ThermoML – an XML-based Approach for Storage and Exchange of Experimental and Critically Evaluated Thermophysical and Thermochemical Property Data. 1. Experimental Data [*]
(Supporting Information)

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Supporting Information

Sample ThermoML Files.

Pure Compound and Mixture Data.

The following ThermoML file contains vapor pressure data for phenol and its mixture with 2-ethoxyethanol as well as vapor-liquid equilibrium data for the same mixture represented as a composition of the vapor phase as a function of the composition of liquid phase at constant temperature[1].

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by Vladimir V. Diky (U. S. Department of Commerce) -->
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      <VariableValue>
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      </VariableValue>
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            <nVarNumber>2</nVarNumber>
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</NumValues>
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      <VariableValue>
            <nVarNumber>1</nVarNumber>
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      </VariableValue>
      <VariableValue>
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      </VariableValue>
      <PropertyValue>
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      </PropertyValue>
</NumValues>
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                  <VariableValue>
                        <nVarNumber>1</nVarNumber>
                        <nVarValue>1</nVarValue>
                  </VariableValue>
                  <VariableValue>
                        <nVarNumber>2</nVarNumber>
                        <nVarValue>363.15</nVarValue>
                  </VariableValue>
                  <PropertyValue>
                        <nPropNumber>1</nPropNumber>
                        <nPropValue>3.424</nPropValue>
                  </PropertyValue>
            </NumValues>
      </PureOrMixtureData>
</DataReport>
```

Reaction Data for Reactions with Initial Thermodynamic State Change.

The following ThermoML file contains the internal energy change data for combustion of 2-methyl-2-oxazoline[2].

```
<?xml version="1.0" encoding="UTF-8"?>
<!-- edited with XML Spy v4.4 U (http://www.xmlspy.com)
```

```
by Vladimir V. Diky (U. S. Department of Commerce) -->
<!--Created by Guided Data Capture (GDC) Software
(http://www.trc.nist.gov)-->
<DataReport xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:noNamespaceSchemaLocation="C:\TRC\ThermoML.xsd">
      <Citation>
            <TRCRefID>
                  <yrYrPub>1976</yrYrPub>
                  <sAuthor1>ham</sAuthor1>
                  <sAuthor2>tho</sAuthor2>
                  <nAuthorn>0</nAuthorn>
            </TRCRefID>
            <eType>journal</eType>
            <eSourceType>Original</eSourceType>
            <sAuthor>Hamilton, W. S.[Walter S.]</sAuthor>
            <sAuthor>Thompson, P.[Patricia]</sAuthor>
            <sAuthor>Pustejovsky, S.[Sharon]</sAuthor>
            <sPubName>J. Chem. Eng. Data</sPubName>
            <yrPubYr>1976</yrPubYr>
            <dateCit>2002-11-08</dateCit>
            <sTitle>The Enthalpies of Combustion and Formation of 2-
Methyl-2-oxazoline and 2-Ethyl-2-oxazoline</sTitle>
            <sKeyword>Enthalpy of combustion</sKeyword>
            <sKeyword>Oxazolines</sKeyword>
            <sVol>21</sVol>
            <sPage>428-9</sPage>
      </Citation>
      <Compound>
            <RegNum>
                  <nCASRNum>1120645</nCASRNum>
            </RegNum>
            <sCommonName>2-methyl-2-oxazoline</sCommonName>
            <sFormulaMolec>C4H7NO</sFormulaMolec>
            <Sample>
                  <nSampleNm>1</nSampleNm>
                  <eSource>Commercial source</eSource>
                  <purity>
                        <nStep>1</nStep>
```

