



Project 2003-009-1-400
**Recommendations for data presentation applicable to
mechanical and rheological measurements of polymers**

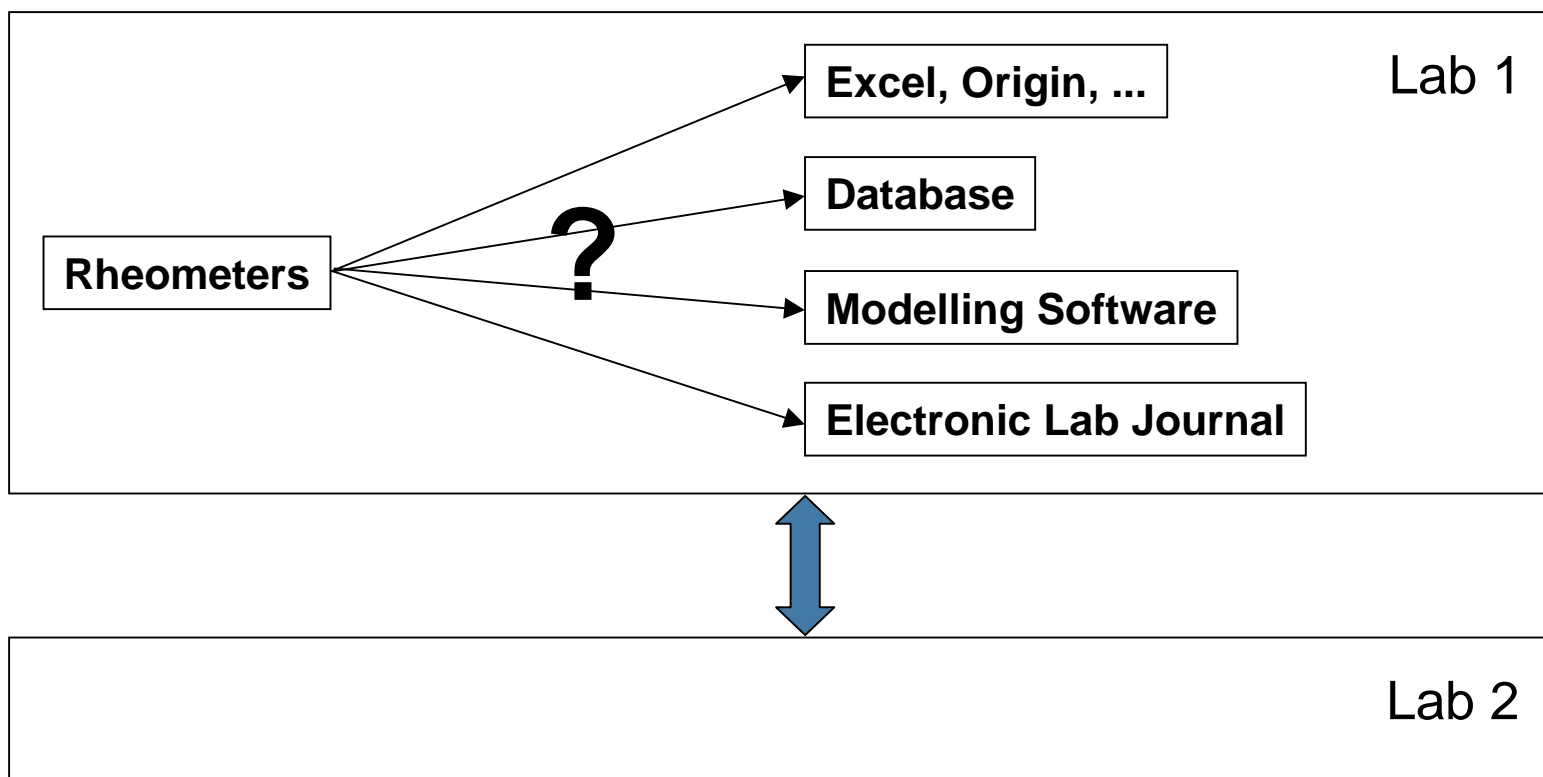
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Dick Dijkstra, Bayer Material Science Leverkusen

IUPAC SC Meeting, Budapest
May 09-11, 2007



What is the problem ?

- Transfer of experimental data from testing equipment to graphics / spreadsheet software still requires a lot of handwork: loss of time



- No common file format to exchange data between different laboratories



IUPAC Approach

- Use impact of IUPAC Sub-Committee with many representatives from industry and academia to introduce a commonly accepted data standard

- Project started in 2003:
 “Recommendations for data presentation applicable to mechanical and rheological measurements of polymers”

- Goal:
 - Store **all relevant** information belonging to **1** measurement on **1** sample

 - No Database-Format to store different measurements on 1 or even more samples (like the ThermoML approach) intended.



Universal Data Exchange Format - Problem & Solution

- Different methods require different information about the setup and different data to be stored (e.g. compare DMA data and capillary rheometry !)
- Thus, a fixed format (i.e. a column and row based interpretation of the file content) of a "universal" file format imposes serious limitations with regard to a generalization.
- Solution: separate data from formatting, instead use descriptive tags to define logical elements within the data file !

e.g. `<Temperature Scale="°C">23</Temperature>`

concept of XML

This information can be easily processed by a computer as well as by a human reader.



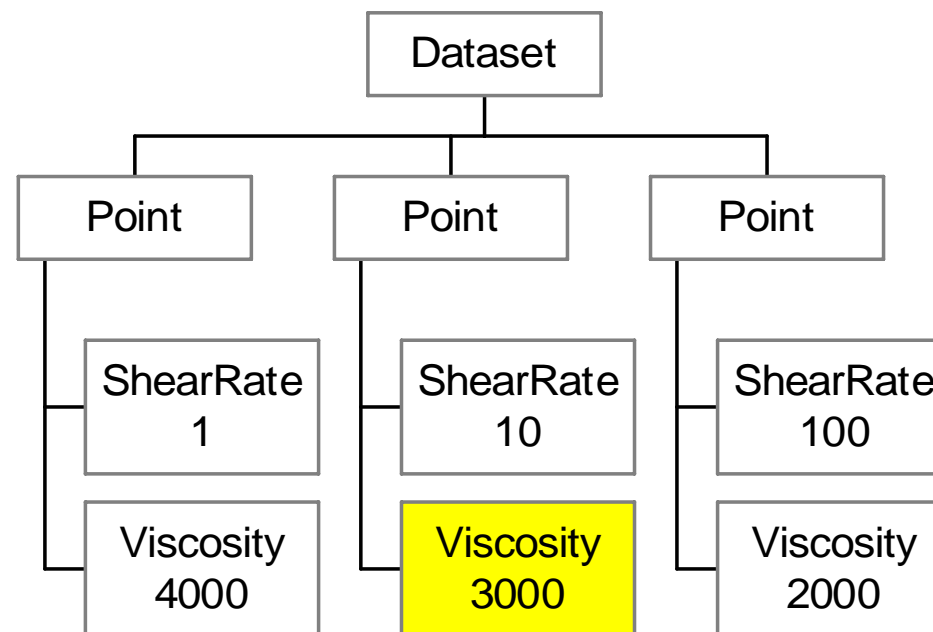
Reasons to use XML format

- XML (eXtensible Markup Language) is an easily adaptable, internationally accepted text-based format.
- XML was developed by an Working Group formed under the auspices of the World Wide Web Consortium (W3C) in 1996: real standard
- XML has some essential benefits: It is system-independent, software independent and proven with HTML on the Web.
- The format can easily be extended by introducing new elements without making old data files invalid !
- (Free) software to create, edit and process XML Files is available.
- XML format included in MS Office 2003, WordPerfect Office, OpenOfficeOrg, ... (unfortunately not directly usable in older versions)



