Pure Appl. Chem.; doi:10.1351/PAC-REC-11-05-01

Supporting information for

EXTENSION OF THERMOML: THE IUPAC STANDARD FOR THERMODYNAMIC DATA COMMUNICATIONS
(IUPAC Recommendations 2011)

Prepared for publication by
MICHAEL FRENKEL, ROBERT D. CHIRICO, VLADIMIR DIKY, PAUL L. BROWN, JOHN H. DYMOND, ROBERT. N. GOLDBERG, ANTHONY R. H. GOODWIN, HEIKO HEERKLOTZ, ERICH KÖNIGSBERGER, JOHN E. LADBURY, KENNETH N. MARSH, DAVID P. REMETA, STEPHEN E. STEIN, WILLIAM A. WAKEHAM, AND PETER A. WILLIAMS

Contents

ThermoML Schema S2
Use Case 01 S72
Use Case 02 S102
Use Case 03 S108
Use Case 04 S117
Use Case 05 S141
Use Case 06 S147
Use Case 07 S151
Use Case 08 S159
Use Case 09 S170
Use Case 10 S177
Use Case 11 S182
Use Case 12 S196
Use Case 13 S203
Use Case 14 S210

********** ThermoML Schema **********

```
<?xml version="1.0" encoding="UTF-8"?>
<!-- edited with XML Spy v4.4 U (http://www.xmlspy.com) by Robert D. Chirico (U. S. Department of Commerce) -->
<xsd:schema targetNamespace="http://www.iupac.org/namespaces/ThermoML" xmlns:tml="http://www.iupac.org/namespaces/ThermoML"
xmlns:xsd="http://www.w3.org/2001/XMLSchema" elementFormDefault="qualified" attributeFormDefault="unqualified">
  <xsd:annotation>
    <xsd:documentation>ThermoML version 4.0</xsd:documentation>
  </xsd:annotation>
  <xsd:element name="DataReport" type="tml:DataReport"/>
  <xsd:complexType name="DataReport">
    <xsd:annotation>
      <xsd:documentation>DataReport complex type</xsd:documentation>
    </xsd:annotation>
    <xsd:sequence>
      <xsd:element name="Version">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="nVersionMajor" type="xsd:integer"/>
            <xsd:element name="nVersionMinor" type="xsd:integer"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <xsd:element name="Citation" type="tml:CitationType"/>
      <xsd:element ref="tml:Compound" minOccurs="0" maxOccurs="unbounded"/>
      <xsd:element ref="tml:PureOrMixtureData" minOccurs="0" maxOccurs="unbounded"/>
      <xsd:element ref="tml:ReactionData" minOccurs="0" maxOccurs="unbounded"/>
    </xsd:sequence>
  </xsd:complexType>
  <!--

  -->
  <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:complexType name="CitationType">
    <xsd:sequence>
      <xsd:element ref="tml:TRCRefID" minOccurs="0"/>
      <xsd:element name="eType" minOccurs="0">
        <xsd:annotation>
          <xsd:documentation>The type of publication</xsd:documentation>
        </xsd:annotation>
        <xsd:simpleType>
          <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:element>
<xsd:element name="eSourceType" minOccurs="0">
    <xsd:annotation>
        <xsd:documentation>The source status type for a citation</xsd:documentation>
    </xsd:annotation>
    <xsd:simpleType>
        <xsd:restriction base="xsd:string">
            <xsd:enumeration value="Original"/>
            <xsd:enumeration value="ChemicalAbstracts"/>
            <xsd:enumeration value="Other"/>
        </xsd:restriction>
    </xsd:simpleType>
</xsd:element>
<xsd:element name="sDocumentOrigin" 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 publication</xsd:documentation>
    </xsd:annotation>
</xsd:element>
<xsd:element name="sPubName" type="xsd:string" minOccurs="0">
    <xsd:annotation>
        <xsd:documentation>Name of the publication.</xsd:documentation>
    </xsd:annotation>
</xsd:element>
<xsd:element name="yrPubYr" type="xsd:gYear" minOccurs="0">
```

```
    <xsd:annotation>
      <xsd:documentation>Publication year</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 publication</xsd:documentation>
    </xsd:annotation>
  </xsd:element>
  <xsd:element name="sAbstract" type="xsd:string" minOccurs="0">
    <xsd:annotation>
      <xsd:documentation>An abstract of the publication</xsd:documentation>
    </xsd:annotation>
  </xsd:element>
  <xsd:element name="sKeyword" type="xsd:string" minOccurs="0" maxOccurs="unbounded"/>
  <xsd:element name="eLanguage" minOccurs="0">
    <xsd:annotation>
      <xsd:documentation>Language of publication</xsd:documentation>
    </xsd:annotation>
    <xsd:simpleType>
      <xsd:restriction base="xsd:string">
        <xsd:enumeration value="Chinese"/>
        <xsd:enumeration value="English"/>
        <xsd:enumeration value="French"/>
        <xsd:enumeration value="German"/>
        <xsd:enumeration value="Japanese"/>
        <xsd:enumeration value="Polish"/>
        <xsd:enumeration value="Russian"/>
        <xsd:enumeration value="Other language"/>
      </xsd:restriction>
    </xsd:simpleType>
  </xsd:element>
  <xsd:element name="sDOI" type="xsd:string" minOccurs="0">
```

```
    <xsd:annotation>
      <xsd:documentation>DOI</xsd:documentation>
    </xsd:annotation>
  </xsd:element>
  <xsd:element name="urlCit" type="xsd:string" minOccurs="0">
    <xsd:annotation>
      <xsd:documentation>URL to the publication</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="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 publication 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:element name="sPublisher" type="xsd:string" minOccurs="0">
              <xsd:annotation>
                <xsd:documentation>Publisher name and city</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 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="nCompIndex" type="xsd:integer" minOccurs="0">
        <xsd:annotation>
          <xsd:documentation>Index to link compounds to data</xsd:documentation>
        </xsd:annotation>
      </xsd:element>
      <xsd:element name="RegNum" minOccurs="0">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="nCASRNum" type="xsd:integer" minOccurs="0"/>
            <xsd:sequence minOccurs="0">
              <xsd:element name="nOrgNum" type="xsd:integer"/>
              <xsd:element name="sOrganization" type="xsd:string" minOccurs="0"/>
            </xsd:sequence>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <xsd:element name="nPubChemID" type="xsd:integer" minOccurs="0"/>
      <xsd:element name="sStandardInChI" type="xsd:string" minOccurs="0">
        <xsd:annotation>
          <xsd:appinfo>Standard InChI string</xsd:appinfo>
          <xsd:documentation>IUPAC International Chemical Identifier</xsd:documentation>
        </xsd:annotation>
      </xsd:element>
      <xsd:element name="sStandardInChIKey" type="xsd:string" minOccurs="0">
        <xsd:annotation>
          <xsd:appinfo>Standard InChI key</xsd:appinfo>
        </xsd:annotation>
      </xsd:element>
      <xsd:element name="sOrgID" minOccurs="0" maxOccurs="unbounded">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="sOrgIdentifier" type="xsd:string"/>
```

```
            <xsd:element name="sOrganization" type="xsd:string"/>
          </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:choice minOccurs="0">
        <xsd:element name="polymer">
          <xsd:complexType>
            <xsd:annotation>
              <xsd:documentation>Polymer-specific information</xsd:documentation>
            </xsd:annotation>
            <xsd:sequence>
              <xsd:element name="nNumberAvgMolMass" type="xsd:float" minOccurs="0">
                <xsd:annotation>
```

```
            <xsd:documentation>Number average molecular mass, kg/kmol</xsd:documentation>
          </xsd:annotation>
        </xsd:element>
        <xsd:element name="nPeakAvgMolMass" type="xsd:float" minOccurs="0">
          <xsd:annotation>
            <xsd:documentation>Peak average molecular mass, kg/kmol</xsd:documentation>
          </xsd:annotation>
        </xsd:element>
        <xsd:element name="nViscosityAvgMolMass" type="xsd:float" minOccurs="0">
          <xsd:annotation>
            <xsd:documentation>Viscosity average molecular mass, kg/kmol</xsd:documentation>
          </xsd:annotation>
        </xsd:element>
        <xsd:element name="nMassAvgMolMass" type="xsd:float" minOccurs="0">
          <xsd:annotation>
            <xsd:documentation>Weight average molecular mass, kg/kmol</xsd:documentation>
          </xsd:annotation>
        </xsd:element>
        <xsd:element name="nZAvgMolMass" type="xsd:float" minOccurs="0">
          <xsd:annotation>
            <xsd:documentation>Z average molecular mass, kg/kmol</xsd:documentation>
          </xsd:annotation>
        </xsd:element>
        <xsd:element name="nMolarMassDispersity" type="xsd:float" minOccurs="0"/>
        <xsd:element name="nDegOfPolymerizationDispersity" type="xsd:float" minOccurs="0"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="ion">
    <xsd:complexType>
      <xsd:annotation>
        <xsd:documentation>Ion-specific information</xsd:documentation>
      </xsd:annotation>
      <xsd:sequence>
        <xsd:element name="nCharge" type="xsd:integer"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
```

```
    <xsd:element name="biomaterial">
      <xsd:complexType>
        <xsd:annotation>
          <xsd:documentation>Bio species information</xsd:documentation>
        </xsd:annotation>
        <xsd:sequence>
          <xsd:element name="sECNumber" type="xsd:string" minOccurs="0"/>
          <xsd:element name="sPDBIdentifier" type="xsd:string" minOccurs="0"/>
        </xsd:sequence>
      </xsd:complexType>
    </xsd:element>
    <xsd:element name="MulticomponentSubstance">
      <xsd:complexType>
        <xsd:sequence>
          <xsd:element name="Component" maxOccurs="unbounded">
            <xsd:complexType>
              <xsd:sequence>
                <xsd:choice>
                  <xsd:element name="nCompIndex" type="xsd:integer"/>
                  <xsd:element ref="tml:RegNum"/>
                </xsd:choice>
                <xsd:element name="nAmount" type="xsd:float"/>
              </xsd:sequence>
            </xsd:complexType>
          </xsd:element>
        </xsd:sequence>
        <xsd:attribute name="type" type="tml:MulticomponentType"/>
        <xsd:attribute name="compositionBasis" type="tml:MulticomponentComposition" use="optional"/>
      </xsd:complexType>
    </xsd:element>
  </xsd:choice>
  <xsd:element name="eSpeciationState" minOccurs="0">
    <xsd:simpleType>
      <xsd:restriction base="xsd:string">
        <xsd:enumeration value="equilibrium"/>
        <xsd:enumeration value="single species"/>
      </xsd:restriction>
    </xsd:simpleType>
```

```
        </xsd:element>
        <xsd:element ref="tml: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="tml:eSampleSource" minOccurs="0"/>
        <xsd:element name="eStatus" type="tml: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="tml:ePurifMethod" minOccurs="0" maxOccurs="unbounded"/>
              <xsd:element name="sPurifMethod" type="xsd:string" minOccurs="0" maxOccurs="unbounded"/>
              <xsd:sequence minOccurs="0">
                <xsd:element name="nPurityMol" type="xsd:float">
                  <xsd:annotation>
                    <xsd:documentation>purity value in mole percent</xsd:documentation>
                  </xsd:annotation>
                </xsd:element>
                <xsd:element name="nPurityMolDigits" type="xsd:integer"/>
              </xsd:sequence>
              <xsd:sequence minOccurs="0">
                <xsd:element name="nPurityMass" type="xsd:float">
                  <xsd:annotation>
                    <xsd:documentation>purity value in mass percent</xsd:documentation>
```

```
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="nPurityMassDigits" type="xsd:integer"/>
  </xsd:sequence>
  <xsd:sequence minOccurs="0">
    <xsd:element name="nPurityVol" type="xsd:float">
      <xsd:annotation>
        <xsd:documentation>purity value in volume percent</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="nPurityVolDigits" type="xsd:integer"/>
  </xsd:sequence>
  <xsd:sequence minOccurs="0">
    <xsd:element name="nUnknownPerCent" type="xsd:float">
      <xsd:annotation>
        <xsd:documentation>purity value in not specified percent</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="nUnknownPerCentDigits" type="xsd:integer"/>
  </xsd:sequence>
  <xsd:sequence minOccurs="0">
    <xsd:element name="nWaterMassPerCent" type="xsd:float">
      <xsd:annotation>
        <xsd:documentation>mass per cent of water</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="nWaterMassPerCentDigits" type="xsd:integer"/>
  </xsd:sequence>
  <xsd:sequence minOccurs="0">
    <xsd:element name="nWaterMolPerCent" type="xsd:float">
      <xsd:annotation>
        <xsd:documentation>mole per cent of water</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="nWaterMolPerCentDigits" type="xsd:integer"/>
  </xsd:sequence>
  <xsd:sequence minOccurs="0">
    <xsd:element name="nHalideMolPerCent" type="xsd:float">
```

```
                <xsd:annotation>
                  <xsd:documentation>mass per cent of halide impurity</xsd:documentation>
                </xsd:annotation>
              </xsd:element>
              <xsd:element name="nHalideMolPerCentDigits" type="xsd:integer"/>
            </xsd:sequence>
            <xsd:sequence minOccurs="0">
              <xsd:element name="nHalideMassPerCent" type="xsd:float">
                <xsd:annotation>
                  <xsd:documentation>mass per cent of halide impurity</xsd:documentation>
                </xsd:annotation>
              </xsd:element>
              <xsd:element name="nHalideMassPerCentDigits" type="xsd:integer"/>
            </xsd:sequence>
            <xsd:element name="eAnalMeth" type="tml: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:element name="ComponentSample" minOccurs="0" maxOccurs="unbounded">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:choice>
              <xsd:element name="nCompIndex" type="xsd:integer"/>
              <xsd:element ref="tml:RegNum"/>
            </xsd:choice>
            <xsd:element name="nSampleNm" type="xsd:integer"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
    </xsd:sequence>
  </xsd:complexType>
</xsd:element>
<!--
```

```
-->
<xsd:element name="PureOrMixtureData">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="nPureOrMixtureDataNumber" type="xsd:integer" minOccurs="0"/>
      <xsd:element name="Component" maxOccurs="unbounded">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:choice>
              <xsd:element name="nCompIndex" type="xsd:integer"/>
              <xsd:element ref="tml:RegNum"/>
            </xsd:choice>
            <xsd:element name="nSampleNm" type="xsd:int" minOccurs="0"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <xsd:element name="AuxiliarySubstance" minOccurs="0" maxOccurs="unbounded">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:choice minOccurs="0">
              <xsd:element name="eFunction">
                <xsd:simpleType>
                  <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="Buffer"/>
                    <xsd:enumeration value="Solvent"/>
                    <xsd:enumeration value="Inert"/>
                  </xsd:restriction>
                </xsd:simpleType>
              </xsd:element>
              <xsd:element name="sFunction" type="xsd:string"/>
            </xsd:choice>
            <xsd:choice>
              <xsd:element name="nCompIndex" type="xsd:integer"/>
              <xsd:element ref="tml:RegNum"/>
            </xsd:choice>
            <xsd:element name="nSampleNm" type="xsd:int" minOccurs="0"/>
          </xsd:sequence>
```

```
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="eExpPurpose" type="tml: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 factor"/>
                                <xsd:enumeration value="Lower consolute temperature, K"/>
                                <xsd:enumeration value="Upper consolute temperature, K"/>
                                <xsd:enumeration value="Lower consolute pressure, kPa"/>
```

```
                <xsd:enumeration value="Upper consolute pressure, kPa"/>
              </xsd:restriction>
            </xsd:simpleType>
          </xsd:element>
          <xsd:choice>
            <xsd:element name="eMethodName">
              <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="Relative permittivity measurements"/>
                  <xsd:enumeration value="Refractive index measurements"/>
                  <xsd:enumeration value="Direct measurement"/>
                  <xsd:enumeration value="Other"/>
                </xsd:restriction>
              </xsd:simpleType>
            </xsd:element>
            <xsd:element name="sMethodName" type="xsd:string"/>
            <xsd:element ref="tml:CriticalEvaluation"/>
            <xsd:element ref="tml:Prediction"/>
          </xsd:choice>
        </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:annotation>
                    <xsd:documentation>Boiling temperature at P=101.325 kPa</xsd:documentation>
```

```
            </xsd:annotation>
          </xsd:enumeration>
          <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:choice>
      <xsd:element name="eMethodName">
        <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="Torsion effusion method"/>
            <xsd:enumeration value="Gas chromatography"/>
            <xsd:enumeration value="Laser pulse heating"/>
            <xsd:enumeration value="Levitation methods"/>
            <xsd:enumeration value="By X=Y"/>
            <xsd:enumeration value="By P(X) extreme"/>
            <xsd:enumeration value="By T(X) extreme"/>
            <xsd:enumeration value="DSC/DTA"/>
            <xsd:enumeration value="Other"/>
          </xsd:restriction>
        </xsd:simpleType>
      </xsd:element>
      <xsd:element name="sMethodName" type="xsd:string"/>
      <xsd:element ref="tml:CriticalEvaluation"/>
```

```
            <xsd:element ref="tml:Prediction"/>
          </xsd:choice>
        </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="Molar enthalpy of transition or fusion, kJ/mol"/>
                <xsd:enumeration value="Molar entropy of transition or fusion, J/K/mol"/>
                <xsd:enumeration value="Cryoscopic constant (mole fraction scale), 1/K"/>
                <xsd:enumeration value="Cryoscopic constant (molality scale), kg/mol/K"/>
                <xsd:enumeration value="Molar enthalpy of vaporization or sublimation, kJ/mol"/>
                <xsd:enumeration value="Molar entropy of vaporization or sublimation, J/K/mol"/>
                <xsd:enumeration value="Molar Gibbs energy 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="Phase boundary pressure, kPa"/>
                <xsd:enumeration value="Eutectic temperature, K"/>
                <xsd:enumeration value="Peritectic temperature, K"/>
                <xsd:enumeration value="Monotectic temperature, K"/>
                <xsd:enumeration value="Molar lattice energy at 0 K, kJ/mol"/>
              </xsd:restriction>
            </xsd:simpleType>
          </xsd:element>
          <xsd:choice>
            <xsd:element name="eMethodName">
              <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 temperature of a dilute solution"/>
                <xsd:enumeration value="AC calorimetry"/>
                <xsd:enumeration value="Resistive pulse heating"/>
                <xsd:enumeration value="Laser pulse heating"/>
                <xsd:enumeration value="Levitation methods"/>
                <xsd:enumeration value="Correlation gas chromatography"/>
                <xsd:enumeration value="Other"/>
              </xsd:restriction>
            </xsd:simpleType>
          </xsd:element>
          <xsd:element name="sMethodName" type="xsd:string"/>
          <xsd:element ref="tml:CriticalEvaluation"/>
          <xsd:element ref="tml:Prediction"/>
        </xsd:choice>
      </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: mole fraction"/>
```

```
      <xsd:enumeration value="Eutectic composition: mass fraction"/>
      <xsd:enumeration value="Eutectic composition: volume fraction"/>
      <xsd:enumeration value="Monotectic composition: mole fraction"/>
      <xsd:enumeration value="Monotectic 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 concentration, kg/m3">
        <xsd:annotation>
          <xsd:documentation>Mass of solute per volume of solution</xsd:documentation>
        </xsd:annotation>
      </xsd:enumeration>
      <xsd:enumeration value="Ratio of amount of solute to mass of solution, mol/kg"/>
      <xsd:enumeration value="Mass ratio of solute to solvent"/>
      <xsd:enumeration value="Molality, mol/kg"/>
      <xsd:enumeration value="Amount concentration (molarity), mol/dm3"/>
      <xsd:enumeration value="Mole fraction"/>
      <xsd:enumeration value="Mole fraction in LLG critical state"/>
      <xsd:enumeration value="Amount ratio of solute to solvent"/>
      <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 of solute to solvent"/>
      <xsd:enumeration value="Mass fraction"/>
      <xsd:enumeration value="Mass fraction in LLG critical state"/>
      <xsd:enumeration value="Henry's Law constant (mole fraction scale), kPa"/>
      <xsd:enumeration value="Henry's Law constant (molality scale), kPa*kg/mol"/>
      <xsd:enumeration value="Henry's Law constant (amount concentration scale), kPa*dm3/mol">
        <xsd:annotation>
          <xsd:documentation>Ratio of partial pressure to molarity</xsd:documentation>
        </xsd:annotation>
      </xsd:enumeration>
      <xsd:enumeration value="Bunsen coefficient"/>
      <xsd:enumeration value="Ostwald coefficient"/>
      <xsd:enumeration value="Partial pressure, kPa"/>
    </xsd:restriction>
  </xsd:simpleType>
```

```
            </xsd:element>
            <xsd:choice>
              <xsd:element name="eMethodName">
                <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="Density calibration data"/>
                    <xsd:enumeration value="Index of refraction calibration data"/>
                    <xsd:enumeration value="Speed of sound calibration data"/>
                    <xsd:enumeration value="Calculated by Gibbs-Duhem equation"/>
                    <xsd:enumeration value="Titration method"/>
                    <xsd:enumeration value="Phase equilibration"/>
                    <xsd:enumeration value="Derived from phase diagram analysis"/>
                    <xsd:enumeration value="Photoacoustic method"/>
                    <xsd:enumeration value="Other"/>
                  </xsd:restriction>
                </xsd:simpleType>
              </xsd:element>
              <xsd:element name="sMethodName" type="xsd:string"/>
              <xsd:element ref="tml:CriticalEvaluation"/>
              <xsd:element ref="tml:Prediction"/>
            </xsd:choice>
          </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="(Relative) activity"/>
                  <xsd:enumeration value="Activity coefficient"/>
                  <xsd:enumeration value="Mean ionic activity coefficient"/>
                  <xsd:enumeration value="Mean ionic activity, (mol/dm3)^n"/>
```

```
                <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:choice>
            <xsd:element name="eMethodName">
              <xsd:simpleType>
                <xsd:restriction base="xsd:string">
                  <xsd:enumeration value="Chromatography"/>
                  <xsd:enumeration value="Differential ebulliometry"/>
                  <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="Potential difference of an electrochemical cell">
                    <xsd:annotation>
                      <xsd:documentation>e.m.f. measurement</xsd:documentation>
                    </xsd:annotation>
                  </xsd:enumeration>
                  <xsd:enumeration value="Other"/>
                </xsd:restriction>
              </xsd:simpleType>
            </xsd:element>
            <xsd:element name="sMethodName" type="xsd:string"/>
            <xsd:element ref="tml:CriticalEvaluation"/>
            <xsd:element ref="tml:Prediction"/>
          </xsd:choice>
        </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="Mass density, kg/m3"/>
        <xsd:enumeration value="Specific volume, m3/kg"/>
        <xsd:enumeration value="Amount density, mol/m3">
          <xsd:annotation>
            <xsd:documentation>Molar density</xsd:documentation>
          </xsd:annotation>
        </xsd:enumeration>
        <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 molar 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="Excess adiabatic compressibility, 1/kPa"/>
        <xsd:enumeration value="Isothermal compressibility, 1/kPa"/>
        <xsd:enumeration value="Excess isothermal compressibility, 1/kPa"/>
        <xsd:enumeration value="Isobaric coefficient of expansion, 1/K"/>
        <xsd:enumeration value="Excess 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:choice>
    <xsd:element name="eMethodName">
      <xsd:simpleType>
        <xsd:restriction base="xsd:string">
          <xsd:enumeration value="Pycnometric method"/>
```

```
                <xsd:enumeration value="X-ray diffraction"/>
                <xsd:enumeration value="Buoyancy - hydrostatic balance"/>
                <xsd:enumeration value="Buoyancy - magnetic float or magnetic suspension"/>
                <xsd:enumeration value="Buoyancy - hydrostatic balance with magnetic float"/>
                <xsd:enumeration value="Buoyancy - hydrostatic balance with magnetic suspension - one sinker"/>
                <xsd:enumeration value="Buoyancy - hydrostatic balance with magnetic suspension - two sinkers"/>
                <xsd:enumeration value="Vibrating tube method"/>
                <xsd:enumeration value="Isochoric PVT measurement"/>
                <xsd:enumeration value="Other PVT measurement"/>
                <xsd:enumeration value="Burnett expansion method"/>
                <xsd:enumeration value="Constant-volume piezometry"/>
                <xsd:enumeration value="Hydrostatic balance"/>
                <xsd:enumeration value="Bellows volumetry"/>
                <xsd:enumeration value="Derived from speed of sound"/>
                <xsd:enumeration value="Resistive pulse heating"/>
                <xsd:enumeration value="Laser pulse heating"/>
                <xsd:enumeration value="Levitation methods"/>
                <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"/>
          <xsd:element ref="tml:CriticalEvaluation"/>
          <xsd:element ref="tml:Prediction"/>
        </xsd:choice>
      </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="Molar heat capacity at constant pressure, J/K/mol"/>
        <xsd:enumeration value="Specific heat capacity at constant pressure, J/K/kg"/>
        <xsd:enumeration value="Heat capacity at constant pressure per volume, J/K/m3"/>
        <xsd:enumeration value="Molar heat capacity at saturation pressure, J/K/mol"/>
        <xsd:enumeration value="Specific heat capacity at saturation pressure, J/K/kg"/>
        <xsd:enumeration value="Heat capacity at saturation pressure per volume, J/K/m3"/>
        <xsd:enumeration value="Molar heat capacity at constant volume, J/K/mol"/>
        <xsd:enumeration value="Specific heat capacity at constant volume, J/K/kg"/>
        <xsd:enumeration value="Heat capacity at constant volume per volume, J/K/m3"/>
        <xsd:enumeration value="Heat capacity ratio cp/cv"/>
        <xsd:enumeration value="Molar entropy, J/K/mol"/>
        <xsd:enumeration value="Molar enthalpy, kJ/mol"/>
        <xsd:enumeration value="Molar enthalpy function {Hm(T)-Hm(0)}/T, J/K/mol"/>
        <xsd:enumeration value="Molar Gibbs energy function {Gm(T)-Hm(0)}/T, J/K/mol"/>
        <xsd:enumeration value="Molar Gibbs energy function {Gm(T)-Hm(298.15)}/T, J/K/mol"/>
        <xsd:enumeration value="Molar Gibbs energy, kJ/mol"/>
        <xsd:enumeration value="Molar Helmholtz energy, kJ/mol"/>
        <xsd:enumeration value="Molar internal energy, kJ/mol"/>
        <xsd:enumeration value="Joule-Thomson coefficient, K/kPa"/>
        <xsd:enumeration value="Pressure coefficient of molar enthalpy, J/kPa/mol"/>
      </xsd:restriction>
    </xsd:simpleType>
  </xsd:element>
  <xsd:choice>
    <xsd:element name="eMethodName">
      <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="Thin-film microcalorimeter"/>
                <xsd:enumeration value="AC calorimetry"/>
                <xsd:enumeration value="Resistive pulse heating"/>
                <xsd:enumeration value="Laser pulse heating"/>
                <xsd:enumeration value="Levitation methods"/>
                <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"/>
          <xsd:element ref="tml:CriticalEvaluation"/>
          <xsd:element ref="tml:Prediction"/>
        </xsd:choice>
      </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 molar enthalpy, kJ/mol"/>
              <xsd:enumeration value="Apparent molar entropy, J/K/mol"/>
              <xsd:enumeration value="Apparent molar Gibbs energy, kJ/mol"/>
              <xsd:enumeration value="Apparent molar heat capacity, J/K/mol"/>
              <xsd:enumeration value="Excess molar enthalpy (molar enthalpy of mixing), kJ/mol">
                <xsd:annotation>
                  <xsd:documentation>Per mol of mixture</xsd:documentation>
                </xsd:annotation>
              </xsd:enumeration>
              <xsd:enumeration value="Molar enthalpy of mixing with solvent, kJ/mol">
                <xsd:annotation>
```

```
                <xsd:documentation>Per mol of solute</xsd:documentation>
              </xsd:annotation>
            </xsd:enumeration>
            <xsd:enumeration value="Molar enthalpy of solution, kJ/mol">
              <xsd:annotation>
                <xsd:documentation>Per mol of solute</xsd:documentation>
              </xsd:annotation>
            </xsd:enumeration>
            <xsd:enumeration value="Molar enthalpy of dilution, kJ/mol">
              <xsd:annotation>
                <xsd:documentation>Per mol of solute</xsd:documentation>
              </xsd:annotation>
            </xsd:enumeration>
            <xsd:enumeration value="Excess molar entropy, J/K/mol"/>
            <xsd:enumeration value="Excess molar Gibbs energy, kJ/mol"/>
            <xsd:enumeration value="Excess molar 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 molar enthalpy, kJ/mol"/>
            <xsd:enumeration value="Standard state molar entropy, J/K/mol"/>
            <xsd:enumeration value="Standard state molar Gibbs energy, kJ/mol"/>
            <xsd:enumeration value="Standard state molar heat capacity, J/K/mol"/>
          </xsd:restriction>
        </xsd:simpleType>
      </xsd:element>
      <xsd:choice>
        <xsd:element name="eMethodName">
          <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="Isoperibol calorimetry"/>
                <xsd:enumeration value="Isothermal displacement"/>
                <xsd:enumeration value="Power-compensation calorimetry"/>
                <xsd:enumeration value="Titration calorimetry"/>
                <xsd:enumeration value="Potential difference of an electrochemical cell"/>
                <xsd:enumeration value="Other"/>
              </xsd:restriction>
            </xsd:simpleType>
          </xsd:element>
          <xsd:element name="sMethodName" type="xsd:string"/>
          <xsd:element ref="tml:CriticalEvaluation"/>
          <xsd:element ref="tml:Prediction"/>
        </xsd:choice>
      </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="Excess 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, m2/s"/>
              <xsd:enumeration value="Self diffusion coefficient, m2/s"/>
              <xsd:enumeration value="Tracer diffusion coefficient, m2/s"/>
              <xsd:enumeration value="Electrical conductivity, S/m"/>
```

```
            <xsd:enumeration value="Molar conductivity, S*m2/mol"/>
            <xsd:enumeration value="Transport number"/>
          </xsd:restriction>
        </xsd:simpleType>
      </xsd:element>
      <xsd:choice>
        <xsd:element name="eMethodName">
          <xsd:simpleType>
            <xsd:restriction base="xsd:string">
              <xsd:enumeration value="Capillary tube (Ostwald; Ubbelohde) 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="Moving piston method"/>
              <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="Hot disk method"/>
              <xsd:enumeration value="Resistive pulse heating"/>
              <xsd:enumeration value="Laser pulse heating"/>
              <xsd:enumeration value="Levitation methods"/>
              <xsd:enumeration value="Alternating current cell with electrodes"/>
              <xsd:enumeration value="Direct current cell with electrodes"/>
              <xsd:enumeration value="Voltage change across transformer (no electrode)"/>
              <xsd:enumeration value="Gouy interferometer"/>
              <xsd:enumeration value="Lamb interferometer"/>
              <xsd:enumeration value="Oscillating sinker"/>
              <xsd:enumeration value="Speed of sound measurements"/>
              <xsd:enumeration value="Other"/>
```

```
                    </xsd:restriction>
                  </xsd:simpleType>
                </xsd:element>
                <xsd:element name="sMethodName" type="xsd:string"/>
                <xsd:element ref="tml:CriticalEvaluation"/>
                <xsd:element ref="tml:Prediction"/>
              </xsd:choice>
            </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="Excess refractive index (Na D-line)"/>
                    <xsd:enumeration value="Refractive index (other wavelength)"/>
                    <xsd:enumeration value="Excess refractive index (other wavelength)"/>
                    <xsd:enumeration value="Relative permittivity at zero frequency"/>
                    <xsd:enumeration value="Excess relative permittivity at zero frequency"/>
                    <xsd:enumeration value="Relative permittivity at various frequencies"/>
                    <xsd:enumeration value="Complex relative permittivity (Real part) at various frequencies"/>
                    <xsd:enumeration value="Complex relative permittivity (Imaginary part) at various frequencies"/>
                    <xsd:enumeration value="Surface tension liquid-gas, N/m"/>
                    <xsd:enumeration value="Excess surface tension liquid-gas, N/m"/>
                    <xsd:enumeration value="Interfacial tension, N/m"/>
                    <xsd:enumeration value="Speed of sound, m/s"/>
                    <xsd:enumeration value="Excess speed of sound, m/s"/>
                  </xsd:restriction>
                </xsd:simpleType>
              </xsd:element>
              <xsd:choice>
                <xsd:element name="eMethodName">
                  <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="Parallel plate capacitor"/>
                <xsd:enumeration value="Coaxial cylinder capacitor"/>
                <xsd:enumeration value="Cross capacitor"/>
