

Example of CMCS WebDav Data Collection: ***Organization of GRI-Mech Thermo***

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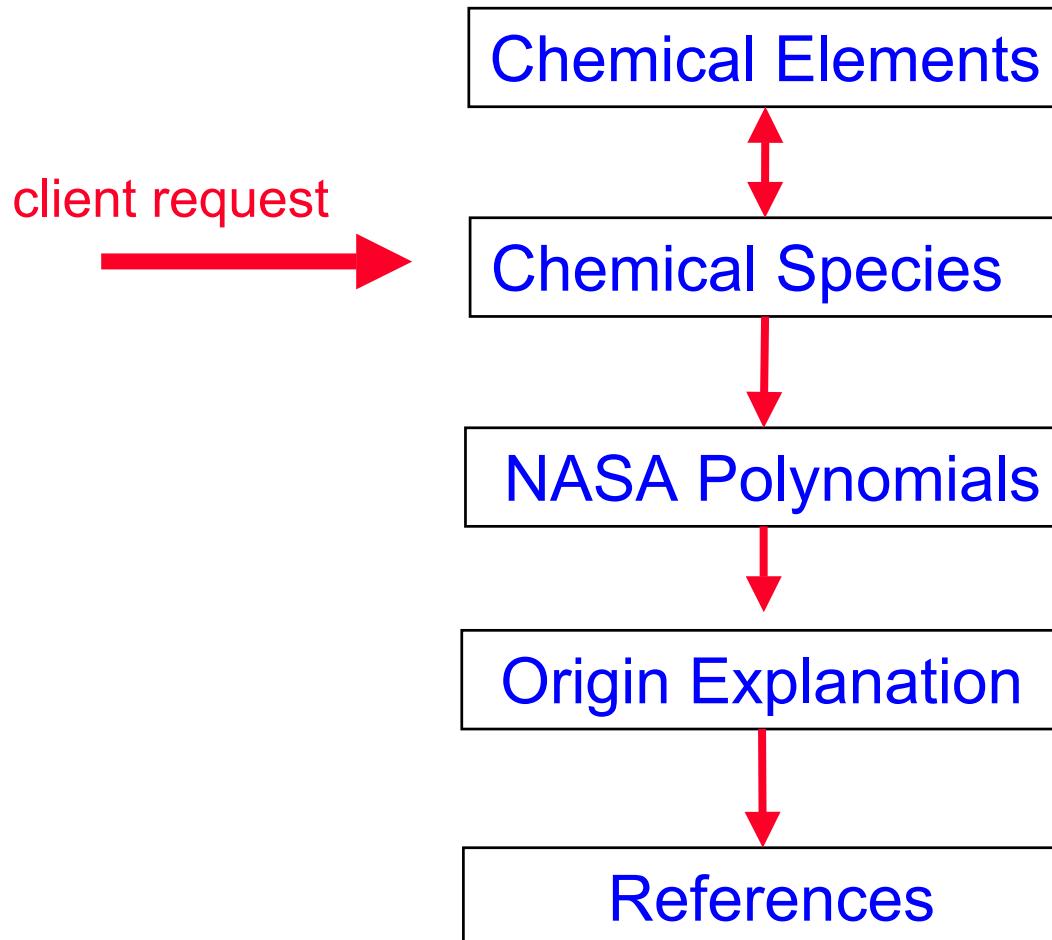
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Sandia National Laboratories



..../grimech/





..../chemSpecies/

ar.xml
c(gr).xml
c.xml
c2h.xml
c2h2.xml
c2h3.xml
c2h4.xml 
• • •

```
<molecule id="c2h4">
  <nomenclature>
    <name type="formula">C2H4</name>
    <name>ethene</name>
    <name>ethylene</name>
  </nomenclature>
  <composition>
    <chemElement id="C">2</chemElement>
    <chemElement id="H">4</chemElement>
  </composition>
</molecule>
```



..chemElements/

argon.xml

carbon.xml

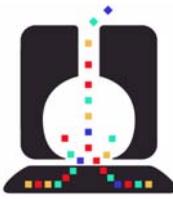
hydrogen.xml

nitrogen.xml

oxygen.xml

• • •

<chemElement id="C">
 <name>carbon</name>
 <symbol>C</symbol>
 <atomicWeight units="g/mol">12.0107</atomicWeight>
 <CASRegistryNo>7440-44-0</CASRegistryNo>
 <refElement>C(GR)</refElement>
 </chemElement>



