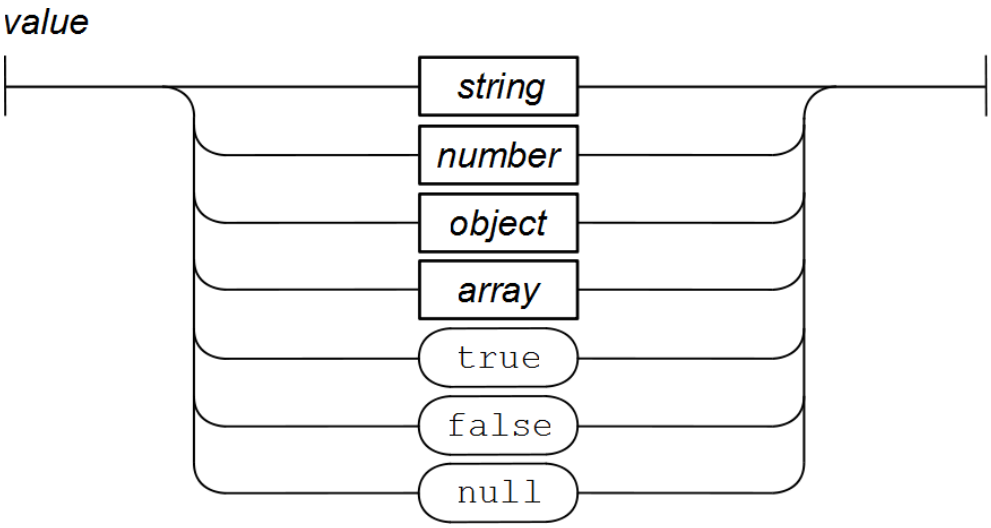

Figure 2-3 Schematic illustration of a value in JSON format (Image from http://json.org (2011-06-27))

A ***string*** can contain Unicode characters and/or control characters which are wrapped in double quotes (").

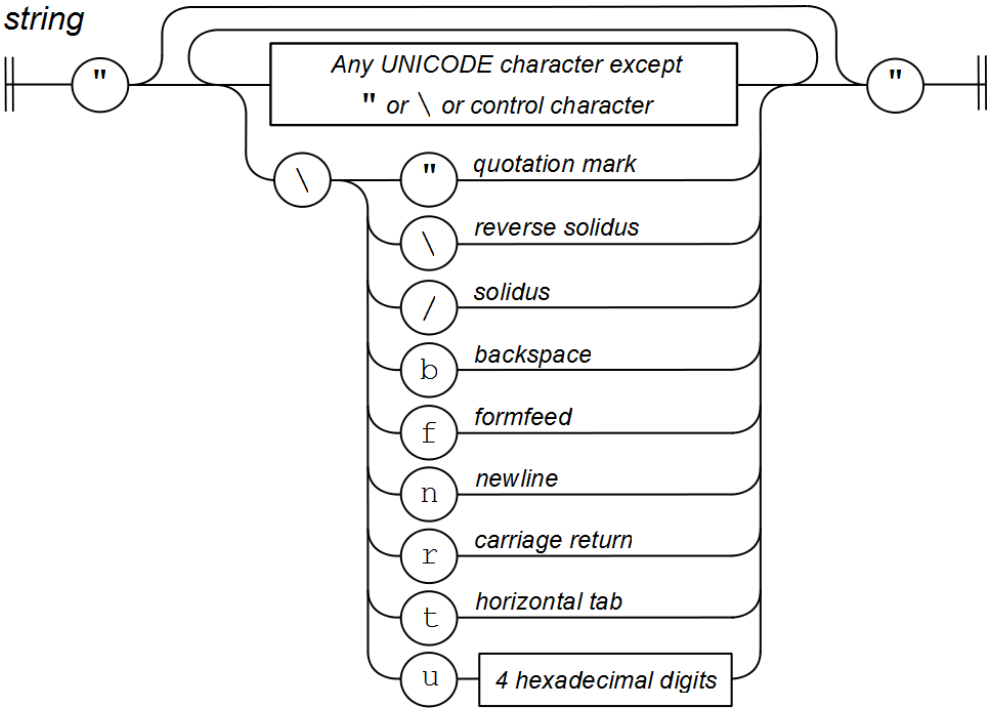

Figure 2-4 Schematic illustration of a string in JSON format (Image from http://json.org (2011-06-27))

Numbers are sequences of digits `0-9` and the point (`.`) used as decimal separator. Furthermore, the sequence can be set as a negative number using a minus sign (`-`). `E` or `e` is used to define terms with an exponent, followed by a sign `+` or `-` and a sequence of digits `0-9`. The octal and hexadecimal formats are not allowed.

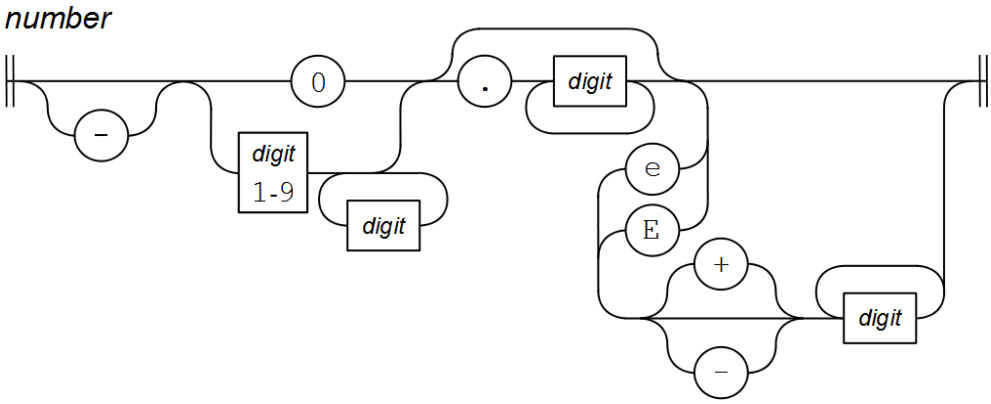

Figure 2-5 Schematic illustration of a number in JSON format (Image from http://json.org (2011-06-27))

Boolean values are represented by the keywords `true` and `false`.

