The RheoML Schema for XML Datafiles

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1 Introduction

The exchange of data between measurement equipment and spreadsheet programs like Microsoft Excel, Sigmaplot or Origin suffers from a non-standardized file format. The content of the data files differ from manufacturer to manufacturer and sometimes mandatory information is not directly contained in the data files. Since handwork is required, a lot of time is wasted to transfer all necessary data.

A similar problem is the exchange of measurement files between different laboratories. Due to the lack of a broadly accepted standard, the files from other sources can usually not directly be used.

Since a long time, the idea of the members of this Subcommittee is to develop a file format to ease the data exchange in order to concentrate on the file content and not the file structure. This file format should not only work for rheological and mechanical data (though this is the main interest of the members), but also for others like data from thermoanalysis or size exclusion chromatography.

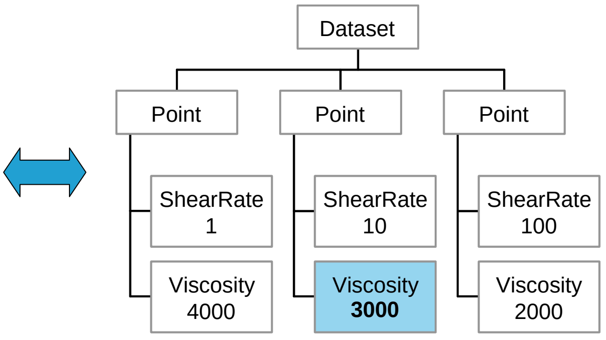
Due to the different specification requirements and data types of different measurement methods, a fixed row and column based table format is not appropriate. Here the XML format which gained more and more attention during the last years offers by far more flexibility and possibilities. The XML is the so called eXtensible Markup Language, which was developed by an Working Group formed under the auspices of the World Wide Web Consortium (W3C) in 1996. The HTML language, which is the standard of the internet, is only one possible application, by the way a very successful on. XML has some essential benefits: It is system-independent, software independent. The impact of XML on the IT world can be seen from the fact, that XML is already implemented in the new Office Programs e.g. from Microsoft. Besides the commercial programs there are a lot of free tools available which can be used to create or edit XML files.

The XML format is a tree-like structure with freely definable keywords, which can perfectly be adapted to the logical structure of measurement data (Fig. 1). It is important for the data exchange project, that it is not necessary to know about the underlying language to use XML files. In principle, the typical user does not have to get in touch with the XML file structure at all. Usually the XML file content will be presented in a very viewer-friendly way.
In order to use XML, a so-called Schema Definition (XSD-File) has to be defined, which contains the tree-like data structure and the allowed keywords (“tags”). The structure is very flexible. In addition the format can easily be extended by introducing new elements without

making old data files invalid! In the following sections the structure of the Schema for the measurement data exchange is introduced. At the moment, the format is limited to data from Dynamic Mechanical Analysis (DMA), Rotational Viscosimetry (RVM) and Capillary Viscosimetry (CVM). However, it is very straightforward to extent the structure to more methods.

Shear Rate	Viscosity
1	4000
10	**3000**
100	2000

Tables
(column/row-based structure)

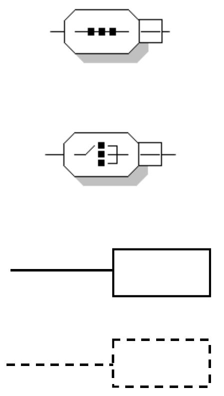


Tree-like structure

Fig. 1: Table vs. tree-like structure

2 XML Schema

The structure of a XML Schema is very flexible. It can contain sequences or selections of different options and elements. The elements can be mandatory, optional or even repeating. In the graphical presentation of the Schema structure the following notation is used:



Sequence of different elements

Selection/switch between different options or elements (only one can be selected)

mandatory element

optional element

The datafile must contain 2 mandatory and can contain 3 optional section:

- **Source**: who/where/when did the measurements
- **Sample**: details about the sample used
- **Equipment**: which machine and setup were used for the measurement
- **Data**: experimental data
- **Evaluation**: data calculated from the experimental data

