NIST Data Programs Supporting the Combustion Cyberinfrastructure

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NIST
National Institute of Standards and Technology
U.S. Department of Commerce

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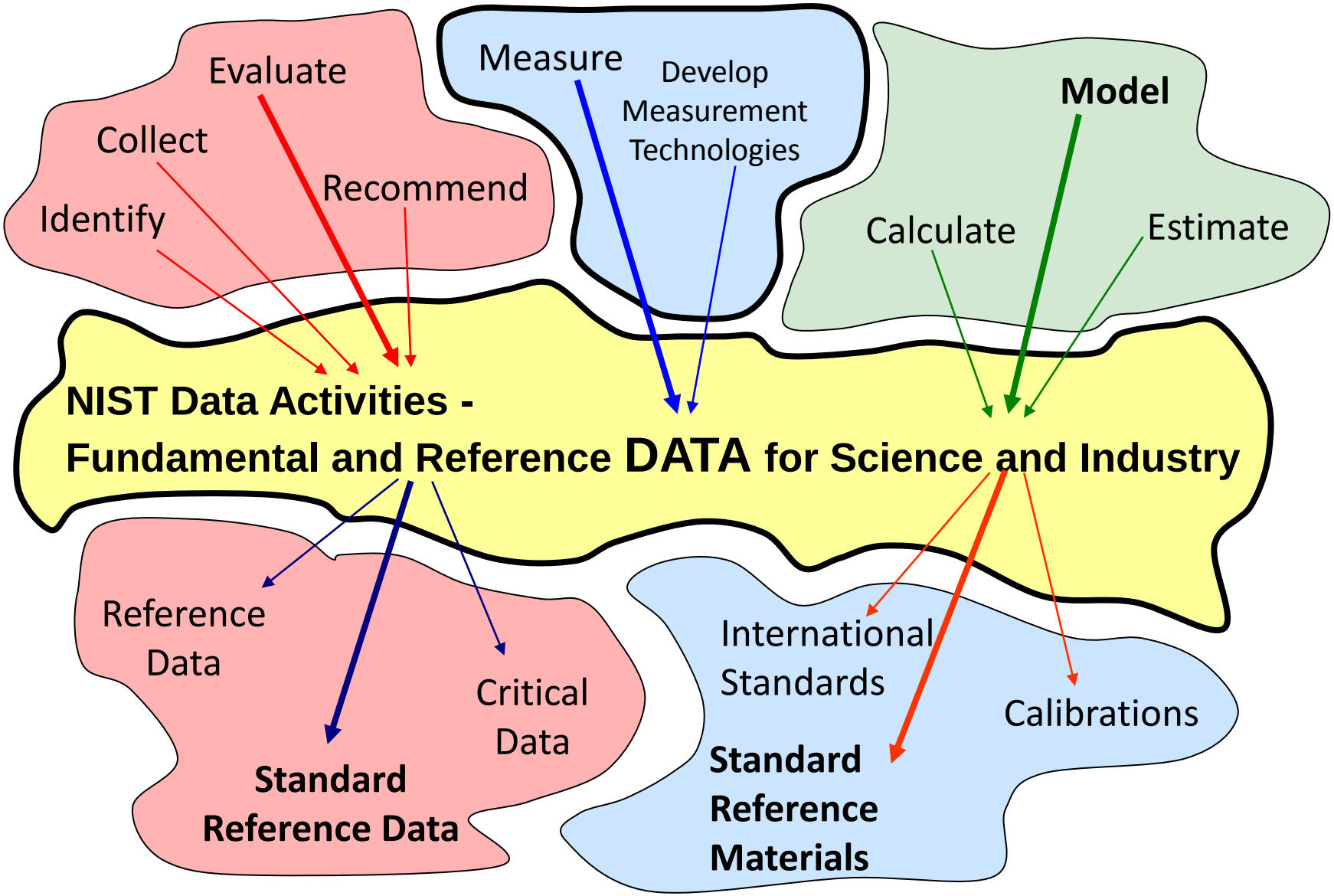
And many more…

Overview

- Current experimental and data efforts
  - What we are doing
- Materials Genome Initiative
  - NIST's role
- SRMDs
  - a new paradigm in reference data
- Future Directions


Evaluate
Collect
Identify
Recommend
Measure
Develop Measurement Technologies
Model
Calculate
Estimate
NIST Data Activities -
Fundamental and Reference DATA for Science and Industry
Reference Data
Critical Data
Standard Reference Data
International Standards
Calibrations
Standard Reference Materials