                <xsd:enumeration value="Reentrant cavity resonator"/>
                <xsd:enumeration value="Coaxial line"/>
                <xsd:enumeration value="Wave guide"/>
                <xsd:enumeration value="Far infrared free space"/>
                <xsd:enumeration value="Single path-length method"/>
                <xsd:enumeration value="Dual path-length method"/>
                <xsd:enumeration value="Multiple path-length method"/>
                <xsd:enumeration value="Cylindrical cavity resonance method"/>
                <xsd:enumeration value="Spherical cavity resonance method"/>
                <xsd:enumeration value="Toroidal cavity resonance method"/>
                <xsd:enumeration value="Levitation methods"/>
                <xsd:enumeration value="Other"/>
              </xsd:restriction>
            </xsd:simpleType>
          </xsd:element>
          <xsd:element name="sMethodName" type="xsd:string"/>
          <xsd:element ref="tml:CriticalEvaluation"/>
          <xsd:element ref="tml:Prediction"/>
        </xsd:choice>
      </xsd:sequence>
```

```
            </xsd:complexType>
          </xsd:element>
          <xsd:element name="BioProperties">
            <xsd:complexType>
              <xsd:sequence>
                <xsd:element name="ePropName">
                  <xsd:simpleType>
                    <xsd:restriction base="xsd:string">
                      <xsd:enumeration value="Temperature of 1/2 conversion, K"/>
                      <xsd:enumeration value="Peak temperature, K"/>
                      <xsd:enumeration value="Zero-Gibbs energy temperature, K"/>
                      <xsd:enumeration value="Heat capacity change at transition, J/K/mol"/>
                      <xsd:enumeration value="van't Hoff enthalpy of transition, kJ/mol"/>
                    </xsd:restriction>
                  </xsd:simpleType>
                </xsd:element>
                <xsd:choice>
                  <xsd:element name="eMethodName">
                    <xsd:simpleType>
                      <xsd:restriction base="xsd:string">
                        <xsd:enumeration value="DSC/DTA"/>
                      </xsd:restriction>
                    </xsd:simpleType>
                  </xsd:element>
                  <xsd:element name="sMethodName" type="xsd:string"/>
                  <xsd:element ref="tml:CriticalEvaluation"/>
                  <xsd:element ref="tml:Prediction"/>
                </xsd:choice>
              </xsd:sequence>
            </xsd:complexType>
          </xsd:element>
        </xsd:choice>
      </xsd:complexType>
    </xsd:element>
    <xsd:choice minOccurs="0">
      <xsd:element name="nCompIndex" type="xsd:integer"/>
      <xsd:element ref="tml:RegNum"/>
    </xsd:choice>
```

```
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="PropPhaseID" minOccurs="0" maxOccurs="unbounded">
    <xsd:annotation>
      <xsd:documentation> CASRN is necessary for mixtures only</xsd:documentation>
    </xsd:annotation>
    <xsd:complexType>
      <xsd:sequence>
        <xsd:element name="ePropPhase" type="tml:ePhaseName"/>
        <xsd:choice minOccurs="0">
          <xsd:element name="eCrystalLatticeType" type="tml:eCrystalLatticeTypeSelection"/>
          <xsd:element name="sPhaseDescription" type="xsd:string"/>
        </xsd:choice>
        <xsd:choice minOccurs="0">
          <xsd:element name="nCompIndex" type="xsd:integer"/>
          <xsd:element ref="tml:RegNum"/>
        </xsd:choice>
        <xsd:choice minOccurs="0">
          <xsd:element name="eBioState">
            <xsd:simpleType>
              <xsd:restriction base="xsd:string">
                <xsd:enumeration value="Native"/>
                <xsd:enumeration value="Denaturated"/>
              </xsd:restriction>
            </xsd:simpleType>
          </xsd:element>
          <xsd:element name="sBioState" type="xsd:string"/>
        </xsd:choice>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="ePresentation" type="tml:ePresentation"/>
  <xsd:element name="eRefStateType" type="tml:eRefStateType" minOccurs="0"/>
  <xsd:sequence minOccurs="0">
    <xsd:element name="nRefTemp" type="xsd:float"/>
    <xsd:element name="nRefTempDigits" type="xsd:integer"/>
  </xsd:sequence>
```

```
<xsd:sequence minOccurs="0">
  <xsd:element name="nRefPressure" type="xsd:float"/>
  <xsd:element name="nRefPressureDigits" type="xsd:integer"/>
</xsd:sequence>
<xsd:element name="RefPhaseID" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation> CASRN is necessary for mixtures only</xsd:documentation>
  </xsd:annotation>
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="eRefPhase" type="tml:ePhaseName"/>
      <xsd:choice minOccurs="0">
        <xsd:element name="eCrystalLatticeType" type="tml:eCrystalLatticeTypeSelection"/>
        <xsd:element name="sPhaseDescription" type="xsd:string"/>
      </xsd:choice>
      <xsd:choice minOccurs="0">
        <xsd:element name="nCompIndex" type="xsd:integer"/>
        <xsd:element ref="tml:RegNum"/>
      </xsd:choice>
    </xsd:sequence>
  </xsd:complexType>
</xsd:element>
<xsd:element ref="tml:Solvent" minOccurs="0"/>
<xsd:element name="eStandardState" minOccurs="0">
  <xsd:simpleType>
    <xsd:restriction base="xsd:string">
      <xsd:enumeration value="Pure compound"/>
      <xsd:enumeration value="Pure liquid solute"/>
      <xsd:enumeration value="Standard molality (1 mol/kg) solute"/>
      <xsd:enumeration value="Standard amount concentration (1 mol/dm3) solute">
        <xsd:annotation>
          <xsd:documentation>Molarity</xsd:documentation>
        </xsd:annotation>
      </xsd:enumeration>
      <xsd:enumeration value="Infinite dilution solute"/>
    </xsd:restriction>
  </xsd:simpleType>
</xsd:element>
```

```
            <xsd:element ref="tml:CombinedUncertainty" minOccurs="0" maxOccurs="unbounded"/>
            <xsd:element name="PropUncertainty" type="tml:PropVarUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
            <xsd:element name="PropRepeatability" type="tml:PropVarRepeatabilityType" minOccurs="0"/>
            <xsd:element name="PropDeviceSpec" type="tml:PropVarDeviceSpecType" minOccurs="0"/>
            <xsd:element ref="tml:CurveDev" minOccurs="0" maxOccurs="unbounded"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="PhaseID" maxOccurs="unbounded">
    <xsd:annotation>
        <xsd:documentation> CASRN is necessary for mixtures only</xsd:documentation>
    </xsd:annotation>
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="ePhase" type="tml:ePhaseName"/>
            <xsd:choice minOccurs="0">
                <xsd:element name="eCrystalLatticeType" type="tml:eCrystalLatticeTypeSelection"/>
                <xsd:element name="sPhaseDescription" type="xsd:string"/>
            </xsd:choice>
            <xsd:choice minOccurs="0">
                <xsd:element name="nCompIndex" type="xsd:integer"/>
                <xsd:element ref="tml:RegNum"/>
            </xsd:choice>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="Constraint" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nConstraintNumber" type="xsd:integer" minOccurs="0"/>
            <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="tml:ConstraintVariableType"/>
                        <xsd:choice minOccurs="0">
```

```
                <xsd:element name="nCompIndex" type="xsd:integer"/>
                <xsd:element ref="tml:RegNum"/>
              </xsd:choice>
            </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="tml:ePhaseName"/>
              <xsd:choice minOccurs="0">
                <xsd:element name="eCrystalLatticeType" type="tml:eCrystalLatticeTypeSelection"/>
                <xsd:element name="sPhaseDescription" type="xsd:string"/>
              </xsd:choice>
              <xsd:choice minOccurs="0">
                <xsd:element name="nCompIndex" type="xsd:integer"/>
                <xsd:element ref="tml:RegNum"/>
              </xsd:choice>
            </xsd:sequence>
          </xsd:complexType>
        </xsd:element>
        <xsd:element ref="tml:Solvent" minOccurs="0"/>
        <xsd:element name="nConstraintValue" type="xsd:float"/>
        <xsd:element name="nConstrDigits" type="xsd:integer"/>
        <xsd:element name="ConstrUncertainty" type="tml:ConstrUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="ConstrRepeatability" type="tml:ConstrRepeatabilityType" minOccurs="0"/>
        <xsd:element name="ConstrDeviceSpec" type="tml:ConstrDeviceSpecType" minOccurs="0"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="Variable" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:element name="nVarNumber" type="xsd:integer"/>
        <xsd:element name="VariableID">
```

```
            <xsd:annotation>
              <xsd:documentation> CASRN is necessary for mixtures only</xsd:documentation>
            </xsd:annotation>
            <xsd:complexType>
              <xsd:sequence>
                <xsd:element name="VariableType" type="tml:ConstraintVariableType"/>
                <xsd:choice minOccurs="0">
                  <xsd:element name="nCompIndex" type="xsd:integer"/>
                  <xsd:element ref="tml:RegNum"/>
                </xsd:choice>
              </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="tml:ePhaseName"/>
                <xsd:choice minOccurs="0">
                  <xsd:element name="eCrystalLatticeType" type="tml:eCrystalLatticeTypeSelection"/>
                  <xsd:element name="sPhaseDescription" type="xsd:string"/>
                </xsd:choice>
                <xsd:choice minOccurs="0">
                  <xsd:element name="nCompIndex" type="xsd:integer"/>
                  <xsd:element ref="tml:RegNum"/>
                </xsd:choice>
              </xsd:sequence>
            </xsd:complexType>
          </xsd:element>
          <xsd:element ref="tml:Solvent" minOccurs="0"/>
          <xsd:element name="VarUncertainty" type="tml:PropVarUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
          <xsd:element name="VarRepeatability" type="tml:PropVarRepeatabilityType" minOccurs="0"/>
          <xsd:element name="VarDeviceSpec" type="tml:PropVarDeviceSpecType" minOccurs="0"/>
        </xsd:sequence>
      </xsd:complexType>
    </xsd:element>
```

```
        <xsd:element ref="tml:NumValues" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element ref="tml:Equation" minOccurs="0" maxOccurs="unbounded"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <!--

      -->
  <xsd:element name="ReactionData">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:element name="nReactionDataNumber" type="xsd:integer" minOccurs="0"/>
        <xsd:element name="Participant" maxOccurs="unbounded">
          <xsd:complexType>
            <xsd:sequence>
              <xsd:choice>
                <xsd:element name="nCompIndex" type="xsd:integer"/>
                <xsd:element ref="tml:RegNum"/>
              </xsd:choice>
              <xsd:element name="nSampleNm" type="xsd:int" minOccurs="0"/>
              <xsd:element name="nStoichiometricCoef" type="xsd:float" minOccurs="0"/>
              <xsd:element name="ePhase" type="tml:ePhaseName"/>
              <xsd:choice minOccurs="0">
                <xsd:element name="eCrystalLatticeType" type="tml:eCrystalLatticeTypeSelection"/>
                <xsd:element name="sPhaseDescription" type="xsd:string"/>
              </xsd:choice>
              <xsd:element name="eStandardState" minOccurs="0">
                <xsd:simpleType>
                  <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="Pure compound"/>
                    <xsd:enumeration value="Pure liquid solute"/>
                    <xsd:enumeration value="Standard molality (1 mol/kg) solute"/>
                    <xsd:enumeration value="Standard amount concentration (1 mol/dm3) solute">
                      <xsd:annotation>
                        <xsd:documentation>Molarity</xsd:documentation>
                      </xsd:annotation>
                    </xsd:enumeration>
                    <xsd:enumeration value="Infinite dilution solute"/>
```

```
            </xsd:restriction>
          </xsd:simpleType>
        </xsd:element>
        <xsd:element name="eCompositionRepresentation" minOccurs="0">
          <xsd:simpleType>
            <xsd:restriction base="xsd:string">
              <xsd:enumeration value="Amount ratio of solvent to participant"/>
              <xsd:enumeration value="Molality - amount of participant per mass of solvent, mol/kg"/>
              <xsd:enumeration value="Amount of participant per mass of solution, mol/kg"/>
              <xsd:enumeration value="Amount concentration - amount of participant per volume of solution, mol/dm3"/>
              <xsd:enumeration value="Amount ratio of participant to solvent"/>
              <xsd:enumeration value="Mass ratio of participant to solvent"/>
              <xsd:enumeration value="Volume ratio of participant to solvent"/>
              <xsd:enumeration value="Mass of participant per volume of solution, kg/m3"/>
            </xsd:restriction>
          </xsd:simpleType>
        </xsd:element>
        <xsd:element name="nNumericalComposition" type="xsd:float" minOccurs="0"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="nElectronNumber" type="xsd:integer" minOccurs="0"/>
  <xsd:element name="AuxiliarySubstance" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:choice minOccurs="0">
          <xsd:element name="eFunction">
            <xsd:simpleType>
              <xsd:restriction base="xsd:string">
                <xsd:enumeration value="Cofactor"/>
                <xsd:enumeration value="Buffer"/>
                <xsd:enumeration value="Inert"/>
              </xsd:restriction>
            </xsd:simpleType>
          </xsd:element>
          <xsd:element name="sFunction" type="xsd:string"/>
        </xsd:choice>
        <xsd:choice>
```

```
            <xsd:element name="nCompIndex" type="xsd:integer"/>
            <xsd:element ref="tml:RegNum"/>
          </xsd:choice>
          <xsd:element name="nSampleNm" type="xsd:int" minOccurs="0"/>
          <xsd:element name="ePhase" type="tml:ePhaseName" minOccurs="0"/>
        </xsd:sequence>
      </xsd:complexType>
    </xsd:element>
    <xsd:element name="Solvent" minOccurs="0" maxOccurs="unbounded">
      <xsd:complexType>
        <xsd:sequence>
          <xsd:choice maxOccurs="unbounded">
            <xsd:element name="nCompIndex" type="xsd:integer"/>
            <xsd:element ref="tml:RegNum"/>
          </xsd:choice>
          <xsd:element name="ePhase" type="tml:ePhaseName"/>
        </xsd:sequence>
      </xsd:complexType>
    </xsd:element>
    <xsd:element name="eReactionFormalism" minOccurs="0">
      <xsd:simpleType>
        <xsd:restriction base="xsd:string">
          <xsd:enumeration value="chemical"/>
          <xsd:enumeration value="biochemical"/>
        </xsd:restriction>
      </xsd:simpleType>
    </xsd:element>
    <xsd:element name="eExpPurpose" type="tml: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 hydrogen 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="Formation of ion"/>
            <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="ReactionStateChangeProp">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="ePropName">
        <xsd:simpleType>
          <xsd:restriction base="xsd:string">
<xsd:enumeration value="Molar enthalpy of reaction, kJ/mol"/>
<xsd:enumeration value="Enthalpy of process, kJ"/>
            <xsd:enumeration value="Specific internal energy of reaction at constant volume, J/g"/>
            <xsd:enumeration value="Molar internal energy of reaction at constant volume, kJ/mol"/>
            <xsd:enumeration value="Molar Gibbs energy of reaction, kJ/mol"/>
            <xsd:enumeration value="Molar entropy of reaction, J/K/mol"/>
            <xsd:enumeration value="Potential difference of an electrochemical cell, V"/>
          </xsd:restriction>
        </xsd:simpleType>
      </xsd:element>
      <xsd:choice maxOccurs="unbounded">
        <xsd:element name="eMethodName">
          <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="Solution calorimetry"/>
              <xsd:enumeration value="Potential difference of an electrochemical cell">
                <xsd:annotation>
                  <xsd:documentation>e.m.f. measurement</xsd:documentation>
                </xsd:annotation>
              </xsd:enumeration>
              <xsd:enumeration value="Anion exchange"/>
              <xsd:enumeration value="Cation exchange"/>
              <xsd:enumeration value="Cell potential with glass electrode"/>
              <xsd:enumeration value="Cell potential with platinum electrode"/>
              <xsd:enumeration value="Cell potential with quinhydrone electrode"/>
              <xsd:enumeration value="Cell potential with redox electrode"/>
              <xsd:enumeration value="Colorimetry"/>
              <xsd:enumeration value="Conductivity measurement"/>
```

```
                <xsd:enumeration value="Coulometry"/>
                <xsd:enumeration value="Cryoscopy"/>
                <xsd:enumeration value="Distribution between two phases"/>
                <xsd:enumeration value="Ion selective electrode"/>
                <xsd:enumeration value="Molar volume determination"/>
                <xsd:enumeration value="Polarography"/>
                <xsd:enumeration value="Potentiometry"/>
                <xsd:enumeration value="Proton relaxation"/>
                <xsd:enumeration value="Rate of reaction"/>
                <xsd:enumeration value="Solubility measurement"/>
                <xsd:enumeration value="Spectrophotometry"/>
                <xsd:enumeration value="Thermal lensing spectrophotometry"/>
                <xsd:enumeration value="Transient conductivity measurement"/>
                <xsd:enumeration value="Solvent extraction"/>
                <xsd:enumeration value="Voltammetry"/>
                <xsd:enumeration value="Other"/>
              </xsd:restriction>
            </xsd:simpleType>
          </xsd:element>
          <xsd:element name="sMethodName" type="xsd:string" maxOccurs="unbounded"/>
          <xsd:element ref="tml:CriticalEvaluation"/>
          <xsd:element ref="tml:Prediction"/>
        </xsd:choice>
      </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="Equilibrium constant in terms of molality, (mol/kg)^n"/>
              <xsd:enumeration value="Equilibrium constant in terms of amount concentration (molarity), (mol/dm3)^n"/>
              <xsd:enumeration value="Equilibrium constant in terms of partial pressure, kPa^n"/>
              <xsd:enumeration value="Equilibrium constant in terms of mole fraction"/>
              <xsd:enumeration value="Natural logarithm of thermodynamic equilibrium constant"/>
```

```
                <xsd:enumeration value="Natural logarithm of equilibrium constant in terms of molality, (mol/kg)^n"/>
                <xsd:enumeration value="Natural logarithm of equilibrium constant in terms of amount concentration (molarity),
(mol/dm3)^n"/>
                <xsd:enumeration value="Natural logarithm of equilibrium constant in terms of partial pressure, kPa^n"/>
                <xsd:enumeration value="Natural logarithm of equilibrium constant in terms of mole fraction"/>
                <xsd:enumeration value="Decadic logarithm of thermodynamic equilibrium constant"/>
                <xsd:enumeration value="Decadic logarithm of equilibrium constant in terms of molality, (mol/kg)^n"/>
                <xsd:enumeration value="Decadic logarithm of equilibrium constant in terms of amount concentration (molarity),
(mol/dm3)^n"/>
                <xsd:enumeration value="Decadic logarithm of equilibrium constant in terms of partial pressure, kPa^n"/>
                <xsd:enumeration value="Decadic logarithm of equilibrium constant in terms of mole fraction"/>
              </xsd:restriction>
            </xsd:simpleType>
          </xsd:element>
          <xsd:choice>
            <xsd:element name="eMethodName">
              <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="Potential difference of an electrochemical cell">
                    <xsd:annotation>
                      <xsd:documentation>e.m.f. measurement</xsd:documentation>
                    </xsd:annotation>
                  </xsd:enumeration>
                  <xsd:enumeration value="Anion exchange"/>
                  <xsd:enumeration value="Cation exchange"/>
                  <xsd:enumeration value="Cell potential with glass electrode"/>
                  <xsd:enumeration value="Cell potential with platinum electrode"/>
                  <xsd:enumeration value="Cell potential with quinhydrone electrode"/>
                  <xsd:enumeration value="Cell potential with redox electrode"/>
                  <xsd:enumeration value="Colorimetry"/>
                  <xsd:enumeration value="Conductivity measurement"/>
```

```
                                <xsd:enumeration value="Coulometry"/>
                                <xsd:enumeration value="Cryoscopy"/>
                                <xsd:enumeration value="Distribution between two phases"/>
                                <xsd:enumeration value="Ion selective electrode"/>
                                <xsd:enumeration value="Molar volume determination"/>
                                <xsd:enumeration value="Polarography"/>
                                <xsd:enumeration value="Potentiometry"/>
                                <xsd:enumeration value="Proton relaxation"/>
                                <xsd:enumeration value="Rate of reaction"/>
                                <xsd:enumeration value="Solubility measurement"/>
                                <xsd:enumeration value="Spectrophotometry"/>
                                <xsd:enumeration value="Thermal lensing spectrophotometry"/>
                                <xsd:enumeration value="Transient conductivity measurement"/>
                                <xsd:enumeration value="Solvent extraction"/>
                                <xsd:enumeration value="Voltammetry"/>
                                <xsd:enumeration value="Other"/>
                              </xsd:restriction>
                            </xsd:simpleType>
                          </xsd:element>
                          <xsd:element name="sMethodName" type="xsd:string" maxOccurs="unbounded"/>
                          <xsd:element ref="tml:CriticalEvaluation"/>
                          <xsd:element ref="tml:Prediction"/>
                        </xsd:choice>
                      </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:choice maxOccurs="unbounded">
              <xsd:element name="nCompIndex" type="xsd:integer"/>
              <xsd:element ref="tml:RegNum"/>
```

```
        </xsd:choice>
        <xsd:element name="ePhase" type="tml:ePhaseName"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="Catalyst" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:choice maxOccurs="unbounded">
          <xsd:element name="nCompIndex" type="xsd:integer"/>
          <xsd:element ref="tml:RegNum"/>
        </xsd:choice>
        <xsd:element name="ePhase" type="tml: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="Pure liquid solute"/>
        <xsd:enumeration value="Standard molality (1 mol/kg) solute"/>
        <xsd:enumeration value="Standard amount concentration (1 mol/dm3) solute">
          <xsd:annotation>
            <xsd:documentation>Molarity</xsd:documentation>
          </xsd:annotation>
        </xsd:enumeration>
        <xsd:enumeration value="Infinite dilution solute"/>
      </xsd:restriction>
    </xsd:simpleType>
  </xsd:element>
  <xsd:sequence minOccurs="0">
    <xsd:element name="nTemperature-K" type="xsd:float">
    </xsd:element>
    <xsd:element name="nTemperatureDigits" type="xsd:integer"/>
  </xsd:sequence>
  <xsd:sequence minOccurs="0">
    <xsd:element name="nPressure-kPa" type="xsd:float">
```

```
            </xsd:element>
            <xsd:element name="nPressureDigits" type="xsd:integer"/>
          </xsd:sequence>
          <xsd:element ref="tml:CombinedUncertainty" minOccurs="0" maxOccurs="unbounded"/>
          <xsd:element name="PropUncertainty" type="tml:PropVarUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
          <xsd:element name="PropRepeatability" type="tml:PropVarRepeatabilityType" minOccurs="0"/>
          <xsd:element name="PropDeviceSpec" type="tml:PropVarDeviceSpecType" minOccurs="0"/>
          <xsd:element ref="tml:CurveDev" minOccurs="0" maxOccurs="unbounded"/>
        </xsd:sequence>
      </xsd:complexType>
    </xsd:element>
    <xsd:element name="Constraint" minOccurs="0" maxOccurs="unbounded">
      <xsd:complexType>
        <xsd:sequence>
          <xsd:element name="nConstraintNumber" type="xsd:integer" minOccurs="0"/>
          <xsd:element name="ConstraintID">
            <xsd:complexType>
              <xsd:sequence>
                <xsd:element name="ConstraintType" type="tml:ConstraintVariableType"/>
                <xsd:choice minOccurs="0">
                  <xsd:element name="nCompIndex" type="xsd:integer"/>
                  <xsd:element ref="tml:RegNum"/>
                </xsd:choice>
              </xsd:sequence>
            </xsd:complexType>
          </xsd:element>
          <xsd:element name="nConstraintValue" type="xsd:float"/>
          <xsd:element name="nConstrDigits" type="xsd:integer"/>
          <xsd:element name="ConstrUncertainty" type="tml:ConstrUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
          <xsd:element name="ConstrRepeatability" type="tml:ConstrRepeatabilityType" minOccurs="0"/>
          <xsd:element name="ConstrDeviceSpec" type="tml:ConstrDeviceSpecType" minOccurs="0"/>
        </xsd:sequence>
      </xsd:complexType>
    </xsd:element>
    <xsd:element name="Variable" minOccurs="0" maxOccurs="unbounded">
      <xsd:complexType>
        <xsd:sequence>
          <xsd:element name="nVarNumber" type="xsd:integer"/>
```

```
            <xsd:element name="VariableID">
              <xsd:complexType>
                <xsd:sequence>
                  <xsd:element name="VariableType" type="tml:ConstraintVariableType"/>
                  <xsd:choice minOccurs="0">
                    <xsd:element name="nCompIndex" type="xsd:integer"/>
                    <xsd:element ref="tml:RegNum"/>
                  </xsd:choice>
                </xsd:sequence>
              </xsd:complexType>
            </xsd:element>
            <xsd:element name="VarPhaseID" minOccurs="0">
              <xsd:complexType>
                <xsd:sequence>
                  <xsd:element name="eVarPhase" type="tml:ePhaseName"/>
                  <xsd:choice minOccurs="0">
                    <xsd:element name="eCrystalLatticeType" type="tml:eCrystalLatticeTypeSelection"/>
                    <xsd:element name="sPhaseDescription" type="xsd:string"/>
                  </xsd:choice>
                  <xsd:choice minOccurs="0">
                    <xsd:element name="nCompIndex" type="xsd:integer"/>
                    <xsd:element ref="tml:RegNum"/>
                  </xsd:choice>
                </xsd:sequence>
              </xsd:complexType>
            </xsd:element>
      <xsd:element ref="tml:Solvent" minOccurs="0"/>
      <xsd:element name="VarUncertainty" type="tml:PropVarUncertaintyType" minOccurs="0" maxOccurs="unbounded"/>
            <xsd:element name="VarRepeatability" type="tml:PropVarRepeatabilityType" minOccurs="0"/>
            <xsd:element name="VarDeviceSpec" type="tml:PropVarDeviceSpecType" minOccurs="0"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <xsd:element ref="tml:NumValues" minOccurs="0" maxOccurs="unbounded"/>
      <xsd:element ref="tml:Equation" minOccurs="0" maxOccurs="unbounded"/>
    </xsd:sequence>
  </xsd:complexType>
</xsd:element>
```

```
<!--

      -->
<xsd:simpleType name="eSampleStatus">
   <xsd:annotation>
      <xsd:documentation>The sample status</xsd:documentation>
   </xsd:annotation>
   <xsd:restriction base="xsd:string">
      <xsd:enumeration value="unknown"/>
      <xsd:enumeration value="notDescribed"/>
      <xsd:enumeration value="previousPaper"/>
      <xsd:enumeration value="noSample"/>
   </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 boiling or ultrasonically"/>
      <xsd:enumeration value="De-gassed by evacuation"/>
      <xsd:enumeration value="De-gassed by freezing and melting in vacuum"/>
      <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 temperatures"/>
```

```
        <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="NMR (proton)"/>
        <xsd:enumeration value="NMR (other)"/>
        <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="Other types of titration"/>
        <xsd:enumeration value="Mass loss on drying"/>
        <xsd:enumeration value="Karl Fischer titration"/>
        <xsd:enumeration value="HPLC"/>
        <xsd:enumeration value="Ion chromatography"/>
        <xsd:enumeration value="Ion-selective electrode"/>
        <xsd:enumeration value="CO2 yield in combustion products"/>
        <xsd:enumeration value="Other"/>
        <xsd:enumeration value="Estimated by the compiler"/>
        <xsd:enumeration value="Stated by supplier"/>
    </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 5"/>
    <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="Smectic liquid crystal 1"/>
    <xsd:enumeration value="Smectic liquid crystal 2"/>
    <xsd:enumeration value="Nematic liquid crystal"/>
    <xsd:enumeration value="Nematic liquid crystal 1"/>
    <xsd:enumeration value="Nematic liquid crystal 2"/>
    <xsd:enumeration value="Cholesteric liquid crystal"/>
    <xsd:enumeration value="Liquid crystal of unknown type"/>
    <xsd:enumeration value="Liquid"/>
    <xsd:enumeration value="Liquid mixture 1"/>
    <xsd:enumeration value="Liquid mixture 2"/>
    <xsd:enumeration value="Liquid mixture 3"/>
    <xsd:enumeration value="Solution"/>
    <xsd:enumeration value="Solution 1"/>
    <xsd:enumeration value="Solution 2"/>
    <xsd:enumeration value="Solution 3"/>
    <xsd:enumeration value="Solution 4"/>
    <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="eCrystalLatticeTypeSelection">
    <xsd:annotation>
        <xsd:documentation>Crystal Lattice Type</xsd:documentation>
    </xsd:annotation>
    <xsd:restriction base="xsd:string">
        <xsd:enumeration value="Cubic"/>
        <xsd:enumeration value="Tetragonal"/>
        <xsd:enumeration value="Hexagonal"/>
        <xsd:enumeration value="Rhombohedral"/>
        <xsd:enumeration value="Orthorhombic"/>
        <xsd:enumeration value="Monoclinic"/>
        <xsd:enumeration value="Triclinic"/>
    </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="Ideal gas at the same amount density, temperature, and composition"/>
    <xsd:enumeration value="Ideal mixture of pure fluid components at the same amount density, temperature, and composition"/>
    <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 fixed 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:choice maxOccurs="unbounded">
            <xsd:element name="nCompIndex" type="xsd:integer"/>
            <xsd:element ref="tml:RegNum"/>
          </xsd:choice>
        </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="Amount concentration (molarity), mol/dm3"/>
            <xsd:enumeration value="Volume fraction"/>
            <xsd:enumeration value="Ratio of amount of solute to mass of solution, mol/kg"/>
            <xsd:enumeration value="Ratio of mass of solute to volume of solution, kg/m3"/>
            <xsd:enumeration value="Amount ratio of solute to solvent"/>
            <xsd:enumeration value="Mass ratio of solute to solvent"/>
            <xsd:enumeration value="Volume ratio of solute to solvent"/>
            <xsd:enumeration value="Initial mole fraction of solute"/>
            <xsd:enumeration value="Final mole fraction of solute"/>
            <xsd:enumeration value="Initial mass fraction of solute"/>
            <xsd:enumeration value="Final mass fraction of solute"/>
            <xsd:enumeration value="Initial molality of solute, mol/kg"/>
            <xsd:enumeration value="Final molality of solute, mol/kg"/>
        </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: Amount concentration (molarity), mol/dm3"/>
            <xsd:enumeration value="Solvent: Amount ratio of component to other component of binary solvent"/>
            <xsd:enumeration value="Solvent: Mass ratio of component to other component of binary solvent"/>
            <xsd:enumeration value="Solvent: Volume ratio of component to other component of binary solvent"/>
            <xsd:enumeration value="Solvent: Ratio of amount of component to mass of solvent, mol/kg"/>
            <xsd:enumeration value="Solvent: Ratio of component mass to volume of solvent, kg/m3"/>
        </xsd:restriction>
    </xsd:simpleType>
</xsd:element>
<xsd:element name="eMiscellaneous">
    <xsd:simpleType>
        <xsd:restriction base="xsd:string">
            <xsd:enumeration value="Wavelength, nm"/>
            <xsd:enumeration value="Frequency, MHz"/>
            <xsd:enumeration value="Molar volume, m3/mol"/>
```

```
            <xsd:enumeration value="Specific volume, m3/kg"/>
            <xsd:enumeration value="Mass density, kg/m3"/>
            <xsd:enumeration value="Amount density, mol/m3">
              <xsd:annotation>
                <xsd:documentation>Molar density</xsd:documentation>
              </xsd:annotation>
            </xsd:enumeration>
            <xsd:enumeration value="Molar entropy, J/K/mol"/>
            <xsd:enumeration value="(Relative) activity"/>
            <xsd:enumeration value="Activity coefficient"/>
          </xsd:restriction>
        </xsd:simpleType>
      </xsd:element>
      <xsd:element name="eBioVariables">
        <xsd:simpleType>
          <xsd:restriction base="xsd:string">
            <xsd:enumeration value="pH"/>
            <xsd:enumeration value="Ionic strength (molality basis), mol/kg"/>
            <xsd:enumeration value="Ionic strength (amount concentration basis), mol/dm3"/>
            <xsd:enumeration value="pC (amount concentration basis)"/>
            <xsd:enumeration value="Solvent: pC (amount concentration basis)"/>
          </xsd:restriction>
        </xsd:simpleType>
      </xsd:element>
  <xsd:element name="eParticipantAmount">
    <xsd:simpleType>
      <xsd:restriction base="xsd:string">
        <xsd:enumeration value="Amount, mol"/>
        <xsd:enumeration value="Mass, kg"/>
      </xsd:restriction>
    </xsd:simpleType>
  </xsd:element>
</xsd:choice>
</xsd:complexType>
<!--

-->
<xsd:complexType name="ConstrDeviceSpecType">
```

