ReSpecTh Kinetics Data Format Specification

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ReSpecTh Kinetics Data Format Specification

The ReSpecTh Kinetics Data Format Specification is a set of specifications for an unambiguous definition and storage of combustion experiments and gas kinetics rate coefficient determinations. It uses an XML-type data format to provide a flexible way of data representation and allow for easy extension of the format specification.

The ReSpecTh Kinetics Data Format Specification (ReSpecTh format for short in this document) is directly based on the PrIMe Experimental Data Format (PrIMe 2.0: https://prime.cki-know.org/, PrIMe 3.0: http://primekinetics.org/), and most of the specification is directly derived from the XML elements and attributes defined in PrIMe. Note, that the PrIMe Experimental Data Format does not specify in details how the data should be interpreted and what is required to completely describe an experiment.

The ReSpecTh format as defined in this document is unambiguous and therefore the corresponding data are well interpretable by computer codes. Specification of the ReSpecTh format also extends the PrIMe format with certain elements (such as ignition type definition). As a consequence, the PrIMe experimental format files are not correct ReSpecTh Format files. However, any PrIMe experimental data file can be easily converted to ReSpecTh format.

An XML file adhering to the ReSpecTh format specification should contain all information required for the proper simulation of an experiment using an arbitrary software package. The main XML file should contain reported values and estimated/calculated properties. Additional information that may be needed by certain simulation codes should not appear in the main XML that describes the experiment. Such information may be stored in an additional XML file, named "*[xmlname]*_info.xml", where *[xmlname]* is the name of the main XML file.

The ReSpecTh format specification provides a set of instructions for the interpretation of XML files. It defines XML elements and attributes, and how they must be interpreted within the ReSpecTh Kinetics Data Format Specification and what types of elements must occur within an XML file to be considered a complete data file. Non-necessary elements in a data file can simply be ignored. Also, further XML nodes can be present in the file which will not be interpreted within the ReSpecTh format specification, but can be used to store auxiliary information.

It is possible to obtain DOI identifiers that are specific to a XML file (in addition to the DOI identifier that belongs to a publication). Please contact the authors of this format specification to request DOIs for the files you create.

Versioning

The versioning of the ReSpecTh format is assigned according to the following guidelines:

- A major and minor version will be assigned to all releases of the ReSpecTh format, which will be represented by the "major.minor" format, e.g. "1.5" for major 1, minor version "5".
- If there is an update to the ReSpecTh format that does not invalidate any file created based on the previous release, the minor version will be incremented and the major version will be unchanged. Such an update could mean the following change: "v1.5" → "v1.6"
- If there is an update to the ReSpecTh format that invalidates any file created based on the previous release, the major version will be incremented and the minor version will be assigned zero. Such an update could mean the following change: "v1.6" → "v2.0"
- For each release of the ReSpecTh format, a new documentation version will be realesed. When the documentation is updated, but no changes are made the specification itself (e.g. typos are corrected, or examples are added to the present documentation), the date of release of the documentation will be altered

Elements of XML files

The ReSpecTh Kinetics Data Format is an XML based format. The present document follows the terminology defined by the Document Object Model (DOM) when discussing the XML format, such as “element”, “attribute” and “node”. For further reference see http://www.w3.org/DOM/.

All data are stored in XML elements and the attributes and text nodes of these elements. This section describes what types of elements are defined within the ReSpecTh Kinetics Data Format Specification and how they are to be interpreted. **Element names** are written in bold, and *attribute names* are written in italics.

Three categories of data are defined: mandatory, allowed, and non-handled.

- Mandatory (M) elements and attributes are required to make the file a valid ReSpecTh Kinetics file.
- Allowed (A) elements and attributes are part of the ReSpecTh Kinetics format and are to be interpreted, but their presence is not necessary for the validity (i.e. completeness) of the ReSpecTh Kinetics file.
- Non-handled (N) data are not interpreted within the ReSpecTh Kinetics format. Every XML element, attribute or other feature that is not described within this document falls into this category. Also, the elements described in the present specification outside their defined context fall into this category.

  Any amount of non-handled data can be present in a ReSpecTh Kinetics file without invalidating it. Non-handled data usually provide information that is not directly relevant to an experiment but it was considered important by the authors of the XML to include it within a file.

In this section the elements of the ReSpecTh Data Format Specification are defined. For each element, its parent, valid children and attributes, and the interpretation of a text child node are defined. Two slightly different schemes are used for the description of indirect (e.g. ignition delay time, laminar burning velocity, etc.) and direct (rate coefficient) measurements. The differences are the name of the root element, and what elements are considered mandatory. In the description of elements that are child elements of the root element, the mandatory/allowed/non-handled state (M/A/N) is given independently for both direct and indirect measurements.

Root elements

Each ReSpecTh Kinetics file must have a single root element with the name **experiment** if the file describes an indirect experiment, and **kdetermination** in the case of measured reaction rate coefficients ("direct measurement") or theoretically determined rate coefficients.