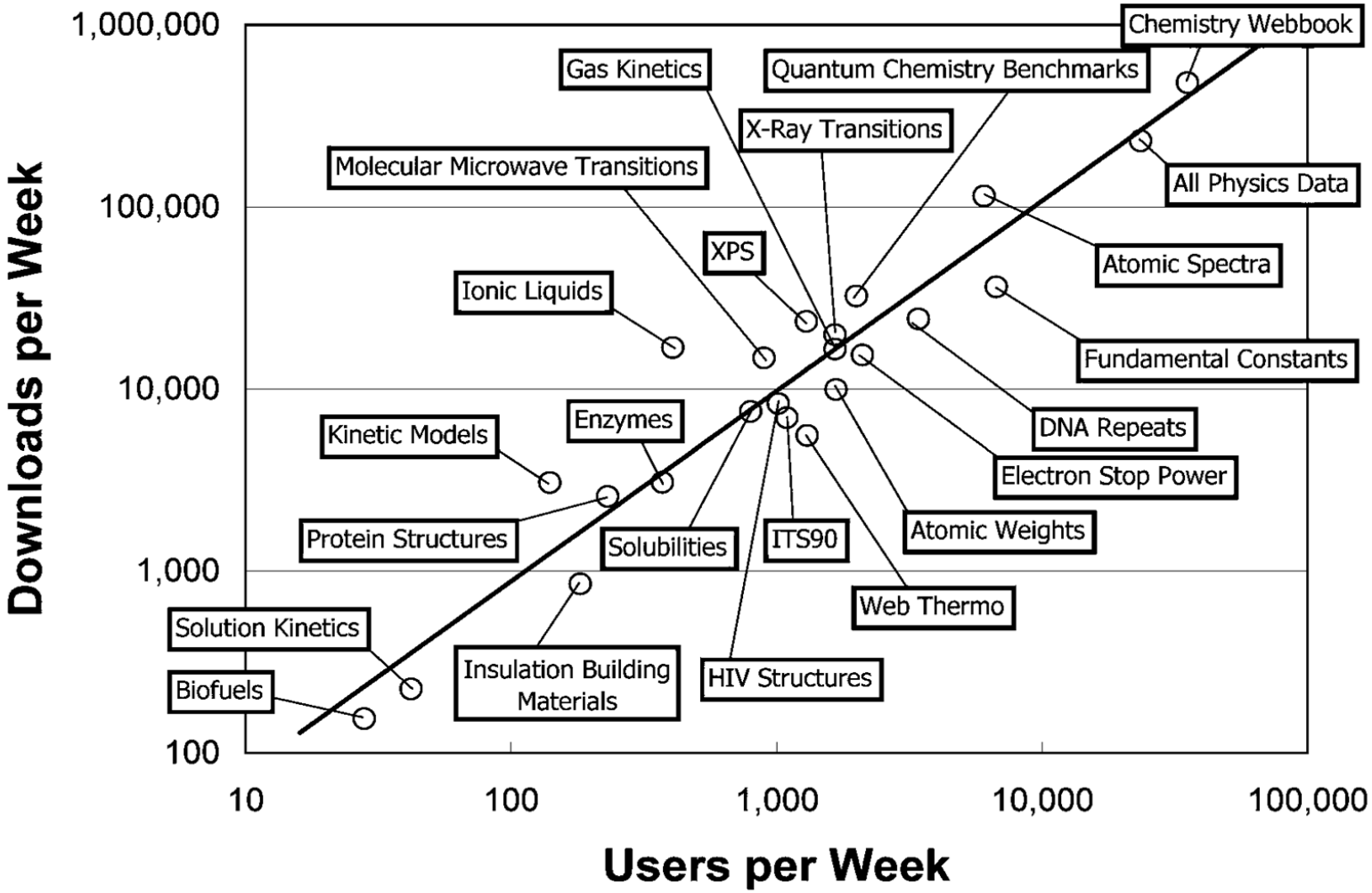
NIST as a Primary Source of Reference Data

- for science & industry
- Provide critical data/measurement technologies enabling the data efforts

Examples of data distributed by NIST

- Atomic Spectroscopic Data [PML]
- Fundamental Physical Constants [PML]
- The Official U.S. Time (atomic clock) [PML,TS]
- Thermochemical Data [MML]
- Chemical Kinetic Data [MML]
- Equation of State for Water (steam tables) [MML]
- NIST/EPA/NIH Mass Spectral Library [MML]
- Phase Equillibria Diagrams Database [MML]
- Crystallographic Structure Databases [MML]
- Heat Transmission Properties of Insulating and Building Materials Database [EL]