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

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

  -->
```

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

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

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

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

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

```
<!--

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

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

-->
<xsd:element name="NumValues">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="VariableValue" minOccurs="0" maxOccurs="unbounded">
```

```
    <xsd:complexType>
      <xsd:sequence>
        <xsd:element name="nVarNumber" type="xsd:integer"/>
        <xsd:element name="nVarValue" type="xsd:float"/>
        <xsd:element name="nVarDigits" type="xsd:integer"/>
        <xsd:element name="VarUncertainty" minOccurs="0" maxOccurs="unbounded">
          <xsd:complexType>
            <xsd:sequence>
              <xsd:element name="nUncertAssessNum" type="xsd:integer"/>
              <xsd:element name="nStdUncertValue" type="xsd:float" minOccurs="0"/>
              <xsd:element name="nExpandUncertValue" type="xsd:float" minOccurs="0"/>
            </xsd:sequence>
          </xsd:complexType>
        </xsd:element>
        <xsd:element name="VarRepeatability" minOccurs="0">
          <xsd:complexType>
            <xsd:sequence>
              <xsd:element name="nVarRepeatValue" type="xsd:float"/>
              <xsd:element name="nRepetitions" type="xsd:integer"/>
            </xsd:sequence>
          </xsd:complexType>
        </xsd:element>
        <xsd:element name="nVarDeviceSpecValue" type="xsd:float" minOccurs="0"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="PropertyValue" maxOccurs="unbounded">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:element name="nPropNumber" type="xsd:integer"/>
        <xsd:choice>
          <xsd:sequence>
            <xsd:element name="nPropValue" type="xsd:float"/>
            <xsd:element name="nPropDigits" type="xsd:integer"/>
          </xsd:sequence>
          <xsd:element name="PropLimit">
            <xsd:complexType>
              <xsd:sequence>
```

```
            <xsd:choice>
              <xsd:element name="nPropUpperLimitValue" type="xsd:float"/>
              <xsd:element name="nPropLowerLimitValue" type="xsd:float"/>
            </xsd:choice>
            <xsd:element name="nPropLimitDigits" type="xsd:integer"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
    </xsd:choice>
    <xsd:element name="CombinedUncertainty" minOccurs="0" maxOccurs="unbounded">
      <xsd:complexType>
        <xsd:sequence>
          <xsd:element name="nCombUncertAssessNum" type="xsd:integer"/>
          <xsd:choice>
            <xsd:sequence>
              <xsd:element name="nCombStdUncertValue" type="xsd:float" minOccurs="0"/>
              <xsd:element name="nCombExpandUncertValue" type="xsd:float" minOccurs="0"/>
            </xsd:sequence>
            <xsd:sequence>
              <xsd:element name="AsymCombStdUncert" type="tml:AsymUncertType" minOccurs="0"/>
              <xsd:element name="AsymCombExpandUncert" type="tml:AsymUncertType" minOccurs="0"/>
            </xsd:sequence>
          </xsd:choice>
        </xsd:sequence>
      </xsd:complexType>
    </xsd:element>
    <xsd:element name="PropUncertainty" minOccurs="0" maxOccurs="unbounded">
      <xsd:complexType>
        <xsd:sequence>
          <xsd:element name="nUncertAssessNum" type="xsd:integer"/>
          <xsd:choice>
            <xsd:sequence>
              <xsd:element name="nStdUncertValue" type="xsd:float" minOccurs="0"/>
              <xsd:element name="nExpandUncertValue" type="xsd:float" minOccurs="0"/>
            </xsd:sequence>
            <xsd:sequence>
              <xsd:element name="AsymStdUncert" type="tml:AsymUncertType" minOccurs="0"/>
              <xsd:element name="AsymExpandUncert" type="tml:AsymUncertType" minOccurs="0"/>
```