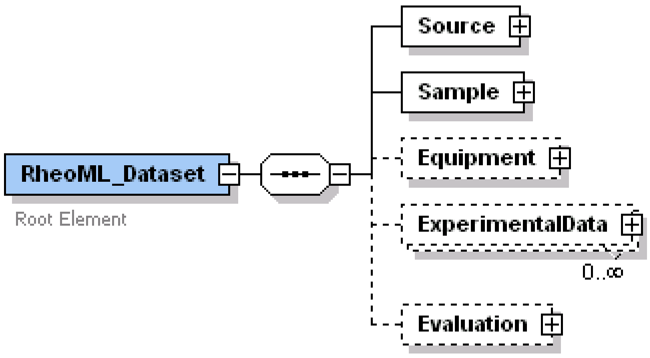


Fig. 2: Root Elements of XML Data Structure

2.1 Source

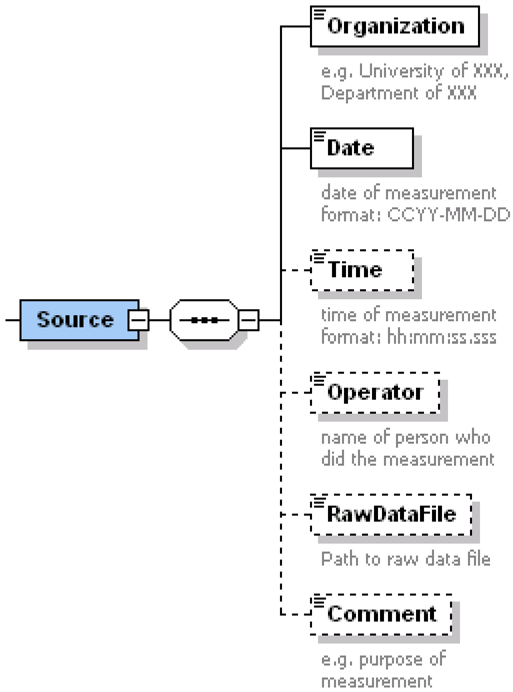


Fig. 3: Source Elements

2.2 Sample

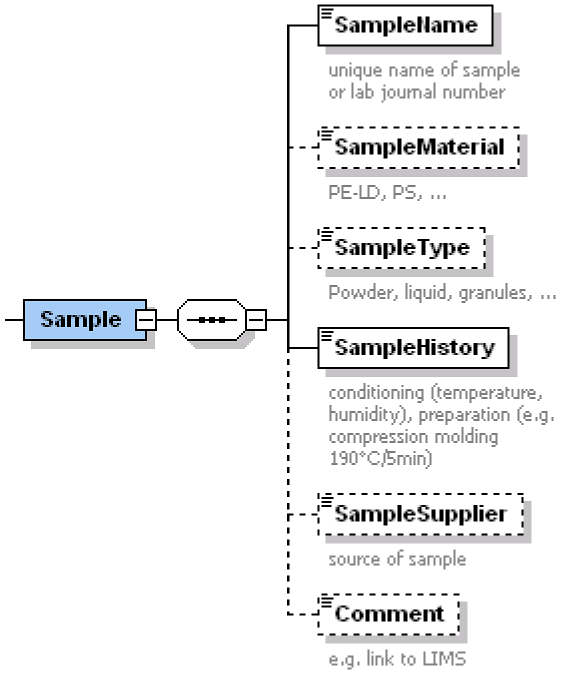


Fig. 4: Specification of Sample

2.3 Equipment