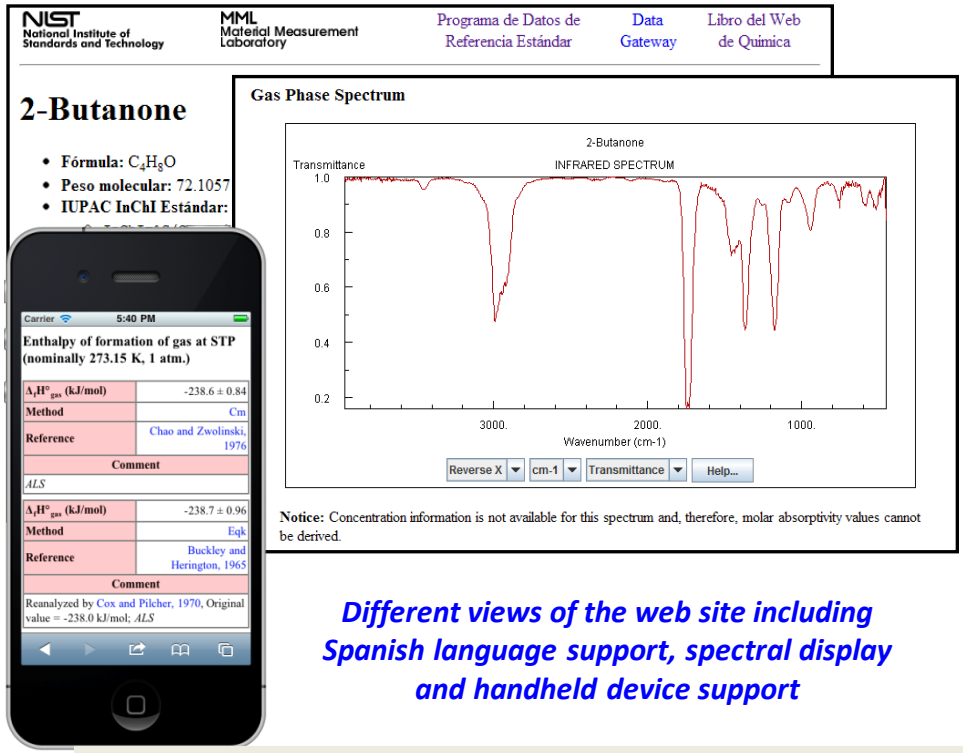
NIST Data - Online



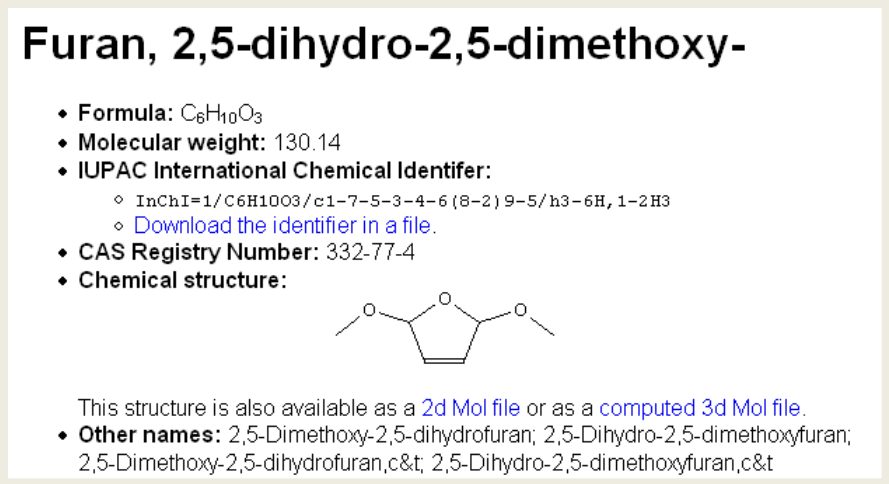
The NIST Chemistry WebBook

http://webbook.nist.gov/chemistry

- Widely used in industry
- Over 3,500 unique users/day
- Over 1,000 literature citations/yr
- Cited in 55 U.S. patents
- Highly ranked by Internet search engines



Different views of the web site including Spanish language support, spectral display and handheld device support



1-Propanol, 2-

webbook.nist.gov/cgi/cbook.cgi?ID=C78831&Units=SI

NIST National Institute of Standards and Technology

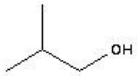
MML Material Measurement Laboratory

1-Propanol, 2-methyl-

- **Formula:** $C_4H_{10}O$
- **Molecular weight:** 74.1216
- **IUPAC Standard InChI:**
  - InChI=1S/C4H10O/c1-4(2)3-5/h4-5H,3H2,1-2H3
  - Download the identifier in a file.

InChI TRUST CERTIFIED 2011

- **IUPAC Standard InChIKey:** ZXEKIIBDNHEJCQ-UHFFFAOYSA-N
- **CAS Registry Number:** 78-83-1
- **Chemical structure:**



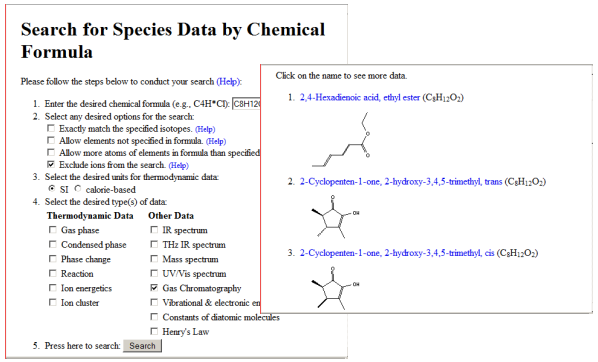
This structure is also available as a 2d Mol file or as a computed 3d Mol file.

- **Other names:** Isobutyl alcohol; Isobutanol; Isopropylcarbinol; 2-Methyl-1-propanol; iso-C4H9O ol; 2-Methylpropanol-1; 2-Methylpropyl alcohol; Butanol-iso; Alcool isobutylique; Isobutylalkoh 2-methyl-1-propanyl alcohol; i-Butanol; Methyl-2 propanol-1; NSC 5708; 2-methylpropanoI
- **Permanent link** for this species. Use this link for bookmarking this species for future reference.
- **Information on this page:**
  - Notes / Error Report
- **Other data available:**
  - Gas phase thermochemistry data
  - Condensed phase thermochemistry data
  - Phase change data
  - Reaction thermochemistry data
  - Henry's Law data
  - Gas phase ion energetics data
  - Ion clustering data
  - IR Spectrum
  - Mass spectrum (electron ionization)
  - Gas Chromatography
- **Data at other public NIST sites:**
  - Computational Chemistry Comparison and Benchmark Database
  - Gas Phase Kinetics Database
- **Options:**
  - Switch to calorie-based units

Data at NIST subscription sites:

Capabilities:

- Searching



Search for Species Data by Chemical Formula

Please follow the steps below to conduct your search (Help):

1. Enter the desired chemical formula (e.g., C4H*Cl): C8H12
2. Select any desired options for the search:
   - ☐ Exactly match the specified isotopes. (Help)
   - ☐ Allow elements not specified in formula. (Help)
   - ☐ Allow more atoms of elements in formula than specified
   - ☑ Exclude ions from the search. (Help)
3. Select the desired units for thermodynamic data:
   - ◉ SI ○ calorie-based
4. Select the desired type(s) of data:

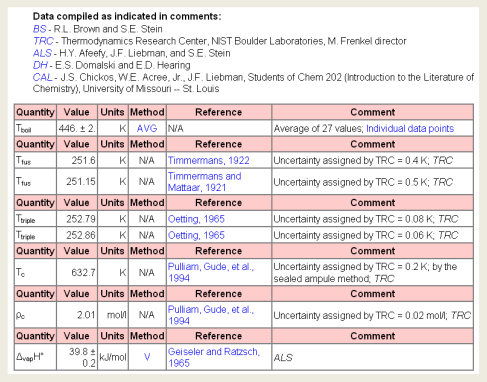
Thermodynamic Data	Other Data
☐ Gas phase	☐ IR spectrum
☐ Condensed phase	☐ THz IR spectrum
☐ Phase change	☐ Mass spectrum
☐ Reaction	☐ UV/Vis spectrum
☐ Ion energetics	☑ Gas Chromatography
☐ Ion cluster	☐ Vibrational & electronic en
	☐ Constants of diatomic molecules
	☐ Henry's Law

5. Press here to search: Search

Click on the name to see more data.