```
                    </xsd:sequence>
                  </xsd:choice>
                </xsd:sequence>
              </xsd:complexType>
            </xsd:element>
            <xsd:element name="PropRepeatability" minOccurs="0">
              <xsd:complexType>
                <xsd:sequence>
                  <xsd:element name="nPropRepeatValue" type="xsd:float"/>
                  <xsd:element name="nRepetitions" type="xsd:integer"/>
                </xsd:sequence>
              </xsd:complexType>
            </xsd:element>
            <xsd:element name="nPropDeviceSpecValue" type="xsd:float" minOccurs="0"/>
            <xsd:element name="CurveDev" minOccurs="0" maxOccurs="unbounded">
              <xsd:complexType>
                <xsd:sequence>
                  <xsd:element name="nCurveDevAssessNum" type="xsd:integer"/>
                  <xsd:element name="nCurveDevValue" type="xsd:float"/>
                </xsd:sequence>
              </xsd:complexType>
            </xsd:element>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
    </xsd:sequence>
  </xsd:complexType>
</xsd:element>
<!--

-->
<xsd:element name="CriticalEvaluation">
  <xsd:complexType>
    <xsd:choice>
      <xsd:element name="SingleProp">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="sEvalSinglePropDescription" type="xsd:string" minOccurs="0"/>
```

```
                <xsd:element name="EvalSinglePropRef" type="tml:CitationType" minOccurs="0" maxOccurs="unbounded"/>
              </xsd:sequence>
            </xsd:complexType>
          </xsd:element>
          <xsd:element name="MultiProp">
            <xsd:complexType>
              <xsd:sequence>
                <xsd:element name="sEvalMultiPropList" type="xsd:string" minOccurs="0"/>
                <xsd:element name="sEvalMultiPropDescription" type="xsd:string" minOccurs="0"/>
                <xsd:element name="EvalMultiPropRef" type="tml:CitationType" minOccurs="0" maxOccurs="unbounded"/>
              </xsd:sequence>
            </xsd:complexType>
          </xsd:element>
          <xsd:element name="EquationOfState">
            <xsd:complexType>
              <xsd:sequence>
                <xsd:element name="sEvalEOSName" type="xsd:string" minOccurs="0"/>
                <xsd:element name="sEvalEOSDescription" type="xsd:string" minOccurs="0"/>
                <xsd:element name="EvalEOSRef" type="tml:CitationType" minOccurs="0" maxOccurs="unbounded"/>
              </xsd:sequence>
            </xsd:complexType>
          </xsd:element>
        </xsd:choice>
      </xsd:complexType>
    </xsd:element>
    <!--

    -->
    <xsd:element name="Prediction">
      <xsd:complexType>
        <xsd:sequence>
          <xsd:element name="ePredictionType">
            <xsd:simpleType>
              <xsd:restriction base="xsd:string">
                <xsd:enumeration value="Ab initio"/>
                <xsd:enumeration value="Molecular dynamics"/>
                <xsd:enumeration value="Semiempirical quantum methods"/>
                <xsd:enumeration value="Molecular mechanics"/>
```

```
                <xsd:enumeration value="Statistical mechanics"/>
                <xsd:enumeration value="Corresponding states"/>
                <xsd:enumeration value="Correlation"/>
                <xsd:enumeration value="Group contribution"/>
              </xsd:restriction>
            </xsd:simpleType>
          </xsd:element>
          <xsd:element name="sPredictionMethodName" type="xsd:string" minOccurs="0"/>
          <xsd:element name="sPredictionMethodDescription" type="xsd:string" minOccurs="0"/>
          <xsd:element name="PredictionMethodRef" type="tml:CitationType" minOccurs="0" maxOccurs="unbounded"/>
        </xsd:sequence>
      </xsd:complexType>
    </xsd:element>
    <!--

    -->
    <xsd:element name="Equation">
      <xsd:complexType>
        <xsd:sequence>
          <xsd:sequence maxOccurs="unbounded">
            <xsd:choice>
              <xsd:element name="eEqName">
                <xsd:simpleType>
                  <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="ThermoML.Antoine.VaporPressure"/>
                    <xsd:enumeration value="ThermoML.CustomExpansion"/>
                    <xsd:enumeration value="ThermoML.Helmholtz3General.EOS"/>
                    <xsd:enumeration value="ThermoML.Helmholtz4General.EOS"/>
                    <xsd:enumeration value="ThermoML.WagnerLinear.VaporPressure"/>
                    <xsd:enumeration value="ThermoML.Wagner25Linear.VaporPressure"/>
                    <xsd:enumeration value="ThermoML.Wagner36Linear.VaporPressure"/>
                    <xsd:enumeration value="ThermoML.PolynomialExpansion"/>
                    <xsd:enumeration value="ThermoML.SpanWagner12Nonpolar.EOS"/>
                    <xsd:enumeration value="ThermoML.SpanWagner12Polar.EOS"/>
                  </xsd:restriction>
                </xsd:simpleType>
              </xsd:element>
              <xsd:element name="sEqName" type="xsd:string"/>
```

```
    </xsd:choice>
    <xsd:element name="urlMathSource" type="xsd:string"/>
  </xsd:sequence>
  <xsd:element name="EqProperty" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:choice minOccurs="0">
          <xsd:element name="nPureOrMixtureDataNumber" type="xsd:integer"/>
          <xsd:element name="nReactionDataNumber" type="xsd:integer"/>
        </xsd:choice>
        <xsd:element name="nPropNumber" type="xsd:integer"/>
        <xsd:element name="sEqSymbol" type="xsd:string"/>
        <xsd:element name="nEqPropIndex" type="xsd:integer" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="sOtherPropUnit" type="xsd:string" minOccurs="0"/>
        <xsd:element name="nEqPropRangeMin" type="xsd:float" minOccurs="0"/>
        <xsd:element name="nEqPropRangeMax" type="xsd:float" minOccurs="0"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="EqConstraint" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:choice minOccurs="0">
          <xsd:element name="nPureOrMixtureDataNumber" type="xsd:integer"/>
          <xsd:element name="nReactionDataNumber" type="xsd:integer"/>
        </xsd:choice>
        <xsd:element name="nConstraintNumber" type="xsd:integer"/>
        <xsd:element name="sEqSymbol" type="xsd:string"/>
        <xsd:element name="nEqConstraintIndex" type="xsd:integer" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="sOtherConstraintUnit" type="xsd:string" minOccurs="0"/>
        <xsd:element name="nEqConstraintRangeMin" type="xsd:float" minOccurs="0"/>
        <xsd:element name="nEqConstraintRangeMax" type="xsd:float" minOccurs="0"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="EqVariable" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
      <xsd:sequence>
```

```
        <xsd:choice minOccurs="0">
          <xsd:element name="nPureOrMixtureDataNumber" type="xsd:integer"/>
          <xsd:element name="nReactionDataNumber" type="xsd:integer"/>
        </xsd:choice>
        <xsd:element name="nVarNumber" type="xsd:integer"/>
        <xsd:element name="sEqSymbol" type="xsd:string"/>
        <xsd:element name="nEqVarIndex" type="xsd:integer" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="sOtherVarUnit" type="xsd:string" minOccurs="0"/>
        <xsd:element name="nEqVarRangeMin" type="xsd:float" minOccurs="0"/>
        <xsd:element name="nEqVarRangeMax" type="xsd:float" minOccurs="0"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="EqParameter" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:element name="nEqParNumber" type="xsd:integer" minOccurs="0"/>
        <xsd:sequence maxOccurs="unbounded">
          <xsd:element name="sEqParSymbol" type="xsd:string"/>
          <xsd:element name="nEqParIndex" type="xsd:integer" minOccurs="0" maxOccurs="unbounded"/>
        </xsd:sequence>
        <xsd:element name="nEqParValue" type="xsd:float"/>
        <xsd:element name="nEqParDigits" type="xsd:integer"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="EqConstant" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:element name="sEqConstantSymbol" type="xsd:string"/>
        <xsd:element name="nEqConstantIndex" type="xsd:integer" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="nEqConstantValue" type="xsd:float"/>
        <xsd:element name="nEqConstantDigits" type="xsd:integer"/>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="Covariance" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
```

```
                <xsd:sequence>
                  <xsd:element name="nEqParNumber1" type="xsd:integer"/>
                  <xsd:element name="nEqParNumber2" type="xsd:integer"/>
                  <xsd:element name="nCovarianceValue" type="xsd:double"/>
                </xsd:sequence>
              </xsd:complexType>
            </xsd:element>
            <xsd:element name="nCovarianceLevOfConfid" type="xsd:float" minOccurs="0"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <!--

      -->
      <xsd:simpleType name="MulticomponentType">
        <xsd:restriction base="xsd:string">
       <xsd:enumeration value="alloy"/>
       <xsd:enumeration value="clathrate"/>
            <xsd:enumeration value="complex"/>
       <xsd:enumeration value="crystal"/>
       <xsd:enumeration value="solution"/>
        </xsd:restriction>
      </xsd:simpleType>
      <!--

      -->
      <xsd:simpleType name="MulticomponentComposition">
        <xsd:restriction base="xsd:string">
            <xsd:enumeration value="number of molecules"/>
            <xsd:enumeration value="mole fraction"/>
            <xsd:enumeration value="mass fraction"/>
        </xsd:restriction>
      </xsd:simpleType>
    </xsd:schema>
```

********** Use Case 01 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<!-- edited with XML Spy v4.4 U (http://www.xmlspy.com) by Robert D. Chirico (U. S. Department of Commerce) -->
<!--Created by Guided Data Capture (GDC) Software (http://www.trc.nist.gov)-->
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>2</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>2001</yrYrPub>
      <sAuthor1>hin</sAuthor1>
      <sAuthor2>sch</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Hinz, H.-J.[Hans-Jurgen]</sAuthor>
    <sAuthor>Schwarz, F. P.[Frederick P.]</sAuthor>
    <sPubName>J. Chem. Thermodyn.</sPubName>
    <yrPubYr>2001</yrPubYr>
    <sTitle>Measurement and analysis of results obtained on  biological substances with d.s.c.</sTitle>
    <sKeyword>differential scanning calorimetry</sKeyword>
    <sKeyword>lipids</sKeyword>
    <sKeyword>phase transition</sKeyword>
    <sKeyword>proteins</sKeyword>
    <sKeyword>transition  enthalpy</sKeyword>
    <sKeyword>transition temperature</sKeyword>
    <sKeyword>unfolding transitions</sKeyword>
    <sVol>33</sVol>
    <sPage>1511-1525</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
```

```
    <sCommonName>lysozyme</sCommonName>
    <sFormulaMolec>{LZ}</sFormulaMolec>
    <biomaterial>
      <sECNumber>3.2.1.17</sECNumber>
    </biomaterial>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
      <purity>
        <nStep>1</nStep>
        <nPurityMass>95</nPurityMass>
        <nPurityMassDigits>2</nPurityMassDigits>
        <eAnalMeth>Stated by supplier</eAnalMeth>
      </purity>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <sCommonName>glycine</sCommonName>
    <sFormulaMolec>C2H5NO2</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <sCommonName>hydrogen chloride</sCommonName>
    <sFormulaMolec>ClH</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>4</nOrgNum>
    </RegNum>
    <sCommonName>water</sCommonName>
    <sFormulaMolec>H2O</sFormulaMolec>
  </Compound>
  <PureOrMixtureData>
```

```
<Component>
  <RegNum>
    <nOrgNum>1</nOrgNum>
  </RegNum>
</Component>
<AuxiliarySubstance>
  <eFunction>Buffer</eFunction>
  <RegNum>
    <nOrgNum>2</nOrgNum>
  </RegNum>
</AuxiliarySubstance>
<AuxiliarySubstance>
  <eFunction>Buffer</eFunction>
  <RegNum>
    <nOrgNum>3</nOrgNum>
  </RegNum>
</AuxiliarySubstance>
<AuxiliarySubstance>
  <eFunction>Solvent</eFunction>
  <RegNum>
    <nOrgNum>4</nOrgNum>
  </RegNum>
</AuxiliarySubstance>
<Property>
  <nPropNumber>1</nPropNumber>
  <Property-MethodID>
    <PropertyGroup>
      <BioProperties>
        <ePropName>Zero-Gibbs energy temperature, K</ePropName>
        <sMethodName>DSC</sMethodName>
      </BioProperties>
    </PropertyGroup>
  </Property-MethodID>
  <PropPhaseID>
    <ePropPhase>Solution</ePropPhase>
    <eBioState>Native</eBioState>
  </PropPhaseID>
  <PropPhaseID>
```

```
        <ePropPhase>Solution</ePropPhase>
        <eBioState>Denaturated</eBioState>
      </PropPhaseID>
      <ePresentation>Direct value, X</ePresentation>
    </Property>
    <Property>
      <nPropNumber>2</nPropNumber>
      <Property-MethodID>
        <PropertyGroup>
          <PhaseTransition>
            <ePropName>Molar entropy of transition or fusion, J/K/mol</ePropName>
            <sMethodName>DSC</sMethodName>
          </PhaseTransition>
        </PropertyGroup>
      </Property-MethodID>
      <PropPhaseID>
        <ePropPhase>Solution</ePropPhase>
        <eBioState>Native</eBioState>
      </PropPhaseID>
      <PropPhaseID>
        <ePropPhase>Solution</ePropPhase>
        <eBioState>Denaturated</eBioState>
      </PropPhaseID>
      <ePresentation>Direct value, X</ePresentation>
    </Property>
    <Property>
      <nPropNumber>3</nPropNumber>
      <Property-MethodID>
        <PropertyGroup>
          <BioProperties>
            <ePropName>van't Hoff enthalpy of transition, kJ/mol</ePropName>
            <sMethodName>DSC</sMethodName>
          </BioProperties>
        </PropertyGroup>
      </Property-MethodID>
      <PropPhaseID>
        <ePropPhase>Solution</ePropPhase>
        <eBioState>Native</eBioState>
```

```
    </PropPhaseID>
    <PropPhaseID>
      <ePropPhase>Solution</ePropPhase>
      <eBioState>Denaturated</eBioState>
    </PropPhaseID>
    <ePresentation>Direct value, X</ePresentation>
  </Property>
  <PhaseID>
    <ePhase>Solution</ePhase>
  </PhaseID>
  <Constraint>
    <ConstraintID>
      <ConstraintType>
        <ePressure>Pressure, kPa</ePressure>
      </ConstraintType>
    </ConstraintID>
    <nConstraintValue>101.325</nConstraintValue>
    <nConstrDigits>6</nConstrDigits>
  </Constraint>
  <Constraint>
    <ConstraintID>
      <ConstraintType>
        <eComponentComposition>Amount concentration (molarity), mol/dm3</eComponentComposition>
      </ConstraintType>
      <RegNum>
        <nOrgNum>2</nOrgNum>
      </RegNum>
    </ConstraintID>
    <nConstraintValue>0.1</nConstraintValue>
    <nConstrDigits>1</nConstrDigits>
  </Constraint>
  <Constraint>
    <ConstraintID>
      <ConstraintType>
        <eComponentComposition>Amount concentration (molarity), mol/dm3</eComponentComposition>
      </ConstraintType>
      <RegNum>
        <nOrgNum>3</nOrgNum>
```

```
        </RegNum>
      </ConstraintID>
      <nConstraintValue>0.1</nConstraintValue>
      <nConstrDigits>1</nConstrDigits>
    </Constraint>
    <Variable>
      <nVarNumber>1</nVarNumber>
      <VariableID>
        <VariableType>
          <eBioVariables>pH</eBioVariables>
        </VariableType>
      </VariableID>
    </Variable>
    <Variable>
      <nVarNumber>2</nVarNumber>
      <VariableID>
        <VariableType>
          <eComponentComposition>Ratio of mass of solute to volume of solution, kg/m3</eComponentComposition>
        </VariableType>
        <RegNum>
          <nOrgNum>1</nOrgNum>
        </RegNum>
      </VariableID>
    </Variable>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>4.81</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>331.4</nPropValue>
```

```
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>393</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>392</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>4.81</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>331.5</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>378</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>391</nPropValue>
        <nPropDigits>3</nPropDigits>
```

```
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>4.81</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.7</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>397</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>406</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>0.97</nVarValue>
```

```
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.6</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>403</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>403</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>0.97</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.6</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>403</nPropValue>
      <nPropDigits>3</nPropDigits>
```

```
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>403</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>0.98</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>331.5</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>406</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>406</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
```

```
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>0.95</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>331.5</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>401</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>402</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>2.28</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>331.5</nPropValue>
        <nPropDigits>4</nPropDigits>
```

```
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>397</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>401</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.28</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.5</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>401</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>402</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
```

```
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>2.3</nVarValue>
    <nVarDigits>2</nVarDigits>
  </VariableValue>
  <VariableValue>
    <nVarNumber>2</nVarNumber>
    <nVarValue>1.00</nVarValue>
    <nVarDigits>3</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>331.3</nPropValue>
    <nPropDigits>4</nPropDigits>
  </PropertyValue>
  <PropertyValue>
    <nPropNumber>2</nPropNumber>
    <nPropValue>401</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
  <PropertyValue>
    <nPropNumber>3</nPropNumber>
    <nPropValue>382</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>2.3</nVarValue>
    <nVarDigits>2</nVarDigits>
  </VariableValue>
  <VariableValue>
    <nVarNumber>2</nVarNumber>
    <nVarValue>2.32</nVarValue>
    <nVarDigits>3</nVarDigits>
```

```
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.6</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>427</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>373</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.3</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.36</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.9</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>434</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
```

```
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>369</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.3</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.36</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.6</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>439</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>368</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.3</nVarValue>
      <nVarDigits>2</nVarDigits>
```

```
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>4.72</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>330.3</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>436</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>363</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.3</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>4.77</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>330.5</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
```

```
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>411</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>373</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.3</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>4.77</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.6</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>401</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>377</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
```

```
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>2.3</nVarValue>
    <nVarDigits>2</nVarDigits>
  </VariableValue>
  <VariableValue>
    <nVarNumber>2</nVarNumber>
    <nVarValue>9.70</nVarValue>
    <nVarDigits>3</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>331.9</nPropValue>
    <nPropDigits>4</nPropDigits>
  </PropertyValue>
  <PropertyValue>
    <nPropNumber>2</nPropNumber>
    <nPropValue>434</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
  <PropertyValue>
    <nPropNumber>3</nPropNumber>
    <nPropValue>366</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>2.3</nVarValue>
    <nVarDigits>2</nVarDigits>
  </VariableValue>
  <VariableValue>
    <nVarNumber>2</nVarNumber>
    <nVarValue>9.70</nVarValue>
    <nVarDigits>3</nVarDigits>
  </VariableValue>
```

```
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.9</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>423</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>373</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>1.00</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.1</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>396</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
```

```
        <nPropNumber>3</nPropNumber>
        <nPropValue>396</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>1.00</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>330.8</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>418</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>418</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
```

```
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>1.00</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.1</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>401</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>403</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.41</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>330.6</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
```

```
        <nPropNumber>2</nPropNumber>
        <nPropValue>386</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>388</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>2.41</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>330.8</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>419</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>418</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
```

```
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.41</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>331.2</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>396</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>398</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>4.81</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
```

```
        <nPropNumber>1</nPropNumber>
        <nPropValue>330.9</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>386</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>388</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>4.81</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>330.8</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>418</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
```

```
        <nPropValue>418</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>10.00</nVarValue>
        <nVarDigits>4</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>331.5</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>396</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>398</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
```

```
        <nVarNumber>2</nVarNumber>
        <nVarValue>10.00</nVarValue>
        <nVarDigits>4</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>330.9</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>415</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>416</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.3</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>2.00</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>330.4</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
```

```
        <nPropValue>402</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>402</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.3</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>3.80</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>330.6</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>401</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>401</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
```

```
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.3</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>2.40</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>329.4</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>381</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>395</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.4</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>3.27</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
```

```
      <nPropValue>331.8</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>419</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>423</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.4</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.79</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>330.5</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>382</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>3</nPropNumber>
      <nPropValue>408</nPropValue>
```

```
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>2.48</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>331.3</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>377</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>3</nPropNumber>
        <nPropValue>404</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
  </PureOrMixtureData>
</DataReport>
```

********** Use Case 02 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<!-- edited with XML Spy v4.4 U (http://www.xmlspy.com) by Robert D. Chirico (U. S. Department of Commerce) -->
<!--Created by Guided Data Capture (GDC) Software (http://www.trc.nist.gov)-->
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>2</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>1998</yrYrPub>
      <sAuthor1>tew</sAuthor1>
      <sAuthor2>che</sAuthor2>
      <nAuthorn>1</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Tewari, Y. B.[Yadu B.]</sAuthor>
    <sAuthor>Chen, J.[Jiangang]</sAuthor>
    <sAuthor>Holden, M. J.[Marcia J.]</sAuthor>
    <sAuthor>Houk, K. N.[Kendall N.]</sAuthor>
    <sAuthor>Goldberg, R. N.[Robert N.]</sAuthor>
    <sPubName>J. Phys. Chem. B</sPubName>
    <yrPubYr>1998</yrPubYr>
    <sTitle>Thermodynamic and Quantum Chemical Study of the Conversion of Chorismate to  (Pyruvate + 4-Hydroxybenzoate)</sTitle>
    <sVol>102</sVol>
    <sPage>8634-8639</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <sCommonName>chorismic acid</sCommonName>
    <sFormulaMolec>C10H10O6</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
```

```
      <eSource>Commercial source</eSource>
      <purity>
        <nStep>1</nStep>
        <nPurityMol>95.1</nPurityMol>
        <nPurityMolDigits>3</nPurityMolDigits>
        <eAnalMeth>HPLC</eAnalMeth>
      </purity>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <sCommonName>chorismate lyase</sCommonName>
    <sFormulaMolec>{CL}</sFormulaMolec>
    <biomaterial>
      <sECNumber>4.1.3.B1</sECNumber>
    </biomaterial>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <sCommonName>p-hydroxybenzoic acid</sCommonName>
    <sFormulaMolec>C7H6O3</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>4</nOrgNum>
    </RegNum>
    <sCommonName>pyruvic acid</sCommonName>
    <sFormulaMolec>C3H4O3</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
    <sCommonName>phosphoric acid</sCommonName>
```