The ***empty value*** is represented by the keyword `NULL`.

Numbers, Boolean values and the empty value `NULL` are not strings therefore they are *not* set in quotes.

Each data type can contain any Unicode-character except the quote sign (`"`), backslash (`\`) or control characters. These excluded characters can nevertheless be entered using the following special format:

Quote sign:	`\"`	Backslash:	`\\`	Slash:	`\/`
Backspace:	`\b`	Formfeed:	`\f`	Newline:	`\n`
Carriage return:	`\r`	Horizontal Tab:	`\t`		

Any special character (i.e. non-Latin characters) can also be entered using the Unicode format by writing `\u`(four-hex-digits), i.e. the small Greek symbol “alpha” (α) is written as `\u03B1`.

Whitespace characters are used arbitrarily, multiple consecutive whitespace characters will be handled as one single whitespace, i.e. the sequence `{"key" : "value"}` will be handled just like `{"key" : "value"}`. Any trailing whitespace is simply ignored, i.e. the sequence `{"key":"value" }` will be handled just like `{"key":"value"}`.

Comments are introduced in JSON using the hash sign (`#`). The comment extends to the line break of the current line. Therefore, all comments are single-line comments. In JSON a multi-line comment can only be built up by several single-line comments. All data types in a comment are ignored by the database. Example:

```
# This comment extends
# over two lines.
```

2.2 THEREDA-specific data structure and definitions

The names of fields in the THEREDA database are designed to be human-readable. Therefore, technical terms, combinations of technical terms and/or abbreviations of these were used as field names. For example, `"molarmass_referenceid"` is the name of the field where the identifier for the reference of the molar mass of a chemical

element is entered. Identical naming of the fields in JSON and PostgreSQL are aimed at as much as possible to facilitate queries.

For a better understanding the reader is advised to follow the documentation below with a JSON-type export from THEREDA at hand.

The THEREDA database is designed as one main JSON object which is divided into four arrays (`"Elements"`, `"Phases"`, `"InteractionPhases"`, and `"Bibliography"`). The order of these arrays is a THEREDA convention.

```
{                                   # main object opening
   "Elements":
   [                                # opening array: "Elements"
     # …                            # content
   ],                               # closing array
   "Phases":
   [                                # opening array: "Phases"
     # …                            # content
   ],                               # closing array
   "InteractionPhases"
   [                                # opening array: "InteractionPhases"
     # …                            # content
   ],                               # closing array
   "Bibliography"
   [                                # opening array: "Bibliography"
     # …                            # content
   ]                                # closing array
}                                   # main object closing
```

2.2.1 The array “Elements”

The array `"Elements"` contains a list of all chemical elements (including the electron) used in the THEREDA database. These elements are ordered by the atomic number of the chemical elements. Since the electron is not a chemical element, it is the first entry in this array per definition.

Every chemical element is an object which contains THEREDA relevant data, such as symbol, name, atomic number, molar mass, entropy, heat capacity, their uncertainties, references and so on. These data are ordered in name/value pairs within the respective object.

```
"Elements":                          # name of the array
[                                    # opening array
  {                                  # opening elements object
    "symbol": "H",                   # chemical symbol
    "name": "Hydrogen",              # element name
    "atomicnumber": 1,               # atomic number
    "molarmass": 1.00794,            # molar mass
    "molarmass_referenceid": "WIE2006",
                                     # reference ID for molar mass
    "s298": 130.68,                  # entropy
    "s298_unctype": "Gauss2s",       # uncertainty calculation type
    "s298_negativeunc": 0.003,       # negative uncertainty
    "s298_positiveunc": 0.003,       # positive uncertainty
    "s298_referenceid": "COX/WAG1989",
                                     # reference ID for entropy value
    "cp298_unctype": "Gauss2s",      # uncertainty calculation type
    "cp298_negativeunc": 0.002,      # positive uncertainty
    "cp298_positiveunc": 0.002,      # negative uncertainty
    "cp298_referenceid": "COX/WAG1989",
                                     # reference ID for entropy value
    "referencestate": "gaseous",     # reference state
    "stoichiometriccoefficient": 2,
                                     # number of atoms per molecular unit in the
                                     # reference state
    "description": "1st example for element",
                                     # description/comment
  },                                 # closing elements object
  { … }                              # next elements object
]                                    # closing  the  array
```

2.2.2 The array “Phases”

The array `"Phases"` includes all the phases (pure and mixed ones) that occur within a chemical system. Each phase is handled as an object.

```
"Phases":                            # name of the array
[                                    # opening array
  {                                  # opening phase-1 object
    # …                              # content
  },                                 # closing phases object
    …                                #
  {                                  # opening phase-(2+n+m) object
    # …                              # content
  }                                  # closing phases object
]                                    # closing the array
```

It is a THEREDA convention that all phases are processed strictly in the following order:

- GAS
- AQUEOUS
- MIXED-PHASE 1 (solid mixed-phase)
- MIXED-PHASE n (solid mixed-phase)
- PHASE-(2+n+1) (pure solid)
- PHASE-(2+n+m) (pure solid)