Basics of XML

Shear Rate	Viscosity
1	4000
10	3000
100	2000



Tables
(column/row-based structure)

Tree-like structure



Example of XML file

```

<?xml version="1.0" encoding="UTF-8"?>
<?xml-stylesheet type='text/xsl' href='IUPAC2html.xsl'?>
<IUPAC_Dataset xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
  xsi:noNamespaceSchemaLocation="Iupac-Schema.v4.xsd" Type="Dynamic Mechanical Analysis">
<Source>
  <SourceLaboratory>BASF AG Ludwigshafen, GKP/R</SourceLaboratory>
  <SourceDate>2002-08-15</SourceDate>
  <SourceOperator>Schweizer, Peter</SourceOperator>
  <SourceComment>02-091</SourceComment>
</Source>
<Sample>
  <SampleName>PS168N</SampleName>
  <SampleMaterial>Polystyrene</SampleMaterial>
  ...
</Sample>
...
<Data>
  <DMA>
    <Time>3</Time>
    <Temperature>210.01</Temperature>
    <AngularFrequency>100</AngularFrequency>
    ...
  
```

File containing the data type definitions

Due to the use of "tags" the file content is easily readable even without knowledge of exact definitions!



Displaying XML files with the Web-Browser

PS168N
Polystyrene - Melt
History: Compression Molding
Supplier: BASF
Comment: no

Equipment

Rheometrics SR2
Measurement Atmosphere: Nitrogen
Measurement Standard: DIN EN ISO 6721-11
Dynamic Mechanical Analyzer
Deformation: *Torsion*
Sample-Geometry: D (mm) = 25, Gap (mm) = 1.02
Comment:

Data

t (s)	T (°C)	ω (rad/s)	Storage Modulus (Pa)	Loss Modulus (Pa)	Strain	Stress (Pa)	Viscosity (Pas)	$\tan \delta$ (δ)	δ (rad)	AngDispl (rad)	TorqueAmpl (Nm)	ForceAmpl (N)	Gap (mm)	PreStrain	Pre (Pa)
3	210.01	100	102800	46606	0.0096177	1085.5	1128.7								
6	210.01	56.234	85677	44139	0.010681	1029.4	1713.9								
10	210.01	31.623	69468	40953	0.012532	1010.6	2550.1								
14	210	17.783	54724	37312	0.015156	1003.9	3724.6								
18	210	10	41288	32785	0.018995	1001.4	5272.1								
22	210	5.6234	30065	28052	0.024332	1000.5	7312.2								
28	210.01	3.1623	20666	22844	0.032468	1000.2	9741.2								
36	210.01	1.7783	13475	17819	0.044763	1000	12563								

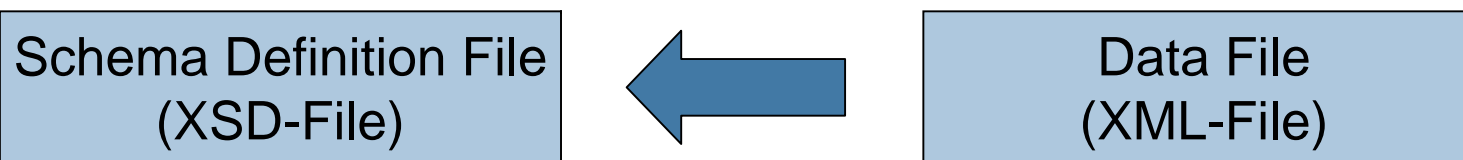
automatic transformation to HTML by use of XSL - eXtensible Stylesheet Language



You do not have to learn XML in order to use it. XML techniques work in background



XSD Schema definition



- Definition of elements:

- Position within tree-like structure
- Data type
- optional/mandatory
- Number of occurrence

- Contains

- data according to defined tree-like structure
 - reference to schema definition file
- Can be validated against schema definition, i.e. is file content OK ?

Output of our project



News

- XML format broadly accepted as new standard
- HAAKE RheoWin software offers XML export which is not compatible, however
- Contact to Procter&Gamble (William Hartt, rheology and mixing central group): they need rotational rheometry
- H.H. Winter started to implement XML into IRIS software. He wants to store more information in file like relaxation time spectrum
- Poster Presentation at AERC 2007 together with H.H. Winter
- Oral Presentation at AERC 2007
- TA instruments (Aly Franck) promised to offer XML export as soon as standard is defined



Changes

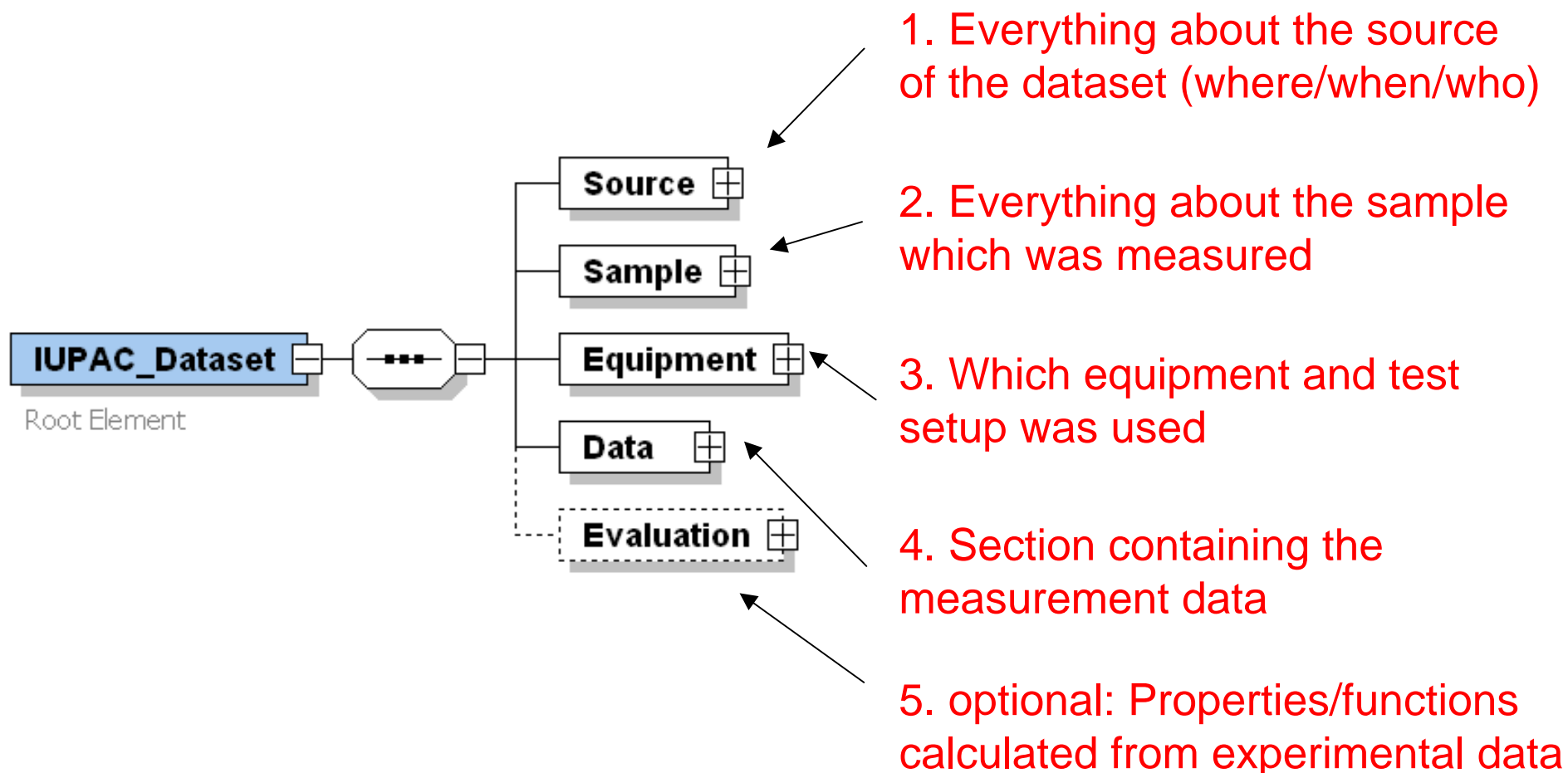
- Rotational Rheometry added
- Data Evaluation section added
- More representative names for Tags (e.g. „ConePlate“ instead of „CP“)
- Use Society of Rheology Nomenclature* (as far as available)