```
    <sFormulaMolec>H3O4P</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>6</nOrgNum>
    </RegNum>
    <sCommonName>phosphoric acid, dipotassium salt</sCommonName>
    <sFormulaMolec>H3K2O4P</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>7</nOrgNum>
    </RegNum>
    <sCommonName>water</sCommonName>
    <sFormulaMolec>H2O</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>8</nOrgNum>
    </RegNum>
    <sCommonName>sodium chloride</sCommonName>
    <sFormulaMolec>NaCl</sFormulaMolec>
  </Compound>
  <ReactionData>
    <Participant>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
      <nStoichiometricCoef>-1</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
      <nStoichiometricCoef>1</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
    </Participant>
```

```
<Participant>
  <RegNum>
    <nOrgNum>4</nOrgNum>
  </RegNum>
  <nStoichiometricCoef>1</nStoichiometricCoef>
  <ePhase>Solution 1</ePhase>
</Participant>
<AuxiliarySubstance>
  <eFunction>Buffer</eFunction>
  <RegNum>
    <nOrgNum>5</nOrgNum>
  </RegNum>
  <ePhase>Solution 1</ePhase>
</AuxiliarySubstance>
<AuxiliarySubstance>
  <eFunction>Buffer</eFunction>
  <RegNum>
    <nOrgNum>6</nOrgNum>
  </RegNum>
  <ePhase>Solution 1</ePhase>
</AuxiliarySubstance>
<AuxiliarySubstance>
  <eFunction>Inert</eFunction>
  <RegNum>
    <nOrgNum>8</nOrgNum>
  </RegNum>
  <ePhase>Solution 1</ePhase>
</AuxiliarySubstance>
<eReactionFormalism>biochemical</eReactionFormalism>
<eReactionType>Other reactions</eReactionType>
<Property>
  <nPropNumber>1</nPropNumber>
  <Property-MethodID>
    <PropertyGroup>
      <ReactionStateChangeProp>
        <ePropName>Molar enthalpy of reaction, kJ/mol</ePropName>
        <sMethodName>Heat-conduction</sMethodName>
      </ReactionStateChangeProp>
```

```
        </PropertyGroup>
      </Property-MethodID>
      <Solvent>
        <RegNum>
          <nOrgNum>7</nOrgNum>
        </RegNum>
        <ePhase>Solution 1</ePhase>
      </Solvent>
      <Catalyst>
        <RegNum>
          <nOrgNum>2</nOrgNum>
        </RegNum>
      </Catalyst>
    </Property>
    <Constraint>
      <ConstraintID>
        <ConstraintType>
          <ePressure>Pressure, kPa</ePressure>
        </ConstraintType>
      </ConstraintID>
      <nConstraintValue>101.3</nConstraintValue>
      <nConstrDigits>4</nConstrDigits>
    </Constraint>
    <Constraint>
      <ConstraintID>
        <ConstraintType>
          <eBioVariables>pH</eBioVariables>
        </ConstraintType>
      </ConstraintID>
      <nConstraintValue>6.98</nConstraintValue>
      <nConstrDigits>3</nConstrDigits>
    </Constraint>
    <Constraint>
      <ConstraintID>
        <ConstraintType>
          <eBioVariables>Ionic strength (molality basis), mol/kg</eBioVariables>
        </ConstraintType>
      </Constraint ID>
```

```
        <nConstraintValue>0.38</nConstraintValue>
        <nConstrDigits>2</nConstrDigits>
      </Constraint>
      <Variable>
        <nVarNumber>1</nVarNumber>
        <VariableID>
          <VariableType>
            <eTemperature>Temperature, K</eTemperature>
          </VariableType>
        </VariableID>
      </Variable>
      <NumValues>
        <VariableValue>
          <nVarNumber>1</nVarNumber>
          <nVarValue>298.15</nVarValue>
          <nVarDigits>5</nVarDigits>
        </VariableValue>
        <PropertyValue>
          <nPropNumber>1</nPropNumber>
          <nPropValue>-144.1</nPropValue>
          <nPropDigits>4</nPropDigits>
        </PropertyValue>
      </NumValues>
    </ReactionData>
</DataReport>
```

********** Use Case 03 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<!-- edited with XML Spy v4.4 U (http://www.xmlspy.com) by Robert D. Chirico (U. S. Department of Commerce) -->
<!--Created by Guided Data Capture (GDC) Software (http://www.trc.nist.gov)-->
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>2</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>2007</yrYrPub>
      <sAuthor1>tod</sAuthor1>
      <sAuthor2>sch</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Todorova, N. A.[Niya A.]</sAuthor>
    <sAuthor>Schwartz, F. P.[Fred P.]</sAuthor>
    <sPubName>J. Chem. Thermodyn.</sPubName>
    <yrPubYr>2007</yrPubYr>
    <sTitle>The role of water in the thermodynamics of drug binding to cyclodextrin</sTitle>
    <sVol>39</sVol>
    <sPage>1038-1048</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <sCommonName>.beta.-cyclodextrin</sCommonName>
    <sFormulaMolec>C42H70O35</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
      <purity>
        <nStep>1</nStep>
```

```
        <nPurityMass>98</nPurityMass>
        <nPurityMassDigits>2</nPurityMassDigits>
        <eAnalMeth>Stated by supplier</eAnalMeth>
      </purity>
      <purity>
        <nStep>2</nStep>
        <ePurifMethod>None used</ePurifMethod>
      </purity>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <sCommonName>2-butanone, 4-(6-methoxy-2-naphthalenyl)-</sCommonName>
    <sFormulaMolec>C15H16O2</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
      <purity>
        <nStep>1</nStep>
        <ePurifMethod>None used</ePurifMethod>
      </purity>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <sCommonName>sodium phosphate</sCommonName>
    <sFormulaMolec>Na3O4P</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
```

```
      <nOrgNum>4</nOrgNum>
    </RegNum>
    <sCommonName>complex, 2-butanone, 4-(6-methoxy-2-naphthalenyl)- with .beta.-cyclodextrin</sCommonName>
    <sFormulaMolec>C57H86O37</sFormulaMolec>
    <MulticomponentSubstance type="complex" compositionBasis="number of molecules">
      <Component>
        <RegNum>
          <nOrgNum>1</nOrgNum>
        </RegNum>
        <nAmount>1</nAmount>
      </Component>
      <Component>
        <RegNum>
          <nOrgNum>2</nOrgNum>
        </RegNum>
        <nAmount>1</nAmount>
      </Component>
    </MulticomponentSubstance>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <ComponentSample>
        <RegNum>
          <nOrgNum>1</nOrgNum>
        </RegNum>
        <nSampleNm>1</nSampleNm>
      </ComponentSample>
      <ComponentSample>
        <RegNum>
          <nOrgNum>2</nOrgNum>
        </RegNum>
        <nSampleNm>1</nSampleNm>
      </ComponentSample>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
```

```
    <sCommonName>phosphoric acid</sCommonName>
    <sFormulaMolec>H3O4P</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <ReactionData>
    <Participant>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
      <nStoichiometricCoef>-1</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>2</nOrgNum>
      </RegNum>
      <nStoichiometricCoef>-1</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>4</nOrgNum>
      </RegNum>
      <nStoichiometricCoef>1</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
    </Participant>
    <AuxiliarySubstance>
      <eFunction>Buffer</eFunction>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
      <ePhase>Solution 1</ePhase>
    </AuxiliarySubstance>
    <AuxiliarySubstance>
      <eFunction>Buffer</eFunction>
```

```
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
    <ePhase>Solution 1</ePhase>
  </AuxiliarySubstance>
  <eReactionFormalism>chemical</eReactionFormalism>
  <eReactionType>Other reactions</eReactionType>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <ReactionEquilibriumProp>
          <ePropName>Equilibrium constant in terms of mole fraction</ePropName>
          <sMethodName>Isothermal titration calorimetry</sMethodName>
        </ReactionEquilibriumProp>
      </PropertyGroup>
    </Property-MethodID>
  </Property>
  <Property>
    <nPropNumber>2</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <ReactionStateChangeProp>
          <ePropName>Molar Gibbs energy of reaction, kJ/mol</ePropName>
          <sMethodName>Isothermal titration calorimetry</sMethodName>
        </ReactionStateChangeProp>
      </PropertyGroup>
    </Property-MethodID>
  </Property>
  <Constraint>
    <ConstraintID>
      <ConstraintType>
        <ePressure>Pressure, kPa</ePressure>
      </ConstraintType>
    </Constraint>
    <nConstraintValue>101.3</nConstraintValue>
    <nConstrDigits>4</nConstrDigits>
  </Constraint>
```

```
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <eComponentComposition>Amount concentration (molarity), mol/dm3</eComponentComposition>
    </ConstraintType>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
  </ConstraintID>
  <nConstraintValue>0.1</nConstraintValue>
  <nConstrDigits>1</nConstrDigits>
</Constraint>
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <eComponentComposition>Amount concentration (molarity), mol/dm3</eComponentComposition>
    </ConstraintType>
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
  </ConstraintID>
  <nConstraintValue>0.1</nConstraintValue>
  <nConstrDigits>1</nConstrDigits>
</Constraint>
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <eBioVariables>pH</eBioVariables>
    </ConstraintType>
  </ConstraintID>
  <nConstraintValue>7.1</nConstraintValue>
  <nConstrDigits>2</nConstrDigits>
</Constraint>
<Variable>
  <nVarNumber>1</nVarNumber>
  <VariableID>
    <VariableType>
      <eTemperature>Temperature, K</eTemperature>
```

```
        </VariableType>
      </VariableID>
    </Variable>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>293.15</nVarValue>
        <nVarDigits>5</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>3.30</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>-19.7</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>298.15</nVarValue>
        <nVarDigits>5</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>3.79</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>-20.4</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
```

```
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>303.15</nVarValue>
      <nVarDigits>5</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>2.94</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>-20.1</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>308.15</nVarValue>
      <nVarDigits>5</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>2.37</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
    <PropertyValue>
      <nPropNumber>2</nPropNumber>
      <nPropValue>-19.9</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>313.15</nVarValue>
      <nVarDigits>5</nVarDigits>
```

```
        </VariableValue>
        <PropertyValue>
          <nPropNumber>1</nPropNumber>
          <nPropValue>1.97</nPropValue>
          <nPropDigits>3</nPropDigits>
        </PropertyValue>
        <PropertyValue>
          <nPropNumber>2</nPropNumber>
          <nPropValue>-19.8</nPropValue>
          <nPropDigits>3</nPropDigits>
        </PropertyValue>
      </NumValues>
    </ReactionData>
</DataReport>
```

********** Use Case 04 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<!-- edited with XML Spy v4.4 U (http://www.xmlspy.com) by Robert D. Chirico (U. S. Department of Commerce) -->
<!--Created by Guided Data Capture (GDC) Software (http://www.trc.nist.gov)-->
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>2</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>1998</yrYrPub>
      <sAuthor1>car</sAuthor1>
      <sAuthor2/>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Carta, R.[Renzo]</sAuthor>
    <sPubName>J. Chem. Thermodyn.</sPubName>
    <yrPubYr>1998</yrPubYr>
    <sTitle>Solubilities of L-cystine, L-tyrosine,  L-leucine, and glycine in sodium chloride  solutions at various pH values</sTitle>
    <sVol>30</sVol>
    <sPage>379-387</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <sCommonName>L-cystine</sCommonName>
    <sFormulaMolec>C6H12N2O4S2</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
      <purity>
        <nStep>1</nStep>
        <nPurityMass>99</nPurityMass>
```

```
        <nPurityMassDigits>2</nPurityMassDigits>
        <eAnalMeth>Stated by supplier</eAnalMeth>
      </purity>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <sCommonName>water</sCommonName>
    <sFormulaMolec>H2O</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
      <purity>
        <nStep>1</nStep>
        <nPurityMol>99.99</nPurityMol>
        <nPurityMolDigits>4</nPurityMolDigits>
        <eAnalMeth>Estimation</eAnalMeth>
      </purity>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <sCommonName>sodium chloride</sCommonName>
    <sFormulaMolec>ClNa</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
      <purity>
        <nStep>1</nStep>
        <nPurityMass>99.9</nPurityMass>
        <nPurityMassDigits>3</nPurityMassDigits>
        <eAnalMeth>Estimation</eAnalMeth>
      </purity>
    </Sample>
```

```
</Compound>
<Compound>
  <RegNum>
    <nOrgNum>4</nOrgNum>
  </RegNum>
  <sCommonName>hydrogen chloride</sCommonName>
  <sFormulaMolec>ClH</sFormulaMolec>
  <Sample>
    <nSampleNm>1</nSampleNm>
    <eSource>Commercial source</eSource>
  </Sample>
</Compound>
<PureOrMixtureData>
  <Component>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <nSampleNm>1</nSampleNm>
  </Component>
  <AuxiliarySubstance>
    <eFunction>Solvent</eFunction>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <nSampleNm>1</nSampleNm>
  </AuxiliarySubstance>
  <AuxiliarySubstance>
    <eFunction>Solvent</eFunction>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <nSampleNm>1</nSampleNm>
  </AuxiliarySubstance>
  <AuxiliarySubstance>
    <eFunction>Solvent</eFunction>
    <RegNum>
      <nOrgNum>4</nOrgNum>
    </RegNum>
```

```
</AuxiliarySubstance>
<Property>
  <nPropNumber>1</nPropNumber>
  <Property-MethodID>
    <PropertyGroup>
      <CompositionAtPhaseEquilibrium>
        <ePropName>Molality, mol/kg</ePropName>
        <sMethodName>gravimetric analysis</sMethodName>
      </CompositionAtPhaseEquilibrium>
    </PropertyGroup>
  </Property-MethodID>
  <PropPhaseID>
    <ePropPhase>Solution</ePropPhase>
  </PropPhaseID>
  <ePresentation>Direct value, X</ePresentation>
</Property>
<PhaseID>
  <ePhase>Solution</ePhase>
</PhaseID>
<PhaseID>
  <ePhase>Crystal</ePhase>
</PhaseID>
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <eTemperature>Temperature, K</eTemperature>
    </ConstraintType>
  </ConstraintID>
  <nConstraintValue>298</nConstraintValue>
  <nConstrDigits>3</nConstrDigits>
</Constraint>
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <ePressure>Pressure, kPa</ePressure>
    </ConstraintType>
  </Constraint>
  <nConstraintValue>101</nConstraintValue>
```

```
    <nConstrDigits>3</nConstrDigits>
  </Constraint>
  <Variable>
    <nVarNumber>1</nVarNumber>
    <VariableID>
      <VariableType>
        <eBioVariables>pH</eBioVariables>
      </VariableType>
    </VariableID>
  </Variable>
  <Variable>
    <nVarNumber>2</nVarNumber>
    <VariableID>
      <VariableType>
        <eSolventComposition>Solvent: Amount concentration (molarity), mol/dm3</eSolventComposition>
      </VariableType>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
    </VariableID>
  </Variable>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>0.00</nVarValue>
      <nVarDigits>0</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>0</nVarValue>
      <nVarDigits>0</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.09412</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
  </NumValues>
```

```
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>1.03</nVarValue>
    <nVarDigits>3</nVarDigits>
  </VariableValue>
  <VariableValue>
    <nVarNumber>2</nVarNumber>
    <nVarValue>0</nVarValue>
    <nVarDigits>0</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>0.01701</nPropValue>
    <nPropDigits>4</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>2.11</nVarValue>
    <nVarDigits>3</nVarDigits>
  </VariableValue>
  <VariableValue>
    <nVarNumber>2</nVarNumber>
    <nVarValue>0</nVarValue>
    <nVarDigits>0</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>0.00145</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>7.81</nVarValue>
```

```
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>0</nVarValue>
        <nVarDigits>0</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.00161</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>10.93</nVarValue>
        <nVarDigits>4</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>0</nVarValue>
        <nVarDigits>0</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.00450</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>12.28</nVarValue>
        <nVarDigits>4</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
```

```
        <nVarValue>0</nVarValue>
        <nVarDigits>0</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.02825</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>0.01</nVarValue>
        <nVarDigits>1</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>0.5</nVarValue>
        <nVarDigits>1</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.10315</nPropValue>
        <nPropDigits>5</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>1.05</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>0.5</nVarValue>
        <nVarDigits>1</nVarDigits>
      </VariableValue>
      <PropertyValue>
```

```
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.02039</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.12</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>0.5</nVarValue>
        <nVarDigits>1</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.00156</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>7.81</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>0.5</nVarValue>
        <nVarDigits>1</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.00169</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
```

```
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>10.93</nVarValue>
    <nVarDigits>4</nVarDigits>
  </VariableValue>
  <VariableValue>
    <nVarNumber>2</nVarNumber>
    <nVarValue>0.5</nVarValue>
    <nVarDigits>1</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>0.00465</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>12.32</nVarValue>
    <nVarDigits>4</nVarDigits>
  </VariableValue>
  <VariableValue>
    <nVarNumber>2</nVarNumber>
    <nVarValue>0.5</nVarValue>
    <nVarDigits>1</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>0.03125</nPropValue>
    <nPropDigits>4</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
```

```
        <nVarValue>0.01</nVarValue>
        <nVarDigits>1</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>1.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.10911</nPropValue>
        <nPropDigits>5</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>1.05</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>1.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.02365</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.14</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
```

```
        <nVarNumber>2</nVarNumber>
        <nVarValue>1.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.00172</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>7.79</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>1.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.00181</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>10.92</nVarValue>
        <nVarDigits>4</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>1.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
```

```
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.00517</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>12.35</nVarValue>
      <nVarDigits>4</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>1.0</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.03392</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>7.79</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>1.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.00211</nPropValue>
      <nPropDigits>3</nPropDigits>
```

```
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>0.02</nVarValue>
      <nVarDigits>1</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>1.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.11864</nPropValue>
      <nPropDigits>5</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>10.90</nVarValue>
      <nVarDigits>4</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>1.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.00552</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
```

```
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.14</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>1.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.00189</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>1.06</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>1.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.02398</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>12.31</nVarValue>
        <nVarDigits>4</nVarDigits>
      </VariableValue>
```

```
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>1.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.03716</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.15</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.0</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.00201</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>10.90</nVarValue>
      <nVarDigits>4</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.0</nVarValue>
      <nVarDigits>2</nVarDigits>
```

```
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.00567</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>7.76</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.0</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.00233</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>0.02</nVarValue>
      <nVarDigits>1</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.0</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.12719</nPropValue>
```

```
        <nPropDigits>5</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>12.30</nVarValue>
        <nVarDigits>4</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>2.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.03722</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>1.06</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>2.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.02401</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
```

```
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>2.17</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.00234</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>0.03</nVarValue>
      <nVarDigits>1</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.14087</nPropValue>
      <nPropDigits>5</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>12.29</nVarValue>
      <nVarDigits>4</nVarDigits>
```

```
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.04087</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>10.88</nVarValue>
      <nVarDigits>4</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.5</nVarValue>
      <nVarDigits>2</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.00593</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>7.79</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>2.5</nVarValue>
```

```
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.00228</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>1.07</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>2.5</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.02447</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>1.08</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>3.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
```

```
        <nPropValue>0.02437</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>2.17</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>3.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.00247</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>7.78</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>3.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.00242</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
```

```
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>10.89</nVarValue>
    <nVarDigits>4</nVarDigits>
  </VariableValue>
  <VariableValue>
    <nVarNumber>2</nVarNumber>
    <nVarValue>3.0</nVarValue>
    <nVarDigits>2</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>0.00596</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>12.32</nVarValue>
    <nVarDigits>4</nVarDigits>
  </VariableValue>
  <VariableValue>
    <nVarNumber>2</nVarNumber>
    <nVarValue>3.0</nVarValue>
    <nVarDigits>2</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>0.04212</nPropValue>
    <nPropDigits>4</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>0.02</nVarValue>
```

```
        <nVarDigits>1</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>3.0</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>0.14399</nPropValue>
        <nPropDigits>5</nPropDigits>
      </PropertyValue>
    </NumValues>
  </PureOrMixtureData>
</DataReport>
```

********** Use Case 05 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<!-- edited with XML Spy v4.4 U (http://www.xmlspy.com) by Robert D. Chirico (U. S. Department of Commerce) -->
<!--Created by Guided Data Capture (GDC) Software (http://www.trc.nist.gov)-->
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>4</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Ortiz, A.[Antonio]</sAuthor>
    <sAuthor>Aranda, F. J.[Francisco J.]</sAuthor>
    <sAuthor>Villalain, J.[Jose]</sAuthor>
    <sAuthor>Gomez-Fernandez, J. C.[Juan C.]</sAuthor>
    <sPubName>Biochimica et Biophysica Acta</sPubName>
    <yrPubYr>1992</yrPubYr>
    <dateCit>2009-07-16</dateCit>
    <sTitle>Influence of retinoids on phosphatidylethanolamine  lipid polymorphism</sTitle>
    <sVol>1112</sVol>
    <sPage>226-234</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <sCommonName>9-Octadecenoic acid, 1-[[[(2-aminoethoxy)hydroxyphosphinyl]oxy]methyl]-1,2-ethanediyl ester, (E,E)-</sCommonName>
    <sFormulaMolec>C41H79NO8P</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>2</nOrgNum>
```

```
    </RegNum>
    <sCommonName>ethylenediaminetetraacetic acid</sCommonName>
    <sFormulaMolec>C10H16N2O8</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <sCommonName>4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid</sCommonName>
    <sFormulaMolec>C8H18N2O4S</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>4</nOrgNum>
    </RegNum>
    <sCommonName>sodium chloride</sCommonName>
    <sFormulaMolec>ClNa</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
    <sCommonName>water</sCommonName>
    <sFormulaMolec>H2O</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
```

```
      <eSource>Commercial source</eSource>
      <purity>
        <nStep>1</nStep>
        <nPurityMol>99.9</nPurityMol>
        <nPurityMolDigits>3</nPurityMolDigits>
        <eAnalMeth>Estimated by the compiler</eAnalMeth>
      </purity>
    </Sample>
  </Compound>
  <PureOrMixtureData>
    <Component>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
    </Component>
    <AuxiliarySubstance>
      <eFunction>Buffer</eFunction>
      <RegNum>
        <nOrgNum>2</nOrgNum>
      </RegNum>
      <nSampleNm>1</nSampleNm>
    </AuxiliarySubstance>
    <AuxiliarySubstance>
      <eFunction>Buffer</eFunction>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
      <nSampleNm>1</nSampleNm>
    </AuxiliarySubstance>
    <AuxiliarySubstance>
      <eFunction>Inert</eFunction>
      <RegNum>
        <nOrgNum>4</nOrgNum>
      </RegNum>
      <nSampleNm>1</nSampleNm>
    </AuxiliarySubstance>
    <AuxiliarySubstance>
      <eFunction>Solvent</eFunction>
```

```
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
    <nSampleNm>1</nSampleNm>
  </AuxiliarySubstance>
  <sCompiler/>
  <sContributor/>
  <dateDateAdded/>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <BioProperties>
          <ePropName>Peak temperature, K</ePropName>
          <sMethodName>DSC</sMethodName>
        </BioProperties>
      </PropertyGroup>
    </Property-MethodID>
    <PropPhaseID>
      <ePropPhase>Solution</ePropPhase>
      <sBioState>1A</sBioState>
    </PropPhaseID>
    <PropPhaseID>
      <ePropPhase>Solution</ePropPhase>
      <sBioState>2AHII</sBioState>
    </PropPhaseID>
    <ePresentation>Direct value, X</ePresentation>
  </Property>
  <Property>
    <nPropNumber>2</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <PhaseTransition>
          <ePropName>Molar enthalpy of transition or fusion, kJ/mol</ePropName>
          <sMethodName>DSC</sMethodName>
        </PhaseTransition>
      </PropertyGroup>
    </Property-MethodID>
```

```
    <PropPhaseID>
      <ePropPhase>Solution</ePropPhase>
      <sBioState>1A</sBioState>
    </PropPhaseID>
    <PropPhaseID>
      <ePropPhase>Solution</ePropPhase>
      <sBioState>2AHII</sBioState>
    </PropPhaseID>
    <ePresentation>Direct value, X</ePresentation>
  </Property>
  <PhaseID>
    <ePhase>Solution</ePhase>
  </PhaseID>
  <Constraint>
    <ConstraintID>
      <ConstraintType>
        <ePressure>Pressure, kPa</ePressure>
      </ConstraintType>
    </ConstraintID>
    <nConstraintValue>101.325</nConstraintValue>
    <nConstrDigits>6</nConstrDigits>
  </Constraint>
  <Variable>
    <nVarNumber>1</nVarNumber>
    <VariableID>
      <VariableType>
        <eBioVariables>pH</eBioVariables>
      </VariableType>
    </VariableID>
  </Variable>
  <Variable>
    <nVarNumber>2</nVarNumber>
    <VariableID>
      <VariableType>
        <eBioVariables>Ionic strength (amount concentration basis), mol/dm3</eBioVariables>
      </VariableType>
    </VariableID>
  </Variable>
```

```
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>7.4</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <VariableValue>
        <nVarNumber>2</nVarNumber>
        <nVarValue>0.20</nVarValue>
        <nVarDigits>2</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>322.4</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
      <PropertyValue>
        <nPropNumber>2</nPropNumber>
        <nPropValue>2.9</nPropValue>
        <nPropDigits>2</nPropDigits>
      </PropertyValue>
    </NumValues>
  </PureOrMixtureData>
</DataReport>
```