<table>
<tr><td colspan="2">experiment</td><td>experiment – M</td><td>kdetermination – N</td></tr>
<tr><td>Child of</td><td>None</td><td>Children</td><td>- fileAuthor – M
- fileDOI – A
- fileVersion – A
- ReSpecThVersion – M
- bibliographyLink – M
- experimentType – M
- apparatus – A
- commonProperties – A
- dataGroup – M
- ignitionType – M/N; see element def.
- timeshift – A/N; see element def.
- comment – A</td></tr>
<tr><td>Attributes</td><td>None</td><td>Text child</td><td>None</td></tr>
<tr><td colspan="4">Description
Root element to describe an indirect experiment. Possible types of indirect experiments are measurements of ignition delay times, laminar burning velocities, concentration profiles measured as a function of time, distance or varying experimental conditions (e.g. reactor temperature).</td></tr>
</table>

kdetermination		experiment – N	kdetermination – M
Child of	None	**Children**	**- fileAuthor** – M **- fileDOI** – A **- fileVersion** – A **- ReSpecThVersion** – M **- reaction** – M **- bibliographyLink** – M **- apparatus** – A/N **- commonProperties** – A **- dataGroup** – M **- method** – N/A **- comment** – A
Attributes	None	**Text child**	None
Description Root element to describe a direct experiment (i.e. a measurement of a reaction rate coefficient) or a theoretical rate determination.			

xmlinfo		experiment – A	kdetermination – A
Child of	None	**Children**	**- fileAuthor** – M **- referenceFileDOI** – A **- referenceXMLFile** – M **- fileVersion** – A **- ReSpecThVersion** – M **- plottingInfo** – A **- modelingInfo** – A **- keywords** – A **- comment** – A
Attributes	None	**Text child**	None
Description Root element for an additional XML file containing information that are not required for a description of an experiment, but may be needed for simulations or further data processing. Note that this root element should only appear in a separate file, the additional XML file named "*[xmlname]*_info.xml", where *[xmlname]* is the name of the main XML file.			

Common data elements

fileAuthor		experiment – M	kdetermination – M
Child of	**- experiment** **- kdetermination** **- xmlinfo**	**Children**	None
Attributes	None	**Text child**	author of the file as a string – M
Description The **fileAuthor** element contains the author of the file (not the data) as the value of the element.			

fileVersion		experiment – A	kdetermination – A
Child of	**- experiment** **- kdetermination** **- xmlinfo**	**Children**	**- major** – A **- minor** – A
Attributes	None	**Text child**	None
Description The **fileVersion** element can be used to track the revisions of a file. While it is not mandatory, it is recommended for users to use the **fileVersion** element for this purpose. Two children elements, major and minor are also provided, to track the major and minor file versions. A version tracking system for the individual files within the ReSpecTh format, as each user might have different preferences. It is recommended to add a **comment** to describe the changes of a file between two file versions.			

ReSpecThVersion		experiment – M	kdetermination – M
Child of	**- experiment** **- kdetermination** **- xmlinfo**	**Children**	**- major** – M **- minor** – M
Attributes	None	**Text child**	None
Description The **ReSpecThVersion** element defines which version of the ReSpecTh Kinetics Data Format Specification a file adheres to. It has two child elements, **major** and **minor**, containing the major and minor version numbers as text nodes respectively.			

Specific data elements of root elements experiment *and* kdetermination

fileDOI		experiment – A	kdetermination – A
Child of	**- experiment** **- kdetermination**	**Children**	None
Attributes	None	**Text child**	DOI of the file as a string – A
Description The **fileDOI** element can be used to specify a unique digital object identifier (DOI) that belongs to the dataset. Please contact the authors of this format specification to request DOIs for the files you create. Do not add prefixes such as "http://dx.doi.org/" to the **fileDOI**.			

bibliographyLink		experiment – M	kdetermination – M
Child of	**- experiment** **- kdetermination**	**Children**	**- description** – M **- referenceDOI** – A **- location** – A **- table** – A **- figure** – A
Attributes	None	**Text child**	None
Description The **bibliographyLink** element contains the bibliographic reference to the source of the experimental data. An unformatted string has to be defined in the child element **description**. This may contain the name of the authors of the corresponding publication, journal name, page numbers etc. The ReSpecTh format specification can be used to encode own, unpublished measurements. In this case, we suggest to provide a meaningful description of the measured data series in the child element **description**. For easier backtracking of the data found in the XML file, it is strongly recommended to add the DOI of the corresponding publication in the child element **referenceDOI**. Do not add prefixes such as "http://dx.doi.org/" to the **referenceDOI**. If the character "<" appears in the DOI, replace it by "#", if the character ">" appears in the DOI, replace it by "$". Additional child elements may help the users of XML files to locate the data in the corresponding publication: **location** (e.g. "Main article" or "Supplementary Material"), **table** (e.g. "Table 1, high-pressure series") and **figure** (e.g. "Figure 2, blue circle"). If data occurs at multiple places within the same paper (e.g. in a summary **table** and a **figure**), we suggest to include both information in the **bibliographyLink**, but indicate the sources which were NOT used for the creation of the XML file (e.g. "Figure 2 (not used)").			

experimentType		experiment – M	kdetermination – N
Child of	- **experiment**	**Children**	None
Attributes	None	**Text child**	experiment type as a string
Description The **experimentType** element defines the experiment type for indirect experiments. The possible values are the following: - ignition delay measurement - laminar burning velocity measurement - outlet concentration measurement - concentration time profile measurement - jet stirred reactor measurement - burner stabilized flame speciation measurement			

apparatus		experiment – A	kdetermination – A/N
Child of	- **experiment** - **kdetermination**	**Children**	- **kind** – A - **mode** – A (multiple instances possible)
Attributes	None	**Text child**	None
Description The **apparatus** element contains the apparatus type, as the text child node of child element **kind,** and the operation mode as the text child node of the **mode** child element(s). The **apparatus** element is used to provide additional information about the experimental apparatus used for experiments described in a file (either indirect experiments with the root element **experiment** or indirect measurements with the root element **kdetermination**).			

method		experiment – N	kdetermination – A
Child of	- **kdetermination**	**Children**	None
Attributes	None	**Text child**	Name of the method as a string – A
Description The **method** element can be used to describe the experimental method that was used in a direct measurement (e.g. “laser photolysis, laser-induced fluorescence”) or the method used in a theoretical determination study (e.g. “VTST”).			

commonProperties		experiment – A	kdetermination – A
Child of	- **experiment** - **kdetermination**	**Children**	- **property** – A
Attributes	None	**Text child**	None

Description

The **commonProperties** element contains **property** elements describing the physical properties that are constant across all experiments within the file. These are the initial conditions for an experimental dataset e.g. the initial gas composition for a flow reactor experiment, or auxiliary data that are required for a full description of the experiment (e.g. rate of pressure rise in a shock tube).