Each phase consists of describing name/value pairs (`"symbol"`, `"modification"`, `"mixedphase"`, and `"description"`) and 1 … k phase constituents. In THEREDA, every constituent is assigned exactly one of four different phase constituent types: `"PrimaryMaster"`, `"SecondaryMaster"`, `"MineralsSolid"` and `"Product"`. In this order, each phase constituent type is declared as object within each phase. Thus, each phase constituent type again is an array.

```
{                                  # opening phase-1 object
  "symbol": "g",                   # symbol
  "modification": "NA",            # modification
  "mixedphase": true,              # mixed  phase: true/false
  "description": NULL,             # description
  "PrimaryMaster":                 # 1st phase constituent type
  [ … ],                           # array
  "SecondaryMaster":               # 2nd phase constituent type
  [ … ],                           # array
  "MineralsSolid":                 # 3rd phase constituent type
  [ … ],                           # array
  "Product":                       # 4th phase constituent type
  [ … ]                            # array
}                                  # closing phase-1 object
```

Within each phase constituent type array there can be several phase constituents. These phase constituents are objects containing the following data blocks in the given order:

- Symbol (name/value pair)
- Declaration (object: `"Declaration"`)
- Oxidation state (array: `"OxidationState"`)
- Composition (array: `"Composition"`)
- (Formation)Reaction (array: `"FormingReaction"`)
- Standard Data (array: `"DataStandard"`)
- p,T-functions: (array: `"DataVariable"`)

```
"Product":                          # name of the array
[                                   # opening array
  {                                 # opening object
    "symbol": "CO2(g)",             # name/value pair
    "Declaration":                  # name of the object
    { … },                          # object
    "OxidationState":,              # name of the array
    [ … ],                          # array
    "Composition":                  # name of the array
    [ … ],                          # array
    "FormingReaction":              # name of the array
    [ … ],                          # array
    "DataStandard":                 # name of the array
    [ … ],                          # array
    "DataVariable":                 # name of the array
    [ … ],                          # array
  },                                # closing object
  { … }                             # next phase constituents object
]                                   # closing array
```

Some elementary characteristics of the phase constituent are stored in the object "Declaration", i.e. charge, molar mass, a possible equilibrium constraint or a Boolean value whether the particular constituent is formed in a redox reaction from a PrimaryMaster.

```
"Declaration":                      # name of the array
{                                   # opening object
  "equilibrium_constraint": "Complete equilibrium",
                                    # equilibrium constraint value
  "charge": 0,                      # name/value pair for charge
  "molarmass": 44.0095,             # name/value pair for molar mass
  "redox": false,                   # false for PrimaryMaster,
                                    # true for SecondaryMaster
  "description": NULL               # name/value pair for description
},                                  # closing object
```

The array `"OxidationState"` contains objects with the two fields `"centralelement"` and `"oxidationnumber"`. Thus, it is possible to allocate more than one central element to each phase constituent.

```
"OxidationState":                   # name of the array
[                                   # opening array
  {                                 # opening object
    "centralelement": "C",          # central element
    "oxidationnumber": 4            # oxidation number value
  }                                 # closing object
]                                   # closing array
```

The array `"Composition"` defines the chemical composition of the phase constituent. There is an object for each chemical element containing two name/value pairs to define

the element and its stoichiometric coefficient of the element within the formula of the phase constituent.

```
"Composition":                    # name of the array
[                                 # opening array
  {                               # opening object
    "element": "C",               # central element
    "numberofelement": 1          # oxidation number value
  },                              # closing object
   {                              # opening object
    "element": "O",               # central element
    "numberofelement": 2          # oxidation number value
  }                               # closing object
]                                 # closing array
```

The array "FormingReaction" defines the (formation) reaction of the phase constituent from the primary and/or secondary master species. For each reactant there is an object in which the reactant and its stoichiometric coefficient for the reaction equation is stored. The stoichiometric coefficient of educts has a negative sign, reaction products have positive values.

```
"FormingReaction":                # name of the array
[                                 # opening array
  {                               # opening object
    "pcon_reactant": "CO2(g)",    # phase constituent reactant
    "coefficient": 1              # stoichiometric coefficient
  },                              # closing object
   {                              # opening object
    "pcon_reactant": "CO3<2->",   # phase constituent reactant
    "numberofelement": -1         # stoichiometric coefficient
  }                               # closing object
  {                               # opening object
    "pcon_reactant": "H<+>",      # phase constituent reactant
    "numberofelement": -2         # stoichiometric coefficient
  }                               # closing object
  {                               # opening object
    "pcon_reactant": "H2O(l)",    # phase constituent reactant
    "numberofelement": 1          # stoichiometric coefficient
  }                               # closing object
]                                 # closing array
```

The array "DataStandard" contains a list of objects for the thermodynamic data at standard conditions. Inside these objects listed name/value pairs describe each thermodynamic data type.

It is a THEREDA convention that these data types are processed strictly in the following order:

- `DFG` ($\Delta_f G°$)
- `DFH` ($\Delta_f H°$)
- `S` ($S°$)
- `CP` ($C_p°$)
- `V` ($V°$)
- `DRG` ($\Delta_r G°$)
- `DRH` ($\Delta_r H°$)
- `DRS` ($\Delta_r S°$)
- `DRCP` ($\Delta_r C_p°$)
- `LOGK` ($\log K°$)

Data valid at standard conditions are marked with “298” appended to the type, e.g. `DFG298`. The `"DataStandard"` array has the following structure:

```
"DataStandard":                    # name of the array
[                                  # opening array
  {                                # opening object
    "datatype": "DFG298",          # data type
    "value": -394372.54795,        # value
    "calcmode": "CGHF",            # calculation mode
    "unctype": "Gauss2s",          # uncertainty calculation mode
    "negativeunc": 133,            # negative uncertainty value
    "positiveunc": 133,            # positive uncertainty value
    "dataclass": -1,               # data class
    "category": "F",               # category
    "dataquality": -1,             # data quality
    "datasource": -1,              # data source
    "value_notallowed": NULL,      # (alternative
    "unctype_notallowed": NULL,    # numerical value
    "negativeunc_notallowed": NULL,# [not subject to
    "positiveunc_notallowed": NULL,# internal calculations])
    "reference_1": "REA1990",      # reference where data is really taken from
    "reference_2": NULL,           # reference where data is origin. published
    "description": NULL,           # description
    "audit_status": "Audit pending"# audit status value
  }                                # closing object
  { … }                            # next object
]                                  # closing array
```

