

**ThermoML – an XML-based Approach for Storage and Exchange of
Experimental and Critically Evaluated Thermophysical and
Thermochemical Property Data. 2. Uncertainties
(Supporting Information)**

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Supporting Information

Sample ThermoML Files.

Pure Compound or Mixture Data.

The following ThermoML file contains density and heat capacity data for a binary mixture of propane and 2-methylpropane accompanied by uncertainties provided by the authors.¹ The experimental results reported by the authors are extensive. Only the first three density and heat-capacity values listed in Tables 3 and 5 of the paper are represented in the ThermoML file.

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Reaction Data.

The following ThermoML file contains the internal energy of reaction for combustion of methhylurea accompanied by *device specification* and *repeatability* information provided by the authors,² as well as expanded and combined uncertainties estimated by TRC.

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    <sAuthor>Kabo, G. J. [Gennady J.]</sAuthor>
    <sAuthor>Frenkel, M. L.[Michael L.]</sAuthor>
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J/g</sCombUncertEvalMethod>
    <nCombUncertLevOfConfid>95</nCombUncertLevOfConfid>
  </CombinedUncertainty>
  <PropUncertainty>
    <nUncertAssessNum>1</nUncertAssessNum>
    <sUncertEvaluator>TRC</sUncertEvaluator>

```

<sUncertEvalMethod>Propagated repeatability multiplied by the coverage factor 1.8946 and device specification</sUncertEvalMethod>

<nUncertLevOfConfid>95</nUncertLevOfConfid>

</PropUncertainty>

<PropRepeatability>

<sRepeatEvaluator>Author</sRepeatEvaluator>

<eRepeatMethod>Standard deviation of the mean</eRepeatMethod>

</PropRepeatability>

<PropDeviceSpec>

<eDeviceSpecMethod>Calibrated by the experimentalist</eDeviceSpecMethod>

<sDeviceSpecMethod>Calculated from the calorimeter constant (14879.54 +- 10.07) J/K</sDeviceSpecMethod>

<nDeviceSpecLevOfConfid>95</nDeviceSpecLevOfConfid>

</PropDeviceSpec>

</Property>

<NumValues>

<PropertyValue>

<nPropNumber>1</nPropNumber>

<nPropValue>-17706.53</nPropValue>

<nPropDigits>7</nPropDigits>

<CombinedUncertainty>

<nCombUncertAssessNum>1</nCombUncertAssessNum>

<nCombExpandUncertValue>15.18</nCombExpandUncertValue>

</CombinedUncertainty>

<PropUncertainty>

<nUncertAssessNum>1</nUncertAssessNum>

<nExpandUncertValue>15.15</nExpandUncertValue>

</PropUncertainty>

<PropRepeatability>

<nPropRepeatValue>4.89</nPropRepeatValue>

<nRepetitions>8</nRepetitions>

```
</PropRepeatability>
  <nPropDeviceSpecValue>11.98</nPropDeviceSpecValue>
</PropertyValue>
</NumValues>
</ReactionData>
</DataReport>
```

Complete Text of ThermoML

```
<?xml version="1.0" encoding="UTF-8"?>
<!-- edited with XML Spy v4.4 U (http://www.xmlspy.com) by Robert D. Chirico (U. S.
Department of Commerce) -->
<xsd:schema xmlns:xsd="http://www.w3.org/2001/XMLSchema"
elementFormDefault="qualified" attributeFormDefault="unqualified">
  <xsd:annotation>
    <xsd:documentation>
      Data report
    </xsd:documentation>
  </xsd:annotation>
  <xsd:element name="DataReport" type="DataReport"/>
  <xsd:complexType name="DataReport">
    <xsd:annotation>
      <xsd:documentation>TRCReport complex type</xsd:documentation>
    </xsd:annotation>
    <xsd:sequence>
      <xsd:element name="Version">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="nVersionMajor" type="xsd:integer"/>
            <xsd:element name="nVersionMinor" type="xsd:integer"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <xsd:element ref="Citation"/>
      <xsd:element ref="Compound" minOccurs="0" maxOccurs="unbounded"/>
      <xsd:element ref="PureOrMixtureData" minOccurs="0"
maxOccurs="unbounded"/>
```



```

        <xsd:element ref="ReactionData" minOccurs="0"
maxOccurs="unbounded"/>
    </xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:simpleType name="ECitationType">
    <xsd:annotation>
        <xsd:documentation>Type of citation</xsd:documentation>
    </xsd:annotation>
    <xsd:restriction base="xsd:string">
        <xsd:enumeration value="book"/>
        <xsd:enumeration value="journal"/>
        <xsd:enumeration value="report"/>
        <xsd:enumeration value="patent"/>
        <xsd:enumeration value="thesis"/>
        <xsd:enumeration value="conferenceProceedings"/>
        <xsd:enumeration value="archivedDocument"/>
        <xsd:enumeration value="personalCorrespondence"/>
        <xsd:enumeration value="publishedTranslation"/>
        <xsd:enumeration value="unspecified"/>
    </xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:simpleType name="ECitationSourceType">
    <xsd:annotation>
        <xsd:documentation>The status type of the citation</xsd:documentation>
    </xsd:annotation>

```

```

<xsd:restriction base="xsd:string">
  <xsd:enumeration value="Original"/>
  <xsd:enumeration value="BiblioBulChemThermo"/>
  <xsd:enumeration value="TRCGeneral"/>
  <xsd:enumeration value="TRCGeneralChecked"/>
  <xsd:enumeration value="TRCDataCard"/>
  <xsd:enumeration value="ChemicalAbstracts"/>
  <xsd:enumeration value="Other"/>
</xsd:restriction>
</xsd:simpleType>
<!--
-->
<xsd:simpleType name="ECitationDataType">
  <xsd:annotation>
    <xsd:documentation>The data type of the citation</xsd:documentation>
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="ReferenceOnly"/>
    <xsd:enumeration value="SomeNumerical"/>
    <xsd:enumeration value="PureOnly"/>
    <xsd:enumeration value="Pure+SomeMixture"/>
    <xsd:enumeration value="MixtureOnly"/>
    <xsd:enumeration value="All"/>
    <xsd:enumeration value="GraphicalOnly"/>
  </xsd:restriction>
</xsd:simpleType>
<!--
-->
<xsd:element name="TRCRefID">

```

```

<xsd:annotation>
  <xsd:documentation>TRC Reference Identifier</xsd:documentation>
</xsd:annotation>
<xsd:complexType>
  <xsd:sequence>
    <xsd:element name="yrYrPub" type="xsd:integer">
      <xsd:annotation>
        <xsd:documentation>Integer year of
publication</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="sAuthor1" type="xsd:string">
      <xsd:annotation>
        <xsd:documentation>First 3 characters of Author 1 last
name</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="sAuthor2" type="xsd:string">
      <xsd:annotation>
        <xsd:documentation>First 3 characters of Author 2 last
name</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="nAuthorn" type="xsd:integer">
      <xsd:annotation>
        <xsd:documentation>Integer identifier to distinguish
conflicts</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
  </xsd:sequence>
</xsd:complexType>

```

```

</xsd:element>
<!--

-->
<xsd:element name="Citation">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element ref="TRCRefID" minOccurs="0"/>
      <xsd:element name="eType" type="ECitationType" minOccurs="0">
        <xsd:annotation>
          <xsd:documentation>The type of citation</xsd:documentation>
        </xsd:annotation>
      </xsd:element>
      <xsd:element name="eSourceType" type="ECitationSourceType"
minOccurs="0">
        <xsd:annotation>
          <xsd:documentation>The source status type for a
citation</xsd:documentation>
        </xsd:annotation>
      </xsd:element>
      <xsd:element name="eDataType" type="ECitationDataType"
minOccurs="0">
        <xsd:annotation>
          <xsd:documentation>The data type of the
citation</xsd:documentation>
        </xsd:annotation>
      </xsd:element>
      <xsd:element name="sCompany" type="xsd:string" minOccurs="0">
        <xsd:annotation>
          <xsd:documentation>Company, institution, or conference
name</xsd:documentation>

```

```

        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sAuthor" type="xsd:string" minOccurs="0"
maxOccurs="unbounded">
        <xsd:annotation>
            <xsd:documentation>Author of citation</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sPubName" type="xsd:string" minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>Name of the publication where the citation
was published.</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="yrPubYr" type="xsd:gYear" minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>Publication year of the
citation</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="dateCit" type="xsd:date" minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>Date of the citation</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sTitle" type="xsd:string" minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>Title of the citation</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sAbstract" type="xsd:string" minOccurs="0">

```

```

        <xsd:annotation>
            <xsd:documentation>An abstract of the
citation</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sKeyword" type="xsd:string" minOccurs="0"
maxOccurs="unbounded"/>
    <xsd:element name="urlCit" type="xsd:string" minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>URL to the citation</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sCASCit" type="xsd:string" minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>The Chemical Abstracts Service
citation</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sBulChemThermoCit" type="xsd:string"
minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>The Bulletin of Chemical Thermodynamics
citation</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sIDNum" type="xsd:string" minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>Identification number, e.g., a patent number
or a document number</xsd:documentation>
        </xsd:annotation>
    </xsd:element>

```

```

<xsd:element name="sLocation" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Reference to a location</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sVol" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Volume number</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sPage" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Page range where the citation can be
found</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:choice minOccurs="0">
  <xsd:element name="book">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:element name="sChapter" type="xsd:string"
minOccurs="0">
          <xsd:annotation>
            <xsd:documentation>Chapter
number</xsd:documentation>
          </xsd:annotation>
        </xsd:element>
        <xsd:element name="sEdition" type="xsd:string"
minOccurs="0">
          <xsd:annotation>

```