```
                        <nPurityVol>99</nPurityVol>
                        <eAnalMeth>Not known</eAnalMeth>
                  </purity>
                  <purity>
                        <nStep>2</nStep>
                        <ePurifMethod>Fractional
distillation</ePurifMethod>
                        <ePurifMethod>Molecular sieve
treatment</ePurifMethod>
                  </purity>
                  <purity>
                        <nStep>2</nStep>
                        <nPurityMass>100</nPurityMass>
                        <eAnalMeth>Gas chromatography</eAnalMeth>
                  </purity>
            </Sample>
      </Compound>
      <Compound>
            <RegNum>
                  <nCASRNum>124389</nCASRNum>
            </RegNum>
            <sCommonName>carbon dioxide</sCommonName>
            <sFormulaMolec>CO2</sFormulaMolec>
      </Compound>
      <Compound>
            <RegNum>
                  <nCASRNum>7727379</nCASRNum>
            </RegNum>
            <sCommonName>nitrogen</sCommonName>
            <sFormulaMolec>N2</sFormulaMolec>
      </Compound>
      <Compound>
            <RegNum>
                  <nCASRNum>7732185</nCASRNum>
            </RegNum>
            <sCommonName>water</sCommonName>
            <sFormulaMolec>H2O</sFormulaMolec>
      </Compound>
```

```
<Compound>
      <RegNum>
            <nCASRNum>7782447</nCASRNum>
      </RegNum>
      <sCommonName>oxygen</sCommonName>
      <sFormulaMolec>O2</sFormulaMolec>
</Compound>
<ReactionData>
      <Participant>
            <RegNum>
                  <nCASRNum>1120645</nCASRNum>
            </RegNum>
            <nSampleNm>1</nSampleNm>
            <nStoichiometricCoef>-1</nStoichiometricCoef>
            <ePhase>Liquid</ePhase>
      </Participant>
      <Participant>
            <RegNum>
                  <nCASRNum>124389</nCASRNum>
            </RegNum>
            <nStoichiometricCoef>4</nStoichiometricCoef>
            <ePhase>Gas</ePhase>
      </Participant>
      <Participant>
            <RegNum>
                  <nCASRNum>7727379</nCASRNum>
            </RegNum>
            <nStoichiometricCoef>0.5</nStoichiometricCoef>
            <ePhase>Gas</ePhase>
      </Participant>
      <Participant>
            <RegNum>
                  <nCASRNum>7732185</nCASRNum>
            </RegNum>
            <nStoichiometricCoef>3.5</nStoichiometricCoef>
            <ePhase>Liquid</ePhase>
      </Participant>
      <Participant>
```

```
                  <RegNum>
                        <nCASRNum>7782447</nCASRNum>
                  </RegNum>
                  <nStoichiometricCoef>-5.25</nStoichiometricCoef>
                  <ePhase>Gas</ePhase>
            </Participant>
            <eExpPurpose>Principal objective of the work</eExpPurpose>
            <sCompiler>RCW</sCompiler>
            <sContributor>TRC</sContributor>
            <dateDateAdded>3/20/1992</dateDateAdded>
            <eReactionType>Combustion with oxygen</eReactionType>
            <Property>
                  <nPropNumber>1</nPropNumber>
                  <Property-MethodID>
                        <PropertyGroup>
                              <EnthalpyInternalEnergyOfReaction>
                                    <ePropName>Internal energy of
reaction (mass basis), J/g</ePropName>
                                    <eMethodName>Other</eMethodName>
                              </EnthalpyInternalEnergyOfReaction>
                        </PropertyGroup>
                  </Property-MethodID>
                  <nTemperature-K>298.15</nTemperature-K>
                  <nPressure-kPa>101.32</nPressure-kPa>
            </Property>
            <NumValues>
                  <PropertyValue>
                        <nPropNumber>1</nPropNumber>
                        <nPropValue>-28236.3516</nPropValue>
                  </PropertyValue>
            </NumValues>
      </ReactionData>
</DataReport>
```

Reaction Data for Reactions in Equilibrium State.

The following ThermoML file contains equilibrium constant data for reaction of formation of 2-methoxy-2methylbutane from methanol and 2-methyl-2-butene[3].