*J.M. Dealy, 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)



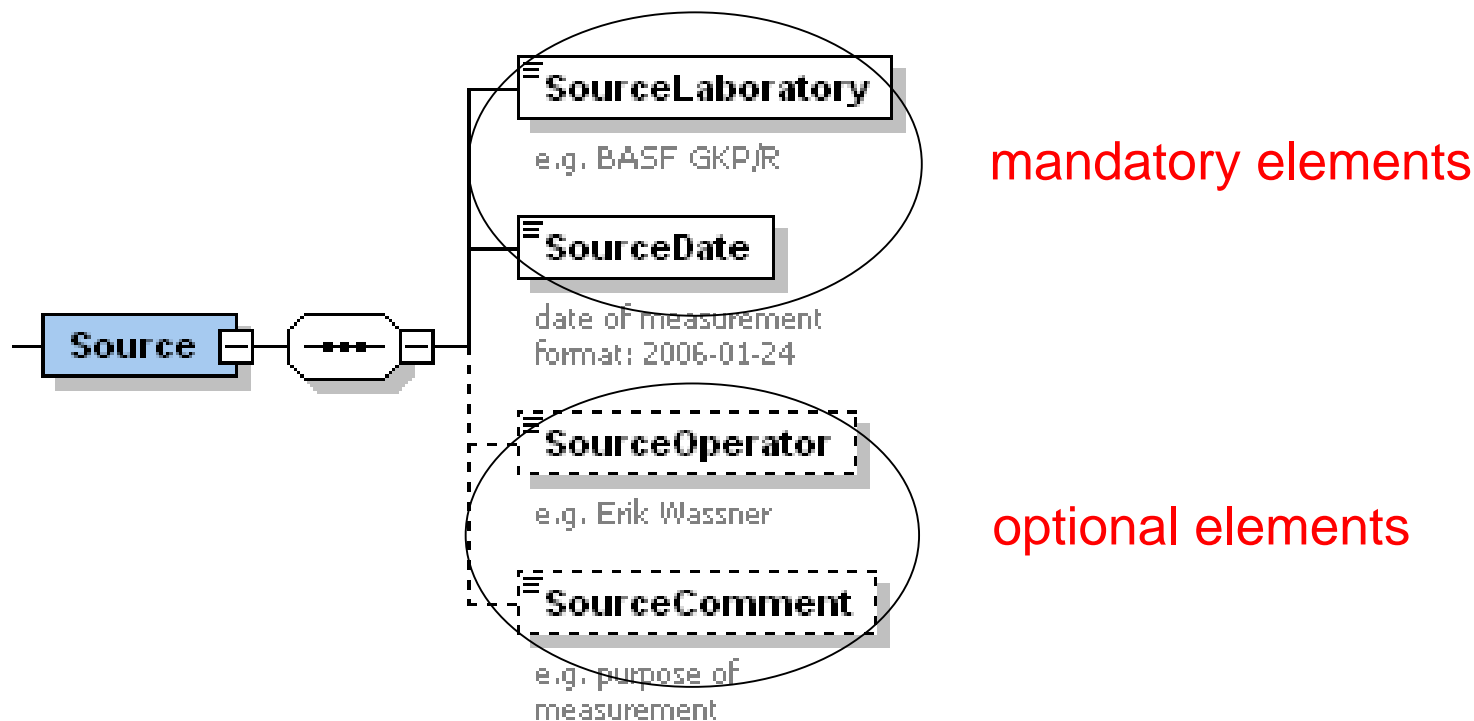
Tentative Structure of IUPAC-XML files - Overview

A dataset contains 5 sections with different information:



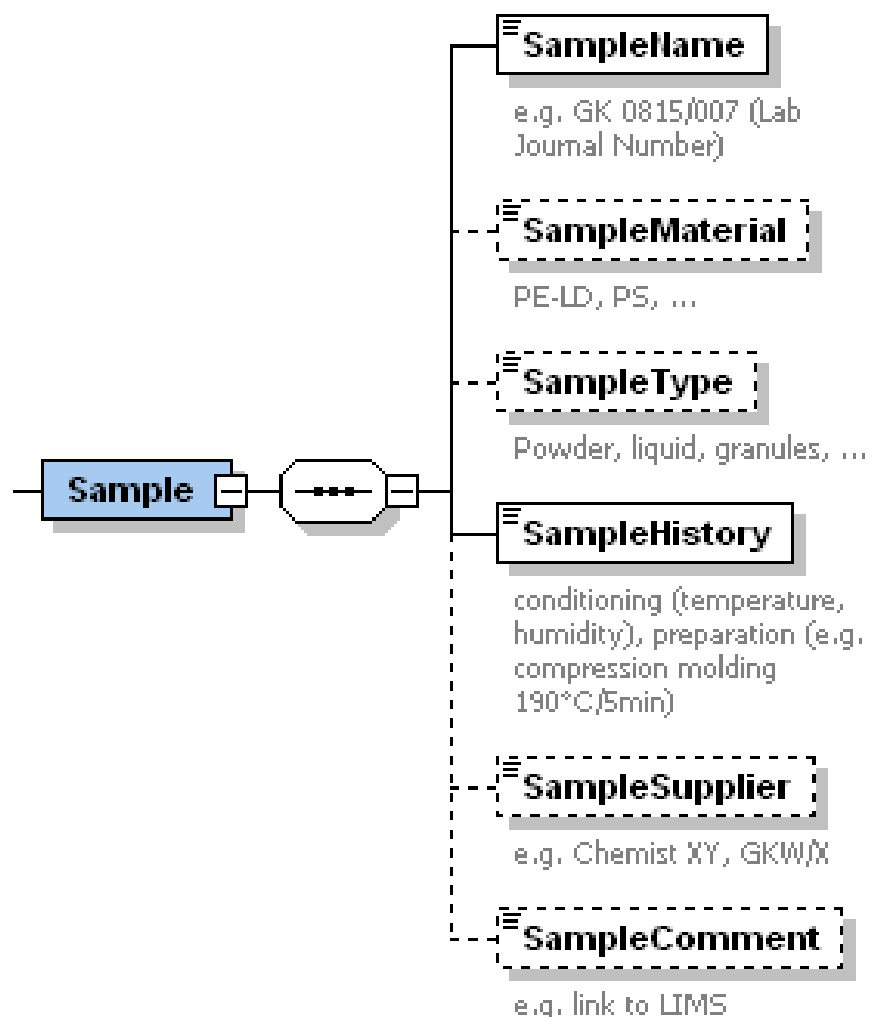


Tentative Structure of IUPAC-XML files – Source





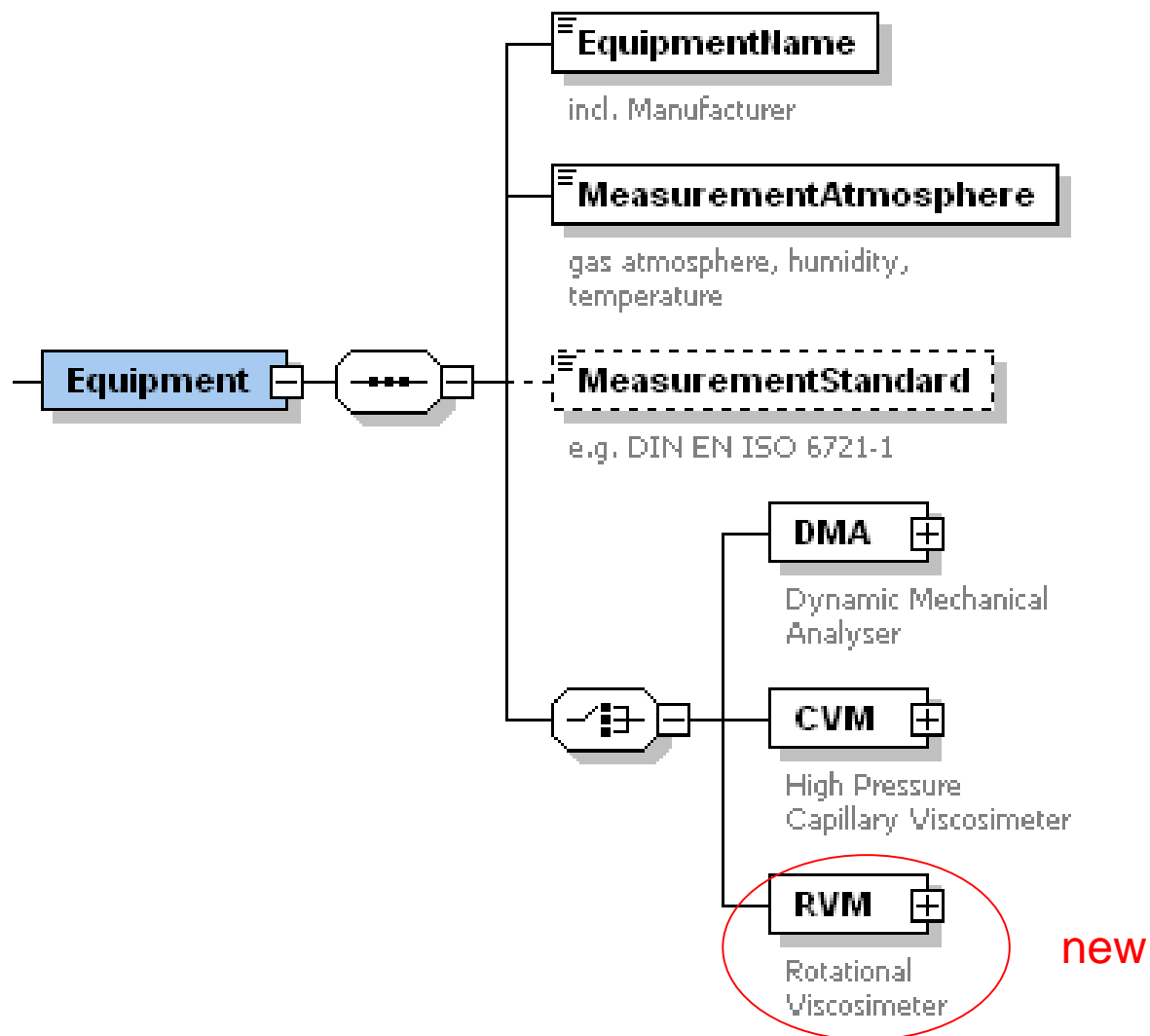
Tentative Structure of IUPAC-XML files – Sample