1. 2,4-Hexadienoic acid, ethyl ester ($C_8H_{12}O_2$)
2. 2-Cyclopenten-1-one, 2-hydroxy-3,4,5-trimethyl, trans ($C_8H_{12}O_2$)
3. 2-Cyclopenten-1-one, 2-hydroxy-3,4,5-trimethyl, cis ($C_8H_{12}O_2$)

- Tabular Data



Data compiled as indicated in comments:

BS - R.L. Brown and S.E. Stein
TRC - Thermodynamics Research Center, NIST Boulder Laboratories, M. Frenkel director
ALS - H.Y. Afeefy, J.F. Liebman, and S.E. Stein
DH - E.S. Domalski and E.D. Hearing
CAL - J.S. Chickos, W.E. Acree, Jr., J.F. Liebman, Students of Chem 202 (Introduction to the Literature of Chemistry), University of Missouri -- St. Louis

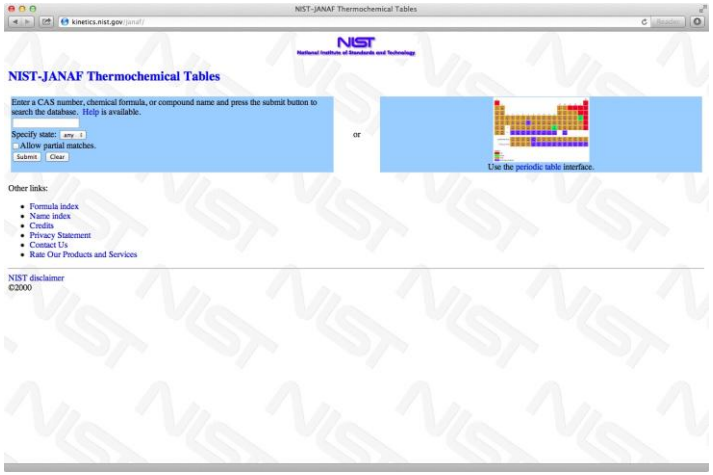
Quantity	Value	Units	Method	Reference	Comment
T_{boil}	446. ± 2.	K	AVG	N/A	Average of 27 values; Individual data points
Quantity	**Value**	**Units**	**Method**	**Reference**	**Comment**
T_{fus}	251.6	K	N/A	Timmermans, 1922	Uncertainty assigned by TRC = 0.4 K; *TRC*
T_{fus}	251.15	K	N/A	Timmermans and Mattaar, 1921	Uncertainty assigned by TRC = 0.5 K; *TRC*
Quantity	**Value**	**Units**	**Method**	**Reference**	**Comment**
T_{triple}	252.79	K	N/A	Oetting, 1965	Uncertainty assigned by TRC = 0.08 K; *TRC*
T_{triple}	252.86	K	N/A	Oetting, 1965	Uncertainty assigned by TRC = 0.06 K; *TRC*
Quantity	**Value**	**Units**	**Method**	**Reference**	**Comment**
T_c	632.7	K	N/A	Pulliam, Gude, et al., 1994	Uncertainty assigned by TRC = 0.2 K; by the sealed ampule method; *TRC*
Quantity	**Value**	**Units**	**Method**	**Reference**	**Comment**
ρ_c	2.01	mol/l	N/A	Pulliam, Gude, et al., 1994	Uncertainty assigned by TRC = 0.02 mol/l; *TRC*
Quantity	**Value**	**Units**	**Method**	**Reference**	**Comment**
$\Delta_{vap}H^\circ$	39.8 ± 0.2	kJ/mol	V	Geiseler and Ratzsch, 1965	*ALS*

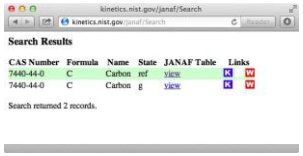
- Spectra

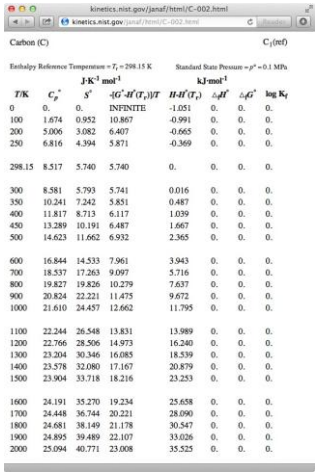
- Models and Tools

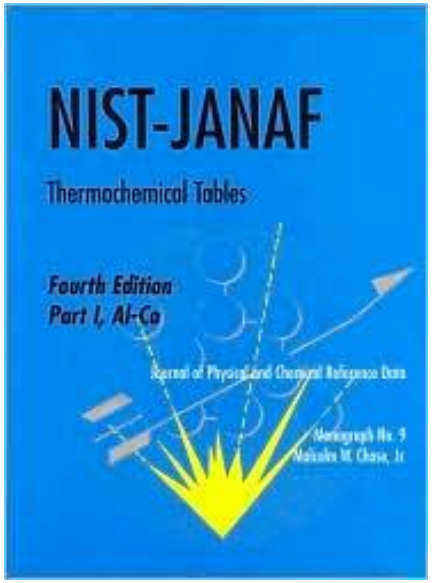
NIST-JANAF Tables

- Thermo data on > 1,850 compounds
- Content of printed volumes available online
- All data will be present in the NIST Chemistry WebBook in a few months



