TRC Metals Alloy Web Services Application Programming Interface (API) Guide

This guide is designed to describe and show examples of Application Programming Interface (API) user functions for the use of the Metals Alloy API web service. These services include retrieving a list of compounds or a list of properties for use in building search queries, retrieving usage/input/output documentation, and submitting a search query to pull TRC metals alloy data.

TRC Metals Alloy API Web Services with Examples

This section covers the web services to perform API functions for the Metals Alloy infrastructure. These functions utilize just one web service to perform the retrieval of compound and property lists, output of documentation, and submission of data search parameters to retrieve TRC metal alloy data.

MetalsAlloyAPI Web Service

The MetalsAlloyAPI web service is the principle and only function to retrieve actual alloy and citation data. Most of the URIs for this web service are available for general use. However some of the URIs do require an authentication key to perform the functions of the web service (to get an authentication key token, please send a request with the user name, email, and user location to TRCalloy@nist.gov). These URIs are:

1. https://trc.nist.gov/MetalsAlloyAPI
2. https://trc.nist.gov/MetalsAlloyAPI/compoundlist
3. https://trc.nist.gov/MetalsAlloyAPI/propertylist
4. https://trc.nist.gov/MetalsAlloyAPI/datafromsavedstate?authkey={user_authkey}
5. https://trc.nist.gov/MetalsAlloyAPI/APIdocumentation/usage
6. https://trc.nist.gov/MetalsAlloyAPI/APIdocumentation/URI
7. https://trc.nist.gov/MetalsAlloyAPI/APIdocumentation/input
8. https://trc.nist.gov/MetalsAlloyAPI/APIdocumentation/output
9. https://trc.nist.gov/MetalsAlloyAPI/search?authkey={user_authkey}

All of the URIs utilize the HTTP GET method for data requests except the /MetalsAlloyAPI/search and /MetalsAlloyAPI/datafromsavedstate URIs which use the HTTP POST method with the default application/x-www-form-urlencoded protocol. Most of the URIs do not require an authentication key passed as a query parameter. The ***search*** and ***datafromsavedstate*** URIs do require an authentication key token and pass JSON input files to be processed to return metals alloy data as JSON.

The first URI is used to get basic URI calls necessary to use the service. It will return a text string that will give the calling user guidance on the URIs to use the web service. An example call to the web service would be:
curl "https://trc.nist.gov/MetalsAlloyAPI"

The second URI is used to pull a specific JSON string that holds the list of compounds in the database and the number of data points that have the compound as a component of the system. This JSON is available to all users and does not need an authentication key as it will be used in both user interface code to list the data coverage and for users to build a compound based input search JSON file.

An example call to the web service URI would be:
curl "https://trc.nist.gov/MetalsAlloyAPI/compoundlist"

The URI will return a JSON string that fits the following format for the compounds in the database:

```
{"compound_list": [
   {"compound_formula": "formula_hill", "compound_name": "preferred_name", "compound_data_count": data_count},
                    .
                    .
   {"compound_formula": "formula_hill", "compound_name": "preferred_name", "compound_data_count": data_count}
  ],
  "number_of_compounds": compound_count
}
```

Example:

```
{"compound_list": [
   {"compound_formula": "Ag","compound_name": "silver","compound_data_count": 63628},
                    .
                    .
   {"compound_formula": "Zr","compound_name": "zirconium","compound_data_count": 38735}
  ],
  "number_of_compounds": 170}
}
```

The third URI is used to pull a specific JSON string that holds the list of properties in the database. This JSON is available to all users and does not need an authentication key as it will be used by users to build a property based input search JSON file.

An example call to the web service URI would be:
curl "https://trc.nist.gov/MetalsAlloyAPI/propertylist"

The URI will return a JSON string that fits the following format for the properties in the database:

```
{"property_list": [
   {"property_code": "code_string", "property_name": "name"},
                    .
                    .
   {"property_code": "code_string", "property_name": "name"}
  ],
  "number_of_properties": property_count
}
```

Example:

```
{"property_list": [
   {"property_code": "AC","property_name": "Activity coefficient"},
                    .
                    .
   {"property_code": "ZC","property_name": "Critical compressibility factor"}
  ],
  "number_of_properties": 138}
}
```

The fourth URI is used mainly by user interfaces to provide a means by which large alloy data retrievals may be broken into multiple pages with a user defined number of citation/alloy data returned per page. This service will make it possible to move through the pages as once the retrieval is requested to be saved as a state (using the "use_cache": "True" JSON parameter in the query) it is possible to pull the data in any combination of citation/alloy data per page and specific page to pull. This URI does use a query parameter for an authkey to insure that the invoking user has permission to load saved state

data. It must be noted that this URI may only be invoked AFTER a search has been performed and the data has been requested to be saved in state! It is also important to note that data retrieval to a state only has a lifetime of 24 hours before the system removes the saved state. The following example shows how to invoke the web service to load a special JSON file holding the information to pull a specific page count (number of citation/alloy data sets per page) and page number for a specific saved state:

curl -X POST -d @saved_state.json "https://trc.nist.gov/MetalsAlloyAPI/datafromsavedstate?authkey=c7d49f8c8ec745e509ed8b928cae927e"

This URI requires an input JSON file in the following format:

```
{
  "page_count": <Number of citations/alloy data per page>,
  "page_number": <Page number to retrieve>,
  "saved_state_hash": <"The MD5 hash of the state; this is returned in the initial output JSON data from the search">
}

example:
{
  "page_count": 5,
  "page_number": 3,
  "saved_state_hash": "78ccf6cbeaef039ae5e09fcbd45bd508"
}
```

The URI will return a JSON string that fits the format found in search output as defined in appendix B but only contain the requested citations/alloy data from the specific page of the saved state.