The values of the properties are stored within **property** elements.

It should be noted that a **commonProperties** element is not mandatory, as it is possible that all experimental conditions were varied within the dataset that is described in a single file and none was kept constant. This is, however, not very likely and files will typically contain this element.

dataGroup		experiment – M	kdetermination – M
Child of	- **experiment** - **kdetermination**	**Children**	- **property** – M - **dataPoint** – M
Attributes	- *id* – M - *label* – A - *dataPointLink* – M/N, see below	**Text child**	None

Description

The **dataGroup** element contains **property** elements describing the physical properties that are varied across the experiments within the file if multiple experiments are recorded in the file, or change within one experiment if the data file describes multiple measurements made during a single experiment.

These properties can be varied initial conditions (e.g. temperature in a series of ignition delay measurements), the independent variable within a single experiment (e.g. reaction time in a flow reactor), and the respective experimental results (e.g. ignition delays, concentrations).

It also contains the corresponding data in the **dataPoint** elements. For the details of the data storage, see the description of **dataPoint**.

The *id* attribute is a mandatory for the **dataGroup** element. The *id* attributes of data groups usually follow the progression "**dg1**", "**dg2**", but can have any other name.

The *label* attribute may contain a string that describes the type of data that is grouped in a dataGroup. This can be useful e.g. to distinguish a **dataGroup** containing the properties volume and time from the primary one containing the measured data.

A data point link has to be provided via the *dataPointLink* attribute, if the non-primary **dataGroup** contains a pressure-time history, volume-time history or temperature-time history. It is by default "all" (which can be specified as such, too). If it shall only be used for selected points of the primary **dataGroup**, the value of this attribute should be specified e.g. as "1" for the 1st point in order of occurrence. Multiple links may be used. In this case, all linked data points have to be separated with a semicolon, e.g. "1;2;5;6;" for the value of the *dataPointLink* attribute.

comment		experiment – A	kdetermination – A
Child of	- **experiment** - **kdetermination**	**Children**	None
Attributes	None	**Text child**	Comment as a string – A

Description

The **comment** element can be used to provide information that are necessary for a complete understanding of the nature or origin of the data described in the XML file (e.g. if parts of the data are taken from another source). It may also be used to provide information about the estimation or calculation of certain properties (e.g. the oxidizer composition used for the calculation of mole fractions from the equivalence ratio).

ignitionType		experiment – M/N; see below	kdetermination – N
Child of	- **experiment**	**Children**	None
Attributes	- *target* – M - *type* – M - *amount* – A - *units* –A - *operation* – A	**Text child**	None

Description

An **ignitionType** element describes how the ignition delay was defined in an ignition delay measurement file. It is mandatory in such a file, and non-handled otherwise.

The attribute *target* defines the physical property on which the ignition delay definition is based. This can be pressure, temperature or the concentration of a species. These are to be denoted by "p", "T", and the name of the species (e.g. OH), respectively. If the ignition delay is defined based on multiple physical properties, e.g. the product of the CO and O_2 mole fractions, the *target* attribute should contain all names separated by semicolons.

The attribute *type* defines which feature of the measured physical property is considered for the ignition delay. Valid values are summarized in the following table:

Valid ignition types	
***type* value**	**Description**
max	The ignition delay is the time at which the maximum of the target physical property was measured
d/dt max	The ignition delay is the time at which the maximum of slope of the target physical property was measured
baseline max intercept from d/dt	Extrapolation to the initial baseline concentration, from the maximum slope. The max/min defines if the slope is negative/positive, therefore if the target species is being depleted/produced respectively.
baseline min intercept from d/dt	
concentration	The ignition delay is the time at which the concentration of the target species reached a specified concentration value
relative concentration	The ignition delay is the time at which the concentration of the target species reached a specified concentration value relative to its maximum concentration

The attribute *amount* defines the absolute or relative concentration value the target species has to reach for ignition to occur. This attribute can only be used when the value of *type* is "concentration" or "relative concentration".

The attribute *units* defines the unit of the concentration value defined in the attribute *amount*. This attribute can only be used when the value of *type* is "concentration" or "relative

concentration". The same units can be used here as for "concentration" or "composition" type properties (e.g. "mole fractions" or "molecule cm-3").

The attribute value *"unitless"* should be assigned to relative fproperties (e.g. a 5% uncertainty has the attributes *units="unitless"* and *kind="relative"*, and the value 0.05).

timeshift		experiment – A/N; see below		kdetermination – N
Child of	- **experiment**	**Children**	None	
Attributes	- *target* – M - *type* – M - *amount* – A	**Text child**	None	

Description

A **timeshift** element describes how the simulated species profile should be shifted in a species profile measurement file. It is mandatory in such a file, and non-handled otherwise.

The time shifting of species profiles is a widely technique used during the interpretation of species profile measurements in flow reactors. To account for an unknown amount of mixing and heating time, the simulated profiles are shifted in time to match a feature (e.g. the time of the half depletion of the fuel) of the experimental profiles. Even if multiple species were measured in a single experiment the same amount is used for each profile.

The attribute *target* defines the physical property on which the time shift is based. This must be the name of a single measured species.