```

        <xsd:documentation>Edition number of the
book</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sEditor" type="xsd:string"
minOccurs="0" maxOccurs="unbounded">
        <xsd:annotation>
            <xsd:documentation>Editor of the
book</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sISBN" type="xsd:string"
minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>The International Standard
Book Number</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="journal">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="sISSN" type="xsd:string"
minOccurs="0">
                <xsd:annotation>
                    <xsd:documentation>The International Standard
Subscription Number</xsd:documentation>
                </xsd:annotation>
            </xsd:element>

```



```

        <xsd:element name="sIssue" type="xsd:string"
minOccurs="0">
            <xsd:annotation>
                <xsd:documentation>Issue number, usually
indicates month</xsd:documentation>
            </xsd:annotation>
        </xsd:element>
        <xsd:element name="sCODEN" type="xsd:string"
minOccurs="0">
            <xsd:annotation>
                <xsd:documentation>The CODEN identification of
the journal</xsd:documentation>
            </xsd:annotation>
        </xsd:element>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="thesis">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="sDeg" type="xsd:string"
minOccurs="0">
                <xsd:annotation>
                    <xsd:documentation>Academic degree designation,
e.g., MS or PhD</xsd:documentation>
                </xsd:annotation>
            </xsd:element>
            <xsd:element name="sDegInst" type="xsd:string"
minOccurs="0">
                <xsd:annotation>

```

```

        <xsd:documentation>Academic degree granting
institution</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sUMIPubNum" type="xsd:string"
minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>University Microfilms
International Publication Number</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<!--
-->
<xsd:element name="Compound">
    <xsd:annotation>
        <xsd:documentation>Material component characteristics that serves to
identify the component    </xsd:documentation>
    </xsd:annotation>
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="RegNum">
                <xsd:complexType>
                    <xsd:sequence>

```

```

        <xsd:element name="nCASRNum" type="xsd:integer"
minOccurs="0"/>
        <xsd:element name="nOrgNum" type="xsd:integer"
minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="sCASName" type="xsd:string" minOccurs="0"/>
<xsd:element name="sIUPACName" type="xsd:string" minOccurs="0">
    <xsd:annotation>
        <xsd:appinfo>IUPAC name, string</xsd:appinfo>
        <xsd:documentation>International Union of Physics and Applied
Chemistry name</xsd:documentation>
    </xsd:annotation>
</xsd:element>
<xsd:element name="sCommonName" type="xsd:string" minOccurs="0"
maxOccurs="unbounded">
    <xsd:annotation>
        <xsd:appinfo>Common name, string</xsd:appinfo>
        <xsd:documentation>Common name</xsd:documentation>
    </xsd:annotation>
</xsd:element>
<xsd:element name="sFormulaMolec" type="xsd:string" minOccurs="0">
    <xsd:annotation>
        <xsd:appinfo>Molecular formula, string</xsd:appinfo>
        <xsd:documentation>Chemical molecular
formula</xsd:documentation>
    </xsd:annotation>
</xsd:element>
<xsd:element name="sSmiles" type="xsd:string" minOccurs="0"
maxOccurs="unbounded">

```

```

        <xsd:annotation>
            <xsd:appinfo>SMILES notation, string</xsd:appinfo>
            <xsd:documentation>SMILES notation</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element ref="Sample" minOccurs="0" maxOccurs="unbounded"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<!--
-->
<xsd:element name="Sample">
    <xsd:annotation>
        <xsd:documentation>sample</xsd:documentation>
    </xsd:annotation>
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nSampleNm" type="xsd:integer"/>
            <xsd:element name="eSource" type="eSampleSource" minOccurs="0"/>
            <xsd:element name="eStatus" type="eSampleStatus" minOccurs="0"/>
            <xsd:element name="purity" minOccurs="0" maxOccurs="unbounded">
                <xsd:annotation>
                    <xsd:documentation>Purity of the sample</xsd:documentation>
                </xsd:annotation>
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:element name="nStep" type="xsd:integer"/>
                        <xsd:element name="ePurifMethod" type="ePurifMethod"
minOccurs="0" maxOccurs="unbounded"/>

```

```

        <xsd:element name="sPurifMethod" type="xsd:string"
minOccurs="0" maxOccurs="unbounded"/>
        <xsd:sequence minOccurs="0">
            <xsd:element name="nPurityMol" type="xsd:float">
                <xsd:annotation>
                    <xsd:documentation>purity value in mole
percent</xsd:documentation>
                </xsd:annotation>
            </xsd:element>
            <xsd:element name="nPurityMolDigits"
type="xsd:integer"/>
        </xsd:sequence>
        <xsd:sequence minOccurs="0">
            <xsd:element name="nPurityMass" type="xsd:float">
                <xsd:annotation>
                    <xsd:documentation>purity value in mass
percent</xsd:documentation>
                </xsd:annotation>
            </xsd:element>
            <xsd:element name="nPurityMassDigits"
type="xsd:integer"/>
        </xsd:sequence>
        <xsd:sequence minOccurs="0">
            <xsd:element name="nPurityVol" type="xsd:float">
                <xsd:annotation>
                    <xsd:documentation>purity value in volume
percent</xsd:documentation>
                </xsd:annotation>
            </xsd:element>
            <xsd:element name="nPurityVolDigits"
type="xsd:integer"/>

```

```

        </xsd:sequence>
        <xsd:sequence minOccurs="0">
            <xsd:element name="nWaterMassPerCent"
type="xsd:float">
                <xsd:annotation>
                    <xsd:documentation>mass per cent of
water</xsd:documentation>
                </xsd:annotation>
            </xsd:element>
            <xsd:element name="nWaterMassPerCentDigits"
type="xsd:integer"/>
        </xsd:sequence>
        <xsd:element name="eAnalMeth" type="ePurityAnalMethod"
minOccurs="0" maxOccurs="unbounded">
            <xsd:annotation>
                <xsd:documentation>Analytical method used to
determine purity</xsd:documentation>
            </xsd:annotation>
        </xsd:element>
        <xsd:element name="sAnalMeth" type="xsd:string"
minOccurs="0" maxOccurs="unbounded"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<!--
-->
<xsd:element name="PureOrMixtureData">

```

```

<xsd:complexType>
  <xsd:sequence>
    <xsd:element name="Component" maxOccurs="unbounded">
      <xsd:complexType>
        <xsd:sequence>
          <xsd:element ref="RegNum"/>
          <xsd:element name="nSampleNm" type="xsd:int"/>
        </xsd:sequence>
      </xsd:complexType>
    </xsd:element>
    <xsd:element name="eExpPurpose" type="eExpPurpose"
minOccurs="0">
      <xsd:annotation>
        <xsd:documentation>Purpose of
measurement</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="sCompiler" type="xsd:string" minOccurs="0"/>
    <xsd:element name="sContributor" type="xsd:string" minOccurs="0"/>
    <xsd:element name="dateDateAdded" minOccurs="0"/>
    <xsd:element name="Property" maxOccurs="unbounded">
      <xsd:complexType>
        <xsd:sequence>
          <xsd:element name="nPropNumber" type="xsd:integer"/>
          <xsd:element name="Property-MethodID">
            <xsd:annotation>
              <xsd:documentation> CASRN is necessary for
mixtures only</xsd:documentation>
            </xsd:annotation>
          </xsd:complexType>
          <xsd:sequence>

```

```

<xsd:element name="PropertyGroup">
  <xsd:complexType>
    <xsd:choice>
      <xsd:element name="Criticals">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element
name="ePropName">
              <xsd:simpleType>
                <xsd:restriction
base="xsd:string">
                  <xsd:enumeration
value="Critical temperature, K"/>
                    <xsd:enumeration
value="Critical pressure, kPa"/>
                      <xsd:enumeration
value="Critical density, kg/m3"/>
                        <xsd:enumeration
value="Critical molar volume, m3/mol"/>
                          <xsd:enumeration
value="Critical specific volume, m3/kg"/>
                            <xsd:enumeration
value="Critical compressibility"/>
                              <xsd:enumeration
value="Lower consolute temperature, K"/>
                                <xsd:enumeration
value="Upper consolute temperature, K"/>
                                  </xsd:restriction>
                                </xsd:simpleType>
                              </xsd:element>

```



```

name="eMethodName" minOccurs="0">
    base="xsd:string">
        value="Visual observation in an unstirred cell"/>
        value="Visual observation in a stirred cell"/>
        value="DSC/DTA"/>
        value="Derived from PVT data"/>
        value="Extrapolated vapor pressure"/>
        value="Rectilinear diameter"/>
        value="Appearance of two phases"/>
        value="Disappearance of two phases"/>
        value="Direct measurement"/>
        value="Other"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>

```