The fifth URI is used to get usage information on using this web service. It will return a JSON string for processing through a user interface. An example call to the web service would be:

curl "https://trc.nist.gov/MetalsAlloyAPI/APIdocumentation/usage"

The sixth URI is used to get URI information on using this web service. It will return a JSON string for processing through a user interface. An example call to the web service would be:

curl "https://trc.nist.gov/MetalsAlloyAPI/APIdocumentation/URI"

The seventh URI is used to get input information and examples on using this web service to make a search request. It will return a JSON string for processing through a user interface. An example call to the web service would be:

curl "https://trc.nist.gov/MetalsAlloyAPI/APIdocumentation/input"

The URI will return a JSON string that fits the format found in the search input and examples as defined in appendix A.

The eighth URI is used to get output information on using this web service. It will return a JSON string for processing through a user interface. An example call to the web service would be:

curl "https://trc.nist.gov/MetalsAlloyAPI/APIdocumentation/output"

The URI will return a JSON string that fits the format found in search output as defined in appendix B.

The ninth and last URI is used to actually search and retrieve data from the web service. It will return a JSON string for processing through a user interface. This URI does use a query parameter for an authkey to insure that the invoking user has permission to search metals alloy data.

The following example shows how to invoke the web service to load a JSON file holding the search parameters (as defined in appendix A) for doing the search and retrieval of data from the web service:

curl -X POST -d @search.json "https://trc.nist.gov/MetalsAlloyAPI/search?authkey=c7d49f8c8ec745e509ed8b928cae927e"

The URI will return a JSON string that fits the format found in search output and examples as defined in appendix B.

Appendix A

This section covers the input search parameter JSON format for use in searching the TRC Metals Alloy database. There will be some examples to show the usage of the input format.

Search Parameters JSON Format

The following is the format for the search parameters JSON file. Note that any comments (denoted by a "//") in the format specification below are not allowed in the actual JSON file but are here to clarify the formatting scheme:

```
{
    // JSON elements for paging/saved state. MUST have this to invoke a saved state
    "use_cache": <string>, //  The string will be either "True" or "False" and nothing else is allowed. This is a search parameter specifies whether to use a disk cache.
    "citations_per_page": <integer>, // The number of citations to display per returned JSON "page".

    // JSON elements for compound search (can not be combined with other searches)
    "exclude_all": <string>, // The string will be either "True" or "False" and nothing else is allowed. This is a search parameter that requires the "required_compounds".
    "required_compounds": [<string>,<string>,...,<string>], // This is the comma separated list of compound names like "Ti", "Al", "Ni" to require as part of the search.
    "required_or": <string>, // The string will be either "True" or "False" and nothing else is allowed. This is a search parameter that requires the "required_compounds"
                             // to use the "compound1 or compound2" rather than the default "compound1 and compound2" database set operation.
    "excluded_compounds": [<string>,<string>,...,<string>], // This is a comma separated list of compound names in which to exclude from a search.
    "optional_compounds": [<string>,<string>,...,<string>], // This is a comma separated list of optional compound names which may be present in an alloy but not required.

    // JSON elements for citation search (can not be combined with other searches)
    "author_full_name": [<string>,<string>,...,<string>], // This is a comma separated list of author full names.
    "author_last_name": [<string>,<string>,...,<string>], // This is a comma separated list of author last names.
    "doi": <string>, // The doi string to find the citation and its data.
    "journal_name": <string>, // The full journal name in which to find citations.
    "journal_abbrev": <string>, // A well known abbreviation of the journal name.
    "keywords": [<string>,<string>,...,<string>] // A comma separated list of keywords.
    "partial_author_match": <string>, // The string will be either "True" or "False" and nothing else is allowed and is used to determine if a fuzzy search is done on
                                      // author last name. This is a search parameter that requires the "author_last_name". Default is false!
    "partial_title_match": <string>, // The string will be either "True" or "False" and nothing else is allowed and is used to determine if a fuzzy search is done on title.
                                     // This is a search parameter that requires the "title". Default is false!
    "title": <string>, // The title string to find the citation and its data.

    // JSON elements for data set searches (can not be combined with other searches)
    "data_set_id": <integer>, // A specific data set identifier to return a specific data set.

    // JSON elements for property searches (can not be combined with other searches)
    "property_search_code": <string>, // A specific property code which to return data.
```

```
    // JSON elements for data reduction by parameters
    "pressure": <double>, // A static pressure value which returned data sets must contain in kPa.
    "start_pressure": <double>, // The start of a pressure range in kPa which returned data sets must contain a pressure in the range. If no end_pressure it is an open
                                // ended range.
    "end_pressure": <double>, // The end of a pressure range in kPa which returned data sets must contain a pressure in the range. If no start_pressure the range
                              // automatically starts at 0 kPa.
    "temperature": <double>, // A static temperature value which returned data sets must contain in K.
    "start_temperature": <double>, // The start of a temperature range in K which returned data sets must contain a temperature in the range. If no end_temperature it is
                                   // an open ended range.
    "end_temperature": <double>, // The end of a temperature range in K which returned data sets must contain a temperature in the range. If no start_temperature the
                                 // range automatically starts at 0 K.
    "year": <integer>, // An exact year which published citations must have this exact publishing date.
    "start_year": <integer>, // The start of a year range which returned citations must be published in the range. If no end_year it is an open ended range.
    "end_year": <integer>, // The end of a year range which returned citations must be published in the range. If no start_year the range is open ended.
    "data_set_type": <string>, // The character will be "Y", "C", "S", "G" for "Data from Experiment", "Data from equation", "Smoothed Data", "Data from Graph"
                               // respectively. Return data must be so categorized.
    "property_reduce_code": <string>, // A specific property code which all return data must contain and is used for compound searches only.

    // JSON elements for use by implementing User Interfaces
    "use_citation_json": <string>, //  The string will be either "True" or "False" and nothing else is allowed and is used to pull only citation identifier, author list, year,
                                   // and title for the purpose of reducing the immediate data requirements of very large data sets from search queries for user
                                   // interfaces. This makes it possible to keep the small sub set of the data from the query in memory for paging and sorting. It
                                   // is then possible in an user interface to use the API call:
                                   //         "http://'API Server':'port'/MetalsAlloyAPI/citation/{citationid}?authkey={authentication_key}"
                                   // to get the full JSON data packet for the specific citation.
}
```

The following are example input parameters in JSON to do searches through the search API web service.