important for interpretation of data

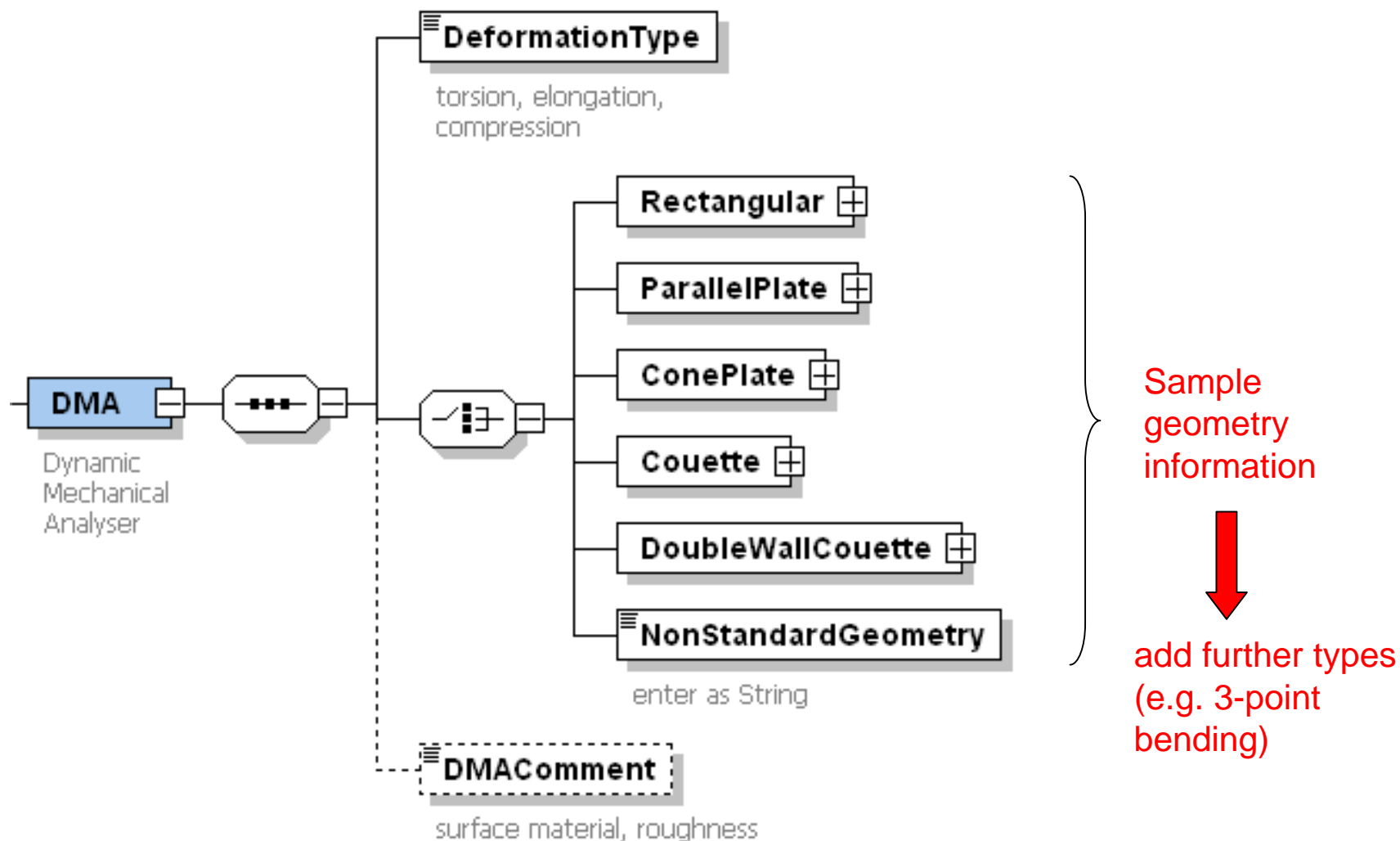


Tentative Structure of IUPAC-XML files – Equipment



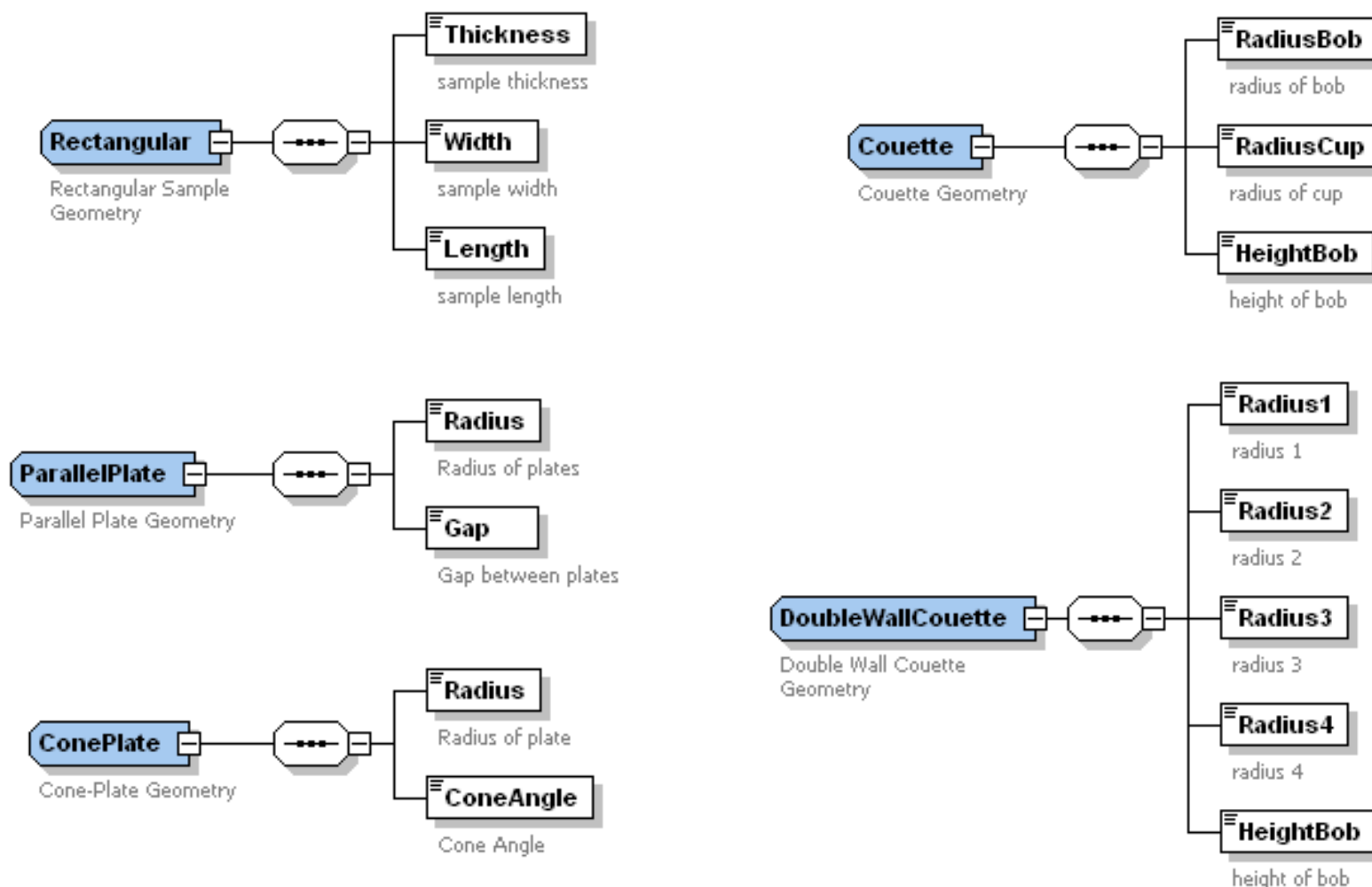


Tentative Structure of IUPAC-XML files – DMA Equipment



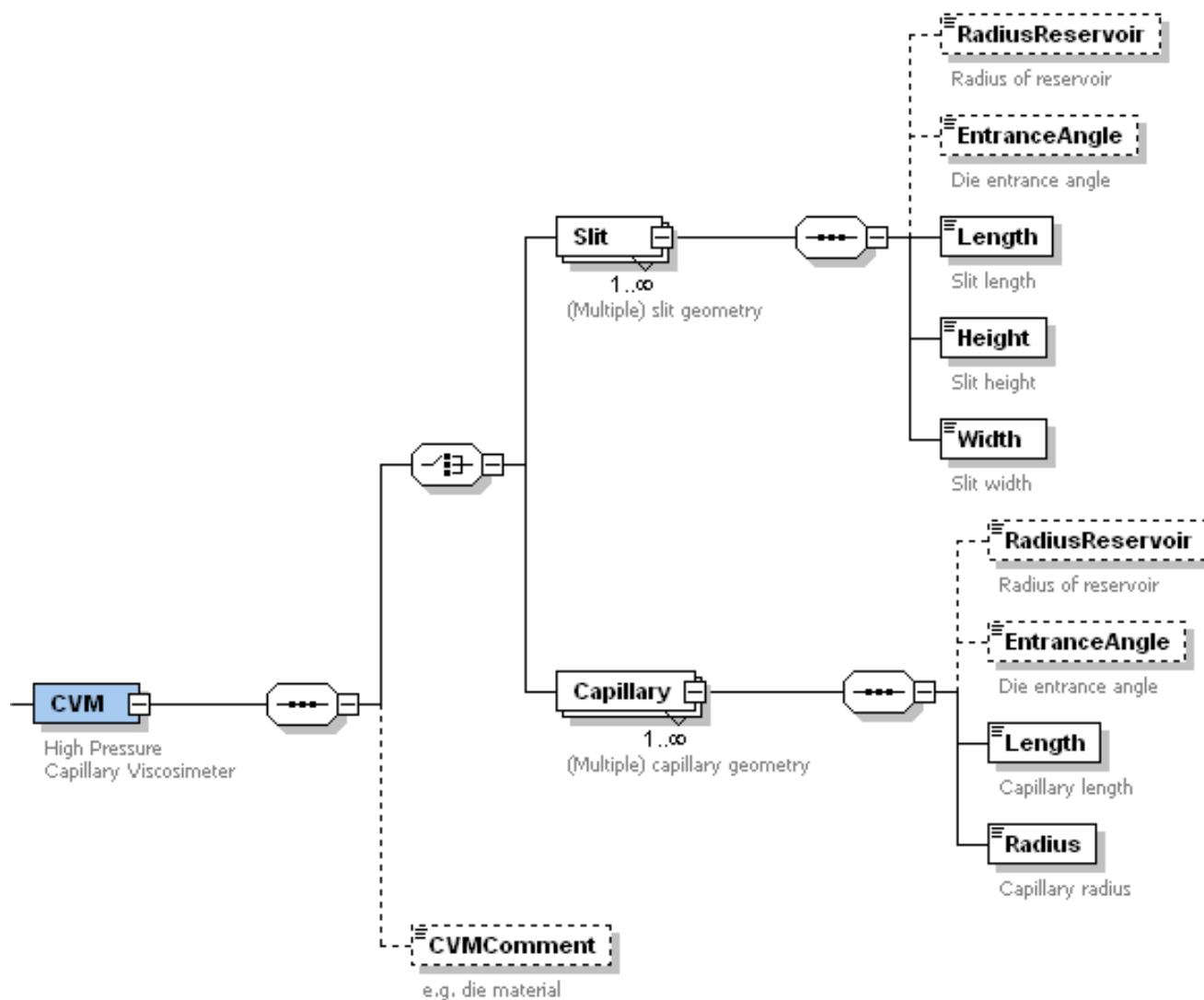


Tentative Structure of IUPAC-XML files – DMA Equipment



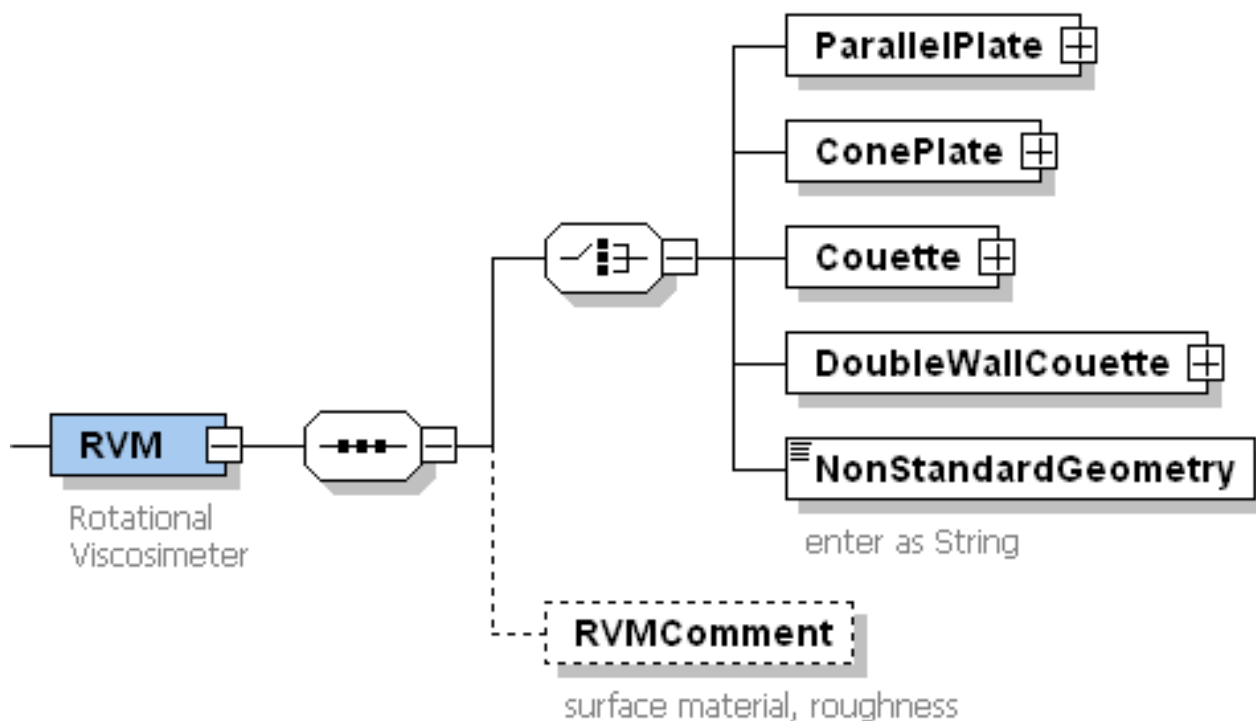


Tentative Structure of IUPAC-XML files – CVM Equipment



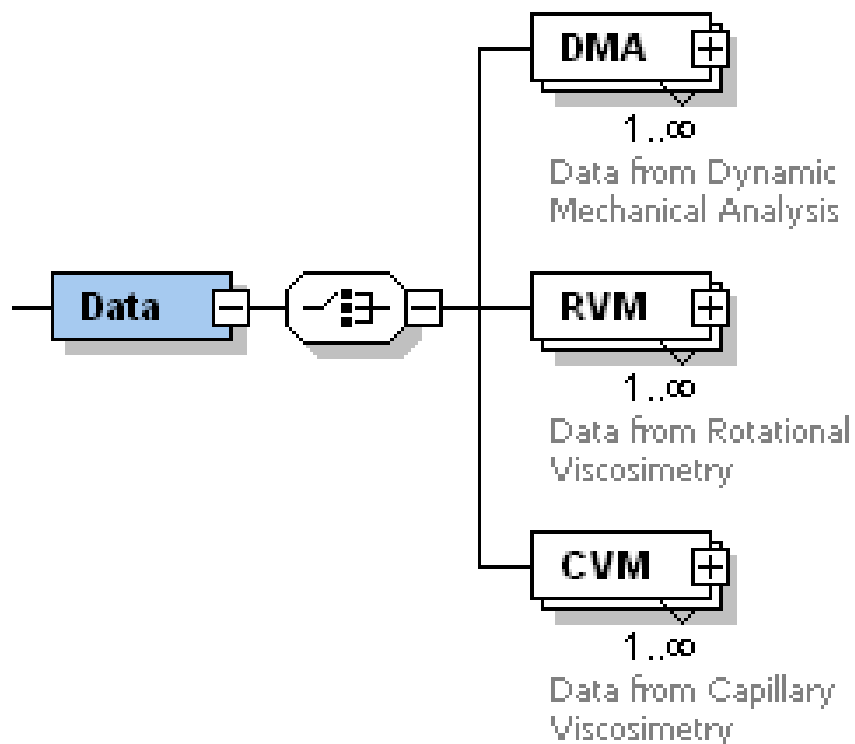