```

        </xsd:complexType>
    </xsd:element>
    <xsd:element
name="VaporPBoilingTAzeotropTandP">
        <xsd:complexType>
            <xsd:sequence>
                <xsd:element
name="ePropName">
                    <xsd:simpleType>
                        <xsd:restriction
base="xsd:string">
                            <xsd:enumeration
value="Vapor or Sublimation pressure, kPa"/>
                                <xsd:enumeration
value="Normal boiling temperature, K"/>
                                    <xsd:enumeration
value="Boiling temperature at pressure P, K"/>
                                        <xsd:enumeration
value="Azeotropic pressure, kPa"/>
                                            <xsd:enumeration
value="Azeotropic temperature, K"/>
                                                </xsd:restriction>
                                                    </xsd:simpleType>
                                                        </xsd:element>
                                                            <xsd:element
name="eMethodName" minOccurs="0">
                        <xsd:simpleType>
                            <xsd:restriction
base="xsd:string">
                                <xsd:enumeration
value="Manometric method"/>

```

value="Closed cell (Static) method"/>	<xsd:enumeration
value="Diaphragm manometer"/>	<xsd:enumeration
value="Inclined piston gauge"/>	<xsd:enumeration
value="Isochoric PVT apparatus"/>	<xsd:enumeration
value="Isoteniscope"/>	<xsd:enumeration
value="Knudsen effusion method"/>	<xsd:enumeration
value="Distillation"/>	<xsd:enumeration
value="Ebulliometric method (Recirculating still)/>	<xsd:enumeration
value="Twin ebulliometer"/>	<xsd:enumeration
value="Transpiration method"/>	<xsd:enumeration
value="Rate of evaporation"/>	<xsd:enumeration
value="By X=Y"/>	<xsd:enumeration
value="By P(X) extreme"/>	<xsd:enumeration
value="By T(X) extreme"/>	<xsd:enumeration
value="Other"/>	<xsd:enumeration
	</xsd:restriction>

```

</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="PhaseTransition">
<xsd:complexType>
<xsd:sequence>
<xsd:element
name="ePropName">
<xsd:simpleType>
<xsd:restriction
base="xsd:string">
<xsd:enumeration
value="Triple point temperature, K"/>
<xsd:enumeration
value="Triple point pressure, kPa"/>
<xsd:enumeration
value="Normal melting temperature, K"/>
<xsd:enumeration
value="Enthalpy of transition or fusion, kJ/mol"/>
<xsd:enumeration
value="Cryoscopic constant, 1/K"/>
<xsd:enumeration
value="Enthalpy of vaporization or sublimation, kJ/mol"/>
<xsd:enumeration
value="Quadruple (quintuple) point temperature, K"/>
<xsd:enumeration
value="Quadruple (quintuple) point pressure, kPa"/>

```

value="Solid-liquid equilibrium temperature, K"/>	<xsd:enumeration
value="Liquid-liquid equilibrium temperature, K"/>	<xsd:enumeration
value="Eutectic temperature, K"/>	<xsd:enumeration
	</xsd:restriction>
	</xsd:simpleType>
	</xsd:element>
	<xsd:element
name="eMethodName" minOccurs="0">	<xsd:simpleType>
	<xsd:restriction
base="xsd:string">	<xsd:enumeration
value="Visual observation"/>	<xsd:enumeration
value="Heating/Cooling curves"/>	<xsd:enumeration
value="DSC/DTA"/>	<xsd:enumeration
value="Adiabatic calorimetry"/>	<xsd:enumeration
value="Large-sample thermal analysis"/>	<xsd:enumeration
value="Drop calorimetry"/>	<xsd:enumeration
value="Drop ice or diphenyl ether calorimetry"/>	<xsd:enumeration
value="Obtained from cryoscopic constant"/>	<xsd:enumeration

```

value="Derived from phase diagram analysis"/>
<xsd:enumeration
value="Static calorimetry"/>
<xsd:enumeration
value="Flow calorimetry"/>
<xsd:enumeration
value="Derived by Second law"/>
<xsd:enumeration
value="Derived by Second law from precise ebulliometry"/>
<xsd:enumeration
value="Depression of a freezing point of a dilute solution"/>
<xsd:enumeration
value="Other"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element
name="CompositionAtPhaseEquilibrium">
<xsd:complexType>
<xsd:sequence>
<xsd:element
name="ePropName">
<xsd:simpleType>
<xsd:restriction
base="xsd:string">

```

value="Azeotropic composition: mole fraction"/>	<xsd:enumeration
value="Azeotropic composition: mass fraction"/>	<xsd:enumeration
value="Eutectic composition: volume fraction"/>	<xsd:enumeration
value="Eutectic composition: mole fraction"/>	<xsd:enumeration
value="Eutectic composition: mass fraction"/>	<xsd:enumeration
value="Lower consolute composition: volume fraction"/>	<xsd:enumeration
value="Lower consolute composition: mole fraction"/>	<xsd:enumeration
value="Lower consolute composition: mass fraction"/>	<xsd:enumeration
value="Mass per volume of solution, kg/m3"/>	<xsd:enumeration
value="Mass ratio to solvent"/>	<xsd:enumeration
value="MolaLity, mol/kg"/>	<xsd:enumeration
value="MolaRity, mol/dm3"/>	<xsd:enumeration
value="Mole fraction"/>	<xsd:enumeration
value="Mole fraction in LLG critical state"/>	<xsd:enumeration
value="Mole ratio to solvent"/>	<xsd:enumeration

```

value="Moles per mass of solution, mol/kg"/>
value="Upper consolute composition: volume fraction"/>
value="Upper consolute composition: mole fraction"/>
value="Upper consolute composition: mass fraction"/>
value="Volume fraction"/>
value="Volume ratio to solvent"/>
value="Mass fraction"/>
value="Mass fraction in LLG critical state"/>
value="Henry's Law constant for mole fraction, kPa"/>
value="Henry's Law constant (molaLity), kPa kg/mol"/>
value="Henry's Law constant (molaRity), kPa l/mol"/>
value="Bunsen coefficient"/>
value="Ostwald coefficient"/>
value="Partial pressure, kPa"/>
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
<xsd:enumeration
</xsd:restriction>
</xsd:simpleType>
</xsd:element>

```


name="eMethodName" minOccurs="0">	<xsd:element
	<xsd:simpleType>
base="xsd:string">	<xsd:restriction
value="By X=Y"/>	<xsd:enumeration
value="By T or P extreme"/>	<xsd:enumeration
value="Chromatography"/>	<xsd:enumeration
value="Spectrophotometry"/>	<xsd:enumeration
value="Determined by refractive index and/or density"/>	<xsd:enumeration
value="Calculated by Gibbs-Duhem equation"/>	<xsd:enumeration
value="Titration method"/>	<xsd:enumeration
value="Static method"/>	<xsd:enumeration
value="Dynamic method"/>	<xsd:enumeration
value="Phase equilibration"/>	<xsd:enumeration
value="Derived from phase diagram analysis"/>	<xsd:enumeration
value="Appearance of two phases"/>	<xsd:enumeration
value="Disappearance of two phases"/>	<xsd:enumeration

```

value="Photoacoustic method"/>
<xsd:enumeration
value="Other"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element
name="ActivityFugacityOsmoticProp">
<xsd:complexType>
<xsd:sequence>
<xsd:element
name="ePropName">
<xsd:simpleType>
<xsd:restriction
base="xsd:string">
<xsd:enumeration
value="Activity"/>
<xsd:enumeration
value="Activity coefficient"/>
<xsd:enumeration
value="Fugacity, kPa"/>
<xsd:enumeration
value="Fugacity coefficient"/>
<xsd:enumeration
value="Osmotic pressure, kPa"/>

```

```

value="Osmotic coefficient"/>
<xsd:enumeration
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="eMethodName" minOccurs="0">
<xsd:simpleType>
<xsd:restriction
base="xsd:string">
<xsd:enumeration
value="Chromatography"/>
<xsd:enumeration
value="Spectroscopy"/>
<xsd:enumeration
value="Mass-spectrometry"/>
<xsd:enumeration
value="NMR spectrometry"/>
<xsd:enumeration
value="Static method"/>
<xsd:enumeration
value="Isopiestic method"/>
<xsd:enumeration
value="Other"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>

```

```

</xsd:element>
<xsd:element name="VolumetricProp">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element
name="ePropName">
          <xsd:simpleType>
            <xsd:restriction
              <xsd:enumeration
value="Specific density, kg/m3"/>
              <xsd:enumeration
value="Specific volume, m3/kg"/>
              <xsd:enumeration
value="Molar density, mol/m3"/>
              <xsd:enumeration
value="Molar volume, m3/mol"/>
              <xsd:enumeration
value="2nd virial coefficient, m3/mol"/>
              <xsd:enumeration
value="2nd acoustic virial coefficient, m3/mol"/>
              <xsd:enumeration
value="3rd virial coefficient, m6/mol2"/>
              <xsd:enumeration
value="3rd acoustic virial coefficient, m6/mol2"/>
              <xsd:enumeration
value="3rd interaction virial coefficient C112, m6/mol2"/>
              <xsd:enumeration
value="3rd interaction virial coefficient C122, m6/mol2"/>
              <xsd:enumeration
value="Excess virial coefficient, m3/mol"/>

```

value="Interaction virial coefficient, m ³ /mol"/>	<xsd:enumeration
value="Excess volume, m ³ /mol"/>	<xsd:enumeration
value="Partial molar volume, m ³ /mol"/>	<xsd:enumeration
value="Relative partial molar volume, m ³ /mol"/>	<xsd:enumeration
value="Apparent molar volume, m ³ /mol"/>	<xsd:enumeration
value="Adiabatic compressibility, 1/kPa"/>	<xsd:enumeration
value="Isothermal compressibility, 1/kPa"/>	<xsd:enumeration
value="Coefficient of expansion, 1/K"/>	<xsd:enumeration
value="Compressibility factor"/>	<xsd:enumeration
value="Thermal pressure coefficient, kPa/K"/>	<xsd:enumeration
	</xsd:restriction>
	</xsd:simpleType>
	</xsd:element>
	<xsd:element
name="eMethodName" minOccurs="0">	<xsd:simpleType>
	<xsd:restriction
base="xsd:string">	<xsd:enumeration
value="Pycnometric method"/>	

```

value="Buoyancy method"/>
value="Vibrating tube method"/>
value="Isochoric PVT measurement"/>
value="Other PVT measurement"/>
value="Burnett expansion technique"/>
value="Constant-volume piesometry"/>
value="Direct dilatometry"/>
value="Derived analytically"/>
value="Derived graphically"/>
value="Calculated with densities of this investigation"/>
value="Calculated with a solvent density reported elsewhere"/>
value="Other"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>

```