The array `"DataVariable"` contains objects with name/value pairs characterizing the pressure and temperature functions (composed from up to six parameters) for each object in the `"DataStandard"` array. It is a THEREDA convention that these objects are processed strictly in the following order:

- `DFGT` ($\Delta_f G^T$)
- `CPT` (C_p^T)
- `VT` (V^T)
- `DRGT` ($\Delta_r G^T$)
- `DRCP` ($\Delta_r C_p^T$)
- `LOGKT` ($\log K^T$)

The "`DataVariable`" array has the following structure:

```
"DataVariable":                    # name of the array
[                                  # opening array
  {                                # opening object
    "datatype": "DRGT",            # data type
    "calcmode": "Entered",         # calculation mode
    "tpfunc": "NEA-extended",      # T,p function
     "a": -1.00239384,             # parameter a value
    "b": 0,                        # parameter b value
    "c": 0,                        # parameter c value
    "d": 0,                        # parameter d value
    "e": 0.001,                    # parameter e value
    "f": 0,                        # parameter f value
    "mintk": 298.15,               # minimum temperature in K
    "maxtk": 393.15,               # maximum temperature in K
    "minpbar": 1.01325,            # minimum pressure in bar
    "maxpbar": 1.01325,            # maximum pressure in bar
    "dataclass": 1,                # data class value
    "category": "R",               # category
    "dataquality": 1,              # data quality value
    "datasource": 6,               # data source value
    "reference_1": "REA1990",      # secondary reference
    "reference_2": NULL,           # primary reference
    "description": NULL,           # description
    "audit_status": "Audit pending"# audit status value
  },                               # closing object
  { … }                            # next object
]                                  # closing array
```

2.2.3 The array “InteractionPhases”

The array "`InteractionPhases`" contains all information for the calculation of chemical interactions in mixed phases (aqueous solution, non-ideal gases, solid solutions) including definition and parameters. The interactions for each phase can be described with completely different interaction models. Because of the very generic structure of the database all interaction models for all phases can be handled within the same framework.

The THEREDA user must select one model to describe the interactions for each mixed phase.

The array "InteractionPhases" is a list of objects, one for each mixed phase.

```
"InteractionPhases":              # name of the array
[                                 # opening array
  {                               # opening mixed-phase-1 object
    # …                           # content
  },                              # closing mixed-phase-1 object
  {                               # opening mixed-phase-2 object
    # …                           # content
  }                               # closing mixed-phase-2 object
]                                 # closing the array
```

Each mixed phase is handled as an object containing name/value pairs for the description of the mixed phase and the chosen interaction model and an array with all the interaction parameters. The following structure is illustrated by the example for the aqueous solution ("aq").

```
{                                 # opening mixed phase object
  "phase": "aq",                  # definition of mixed phase
  "interactionmodel": "Pitzer",   # chosen interaction model
  "interaction":                  # name of the array
  [ … ]                           # array
}                                 # closing mixed phase object
```

In this array, every interaction parameter is described as an object. Inside these objects three different objects define the interaction parameter. The first object ("Declaration") describes the type of interaction parameter (i.e. "Pitzer_binary") and the interacting phase constituents. The second object ("IP298") describes the parameter values and their uncertainties for the interaction at the standard temperature. The third object contains parameters for the temperature function of the interaction.

```
"Interaction":                    # name of the array
[                                 # opening array
  {                               # opening interaction param. object
    "Declaration":                # name of object
    { … }                         # object
    "IP298":                      # name of object
    { … }                         # object
    "IPT":                        # name of object
    { … }                         # object
  },                              # closing interaction param. object
  { … }                           # next object
]                                 # closing array
```

The object "Declaration" contains the interacting phase constituents as name /value pairs. Therefore it is possible to define binary or ternary parameters (as defined in the table “interactiontype”) within the same format.

```
"Declaration":                    # name of the array
{                                 # opening object
  "interactiontype": "Pitzer_binary",
                                  # name/value pair for param. type
  "pcon_1": "K<+>",               # 1st phase constituent
  "pcon_2": "Cl<->",              # 2nd phase constituent
  "pcon_3": NULL,                 # 3rd phase constituent (of course not used
                                  # for binary interactions, but required as the
                                  # interactions are defined in a generic way)
  "description": NULL             # description
},                                # closing object
```

The object "IP298" contains a list with up to six interaction parameters, their uncertainties, data quality and data source values and reference entries for the standard temperature. This information is stored as name/value pairs. In the example below the names ip298_1 to ip298_6 stand for $\beta^{(0)}$, $\beta^{(1)}$, $\beta^{(2)}$, C^{ϕ}, $\alpha^{(1)}$, $\alpha^{(2)}$. Presently, the meaning and order of the various interaction parameters per model is only defined in the description field of the table “interactiontype”. For more detailed information please refer to the Technical Paper "Technical Documentation of THEREDA: Databank".

```
"IP298":                          # name of the array
{                                 # opening object
  "ip298_1": 0.0480802587884002,  # 1st interaction parameter
  "ip298_1_unctype": NULL,        # uncertainty type
  "ip298_1_negativeunc": 0,       # negative uncertainty value
  "ip298_1_positiveunc": 0,       # positive uncertainty value
  "ip298_2": 0.218076817366779,   # 2nd interaction parameter
  "ip298_2_unctype": NULL,        # …
  "ip298_2_negativeunc": 0,       #
  "ip298_2_positiveunc": 0,       #
  "ip298_3": 0,                   #
  "ip298_3_unctype": NULL,        #
  "ip298_3_negativeunc": 0,       #
  "ip298_3_positiveunc": 0,       #
  "ip298_4": -0.000787989096430533, #
  "ip298_4_unctype": NULL,        #
  "ip298_4_negativeunc": 0,       #
  "ip298_4_positiveunc": 0,       #
  "ip298_5": 2,                   #
  "ip298_5_unctype": NULL,        #
  "ip298_5_negativeunc": 0,       #
  "ip298_5_positiveunc": 0,       #
  "ip298_6": 0,                   #
  "ip298_6_unctype": NULL,        #
  "ip298_6_negativeunc": 0,       #
  "ip298_6_positiveunc": 0,       #
```

```
  "calcmode": "CTPFUNC",          # calculation mode
  "dataquality": -1,              # data quality value
  "datasource": -1,               # data source value
  "reference_1": "REA1990",       # reference where data is really taken from
  "reference_2": NULL,            # reference where data is origin. published
  "description": NULL             # description
},                                # closing object
```