********** Use Case 06 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>2</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>1989</yrYrPub>
      <sAuthor1>chi</sAuthor1>
      <sAuthor2>hos</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Chirico, R. D.[Robert D.]</sAuthor>
    <sAuthor>Hossenlopp, I. A.</sAuthor>
    <sAuthor>Nguyen, A.</sAuthor>
    <sAuthor>Steele, W. V.[William V.]</sAuthor>
    <sAuthor>Gammon, B. E.[Bruce E.]</sAuthor>
    <sPubName>J. Chem. Thermodyn.</sPubName>
    <yrPubYr>1989</yrPubYr>
    <dateCit>2010-06-08</dateCit>
    <sTitle>The thermodynamic properties of 4-methylphenanthrene</sTitle>
    <sVol>21</sVol>
    <sPage>179-201</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <sCommonName>4-methylphenanthrene</sCommonName>
    <sFormulaMolec>C15H12</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Synthesized by the authors</eSource>
```

```
      <purity>
        <nStep>1</nStep>
        <nPurityMol>98</nPurityMol>
        <nPurityMolDigits>2</nPurityMolDigits>
        <eAnalMeth>Gas chromatography</eAnalMeth>
      </purity>
      <purity>
        <nStep>2</nStep>
        <ePurifMethod>Crystallization from solution</ePurifMethod>
        <ePurifMethod>Fractional distillation</ePurifMethod>
      </purity>
      <purity>
        <nStep>2</nStep>
        <nPurityMol>99.92</nPurityMol>
        <nPurityMolDigits>4</nPurityMolDigits>
        <eAnalMeth>Fraction melting in an adiabatic calorimeter</eAnalMeth>
      </purity>
      <purity>
        <nStep>2</nStep>
        <nPurityMol>99.96</nPurityMol>
        <nPurityMolDigits>4</nPurityMolDigits>
        <eAnalMeth>Gas chromatography</eAnalMeth>
      </purity>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <sCommonName>carbon</sCommonName>
    <sFormulaMolec>C</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <sCommonName>hydrogen</sCommonName>
    <sFormulaMolec>H2</sFormulaMolec>
```

```
  </Compound>
  <ReactionData>
    <Participant>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
      <nSampleNm>1</nSampleNm>
      <nStoichiometricCoef>1</nStoichiometricCoef>
      <ePhase>Crystal</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>2</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>-15</nStoichiometricCoef>
      <ePhase>Crystal</ePhase>
      <sPhaseDescription>graphite</sPhaseDescription>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>-6</nStoichiometricCoef>
      <ePhase>Ideal gas</ePhase>
    </Participant>
    <eExpPurpose>Principal objective of the work</eExpPurpose>
    <sCompiler>VVD</sCompiler>
    <sContributor>TRC</sContributor>
    <dateDateAdded>6/8/2010</dateDateAdded>
    <eReactionType>Formation of a compound from elements in their stable state</eReactionType>
    <Property>
      <nPropNumber>1</nPropNumber>
      <Property-MethodID>
        <PropertyGroup>
          <ReactionStateChangeProp>
            <ePropName>Molar enthalpy of reaction, kJ/mol</ePropName>
```

```
            <eMethodName>Static bomb calorimetry</eMethodName>
          </ReactionStateChangeProp>
        </PropertyGroup>
      </Property-MethodID>
      <nTemperature-K>298.15</nTemperature-K>
      <nTemperatureDigits>5</nTemperatureDigits>
      <nPressure-kPa>101.325</nPressure-kPa>
      <nPressureDigits>6</nPressureDigits>
    </Property>
    <NumValues>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>102.42</nPropValue>
        <nPropDigits>5</nPropDigits>
      </PropertyValue>
    </NumValues>
  </ReactionData>
</DataReport>
```

********** Use Case 07 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>2</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>2006</yrYrPub>
      <sAuthor1>rak</sAuthor1>
      <sAuthor2>par</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Rakshit, S. K.</sAuthor>
    <sAuthor>Parida, S. C.</sAuthor>
    <sAuthor>Dash, S.</sAuthor>
    <sAuthor>Singh, Z.[Ziley]</sAuthor>
    <sAuthor>Venugopal, V.</sAuthor>
    <sPubName>Thermochim. Acta</sPubName>
    <yrPubYr>2006</yrPubYr>
    <dateCit>2010-05-13</dateCit>
    <sTitle>Thermodynamics of BaNd2Fe2O7(s) and BaNdFeO4(s) in the system Ba Nd Fe O</sTitle>
    <sKeyword>Quaternary oxides</sKeyword>
    <sKeyword>Thermodynamic properties</sKeyword>
    <sKeyword>Heat capacity</sKeyword>
    <sKeyword>Solid-state electrochemical cell</sKeyword>
    <sKeyword>Differential scanning calorimetry</sKeyword>
    <sVol>443</sVol>
    <sPage>98-104</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
```

```
    <sCommonName>calcium oxide</sCommonName>
    <sFormulaMolec>CaO</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <sCommonName>BaNd2Fe2O7</sCommonName>
    <sFormulaMolec>BaFe2Nd2O7</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Synthesized by the authors</eSource>
      <purity>
        <nStep>1</nStep>
        <nPurityMol>98</nPurityMol>
        <nPurityMolDigits>2</nPurityMolDigits>
        <eAnalMeth>Estimated by the compiler</eAnalMeth>
      </purity>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <sCommonName>BaNdFeO4</sCommonName>
    <sFormulaMolec>BaFeNdO4</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Synthesized by the authors</eSource>
      <purity>
        <nStep>1</nStep>
        <nPurityMol>98</nPurityMol>
        <nPurityMolDigits>2</nPurityMolDigits>
        <eAnalMeth>Estimated by the compiler</eAnalMeth>
      </purity>
    </Sample>
  </Compound>
  <Compound>
```

```
    <RegNum>
      <nOrgNum>4</nOrgNum>
    </RegNum>
    <sCommonName>barium fluoride (BaF2)</sCommonName>
    <sFormulaMolec>BaF2</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
    <sCommonName>calcium fluoride</sCommonName>
    <sFormulaMolec>CaF2</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>6</nOrgNum>
    </RegNum>
    <sCommonName>NdFeO3</sCommonName>
    <sFormulaMolec>FeNdO3</sFormulaMolec>
  </Compound>
  <ReactionData>
    <Participant>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>-1</nStoichiometricCoef>
      <ePhase>Crystal</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>4</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>-1</nStoichiometricCoef>
      <ePhase>Crystal</ePhase>
    </Participant>
    <Participant>
```

```
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
    <nSampleNm>0</nSampleNm>
    <nStoichiometricCoef>1</nStoichiometricCoef>
    <ePhase>Crystal</ePhase>
  </Participant>
  <Participant>
    <RegNum>
      <nOrgNum>6</nOrgNum>
    </RegNum>
    <nSampleNm>0</nSampleNm>
    <nStoichiometricCoef>-2</nStoichiometricCoef>
    <ePhase>Crystal</ePhase>
  </Participant>
  <Participant>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <nSampleNm>1</nSampleNm>
    <nStoichiometricCoef>1</nStoichiometricCoef>
    <ePhase>Crystal</ePhase>
  </Participant>
  <nElectronNumber>2</nElectronNumber>
  <eExpPurpose>Principal objective of the work</eExpPurpose>
  <sCompiler>VVD</sCompiler>
  <sContributor>TRC</sContributor>
  <dateDateAdded>5/13/2010</dateDateAdded>
  <eReactionType>Other reactions</eReactionType>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <ReactionStateChangeProp>
          <ePropName>Potential difference of an electrochemical cell, V</ePropName>
          <eMethodName>Potential difference of an electrochemical cell</eMethodName>
        </ReactionStateChangeProp>
      </PropertyGroup>
```

```
    </Property-MethodID>
    <eStandardState>Pure compound</eStandardState>
  </Property>
  <Constraint>
    <ConstraintID>
      <ConstraintType>
        <ePressure>Pressure, kPa</ePressure>
      </ConstraintType>
    </ConstraintID>
    <nConstraintValue>101.325</nConstraintValue>
    <nConstrDigits>6</nConstrDigits>
  </Constraint>
  <Variable>
    <nVarNumber>1</nVarNumber>
    <VariableID>
      <VariableType>
        <eTemperature>Temperature, K</eTemperature>
      </VariableType>
    </VariableID>
  </Variable>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>861</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>0.0213</nPropValue>
      <nPropDigits>4</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>995</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
```

```
        <PropertyValue>
          <nPropNumber>1</nPropNumber>
          <nPropValue>0.0725</nPropValue>
          <nPropDigits>3</nPropDigits>
        </PropertyValue>
      </NumValues>
    </ReactionData>
    <ReactionData>
      <Participant>
        <RegNum>
          <nOrgNum>1</nOrgNum>
        </RegNum>
        <nSampleNm>0</nSampleNm>
        <nStoichiometricCoef>-1</nStoichiometricCoef>
        <ePhase>Crystal</ePhase>
      </Participant>
      <Participant>
        <RegNum>
          <nOrgNum>4</nOrgNum>
        </RegNum>
        <nSampleNm>0</nSampleNm>
        <nStoichiometricCoef>-1</nStoichiometricCoef>
        <ePhase>Crystal</ePhase>
      </Participant>
      <Participant>
        <RegNum>
          <nOrgNum>5</nOrgNum>
        </RegNum>
        <nSampleNm>0</nSampleNm>
        <nStoichiometricCoef>1</nStoichiometricCoef>
        <ePhase>Crystal</ePhase>
      </Participant>
      <Participant>
        <RegNum>
          <nOrgNum>6</nOrgNum>
        </RegNum>
        <nSampleNm>0</nSampleNm>
        <nStoichiometricCoef>-2</nStoichiometricCoef>
```

```
    <ePhase>Crystal</ePhase>
  </Participant>
  <Participant>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <nSampleNm>1</nSampleNm>
    <nStoichiometricCoef>1</nStoichiometricCoef>
    <ePhase>Crystal</ePhase>
  </Participant>
  <nElectronNumber>2</nElectronNumber>
  <eExpPurpose>Principal objective of the work</eExpPurpose>
  <sCompiler>VVD</sCompiler>
  <sContributor>TRC</sContributor>
  <dateDateAdded>5/13/2010</dateDateAdded>
  <eReactionType>Other reactions</eReactionType>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <ReactionStateChangeProp>
          <ePropName>Molar Gibbs energy of reaction, kJ/mol</ePropName>
          <eMethodName>Potential difference of an electrochemical cell</eMethodName>
        </ReactionStateChangeProp>
      </PropertyGroup>
    </Property-MethodID>
    <eStandardState>Pure compound</eStandardState>
  </Property>
  <Constraint>
    <ConstraintID>
      <ConstraintType>
        <ePressure>Pressure, kPa</ePressure>
      </ConstraintType>
    </Constraint>
    <nConstraintValue>101.325</nConstraintValue>
    <nConstrDigits>6</nConstrDigits>
  </Constraint>
  <Variable>
```

```
        <nVarNumber>1</nVarNumber>
        <VariableID>
          <VariableType>
            <eTemperature>Temperature, K</eTemperature>
          </VariableType>
        </VariableID>
      </Variable>
      <NumValues>
        <VariableValue>
          <nVarNumber>1</nVarNumber>
          <nVarValue>861</nVarValue>
          <nVarDigits>3</nVarDigits>
        </VariableValue>
        <PropertyValue>
          <nPropNumber>1</nPropNumber>
          <nPropValue>4.17</nPropValue>
          <nPropDigits>4</nPropDigits>
        </PropertyValue>
      </NumValues>
      <NumValues>
        <VariableValue>
          <nVarNumber>1</nVarNumber>
          <nVarValue>995</nVarValue>
          <nVarDigits>3</nVarDigits>
        </VariableValue>
        <PropertyValue>
          <nPropNumber>1</nPropNumber>
          <nPropValue>14.03</nPropValue>
          <nPropDigits>4</nPropDigits>
        </PropertyValue>
      </NumValues>
    </ReactionData>
</DataReport>
```

********** Use Case 08 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>2</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>2009</yrYrPub>
      <sAuthor1>ham</sAuthor1>
      <sAuthor2>ver</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Hamborg, E. S.[Espen S.]</sAuthor>
    <sAuthor>Versteeg, G. F.[Geert F.]</sAuthor>
    <sPubName>J. Chem. Eng. Data</sPubName>
    <yrPubYr>2009</yrPubYr>
    <dateCit>2010-04-21</dateCit>
    <sTitle>Dissociation Constants and Thermodynamic Properties of Amines and Alkanolamines from (293 to 353) K</sTitle>
    <sDOI>10.1021/je800897v</sDOI>
    <sVol>54</sVol>
    <sPage>1318-1328</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <sCommonName>piperazine</sCommonName>
    <sFormulaMolec>C4H10N2</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
    </Sample>
  </Compound>
  <Compound>
```

```
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <sCommonName>piperazonium</sCommonName>
    <sFormulaMolec>C4H11N2</sFormulaMolec>
    <ion>
      <nCharge>1</nCharge>
    </ion>
    <Sample>
      <nSampleNm>1</nSampleNm>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <sCommonName>piperazinedionium</sCommonName>
    <sFormulaMolec>C4H12N2</sFormulaMolec>
    <ion>
      <nCharge>2</nCharge>
    </ion>
    <Sample>
      <nSampleNm>1</nSampleNm>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>4</nOrgNum>
    </RegNum>
    <sCommonName>water</sCommonName>
    <sFormulaMolec>H2O</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
      <purity>
        <nStep>1</nStep>
        <nPurityMol>99.9</nPurityMol>
        <nPurityMolDigits>3</nPurityMolDigits>
```

```
        <eAnalMeth>Estimated by the compiler</eAnalMeth>
      </purity>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
    <sCommonName>hydroxonium ion</sCommonName>
    <sFormulaMolec>H3O</sFormulaMolec>
    <ion>
      <nCharge>1</nCharge>
    </ion>
    <Sample>
      <nSampleNm>1</nSampleNm>
    </Sample>
  </Compound>
  <ReactionData>
    <Participant>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
      <nSampleNm>1</nSampleNm>
      <nStoichiometricCoef>-1</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>5</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>2</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
```

```
    <nSampleNm>0</nSampleNm>
    <nStoichiometricCoef>1</nStoichiometricCoef>
    <ePhase>Solution 1</ePhase>
  </Participant>
  <Participant>
    <RegNum>
      <nOrgNum>4</nOrgNum>
    </RegNum>
    <nSampleNm>0</nSampleNm>
    <nStoichiometricCoef>-2</nStoichiometricCoef>
    <ePhase>Solution 1</ePhase>
  </Participant>
  <eExpPurpose>Principal objective of the work</eExpPurpose>
  <sCompiler>TRC</sCompiler>
  <sContributor>VVD</sContributor>
  <dateDateAdded>4/21/2010</dateDateAdded>
  <eReactionType>Other reactions</eReactionType>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <ReactionEquilibriumProp>
          <ePropName>Thermodynamic equilibrium constant</ePropName>
          <eMethodName>Cell potential with glass electrode</eMethodName>
        </ReactionEquilibriumProp>
      </PropertyGroup>
    </Property-MethodID>
    <Solvent>
      <RegNum>
        <nOrgNum>4</nOrgNum>
      </RegNum>
      <ePhase>Solution 1</ePhase>
    </Solvent>
    <eStandardState>Infinite dilution solute</eStandardState>
  </Property>
  <Constraint>
    <ConstraintID>
      <ConstraintType>
```

```
            <ePressure>Pressure, kPa</ePressure>
        </ConstraintType>
    </ConstraintID>
    <nConstraintValue>100</nConstraintValue>
    <nConstrDigits>3</nConstrDigits>
  </Constraint>
  <Variable>
    <nVarNumber>1</nVarNumber>
    <VariableID>
        <VariableType>
            <eTemperature>Temperature, K</eTemperature>
        </VariableType>
    </VariableID>
  </Variable>
  <NumValues>
    <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>293.15</nVarValue>
        <nVarDigits>5</nVarDigits>
    </VariableValue>
    <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>3.11E-06</nPropValue>
        <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>298.15</nVarValue>
        <nVarDigits>5</nVarDigits>
    </VariableValue>
    <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>3.92E-06</nPropValue>
        <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
```

```
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>303.15</nVarValue>
    <nVarDigits>5</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>4.83E-06</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>308.15</nVarValue>
    <nVarDigits>5</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>5.96E-06</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>313.15</nVarValue>
    <nVarDigits>5</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>7.28E-06</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
```

```
        <nVarNumber>1</nVarNumber>
        <nVarValue>318.15</nVarValue>
        <nVarDigits>5</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>8.90E-06</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>323.15</nVarValue>
        <nVarDigits>5</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>1.09E-05</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
  </ReactionData>
  <ReactionData>
    <Participant>
      <RegNum>
        <nOrgNum>2</nOrgNum>
      </RegNum>
      <nSampleNm>1</nSampleNm>
      <nStoichiometricCoef>-1</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
      <eStandardState>Infinite dilution solute</eStandardState>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>5</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
```

```
    <nStoichiometricCoef>1</nStoichiometricCoef>
    <ePhase>Solution 1</ePhase>
    <eStandardState>Infinite dilution solute</eStandardState>
  </Participant>
  <Participant>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <nSampleNm>0</nSampleNm>
    <nStoichiometricCoef>1</nStoichiometricCoef>
    <ePhase>Solution 1</ePhase>
    <eStandardState>Infinite dilution solute</eStandardState>
  </Participant>
  <Participant>
    <RegNum>
      <nOrgNum>4</nOrgNum>
    </RegNum>
    <nSampleNm>0</nSampleNm>
    <nStoichiometricCoef>-1</nStoichiometricCoef>
    <ePhase>Solution 1</ePhase>
    <eStandardState>Infinite dilution solute</eStandardState>
  </Participant>
  <eExpPurpose>Principal objective of the work</eExpPurpose>
  <sCompiler>TRC</sCompiler>
  <sContributor>VVD</sContributor>
  <dateDateAdded>4/21/2010</dateDateAdded>
  <eReactionType>Other reactions</eReactionType>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <ReactionEquilibriumProp>
          <ePropName>Natural logarithm of thermodynamic equilibrium constant</ePropName>
          <eMethodName>Cell potential with glass electrode</eMethodName>
        </ReactionEquilibriumProp>
      </PropertyGroup>
    </Property-MethodID>
    <Solvent>
```

```
        <RegNum>
          <nOrgNum>4</nOrgNum>
        </RegNum>
        <ePhase>Solution 1</ePhase>
      </Solvent>
    </Property>
    <Constraint>
      <ConstraintID>
        <ConstraintType>
          <ePressure>Pressure, kPa</ePressure>
        </ConstraintType>
      </ConstraintID>
      <nConstraintValue>100</nConstraintValue>
      <nConstrDigits>3</nConstrDigits>
    </Constraint>
    <Variable>
      <nVarNumber>1</nVarNumber>
      <VariableID>
        <VariableType>
          <eTemperature>Temperature, K</eTemperature>
        </VariableType>
      </VariableID>
    </Variable>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>293.15</nVarValue>
        <nVarDigits>5</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>-22.66</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
```

```
        <nVarValue>298.15</nVarValue>
        <nVarDigits>5</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>-22.37</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>303.15</nVarValue>
        <nVarDigits>5</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>-22.08</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>308.15</nVarValue>
        <nVarDigits>5</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>-21.80</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>313.15</nVarValue>
        <nVarDigits>5</nVarDigits>
```