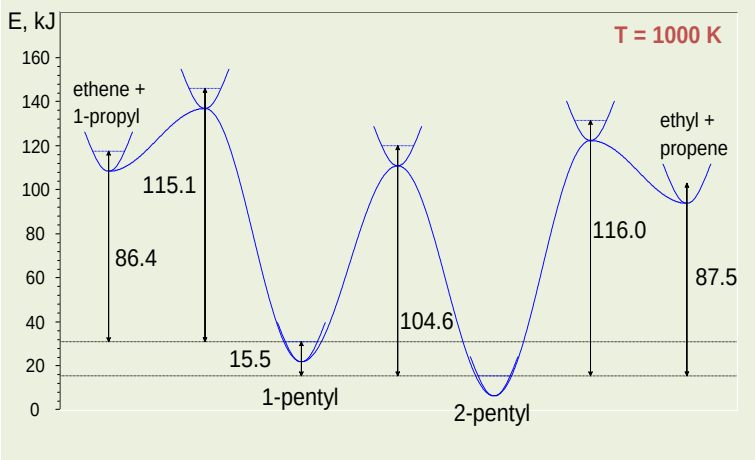






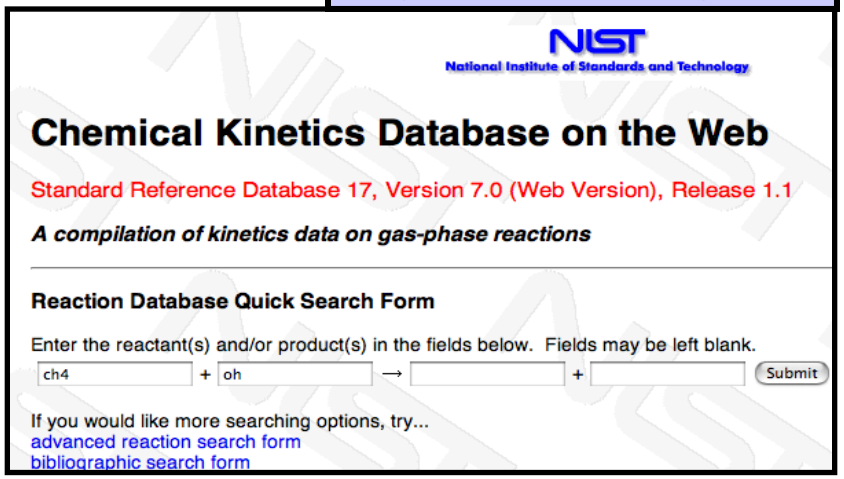
NIST Chemical Kinetics Database

- Collection of rate coefficient data for gas-phase chemical reactions – branching ratios
- Abstracted from literature
- At present, database contains:
  - 17,500 bibliographic entries
  - 54,500 rate coefficients
  - 12,873 chemical species



Primary Kinetic Reference Database used by **Atmospheric and Combustion Chemists and Evaluation Committees** (e.g. NASA JPL Panel, IUPAC Panel, Baulch Combustion Kinetics Evaulations, etc.)

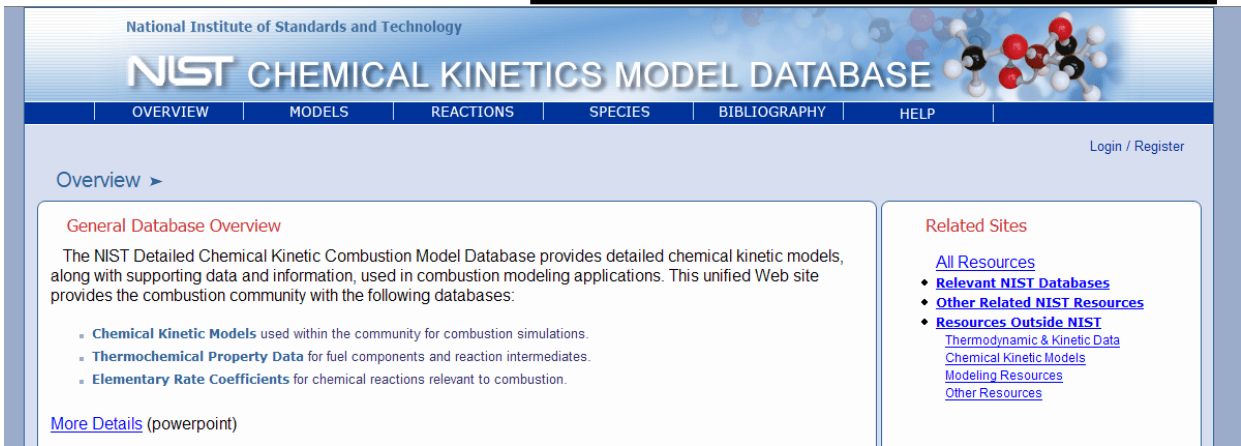
http://kinetics.nist.gov/



NIST Chemical Kinetics Model Database

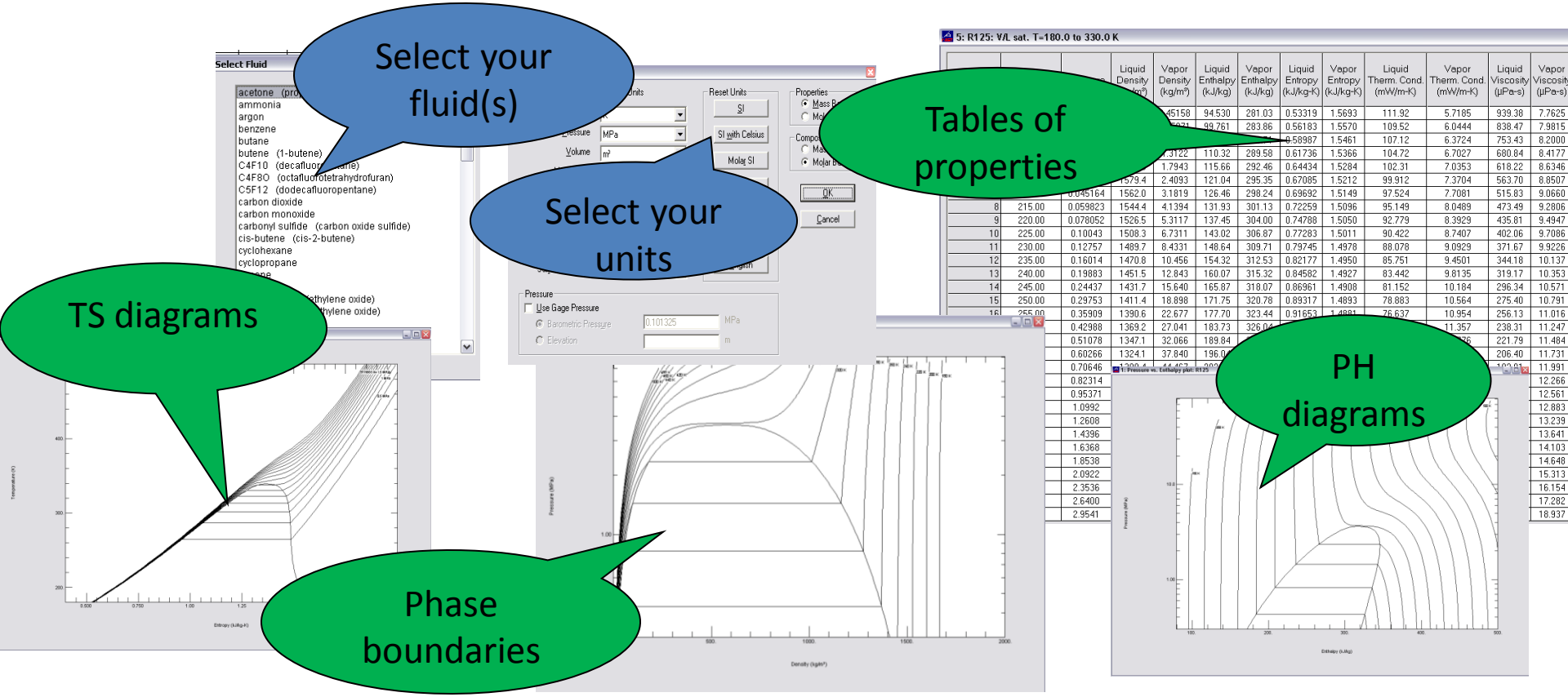
- Collection of Available Electronic Models from Literature (User upload of CHEMKIN models)
- Chemical identifier translation to NIST standard
- Tools to compare models (rxns, rates, thermodynamics)
- Species linked to NIST Webook & NIST Kinetics Database
- Bibliographic information