```

</xsd:element>
<xsd:element
name="HeatCapacityAndDerivedProp">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element
name="ePropName">
                <xsd:simpleType>
                    <xsd:restriction
base="xsd:string">
                        <xsd:enumeration
value="Heat capacity at constant pressure Cp, J/K/mol"/>
                            <xsd:enumeration
value="Heat capacity at vapor saturation pressure Csat, J/K/mol"/>
                                <xsd:enumeration
value="Heat capacity at constant volume Cv, J/K/mol"/>
                                    <xsd:enumeration
value="Heat capacity at constant pressure Cp per unit mass, J/K/kg"/>
                                        <xsd:enumeration
value="Heat capacity at constant pressure Cp per unit volume, J/K/m3"/>
                                            <xsd:enumeration
value="Heat capacity at constant volume Cv per unit mass, J/K/kg"/>
                                                <xsd:enumeration
value="Heat capacity at constant volume Cv per unit volume, J/K/m3"/>
                                                    <xsd:enumeration
value="Heat capacity ratio Cp/Cv"/>
                                                        <xsd:enumeration
value="Entropy, J/K/mol"/>
                                                            <xsd:enumeration
value="Enthalpy, kJ/mol"/>

```

value="Enthalpy function $\{H(T)-H(0)\}/T$, J/K/mol"/>	<xsd:enumeration
value="Gibbs energy function $\{G(T)-H(0)\}/T$, J/K/mol"/>	<xsd:enumeration
value="Gibbs energy, kJ/mol"/>	<xsd:enumeration
value="Helmholtz energy, kJ/mol"/>	<xsd:enumeration
value="Internal energy, kJ/mol"/>	<xsd:enumeration
value="Joule-Thomson coefficient, K/kPa"/>	<xsd:enumeration
value="Pressure coefficient of enthalpy, J/mol/kPa"/>	<xsd:enumeration
	</xsd:restriction>
	</xsd:simpleType>
	</xsd:element>
	<xsd:element
name="eMethodName" minOccurs="0">	<xsd:simpleType>
	<xsd:restriction
base="xsd:string">	<xsd:enumeration
value="Vacuum adiabatic calorimetry"/>	<xsd:enumeration
value="Small (less than 1 g) adiabatic calorimetry"/>	<xsd:enumeration
value="Flow calorimetry"/>	<xsd:enumeration
value="Large sample (1 g) DSC"/>	<xsd:enumeration


```

value="Small sample (50 mg) DSC"/>
<xsd:enumeration
value="Drop calorimetry"/>
<xsd:enumeration
value="Drop ice or diphenyl ether calorimetry"/>
<xsd:enumeration
value="Open cup calorimetry"/>
<xsd:enumeration
value="Closed cup calorimetry"/>
<xsd:enumeration
value="Differential flow calorimetry"/>
<xsd:enumeration
value="Extra sensitive DSC"/>
<xsd:enumeration
value="Twin closed calorimetry"/>
<xsd:enumeration
value="Derived from speed of sound"/>
<xsd:enumeration
value="Derived from equation of state"/>
<xsd:enumeration
value="Expansion technique"/>
<xsd:enumeration
value="Other"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>

```

```

</xsd:element>
<xsd:element
name="ExcessPartialApparentEnergyProp">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element
name="ePropName">
        <xsd:simpleType>
          <xsd:restriction
base="xsd:string">
            <xsd:enumeration
value="Apparent enthalpy, kJ/mol"/>
            <xsd:enumeration
value="Apparent entropy, J/K/mol"/>
            <xsd:enumeration
value="Apparent Gibbs energy, kJ/mol"/>
            <xsd:enumeration
value="Apparent molar heat capacity, J/K/mol"/>
            <xsd:enumeration
value="Enthalpy of mixing with a binary solvent, kJ/mol"/>
            <xsd:enumeration
value="Excess enthalpy, kJ/mol"/>
            <xsd:enumeration
value="Enthalpy of mixing with binary solvent, kJ/mol"/>
            <xsd:enumeration
value="Excess entropy, J/K/mol"/>
            <xsd:enumeration
value="Excess Gibbs energy, kJ/mol"/>
            <xsd:enumeration
value="Excess heat capacity, J/K/mol"/>

```

value="Partial molar enthalpy, kJ/mol"/>	<xsd:enumeration
value="Partial molar entropy, J/K/mol"/>	<xsd:enumeration
value="Partial molar Gibbs energy, kJ/mol"/>	<xsd:enumeration
value="Partial molar heat capacity, J/K/mol"/>	<xsd:enumeration
value="Relative partial molar enthalpy, kJ/mol"/>	<xsd:enumeration
value="Relative partial molar entropy, J/K/mol"/>	<xsd:enumeration
value="Relative partial molar Gibbs energy, kJ/mol"/>	<xsd:enumeration
value="Relative partial molar heat capacity, J/K/mol"/>	<xsd:enumeration
value="Standard state enthalpy, kJ/mol"/>	<xsd:enumeration
value="Standard state entropy, J/K/mol"/>	<xsd:enumeration
value="Standard state Gibbs energy, kJ/mol"/>	<xsd:enumeration
value="Standard state heat capacity, J/K/mol"/>	<xsd:enumeration
value=""/>	</xsd:restriction>
	</xsd:simpleType>
	</xsd:element>
	<xsd:element
name="eMethodName" minOccurs="0">	

```

        <xsd:simpleType>
            <xsd:restriction
                base="xsd:string">
                <xsd:enumeration
                    value="Vacuum adiabatic calorimetry"/>
                <xsd:enumeration
                    value="Small (less than 1 g) adiabatic calorimetry"/>
                <xsd:enumeration
                    value="Flow calorimetry"/>
                <xsd:enumeration
                    value="Differential flow calorimetry"/>
                <xsd:enumeration
                    value="Calvet calorimetry"/>
                <xsd:enumeration
                    value="Large sample (1 g) DSC"/>
                <xsd:enumeration
                    value="Small sample (50 mg) DSC"/>
                <xsd:enumeration
                    value="Extra sensitive DSC"/>
                <xsd:enumeration
                    value="Twin closed calorimetry"/>
                <xsd:enumeration
                    value="Other"/>
            </xsd:restriction>
        </xsd:simpleType>
    </xsd:element>
<xsd:element
    name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>

```

```

name="ePropName">
    <xsd:element name="TransportProp">
        <xsd:complexType>
            <xsd:sequence>
                <xsd:element
                    name="ePropName">
                        <xsd:simpleType>
                            <xsd:restriction
                                base="xsd:string">
                                    <xsd:enumeration
                                        value="Viscosity, Pa*s"/>
                                        <xsd:enumeration
                                        value="Kinematic viscosity, m2/s"/>
                                        <xsd:enumeration
                                        value="Fluidity, 1/Pa*s"/>
                                        <xsd:enumeration
                                        value="Thermal conductivity, W/m/K"/>
                                        <xsd:enumeration
                                        value="Thermal diffusivity, m2/s"/>
                                        <xsd:enumeration
                                        value="Binary diffusion coefficient, 1e-9 m2/s"/>
                                        <xsd:enumeration
                                        value="Self diffusion coefficient, 1e-9 m2/s"/>
                                        <xsd:enumeration
                                        value="Tracer diffusion coefficient, 1e-9 m2/s"/>
                                    </xsd:restriction>
                                </xsd:simpleType>
                            </xsd:element>
                        <xsd:element
                            name="eMethodName" minOccurs="0">
                                <xsd:simpleType>

```

base="xsd:string">

value="Capillary tube (Ostwald; Ubbelohde) method"/>

value="Cone and plate viscometry"/>

value="Concentric cylinders viscometry"/>

value="Falling or rolling sphere viscometry"/>

value="Oscillating disk viscometry"/>

value="Vibrating wire viscometry"/>

value="Parallel plate method"/>

value="Coaxial cylinder method"/>

value="Hot wire method"/>

value="Optical interferometry"/>

value="Dispersion"/>

value="Diaphragm Cell"/>

value="Open capillary"/>

value="Closed capillary"/>

<xsd:restriction

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

<xsd:enumeration

```

value="Taylor dispersion method"/>
<xsd:enumeration
value="NMR spin-echo technique"/>
<xsd:enumeration
value="Other"/>
<xsd:enumeration
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element
name="RefractionSurfaceTensionSoundSpeed">
<xsd:complexType>
<xsd:sequence>
<xsd:element
name="ePropName">
<xsd:simpleType>
<xsd:restriction
base="xsd:string">
<xsd:enumeration
value="Refractive index (Na D-line)"/>
<xsd:enumeration
value="Refractive index (other wavelength)"/>
<xsd:enumeration
value="Surface tension liquid-gas, N/m"/>
<xsd:enumeration
value="Interfacial tension, N/m"/>

```

value="Speed of sound, m/s"/>	<xsd:enumeration
	</xsd:restriction>
	</xsd:simpleType>
	</xsd:element>
	<xsd:element
name="eMethodName" minOccurs="0">	
	<xsd:simpleType>
	<xsd:restriction
base="xsd:string">	
	<xsd:enumeration
value="Standard Abbe refractometry"/>	
	<xsd:enumeration
value="Precision Abbe refractometry"/>	
	<xsd:enumeration
value="Dipping refractometry (monochromatic)/>	
	<xsd:enumeration
value="Interferometer"/>	
	<xsd:enumeration
value="Capillary rise"/>	
	<xsd:enumeration
value="Drop weight"/>	
	<xsd:enumeration
value="Drop volume"/>	
	<xsd:enumeration
value="Maximal bubble pressure"/>	
	<xsd:enumeration
value="Pendant drop shape"/>	
	<xsd:enumeration
value="Ring tensiometer"/>	