The object "IPT" holds the information for the temperature function of the interaction parameters, the range of validity in terms of pressure and temperature as name/value pairs, data quality and data source values and reference entries. As for the object "IP298" the meaning and order of the various interaction parameters per model is only defined in the description field of the table “interactiontype”.

```
"IPT":                            # name of the array
{                                 # opening object
  "tpfunc": "Pitzer-function",    # T-function defined
  "ip_1_a": -758.476330506946,    # 1st T param. of 1st inter. param.
  "ip_1_b": 26.7372347224728,     # 2nd T param. of 1st inter. param.
  "ip_1_c": -4.70618514763365,    # 3rd T param. of 1st inter. param.
  "ip_1_d": 0.0100719838607252,   # 4th T param. of 1st inter. param.
  "ip_1_e": -0.00000375989815382765,# 5th T param. of 1st inter. param.
  "ip_1_f": 0,                    # 6th T param. of 1st inter. param.
  "ip_2_a": 112193.168416622,     # 1st T param. of 2nd inter. param.
  "ip_2_b": -2804.03483552829,    # 2nd T param. of 2nd inter. param.
  "ip_2_c": 478.32163208852,      # 3rd T param. of 2nd inter. param.
  "ip_2_d": -0.907183089061278,   # 4th T param. of 2nd inter. param.
  "ip_2_e": 0.000323929103974983,# 5th T param. of 2nd inter. param.
  "ip_2_f": -4946661.79806362,    # 6th T param. of 2nd inter. param.
                                  #
  …                               # skipped identically formatted entries
                                  #
  "ip_6_a": 0,                    # 1st T param. of 6th inter. param.
  "ip_6_b": 0,                    # 2nd T param. of 6th inter. param.
  "ip_6_c": 0,                    # 3rd T param. of 6th inter. param.
  "ip_6_d": 0,                    # 4th T param. of 6th inter. param.
  "ip_6_e": 0,                    # 5th T param. of 6th inter. param.
  "ip_6_f": 0,                    # 6th T param. of 6th inter. param.
  "mintk": 273.15,                # minimum temperature in K
  "maxtk": 393.15,                # maximum temperature in K
  "minpbar": 1.01325,             # minimum pressure in bar
  "maxpbar": 1.01325,             # maximum pressure in bar
  "calcmode": "Entered",          # calculation mode
  "dataquality": 1,               # data quality value
  "datasource": 6,                # data source value
  "reference_1": "REA1990",       # secondary reference
  "reference_2": NULL,            # primary reference
  "description": NULL             # description
},                                # closing object
```

2.2.4 The array “Bibliography”

Each literature reference from the datasets above will be listed here. The array "`Bibliography`" contains a list of all references and their according data. Every reference is an object containing several name/value pairs. Unneeded fields are left blank.

```
"Bibliography":                    # name of the array
[                                  # opening array
  {                                # opening elements object
    "ID": "COX\/WAG1989",          # reference code
    "type": "Book",                # reference type
    "pubname": NULL,               # name of journal
    "origin": NULL,                # origin
    "title": " CODATA Key Values for Thermodynamics ",
                                   # title of reference
    "author": " Cox, J. D., Wagman, D. D., Medvedev, V. A.",
                                   # author(s) name(s)
    "year": 1989,                  # year
    "volume": NULL,                # volume
    "page": NULL,                  # page(s)
    "editors": NULL,               # name(s) of editor(s)
    "language": "English",         # language
    "publisher": "Hemisphere Publ. Corp.",
                                   # publisher
    "ISBN_ISSN": NULL              # ISBN or ISSN number
    "citedinid": NULL,             # ID of citing reference
    "citationmetainfo": NULL,      # additional information of reference
    "doi": NULL,                   # Digital Object Identifier (DOI)
    "puburl": NULL,                # URL to reference
    "cascit": NULL,                # Chemical abstracts service citation
    "chapter": NULL,               # chapter number
    "edition": NULL,               # edition number
    "location": "New York",        # location of publisher
    "thesisdeg": NULL,             # PhD / Diploma / MSc / BSc
    "thesisumipubnum": NULL        # University Microfilm Publication Number
  },                               # closing elements object
  { … }                            # next object
]                                  # closing the array
```

3 Conclusion

The JSON export format for THEREDA is intended to facilitate the import with other computer codes and to promote the usage of the database. In this spirit, any proposals and remarks, which help to improve our JSON export format for THEREDA are most welcome.