```
        </VariableValue>
        <PropertyValue>
          <nPropNumber>1</nPropNumber>
          <nPropValue>-21.53</nPropValue>
          <nPropDigits>3</nPropDigits>
        </PropertyValue>
      </NumValues>
      <NumValues>
        <VariableValue>
          <nVarNumber>1</nVarNumber>
          <nVarValue>318.15</nVarValue>
          <nVarDigits>5</nVarDigits>
        </VariableValue>
        <PropertyValue>
          <nPropNumber>1</nPropNumber>
          <nPropValue>-21.27</nPropValue>
          <nPropDigits>3</nPropDigits>
        </PropertyValue>
      </NumValues>
      <NumValues>
        <VariableValue>
          <nVarNumber>1</nVarNumber>
          <nVarValue>323.15</nVarValue>
          <nVarDigits>5</nVarDigits>
        </VariableValue>
        <PropertyValue>
          <nPropNumber>1</nPropNumber>
          <nPropValue>-21.01</nPropValue>
          <nPropDigits>3</nPropDigits>
        </PropertyValue>
      </NumValues>
    </ReactionData>
</DataReport>
```

********** Use Case 09 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>2</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>2008</yrYrPub>
      <sAuthor1>cia</sAuthor1>
      <sAuthor2>eli</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Ciavatta, L.</sAuthor>
    <sAuthor>Elia, V.</sAuthor>
    <sAuthor>Napoli, E.</sAuthor>
    <sAuthor>Niccoli, M.</sAuthor>
    <sPubName>J. Solution Chem.</sPubName>
    <yrPubYr>2008</yrPubYr>
    <dateCit>2010-06-09</dateCit>
    <sTitle>New Physico-Chemical Properties of Extremely Diluted  Solutions. Electromotive Force Measurements  of Galvanic Cells Sensible to the Activity of
NaCl at 25 deg C</sTitle>
    <sDOI>10.1007/s10953-008-9299-6</sDOI>
    <sVol>37</sVol>
    <sPage>1037-1049</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <sCommonName>water</sCommonName>
    <sFormulaMolec>H2O</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
```

```
        <eSource>Commercial source</eSource>
        <purity>
          <nStep>1</nStep>
          <ePurifMethod>Fractional distillation</ePurifMethod>
        </purity>
      </Sample>
    </Compound>
    <Compound>
      <RegNum>
        <nOrgNum>2</nOrgNum>
      </RegNum>
      <sCommonName>sodium chloride</sCommonName>
      <sFormulaMolec>ClNa</sFormulaMolec>
      <Sample>
        <nSampleNm>1</nSampleNm>
        <eSource>Commercial source</eSource>
        <purity>
          <nStep>1</nStep>
          <ePurifMethod>Dried by oven heating</ePurifMethod>
        </purity>
      </Sample>
    </Compound>
    <PureOrMixtureData>
      <Component>
        <RegNum>
          <nOrgNum>2</nOrgNum>
        </RegNum>
        <nSampleNm>1</nSampleNm>
      </Component>
      <Component>
        <RegNum>
          <nOrgNum>1</nOrgNum>
        </RegNum>
        <nSampleNm>1</nSampleNm>
      </Component>
      <eExpPurpose>Principal objective of the work</eExpPurpose>
      <sCompiler>VVD</sCompiler>
      <sContributor>TRC</sContributor>
```

```
<dateDateAdded>6/9/2010</dateDateAdded>
<Property>
  <nPropNumber>1</nPropNumber>
  <Property-MethodID>
    <PropertyGroup>
      <ActivityFugacityOsmoticProp>
        <ePropName>Mean ionic activity, (mol/dm3)^n</ePropName>
        <eMethodName>Potential difference of an electrochemical cell</eMethodName>
      </ActivityFugacityOsmoticProp>
    </PropertyGroup>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
  </Property-MethodID>
  <PropPhaseID>
    <ePropPhase>Liquid</ePropPhase>
  </PropPhaseID>
  <ePresentation>Direct value, X</ePresentation>
  <eStandardState>Infinite dilution solute</eStandardState>
</Property>
<PhaseID>
  <ePhase>Liquid</ePhase>
</PhaseID>
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <eTemperature>Temperature, K</eTemperature>
    </ConstraintType>
  </ConstraintID>
  <nConstraintValue>298.15</nConstraintValue>
  <nConstrDigits>5</nConstrDigits>
</Constraint>
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <ePressure>Pressure, kPa</ePressure>
    </ConstraintType>
  </Constraint>
```

```
      <nConstraintValue>101.325</nConstraintValue>
      <nConstrDigits>6</nConstrDigits>
    </Constraint>
    <Variable>
      <nVarNumber>1</nVarNumber>
      <VariableID>
        <VariableType>
          <eComponentComposition>Amount concentration (molarity), mol/dm3</eComponentComposition>
        </VariableType>
        <RegNum>
          <nOrgNum>2</nOrgNum>
        </RegNum>
      </VariableID>
      <VarPhaseID>
        <eVarPhase>Liquid</eVarPhase>
      </VarPhaseID>
    </Variable>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>.9899</nVarValue>
        <nVarDigits>4</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>.6464</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
    </NumValues>
  </PureOrMixtureData>
  <PureOrMixtureData>
    <Component>
      <RegNum>
        <nOrgNum>2</nOrgNum>
      </RegNum>
      <nSampleNm>1</nSampleNm>
    </Component>
    <Component>
```

```
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <nSampleNm>1</nSampleNm>
  </Component>
  <eExpPurpose>Principal objective of the work</eExpPurpose>
  <sCompiler>VVD</sCompiler>
  <sContributor>TRC</sContributor>
  <dateDateAdded>6/9/2010</dateDateAdded>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <ActivityFugacityOsmoticProp>
          <ePropName>Mean ionic activity coefficient</ePropName>
          <eMethodName>Potential difference of an electrochemical cell</eMethodName>
        </ActivityFugacityOsmoticProp>
      </PropertyGroup>
      <RegNum>
        <nOrgNum>2</nOrgNum>
      </RegNum>
    </Property-MethodID>
    <PropPhaseID>
      <ePropPhase>Liquid</ePropPhase>
    </PropPhaseID>
    <ePresentation>Direct value, X</ePresentation>
    <eStandardState>Infinite dilution solute</eStandardState>
  </Property>
  <PhaseID>
    <ePhase>Liquid</ePhase>
  </PhaseID>
  <Constraint>
    <ConstraintID>
      <ConstraintType>
        <eTemperature>Temperature, K</eTemperature>
      </Constraint Type>
    </ConstraintID>
    <nConstraintValue>298.15</nConstraintValue>
```

```
      <nConstrDigits>5</nConstrDigits>
    </Constraint>
    <Constraint>
      <ConstraintID>
        <ConstraintType>
          <ePressure>Pressure, kPa</ePressure>
        </ConstraintType>
      </ConstraintID>
      <nConstraintValue>101.325</nConstraintValue>
      <nConstrDigits>6</nConstrDigits>
    </Constraint>
    <Variable>
      <nVarNumber>1</nVarNumber>
      <VariableID>
        <VariableType>
          <eComponentComposition>Amount concentration (molarity), mol/dm3</eComponentComposition>
        </VariableType>
        <RegNum>
          <nOrgNum>2</nOrgNum>
        </RegNum>
      </VariableID>
      <VarPhaseID>
        <eVarPhase>Liquid</eVarPhase>
      </VarPhaseID>
    </Variable>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>.9899</nVarValue>
        <nVarDigits>4</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>.6530</nPropValue>
        <nPropDigits>4</nPropDigits>
      </PropertyValue>
    </NumValues>
  </PureOrMixtureData>
```

</DataReport>

********** Use Case 10 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>2</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>1938</yrYrPub>
      <sAuthor1>lon</sAuthor1>
      <sAuthor2>mac</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Longsworth, L. G.</sAuthor>
    <sAuthor>MacInnes, D. A.</sAuthor>
    <sPubName>J. Am. Chem. Soc.</sPubName>
    <yrPubYr>1938</yrPubYr>
    <dateCit>2010-06-23</dateCit>
    <sTitle>Transference Numbers of Lanthanum Chloride at 25 C by the Moving Boundary Method</sTitle>
    <sVol>60</sVol>
    <sPage>3070-3074</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <sCommonName>water</sCommonName>
    <sFormulaMolec>H2O</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <Compound>
```

```
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <sCommonName>lanthanum chloride</sCommonName>
    <sFormulaMolec>Cl3La</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <sCommonName>lanthanum ion</sCommonName>
    <sFormulaMolec>La</sFormulaMolec>
    <ion>
      <nCharge>3</nCharge>
    </ion>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>No sample used</eSource>
    </Sample>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>4</nOrgNum>
    </RegNum>
    <sCommonName>chloride ion</sCommonName>
    <sFormulaMolec>Cl</sFormulaMolec>
    <ion>
      <nCharge>-1</nCharge>
    </ion>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>No sample used</eSource>
    </Sample>
  </Compound>
```

```
<PureOrMixtureData>
  <Component>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <nSampleNm>1</nSampleNm>
  </Component>
  <Component>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <nSampleNm>1</nSampleNm>
  </Component>
  <eExpPurpose>Principal objective of the work</eExpPurpose>
  <sCompiler>VVD</sCompiler>
  <sContributor>TRC</sContributor>
  <dateDateAdded>6/23/2010</dateDateAdded>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <TransportProp>
          <ePropName>Transport number</ePropName>
          <sMethodName>moving boundary</sMethodName>
        </TransportProp>
      </PropertyGroup>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
    </Property-MethodID>
    <PropPhaseID>
      <ePropPhase>Liquid</ePropPhase>
    </PropPhaseID>
    <ePresentation>Direct value, X</ePresentation>
  </Property>
  <PhaseID>
    <ePhase>Liquid</ePhase>
  </PhaseID>
```

```
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <eTemperature>Temperature, K</eTemperature>
    </ConstraintType>
  </ConstraintID>
  <nConstraintValue>298.15</nConstraintValue>
  <nConstrDigits>5</nConstrDigits>
</Constraint>
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <ePressure>Pressure, kPa</ePressure>
    </ConstraintType>
  </ConstraintID>
  <nConstraintValue>101.325</nConstraintValue>
  <nConstrDigits>6</nConstrDigits>
</Constraint>
<Variable>
  <nVarNumber>1</nVarNumber>
  <VariableID>
    <VariableType>
      <eComponentComposition>Amount concentration (molarity), mol/dm3</eComponentComposition>
    </VariableType>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
  </VariableID>
  <VarPhaseID>
    <eVarPhase>Liquid</eVarPhase>
  </VarPhaseID>
</Variable>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>0.0025</nVarValue>
    <nVarDigits>2</nVarDigits>
  </VariableValue>
```

```
        <PropertyValue>
          <nPropNumber>1</nPropNumber>
          <nPropValue>0.4641</nPropValue>
          <nPropDigits>4</nPropDigits>
        </PropertyValue>
      </NumValues>
    </PureOrMixtureData>
</DataReport>
```

********** Use Case 11 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>2</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>1982</yrYrPub>
      <sAuthor1>wag</sAuthor1>
      <sAuthor2>eva</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Wagman, D. D.</sAuthor>
    <sAuthor>Evans, W. H.</sAuthor>
    <sAuthor>Parker, V. B.[Vivian Barfield]</sAuthor>
    <sAuthor>Schumm, P.</sAuthor>
    <sAuthor>Halow, I.</sAuthor>
    <sAuthor>Bailey, S. M.</sAuthor>
    <sAuthor>Churney, K. L.[Kenneth L.]</sAuthor>
    <sAuthor>Nuttall, R. L.</sAuthor>
    <sPubName>J. Phys. Chem. Ref. Data</sPubName>
    <yrPubYr>1982</yrPubYr>
    <dateCit>2010-04-21</dateCit>
    <sTitle>The NBS tables of chemical thermodynamic properties</sTitle>
    <sVol>11</sVol>
    <sPage>2-1</sPage>
  </Citation>
  <Compound>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <sCommonName>sulfate ion</sCommonName>
    <sFormulaMolec>O4S</sFormulaMolec>
```

```
    <ion>
      <nCharge>-2</nCharge>
    </ion>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>2</nOrgNum>
    </RegNum>
    <sCommonName>sulfur cation</sCommonName>
    <sFormulaMolec>S</sFormulaMolec>
    <ion>
      <nCharge>1</nCharge>
    </ion>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
    <sCommonName>oxygen</sCommonName>
    <sFormulaMolec>O2</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>4</nOrgNum>
    </RegNum>
    <sCommonName>sulfur</sCommonName>
    <sFormulaMolec>S</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
    <sCommonName>water</sCommonName>
    <sFormulaMolec>H2O</sFormulaMolec>
  </Compound>
  <Compound>
    <RegNum>
      <nOrgNum>6</nOrgNum>
```

```
      </RegNum>
      <sCommonName>electron</sCommonName>
      <sFormulaMolec>e</sFormulaMolec>
      <ion>
        <nCharge>-1</nCharge>
      </ion>
    </Compound>
    <Compound>
      <RegNum>
        <nOrgNum>7</nOrgNum>
      </RegNum>
      <sCommonName>hydrohen ion</sCommonName>
      <sFormulaMolec>H</sFormulaMolec>
      <ion>
        <nCharge>1</nCharge>
      </ion>
    </Compound>
    <Compound>
      <RegNum>
        <nOrgNum>8</nOrgNum>
      </RegNum>
      <sCommonName>hydrohen</sCommonName>
      <sFormulaMolec>H2</sFormulaMolec>
    </Compound>
  <PureOrMixtureData>
    <Component>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
    </Component>
    <Component>
      <RegNum>
        <nOrgNum>5</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
    </Component>
    <eExpPurpose>Principal objective of the work</eExpPurpose>
```

```
<sCompiler>TRC</sCompiler>
<sContributor>VVD</sContributor>
<dateDateAdded>4/22/2010</dateDateAdded>
<Property>
 <nPropNumber>1</nPropNumber>
 <Property-MethodID>
  <PropertyGroup>
   <ExcessPartialApparentEnergyProp>
    <ePropName>Standard state molar entropy, J/K/mol</ePropName>
    <sMethodName>Other</sMethodName>
   </ExcessPartialApparentEnergyProp>
  </PropertyGroup>
  <RegNum>
   <nOrgNum>1</nOrgNum>
  </RegNum>
 </Property-MethodID>
 <PropPhaseID>
  <ePropPhase>Liquid</ePropPhase>
 </PropPhaseID>
 <ePresentation>Direct value, X</ePresentation>
 <Solvent>
  <RegNum>
   <nOrgNum>3</nOrgNum>
  </RegNum>
 </Solvent>
 <eStandardState>Infinite dilution solute</eStandardState>
</Property>
<PhaseID>
 <ePhase>Liquid</ePhase>
</PhaseID>
<Constraint>
 <ConstraintID>
  <ConstraintType>
   <eTemperature>Temperature, K</eTemperature>
  </ConstraintType>
 </ConstraintID>
 <nConstraintValue>298.15</nConstraintValue>
 <nConstrDigits>5</nConstrDigits>
```

```
  </Constraint>
  <Constraint>
    <ConstraintID>
      <ConstraintType>
        <ePressure>Pressure, kPa</ePressure>
      </ConstraintType>
    </ConstraintID>
    <nConstraintValue>100</nConstraintValue>
    <nConstrDigits>3</nConstrDigits>
  </Constraint>
  <Variable>
    <nVarNumber>1</nVarNumber>
    <VariableID>
      <VariableType>
        <eComponentComposition>Molality, mol/kg</eComponentComposition>
      </VariableType>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
    </VariableID>
    <VarPhaseID>
      <eVarPhase>Liquid</eVarPhase>
    </VarPhaseID>
    <Solvent>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
    </Solvent>
  </Variable>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>1</nVarValue>
      <nVarDigits>1</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>20.1</nPropValue>
```

```
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
</PureOrMixtureData>
<PureOrMixtureData>
  <Component>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
    <nSampleNm>0</nSampleNm>
  </Component>
  <Component>
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
    <nSampleNm>0</nSampleNm>
  </Component>
  <eExpPurpose>Principal objective of the work</eExpPurpose>
  <sCompiler>TRC</sCompiler>
  <sContributor>VVD</sContributor>
  <dateDateAdded>4/22/2010</dateDateAdded>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <ExcessPartialApparentEnergyProp>
          <ePropName>Standard state molar heat capacity, J/K/mol</ePropName>
          <sMethodName>Other</sMethodName>
        </ExcessPartialApparentEnergyProp>
      </PropertyGroup>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
    </Property-MethodID>
    <PropPhaseID>
      <ePropPhase>Liquid</ePropPhase>
    </PropPhaseID>
    <ePresentation>Direct value, X</ePresentation>
```

```
  <Solvent>
    <RegNum>
      <nOrgNum>3</nOrgNum>
    </RegNum>
  </Solvent>
  <eStandardState>Infinite dilution solute</eStandardState>
</Property>
<PhaseID>
  <ePhase>Liquid</ePhase>
</PhaseID>
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <eTemperature>Temperature, K</eTemperature>
    </ConstraintType>
  </ConstraintID>
  <nConstraintValue>298.15</nConstraintValue>
  <nConstrDigits>5</nConstrDigits>
</Constraint>
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <ePressure>Pressure, kPa</ePressure>
    </ConstraintType>
  </ConstraintID>
  <nConstraintValue>100</nConstraintValue>
  <nConstrDigits>3</nConstrDigits>
</Constraint>
<Variable>
  <nVarNumber>1</nVarNumber>
  <VariableID>
    <VariableType>
      <eComponentComposition>Molality, mol/kg</eComponentComposition>
    </VariableType>
    <RegNum>
      <nOrgNum>1</nOrgNum>
    </RegNum>
  </VariableID>
```

```
    <VarPhaseID>
      <eVarPhase>Liquid</eVarPhase>
    </VarPhaseID>
    <Solvent>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
    </Solvent>
  </Variable>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>1</nVarValue>
      <nVarDigits>1</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>-293</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
</PureOrMixtureData>
<ReactionData>
    <Participant>
        <RegNum>
            <nOrgNum>2</nOrgNum>
        </RegNum>
        <nSampleNm>0</nSampleNm>
        <nStoichiometricCoef>1</nStoichiometricCoef>
        <ePhase>Ideal gas</ePhase>
    </Participant>
    <Participant>
        <RegNum>
            <nOrgNum>6</nOrgNum>
        </RegNum>
        <nSampleNm>0</nSampleNm>
        <nStoichiometricCoef>1</nStoichiometricCoef>
        <ePhase>Ideal gas</ePhase>
```

```
</Participant>
<Participant>
  <RegNum>
    <nOrgNum>4</nOrgNum>
  </RegNum>
  <nSampleNm>0</nSampleNm>
  <nStoichiometricCoef>-1</nStoichiometricCoef>
  <ePhase>Crystal</ePhase>
</Participant>
<eExpPurpose>Principal objective of the work</eExpPurpose>
<sCompiler>TRC</sCompiler>
<sContributor>VVD</sContributor>
<dateDateAdded>4/21/2010</dateDateAdded>
<eReactionType>Formation of ion</eReactionType>
<Property>
  <nPropNumber>1</nPropNumber>
  <Property-MethodID>
    <PropertyGroup>
      <ReactionStateChangeProp>
        <ePropName>Molar enthalpy of reaction, kJ/mol</ePropName>
        <CriticalEvaluation>
          <SingleProp/>
        </CriticalEvaluation>
      </ReactionStateChangeProp>
    </PropertyGroup>
  </Property-MethodID>
  <nTemperature-K>1</nTemperature-K>
  <nTemperatureDigits>1</nTemperatureDigits>
  <nPressure-kPa>100</nPressure-kPa>
  <nPressureDigits>3</nPressureDigits>
</Property>
<NumValues>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>1276.133</nPropValue>
    <nPropDigits>7</nPropDigits>
  </PropertyValue>
</NumValues>
```

```
  </ReactionData>
  <ReactionData>
    <Participant>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>1</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
      <eCompositionRepresentation>Molality - amount of participant per mass of solvent, mol/kg</eCompositionRepresentation>
      <nNumericalComposition>0</nNumericalComposition>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>7</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>-2</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>4</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>-1</nStoichiometricCoef>
      <ePhase>Crystal</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>-2</nStoichiometricCoef>
      <ePhase>Ideal gas</ePhase>
    </Participant>
    <Participant>
      <RegNum>
```

```
      <nOrgNum>8</nOrgNum>
    </RegNum>
    <nSampleNm>0</nSampleNm>
    <nStoichiometricCoef>-1</nStoichiometricCoef>
    <ePhase>Ideal gas</ePhase>
  </Participant>
  <eExpPurpose>Principal objective of the work</eExpPurpose>
  <sCompiler>TRC</sCompiler>
  <sContributor>VVD</sContributor>
  <dateDateAdded>4/21/2010</dateDateAdded>
  <eReactionType>Formation of ion</eReactionType>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <ReactionStateChangeProp>
          <ePropName>Molar enthalpy of reaction, kJ/mol</ePropName>
          <CriticalEvaluation>
            <SingleProp/>
          </CriticalEvaluation>
        </ReactionStateChangeProp>
      </PropertyGroup>
    </Property-MethodID>
    <Solvent>
      <RegNum>
        <nOrgNum>5</nOrgNum>
      </RegNum>
      <ePhase>Solution 1</ePhase>
    </Solvent>
    <nTemperature-K>298.15</nTemperature-K>
    <nTemperatureDigits>5</nTemperatureDigits>
    <nPressure-kPa>100</nPressure-kPa>
    <nPressureDigits>3</nPressureDigits>
  </Property>
  <NumValues>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>-909.27</nPropValue>
```

```
        <nPropDigits>5</nPropDigits>
      </PropertyValue>
    </NumValues>
  </ReactionData>
  <ReactionData>
    <Participant>
      <RegNum>
        <nOrgNum>1</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>1</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
      <eCompositionRepresentation>Molality - amount of participant per mass of solvent, mol/kg</eCompositionRepresentation>
      <nNumericalComposition>1</nNumericalComposition>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>7</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>-2</nStoichiometricCoef>
      <ePhase>Solution 1</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>4</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>-1</nStoichiometricCoef>
      <ePhase>Crystal</ePhase>
    </Participant>
    <Participant>
      <RegNum>
        <nOrgNum>3</nOrgNum>
      </RegNum>
      <nSampleNm>0</nSampleNm>
      <nStoichiometricCoef>-2</nStoichiometricCoef>
      <ePhase>Ideal gas</ePhase>
```

```
</Participant>
<Participant>
  <RegNum>
    <nOrgNum>8</nOrgNum>
  </RegNum>
  <nSampleNm>0</nSampleNm>
  <nStoichiometricCoef>-1</nStoichiometricCoef>
  <ePhase>Ideal gas</ePhase>
</Participant>
<eExpPurpose>Principal objective of the work</eExpPurpose>
<sCompiler>TRC</sCompiler>
<sContributor>VVD</sContributor>
<dateDateAdded>4/21/2010</dateDateAdded>
<eReactionType>Formation of ion</eReactionType>
<Property>
  <nPropNumber>1</nPropNumber>
  <Property-MethodID>
    <PropertyGroup>
      <ReactionStateChangeProp>
        <ePropName>Molar Gibbs energy of reaction, kJ/mol</ePropName>
        <CriticalEvaluation>
          <SingleProp/>
        </CriticalEvaluation>
      </ReactionStateChangeProp>
    </PropertyGroup>
  </Property-MethodID>
  <Solvent>
    <RegNum>
      <nOrgNum>5</nOrgNum>
    </RegNum>
    <ePhase>Solution 1</ePhase>
  </Solvent>
  <eStandardState>Infinite dilution solute</eStandardState>
  <nTemperature-K>298.15</nTemperature-K>
  <nTemperatureDigits>5</nTemperatureDigits>
  <nPressure-kPa>100</nPressure-kPa>
  <nPressureDigits>3</nPressureDigits>
</Property>
```

```
      <NumValues>
        <PropertyValue>
          <nPropNumber>1</nPropNumber>
          <nPropValue>-744.53</nPropValue>
          <nPropDigits>5</nPropDigits>
        </PropertyValue>
      </NumValues>
    </ReactionData>
</DataReport>
```