http://kinetics.nist.gov/CKMech



Reference Fluid Thermodynamic and Transport Properties (REFPROP)

uses equations for the thermodynamic and transport properties to calculate the state points of the fluid or mixture.



NIST Computational Chemistry Comparison and Benchmark Database

http://cccbdb.nist.gov

The source for *ab initio* and experimental ideal-gas thermochemical properties

- Data for 15000 molecules
- Data includes: enthalpies, geometries, vibrational frequencies, dipole moments, quadrupoles, and polarizabilities
- Over 200 computational methods per molecule; a wide variety of quantum chemical methodologies

Used for:

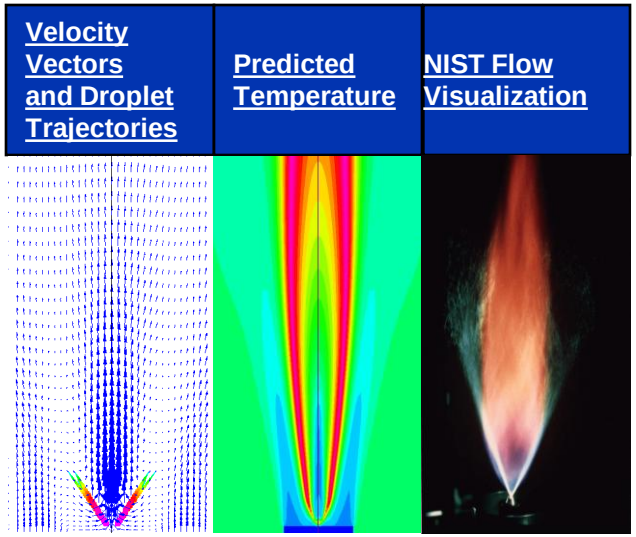
- Comparing experimental data
- Comparing experiment to theory
- Benchmarking new methods
- Assigning uncertainties to calculated results

50,000 – 100,000 users per year

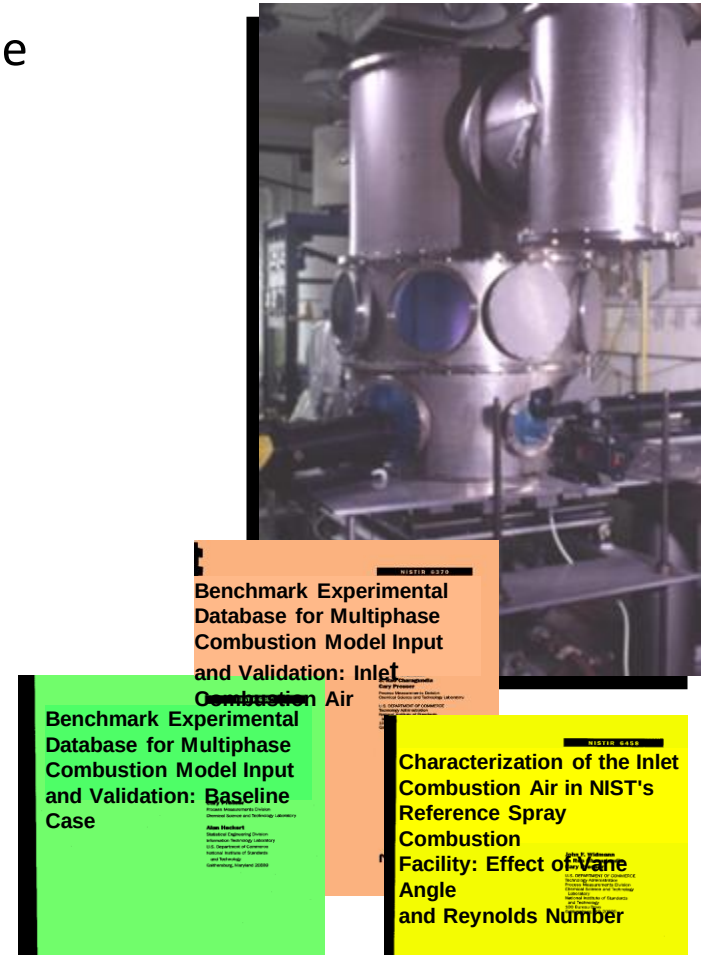
Benchmark Spray Combustion Data

– Spray Combustion Facility with state-of-the-art combustion diagnostics provided a well-controlled environment for model validation