The attribute *type* defines which part of the specified species profile is matched with the experiments. The valid types are summarized in the following table.

Valid timeshift types

***type* value**	**Description**
half	The half concentration relative to the maximum concentration of the specified species is matched between the experiment and simulation.
inflexion	The inflexion point of the specified profile is matched between the experiment and simulation.
relative	A concentration relative to the maximum concentration of the specified species is matched between the experiment and simulation. In this case an *amount* attribute is mandatory and contains the value of the relative concentration that is matched.

Note

The *type* value also has to be followed by "increase" or "decrease". This defines if the target species is being produced or depleted respectively.

Therefore a valid *type* value would be "half decrease" if the half depletion of the species is used for the time shifting.

The attribute *amount* defines the relative concentration value of the target species that is used to match the experiment and the simulation. This attribute can only be used when the value of *type* is “relative increase” or “relative decrease”.

In the current version of the ReSpecTh Kinetics Data Format Specification, it is not possible to define a fixed (i.e. absolute) time shift.

reaction		experiment – N	kdetermination – M
Child of	- **kdetermination**	**Children**	None
Attributes	- *preferredKey* – M - *order* – M - *bulkgas*– M	**Text child**	None

Description

The **reaction** element defines the reaction for which the rate coefficients that are recorded in a file were measured.

The *preferredKey* attribute contains the reaction string which defines the reaction. The reaction string must contain “LP” or “HP” before the first species separated by a space, if the rate coefficients measured are at the low pressure or high pressure limit respectively, for pressure dependent reaction rate coefficients. (e.g. “LP H+O2+M=HO2+M”)

The reaction string can contain the word “PRODUCTS” in place of the actual products. In this case, the rate coefficient is be interpreted as the sum of all reaction channels with the same reactants. (e.g. “C2H5OH+M=PRODUCTS” means all ethanol decomposition channels)

The *order* attribute contains the order of the reaction.

The *bulkgas* attribute defines the bath gas (as the name of the species) in which rate coefficient was measured. It is possible to provide a detailed experimental gas composition using appropriate **property** elements in the **commonProperties** or **dataGroup** elements. If this is provided then the detailed composition must be considered, and the *bulkgas* attribute must be ignored.

However, in many cases this information is not available, yet it is important to know the bath gas to account for third body collision effects. Also, for non-pressure dependent rate coefficients the detailed gas composition has no influence on the rate coefficients.

Multiple **reaction** elements can be present in a single file. In this case the sum of the reaction rate coefficients of all **reactions** defined in all **reaction** elements are recorded in the file.

property			
Child of	- **commonProperties** - **dataGroup**	**Children**	- **value** – M/N; see below - **component** – M/N; see below - **speciesLink** – M/N; see below
Attributes	- *id* – M/N; see below - *label* – A - *name* – M - *sourcetype* – M - *units* – M/N; see below - *reference* – M/N; see below - *kind* – M/A/N; see below - *bound* – M/N; see below	**Text child**	None

Description

A **property** element describes a physical property that was measured during the experiment or was one of the initial conditions that was set for the experiment. A **property** element can occur in a **commonProperties** element, where it describes an initial condition of the experiment, and its numerical value has to be given as the value of the element.

If a **property** element occurs as the child of the **commonProperties** element, and its type (*name* value) is not „initial composition", it must have a **value** child element, which contains its numeric value as a text child node. If it is an „initial composition" property, then it must have **component** children elements that define the component species of the initial composition.

A property element can also occur in a **dataGroup** element, where it defines a physical property that was varied between experiments or is measured as a function of another **property** within a single experiment. The numerical values will be given in the **dataPoint** children elements of the current **dataGroup**, in children elements with names corresponding to the *id* values of the **property** elements of the **dataGroup**.

If a property element occurs as the child of the **dataGroup** element, and it describes data corresponding to a species (a "concentration" or "composition" type property), then a **speciesLink** child element is mandatory, which defines the species to which the **property** corresponds.

The *id* attribute is mandatory only if the property element is the child of a **dataGroup** element, otherwise it is non-handled. It contains the name of the child element of the **dataPoint** elements in which the corresponding numerical values will appear. The *id* attributes within a **dataGroup** usually follow the progression "**x1**", "**x2**", "**x3**", but can have any other name.

The *label* attribute contains a string that is the short notation of the physical property, e.g. for a temperature property, the *label* is usually "T".

The *name* attribute is a string that defines the type of the physical property. The accepted values are summarized in the following table:

The *kind* attribute is a string that can be used to define the nature of a physical property (e.g. if a pressure rise is "relative"). It is mandatory for the property *name* "uncertainty", and an allowed or non-handled attribute for all other properties.

Valid property *name* types (M/N depending on the **experimentType**; "uncertainty" and "equivalence ratio" are always A)	
temperature	length
pressure	density
volume	flow rate
time	laminar burning velocity
residence time	initial composition
distance	composition
ignition delay	concentration
rate coefficient	uncertainty
equivalence ratio	

If the property *name* type is "uncertainty", three more attributes are mandatory:

- The attribute *reference* contains the *name* of the property to which the specified uncertainty refers.
- The attribute *kind* describes the kind of uncertainty. It can have the values "absolute" and "relative"
- The attribute *bound* specifies the type of uncertainty bound(s): "plus", "minus" or "plusminus"

The property *name* type "equivalence ratio" is often reported in the literature. An exact knowledge of the composition of the oxidizer as well as information regarding the dilution of the mixture with additional gases is required. Although there is a potential for redundancy, the parallel definition of *equivalence ratio* and *composition* (or *concentration*) is legal, as long as the *type* attributes differ (see next paragraph).