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Appendices

Table of Contents

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Appendix B: Complete example of the "`InteractionPhases`" array XIII

Appendix A: Complete example of the "`Phases`" array


```
"Phases":
[
  {
    "symbol": "g",
    "modification": "NA",
    "mixedphase": true,
    "description": NULL,
    "PrimaryMaster":
    [
      {
        "symbol": "H2(g)",
        "Declaration":
        {
          "equilibrium_constraint": "Complete equilibrium",
          "charge": 0,
          "molarmass": 2.01588,
          "centralelement": "EA",
          "oxidationnumber": 0,
          "redox": false,
          "description": NULL
        },
        "Composition":
        [
          {
            "element": "H",
            "numberofelement": 2
          }
        ],
        "FormingReaction": [ ],
        "DataStandard":
        [
          {
            "datatype": "DFG298",
            "value": 0,
            "calcmode": "CGHF",
            "unctype": NULL,
            "negativeunc": NULL,
            "positiveunc": NULL,
            "dataclass": 0,
            "category": "F",
            "dataquality": 0,
            "datasource": 0,
            "value_notallowed": NULL,
            "unctype_notallowed": NULL,
            "negativeunc_notallowed": NULL,
            "positiveunc_notallowed": NULL,
            "reference_1": "Definition\/Convention",
            "reference_2": NULL,
            "description": NULL,
            "audit_result": "Auditing not yet initiated"
          },
          {
            "datatype": "DFH298",
            "value": 0,
            "calcmode": "Entered",
```

```
        "unctype": NULL,
        "negativeunc": NULL,
        "positiveunc": NULL,
        "dataclass": 0,
        "category": "F",
        "dataquality": 0,
        "datasource": 0,
        "value_notallowed": NULL,
        "unctype_notallowed": NULL,
        "negativeunc_notallowed": NULL,
        "positiveunc_notallowed": NULL,
        "reference_1": "Definition\/Convention",
        "reference_2": NULL,
        "description": NULL,
        "audit_result": "Auditing not yet initiated"
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        "calcmode": "Entered",
        "unctype": "Gauss2s",
        "negativeunc": 0.003,
        "positiveunc": 0.003,
        "dataclass": -1,
        "category": "F",
        "dataquality": -1,
        "datasource": -1,
        "value_notallowed": NULL,
        "unctype_notallowed": NULL,
        "negativeunc_notallowed": NULL,
        "positiveunc_notallowed": NULL,
        "reference_1": "GUI\/FAN2003",
        "reference_2": "COX\/WAG1989",
        "description": NULL,
        "audit_result": "Auditing not yet initiated"
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        "calcmode": "Entered",
        "unctype": "Gauss2s",
        "negativeunc": 0.002,
        "positiveunc": 0.002,
        "dataclass": -1,
        "category": "F",
        "dataquality": -1,
        "datasource": -1,
        "value_notallowed": NULL,
        "unctype_notallowed": NULL,
        "negativeunc_notallowed": NULL,
        "positiveunc_notallowed": NULL,
        "reference_1": "GUI\/FAN2003",
        "reference_2": "COX\/WAG1989",
        "description": NULL,
        "audit_result": "Auditing not yet initiated"
      }
    ],
    "DataVariable": [ ]
  }
],
"SecondaryMaster":
```

```
[
  {
    "symbol": "O2(g)",
    "Declaration":
    {
      "equilibrium_constraint": "Complete equilibrium",
      "charge": 0,
      "molarmass": 31.9988,
      "centralelement": "O",
      "oxidationnumber": 0,
      "redox": true,
      "description": NULL
    },
    "Composition":
    [
      {
        "element": "O",
        "numberofelement": 2
      }
    ],
    "FormingReaction":
    [
      {
        "pcon_reactant": "H2(g)",
        "coefficient": 2
      },
      {
        "pcon_reactant": "H2O(l)",
        "coefficient": -2
      },
      {
        "pcon_reactant": "O2(g)",
        "coefficient": 1
      }
    ],
    "DataStandard":
    [
      {
        "datatype": "DFG298",
        "value": -0.002071,
        "calcmode": "CRLOGK",
        "unctype": NULL,
        "negativeunc": NULL,
        "positiveunc": NULL,
        "dataclass": -1,
        "category": "R",
        "dataquality": -1,
        "datasource": -1,
        "value_notallowed": NULL,
        "unctype_notallowed": NULL,
        "negativeunc_notallowed": NULL,
        "positiveunc_notallowed": NULL,
        "reference_1": "REA1990",
        "reference_2": NULL,
        "description": NULL,
        "audit_result": "Auditing not yet initiated"
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        "value": 0,
        "calcmode": "CR",
```

```
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  "negativeunc": NULL,
  "positiveunc": NULL,
  "dataclass": -1,
  "category": "R",
  "dataquality": -1,
  "datasource": -1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "REA1990",
  "reference_2": NULL,
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
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{
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  "calcmode": "CR",
  "unctype": NULL,
  "negativeunc": NULL,
  "positiveunc": NULL,
  "dataclass": -1,
  "category": "R",
  "dataquality": -1,
  "datasource": -1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "InternallyCalculated",
  "reference_2": NULL,
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
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  "value": 474280.6322,
  "calcmode": "CGHR",
  "unctype": NULL,
  "negativeunc": NULL,
  "positiveunc": NULL,
  "dataclass": -1,
  "category": "R",
  "dataquality": -1,
  "datasource": -1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "InternallyCalculated",
  "reference_2": NULL,
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
},
{
  "datatype": "DRH298",
  "value": 571660,
  "calcmode": "Entered",
  "unctype": "Gauss2s",
```

```
        "negativeunc": 80,
        "positiveunc": 80,
        "dataclass": 1,
        "category": "F",
        "dataquality": 1,
        "datasource": 1,
        "value_notallowed": NULL,
        "unctype_notallowed": NULL,
        "negativeunc_notallowed": NULL,
        "positiveunc_notallowed": NULL,
        "reference_1": "COX\/WAG1989",
        "reference_2": NULL,
        "description": NULL,
        "audit_result": "Auditing not yet initiated"
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        "datatype": "DRS298",
        "value": 326.612,
        "calcmode": "Entered",
        "unctype": "Gauss2s",
        "negativeunc": 71,
        "positiveunc": 71,
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        "category": "F",
        "dataquality": 1,
        "datasource": 1,
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        "unctype_notallowed": NULL,
        "negativeunc_notallowed": NULL,
        "positiveunc_notallowed": NULL,
        "reference_1": "COX\/WAG1989",
        "reference_2": NULL,
        "description": NULL,
        "audit_result": "Auditing not yet initiated"
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      {
        "datatype": "LOGK298",
        "value": -83.089898,
        "calcmode": "CR",
        "unctype": NULL,
        "negativeunc": NULL,
        "positiveunc": NULL,
        "dataclass": -1,
        "category": "R",
        "dataquality": -1,
        "datasource": -1,
        "value_notallowed": NULL,
        "unctype_notallowed": NULL,
        "negativeunc_notallowed": NULL,
        "positiveunc_notallowed": NULL,
        "reference_1": "InternallyCalculated",
        "reference_2": NULL,
        "description": NULL,
        "audit_result": "Auditing not yet initiated"
      }
    ],
    "DataVariable": [ ]
  }
],
"Product":
[
```

```
{
  "symbol": "CO2(g)",
  "Declaration":
  {
    "equilibrium_constraint": "Complete equilibrium",
    "charge": 0,
    "molarmass": 44.0095,
    "centralelement": NULL,
    "oxidationnumber": NULL,
    "redox": false,
    "description": NULL
  },
  "Composition":
  [
    {
      "element": "C",
      "numberofelement": 1
    },
    {
      "element": "O",
      "numberofelement": 2
    }
  ],
  "FormingReaction":
  [
    {
      "pcon_reactant": "CO2(g)",
      "coefficient": 1
    },
    {
      "pcon_reactant": "CO3<2->",
      "coefficient": -1
    },
    {
      "pcon_reactant": "H<+>",
      "coefficient": -2
    },
    {
      "pcon_reactant": "H2O(l)",
      "coefficient": 1
    }
  ],
  "DataStandard":
  [
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      "datatype": "DFG298",
      "value": -394372.54795,
      "calcmode": "CGHF",
      "unctype": "Gauss2s",
      "negativeunc": 133,
      "positiveunc": 133,
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      "category": "F",
      "dataquality": -1,
      "datasource": -1,
      "value_notallowed": NULL,
      "unctype_notallowed": NULL,
      "negativeunc_notallowed": NULL,
      "positiveunc_notallowed": NULL,
      "reference_1": "InternallyCalculated",
      "reference_2": NULL,
```