Tentative Structure of IUPAC-XML files – RVM Equipment



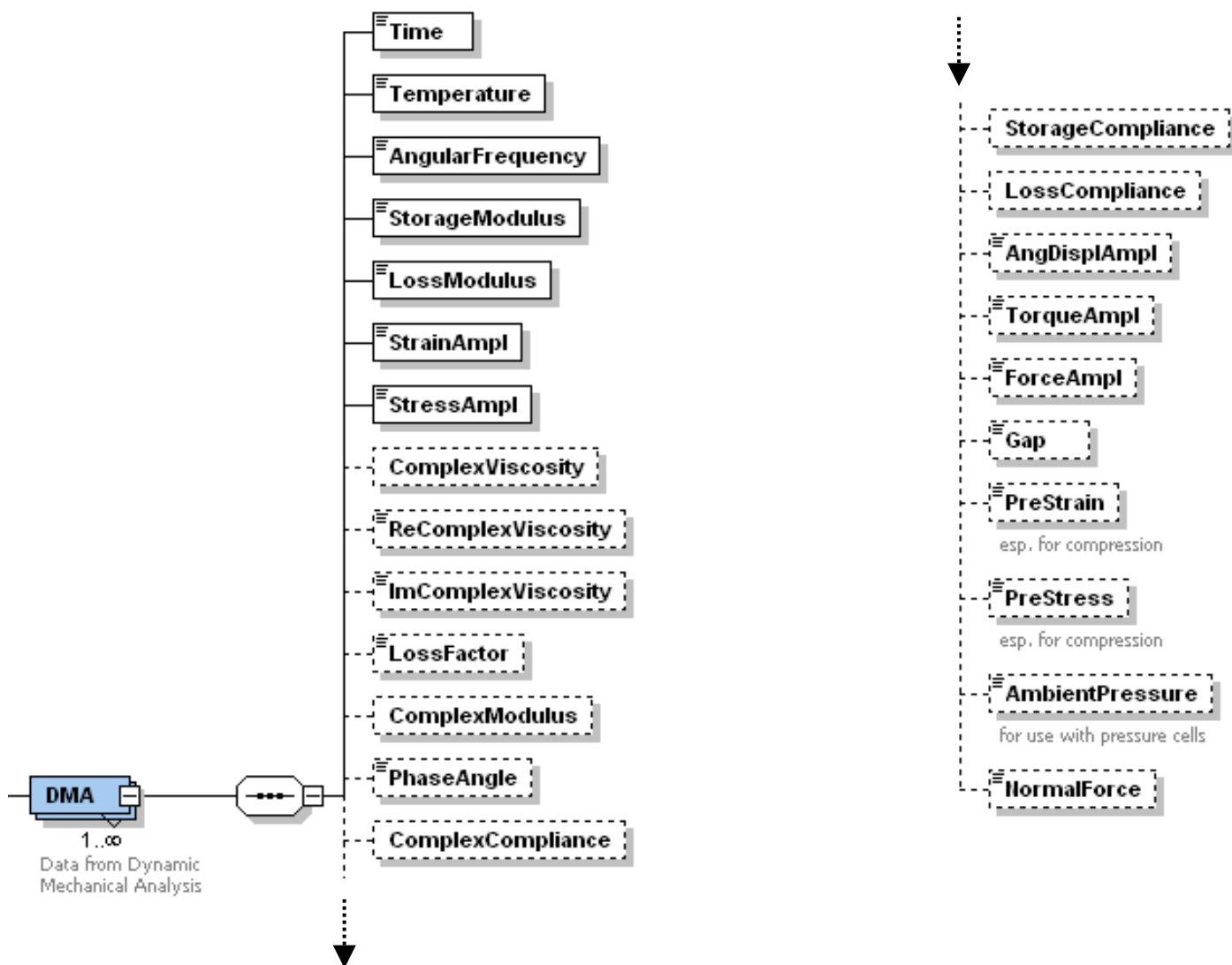


Tentative Structure of IUPAC-XML files – Data



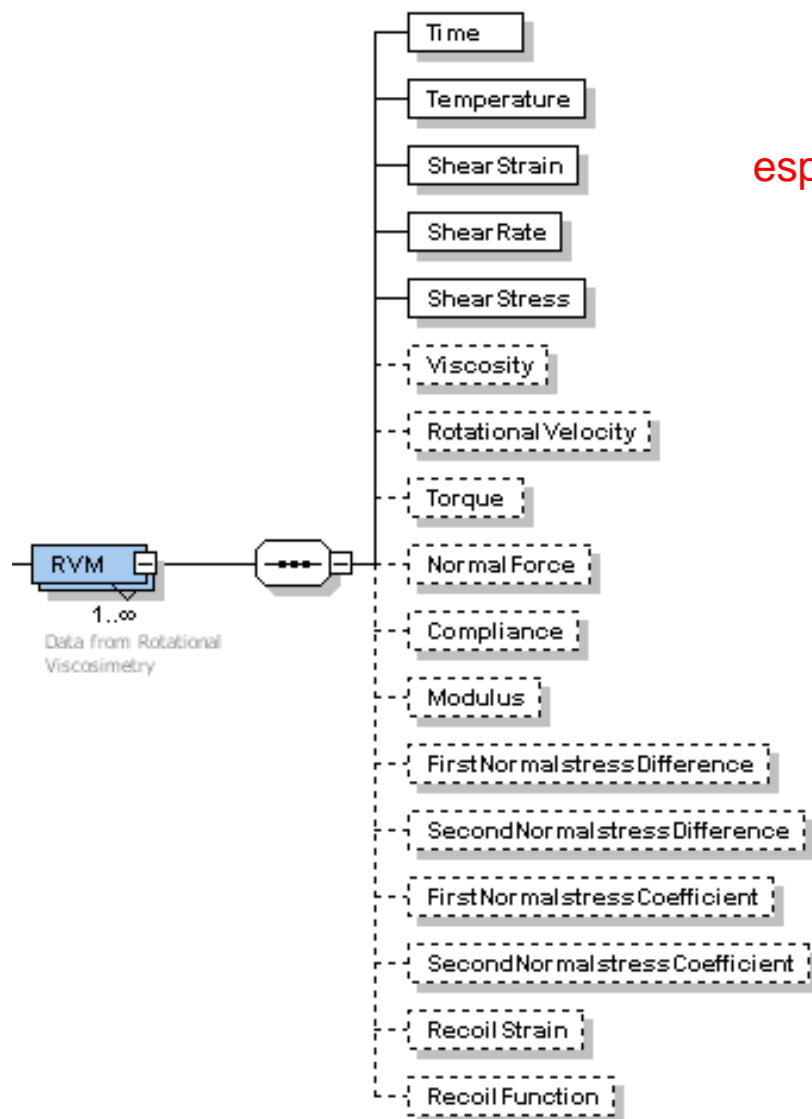


Tentative Structure of IUPAC-XML files – DMA Data





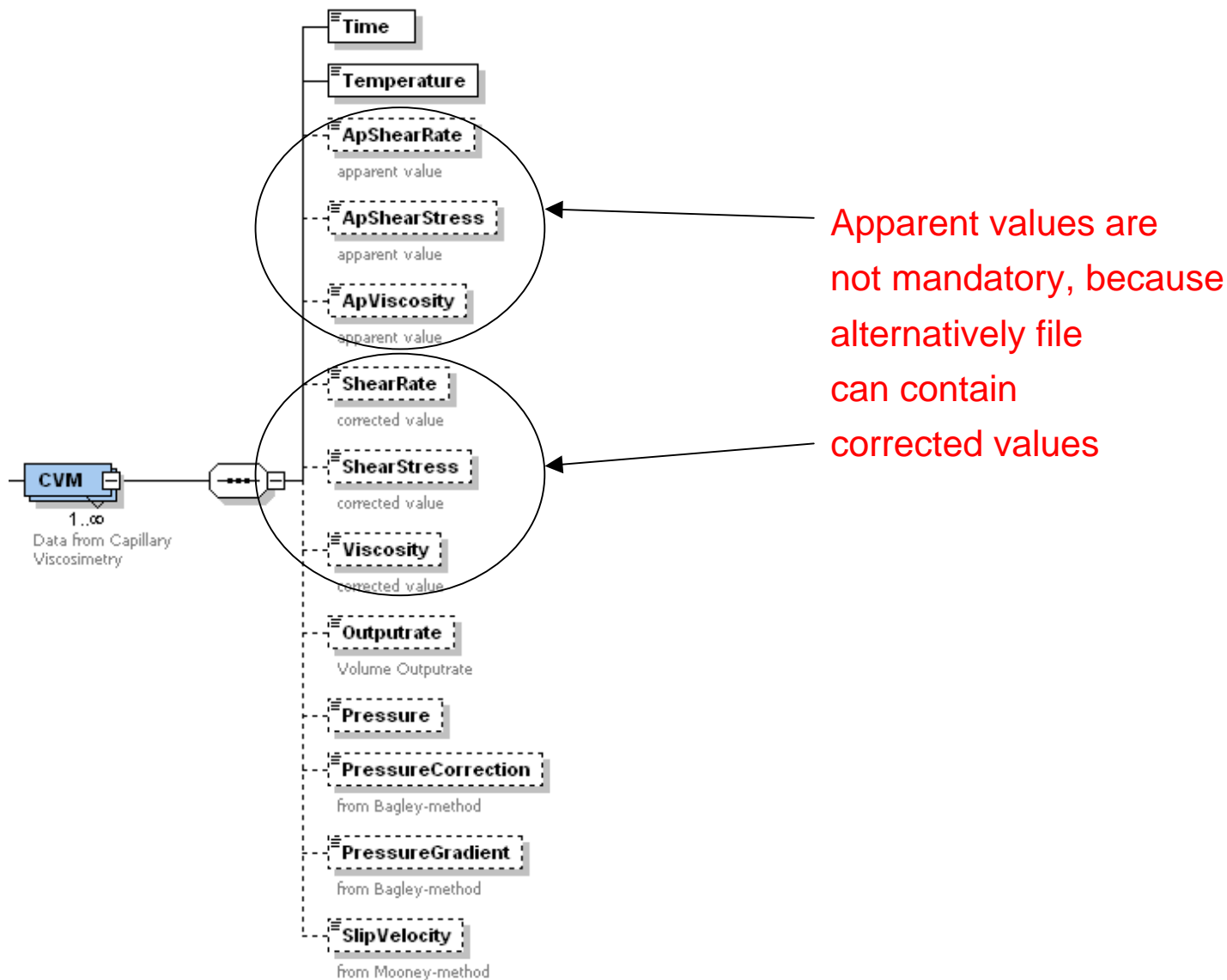
Tentative Structure of IUPAC-XML files – RVM Data



esp. for stress relaxation experiments

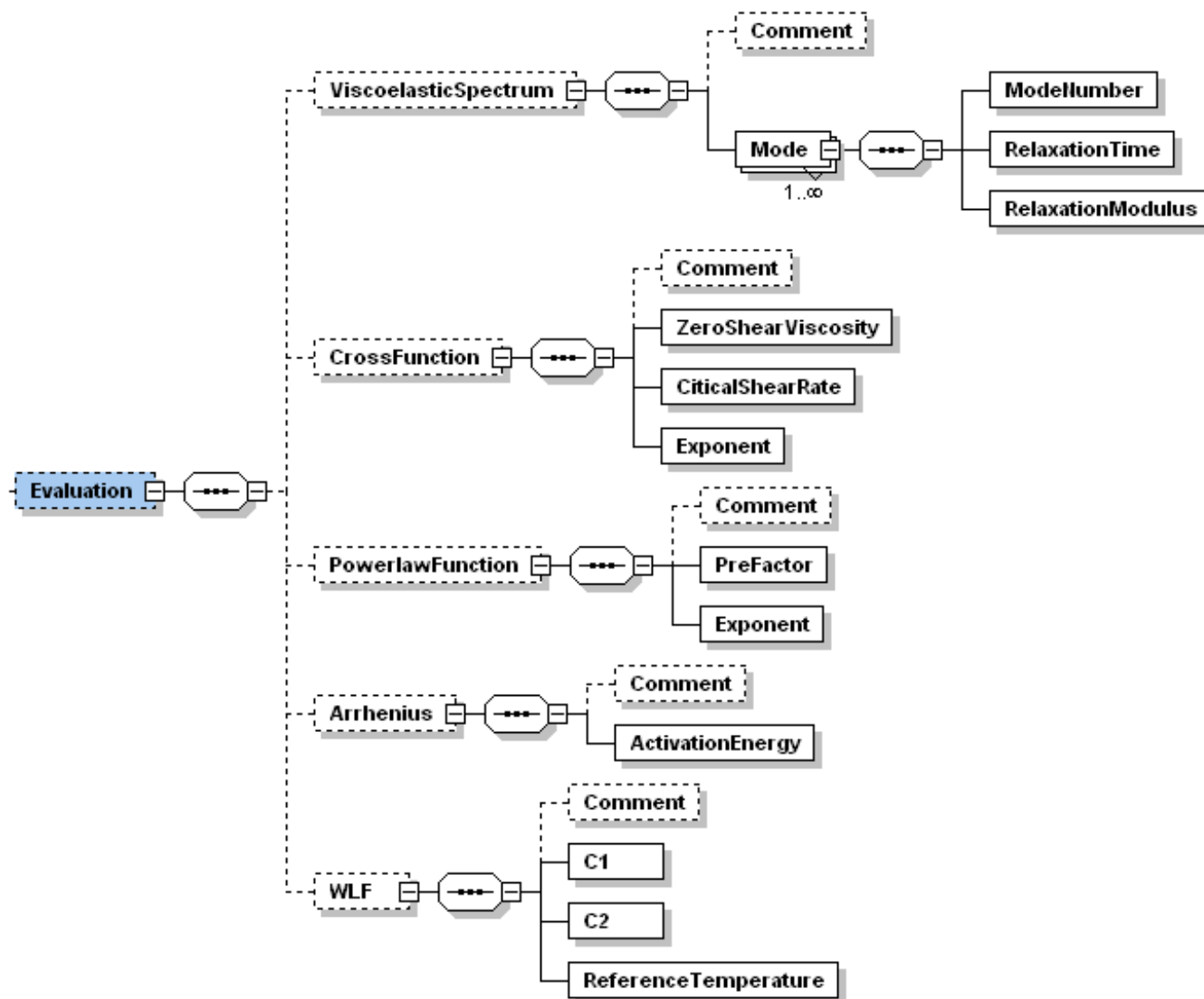


Tentative Structure of IUPAC-XML files – CVM Data





Tentative Structure of IUPAC-XML files – Evaluation





Unit System

- Use SI units ?
- Alternatives:
 - Fixed units for all measurement entities, e.g. stress only in Pa, not MPa
 advantage: very easy to implement, avoids confusion
 disadvantage: units only specified in reference document
 - Units can be defined for each measurement entity (column)
 advantage: higher flexibility
 disadvantage: more difficult to implement in XML
 - Units can be defined for each datapoint
 advantage: easy to implement, units are attributes of elements
 disadvantage: more disk space, confusion likely



To-Do's

- Define final file structure: XSD Schema
- Define unit system
- Write and publish document with specification (work already started)
- Continuation of standardization activities:
 - Further methods beyond rheology
 - Make XML format an ISO standard ? contacts necessary, long term
 - H.H. Winter proposed to continue work within ACCESS* project

*Amherst Cyberinfrastructure Consortium for Engineering and Science Synergy (ACCESS)

I U P A C

Advancing Worldwide Chemistry