The *sourcetype* attribute can be either "reported" (if the **property** was found in the corresponding literature reference), "digitized" (if the **property** was reported, but had to be digitized from a plot by the creator of the XML file), "calculated" (if the **property** was calculated during data processing, e.g. as a result of unit conversion) or "estimated" (if the **property** was estimated during data processing using some kind of assumption, e.g. a composition calculated using the not explicitly reported composition of air).

The *units* attribute contains the physical unit of the numeric values corresponding to the **property**. It is mandatory in all cases, except if its type (*name* value) is „initial composition", where it is non-handled.

In this case, the units are defined within each **component** child element.

component			
Child of	- **property**	**Children**	- **amount** – M - **speciesLink** – M
Attributes	None	**Text child**	None

Description

The **component** element can only occur as a child element of an "initial composition" **property** element as a host for a **speciesLink** element, and a corresponding **amount** element. The **speciesLink** is used to identify the species and the **amount** element is used to define the amount of the species in the initial composition.

speciesLink			
Child of	- **property** - **component**	**Children**	None
Attributes	- *preferredKey* – M - *CAS* – A - *InChI* – A - *SMILES* – A - *chemName* – A	**Text child**	None

Description

The **speciesLink** element is used to identify the species to which a "composition" or "concentration" type **property** element or a **component** element refers. It is also necessary when a **property** "uncertainty" has the *reference* "composition" or "concentration".

If a **property** shall be defined as the sum of several species, multiple **speciesLink** blocks occurring after one another should be specified.

The name of the species is stored within the *preferredKey* attribute as a string. The *CAS* attribute serves as an unambiguous form of identification of chemical species. The CAS Registry Number of the species is stored within the *CAS* attribute as a string. Such identification numbers can be found in various online databases, e.g. http://www.commonchemistry.org/index.aspx.

As alternatives to *CAS*, the *InChI* and *SMILES* identifiers can be used to identify species. Note that the standard InChI string should be used, not the InChIKey which is a hashed version of the standard InChI string. If the user prefers using SMILES identifiers, a canonical identifier should be used. Note that typically, a number of equally valid SMILES strings can be written for a single molecule which may cause ambiguity.

In addition to the mandatory *preferredKey* and the allowed attributes *CAS*, *InChI* and *chemName* may be used to denote the chemical name of a certain species.

Example:

<speciesLink preferredKey="C2H5OH" chemName="ethanol" CAS="64-17-5"
InChI="1S/C2H6O/c1-2-3/h3H,2H2,1H3 " SMILES="CCO"/>

dataPoint			
Child of	**- dataGroup**	**Children**	see below
Attributes	None	**Text child**	None

Description

Contains as many children elements as many properties were defined in the **dataGroup** of which the **dataPoint** is a child of. These children have names corresponding to the *id* attributes of the **property** elements contained in the **dataGroup**. In each **dataPoint** the numeric values of the corresponding properties are stored in the corresponding child element. Each **dataPoint** corresponds to a measured data point, which can represent an experiment by itself, or a single point measured during the course of an experiment. Contains the values of both the independent and dependent variables of the experiment, and the content of the corresponding **property** elements contain the relevant information.

Specific data elements of root element **xmlinfo**

referenceFileDOI		experiment – A	kdetermination – A
Child of	**- xmlinfo**	**Children**	None
Attributes	None	**Text child**	DOI of the related main XML file as a string – A
Description The **referenceFileDOI** element is the counterpart of **fileDOI** that should have the same content as a text child. A distinction is made here to avoid the false assumption that a separate DOI should be requested/assigned for an addition XML file.			

referenceXMLFile		experiment – M	kdetermination – M
Child of	**- xmlinfo**	**Children**	None
Attributes	None	**Text child**	Name of the related XML file as a string – M
Description The **referenceXMLFile** element is mandatory if an additional XML file exists. The naming scheme "*[xmlname]*_info.xml" isrecommended. The element should contain the string "*[xmlname]*.xml" as its text child.			

keywords		experiment – A	kdetermination – A
Child of	**- xmlinfo**	**Children**	**- item** (multiple instances possible)
Attributes	None	**Text child**	Keyword(s) as a string in the child element – A
Description The **keywords** element may contain keywords associated with the experiment or the publication.			

modelingInfo		experiment – A	kdetermination – A
Child of	**- xmlinfo**	**Children**	**- item** (multiple instances possible)
Attributes	None	**Text child**	Comment as a string in the child element – A
Description The **modelingInfo** element may be used to provide solver-specific information.			

plottingInfo		experiment – A	kdetermination – A
Child of	- **xmlinfo**	**Children**	- **Xaxis** – M/N; see below - **Yaxis** – M/N; see below - **speciesLink** – M/N; see below
Attributes	No attributes of the main element. Attributes of the child elements are: - *name* – M - *units* – M - *scale* – M - *label* – A - *reference* – M/N; see below - *kind* – M/N; see below - *bound* – M/N; see below	**Text child**	None

Description

The element **plottingInfo** and its children can be used to specify which **property** names appearing in the main XML file should be plotted. If the element is specified, *name, units* and *scale* are mandatory.

While *name* has to match the *name* of a **property** in the main XML file, *units* can have a different value depending on the type of property (see Section "Summary of valid units"). The attribute *scale* can take the values "lin" (linear axis), "inv" (inverse axis), "log10" (decadic logarithmic axis) and "ln" (natural logarithmic axis).

The *label* attribute contains a string that is the short notation of the physical property and may be used as the label in case of plotting, e.g. for a temperature property, the *label* is usually "T".