Example one:

```
{
   "required_compounds": ["Ti","Ni"],
   "excluded_compounds": ["Cu"],
   "use_citation_json": "True"
}
```

Example two:

```
{
   "exclude_all": "True",
   "required_compounds": ["Ti","Ni"],
   "optional_compounds": ["Al"],
   "required_or": "True"
}
```

Example three:

```
{
    "author_last_name": ["Wilthan"],
    "doi": "10.1007/s10765-005-6682-z",
    "property_reduce_code": "H",
    "year": 2005
}
```

Example four:

```
{
    "citations_per_page": 20,
    "property_search_code":"H",
    "start_year": 1955,
    "end_year": 2016
}
```

Example five:

```
{
    "citations_per_page": 20,
    "exclude_all": "True",
    "required_compounds": ["Fe","Ni"],
    "property_reduce_code": "H",
    "start_year": 1901,
    "end_year": 2019,
    "start_temperature": 900,
    "end_temperature": 2200
}
```

Example six:

```
{
    "required_compounds": ["Fe","Ni"],
    "excluded_compounds": ["Cu"],
    "required_or": "True",
    "data_set_type": "G",
    "start_year": 1901,
    "end_year": 2019,
    "start_temperature": 900,
    "end_temperature": 2200
}
```

Appendix B

This section covers the output JSON format for holding TRC Metals Alloy data. There will be some examples following the format scheme definition.