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  "description": NULL,
  "audit_result": "Auditing not yet initiated"
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{
  "datatype": "DFH298",
  "value": -393510,
  "calcmode": "Entered",
  "unctype": "Gauss2s",
  "negativeunc": 130,
  "positiveunc": 130,
  "dataclass": 1,
  "category": "F",
  "dataquality": 1,
  "datasource": 1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "GUI\/FAN2003",
  "reference_2": "COX\/WAG1989",
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
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{
  "datatype": "S298",
  "value": 213.785,
  "calcmode": "Entered",
  "unctype": "Gauss2s",
  "negativeunc": 0.01,
  "positiveunc": 0.01,
  "dataclass": 1,
  "category": "F",
  "dataquality": 1,
  "datasource": 1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "GUI\/FAN2003",
  "reference_2": "COX\/WAG1989",
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
},
{
  "datatype": "CP298",
  "value": 37.135,
  "calcmode": "Entered",
  "unctype": "Gauss2s",
  "negativeunc": 0.002,
  "positiveunc": 0.002,
  "dataclass": 1,
  "category": "F",
  "dataquality": 1,
  "datasource": 1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "GUI\/FAN2003",
  "reference_2": "COX\/WAG1989",
  "description": NULL,
```

```
  "audit_result": "Auditing not yet initiated"
},
{
  "datatype": "DRG298",
  "value": -103629.503071,
  "calcmode": "CRLOGK",
  "unctype": "Gauss2s",
  "negativeunc": 199,
  "positiveunc": 199,
  "dataclass": -1,
  "category": "R",
  "dataquality": -1,
  "datasource": -1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "InternallyCalculated",
  "reference_2": NULL,
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
},
{
  "datatype": "DRH298",
  "value": NULL,
  "calcmode": "NotApplicable",
  "unctype": NULL,
  "negativeunc": NULL,
  "positiveunc": NULL,
  "dataclass": 6,
  "category": "NA",
  "dataquality": 6,
  "datasource": 6,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": NULL,
  "reference_2": NULL,
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
},
{
  "datatype": "DRS298",
  "value": NULL,
  "calcmode": "NotApplicable",
  "unctype": NULL,
  "negativeunc": NULL,
  "positiveunc": NULL,
  "dataclass": 6,
  "category": "NA",
  "dataquality": 6,
  "datasource": 6,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": NULL,
  "reference_2": NULL,
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
```