– Benchmark experimental data of the baseline case available on the web

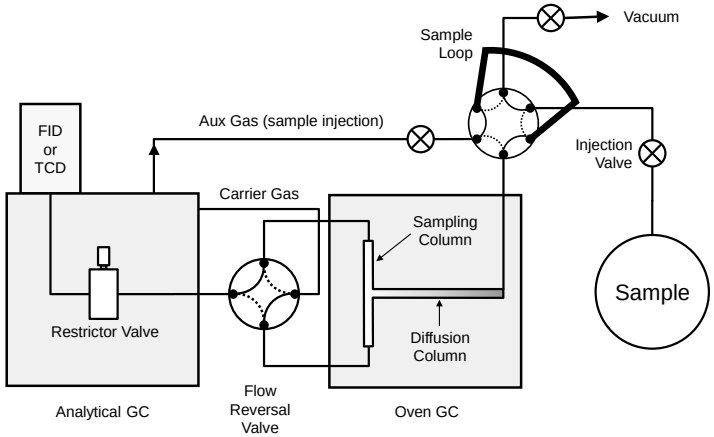


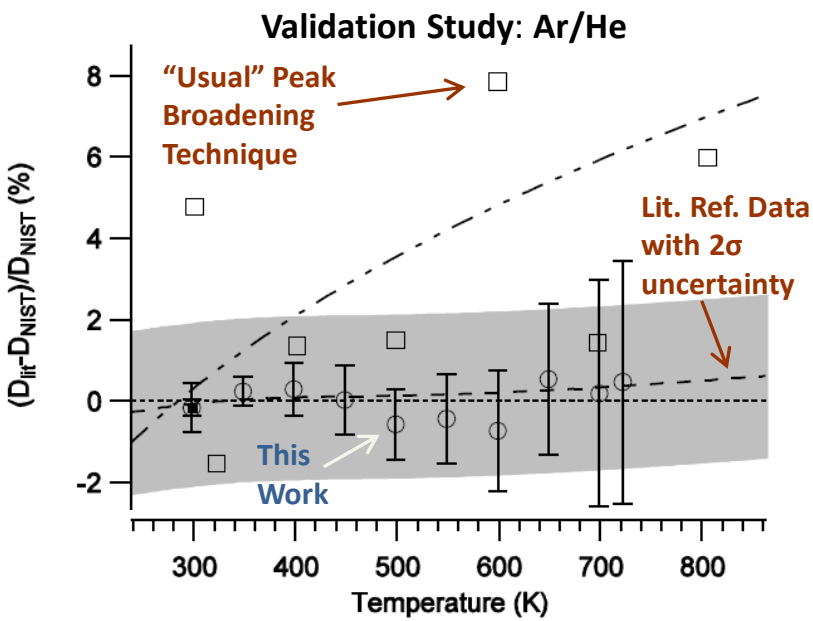
Database with quantitative uncertainties is allowing validation of established and proposed models. Simulation courtesy of CFD Research Corporation.



Binary Diffusion Coefficients of Fuels

- Binary diffusion coefficients are important parameters in combustion simulations.
- Accurate reference data over extended temperature range is needed



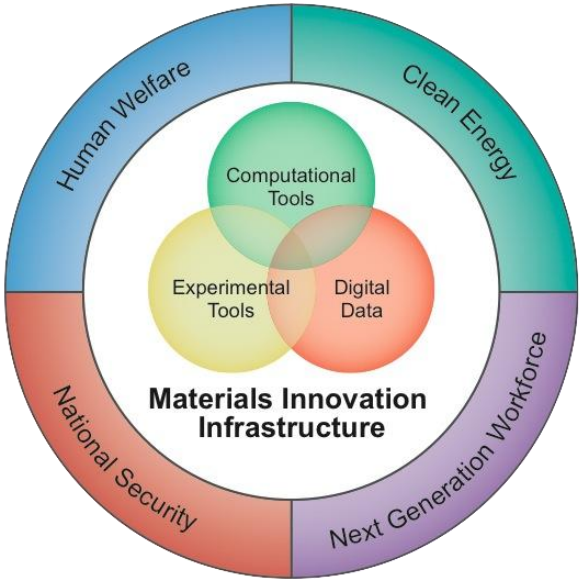


- Developed & validated apparatus for measurements to 725 K.
- Precision and accuracy of *ca.* (1 to 2)%
- 5x to 10x improvement
- Collaborating with theoreticians to better understand & extrapolate over *P, T*.

Materials Genome Initiative
for Global Competitiveness

Accelerate advanced materials discovery and deployment

Through new integrated computational, experimental, and data informatics tools.



Tools to:

- Span the entire materials continuum
- Use an open platform
- Improve predictive capabilities
- Adhere to newly created standards for quick integration of digital information.

Materials Genome Initiative

- Address issues with current approach in materials design
  - High barrier to adoption of methods and results
  - Extra expense due to duplication of effort
  - Lost opportunities to enable discovery & further science