If the specified *name* is "uncertainty", additional attributes of the child element are mandatory:

- *reference* containing the *name* of the property to which the specified uncertainty refers.
- *kind* describing the kind of uncertainty. It can have the values "absolute" and "relative"
- *bound* specifying the type of uncertainty bound(s): "plus", "minus" or "plusminus"

Note that several **Yaxis** child elements may be specified, e.g. for different species to be plotted, or when an uncertainty information corresponding to a certain property shall be added to the plot.

If a **property** element to be plotted describes data corresponding to a species (a "concentration" or "composition" type property), then a **speciesLink** child element is mandatory, which defines the species to which the property corresponds. If a property shall be defined as the sum of several species, multiple **speciesLink** blocks occurring after one another have to be specified.

Several **Xaxis** elements may only be used for a selected property and its related uncertainty. If you wish to create plots with different **Xaxis** properties, please use separate **plottingInfo** blocks.

dataGroup		experiment – A	kdetermination – A
Child of	- **xmlinfo**	**Children**	- **property** – M - **dataPoint** – M
Attributes	- *id* – M - *label* – A - *dataPointLink* – M/N, see below	**Text child**	None

Description

The **dataGroup** element as a child of **xmlinfo** should only be used for reported information that are too large for an efficient handling of the main XML file, e.g. pressure–time histories. Volume–time histories, which were converted from pressure–time histories (and potentially smoothened and/or sampled) should occur in the main XML file.

The **dataGroup** element contains **property** elements. It also contains the corresponding data in the **dataPoint** elements. For the details of the data storage, see the description of **dataPoint**.

The *id* attribute is mandatory in **xmlinfo** files and has to match the *id* attribute of the corresponding **dataGroup** in the main XML file. These *id* attributes of data groups also usually follow the progression "**dg1**", "**dg2**", but can have any other name.

The *label* attribute may contain a string that describes the type of data that is grouped in a dataGroup. This can be useful e.g. to distinguish a **dataGroup** containing the properties volume and time from the primary one containing the measured data.

A data point link has to be provided via the *dataPointLink* attribute, if the non-primary **dataGroup** contains a pressure-time history, volume-time history or temperature-time-history. It is by default "all" (which can be specified as such, too). If it shall only be used for selected points of the primary **dataGroup**, the value of this attribute should be specified e.g. as "1" for the 1st point in order of occurrence. Multiple links may be used. In this case, all linked data points have to be separated with a semicolon, e.g. "1;2;5;6;" for the value of the *dataPointLink* attribute.

Description of the XML structure for different experiment types

The ReSpecTh Kinetics Data Format can be used to describe ignition delay, laminar burning velocity measurements, concentration profiles measured as a function of time, distance or varying experimental conditions (e.g. reactor temperature). These types altogether are called "indirect experiment types". Reaction rate coefficients can also be stored using the ReSpecTh Kinetics Format, and these are called "direct measurements" or "theoretical rate determinations".

This section describes which data are mandatory and allowed for each experiment type.

Common features

Data files describing indirect experiment types must have a root element named **experiment**, and those describing direct data files must have a root element named **kdetermination**.

The root element must have the following children elements (for details see section *Elements of the data format*)

- **fileAuthor** – Author of the file (not the data)
- **ReSpecThVersion** – ReSpecTh specification version followed by the file
- **bibliographyLink** – Bibliographic data of the source publication
- **dataGroup** – The measured dataset (experimental conditions, measured values)

A **commonProperties** element is also almost always present in all files. This contains the experimental conditions that are constant over the whole dataset.

The **ReSpecThVersion** element defines which version of the ReSpecTh Kinetics Data Format Specification a file was created. This way even if the ReSpecTh format is modified in a non-backwards compatible way, the correct way for interpretation can be identified for any file.

For indirect experimental files, an **experimentType** and **apparatus** element is also necessary, which are non-handled for direct experiments. These define the type of the experiment and experimental apparatus respectively.

In the following subsections the mandatory and allowed types of physical properties are listed and how they are to be interpreted. All physical properties have to be defined in **property** elements, as children of either the **commonProperties** or **dataGroup** elements. Properties in the **commonProperties** element describe the experimental conditions common for all experiments described in the data files, and those in the **dataGroup** element correspond to those experimental conditions that were varied between the experiments and the measured values.

For each property it is specified whether it can occur in the **commonProperties** (C for "constant"), **dataGroup** (V for "variable") or both (C/V). It should be noted that a composition type **property** in the **commonProperties** is defined differently from all other **property** elements. For details, see the detailed description of the **property** element. The possible units are also given for each type property in a summarized form in the "Summary of valid units" section.

experiment: *ignition delay measurement*

Ignition delay measurements can describe data measured in shock tubes or rapid compression machines (RCMs). The initial state of the reactive mixture must be defined by the temperature, pressure and composition. If it is known that the system cannot be described adiabatically, e.g. due to pressure rise in a shock tube, or heat losses in a rapid compression machine, an equivalent volume–time history can also be defined that describes these effects, or a constant pressure rise factor. The measured values are ignition delays, and the definition of the ignition must be defined in the **ignitionType** child element of the root element.

For shock tube data, the initial state defined in the file should correspond to the state behind the reflected shock wave (usually denoted by p_5 and T_5). It is useful to encapsulate this information in the **apparatus** element

Example: For a reflected shock tube measurement, the child element **kind** should be specified as "shock tube", and the **mode** should be "reflected". Accordingly, the **mode** of an experiment at incident shock wave should be "incident".

For rapid compression machine data the initial state should correspond to the beginning of the corresponding volume–time history. The volume–time history can begin before the start of the compression phase of the experiment or to the state at the end of the compression phase. In either case the ignition delay should be interpreted as the delay compared to the end of the compression phase.