```
<?xml version="1.0" encoding="UTF-8"?>
```

```
<!-- edited with XML Spy v4.4 U (http://www.xmlspy.com)
by Vladimir V. Diky (U. S. Department of Commerce) -->
<!--Created by Guided Data Capture (GDC) Software
(http://www.trc.nist.gov)-->
<DataReport xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:noNamespaceSchemaLocation="C:\TRC\ThermoML.xsd">
      <Citation>
            <TRCRefID>
                  <yrYrPub>1994</yrYrPub>
                  <sAuthor1>rih</sAuthor1>
                  <sAuthor2>lin</sAuthor2>
                  <nAuthorn>0</nAuthorn>
            </TRCRefID>
            <eType>journal</eType>
            <eSourceType>Original</eSourceType>
            <sAuthor>Rihko, L. K.[Liisa K.]</sAuthor>
            <sAuthor>Linnekoski, J. A.[Juha A.]</sAuthor>
            <sAuthor>Krause, A. O. I.[A. Outi I.]</sAuthor>
            <sPubName>J. Chem. Eng. Data</sPubName>
            <yrPubYr>1994</yrPubYr>
            <dateCit>2002-11-07</dateCit>
            <sTitle>Reaction Equilibria in the Synthesis of 2-Methoxy-
2-methylbutane and 2-Ethoxy-2-methylbutane in the Liquid Phase</sTitle>
            <sKeyword>TAME</sKeyword>
            <sKeyword>TAEE</sKeyword>
            <sKeyword>Synthesis</sKeyword>
            <sKeyword>Equilibrium</sKeyword>
            <sVol>39</sVol>
            <sPage>700-4</sPage>
      </Citation>
      <Compound>
            <RegNum>
                  <nCASRNum>994058</nCASRNum>
            </RegNum>
            <sCommonName>tert-amyl methyl ether</sCommonName>
            <sFormulaMolec>C6H14O</sFormulaMolec>
            <Sample>
                  <nSampleNm>1</nSampleNm>
```

```
            <eSource>Commercial source</eSource>
            <purity>
                  <nStep>1</nStep>
                  <nPurityMass>97.2</nPurityMass>
                  <eAnalMeth>Not known</eAnalMeth>
            </purity>
      </Sample>
</Compound>
<Compound>
      <RegNum>
            <nCASRNum>513359</nCASRNum>
      </RegNum>
      <sCommonName>2-methyl-2-butene</sCommonName>
      <sFormulaMolec>C5H10</sFormulaMolec>
      <Sample>
            <nSampleNm>1</nSampleNm>
            <eSource>Commercial source</eSource>
            <purity>
                  <nStep>1</nStep>
                  <nPurityMass>99.3</nPurityMass>
                  <eAnalMeth>Not known</eAnalMeth>
            </purity>
      </Sample>
</Compound>
<Compound>
      <RegNum>
            <nCASRNum>67561</nCASRNum>
      </RegNum>
      <sCommonName>methanol</sCommonName>
      <sFormulaMolec>CH4O</sFormulaMolec>
      <Sample>
            <nSampleNm>1</nSampleNm>
            <eSource>Commercial source</eSource>
            <purity>
                  <nStep>1</nStep>
                  <nPurityMass>99.8</nPurityMass>
                  <eAnalMeth>Not known</eAnalMeth>
            </purity>
```