********** Use Case 12 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
 <Version>
    <nVersionMajor>4</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>1986</yrYrPub>
      <sAuthor1>cha</sAuthor1>
      <sAuthor2>hal</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Chao, J.[Jing]</sAuthor>
    <sAuthor>Hall, K. R.[Kenneth R.]</sAuthor>
    <sAuthor>Marsh, K. N.[Kenneth N.]</sAuthor>
    <sAuthor>Wilhoit, R. C.[Randolph C.]</sAuthor>
    <sPubName>J. Phys. Chem. Ref. Data</sPubName>
    <yrPubYr>1986</yrPubYr>
    <dateCit>2011-03-29</dateCit>
    <sTitle>Thermodynamic Properties of Key Organic Oxygen Compounds in the  Carbon Range C1 to C4</sTitle>
    <sVol>15</sVol>
    <sPage>1369</sPage>
  </Citation>
 <Compound>
   <nCompIndex>1</nCompIndex>
  <sCommonName>acetic acid</sCommonName>
  <sFormulaMolec>C2H4O2</sFormulaMolec>
  <Sample>
    <nSampleNm>1</nSampleNm>
  </Sample>
 </Compound>
 <Compound>
  <nCompIndex>2</nCompIndex>
```

```
  <sCommonName>acetic acid monomer</sCommonName>
  <sFormulaMolec>C2H4O2</sFormulaMolec>
  <eSpeciationState>single species</eSpeciationState>
  <Sample>
    <nSampleNm>1</nSampleNm>
  </Sample>
</Compound>
<Compound>
  <nCompIndex>3</nCompIndex>
  <sCommonName>acetic acid dimer</sCommonName>
     <sFormulaMolec>C4H8O4</sFormulaMolec>
  <eSpeciationState>single species</eSpeciationState>
  <Sample>
    <nSampleNm>1</nSampleNm>
     </Sample>
  </Compound>
  <PureOrMixtureData>
     <Component>
    <nCompIndex>1</nCompIndex>
    <nSampleNm>1</nSampleNm>
     </Component>
     <eExpPurpose>Principal objective of the work</eExpPurpose>
     <sCompiler>VVD</sCompiler>
     <sContributor>TRC</sContributor>
     <dateDateAdded>3/29/2011</dateDateAdded>
     <Property>
        <nPropNumber>1</nPropNumber>
        <Property-MethodID>
           <PropertyGroup>
              <HeatCapacityAndDerivedProp>
                 <ePropName>Molar entropy, J/K/mol</ePropName>
        <CriticalEvaluation>
          <MultiProp>
          </MultiProp>
        </CriticalEvaluation>
      </HeatCapacityAndDerivedProp>
           </PropertyGroup>
        </Property-MethodID>
```

```
      <PropPhaseID>
        <ePropPhase>Ideal gas</ePropPhase>
      </PropPhaseID>
      <ePresentation>Direct value, X</ePresentation>
    </Property>
    <PhaseID>
        <ePhase>Ideal gas</ePhase>
    </PhaseID>
    <Constraint>
      <ConstraintID>
        <ConstraintType>
          <ePressure>Pressure, kPa</ePressure>
        </ConstraintType>
      </ConstraintID>
      <nConstraintValue>101.325</nConstraintValue>
      <nConstrDigits>6</nConstrDigits>
    </Constraint>
    <Variable>
      <nVarNumber>1</nVarNumber>
      <VariableID>
        <VariableType>
          <eTemperature>Temperature, K</eTemperature>
        </VariableType>
      </VariableID>
    </Variable>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>298.15</nVarValue>
        <nVarDigits>5</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>208.85</nPropValue>
        <nPropDigits>5</nPropDigits>
      </PropertyValue>
    </NumValues>
  </PureOrMixtureData>
```

```
<PureOrMixtureData>
 <Component>
  <nCompIndex>2</nCompIndex>
  <nSampleNm>1</nSampleNm>
 </Component>
 <eExpPurpose>Principal objective of the work</eExpPurpose>
 <sCompiler>VVD</sCompiler>
 <sContributor>TRC</sContributor>
 <dateDateAdded>3/29/2011</dateDateAdded>
 <Property>
  <nPropNumber>1</nPropNumber>
  <Property-MethodID>
   <PropertyGroup>
    <HeatCapacityAndDerivedProp>
     <ePropName>Molar entropy, J/K/mol</ePropName>
     <CriticalEvaluation>
      <MultiProp>
      </MultiProp>
     </CriticalEvaluation>
    </HeatCapacityAndDerivedProp>
   </PropertyGroup>
  </Property-MethodID>
  <PropPhaseID>
   <ePropPhase>Ideal gas</ePropPhase>
  </PropPhaseID>
  <ePresentation>Direct value, X</ePresentation>
 </Property>
 <PhaseID>
  <ePhase>Ideal gas</ePhase>
 </PhaseID>
 <Constraint>
  <ConstraintID>
   <ConstraintType>
    <ePressure>Pressure, kPa</ePressure>
   </ConstraintType>
  </Constraint>
  <nConstraintValue>101.325</nConstraintValue>
  <nConstrDigits>6</nConstrDigits>
```

```
  </Constraint>
  <Variable>
    <nVarNumber>1</nVarNumber>
    <VariableID>
      <VariableType>
        <eTemperature>Temperature, K</eTemperature>
      </VariableType>
    </VariableID>
  </Variable>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>298.15</nVarValue>
      <nVarDigits>5</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>283.47</nPropValue>
      <nPropDigits>5</nPropDigits>
    </PropertyValue>
  </NumValues>
</PureOrMixtureData>
<PureOrMixtureData>
  <Component>
    <nCompIndex>3</nCompIndex>
    <nSampleNm>1</nSampleNm>
  </Component>
  <eExpPurpose>Principal objective of the work</eExpPurpose>
  <sCompiler>VVD</sCompiler>
  <sContributor>TRC</sContributor>
  <dateDateAdded>3/29/2011</dateDateAdded>
  <Property>
    <nPropNumber>1</nPropNumber>
    <Property-MethodID>
      <PropertyGroup>
        <HeatCapacityAndDerivedProp>
          <ePropName>Molar entropy, J/K/mol</ePropName>
          <CriticalEvaluation>
```

```
        <MultiProp>
        </MultiProp>
       </CriticalEvaluation>
      </HeatCapacityAndDerivedProp>
    </PropertyGroup>
  </Property-MethodID>
  <PropPhaseID>
    <ePropPhase>Ideal gas</ePropPhase>
  </PropPhaseID>
  <ePresentation>Direct value, X</ePresentation>
</Property>
<PhaseID>
  <ePhase>Ideal gas</ePhase>
</PhaseID>
<Constraint>
  <ConstraintID>
    <ConstraintType>
      <ePressure>Pressure, kPa</ePressure>
    </ConstraintType>
  </ConstraintID>
  <nConstraintValue>101.325</nConstraintValue>
  <nConstrDigits>6</nConstrDigits>
</Constraint>
<Variable>
  <nVarNumber>1</nVarNumber>
  <VariableID>
    <VariableType>
      <eTemperature>Temperature, K</eTemperature>
    </VariableType>
  </VariableID>
</Variable>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>298.15</nVarValue>
    <nVarDigits>5</nVarDigits>
  </VariableValue>
  <PropertyValue>
```

```
      <nPropNumber>1</nPropNumber>
      <nPropValue>414.39</nPropValue>
      <nPropDigits>5</nPropDigits>
    </PropertyValue>
  </NumValues>
 </PureOrMixtureData>
</DataReport>
```

********** Use Case 13 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>4</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Kuznetsov, A. Y.</sAuthor>
    <sAuthor>Kudin, L. S.</sAuthor>
    <sAuthor>Pogrebnoi, A. M.</sAuthor>
    <sAuthor>Butman, M. F.</sAuthor>
    <sAuthor>Burdukovskaya, G. G.</sAuthor>
    <sPubName>Zh. Fiz. Khim.</sPubName>
    <yrPubYr>1999</yrPubYr>
    <dateCit>2011-03-28</dateCit>
    <sTitle>Thermodynamic Properties of Neutral and Ionic Components of Holmium Trichloride Vapor</sTitle>
    <sVol>73</sVol>
    <sPage>566-569</sPage>
  </Citation>
  <Compound>
    <nCompIndex>1</nCompIndex>
    <sCommonName>holmium trichloride</sCommonName>
    <sFormulaMolec>Cl3Ho</sFormulaMolec>
    <eSpeciationState>equilibrium</eSpeciationState>
    <Sample>
      <nSampleNm>1</nSampleNm>
    </Sample>
  </Compound>
  <Compound>
    <nCompIndex>2</nCompIndex>
    <sCommonName>holmium trichloride</sCommonName>
    <sFormulaMolec>Cl3Ho</sFormulaMolec>
    <eSpeciationState>single species</eSpeciationState>
    <Sample>
```

```
      <nSampleNm>1</nSampleNm>
    </Sample>
  </Compound>
  <Compound>
    <nCompIndex>3</nCompIndex>
    <sCommonName>diholmium hexachloride</sCommonName>
    <sFormulaMolec>Cl6Ho2</sFormulaMolec>
    <eSpeciationState>single species</eSpeciationState>
    <Sample>
      <nSampleNm>1</nSampleNm>
    </Sample>
  </Compound>
  <PureOrMixtureData>
    <Component>
      <nCompIndex>1</nCompIndex>
      <nSampleNm>1</nSampleNm>
    </Component>
    <eExpPurpose>Principal objective of the work</eExpPurpose>
    <sCompiler>VVD</sCompiler>
    <sContributor>TRC</sContributor>
    <dateDateAdded>3/28/2011</dateDateAdded>
    <Property>
      <nPropNumber>1</nPropNumber>
      <Property-MethodID>
        <PropertyGroup>
          <VaporPBoilingTAzeotropTandP>
            <ePropName>Vapor or sublimation pressure, kPa</ePropName>
            <sMethodName>mass spectrometry</sMethodName>
          </VaporPBoilingTAzeotropTandP>
        </PropertyGroup>
        <nCompIndex>2</nCompIndex>
      </Property-MethodID>
      <PropPhaseID>
        <ePropPhase>Crystal</ePropPhase>
      </PropPhaseID>
      <ePresentation>Direct value, X</ePresentation>
    </Property>
    <PhaseID>
```

```
        <ePhase>Crystal</ePhase>
    </PhaseID>
    <PhaseID>
        <ePhase>Gas</ePhase>
    </PhaseID>
    <Variable>
      <nVarNumber>1</nVarNumber>
      <VariableID>
        <VariableType>
          <eTemperature>Temperature, K</eTemperature>
        </VariableType>
      </VariableID>
    </Variable>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>938</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>.000089469975</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
      <VariableValue>
        <nVarNumber>1</nVarNumber>
        <nVarValue>959</nVarValue>
        <nVarDigits>3</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>.00017529225</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
    <NumValues>
```

```
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>983</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>.00051169125</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>997</nVarValue>
      <nVarDigits>3</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>.0011449725</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
      <nVarValue>1027</nVarValue>
      <nVarDigits>4</nVarDigits>
    </VariableValue>
    <PropertyValue>
      <nPropNumber>1</nPropNumber>
      <nPropValue>.0022392825</nPropValue>
      <nPropDigits>3</nPropDigits>
    </PropertyValue>
  </NumValues>
  <NumValues>
    <VariableValue>
      <nVarNumber>1</nVarNumber>
```

```
        <nVarValue>1051</nVarValue>
        <nVarDigits>4</nVarDigits>
      </VariableValue>
      <PropertyValue>
        <nPropNumber>1</nPropNumber>
        <nPropValue>.003465315</nPropValue>
        <nPropDigits>3</nPropDigits>
      </PropertyValue>
    </NumValues>
  </PureOrMixtureData>
  <PureOrMixtureData>
    <Component>
      <nCompIndex>1</nCompIndex>
      <nSampleNm>1</nSampleNm>
    </Component>
    <eExpPurpose>Principal objective of the work</eExpPurpose>
    <sCompiler>VVD</sCompiler>
    <sContributor>TRC</sContributor>
    <dateDateAdded>3/28/2011</dateDateAdded>
    <Property>
      <nPropNumber>1</nPropNumber>
      <Property-MethodID>
        <PropertyGroup>
          <VaporPBoilingTAzeotropTandP>
            <ePropName>Vapor or sublimation pressure, kPa</ePropName>
            <sMethodName>mass spectrometry</sMethodName>
          </VaporPBoilingTAzeotropTandP>
        </PropertyGroup>
        <nCompIndex>3</nCompIndex>
      </Property-MethodID>
      <PropPhaseID>
        <ePropPhase>Crystal</ePropPhase>
      </PropPhaseID>
      <ePresentation>Direct value, X</ePresentation>
    </Property>
    <PhaseID>
        <ePhase>Crystal</ePhase>
    </PhaseID>
```

```
<PhaseID>
    <ePhase>Gas</ePhase>
</PhaseID>
<Variable>
  <nVarNumber>1</nVarNumber>
  <VariableID>
    <VariableType>
      <eTemperature>Temperature, K</eTemperature>
    </VariableType>
  </VariableID>
</Variable>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>940</nVarValue>
    <nVarDigits>3</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>.000002776305</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
    <nVarValue>959</nVarValue>
    <nVarDigits>3</nVarDigits>
  </VariableValue>
  <PropertyValue>
    <nPropNumber>1</nPropNumber>
    <nPropValue>.00000514731</nPropValue>
    <nPropDigits>3</nPropDigits>
  </PropertyValue>
</NumValues>
<NumValues>
  <VariableValue>
    <nVarNumber>1</nVarNumber>
```

```
            <nVarValue>997</nVarValue>
            <nVarDigits>3</nVarDigits>
          </VariableValue>
          <PropertyValue>
            <nPropNumber>1</nPropNumber>
            <nPropValue>.000064746675</nPropValue>
            <nPropDigits>3</nPropDigits>
          </PropertyValue>
        </NumValues>
        <NumValues>
          <VariableValue>
            <nVarNumber>1</nVarNumber>
            <nVarValue>1027</nVarValue>
            <nVarDigits>4</nVarDigits>
          </VariableValue>
          <PropertyValue>
            <nPropNumber>1</nPropNumber>
            <nPropValue>.0001276695</nPropValue>
            <nPropDigits>3</nPropDigits>
          </PropertyValue>
        </NumValues>
        <NumValues>
          <VariableValue>
            <nVarNumber>1</nVarNumber>
            <nVarValue>1051</nVarValue>
            <nVarDigits>4</nVarDigits>
          </VariableValue>
          <PropertyValue>
            <nPropNumber>1</nPropNumber>
            <nPropValue>.0001925175</nPropValue>
            <nPropDigits>3</nPropDigits>
          </PropertyValue>
        </NumValues>
      </PureOrMixtureData>
    </DataReport>
```

********** Use Case 14 **********


```
<?xml version="1.0" encoding="UTF-8"?>
<DataReport xmlns="http://www.iupac.org/namespaces/ThermoML" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.iupac.org/namespaces/ThermoML ThermoML.xsd">
  <Version>
    <nVersionMajor>4</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <Citation>
    <TRCRefID>
      <yrYrPub>2001</yrYrPub>
      <sAuthor1>dem</sAuthor1>
      <sAuthor2>yan</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>De Miguel, E. M.[Ernestina Munoz]</sAuthor>
    <sAuthor>Yanes, C.[Cayetano]</sAuthor>
    <sAuthor>Maestre, A.[Alfredo]</sAuthor>
    <sPubName>J. Chem. Eng. Data</sPubName>
    <yrPubYr>2001</yrPubYr>
    <dateCit>2011-03-29</dateCit>
    <sTitle>Mixing Enthalpies of Alkylureas with Electrolytes in Water at 298.15  K</sTitle>
    <sVol>46</sVol>
    <sPage>423</sPage>
  </Citation>
  <Compound>
    <nCompIndex>1</nCompIndex>
    <sCommonName>methylurea</sCommonName>
    <sFormulaMolec>C2H6N2O</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <Compound>
    <nCompIndex>2</nCompIndex>
```

```
    <sCommonName>sodium chloride</sCommonName>
    <sFormulaMolec>ClNa</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <Compound>
    <nCompIndex>3</nCompIndex>
    <sCommonName>water</sCommonName>
    <sFormulaMolec>H2O</sFormulaMolec>
    <Sample>
      <nSampleNm>1</nSampleNm>
      <eSource>Commercial source</eSource>
    </Sample>
  </Compound>
  <ReactionData>
    <Participant>
      <nCompIndex>1</nCompIndex>
      <nSampleNm>1</nSampleNm>
      <ePhase>Solution 1</ePhase>
    </Participant>
    <Participant>
      <nCompIndex>2</nCompIndex>
      <nSampleNm>1</nSampleNm>
      <ePhase>Solution 2</ePhase>
    </Participant>
    <Participant>
      <nCompIndex>1</nCompIndex>
      <nSampleNm>1</nSampleNm>
      <ePhase>Solution 3</ePhase>
    </Participant>
    <Participant>
      <nCompIndex>2</nCompIndex>
      <nSampleNm>1</nSampleNm>
      <ePhase>Solution 3</ePhase>
    </Participant>
    <Solvent>
```

```
      <nCompIndex>3</nCompIndex>
      <ePhase>Solution 1</ePhase>
    </Solvent>
    <Solvent>
      <nCompIndex>3</nCompIndex>
      <ePhase>Solution 2</ePhase>
    </Solvent>
    <Solvent>
      <nCompIndex>3</nCompIndex>
      <ePhase>Solution 3</ePhase>
    </Solvent>
    <eExpPurpose>Principal objective of the work</eExpPurpose>
    <sCompiler>VVD</sCompiler>
    <sContributor>TRC</sContributor>
    <dateDateAdded>3/29/2011</dateDateAdded>
    <eReactionType>Other reactions</eReactionType>
    <Property>
      <nPropNumber>1</nPropNumber>
      <Property-MethodID>
        <PropertyGroup>
          <ReactionStateChangeProp>
            <ePropName>Enthalpy of process, kJ</ePropName>
            <sMethodName>Fow calorimetry</sMethodName>
          </ReactionStateChangeProp>
        </PropertyGroup>
      </Property-MethodID>
      <nTemperature-K>298.15</nTemperature-K>
      <nTemperatureDigits>5</nTemperatureDigits>
      <nPressure-kPa>101.325</nPressure-kPa>
      <nPressureDigits>6</nPressureDigits>
    </Property>
  <Variable>
   <nVarNumber>1</nVarNumber>
   <VariableID>
    <VariableType>
     <eParticipantAmount>Amount, mol</eParticipantAmount>
    </VariableType>
    <nCompIndex>1</nCompIndex>
```

```
    </VariableID>
    <VarPhaseID>
      <eVarPhase>Liquid mixture 1</eVarPhase>
    </VarPhaseID>
  </Variable>
  <Variable>
    <nVarNumber>2</nVarNumber>
    <VariableID>
      <VariableType>
        <eParticipantAmount>Amount, mol</eParticipantAmount>
      </VariableType>
      <nCompIndex>2</nCompIndex>
    </VariableID>
    <VarPhaseID>
      <eVarPhase>Liquid mixture 2</eVarPhase>
    </VarPhaseID>
  </Variable>
  <Variable>
    <nVarNumber>3</nVarNumber>
    <VariableID>
      <VariableType>
        <eParticipantAmount>Amount, mol</eParticipantAmount>
      </VariableType>
      <nCompIndex>1</nCompIndex>
    </VariableID>
    <VarPhaseID>
      <eVarPhase>Liquid mixture 3</eVarPhase>
    </VarPhaseID>
  </Variable>
  <Variable>
    <nVarNumber>4</nVarNumber>
    <VariableID>
      <VariableType>
        <eParticipantAmount>Amount, mol</eParticipantAmount>
      </VariableType>
      <nCompIndex>2</nCompIndex>
    </VariableID>
    <VarPhaseID>
```

```
    <eVarPhase>Liquid mixture 3</eVarPhase>
  </VarPhaseID>
</Variable>
<Variable>
    <nVarNumber>5</nVarNumber>
    <VariableID>
      <VariableType>
        <eComponentComposition>Molality, mol/kg</eComponentComposition>
      </VariableType>
      <nCompIndex>1</nCompIndex>
    </VariableID>
    <VarPhaseID>
      <eVarPhase>Liquid mixture 1</eVarPhase>
    </VarPhaseID>
    <Solvent>
      <nCompIndex>3</nCompIndex>
    </Solvent>
  </Variable>
  <Variable>
    <nVarNumber>6</nVarNumber>
    <VariableID>
      <VariableType>
        <eComponentComposition>Molality, mol/kg</eComponentComposition>
      </VariableType>
      <nCompIndex>2</nCompIndex>
    </VariableID>
    <VarPhaseID>
      <eVarPhase>Liquid mixture 2</eVarPhase>
    </VarPhaseID>
    <Solvent>
      <nCompIndex>3</nCompIndex>
    </Solvent>
  </Variable>
  <NumValues>
 <VariableValue>
  <nVarNumber>1</nVarNumber>
  <nVarValue>-0.1258</nVarValue>
  <nVarDigits>6</nVarDigits>
```

```
    </VariableValue>
    <VariableValue>
      <nVarNumber>2</nVarNumber>
      <nVarValue>-0.1252</nVarValue>
      <nVarDigits>6</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>3</nVarNumber>
      <nVarValue>0.1258</nVarValue>
      <nVarDigits>6</nVarDigits>
    </VariableValue>
    <VariableValue>
      <nVarNumber>4</nVarNumber>
      <nVarValue>0.1252</nVarValue>
      <nVarDigits>6</nVarDigits>
    </VariableValue>
    <VariableValue>
            <nVarNumber>5</nVarNumber>
            <nVarValue>0.2581</nVarValue>
            <nVarDigits>6</nVarDigits>
        </VariableValue>
        <VariableValue>
            <nVarNumber>6</nVarNumber>
            <nVarValue>0.2442</nVarValue>
            <nVarDigits>6</nVarDigits>
        </VariableValue>
        <PropertyValue>
            <nPropNumber>1</nPropNumber>
            <nPropValue>-.0047</nPropValue>
            <nPropDigits>2</nPropDigits>
        </PropertyValue>
      </NumValues>
   </ReactionData>
</DataReport>
```