```

value="Linear variable-path acoustic interferometer"/>
<xsd:enumeration
value="Sing-around technique in a fixed-path interferometer"/>
<xsd:enumeration
value="Annular interferometer"/>
<xsd:enumeration
value="Pulse-echo method"/>
<xsd:enumeration
value="Spherical resonator"/>
<xsd:enumeration
value="Light diffraction method"/>
<xsd:enumeration
value="Other"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
</xsd:choice>
</xsd:complexType>
</xsd:element>
<xsd:element ref="RegNum" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="PropPhaseID" minOccurs="0">
<xsd:annotation>

```

```

        <xsd:documentation> CASRN is necessary for
mixtures only</xsd:documentation>
    </xsd:annotation>
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="ePropPhase"
type="ePhaseName"/>
            <xsd:element ref="RegNum" minOccurs="0">
                <xsd:annotation>
                    <xsd:documentation> CASRN is necessary
for mixtures only</xsd:documentation>
                </xsd:annotation>
            </xsd:element>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="ePresentation" type="ePresentation"/>
<xsd:element name="eRefStateType" type="eRefStateType"
minOccurs="0"/>
    <xsd:sequence minOccurs="0">
        <xsd:element name="nRefTemp" type="xsd:float"/>
        <xsd:element name="nRefTempDigits"
type="xsd:integer"/>
    </xsd:sequence>
    <xsd:sequence minOccurs="0">
        <xsd:element name="nRefPressure" type="xsd:float"/>
        <xsd:element name="nRefPressureDigits"
type="xsd:integer"/>
    </xsd:sequence>
    <xsd:element name="RefPhaseID" minOccurs="0">
        <xsd:annotation>

```

```

        <xsd:documentation> CASRN is necessary for
mixtures only</xsd:documentation>
    </xsd:annotation>
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="eRefPhase"
type="ePhaseName"/>
            <xsd:element ref="RegNum" minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element ref="Solvent" minOccurs="0"/>
<xsd:element name="eStandardState" minOccurs="0">
    <xsd:simpleType>
        <xsd:restriction base="xsd:string">
            <xsd:enumeration value="Pure compound"/>
            <xsd:enumeration value="Hypothetical pure
solute"/>
            <xsd:enumeration value="Hypothetical unit
molality solute"/>
            <xsd:enumeration value="Hypothetical unit
molarity solute"/>
            <xsd:enumeration value="Infinite dilution solute"/>
        </xsd:restriction>
    </xsd:simpleType>
</xsd:element>
<xsd:element ref="CombinedUncertainty" minOccurs="0"
maxOccurs="unbounded"/>
    <xsd:element name="PropUncertainty"
type="PropVarUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>

```

```

        <xsd:element name="PropRepeatability"
type="PropVarRepeatabilityType" minOccurs="0"/>
        <xsd:element name="PropDeviceSpec"
type="PropVarDeviceSpecType" minOccurs="0"/>
        <xsd:element ref="CurveDev" minOccurs="0"
maxOccurs="unbounded"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="PhaseID" maxOccurs="unbounded">
    <xsd:annotation>
        <xsd:documentation> CASRN is necessary for mixtures
only</xsd:documentation>
    </xsd:annotation>
</xsd:complexType>
    <xsd:sequence>
        <xsd:element name="ePhase" type="ePhaseName"/>
        <xsd:element ref="RegNum" minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="Constraint" minOccurs="0"
maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="ConstraintID">
                <xsd:annotation>
                    <xsd:documentation> CASRN is necessary for
mixtures only</xsd:documentation>
                </xsd:annotation>
            </xsd:complexType>

```

```

        <xsd:sequence>
            <xsd:element name="ConstraintType"
type="ConstraintVariableType"/>
            <xsd:element ref="RegNum" minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="ConstraintPhaseID" minOccurs="0">
    <xsd:annotation>
        <xsd:documentation> CASRN is necessary for
mixtures only</xsd:documentation>
    </xsd:annotation>
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="eConstraintPhase"
type="ePhaseName"/>
            <xsd:element ref="RegNum" minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element ref="Solvent" minOccurs="0"/>
<xsd:element name="nConstraintValue" type="xsd:float"/>
<xsd:element name="nConstrDigits" type="xsd:integer"/>
<xsd:element name="ConstrUncertainty"
type="ConstrUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
    <xsd:element name="ConstrRepeatability"
type="ConstrRepeatabilityType" minOccurs="0"/>
    <xsd:element name="ConstrDeviceSpec"
type="ConstrDeviceSpecType" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>

```

```

        </xsd:element>
        <xsd:element name="Variable" minOccurs="0"
maxOccurs="unbounded">
            <xsd:complexType>
                <xsd:sequence>
                    <xsd:element name="nVarNumber" type="xsd:integer"/>
                    <xsd:element name="VariableID">
                        <xsd:annotation>
                            <xsd:documentation> CASRN is necessary for
mixtures only</xsd:documentation>
                        </xsd:annotation>
                    <xsd:complexType>
                        <xsd:sequence>
                            <xsd:element name="VariableType"
type="ConstraintVariableType"/>
                            <xsd:element ref="RegNum" minOccurs="0"/>
                        </xsd:sequence>
                    </xsd:complexType>
                </xsd:element>
                <xsd:element name="VarPhaseID" minOccurs="0">
                    <xsd:annotation>
                        <xsd:documentation> CASRN is necessary for
mixtures only</xsd:documentation>
                    </xsd:annotation>
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:element name="eVarPhase"
type="ePhaseName"/>
                        <xsd:element ref="RegNum" minOccurs="0"/>
                    </xsd:sequence>
                </xsd:complexType>
            </xsd:complexType>
        </xsd:element>

```

```

        </xsd:element>
        <xsd:element ref="Solvent" minOccurs="0"/>
        <xsd:element name="VarUncertainty"
type="PropVarUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="VarRepeatability"
type="PropVarRepeatabilityType" minOccurs="0"/>
        <xsd:element name="VarDeviceSpec"
type="PropVarDeviceSpecType" minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
    <xsd:element ref="NumValues" minOccurs="0"
maxOccurs="unbounded"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<!--
-->
<xsd:element name="ReactionData">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="Participant" maxOccurs="unbounded">
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:element ref="RegNum"/>
                        <xsd:element name="nSampleNm" type="xsd:int"
minOccurs="0"/>
                        <xsd:element name="nStoichiometricCoef" type="xsd:float"/>
                        <xsd:element name="ePhase" type="ePhaseName"/>

```

```

        <xsd:element name="eCompositionRepresentation"
minOccurs="0">
            <xsd:annotation>
                <xsd:documentation>Only for reactions with the initial
state change</xsd:documentation>
            </xsd:annotation>
            <xsd:simpleType>
                <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="Mole ratio of solvent to
participant"/>
                    <xsd:enumeration value="Molality (moles of
participant per kilogram of solvent)"/>
                    <xsd:enumeration value="Moles of participant per
kilogram of solution"/>
                    <xsd:enumeration value="Molarity (moles of
participant per liter of solution)"/>
                    <xsd:enumeration value="Mole ratio (moles of
participant per mole of solvent)"/>
                    <xsd:enumeration value="Mass ratio (mass of
participant per mass of solvent)"/>
                    <xsd:enumeration value="Volume ratio (volume of
participant per volume of solvent)"/>
                    <xsd:enumeration value="Mass of participant (kg)
per volume of solution (m-3)"/>
                </xsd:restriction>
            </xsd:simpleType>
        </xsd:element>
        <xsd:element name="nNumericalComposition"
type="xsd:float" minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>

```



```

    </xsd:element>
    <xsd:element name="eExpPurpose" type="eExpPurpose"
minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>Purpose of
measurement</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sCompiler" type="xsd:string" minOccurs="0"/>
    <xsd:element name="sContributor" type="xsd:string" minOccurs="0"/>
    <xsd:element name="dateDateAdded" minOccurs="0"/>
    <xsd:element name="eReactionType">
        <xsd:simpleType>
            <xsd:restriction base="xsd:string">
                <xsd:enumeration value="Combustion with oxygen"/>
                <xsd:enumeration value="Addition of various compounds to
unsaturated compounds"/>
                <xsd:enumeration value="Addition of water to a liquid or solid
to produce a hydrate"/>
                <xsd:enumeration value="Atomization (or formation from
atoms)/>
                <xsd:enumeration value="Combustion with other elements or
compounds"/>
                <xsd:enumeration value="Esterification"/>
                <xsd:enumeration value="Exchange of alkyl groups"/>
                <xsd:enumeration value="Exchange of hydrogen (atoms) with
other groups"/>
                <xsd:enumeration value="Formation of a compound from
elements in their stable state"/>
                <xsd:enumeration value="Halogenation (addition of or
replacement by a halogen)"/>
            </xsd:restriction>
        </xsd:simpleType>
    </xsd:element>

```