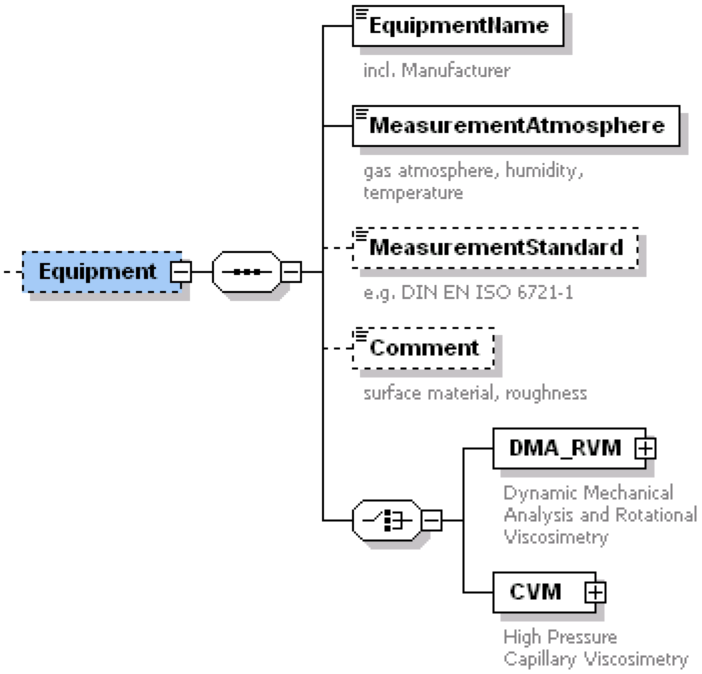


Fig. 5: Specification of Equipment

2.4 Dynamic Mechanical Analysis and Rotational Viscosimeter

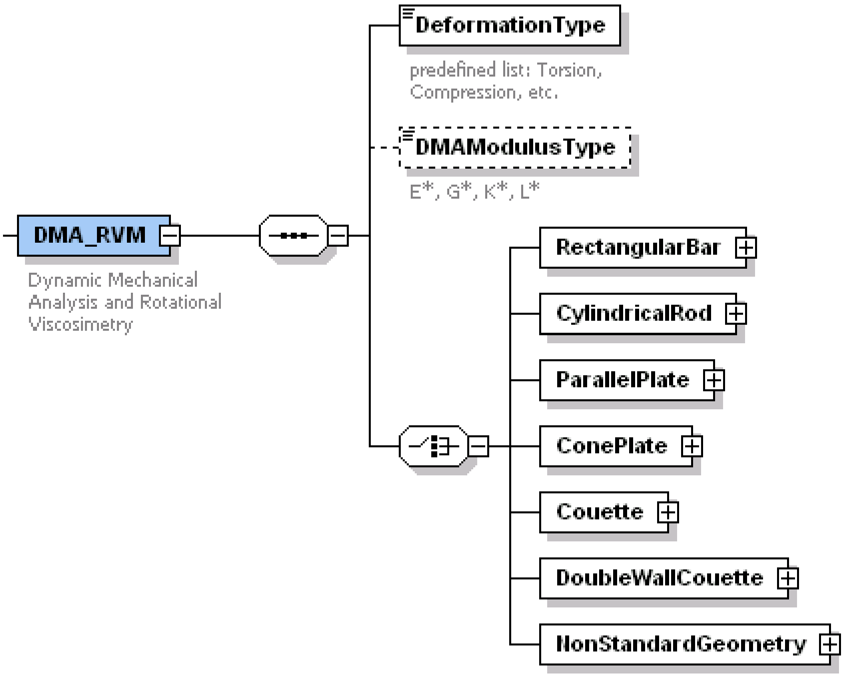
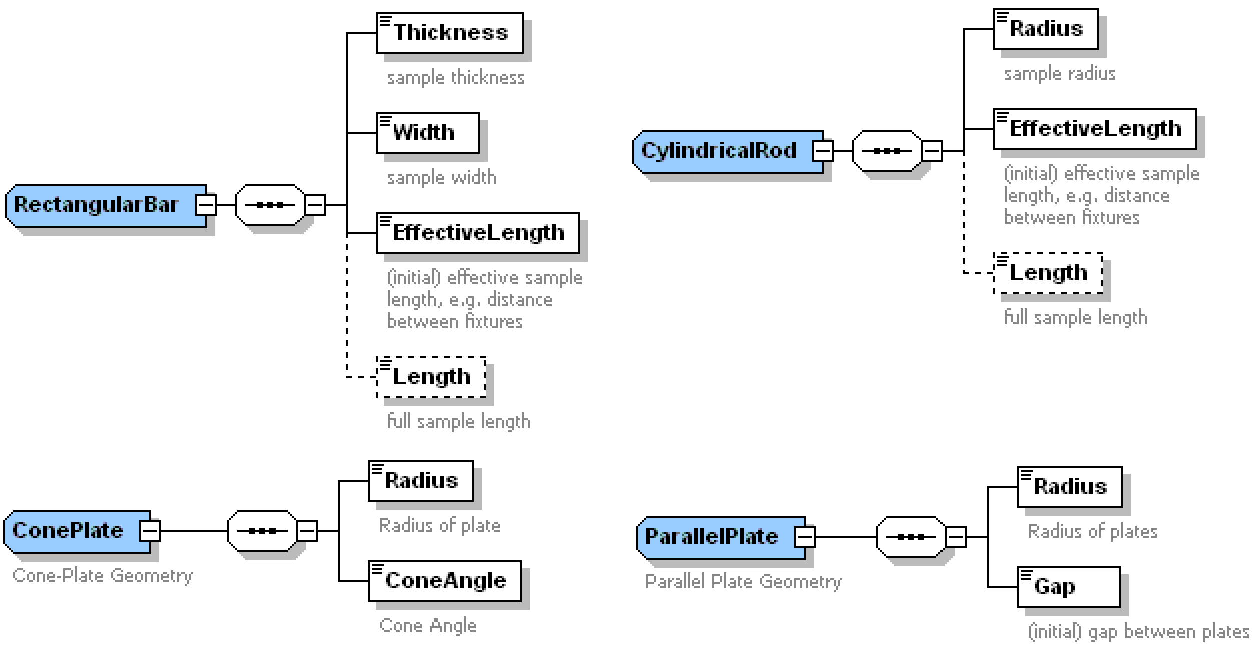
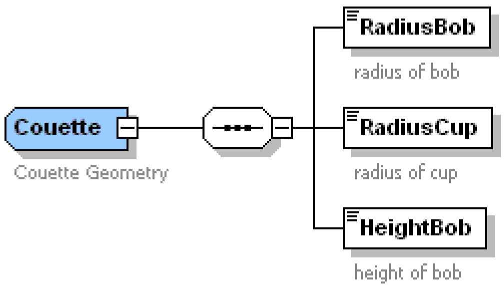
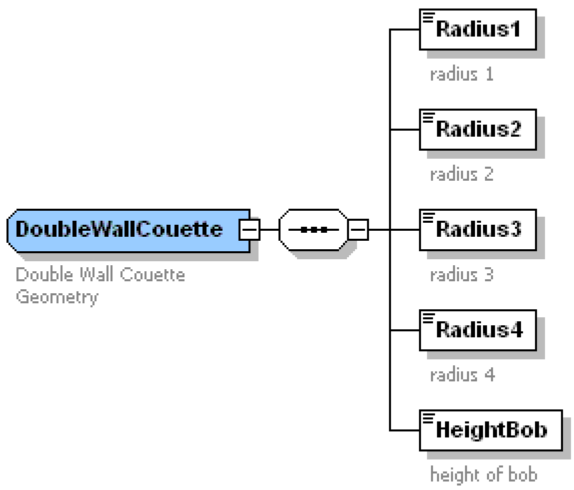