TRC JSON Format for Metals Alloy Data Scheme

The following is the format for the TRC Metals Alloy JSON file. Note that any comments (denoted by a "//") in the format specification are not allowed in the actual JSON file but are here to clarify the formatting scheme:

```
{ // Required. Main trunk object
  "TRC_data": [ // Required. A JSON array of Data objects with each object being a citation and data
                // All comments are NOT a part of the actual data specification.
                // Note that most of the top level branches are require elements
    { // Required. A JSON Data object. One citation with all of the captured data for that citation
      "citation": { // Required. A JSON object
        // Specify general citation elements below
        "abstract": "<string>", // Optional. A UTF8, UTF16, UTF32, or some wide string capable of holding I18N strings
        "authors": [ // Required. A JSON array holding one or more strings of author names
          "<string>", // Required. A string of the format "Last Name, FI., MI." or "Last Name, First Name, MI." or "Last Name, First Name, Middle Name"
                      // using the western definition of "Last Name"
                .
                .
                .
          "<string>"
        ],
        "cas_citation": "<string>", // Optional. The Chemical Abstracts Service citation string
        "citation_id": <integer>, // Required. The unique identifier number for this citation array element
        "citation_key": { // Required. A JSON object used for uniquely defining citations and associated system elements
          "author1": "<string>", // Required. The author1 string which is the first 2 or 3 letters of the principle authors last name
          "author2": "<string>", // required if exists. The author2 string if it exists and is the first 2 or 3 letters of the last name
          "authorn": <integer>, // Required. A specific uniquely identifying integer for citation differentiation
          "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
          "version": "<string>", // Optional. A version or comment string specifying a version for a specific citation entry
          "year": <integer> // Required. The identifying year the citation was either published, submitted, or written
        },
        "citation_tag": [ // Optional. A JSON array holding citation tag information used for searching citations by a tag
          { // Required. A JSON object
            "description": "<string>", // Optional. A string holding a descriptive text describing the tag
            "id": <integer>, // Required. A unique integer holding the tag identifier for the specific tag stored in this citation
```

```
    "name": "<string>" // Required. A string holding the name of the tag which is required as this is the search term for the tag
  },

        .
        .
        .
  {...}
],
"citation_string": "<string>", // Optional. The raw citation string that could have been used to
                               // generate the citation entry
"date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY;
                          // MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
"document_type": "<string>", // Required. A string which specifies the type of document for which
                             // this citation object is storing data
"doi": "<string>", // Optional. The DOI of the citation if it exists
"editors": [ // Optional. A JSON array holding one or more strings of editor names
  "<string>", // Required. A string of the format "Last Name, FI., MI." or "Last Name, First Name, MI." or "Last Name, First Name, Middle Name"
                    // using the western definition of “Last Name"
           .
           .
           .
  "<string>"
],
"item_number": "<string>", // Optional. A string holding the citation item number
"keywords": "<string>", // Optional. A string holding any defined keywords
"language": "<string>", // Optional. A string holding the language of the document
"location": "<string>", // Optional. A string holding the publishing location or address
"note": "<string>", // Optional. A string holding any notes gathered during the capture of this citation information
"organization": "<string>", // Optional. A string holding the organization for producing the citation for reports and conferences
"pages": "<string>", // Optional. The page numbers of an article or report that were captured for this citation
"source_title": "<string>", // Optional. The title specified by the original source citation which might be in any language
"temperature_scale": "<string>", // Optional. An international temperature scale specified for all data in the citation
"title": "<string>", // Optional. A string specifying the citation's actual title as specified by the captured document
"total_pages": <integer>, // Optional. An integer specifying the total number of pages in the captured document
"translation_of": <integer>, // Optional. An integer specifying the citation identifier of a cited work of which this citation is a translation
"url": "<string>", // Optional. A string holding the URL necessary to retrieve electronic version of this cited work
"volume": "<string>", // Optional. A string specifying a volume as defined for articles, reports, or conference proceedings
"year": <integer>, // Required. The identifying year the citation was either published, submitted, or written

// Specify Article/Journal specific citation elements below
"coden": "<string>", // Optional. A string holding the CODEN identification of the journal
"erratum_of": <integer>, // Optional. An integer holding the article citation identifier of a cited work of which this article is an erratum
```

```
  "issue": "<string>", // Optional. A string holding the articles Journal issue for the specific citation referenced
  "journal_abbreviation": "<string>", // optional/Required. The abbreviated name of the journal in which the article was published. This element or the
                                      // journal_full must be specified to create a link to either a database journal entry or a journal entry below
  "journal_fullname": "<string>", // optional/Required. The full name of the journal in which the article was published. This element or the journal_abbr must
                                  // be specified to create a link to either a database journal entry or a journal entry below

  // Specify Book specific citation elements below
  "book_title": "<string>", // Optional. The book title which may be different than the citation title
  "chapter": "<string>", // Optional. A string holding the chapter number/name for the book citation referenced
  "edition": "<string>", // Optional. A string holding the edition of the book cited
  "isbn": "<string>", // Optional. A string holding the International Standard Book Number (ISBN) which is a 10-13 digit number used to identify books or citations
  "publisher": "<string>", // Optional. A string holding the name of the publishing company

  // Specify Conference Proceedings specific citation elements below
  "conference_title": "<string>", // Optional. A string holding the name for the conference the proceeding document covers
  "end_date": "<string>", // Optional. The end date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
  "end_month": <integer>, // Optional. An integer holding the end month (1-12) for the conference the proceeding document covers
  "start_date": "<string>", // Optional. The start date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
  "start_month": <integer>, // Optional. An integer holding the start month (1-12) for the conference the proceeding document covers

  // Specify Patent specific citation elements below; patent_country and patent_number are required only if the citation is a patent
  "patent_country": "<string>", // Optional. A string holding the name or abbreviated name of the country issuing the patent
  "patent_end_date": "<string>", // Optional. The end date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
  "patent_holder": "<string>", // Optional. The institution or individuals who hold the rights to the patents
  "patent_number": "<string>", // Optional. A string holding the patent number issued by the country the patent was granted
  "patent_start_date": "<string>", // Optional. The start date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD

  // Specify Thesis specific citation elements below
  "degree": "<string>", // Optional. A string holding the degree granted to the author of the thesis
  "thesis_type": "<string>", // Optional. A string holding the type of thesis document this citation covers
  "umi_publication_number": <integer> // Optional. An integer holding the University Microfilms International (UMI) Publication Number identifying the
                                      // thesis publication
},// End of citation object
"compounds":[ // Required. A JSON array and will contain one or more elements
  { // Required. A JSON object