```

        <xsd:enumeration value="Hydrogenation (addition of H2 to
unsaturated compounds)"/>
        <xsd:enumeration value="Hydrohalogenation"/>
        <xsd:enumeration value="Hydrolysis of ions"/>
        <xsd:enumeration value="Other reactions with water"/>
        <xsd:enumeration value="Ion exchange"/>
        <xsd:enumeration value="Neutralization (reaction of an acid
with a base)"/>
        <xsd:enumeration value="Oxidation with oxidizing agents
other than oxygen"/>
        <xsd:enumeration value="Oxidation with oxygen (not
complete)"/>
        <xsd:enumeration value="Polymerization (all other types)"/>
        <xsd:enumeration value="Homonuclear dimerization"/>
        <xsd:enumeration value="Solvolysis (solvents other than
water)"/>
        <xsd:enumeration value="Stereoisomerism"/>
        <xsd:enumeration value="Structural isomerization"/>
        <xsd:enumeration value="Other reactions"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="Property" maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nPropNumber" type="xsd:integer"/>
            <xsd:element name="Property-MethodID">
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:element name="PropertyGroup">
                            <xsd:complexType>

```

```

                                <xsd:choice>
                                    <xsd:element
name="EnthalpyInternalEnergyOfReaction">
                                <xsd:complexType>
                                    <xsd:sequence>
                                        <xsd:element
name="ePropName">
                                            <xsd:simpleType>
                                                <xsd:restriction
base="xsd:string">
                                                    <xsd:enumeration
value="Enthalpy of reaction, kJ/mol"/>
                                                        <xsd:enumeration
value="Internal energy of reaction (mass basis), J/g"/>
                                                            <xsd:enumeration
value="Internal energy of reaction (mole basis), kJ/mol"/>
                                                                </xsd:restriction>
                                                                    </xsd:simpleType>
                                                                </xsd:element>
                                                            <xsd:element
name="eMethodName" minOccurs="0">
                                            <xsd:simpleType>
                                                <xsd:restriction
base="xsd:string">
                                                    <xsd:enumeration
value="Static bomb calorimetry"/>
                                                        <xsd:enumeration
value="Rotating bomb calorimetry"/>
                                                            <xsd:enumeration
value="Micro-bomb calorimetry"/>

```

```

value="Flame calorimetry"/>
<xsd:enumeration
value="Other"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element
name="ReactionEquilibriumProp">
<xsd:complexType>
<xsd:sequence>
<xsd:element
name="ePropName">
<xsd:simpleType>
<xsd:restriction
base="xsd:string">
<xsd:enumeration
value="Thermodynamic equilibrium constant"/>
<xsd:enumeration
value="Apparent equilibrium constant in terms of molality, (mol/kg)^n"/>
<xsd:enumeration
value="Apparent equilibrium constant in terms of molarity, (mol/dm3)^n"/>
<xsd:enumeration
value="Apparent equilibrium constant in terms of pressure, kPa^n"/>
<xsd:enumeration
value="Apparent equilibrium constant in terms of mole fraction X"/>

```

```

</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="eMethodName" minOccurs="0">
<xsd:simpleType>
<xsd:restriction
base="xsd:string">
<xsd:enumeration
value="Static equilibration"/>
<xsd:enumeration
value="Dynamic equilibration"/>
<xsd:enumeration
value="Chromatography"/>
<xsd:enumeration
value="IR spectrometry"/>
<xsd:enumeration
value="UV spectroscopy"/>
<xsd:enumeration
value="NMR spectrometry"/>
<xsd:enumeration
value="Titration"/>
<xsd:enumeration
value="Other"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element
name="sMethodName" type="xsd:string" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>

```

```

                </xsd:element>
            </xsd:choice>
        </xsd:complexType>
    </xsd:element>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="Solvent" minOccurs="0">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element ref="RegNum"/>
            <xsd:element name="ePhase"
type="ePhaseName"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="Catalyst" minOccurs="0">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element ref="RegNum"/>
            <xsd:element name="ePhase" type="ePhaseName"
minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="eStandardState" minOccurs="0">
    <xsd:simpleType>
        <xsd:restriction base="xsd:string">
            <xsd:enumeration value="Pure compound"/>
            <xsd:enumeration value="Hypothetical pure
solute"/>
        </xsd:restriction>
    </xsd:simpleType>
</xsd:element>

```

```

        <xsd:enumeration value="Hypothetical unit
molality solute"/>
        <xsd:enumeration value="Hypothetical unit
molarity solute"/>
        <xsd:enumeration value="Infinite dilution solute"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:sequence minOccurs="0">
    <xsd:element name="nTemperature-K" type="xsd:float">
        <xsd:annotation>
            <xsd:documentation> Only for reactions with the
initial state change</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="nTemperatureDigits"
type="xsd:integer"/>
</xsd:sequence>
<xsd:sequence minOccurs="0">
    <xsd:element name="nPressure-kPa" type="xsd:float">
        <xsd:annotation>
            <xsd:documentation> Only for reactions with the
initial state change</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="nPressureDigits"
type="xsd:integer"/>
</xsd:sequence>
    <xsd:element ref="CombinedUncertainty" minOccurs="0"
maxOccurs="unbounded"/>

```

```

        <xsd:element name="PropUncertainty"
type="PropVarUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="PropRepeatability"
type="PropVarRepeatabilityType" minOccurs="0"/>
        <xsd:element name="PropDeviceSpec"
type="PropVarDeviceSpecType" minOccurs="0"/>
        <xsd:element ref="CurveDev" minOccurs="0"
maxOccurs="unbounded"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="Constraint" minOccurs="0"
maxOccurs="unbounded">
    <xsd:annotation>
        <xsd:documentation>Only for reactions in
equilibrium</xsd:documentation>
    </xsd:annotation>
</xsd:complexType>
    <xsd:sequence>
        <xsd:element name="ConstraintID">
            <xsd:complexType>
                <xsd:sequence>
                    <xsd:element name="ConstraintType"
type="ConstraintVariableType"/>
                    <xsd:element ref="RegNum" minOccurs="0"/>
                </xsd:sequence>
            </xsd:complexType>
        </xsd:element>
        <xsd:element name="nConstraintValue" type="xsd:float"/>
        <xsd:element name="nConstrDigits" type="xsd:integer"/>
    </xsd:sequence>
</xsd:element>

```



```

        <xsd:element name="ConstrUncertainty"
type="ConstrUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="ConstrRepeatability"
type="ConstrRepeatabilityType" minOccurs="0"/>
        <xsd:element name="ConstrDeviceSpec"
type="ConstrDeviceSpecType" minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="Variable" minOccurs="0"
maxOccurs="unbounded">
    <xsd:annotation>
        <xsd:documentation>Only for reactions in
equilibrium</xsd:documentation>
    </xsd:annotation>
<xsd:complexType>
    <xsd:sequence>
        <xsd:element name="nVarNumber" type="xsd:integer"/>
        <xsd:element name="VariableID">
            <xsd:complexType>
                <xsd:sequence>
                    <xsd:element name="VariableType"
type="ConstraintVariableType"/>
                    <xsd:element ref="RegNum" minOccurs="0"/>
                </xsd:sequence>
            </xsd:complexType>
        </xsd:element>
        <xsd:element name="VarUncertainty"
type="PropVarUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="VarRepeatability"
type="PropVarRepeatabilityType" minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>

```

```

        <xsd:element name="VarDeviceSpec"
type="PropVarDeviceSpecType" minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
    <xsd:element ref="NumValues" minOccurs="0"
maxOccurs="unbounded"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<!--
-->
<xsd:simpleType name="eSampleStatus">
    <xsd:annotation>
        <xsd:documentation>The sample status</xsd:documentation>
    </xsd:annotation>
    <xsd:restriction base="xsd:string">
        <xsd:enumeration value="unknown"/>
        <xsd:enumeration value="notDescribed"/>
        <xsd:enumeration value="previousPaper"/>
        <xsd:enumeration value="compilation"/>
    </xsd:restriction>
</xsd:simpleType>
<!--
-->
<xsd:simpleType name="eSampleSource">
    <xsd:annotation>
        <xsd:documentation>Source(s) of the sample</xsd:documentation>
    </xsd:annotation>

```

```

<xsd:restriction base="xsd:string">
  <xsd:enumeration value="Commercial source"/>
  <xsd:enumeration value="Synthesized by the authors"/>
  <xsd:enumeration value="Synthesized by others"/>
  <xsd:enumeration value="Standard Reference Material (SRM)"/>
  <xsd:enumeration value="Isolated from a natural product"/>
  <xsd:enumeration value="Not stated in the document"/>
  <xsd:enumeration value="No sample used"/>
</xsd:restriction>
</xsd:simpleType>
<!--
-->
<xsd:simpleType name="ePurifMethod">
  <xsd:annotation>
    <xsd:documentation>Purification method(s) used to purify
sample</xsd:documentation>
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="Impurity adsorption"/>
    <xsd:enumeration value="Vacuum degasification"/>
    <xsd:enumeration value="Chemical reagent treatment"/>
    <xsd:enumeration value="Crystallization from melt"/>
    <xsd:enumeration value="Crystallization from solution"/>
    <xsd:enumeration value="Liquid chromatography"/>
    <xsd:enumeration value="Dried with chemical reagent"/>
    <xsd:enumeration value="Dried in a desiccator"/>
    <xsd:enumeration value="Dried by oven heating"/>
    <xsd:enumeration value="Dried by vacuum heating"/>
    <xsd:enumeration value="De-gassed by freezing and melting in vacuum"/>
    <xsd:enumeration value="De-gassed by boiling or ultrasonically"/>
  </xsd:restriction>
</xsd:simpleType>

```