Fig. 6 Specification of DMA-Equipment

Table 1: Geometry Types







2.4.1 Capillary Viscosimeter

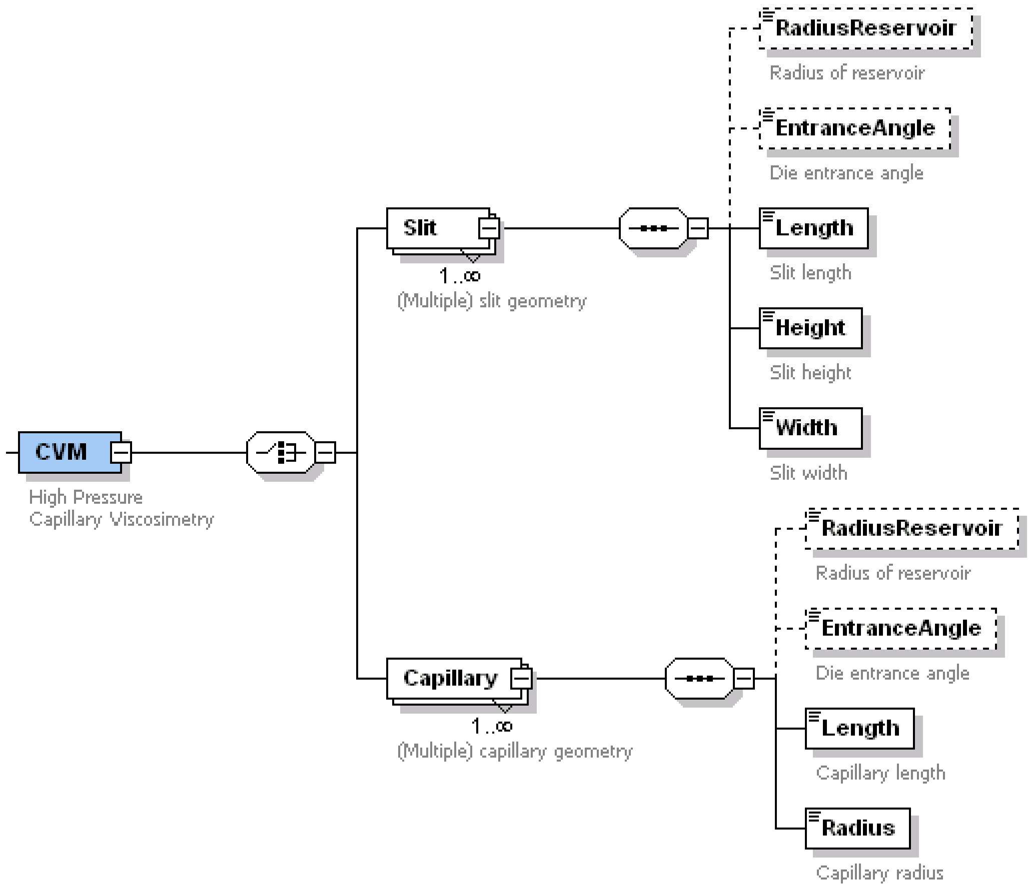


Fig. 7: Specification of Capillary Viscosimeter-Equipment

2.5 Experimental Data

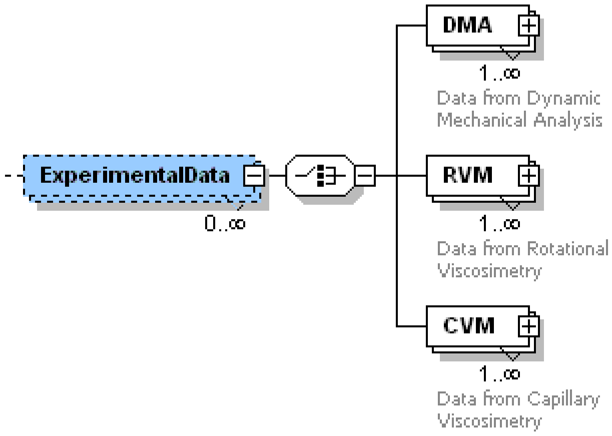


Fig. 8: Specification of Experimental Data

2.5.1 Dynamic Mechanical Analysis

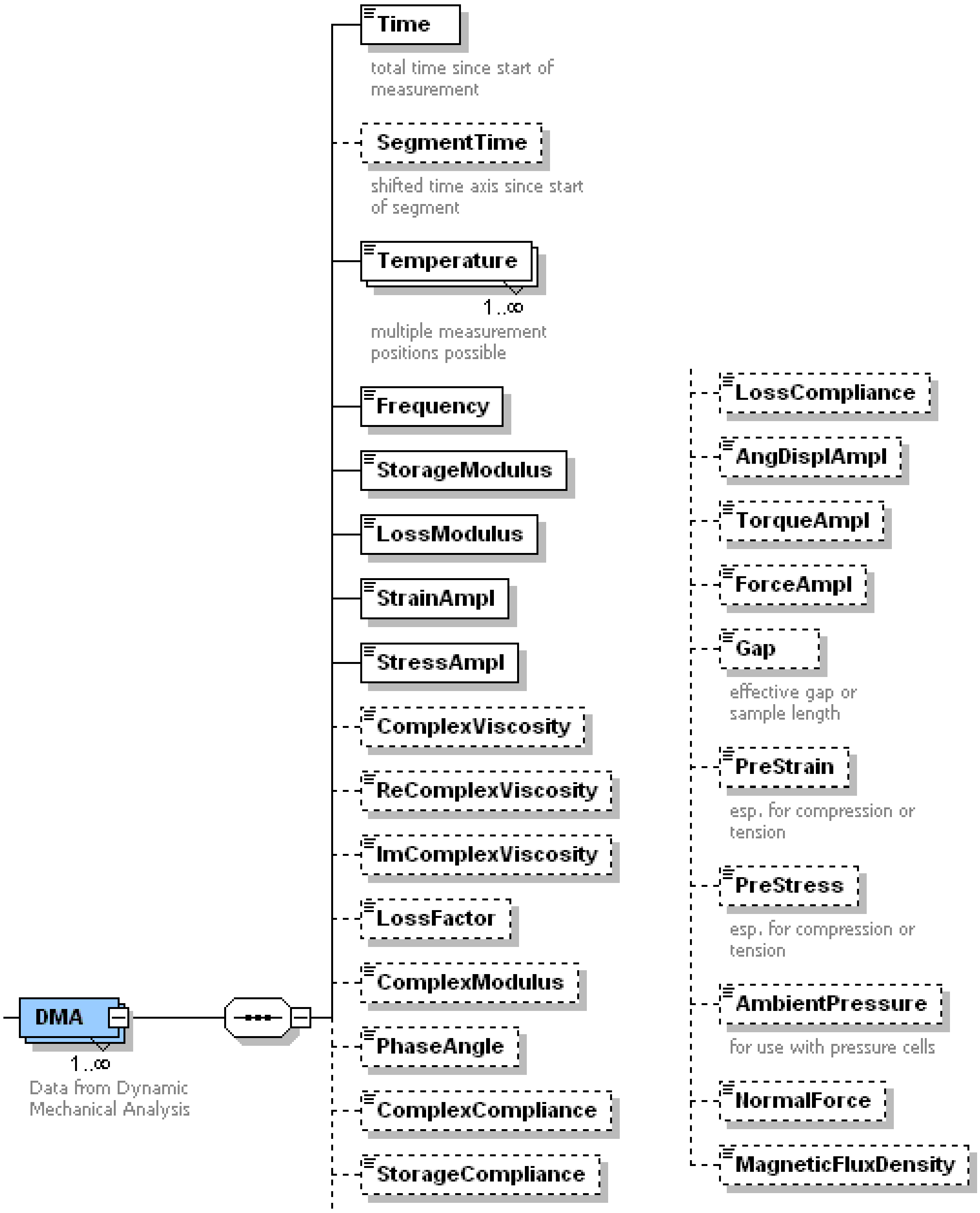


Fig. 9: Mandatory and optional elements for DMA data