```
            </Sample>
      </Compound>
      <ReactionData>
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                  </RegNum>
                  <nSampleNm>1</nSampleNm>
                  <nStoichiometricCoef>-1</nStoichiometricCoef>
                  <ePhase>Liquid</ePhase>
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            <Participant>
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                  </RegNum>
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                  <ePhase>Liquid</ePhase>
            </Participant>
            <Participant>
                  <RegNum>
                        <nCASRNum>994058</nCASRNum>
                  </RegNum>
                  <nSampleNm>1</nSampleNm>
                  <nStoichiometricCoef>1</nStoichiometricCoef>
                  <ePhase>Liquid</ePhase>
            </Participant>
            <eExpPurpose>Principal objective of the work</eExpPurpose>
            <sCompiler>VVD</sCompiler>
            <sContributor>TRC</sContributor>
            <dateDateAdded>11/7/2002</dateDateAdded>
            <eReactionType>Addition of various compounds to unsaturated
compounds</eReactionType>
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                  <nPropNumber>1</nPropNumber>
                  <Property-MethodID>
                        <PropertyGroup>
                              <ReactionEquilibriumProp>
```

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                                    <ePropName>Thermodynamic
equilibrium constant</ePropName>
                              </ReactionEquilibriumProp>
                        </PropertyGroup>
                  </Property-MethodID>
            </Property>
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                  <ConstraintID>
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                              <ePressure>Pressure, kPa</ePressure>
                        </ConstraintType>
                  </ConstraintID>
                  <nConstraintValue>700</nConstraintValue>
            </Constraint>
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K</eTemperature>
                        </VariableType>
                  </VariableID>
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      </PropertyValue>
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      <VariableValue>
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            <nPropValue>4.4</nPropValue>
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      </PropertyValue>
</NumValues>
<NumValues>
      <VariableValue>
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      <PropertyValue>
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      </PropertyValue>
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      <VariableValue>
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      </VariableValue>
      <PropertyValue>
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      </PropertyValue>
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<NumValues>
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      <PropertyValue>
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      <VariableValue>
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      </PropertyValue>
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      </VariableValue>
      <PropertyValue>
            <nPropNumber>1</nPropNumber>
            <nPropValue>4.9</nPropValue>
      </PropertyValue>
```

```
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      </VariableValue>
      <PropertyValue>
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            <nPropValue>4.4</nPropValue>
      </PropertyValue>
</NumValues>
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      <VariableValue>
            <nVarNumber>1</nVarNumber>
            <nVarValue>353</nVarValue>
      </VariableValue>
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      </PropertyValue>
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            <nVarValue>353</nVarValue>
      </VariableValue>
      <PropertyValue>
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            <nPropValue>2.3</nPropValue>
      </PropertyValue>
</NumValues>
<NumValues>
      <VariableValue>
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            <nVarValue>353</nVarValue>
      </VariableValue>
      <PropertyValue>
            <nPropNumber>1</nPropNumber>
```

```
                        <nPropValue>2.7</nPropValue>
                  </PropertyValue>
            </NumValues>
            <NumValues>
                  <VariableValue>
                        <nVarNumber>1</nVarNumber>
                        <nVarValue>353</nVarValue>
                  </VariableValue>
                  <PropertyValue>
                        <nPropNumber>1</nPropNumber>
                        <nPropValue>2.6</nPropValue>
                  </PropertyValue>
            </NumValues>
            <NumValues>
                  <VariableValue>
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                        <nVarValue>353</nVarValue>
                  </VariableValue>
                  <PropertyValue>
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                        <nPropValue>2.7</nPropValue>
                  </PropertyValue>
            </NumValues>
            <NumValues>
                  <VariableValue>
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                        <nVarValue>363</nVarValue>
                  </VariableValue>
                  <PropertyValue>
                        <nPropNumber>1</nPropNumber>
                        <nPropValue>1.92</nPropValue>
                  </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 Vladimir V. Diky (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 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:element
name="nPurityMol" type="xsd:float" minOccurs="0">
                                                <xsd:annotation>

      <xsd:documentation>purity value in mole
percent</xsd:documentation>
                                                </xsd:annotation>
                                          </xsd:element>
                                          <xsd:element
name="nPurityMass" type="xsd:float" minOccurs="0">
                                                <xsd:annotation>
```

```
      <xsd:documentation>purity value in mass
percent</xsd:documentation>
                                                </xsd:annotation>
                                          </xsd:element>
                                          <xsd:element
name="nPurityVol" type="xsd:float" minOccurs="0">
                                                <xsd:annotation>

      <xsd:documentation>purity value in volume
percent</xsd:documentation>
                                                </xsd:annotation>
                                          </xsd:element>
                                          <xsd:element
name="nWaterMassPerCent" type="xsd:float" minOccurs="0">