```

    <xsd:enumeration value="Fractional crystallization"/>
    <xsd:enumeration value="Fractional distillation"/>
    <xsd:enumeration value="Molecular sieve treatment"/>
    <xsd:enumeration value="Unspecified"/>
    <xsd:enumeration value="Preparative gas chromatography"/>
    <xsd:enumeration value="Sublimation"/>
    <xsd:enumeration value="Steam distillation"/>
    <xsd:enumeration value="Solvent extraction"/>
    <xsd:enumeration value="Salting out of solution"/>
    <xsd:enumeration value="Zone refining"/>
    <xsd:enumeration value="Other"/>
    <xsd:enumeration value="None used"/>
  </xsd:restriction>
</xsd:simpleType>
<!--
-->
<xsd:simpleType name="ePurityAnalMethod">
  <xsd:annotation>
    <xsd:documentation>Analytical method used to measure
purity.</xsd:documentation>
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="Chemical analysis"/>
    <xsd:enumeration value="Difference between bubble and dew points"/>
    <xsd:enumeration value="Density"/>
    <xsd:enumeration value="DSC"/>
    <xsd:enumeration value="Estimation"/>
    <xsd:enumeration value="Gas chromatography"/>
    <xsd:enumeration value="Fraction melting in an adiabatic calorimeter"/>
    <xsd:enumeration value="Mass spectrometry"/>
  </xsd:restriction>

```

```

        <xsd:enumeration value="Not known"/>
        <xsd:enumeration value="Spectroscopy"/>
        <xsd:enumeration value="Thermal analysis using temperature-time
measurement"/>
        <xsd:enumeration value="Acid-base titration"/>
        <xsd:enumeration value="Mass loss on drying"/>
        <xsd:enumeration value="HPLC"/>
        <xsd:enumeration value="CO2 yield in combustion products"/>
        <xsd:enumeration value="Other"/>
        <xsd:enumeration value="Estimated by the compiler"/>
    </xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:simpleType name="eExpPurpose">
    <xsd:annotation>
        <xsd:documentation>Purpose of measurement</xsd:documentation>
    </xsd:annotation>
    <xsd:restriction base="xsd:string">
        <xsd:enumeration value="Principal objective of the work"/>
        <xsd:enumeration value="Secondary purpose (by-product of other
objective)"/>
        <xsd:enumeration value="Determined for identification of a synthesized
compound"/>
    </xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:simpleType name="ePhaseName">

```

```

<xsd:annotation>
  <xsd:documentation>Phase description</xsd:documentation>
</xsd:annotation>
<xsd:restriction base="xsd:string">
  <xsd:enumeration value="Crystal 4"/>
  <xsd:enumeration value="Crystal 3"/>
  <xsd:enumeration value="Crystal 2"/>
  <xsd:enumeration value="Crystal 1"/>
  <xsd:enumeration value="Crystal"/>
  <xsd:enumeration value="Crystal of unknown type"/>
  <xsd:enumeration value="Crystal of intercomponent compound 1"/>
  <xsd:enumeration value="Crystal of intercomponent compound 2"/>
  <xsd:enumeration value="Crystal of intercomponent compound 3"/>
  <xsd:enumeration value="Metastable crystal"/>
  <xsd:enumeration value="Glass"/>
  <xsd:enumeration value="Smectic liquid crystal"/>
  <xsd:enumeration value="Nematic liquid crystal"/>
  <xsd:enumeration value="Cholesteric liquid crystal"/>
  <xsd:enumeration value="Liquid"/>
  <xsd:enumeration value="Liquid mixture 1"/>
  <xsd:enumeration value="Liquid mixture 2"/>
  <xsd:enumeration value="Solution 1"/>
  <xsd:enumeration value="Solution 2"/>
  <xsd:enumeration value="Fluid (supercritical or subcritical phases)"/>
  <xsd:enumeration value="Ideal gas"/>
  <xsd:enumeration value="Gas"/>
  <xsd:enumeration value="Air at 1 atmosphere"/>
</xsd:restriction>
</xsd:simpleType>
<xsd:simpleType name="ePresentation">
  <xsd:annotation>

```

```

        <xsd:documentation>Means of property presentation</xsd:documentation>
    </xsd:annotation>
    <xsd:restriction base="xsd:string">
        <xsd:enumeration value="Direct value, X"/>
        <xsd:enumeration value="Difference between upper and lower temperature,
X(T2)-X(T1)"/>
        <xsd:enumeration value="Difference between upper and lower pressure,
X(P2)-X(P1)"/>
        <xsd:enumeration value="Mean between upper and lower temperature,
[X(T2)+X(T1)]/2"/>
        <xsd:enumeration value="Difference with the reference state, X-X(REF)"/>
        <xsd:enumeration value="Ratio with the reference state, X/X(REF)"/>
        <xsd:enumeration value="Ratio of difference with the reference state to the
reference state, [X-X(REF)]/X(REF)"/>
    </xsd:restriction>
</xsd:simpleType>
<!--
-->
<xsd:simpleType name="eRefStateType">
    <xsd:annotation>
        <xsd:documentation>Type of reference state</xsd:documentation>
    </xsd:annotation>
    <xsd:restriction base="xsd:string">
        <xsd:enumeration value="Reference phase with the same composition at fixed
temperature and pressure"/>
        <xsd:enumeration value="Reference phase with the same composition,
temperature and pressure"/>
        <xsd:enumeration value="Reference phase at fixed temperature and the same
pressure"/>
    </xsd:restriction>

```

```

        <xsd:enumeration value="Reference phase at the same temperature and fixed
pressure"/>
        <xsd:enumeration value="Phase in equilibrium with primary phase at the
same temperature and pressure"/>
        <xsd:enumeration value="Pure components in the same proportion at the
same temperature and pressure"/>
        <xsd:enumeration value="Pure solvent at the temperature of the same phase
equilibrium"/>
        <xsd:enumeration value="Pure solvent at the same temperature and
pressure"/>
        <xsd:enumeration value="Pure solute at the same temperature and pressure"/>
    </xsd:restriction>
</xsd:simpleType>
<!--
-->
<xsd:element name="RegNum">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nCASRNum" type="xsd:integer" minOccurs="0"/>
            <xsd:element name="nOrgNum" type="xsd:integer" minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<!--
-->
<xsd:element name="Solvent">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element ref="RegNum" maxOccurs="unbounded"/>

```



```

        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<!--

-->
<xsd:complexType name="ConstraintVariableType">
    <xsd:choice>
        <xsd:element name="eTemperature">
            <xsd:simpleType>
                <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="Temperature, K"/>
                    <xsd:enumeration value="Upper temperature, K"/>
                    <xsd:enumeration value="Lower temperature, K"/>
                </xsd:restriction>
            </xsd:simpleType>
        </xsd:element>
        <xsd:element name="ePressure">
            <xsd:simpleType>
                <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="Pressure, kPa"/>
                    <xsd:enumeration value="Partial pressure, kPa"/>
                    <xsd:enumeration value="Upper pressure, kPa"/>
                    <xsd:enumeration value="Lower pressure, kPa"/>
                </xsd:restriction>
            </xsd:simpleType>
        </xsd:element>
        <xsd:element name="eComponentComposition">
            <xsd:simpleType>
                <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="Mole fraction"/>

```

```

    <xsd:enumeration value="Mass fraction"/>
    <xsd:enumeration value="MolaLity, mol/kg"/>
    <xsd:enumeration value="MolaRity, mol/dm3"/>
    <xsd:enumeration value="Volume fraction"/>
    <xsd:enumeration value="Moles per mass of solution, mol/kg"/>
    <xsd:enumeration value="Mass per volume of solution, kg/m3"/>
    <xsd:enumeration value="Mole ratio to solvent"/>
    <xsd:enumeration value="Mass ratio to solvent"/>
    <xsd:enumeration value="Volume ratio to solvent"/>
    <xsd:enumeration value="Activity"/>
    <xsd:enumeration value="Activity coefficient"/>
    <xsd:enumeration value="Initial mole fraction"/>
    <xsd:enumeration value="Initial mass fraction"/>
  </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="eSolventComposition">
  <xsd:simpleType>
    <xsd:restriction base="xsd:string">
      <xsd:enumeration value="Solvent: Mole fraction"/>
      <xsd:enumeration value="Solvent: Mass fraction"/>
      <xsd:enumeration value="Solvent: Volume fraction"/>
      <xsd:enumeration value="Solvent: MolaLity, mol/kg"/>
      <xsd:enumeration value="Solvent: MolaRity, mol/dm3"/>
      <xsd:enumeration value="Solvent: Mole ratio to other component
of binary solvent"/>
      <xsd:enumeration value="Solvent: Mass ratio to other component
of binary solvent"/>
      <xsd:enumeration value="Solvent: Volume ratio to other
component of binary solvent"/>
    </xsd:restriction>
  </xsd:simpleType>
</xsd:element>

```

```

        <xsd:enumeration value="Solvent: Moles per mass of solvent,
mol/kg"/>
        <xsd:enumeration value="Solvent: Mass per volume of solvent,
kg/m3"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="eMiscellaneous">
    <xsd:simpleType>
        <xsd:restriction base="xsd:string">
            <xsd:enumeration value="Wavelength, nm"/>
            <xsd:enumeration value="Molar volume, m3/mol"/>
            <xsd:enumeration value="Specific volume, m3/kg"/>
            <xsd:enumeration value="Density, kg/m3"/>
            <xsd:enumeration value="Molar density, mol/m3"/>
            <xsd:enumeration value="Entropy, J/K/mol"/>
        </xsd:restriction>
    </xsd:simpleType>
</xsd:element>
</xsd:choice>
</xsd:complexType>
<!--
-->
<xsd:complexType name="ConstrDeviceSpecType">
    <xsd:sequence>
        <xsd:element name="sDeviceSpecEvaluator" type="xsd:string"
minOccurs="0"/>
        <xsd:element name="eDeviceSpecMethod">
            <xsd:simpleType>
                <xsd:restriction base="xsd:string">

```