2.5.2 Rotational Viscosimetry

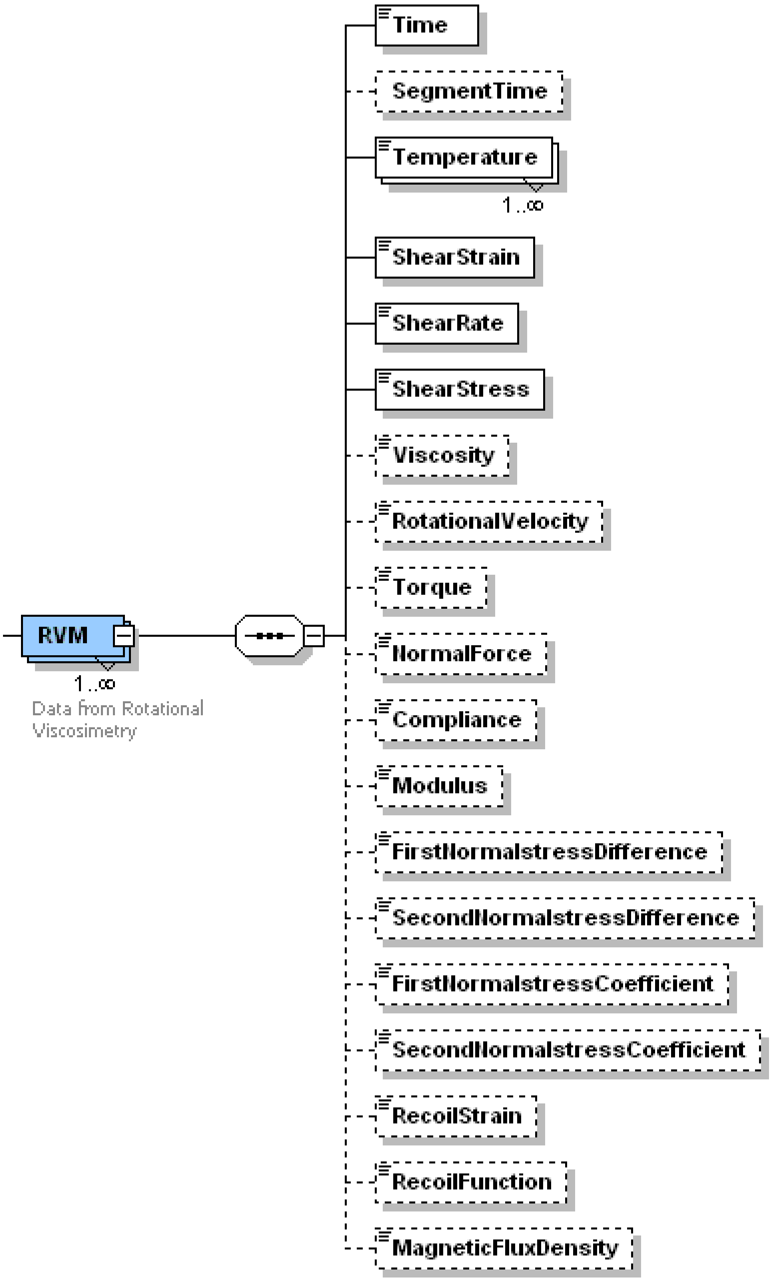


Fig. 10: Mandatory and optional elements for rotational viscosimetry data

2.6 Capillary Viscosimetry

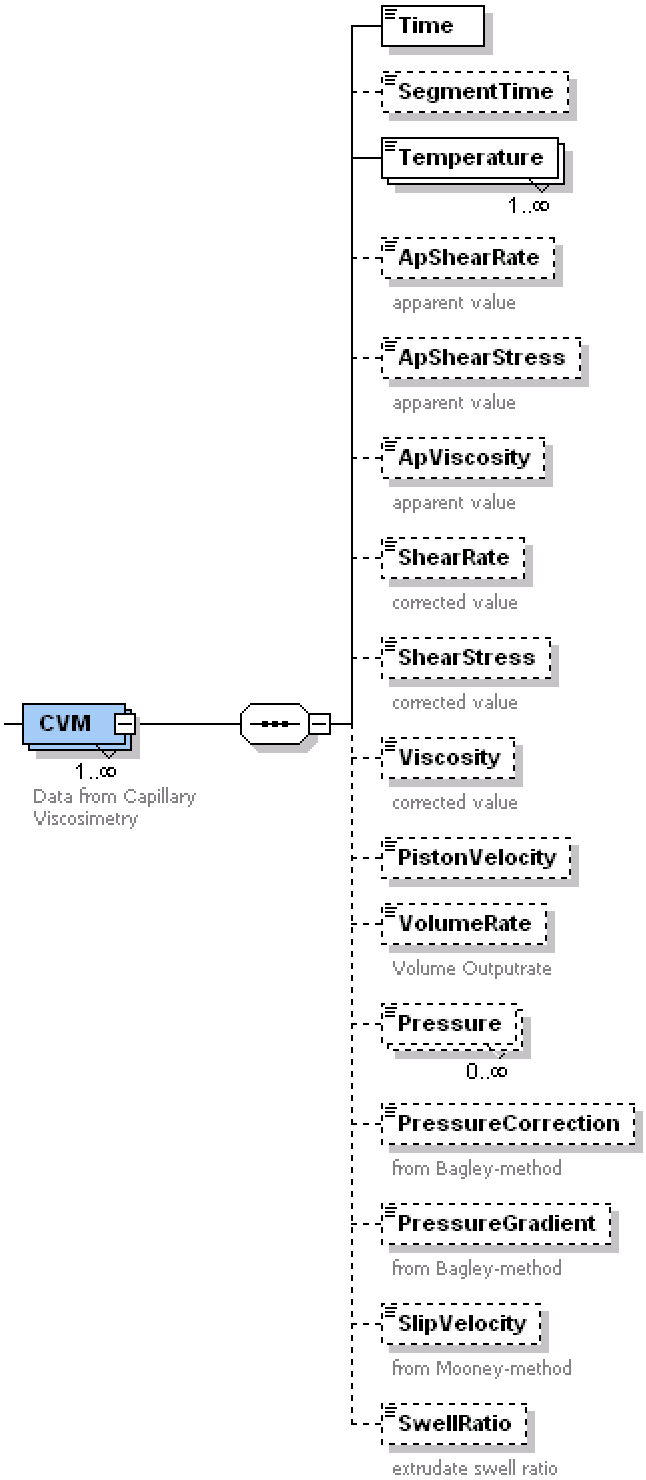


Fig. 11: Mandatory and optional elements for capillary viscosimetry data

2.7 *Evaluation*

Often, the rheometer software is used to perform further calculations with the experimental data, like the fitting of viscosity functions. To support the easy transfer of the results of such calculations, the IUPAC XML file can contain an optional *Evaluation* section, where the calculated parameters can be stored. So far, only few functions are supported, since this possibility was not part of the initial scope of the project. The extension of this *Evaluation* section will be a central part of future activities.