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C/V	The temperature behind the reflected shock wave in a shock tube experiment. For an RCM experiment this can be the temperature before the start of the compression, or the temperature at the end of compression, depending on the accompanying volume–time history.
pressure	C/V	The pressure behind the reflected shock wave in a shock tube experiment. For an RCM experiment this can be the pressure before the start of the compression, or the pressure at the end of compression, depending on the accompanying volume–time history.
composition	C/V	The composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
ignition delay	V	The measured ignition delay. For an RCM experiment the delay should be given compared to the end of compression, even if a volume–time history is available from the beginning of compression.

Allowed properties		
Property	**C/V**	**Notes**
volume	V	A volume **property** can be given in a **dataGroup** separate from the primary one, to provide a volume–time history for an ignition experiment. It has to be accompanied by a time property in the same **dataGroup**, to provide the corresponding time values. A data point link has to be provided via the *dataPointLink* attribute, which is by default "all" (which can be specified as such, too). If a volume–time histories shall only be used for selected points of the primary **dataGroup**, the value of this attribute should be specified e.g. as "1" for the 1st point in order of occurrence. Multiple links may be used. In this case, all linked data points have to be separated with a semicolon, e.g. "1;2;5;6;" for the value of the *dataPointLink* attribute. A volume–time history cannot be used together with a constant pressure rise value.
temperature	C/V	A temperature **property** can be given in a **dataGroup** separate from the primary one, to provide a temperature–time history for a concentration experiment. It has to be accompanied by a time property in the same **dataGroup**, to provide the corresponding time values. A *dataPointLink* attribute link has to be provided. For details, see the above description of the property "volume".
pressure	C/V	A pressure **property** can be given in a **dataGroup** separate from the primary one, to provide a pressure–time histoprery for a concentration experiment. It has to be accompanied by a time property in the same **dataGroup**, to provide the corresponding time values. A pressure–time history cannot be used together with a temperature–time history in certain simulation codes (*e.g.* CHEMKIN-II). A *dataPointLink* attribute link has to be provided. For details, see the above description of the property "volume".
time	V	The time values for a volume–time history.
pressure rise	C	A constant pressure rise can be defined to represent the pressure rise behind the reflected shock wave due to shock attenuation. A constant rise can be defined relative to the initial pressure. *Example:* <property label="dp/dt" name="pressure rise" sourcetype="reported" units="ms-1" kind="relative"> <value>0.05</value></property> At an initial pressure of 2 bar, a relative pressure rise value of 0.05 ms^{-1} means that the pressure rises by 0.1 bar every millisecond. A pressure rise cannot be used together with a volume–time history.

experiment: *laminar burning velocity measurement*

To describe laminar burning velocity measurement data the composition and state of the initial gas mixture has to be defined, and the corresponding measured laminar burning velocity.

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C/V	Unburned gas temperature.
pressure	C/V	Inlet gas pressure.
composition	C/V	The composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
laminar burning velocity	V	The measured laminar burning velocity.

experiment: *concentration time profile measurement*

Concentration time profile measurements describe concentration values measured as a function of the reaction time, typically in a flow reactor or other reactor that can be described by homogeneous kinetics. The state and composition of the inlet or initial gas mixture has to be defined, along with the measured time – concentration values.

If the measurements should be interpreted with a time shifting compared to the simulated values, this can be defined with a **timeshift** child element of the root element.

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C	Inlet gas temperature.
pressure	C	Inlet gas pressure.
initial composition	C	The composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
time	V	The time values at which concentrations were measured.
composition	V	The measured species mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.

experiment: *outlet concentration measurement*

Outlet concentration measurements describe concentration values that were measured as the outlet of an adiabatic homogeneous reactor (e.g. final product distributions measured from turbulent flow reactors or shock tubes). Jet-stirred reactor outlet (i.e. end) concentrations are handled as a separate case (see below). The initial state and composition of the gas must be defined and the measured outlet concentrations after a given residence time.

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C/V	Inlet gas temperature.
pressure	C/V	Inlet gas pressure.
residence time	C/V	Residence time of the reactive mixture in the reactor.
initial composition	C	The composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
composition	V	The measured species mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.

experiment: *burner stabilized flame speciation measurement*

Burner stabilized flame speciation measurements describe speciated flame measurements. The inlet gas state, composition and flow rate must be defined, and the measured concentrations have to be defined as a function of the distance from the burner.

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C	Inlet gas temperature.
pressure	C	Inlet gas pressure.
flow rate	C	Mass flow rate of the inlet gases
initial composition	C	The composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
distance	V	The distance values from the burner at which the species concentrations were measured.
composition	V	The measured species mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.

experiment: *jet-stirred reactor measurement*

Jet-stirred reactor measurements describe concentration values that were measured at the outlet of a jet-stirred reactor (or perfectly stirred reactor), i.e. they represent end concentrations. The initial state and composition of the gas must be defined, along with the reactor volume and the measured outlet concentrations after a given residence time.

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C/V	Inlet gas temperature.
pressure	C/V	Inlet gas pressure.
residence time	C/V	Residence time of the reactive mixture in the reactor.
volume	C/V	Volume of the reactor
initial composition	C	The initial composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
composition	V	The measured species mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.

kdetermination: *Rate coefficient determinations*

Reaction rate coefficient measurement files contain for a given reaction the rate coefficients measured at various temperatures, pressures and gas compositions. Defining the pressure and gas composition in a data file is not necessary, as these are only relevant for pressure dependent reactions.

The reaction for which the data are contained in the file is stored in a **reaction** element. If the sum of the rate coefficient of two or more reactions is to be stored in a file, these reactions should be stored in separate **reaction** elements. Alternately, a single **reaction** element can define the sum of all (or selected) branches for a given set of reactants. For details on defining the reaction, see the description of the **reaction** element.