```

        <xsd:enumeration value="Specified by the manufacturer"/>
        <xsd:enumeration value="Certified or calibrated by a third
party"/>
        <xsd:enumeration value="Calibrated by the experimentalist"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="sDeviceSpecMethod" type="xsd:string"
minOccurs="0"/>
    <xsd:element name="nDeviceSpecValue" type="xsd:float" minOccurs="0"/>
    <xsd:element name="nDeviceSpecLevOfConfid" type="xsd:float"
minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
<!--
-->
<xsd:complexType name="PropVarDeviceSpecType">
    <xsd:sequence>
        <xsd:element name="sDeviceSpecEvaluator" type="xsd:string"
minOccurs="0"/>
        <xsd:element name="eDeviceSpecMethod">
            <xsd:simpleType>
                <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="Specified by the manufacturer"/>
                    <xsd:enumeration value="Certified or calibrated by a third
party"/>
                    <xsd:enumeration value="Calibrated by the experimentalist"/>
                </xsd:restriction>
            </xsd:simpleType>
        </xsd:element>

```

```

        <xsd:element name="sDeviceSpecMethod" type="xsd:string"
minOccurs="0"/>
        <xsd:element name="nDeviceSpecLevOfConfid" type="xsd:float"
minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:complexType name="ConstrRepeatabilityType">
    <xsd:sequence>
        <xsd:element name="sRepeatEvaluator" type="xsd:string" minOccurs="0"/>
        <xsd:element name="eRepeatMethod">
            <xsd:simpleType>
                <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="Standard deviation of a single value
(biased)"/>
                    <xsd:enumeration value="Standard deviation of a single value
(unbiased)"/>
                    <xsd:enumeration value="Standard deviation of the mean"/>
                    <xsd:enumeration value="Other"/>
                </xsd:restriction>
            </xsd:simpleType>
        </xsd:element>
        <xsd:element name="sRepeatMethod" type="xsd:string" minOccurs="0"/>
        <xsd:element name="nRepeatValue" type="xsd:float" minOccurs="0"/>
        <xsd:element name="nRepetitions" type="xsd:integer" minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
<!--

```

```

-->
<xsd:complexType name="PropVarRepeatabilityType">
  <xsd:sequence>
    <xsd:element name="sRepeatEvaluator" type="xsd:string" minOccurs="0"/>
    <xsd:element name="eRepeatMethod">
      <xsd:simpleType>
        <xsd:restriction base="xsd:string">
          <xsd:enumeration value="Standard deviation of a single value
(biased)"/>
          <xsd:enumeration value="Standard deviation of a single value
(unbiased)"/>
          <xsd:enumeration value="Standard deviation of the mean"/>
          <xsd:enumeration value="Other"/>
        </xsd:restriction>
      </xsd:simpleType>
    </xsd:element>
    <xsd:element name="sRepeatMethod" type="xsd:string" minOccurs="0"/>
  </xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:element name="CurveDev">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="nCurveDevAssessNum" type="xsd:integer"/>
      <xsd:element name="sCurveDevEvaluator" type="xsd:string"
minOccurs="0"/>
      <xsd:element name="sCurveSpec" type="xsd:string"/>
      <xsd:element name="nCurveRmsDevValue" type="xsd:float"
minOccurs="0"/>

```

```

        <xsd:element name="nCurveRmsRelativeDevValue" type="xsd:float"
minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<!--

-->
<xsd:complexType name="ConstrUncertaintyType">
    <xsd:sequence>
        <xsd:element name="sUncertEvaluator" type="xsd:string" minOccurs="0"/>
        <xsd:element name="sUncertEvalMethod" type="xsd:string"
minOccurs="0"/>
        <xsd:element name="nStdUncertValue" type="xsd:float" minOccurs="0"/>
        <xsd:element name="nCoverageFactor" type="xsd:float" minOccurs="0"/>
        <xsd:element name="nExpandUncertValue" type="xsd:float"
minOccurs="0"/>
        <xsd:element name="nUncertLevOfConfid" type="xsd:float"
minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:complexType name="PropVarUncertaintyType">
    <xsd:sequence>
        <xsd:element name="nUncertAssessNum" type="xsd:integer"/>
        <xsd:element name="sUncertEvaluator" type="xsd:string" minOccurs="0"/>
        <xsd:element name="sUncertEvalMethod" type="xsd:string"
minOccurs="0"/>
        <xsd:element name="nCoverageFactor" type="xsd:float" minOccurs="0"/>

```

```

        <xsd:element name="nUncertLevOfConfid" type="xsd:float"
minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:complexType name="AsymUncertType">
    <xsd:sequence>
        <xsd:element name="nPositiveValue" type="xsd:float" minOccurs="0"/>
        <xsd:element name="nNegativeValue" type="xsd:float" minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:element name="CombinedUncertainty">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nCombUncertAssessNum" type="xsd:integer"/>
            <xsd:element name="sCombUncertEvaluator" type="xsd:string"
minOccurs="0"/>
            <xsd:element name="eCombUncertEvalMethod">
                <xsd:simpleType>
                    <xsd:restriction base="xsd:string">
                        <xsd:enumeration value="Propagation of evaluated standard
uncertainties"/>
                        <xsd:enumeration value="Comparison with reference property
values"/>
                    </xsd:restriction>
                </xsd:simpleType>

```



```

        </xsd:element>
        <xsd:element name="sCombUncertEvalMethod" type="xsd:string"
minOccurs="0"/>
        <xsd:element name="nCombCoverageFactor" type="xsd:float"
minOccurs="0"/>
        <xsd:element name="nCombUncertLevOfConfid" type="xsd:float"
minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="NumValues">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="VariableValue" minOccurs="0"
maxOccurs="unbounded">
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:element name="nVarNumber" type="xsd:integer"/>
                        <xsd:element name="nVarValue" type="xsd:float"/>
                        <xsd:element name="nVarDigits" type="xsd:integer"/>
                        <xsd:element name="VarUncertainty" minOccurs="0"
maxOccurs="unbounded">
                                <xsd:complexType>
                                    <xsd:sequence>
                                        <xsd:element name="nUncertAssessNum"
type="xsd:integer"/>
                                        <xsd:element name="nStdUncertValue"
type="xsd:float" minOccurs="0"/>
                                        <xsd:element name="nExpandUncertValue"
type="xsd:float" minOccurs="0"/>
                                    </xsd:sequence>
                                </xsd:complexType>
                            </xsd:element>
                    </xsd:sequence>
                </xsd:complexType>
            </xsd:element>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>

```

```

        </xsd:complexType>
    </xsd:element>
    <xsd:element name="VarRepeatability" minOccurs="0">
        <xsd:complexType>
            <xsd:sequence>
                <xsd:element name="nVarRepeatValue"
type="xsd:float"/>
                <xsd:element name="nRepetitions"
type="xsd:integer"/>
            </xsd:sequence>
        </xsd:complexType>
    </xsd:element>
    <xsd:element name="nVarDeviceSpecValue" type="xsd:float"
minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="PropertyValue" maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nPropNumber" type="xsd:integer"/>
            <xsd:choice>
                <xsd:sequence>
                    <xsd:element name="nPropValue" type="xsd:float"/>
                    <xsd:element name="nPropDigits"
type="xsd:integer"/>
                </xsd:sequence>
            <xsd:element name="PropLimit">
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:choice>

```

```

                <xsd:element
name="nPropUpperLimitValue" type="xsd:float"/>
                <xsd:element
name="nPropLowerLimitValue" type="xsd:float"/>
            </xsd:choice>
            <xsd:element name="nPropLimitDigits"
type="xsd:integer"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
</xsd:choice>
<xsd:element name="CombinedUncertainty" minOccurs="0"
maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nCombUncertAssessNum"
type="xsd:integer"/>
            <xsd:choice>
                <xsd:sequence>
                    <xsd:element
name="nCombStdUncertValue" type="xsd:float" minOccurs="0"/>
                    <xsd:element
name="nCombExpandUncertValue" type="xsd:float" minOccurs="0"/>
                </xsd:sequence>
                <xsd:sequence>
                    <xsd:element
name="AsymCombStdUncert" type="AsymUncertType" minOccurs="0"/>
                    <xsd:element
name="AsymCombExpandUncert" type="AsymUncertType" minOccurs="0"/>
                </xsd:sequence>
            </xsd:choice>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>

```

```

        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="PropUncertainty" minOccurs="0"
maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nUncertAssessNum"
type="xsd:integer"/>
            <xsd:choice>
                <xsd:sequence>
                    <xsd:element name="nStdUncertValue"
type="xsd:float" minOccurs="0"/>
                    <xsd:element name="nExpandUncertValue"
type="xsd:float" minOccurs="0"/>
                </xsd:sequence>
                <xsd:sequence>
                    <xsd:element name="AsymStdUncert"
type="AsymUncertType" minOccurs="0"/>
                    <xsd:element name="AsymExpandUncert"
type="AsymUncertType" minOccurs="0"/>
                </xsd:sequence>
            </xsd:choice>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="PropRepeatability" minOccurs="0">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nPropRepeatValue"
type="xsd:float"/>

```


Literature Cited

- (1) H. A. Duarte-Garza and J. W. Magee. Isochoric p - v - T and Heat Capacity C_v Measurements on $\{x \text{ C}_3\text{H}_8 + (1-x) \text{ i-C}_4\text{H}_{10}, x = 0.7, 0.3\}$ from 200 to 400 K at Pressures to 35 MPa. *J. Chem. Eng. Data*, **1999**, *44*, 1048 - 1054.
- (2) V. V. Simirsky, G. J. Kabo, and M. L. Frenkel. Additivity of the enthalpies of formation of urea derivatives in the crystalline state. *J. Chem. Thermodyn.* **1987**, *19*, 1121-1127.