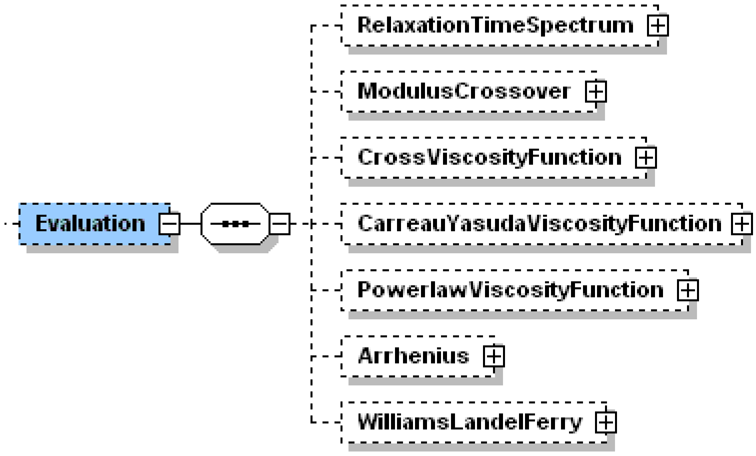
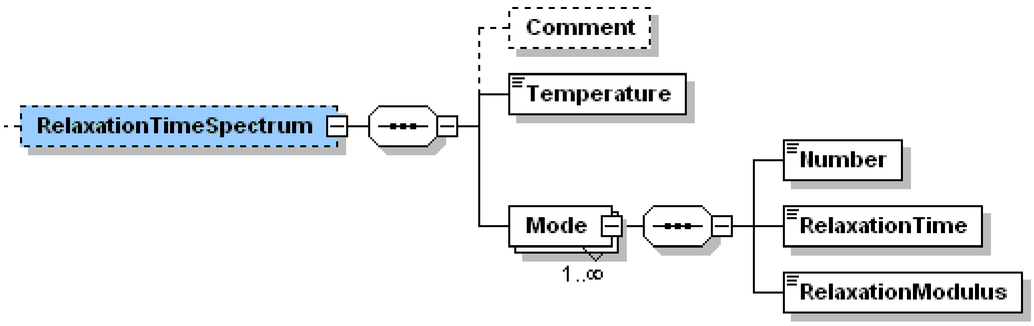


Fig. 12: Optional elements for data evaluation

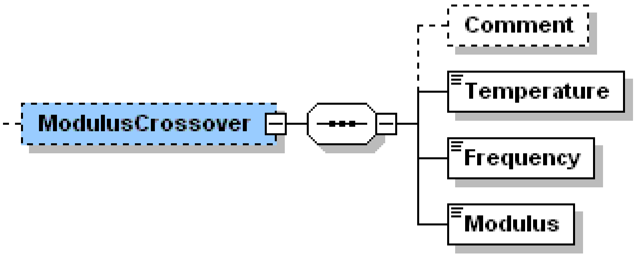
2.7.1 Relaxation Time Spectrum

Viscoelastic relaxation time spectrum



2.7.2 Modulus Crossover

Angular frequency and modulus at the cross-over of storage and loss modulus.

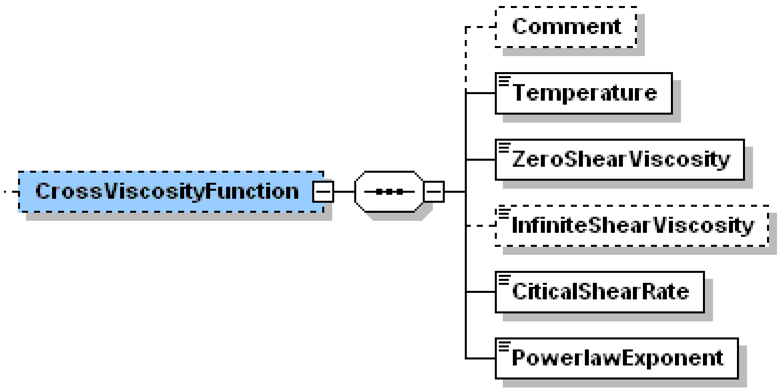


2.7.3 Cross Viscosity Function

Viscosity function according to Cross:

$$\eta = \eta_\infty + \frac{\eta_0 - \eta_\infty}{1 + \left(\frac{\dot{\gamma}}{\dot{\gamma}_c}\right)^m}$$

with:	η_0	ZeroShearViscosity
	η_∞	InfiniteShearViscosity
	$\dot{\gamma}_c$	CriticalShearRate
	m	PowerlawExponent

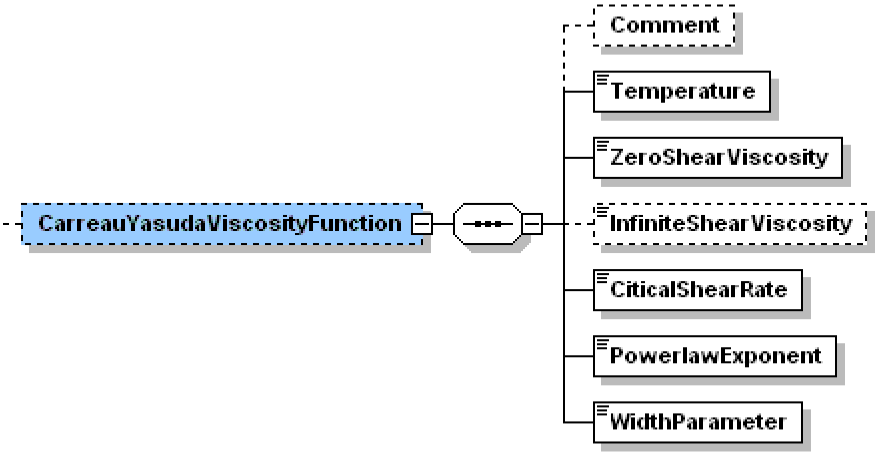


2.7.4 Carreau Yasuda Viscosity Function

Viscosity function according to Carreau-Yasuda:

$$\eta = \eta_\infty + \frac{\eta_0 - \eta_\infty}{\left[1 + \left(\frac{\dot{\gamma}}{\dot{\gamma}_c}\right)^a\right]^{\frac{1-n}{a}}}$$

with: η_0 ZeroShearViscosity
η_∞ InfiniteShearViscosity
$\dot{\gamma}_c$ CriticalShearRate
n PowerlawExponent
a WidthParameter