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C/V	Temperature at which the rate coefficient was measured.
rate coefficient	V	Inlet gas pressure.

Allowed properties		
Property	**C/V**	**Notes**
pressure	C/V	Pressure at which the rate coefficient was measured. This is only relevant for pressure dependent reactions, but can be defined in any case.
composition	C/V	The gas composition in which the rate coefficient was measured. This is only relevant for pressure dependent reactions, but can be defined in any case.

Summary of valid units

In the following table a summary of the unit strings that are currently handled within the ReSpecTh Kinetics Data Format Specification is given. Here all strings are given in the exact way as it should appear in the file. This means that exponents are not typed as superscript, and the micro (μ) prefix should be typed as "u" to guarantee that these can be typed in plain text files.

Property type	Valid units
temperature	K
pressure	Pa, kPa, MPa, Torr, torr, bar, mbar, atm
volume	m3, dm3, cm3, mm3, L
time	s, ms, us, ns, min
residence time	s, ms, us, ns, min
time	s, ms, us, ns, min
distance	m, dm, cm, mm
ignition delay	s, ms, us, ns, min
length	m, dm, cm, mm
density	g m-3, g dm-3, g cm-3, g mm-3, kg m-3, kg dm-3, kg cm-3, kg mm-3
flow rate	g m-2 s-1, g dm-2 s-1, g cm-2 s-1, g mm-2 s-1, kg m-2 s-1, kg dm-2 s-1, kg cm-2 s-1, kg mm-2 s-1
laminar burning velocity	m/s, dm/s, cm/s, mm/s, m s-1, dm s-1, cm s-1, mm s-1
composition	mole fraction, percent, ppm, ppb
concentration	mol/m3, mol/dm3, mol/cm3, mol m-3, mol dm-3, mol cm-3, molecule/m3, molecule/dm3, molecule/cm3, molecule m-3, molecule dm-3, molecule cm-3
rate coefficient	s-1, m3 mol-1 s-1, dm3 mol-1 s-1, cm3 mol-1 s-1, m3 molecule-1 s-1, dm3 molecule-1 s-1, cm3 molecule-1 s-1, m6 mol-3 s-1, dm6 mol-2 s-1, cm6 mol-2 s-1, m6 molecule-2 s-1, dm6 molecule-2 s-1, cm6 molecule-2 s-1
pressure rise	ms-1, s-1
all relative properties	unitless

Change log

v1.0 to v2.0

- The root element **kmeasurement** was renamed to **kdetermination**, which allows to encode the results of theoretical reaction rate determinations in a similar manner
- The allowed child **method** was introduced for **kdetermination**
- Instead of the labels “indirect” and “direct”, now the labels “experiment” and “kdetermination” are used throughout the manual
- The root element **xmlinfo** was introduced, which should appear in a separate file named “*[xmlname]*_info.xml”. Other than the common data elements, it has the following unique children: **referenceFileDOI, referenceXMLFile, keywords, plottingInfo, modelingInfo**
- The structure of the mandatory element **bibliographyLink** was changed, which necessitated a major version update:
    - The attribute *preferredKey* was replaced by the mandatory child **description**
    - Allowed children were added: **referenceDOI**, **location**, **table**, **figure**
- The following allowed elements were added:
    - **fileDOI**
    - **comment**
- New *name* types were added to the mandatory element **property**:
    - “uncertainty”
    - “equivalence ratio”
- The *name* type “flame speed” was renamed to “laminar burning velocity”
- New attributes were added to the mandatory element **property**:
    - *sourcetype* (mandatory)
    - *reference, kind, bound* (mandatory if the **property** *name* is “uncertainty”)
- The allowed text children of **experimentType** were revised:
    - All text children now start with lower case letters (e.g. “ignition delay measurement” instead of “Ignition delay measurement”) in accordance with other specifications
    - “Laminar flame speed measurement” was renamed to “laminar burning velocity measurement”, as this term describes the measured quantity more accurately
- The attribute *description* of the property “pressure rise” was renamed to *kind*
- The allowed attributes *CAS, InChI, SMILES* and *chemName* were added to the **speciesLink** element specification
- The initial composition of a concentration measurements has to be defined as “initial composition” – in the old format specification, this was not stated explicitly
- The role *dataPointLink* in **dataGroup** elements is now detailed in a more consistent manner
- Some missing explanations of already existing features were added, others were corrected. If you notice others missing in this manual, please contact the authors! ☺
- The policy of documentation versioning was changed to avoid confusion

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Appendix: Example files

Example files for each type of **experiment** and **kdetermination** can be found in the ZIP archive "example_files.zip", alongside some additional XML files containing **xmlinfo** blocks.

These contain published data and can be found on http://respecth.hu.

Note that the values of the elements **fileDOI**, **modelingInfo** and **keywords** contain dummy values.

Type of data	Example file (with info file)
experiment	
ignition delay measurement (shock tube)	x10003006.xml (x10003006_info.xml)
ignition delay measurement (RCM)	x40003002.xml (x40003002_info.xml)
laminar burning velocity measurement	x23003038.xml (x23003038_info.xml)
outlet concentration measurement	x30003004.xml (x30003004_info.xml)
concentration time profile measurement (flow reactor)	x30003001.xml
concentration time profile measurement (shock tube)	x50003002.xml
jet stirred reactor measurement	x00003001.xml
burner stabilized flame speciation measurement	x60003002.xml
kdetermination	
Experimental/direct rate determination	k10003002.xml (k10003002_info.xml)
Theoretical rate determination	t10003001.xml (t10003001_info.xml)