    "ambiguity_flag": "<string>", // Optional. A string holding a code for compound ambiguity
    "cas_number": "<string>", // Optional. A string holding the registered Chemical Abstracts Service (CAS) number for the compound if it is known or defined
    "charge": <integer>, // Optional. A signed integer holding the charge of the compound
    "compound_id": <integer>, // Required. A unique integer identifier for this compound
    "compound_name": [ // Required. An array of objects holding the name and preferred name flag
      {
        "name": "<string>", // Required. A string holding a name of the compound
```

```
      "preferred": <integer> // Required. An integer holding the preferred flag for the name. If 1 then this name is preferred
     },
          .
          .
          .
     {...}
   ], // End of Compound Name array
   "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
   "formula_extended": "<string>", // Optional. A string holding the extended version of the compound formula
   "formula_hill": "<string>", // Optional. A string holding the Hill system formula of the compound
   "inchi_key": "<string>", // Optional. A string holding the inchi key for this specific compound
   "molecular_weight": <double> // Optional. A double holding the calculated molecular weight of the compound
  },
     .
     .
     .
  {...} // Required. A JSON object
], // End of Compounds array
"journals": [ // Optional. A JSON array and will contain one or more elements
  { // Required. A JSON object
   "abbreviated_name": "<string>", // Optional. A string holding the abbreviated name of the journal
   "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
   "english_name": "<string>", // Optional. The english equivalent of the journal name if it differs from the full name
   "issn_online": "<string>", // Optional. A string holding the journals online International Standard Serial Number if known
   "issn_print": "<string>", // Optional. A string holding the journals print International Standard Serial Number if known
   "journal_id": <integer>, // Required. A unique integer identifier for this journal
   "name": "<string>", // Required. A string holding the full name of the journal
   "note": "<string>", // Optional. A string holding any notes gathered during the capture of this journal entry
   "url": "<string>", // Optional. A string holding the URL necessary to retrieve issues of this journal
   "year_end": <integer>, // Optional. An integer holding the year this journal stopped publishing
   "year_start": <integer> // Optional. An integer holding the year this journal started publishing
  },
     .
     .
     .
  {...} // Required. A JSON object
], // End of Journals array
"specimens": [ // Required. A JSON array and will contain one or more elements
  { // Required. A JSON object
   "compound_ids": [ // Required. A JSON array of compound identifiers which comprise this specimen
     <integer>, // Required. An integer holding a unique compound identifier for a compound object
          .
          .
```

```
          .
    <integer>
   ], // End of Compound Identifiers array
   "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
   "description": { // Optional. A JSON object that holds "key": "value" pairs where the "key" is not apriori known and specifies different processing steps performed
                    // on the specimen. Keys could include "initial", or "final" for step descriptors
    "<string>": "<string>",
          .
          .
          .
    "<string>": "<string>"
   }, // End of Description object
   "history": { // Optional. A JSON object of "key": "value" pairs
    "history_id": <integer>, // Required. An integer holding a unique system history identifier for a history entry
    "history_name": "<string>", // Optional. A string holding holding the name of this history entry
    "history_string": "<string>" // Required. A string holding the processing history of the system
   }, // End of History object
   "impurity": [ // Optional. A JSON array of objects
    { // Required. A JSON object holding impurity "key": "value" pairs
     "amount": <double>, // Required. A double holding the amount of the compound in the impurity
     "attribute", "<string>", // Optional. A string holding an attribute code for the impurity
     "compound_id": <integer>, // Required. The unique identifier to a compound object that this impurity applies
     "method": "<string>", // Optional. A string that states the name or description of the method used to determine the impurities from the specimen
     "representation": "<string>" // Optional. A string detailing how the amount is represented: i.e. %, weight %, mass %
    },
          .
          .
          .
    {...}
   ], // End of Impurity array
   "name": "<string>", // Optional. A string holding the cleaned up name of this specimen
   "note": "<string>", // Optional. A string holding any notes gathered during the capture of this specimen object
   "parent_id": <integer>, // Optional. An integer that specifies a unique identifier for a parent specimen
   "phase_purity": <double>, // Optional. A double holding the phase purity of the specimen
   "single_crystal": "<string>", // Optional. A string holding the "T" or "F" for true or false if it is a single crystal specimen
   "specimen_id": <integer> // Required. A unique integer identifier for this specimen object
  },
     .
     .
     .
  {...} // Required. A JSON object
 ], // End of Specimens array
 "systems": [ // Required. A JSON array and will contain one or more elements
```

```
{ // Required. A JSON object
 "compound_ids": [ // Required. A JSON array of compound identifiers which comprise this system
   <integer>, // Required. An integer holding a unique compound identifier for a compound object
          .
          .
          .
   <integer>
 ], // End of Compound Identifiers array
 "data_sets": [ // Required. A JSON array of data set objects
  { // Required. A JSON object
   "atmosphere": "<string>", // Optional. A string holding the crucible atmosphere used in the experiment
   "compiler": "<string>", // Optional. A string holding the name/initials of the person who compiled the data
   "contributor":"<string>", // Optional. A string specifying a particular person, project, institution, or general source of the data
   "crucible": "<string>", // Optional. A string holding the material that comprises the crucible
   "data": [ // Required. A JSON array holding JSON objects of data_value and variable_id
    { // Required. A JSON object
     "data_values": [ // Required. A JSON array holding JSON objects of value and uncertainty
      { // Required. A JSON object
       "flawed": "<string>", // Optional. A string holding either "true" or "false" to set the flawed flag on the data value
       "uncertainty": <double>, // Optional. A double holding an uncertainty measurement for the data value
       "value": <integer> or <double> or "<string>" // Optional. A captured data value
      }
              .
              .
              .
      {} // Required. A JSON object
     ], // End of Data Values array
     "variable_id": <integer> // Required. An integer holding the unique variable identifier to a variable object
    },
         .
         .
         .
    {} // Required. A JSON object
   ], // End of Data array
   "data_comment": "<string>", // Optional. A string holding the comments added by the compiler during data capture
   "data_set_id": <integer>, // Required. An integer holding a unique system data set identifier for a dataset object
   "data_set_type": "<string>", // Optional. A string holding the code for the type of data entered: 'C' => "From Equation", 'Y' => "Experimental",
                                // 'S' => "Smoothed", 'G' => "From Graph"
   "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
   "description": "<string>", // Optional. A string specifying the description or purpose of measurement
   "flawed": "<string>", // Optional. A string holding either "true" or "false" to set the flawed flag on the entire data set
   "instrumentation": [ // Optional. A JSON array of JSON objects holding instrumentation object data
    { // Required. A JSON object holding instrumentation object data
```

```
    "brand": "<string>", // Optional. A string holding the instrument "brand" used for measuring the data
    "city": "<string>", // Optional. A string holding the name of the city of the manufacturer
    "country": "<string>", // Optional. A string holding the country of the manufacturer
    "customization": "<string>", // Optional. A string holding any user specific customization done to the instrument outside of the manufacturer
    "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
    "instrumentation_id": <integer>, // Required. An integer holding a unique system instrumentation identifier for an instrumentation object
    "instrument_name": "<string>", // Optional. A string holding the full name of the instrument
    "instrument_short_name": "<string>", // Optional. A string holding the short name or acronym of the instrument if one exists