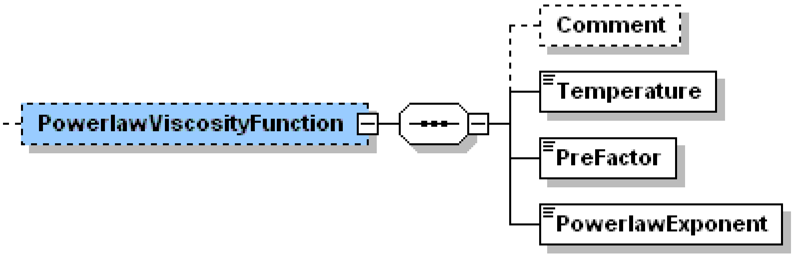


2.7.5 Powerlaw Viscosity Function

Viscosity function according to Ostwald-de Waele:

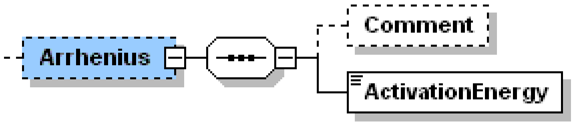
$$\eta = K \cdot \dot{\gamma}^n$$

with: K PreFactor
n PowerlawExponent



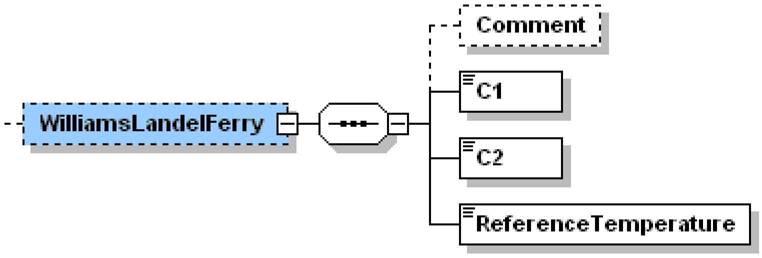
2.7.6 Arrhenius

Activation energy of the Arrhenius function



2.7.7 Williams Landel Ferry

Parameters of the Williams Landel Ferry (WLF) Function:



3 References

[1] Leaderman, H., “Proposed nomenclature for linear viscoelastic behavior,” Transactions of The Society of Rheology, 1, 213-222 (1957).

[2] Sieglaff, C. L., “Proposed nomenclature for steady shear flow and linear viscoelastic behavior,” Transactions of The Society of Rheology, 20:2, 311-317 (1976).

[3] Dealy, J. M., “Official nomenclature for material functions describing the response of a viscoelastic fluid to various shearing and extensional deformations,” J. Rheol., 39:1, 253-265 (1995).

4 Appendix

4.1 Unit System

The schema does not use fixed units. However, the units for each entity can be selected from a pre-defined list, only, to avoid misunderstanding. Further units can be included later if necessary! In the following list, all possible units are summarized.

Entity	Possible units
Acceleration	m/s^2, cm/s^2, mm/s^2, $\mu m/s^2$,
ActivationEnergy	kJ/mol, J/mol
Angle	°, rad
AngularVelocity	rad/s
Area	m^2, cm^2, mm^2, μm^2, nm^2, in^2
Compliance	1/Pa, 1/MPa, 1/mPa
Density	kg/m^3, g/cm^3, mg/cm^3, $\mu g/cm^3$
Energy	J, Nm, kJ, mJ
Force	kN, N, cN, mN, µN
Frequency	Hz, s-1, 1/s
Length	m, cm, mm, µm, nm
MagneticFluxDensity	T, Wb/m^2
Mass	kg, g, mg, µg
MassRate	kg/s, kg/h, g/s, mg/s, µg/s
Modulus	Pa, MPa, mPa, dyn/cm^2, dyn/in^2
NormalStressCoefficient	$Pa \cdot s^2$, $mPa \cdot s^2$, $dyn \cdot s^2/cm^2$
Pressure	mbar, bar, Pa, MPa, mPa, dyn/cm^2, dyn/in^2
PressureGradient	mbar/mm, bar/mm, Pa/mm, MPa/mm, mPa/mm
Rate	s-1, 1/s
Stress	Pa, MPa, mPa, dyn/cm^2, dyn/in^2
Temperature	°C, °F, K, Kelvin
Torque	Nm, mNm, µNm, nNm
Time	h, min, s, ms, µs, ns
Velocity	m/s, cm/s, mm/s, µm/s, nm/s, km/h
Viscosity	Pa·s, mPa·s, P, cP
Volume	mm^3, cm^3, dm^3, m^3, l
VolumeRate	mm^3/s, cm^3/s, dm^3/s, m^3/s, l/s