                                                <xsd:annotation>

      <xsd:documentation>mass per cent of water</xsd:documentation>
                                                </xsd:annotation>
                                          </xsd:element>
                                          <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>

                            <xsd:element name="eMethodName" minOccurs="0">

                                <xsd:simpleType>

                                    <xsd:restriction base="xsd:string">

                                        <xsd:enumeration
value="Visual observation in an unstirred cell"/>

                                        <xsd:enumeration
value="Visual observation in a stirred cell"/>

                                        <xsd:enumeration
value="DSC/DTA"/>

                                        <xsd:enumeration
value="Derived from PVT data"/>
```

```
                                        <xsd:enumeration
value="Extrapolated vapor pressure"/>

                                        <xsd:enumeration
value="Rectilinear diameter"/>

                                        <xsd:enumeration
value="Appearance of two phases"/>

                                        <xsd:enumeration
value="Disappearance of two phases"/>

                                        <xsd:enumeration
value="Direct measurement"/>

                                        <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="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"/>
```

```
                                        <xsd:enumeration
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: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"/>

                                        <xsd:enumeration
value="Solid-liquid equilibrium temperature, K"/>

                                        <xsd:enumeration
value="Liquid-liquid equilibrium temperature, K"/>

                                        <xsd:enumeration
value="Eutectic temperature, K"/>

                                    </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">
                                <xsd:enumeration
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"/>

                                        <xsd:enumeration value="Upper
consolute composition: volume fraction"/>

                                        <xsd:enumeration value="Upper
consolute composition: mole fraction"/>

                                        <xsd:enumeration value="Upper
consolute composition: mass fraction"/>

                                        <xsd:enumeration
value="Volume fraction"/>

                                        <xsd:enumeration
value="Volume ratio to solvent"/>

                                        <xsd:enumeration value="Mass
fraction"/>

                                        <xsd:enumeration value="Mass
fraction in LLG critical state"/>
```

```
                                        <xsd:enumeration
value="Henry's Law constant for mole fraction, kPa"/>

                                        <xsd:enumeration
value="Henry's Law constant (molaLity), kPa kg/mol"/>

                                        <xsd:enumeration
value="Henry's Law constant (molaRity), kPa l/mol"/>

                                        <xsd:enumeration
value="Bunsen coefficient"/>

                                        <xsd:enumeration
value="Ostwald coefficient"/>

                                        <xsd:enumeration
value="Partial pressure, kPa"/>

                                    </xsd:restriction>

                               </xsd:simpleType>

                          </xsd:element>

                          <xsd:element name="eMethodName" minOccurs="0">

                               <xsd:simpleType>

                                    <xsd:restriction base="xsd:string">

                                        <xsd:enumeration 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="Chromatography"/>
```

```
                                        <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"/>

                                        <xsd:enumeration
value="Osmotic coefficient"/>

                                    </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 base="xsd:string">
                                        <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"/>
                                        <xsd:enumeration
value="Interaction virial coefficient, m3/mol"/>
```

```
                                        <xsd:enumeration
value="Excess volume, m3/mol"/>

                                        <xsd:enumeration
value="Partial molar volume, m3/mol"/>

                                        <xsd:enumeration
value="Relative partial molar volume, m3/mol"/>

                                        <xsd:enumeration
value="Apparent molar volume, m3/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:restriction>

                                </xsd:simpleType>

                            </xsd:element>

                            <xsd:element name="eMethodName" minOccurs="0">

                                <xsd:simpleType>
```

```
                                <xsd:restriction base="xsd:string">
                                    <xsd:enumeration
value="Pycnometric method"/>
                                    <xsd:enumeration
value="Buoyancy method"/>
                                    <xsd:enumeration
value="Vibrating tube method"/>
                                    <xsd:enumeration
value="Isochoric PVT measurement"/>
                                    <xsd:enumeration value="Other
PVT measurement"/>
                                    <xsd:enumeration
value="Burnett expansion technique"/>
                                    <xsd:enumeration
value="Constant-volume piesometry"/>
                                    <xsd:enumeration
value="Direct dilatometry"/>
                                    <xsd:enumeration
value="Derived analytically"/>
                                    <xsd:enumeration
value="Derived graphically"/>
                                    <xsd:enumeration
value="Calculated with densities of this investigation"/>
                                    <xsd:enumeration
value="Calculated with a solvent density reported elsewhere"/>
```

```
                                        <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="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="Standard entropy S(T)-S(0), J/K/mol"/>

                                        <xsd:enumeration
value="Standard enthalpy H(T)-H(0), kJ/mol"/>

                                        <xsd:enumeration
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 G(T)-H(0), kJ/mol"/>

                                        <xsd:enumeration
value="Helmholtz energy A(T)-E(0), kJ/mol"/>
```

```
                                        <xsd:enumeration
value="Internal energy E(T)-E(0), kJ/mol"/>

                                        <xsd:enumeration
value="Joule-Thompson coefficient, K/kPa"/>