    "instrument_type": "<string>", // Optional. A string describing the type of instrument
    "manufacturer": "<string>", // Optional. A string holding the name of the instrument manufacturer
    "model": "<string>", // Optional. A string holding the model or version of the specific instrument used
    "notes": "<string>", // Optional. A string holding any other miscellaneous notes about the instrument such as serial numbers, performance metrics, etc
    "organization_name": "<string>", // Optional. A string holding the name of the organization that used the instrument in the study
    "organization_short_name": "<string>", // Optional. A string holding the short name or acronym of the organization that used the instrument in the study
    "province": "<string>", // Optional. A string holding any province name for the location of the manufacturer
    "region": "<string>", // Optional. A string holding any region name for the location of the manufacturer
    "state": "<string>" // Optional. A string holding any state name for the location of the manufacturer
  },
            .
            .
            .
  {} // Required. A JSON object holding instrumentation object data
], // End of Instrumentation array
"lines": [ // Optional. A JSON array holding the line object identifiers that link the line objects to the data set
  <integer>, // Required. An integer for a line identifier for a line object
            .
            .
            .
  <integer>
], // End of Line Identifiers array
"method": "<string>", // Optional. A string holding a general method for an entire data set
"phase_fields": [ // Optional. A JSON array holding the phase field object identifiers that link the phase_field objects to the data set
  <integer>, // Required. An integer for a phase field identifier for a phase_field object
            .
            .
            .
  <integer>
], // End of Line Identifiers array
"reference_pressure_maximum": <double>, // Optional. A double holding the maximum reference pressure for the experiment
"reference_pressure_minimum": <double>, // Optional. A double holding the minimum reference pressure for the experiment
"reference_pressure_units": "<string>", // Optional. A string holding the units for the pressure temperature for the experiment
"reference_temperature_maximum": <double>, // Optional. A double holding the maximum reference temperature for the experiment
"reference_temperature_minimum": <double>, // Optional. A double holding the minimum reference temperature for the experiment
```

```
"reference_temperature_units": "<string>", // Optional. A string holding the units for the reference temperature for the experiment
"regions": [ // Optional. A JSON array holding the region object identifiers that link the region objects to the data set
  <integer>, // Required. An integer for a region identifier for a region object
          .
          .
          .
  <integer>
], // End of Region Identifiers array
"states": [ // Required. A JSON array of JSON objects holding state object data
  { // Required. A JSON object holding state object data
    "attribute": "<string>", // Optional. A string holding either a code or a full string for the state "Equilibrium" attribute
    "compound_id": <integer>, // Optional. An integer for a compound identifier for a compound object
    "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
    "description": "<string>", // Optional. A string holding a description of the state
    "error_flag": "<string>", // Optional. A string holding either "true" or "false" specifying whether or not the state is viewed as having an error in definition.
                                  // Defaults to false
    "metastable_phase_flag": "<string>", // Optional. A string holding either "true" or "false" specifying whether or not the phase is a metastable phase.
                                            // Defaults to false
    "partially_known_phase_flag": "<string>", // Optional. A string holding either "true" or "false" specifying whether or not the phase for the state is only
                                                 // partially known. Defaults to false
    "phase_basis": "<string>", // Optional. A string holding either a code or a full string specifying an assignment basis for the phase of the state
    "phase_id": <integer>, // Optional. An integer for a phase identifier for a phase object
    "phase_method": "<string>", // Optional. A string holding either a code or a full string specifying the method used to measure the phase
    "phase_state": "<string>", // Optional. A string holding either a phase type code or an arbitrary string defining a phase
    "region_id": <integer>, // Optional. An integer for a region identifier for a region object
    "solvents": [ // Optional. A JSON array of "<string>" specifying solvents used in the experiment
      "<string>", // Required. A string holding a solvent used in the experiment
                .
                .
                .
      "<string>"
    ], // End of Solvents array
    "specimen_id": <integer>, // Optional. An integer for a specimen identifier for a specimen object
    "state_id": <integer>, // Required. An integer holding a unique system state identifier for a state object
    "state_role": "<string>" // Optional. A string holding either a code or a full string of the state object's current role in the system
  },
          .
          .
          .
  {} // Required. A JSON object holding state object data
], // End of States array
"variables": [ // Required. A JSON array of JSON objects holding variable (metadata) object data
  { // Required. A JSON object holding variable (metadata) object data
```

```
  "attribute_name": "<string>", // Optional. A string holding the name of the attribute which is used to hold static extra data associated
                                // with the variable such as wavelength for radiance temperature data
  "attribute_value": <double>, // Optional. A double holding the value of the attribute which is used to hold extra static data
  "component_compound_id": <integer>, // Optional. An integer for a compound identifier to a compound object
  "confidence": <integer>, // Optional. An integer holding the coverage factor percentage
  "data_type": "<string>", // Required. A string holding the data type for the data associate with this variable  and may be "integer" or
                           // "double" for numeric data types and "string" or "bool" for non-numeric data types
  "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
  "derived_from_id": <integer>, // Optional. An integer holding the variable identifier of the variable from which these values are derived
  "instrumentation_id": <integer>, // Optional. An integer for a instrumentation identifier to an instrumentation object
  "method": "<string>", // Optional. A string holding the name/description of the method used to obtain data
  "method_details": "<string>", // Optional. A string holding additional information to include about the method used to determine the data
  "per_component_compound_id": <integer>, // Optional. An integer for a compound identifier to a compound object
  "per_state_id": <integer>, // Optional. An integer for a state identifier for a state object
  "reference_pressure": <double>, // Optional. A double holding the reference pressure used for a control pressure in experimental measurements
  "reference_pressure_units": "<string>", // Optional. A string holding the reference pressure units
  "reference_state_description": "<string>", // Optional. A string holding the description for the reference state for attribute
  "reference_state_id": <integer>, // Optional. An integer for a state identifier for a state object
  "reference_temperature": <double>, // Optional. A double holding the reference temperature used for a control temperature in experimental measurements
  "reference_temperature_units": "<string>", // Optional. A string holding the reference temperature units
  "repetitions": <integer>, // Optional. An integer holding the number of measurements performed that affect uncertainty
  "representation": "<string">, // Optional. A string holding the representation of the measurement
  "solvent_used": "<string>", // Optional. A string holding either "true" or "false" specifying whether or not the primary compound has been
                              // dissolved in a solvent
  "solvents": [ // Optional. A JSON array of "<string>" specifying solvents used in the experiment
    "<string>", // Required. A string holding a solvent used in the experiment
            .
            .
            .
    "<string>"
  ], // End of Solvent array
  "standard_state_description": "<string>", // Optional. A string holding the definition or description of the standard state of the measurement
  "standard_state_id": <integer>, // Optional. An integer for a state identifier for a state object
  "state_id": <integer>, // Optional. An integer for a state identifier for a state object