...thermo/

- ar.xml
- c(gr).xml
- c.xml
- c2h.xml
- c2h2.xml
- c2h3.xml
- c2h4.xml
- • •

Each of these individual files has pedigree information attached to it

```
<thermo type="polyFit" id="c2h4" source="GRI-Mech 3.0" pedigree="c2h4">
  <coef type="nasa" TempRange="200 1000">3.9592015e+00 ...
  <coef type="nasa" TempRange="1000 3500">2.0361112e+00 ...
  <coef type="nasaF" TempRange="200 1000">-1.0771662e-01 ...
  <coef type="nasaF" TempRange="1000 5000">-7.5498320e+00 ...
</thermo>
```





..../description/

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hccn.xml

hco.xml

hcn.xml

hcno.xml

nasaThermo.xml

nh.xml

• • •



```
<description id="hcn" xmlns:xlink="http://www.w3.org/1999/xlink">
<p>The polynomial coefficients for heat capacity and entropy are from
<reference xlink:href="technion93">Burcat and McBride (1993).</reference>
</p>
<h2>Enthalpy of Formation</h2>
<p>The JANAF value of the enthalpy of formation for HCN was used in the
Sandia database and for GRI-Mech 2.11 and the base mechanism in the
GRI-Mech 3.0 optimization. It is the average of differing calorimetric
measurements and is assigned a large error bar of +/- 2.0 kcal/mole.
Therefore the HCN enthalpy was chosen as an optimization variable
for those GRI-Mech targets to which it is sensitive.</p>
<p>The following values of H_298 (in kcal/mol) for HCN have been reported:</p>
<ul>
<li>32.3<reference xlink:href="janaf3">JANAF tables (1985)</reference></li>
<li>31.1<reference xlink:href="trc91">TRC tables (1991)</reference></li>
<li>30.5<reference xlink:href="mlarw92">Morley et al (1992)</reference></li>
<li>31.0<reference xlink:href="martin96">Martin (1996)</reference></li>
<li>30.8<reference xlink:href="cwlpbkdkbe98">Clifford et al (1998)</reference></li>
</ul>
<p>GRI-Mech 3.0 adopts a value of 31.3 kcal/mole for H_298, near the more
recent consensus for this number and at the low end of the polynomial
range afforded in the optimization. This value was fixed in the optimization.
It corresponds to the enthalpy reported by
<reference xlink:href="hyk51">Horiuchi, Yano, and Kanai (1951),</reference>
one of the two differing values cited by JANAF.</p>
</description>
```



..../references/

• • •

dean_bozzelli.xml

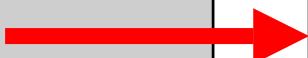
gurvich89.xml

janaf3.xml

sandia90.xml

technion95.xml

• • •



```
<reference id="sandia90">
  <type>report</type>
  <author>Kee, R. J.</author>
  <author>Rupley, F. M.</author>
  <author>Miller, J. A.</author>
  <year>1990</year>
  <title>The Chemkin Thermodynamic Data Base</title>
  <city>Livermore, CA</city>
  <institution>Sandia National Laboratories</institution>
  <pages />
  <edition />
  <date />
  <type />
  <shortTitle />
  <reportNumber>SAND87-8215B</reportNumber>
  <accessionNumber />
  <callNumber />
  <label />
  <keywords>thermodynamics,data</keywords>
  <abstract />
  <notes />
  <url />
  <authorAddress />
</reference>
```



Client Application Demo

A CMCS Example - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Search Favorites History Go Links >

Address http://www.me.berkeley.edu/gri_mech/plus/test5dav.html

T	Cp	S	delta-H_f
K	cal/mol K	kcal/mol	
300	7.14	43.95	9.4
400	7.07	46	9.41
500	7.05	47.57	9.4
600	7.06	48.86	9.38
700	7.09	49.95	9.35
800	7.15	50.9	9.31
900	7.23	51.74	9.26
1000	7.34	52.51	9.22
1100	7.45	53.21	9.17
1200	7.56	53.87	9.13

Begin by selecting a species from the drop-down menu on the left.

OH names mol weight show xml file

Temperature 300:100:3000 K calculate units cal

(e.g. 1200 or 1200:100:2000)

[View DAV grimech directory](#) [Explanations](#)

Done Internet