

```

<module version="1.0" encoding="utf-8"?>
  <module convention="convention:compchem"
    xmlns="http://www.xml-cml.org/schema"
    xmlns:iupac="http://www.iupac.org/"
    xmlns:xsd="http://www.w3.org/2001/XMLSchema"
    xmlns:si="http://www.xml-cml.org/unit/si/"
  >
    <module dictRef="cc:jobList">
      <module dictRef="cc:job">
        <module dictRef="cc:initialization">
          <molecule convention="convention:molecular" id="mol-init-1" formalCharge="0" spinMultiplicity="1">
            ...
          </molecule>
          <parameterList>
            <parameter dictRef="cc:basis">
              <scalar dataType="xsd:string">6-311+G(d,p)</scalar>
            </parameter>
            <parameter dictRef="cc:method">
              <scalar dataType="xsd:string">UB971</scalar>
            </parameter>
            <parameter dictRef="g:goal">
              <scalar dataType="xsd:string">FOpt</scalar>
            </parameter>
            <parameter dictRef="cc:goal">
              <scalar dataType="xsd:string">Geometry optimization</scalar>
            </parameter>
            <parameter dictRef="g:route">
              <scalar dataType="xsd:string">#p uB971/6-311+G(d,p) Opt=(Tight, NewEstmFC, MaxCyc = 200) GFInput
                Freq=(HinderedRotor) Population=None Integral(Grid=UltraFine) Guess=Mix NoSymmetry</scalar>
            </parameter>
          </parameterList>
        </module>
      <module dictRef="cc:finalization">
        ...
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    </module>
  </module>
  <module dictRef="cc:job">
    <module dictRef="cc:initialization">
      <molecule convention="convention:molecular" id="mol-init-3" formalCharge="0" spinMultiplicity="1">
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        ...
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    </module>
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      <molecule convention="convention:molecular" id="mol-final-4" formalCharge="0" spinMultiplicity="1">
        <atomArray>
          <atom id="a1" elementType="O" x3="-2.071636" y3="1.038054" z3="-0.6913" />
          <atom id="a2" elementType="Ti" x3="-0.924385" y3="0.140554" z3="0.051605" />
          <atom id="a3" elementType="O" x3="-0.180469" y3="-0.872918" z3="-0.993896" />
        </atomArray>
        <bondArray>
          <bond atomRefs2="a1 a2" id="a1_a2" order="D" />
          <bond atomRefs2="a2 a3" id="a2_a3" order="D" />
        </bondArray>
      </molecule>
      <propertyList>
        <property dictRef="cc:scfenergy">
          <scalar dataType="xsd:double" units="nonSi:hartree">-999.862822916</scalar>
        </property>
        <property dictRef="cc:vibrations">
          <table>
            <array dataType="xsd:string" size="3" dictRef="cc:labels">f1 f2 f3</array>
            <array dataType="xsd:double" size="3" units="nonSi:amu" dictRef="cc:reduced_masses">
              18.3734 20.219 18.5392</array>
            <array dataType="xsd:double" size="3" units="nonSi:mDyne.A^-1" dictRef="cc:force_consts">
              1.2673 11.5369 11.6911</array>
            <array dataType="xsd:double" size="3" units="nonSi:GHz" dictRef="cc:frequencies">342.1553
              984.1014 1034.5665</array>
          </table>
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        <property dictRef="cc:rotational_symmetry">
          <scalar dataType="xsd:integer" units="si:none">1</scalar>
        </property>
      </propertyList>
    </module>
  </module>
</module>

```