  "temperature_scale": "<string>", // Optional. A string holding the temperature scale defined for the temperature measurements
  "to_component_compound_id": <integer>, // Optional. An integer for a compound identifier to a compound object
  "uncertainty_type": "<string>", // Optional. A string holding the uncertainty type (such as calculated from standard deviation)
  "units": "<string>", // Optional. A string holding the units for the variable
  "variable_id": <integer>, // Required. An integer holding a unique system variable identifier for a variable object
  "variable_name": "<string>", // Required. A string holding the name of the variable
  "variable_role": "<string>", // Required. A string holding the role of the variable this object defines, either "property" or "variable" or "constraint"
  "variable_type": "<string>" // Optional. A string holding the type of variable this object defines; either "fixed" or "varying"
},
```

```
                .
                .
                .
    {} // Required. A JSON object holding variable (metadata) object data
   ] // End of Variables array
  },
       .
       .
       .
  {...} // Required. A JSON object
], // End of DataSets array
"date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
"history": [ // Optional. A JSON array
  { // Required. A JSON object of "key": "value" pairs
    "history_id": <integer>, // Required. An integer holding a unique system history identifier for a history entry
    "history_name": "<string>", // Optional. A string holding holding the name of this history entry
    "history_string": "<string>" // Required. A string holding the processing history of the system
  },
      .
      .
      .
  {...} // Required. A JSON object
], // End of History array
"lines": [ // Optional. A JSON array of line objects
  { // Required. A JSON object of "key": "value" pairs
    "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
    "hight": "<string>", // Optional. A string holding either "true" or "false" to determine if the region ID 2 specifies the High Temperature (High T) value
    "line_attributes": "<string>", // Optional. A string holding optional attribute information about the line
    "line_basis": "<string>", // Optional. A string holding the line basis information
    "line_id": <integer>, // Required. An integer holding a unique system line identifier for a line object
    "line_name": "<string>", // Optional. A string holding the given name for the line object
    "invariant_line": "<string>", // Optional. A string holding either "true" or "false" to determine if the line is invariant (a collapsed region). Default is false
    "region_ids": [ // Required. A JSON array of region identifiers (usually will hold 1 or 2 region identifiers)
      <integer>, // Required. An integer holding a unique region identifier for a region object
                .
                .
                .
      <integer>
    ] // End of Region Identifiers array
  },
       .
       .
       .
```

```
  {...} // Required. A JSON object
], // End of Lines array
"phases": [ // Optional. A JSON array of phase objects
  { // Required. A JSON object of "key": "value" pairs
    "common_name": "<string>", // Optional. A string holding the common name for the phase object
    "compound_ids": [ // Optional. A JSON array of compound identifiers
      <integer>, // Required. An integer holding a unique compound identifier for a compound object
            .
            .
            .
      <integer>
    ], // End of Compound Identifiers array
    "crystal_lattice": "<string>", // Optional. A string holding the determined crystal structure, e.g. cubic, rhombahedral, triclinic, etc.
    "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
    "magnetic_state": "<string>", // Optional. A string holding the name/code of the magnetic state of the phase
    "meta_stable": "<string>", // Optional.  A string holding either "true" or "false" indicating the instability of phase
    "pearson_symbol": "<string>", // Optional. A string holding a description of the crystallographic structure
    "phase_id": <integer>, // Required. An integer holding a unique system phase identifier for a phase object
    "phase_name": "<string>", // Optional. A string holding the name of the phase object
    "sgte_name": "<string>", // Optional. A string holding the codes used in the CALPHAD community to identify specific phases for metal alloy data
    "space_group": "<string>", // Optional. A string holding the description of symmetry of phase using space group
    "space_group_number": <integer>, // Optional. An integer specifying the assignment of symmetry in crystal by space group number
    "strukturbericht": "<string>", // Optional. A string specifying the classification of phase according to Strukturbericht journal
    "super_conductive": "<string>", // Optional. A string holding either "true" or "false" indicating if the phase is in a super conductive state
    "type": "<string>", // Required. A string holding the code or decoded string of the type of phase. I.E. "L" for a liquid phase
    "wyckoff_sequence": "<string>" // Optional. A string specifying the description of atom locations in the phase
  },
        .
        .
        .
  {...} // Required. A JSON object
], //End of Phases array
"phase_fields": [ // Optional. A JSON array of phase_field objects
  { // Required. A JSON object of "key": "value" pairs
    "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY; YYYY-MM-DD
    "phases": [ // Required. A JSON array holding the JSON object of phase_id and zero_phase_fraction
      { // Required. A JSON object of "key": "value" pairs of phase_id and zero_phase_fraction
        "phase_id": <integer>, // Required. An integer holding the unique phase identifier for a phase object
        "zero_phase_fraction": "<string>" // Required. A string  holding either "true" or “false” indicating whether this phase is in a zero
                                          // phase fraction status (I.E. on a boundry)
      },
            .
            .
```

```
                .
      {} // Required. A JSON object of "key": "value" pairs of phase_id and zero_phase_fraction
     ], // End of Phase and Zero Phase Fraction Identifiers array
     "phase_field_id": <integer>, // Required.  An integer holding a unique system phase_field identifier for a phase field object
     "point": "<string>" // Optional. A string  holding either "true" or "false" indicating whether the phase_field defines a point like a Eutectic,
                                 // Eutectoid, or Peritectoid
   },
          .
          .
          .
   {...} // Required. A JSON object
  ], // End of PhaseFields array
  "regions": [ // Optional. A JSON array of region objects
   { // Required. A JSON object of "key": "value" pairs
    "complete": "<string>", // Optional. A string holding either "true" or "false" indicating if the region has been defined completely
    "date_added": "<string>", // Optional. A date string in one of four formats: Month DD, YYYY; MM/DD/YYYY; Mon-DD-YYYY;  YYYY-MM-DD
    "phase_ids": [ // Required. A JSON array of phase identifiers
     <integer>, // Required. An integer holding a unique phase identifier for a phase object
          .
          .
          .
     <integer>
    ], // End of Phase Identifiers array
    "region_id": <integer>, // Required. An integer holding a unique system region identifier for a region object
    "region_name": "<string>", // Optional. A string holding the name of the region object
    "region_role": "<string>" // Optional. A string holding either the full string description or the code for the role (full region or invariant line/collapsed region)
   },
          .
          .
          .
   {...} // Required. A JSON object
  ], // End of Regions array
  "specimen_ids": [ // Optional. A JSON array of specimen identifiers
   <integer>, // Required. An integer holding a unique specimen identifier for a specimen object
          .
          .
          .
   <integer>
  ], // End of Specimen Identifiers array
  "system_id": <integer> // Required. A unique integer identifier for this system object
},
   .
   .
```

```
        .
      {...} // Required. A JSON object
    ], // End of System array
    "version": { // Optional. A JSON object
      "datetime_added": "<string>", // Required. A datetime string in the format: YYYY-MM-DD HH:Min:Sec
      "notes": "<string>", // Optional. A string holding any notes added to describe the state of the data in this JSON file
      "md5_hash": "<string>" // Required. A generated MD5 hash to uniquely define this specific version of the JSON file
    } // End of Version object
  } // End of Data object
    .
    .
    .
  {...} // Required. A JSON object
 ], // End of Data array
 "number_of_citations": <integer>, // Required. An integer holding the number of elements in the array above
 "saved_state_hash": <string> // Optional. The MD5 hash name of the saved state used to do paging and state operations if paging is requested
} // End of main trunk
```