                                        <xsd:enumeration
value="Pressure coefficient of enthalpy, J/mol/kPa"/>

                                    </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"/>

                                        <xsd:enumeration
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>

            <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>

                                    <xsd:restriction base="xsd:string">

                                          <xsd:enumeration
value="Capillary tube (Ostwald; Ubellohde) method"/>

                                          <xsd:enumeration value="Cone
and plate viscometry"/>

                                          <xsd:enumeration
value="Concentric cylinders viscometry"/>

                                          <xsd:enumeration
value="Falling or rolling sphere viscometry"/>

                                          <xsd:enumeration
value="Oscillating disk viscometry"/>

                                          <xsd:enumeration
value="Vibrating wire viscometry"/>

                                          <xsd:enumeration
value="Parallel plate method"/>

                                          <xsd:enumeration
value="Coaxial cylinder method"/>

                                          <xsd:enumeration value="Hot
wire method"/>

                                          <xsd:enumeration
value="Optical interferometry"/>
```

```
                                        <xsd:enumeration
value="Dispersion"/>

                                        <xsd:enumeration
value="Diaphragm Cell"/>

                                        <xsd:enumeration value="Open
capillary"/>

                                        <xsd:enumeration
value="Closed capillary"/>

                                        <xsd:enumeration
value="Taylor dispersion method"/>

                                        <xsd:enumeration value="NMR
spin-echo 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="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"/>
                                          <xsd:enumeration value="Speed
of sound, m/s"/>
                                    </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"/>

                                        <xsd:enumeration
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:element name="nRefTemp"
type="xsd:float" minOccurs="0"/>
                                          <xsd:element
name="nRefPressure" type="xsd:float" minOccurs="0"/>
                                          <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: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: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:element>
                                          <xsd:element ref="Solvent"
minOccurs="0"/>
                                    </xsd:sequence>
                              </xsd:complexType>
                        </xsd:element>
                        <xsd:element name="NumValues" minOccurs="0"
maxOccurs="unbounded">
                              <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:sequence>
                                                </xsd:complexType>
                                          </xsd:element>
                                          <xsd:element
name="PropertyValue" maxOccurs="unbounded">
                                                <xsd:complexType>
                                                      <xsd:sequence>

      <xsd:element name="nPropNumber" type="xsd:integer"/>

      <xsd:element name="nPropValue" type="xsd:float"/>
                                                      </xsd:sequence>
                                                </xsd:complexType>
                                          </xsd:element>
                                    </xsd:sequence>
                              </xsd:complexType>
                        </xsd:element>
                  </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: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="Solvolyis (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"/>

                                          <xsd:enumeration 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: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
name="nTemperature-K" type="xsd:float" minOccurs="0">
                                              <xsd:annotation>

      <xsd:documentation> Only for reactions with the initial state
change</xsd:documentation>
                                              </xsd:annotation>
                                        </xsd:element>
                                        <xsd:element name="nPressure-
kPa" type="xsd:float" minOccurs="0">
                                              <xsd:annotation>

      <xsd:documentation> Only for reactions with the initial state
change</xsd:documentation>
                                              </xsd:annotation>
                                        </xsd:element>
                                  </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: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:sequence>
                                </xsd:complexType>
                          </xsd:element>
                          <xsd:element name="NumValues" minOccurs="0"
maxOccurs="unbounded">
                                <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:sequence>
                                                  </xsd:complexType>
                                            </xsd:element>
                                            <xsd:element
name="PropertyValue" maxOccurs="unbounded">
                                                  <xsd:complexType>
                                                        <xsd:sequence>

      <xsd:element name="nPropNumber" type="xsd:integer"/>

      <xsd:element name="nPropValue" type="xsd:float"/>
                                                        </xsd:sequence>
                                                  </xsd:complexType>
                                            </xsd:element>
                                      </xsd:sequence>
```

```
                              </xsd:complexType>
                        </xsd:element>
                  </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: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: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: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: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: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:schema>
```

Literature Cited

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(2) Hamilton, W. S.; Thompson, P.; Pustejovsky, S. The Enthalpies of Combustion and Formation of 2-Methyl-2-oxazoline and 2-Ethyl-2-oxazoline. *J. Chem. Eng. Data*, **1976**, *21*, 428-429.

(3) Rihko, L. K.; Linnekoski, J. A.; Krause, A. O. Reaction Equilibria in the Synthesis of 2-Methoxy-2-methylbutane and 2-Ethoxy-2-methylbutane in the Liquid Phase. *J. Chem. Eng. Data*, **1994**, *39*, 700-704.