```
          },
          {
            "datatype": "LOGK298",
            "value": 18.155,
            "calcmode": "Entered",
            "unctype": "Gauss2s",
            "negativeunc": 0.035,
            "positiveunc": 0.035,
            "dataclass": 1,
            "category": "R",
            "dataquality": 1,
            "datasource": 1,
            "value_notallowed": NULL,
            "unctype_notallowed": NULL,
            "negativeunc_notallowed": NULL,
            "positiveunc_notallowed": NULL,
            "reference_1": "GUI\/FAN2003",
            "reference_2": NULL,
            "description": "original equation: CO2(aq) = CO2(g).
original value 1.472+-0.020",
            "audit_result": "Auditing not yet initiated"
          }
        ],
        "DataVariable": [ ]
      },
      {
        "symbol": "H2O(g)",
        "Declaration":
        {
          "equilibrium_constraint": "Complete equilibrium",
          "charge": 0,
          "molarmass": 18.01528,
          "centralelement": NULL,
          "oxidationnumber": NULL,
          "redox": false,
          "description": NULL
        },
        "Composition":
        [
          {
            "element": "H",
            "numberofelement": 2
          },
          {
            "element": "O",
            "numberofelement": 1
          }
        ],
        "FormingReaction":
        [
          {
            "pcon_reactant": "H2O(g)",
            "coefficient": 1
          },
          {
            "pcon_reactant": "H2O(l)",
            "coefficient": -1
          }
        ],
        "DataStandard":
        [
```

```
{
  "datatype": "DFG298",
  "value": -228581.87885,
  "calcmode": "CGHF",
  "unctype": "Gauss2s",
  "negativeunc": 400,
  "positiveunc": 400,
  "dataclass": -1,
  "category": "F",
  "dataquality": -1,
  "datasource": -1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "InternallyCalculated",
  "reference_2": NULL,
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
},
{
  "datatype": "DFH298",
  "value": -241826,
  "calcmode": "CR",
  "unctype": "Gauss2s",
  "negativeunc": 80,
  "positiveunc": 80,
  "dataclass": -1,
  "category": "F",
  "dataquality": -1,
  "datasource": -1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "InternallyCalculated",
  "reference_2": "COX\/WAG1989",
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
},
{
  "datatype": "S298",
  "value": 188.835,
  "calcmode": "CR",
  "unctype": "Gauss2s",
  "negativeunc": 40,
  "positiveunc": 40,
  "dataclass": -1,
  "category": "F",
  "dataquality": -1,
  "datasource": -1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "InternallyCalculated",
  "reference_2": "COX\/WAG1989",
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
},
{
```

```
  "datatype": "CP298",
  "value": 33.609,
  "calcmode": "NotYetDetermined",
  "unctype": "Gauss2s",
  "negativeunc": 0.03,
  "positiveunc": 0.03,
  "dataclass": 6,
  "category": "NA",
  "dataquality": 6,
  "datasource": 6,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": NULL,
  "reference_2": "COX\/WAG1989",
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
},
{
  "datatype": "DRG298",
  "value": 8558.43725,
  "calcmode": "CGHR",
  "unctype": NULL,
  "negativeunc": NULL,
  "positiveunc": NULL,
  "dataclass": 1,
  "category": "F",
  "dataquality": 1,
  "datasource": 1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "GUI\/FAN2003",
  "reference_2": "COX\/WAG1989",
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
},
{
  "datatype": "DRH298",
  "value": 44004,
  "calcmode": "Entered",
  "unctype": NULL,
  "negativeunc": NULL,
  "positiveunc": NULL,
  "dataclass": 1,
  "category": "F",
  "dataquality": 1,
  "datasource": 1,
  "value_notallowed": NULL,
  "unctype_notallowed": NULL,
  "negativeunc_notallowed": NULL,
  "positiveunc_notallowed": NULL,
  "reference_1": "GUI\/FAN2003",
  "reference_2": "COX\/WAG1989",
  "description": NULL,
  "audit_result": "Auditing not yet initiated"
},
{
  "datatype": "DRS298",
```

```
            "value": 118.885,
            "calcmode": "Entered",
            "unctype": NULL,
            "negativeunc": NULL,
            "positiveunc": NULL,
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            "category": "F",
            "dataquality": 1,
            "datasource": 1,
            "value_notallowed": NULL,
            "unctype_notallowed": NULL,
            "negativeunc_notallowed": NULL,
            "positiveunc_notallowed": NULL,
            "reference_1": "GUI\/FAN2003",
            "reference_2": "COX\/WAG1989",
            "description": NULL,
            "audit_result": "Auditing not yet initiated"
          },
          {
            "datatype": "LOGK298",
            "value": -1.499365,
            "calcmode": "CR",
            "unctype": NULL,
            "negativeunc": NULL,
            "positiveunc": NULL,
            "dataclass": -1,
            "category": "F",
            "dataquality": -1,
            "datasource": -1,
            "value_notallowed": NULL,
            "unctype_notallowed": NULL,
            "negativeunc_notallowed": NULL,
            "positiveunc_notallowed": NULL,
            "reference_1": "InternallyCalculated",
            "reference_2": NULL,
            "description": NULL,
            "audit_result": "Auditing not yet initiated"
          }
        ],
        "DataVariable": [ ]
      }
    ],
    "MineralsSolids": [ ]
  },
]
```

Appendix B: Complete example of the "`InteractionPhases`" array


```
"InteractionPhases":
[
  {
    "phase": "aq",
    "interactionmodel": "Pitzer",
    "interaction":
    [
      {
        "Declaration":
        {
          "interactiontype": "Pitzer_binary",
          "pcon_1": "ClO4<->",
          "pcon_2": "H<+>",
          "pcon_3": NULL,
          "description": NULL
        },
        "IP298": NULL,
        "IPT": NULL
      },
      {
        "Declaration":
        {
          "interactiontype": "Pitzer_binary",
          "pcon_1": "Na<+>",
          "pcon_2": "Cl<->",
          "pcon_3": NULL,
          "description": NULL
        },
        "IP298":
        {
          "ip298_1": 0.0752804438551031,
          "ip298_1_unctype": NULL,
          "ip298_1_negativeunc": 0,
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  },
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{
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    "description": NULL
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  "IPT": NULL
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        "description": NULL
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      "IPT": NULL
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        "pcon_3": "Na<+>",
        "description": NULL
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      "IPT": NULL
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        "description": NULL
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      "IP298": NULL,
      "IPT": NULL
    }
  ]
}
```

```
],
```