An example of the output JSON:


```
{
  "TRC_data": [
    {
      "citation": {
        "abstract": "Sections of the phase diagram Al-Mg-Si with up to 35 at.% magnesium and 35 at.% silicon are constructed. The thermodynamic calculation and experimental analysis have shown that the conode of three-phase eutectic equilibrium, corresponding to the maximum temperature of eutectic transformation, does not coincide with the stoichiometric cross section between Al and Mg2Si in the Al-Mg-Si ternary system, but rather occurs toward the magnesium rich side of the ternary diagram. A polythermal cross section, corresponding to this conode, has been constructed. Concentration-temperature parameters of the univariant eutectic transformation, as well as the boundaries of the domain of existence of alloys crystallizing with the formation of only two phases, namely, alpha-Al and Mg2Si, were determined. Modeling of phase equilibria involving solid and liquid phases in the ternary system Al-Mg-Si was carried out. The topology of the phase diagram is stable against a wide range variation of the adjustable parameters; the inherent form of the diagram seems well established. The reasons for this are discussed.",
        "authors": [
          "Barabash, O. M.",
          "Sulgenko, O. V.",
          "Legkaya, T. N.",
          "Korzhova, N. P."
        ],
        "citation_id": 1,
        "citation_key": {
          "author1": "bar",
          "author2": "sul",
```

```
    "authorn": 5,
    "year": 2001
   },
   "citation_string": "@J. Phase Equilib.@ $22$(1), 5 - 11",
   "document_type": "article",
   "doi": "10.1007/s11669-001-0049-3",
   "item_number": "1",
   "journal_abbreviation": "J. Phase Equilib.",
   "journal_fullname": "Journal of Phase Equilibria",
   "status": "captured",
   "title": "Experimental analysis and thermodynamic calculation of the structural regularities in the fusion diagram of the system of alloys Al-Mg-Si",
   "volume": "22",
   "year": 2001
  },
  "compounds": [
   {
    "cas_number": "7429905",
    "compound_id": 24088,
    "compound_name": [
     {
      "name": "aluminum",
      "preferred": 1
     }
    ],
    "formula_extended": "Al",
    "formula_hill": "Al",
    "inchi_key": "XAGFODPZIPBFFR-UHFFFAOYSA-N",
    "molecular_weight": 26.981538
   },
   {
    "cas_number": "7439954",
    "compound_id": 24090,
    "compound_name": [
     {
      "name": "magnesium",
      "preferred": 1
     }
    ],
    "formula_extended": "Mg",
    "formula_hill": "Mg",
    "inchi_key": "FYYHWMGAXLPEAU-UHFFFAOYSA-N",
    "molecular_weight": 24.305
   },
```

```
  {
   "cas_number": "7440213",
   "compound_id": 10879,
   "compound_name": [
    {
     "name": "silicon",
     "preferred": 1
    }
   ],
   "formula_extended": "Si",
   "formula_hill": "Si",
   "inchi_key": "XUIMIQQOPSSXEZ-UHFFFAOYSA-N",
   "molecular_weight": 28.085
  },
  {
   "cas_number": "22831396",
   "compound_id": 29440,
   "compound_name": [
    {
     "name": "magnesium silicide (Mg2Si)",
     "preferred": 1
    }
   ],
   "formula_extended": "Mg_{2}Si",
   "formula_hill": "Mg2Si",
   "inchi_key": "YTHCQFKNFVSQBC-UHFFFAOYSA-N",
   "molecular_weight": 76.695
  }
 ],
 "specimens": [
  {
   "compound_id": [
    24088
   ],
   "description": {
    "initial": "not stated"
   },
   "name": "Al1",
   "specimen_id": 1
  },
  {
   "compound_id": [
    24090
```

```
    ],
    "description": {
      "initial": "not stated"
    },
    "name": "Mg1",
    "specimen_id": 2
  },
  {
    "compound_id": [
      10879
    ],
    "description": {
      "initial": "not stated"
    },
    "name": "Si1",
    "specimen_id": 3
  },
  {
    "compound_id": [
      24088,
      24090,
      10879
    ],
    "history": {
      "history_id": 0,
      "history_string": "Op=T+melt+,mat=Al2O3;Op=P+mcast+cast,mat=copper;Op=H+quen+water;"
    },
    "name": "Al-Mg-Si",
    "parent_id": [
      1,
      2,
      3
    ],
    "phase_purity": 0.0,
    "single_crystal": "false",
    "specimen_id": 4
  }
],
"systems": [
  {
    "compound_ids": [
      24088,
      24090,
```

```
  10879
],
"data_sets": [
  {
    "compiler": "MAT",
    "contributor": "XXX",
    "data": [
      {
        "data_values": [
          {
            "value": 0.00042
          },
          {
            "value": 0.00053
          },
          {
            "value": 0.002549
          },
          {
            "value": 0.00418
          },
          {
            "value": 0.01507
          }
        ],
        "variable_id": 1
      },
      {
        "data_values": [
          {
            "value": 0.02652
          },
          {
            "value": 0.02673
          },
          {
            "value": 0.03055
          },
          {
            "value": 0.03364
          },
          {
            "value": 0.05424
```

```
    }
   ],
   "variable_id": 2
  },
  {
   "data_values": [
    {
     "value": 4
    },
    {
     "value": 4
    },
    {
     "value": 4
    },
    {
     "value": 4
    },
    {
     "value": 4
    }
   ],
   "variable_id": 3
  },
  {
   "data_values": [
    {
     "uncertainty": 10.0,
     "uncertainty_type": "uncertainty",
     "value": 655.39
    },
    {
     "uncertainty": 10.0,
     "uncertainty_type": "uncertainty",
     "value": 645.21
    },
    {
     "uncertainty": 10.0,
     "uncertainty_type": "uncertainty",
     "value": 652.32
    },
    {
     "uncertainty": 10.0,
```

```
        "uncertainty_type": "uncertainty",
        "value": 648.6
       },
       {
        "uncertainty": 10.0,
        "uncertainty_type": "uncertainty",
        "value": 630.93
       }
     ],
     "variable_id": 4
    },
    {
     "data_values": [
       {
        "value": 1
       },
       {
        "value": 1
       },
       {
        "value": 1
       },
       {
        "value": 1
       },
       {
        "value": 1
       },
       {
        "value": 1
       }
     ],
     "variable_id": 5
    }
  ],
  "data_set_id": 1,
  "data_set_type": "G",
  "date_added": "7/16/2015",
  "description": "Fig.6",
  "lines": [
    4,
    12,
    11
  ],
  "phase_fields": [
    1,
```

```
  2
],
"states": [
  {
    "description": "Crystal",
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      "region_role": "Region"
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      "region_role": "Region"
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