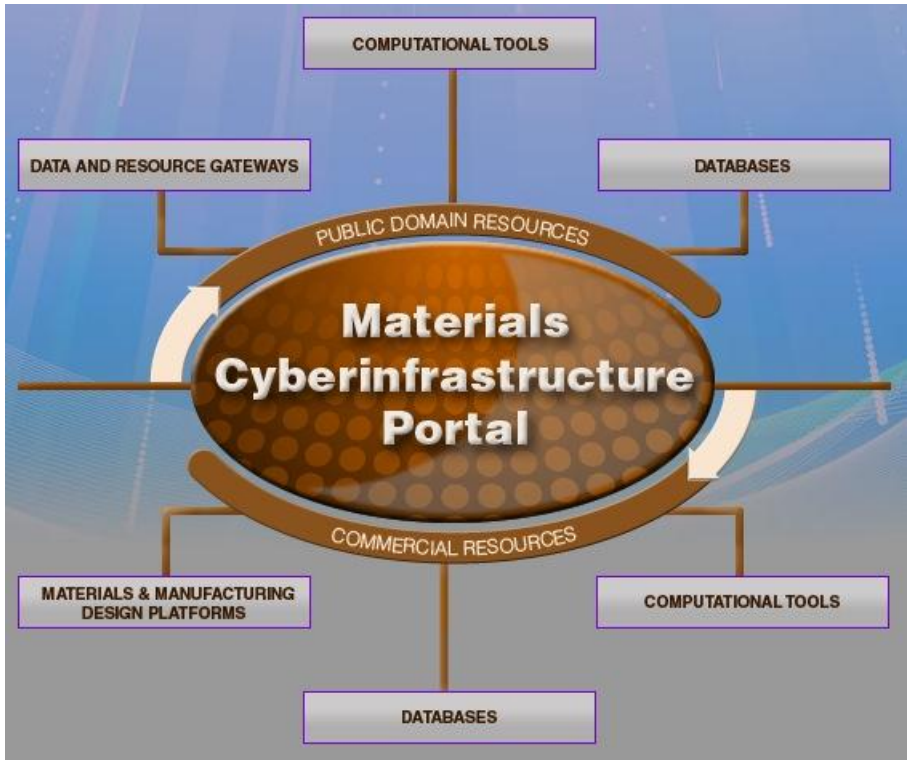
New Challenges

- The data landscape is changing at an incredible pace
- Increased demand for more physical & chemical properties data & SRMs
  - Particularly true in the case of complex advanced materials and biological mixtures
- No single institute/research group can provide all required measurements/data
  - Resources limitations
  - Hard to predict what new properties will be relevant to the scientific community
- Data should be reliable, and easily accessible

Materials Genome Initiative

NIST effort includes

- experiment
- theory
- data
- infrastructure



WebBook Enhancements

- Provide “one-stop shopping” for a wide range of data
- Data mining
- Software tools
- Build on content management system (CMS)
- Share data broadly
- Simplify access to data
- New data in targeted areas (e.g. materials, GWP, etc)
- Computed structures for all molecules

Future Directions…

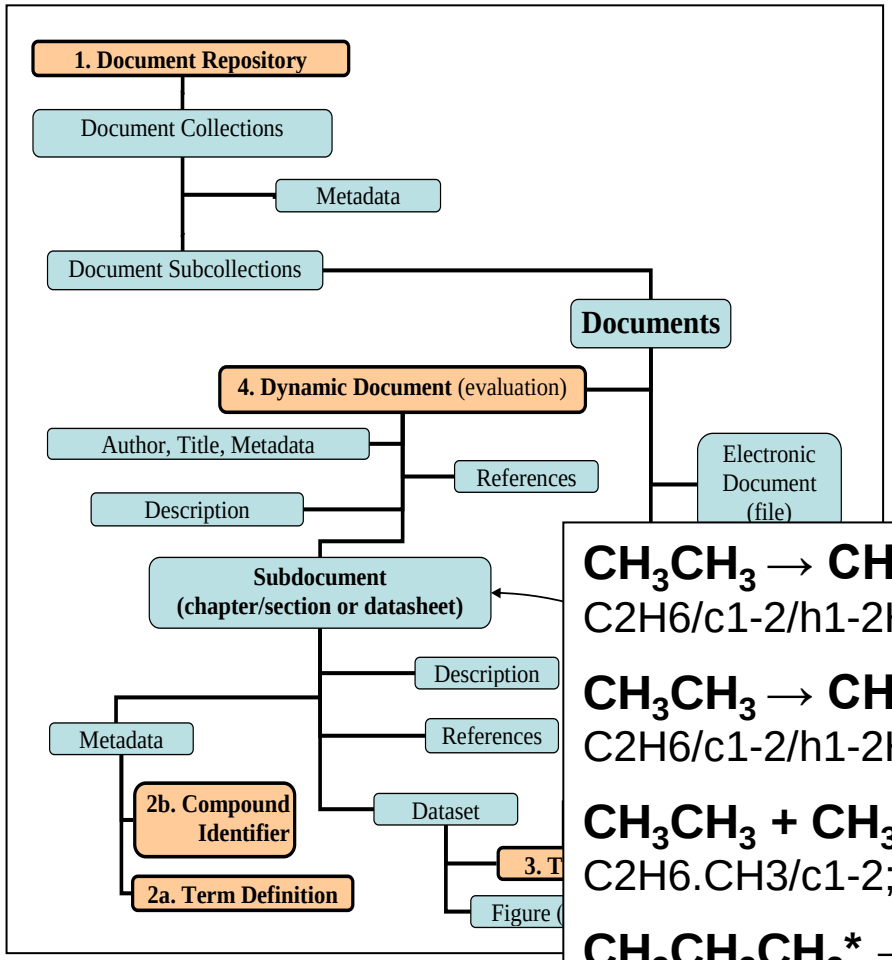
- Crowd-sourced data review
- User contributions
- Interface with publicly available/open source efforts
- Machine learning

Extending information management

Document Repository and Metadata Standards for Documents, Compounds, and Reactions

- **Unified Modeling Language (UML) based**
  - **Object Oriented**
- **Develop a platform for facile collection, indexing, and cataloging**
  - **Enables efficient discovery and rapid dissemination**
    - Documents: Manuscripts, Tables, Figures, etc.
    - Static Documents (files)
    - Dynamic Documents (editable collections of documents)
- **Provide functionalities to aid in tagging records with metadata**
  - Data models, Ontologies, Definition of Terms, Indexes, Compound Identifiers, Reaction Identifiers, and other Scientific Identifiers
- **Provide the ability to generate collections of summary tables with support for detailed tables with that are discoverable by users and editable by evaluators**

Examples – information management

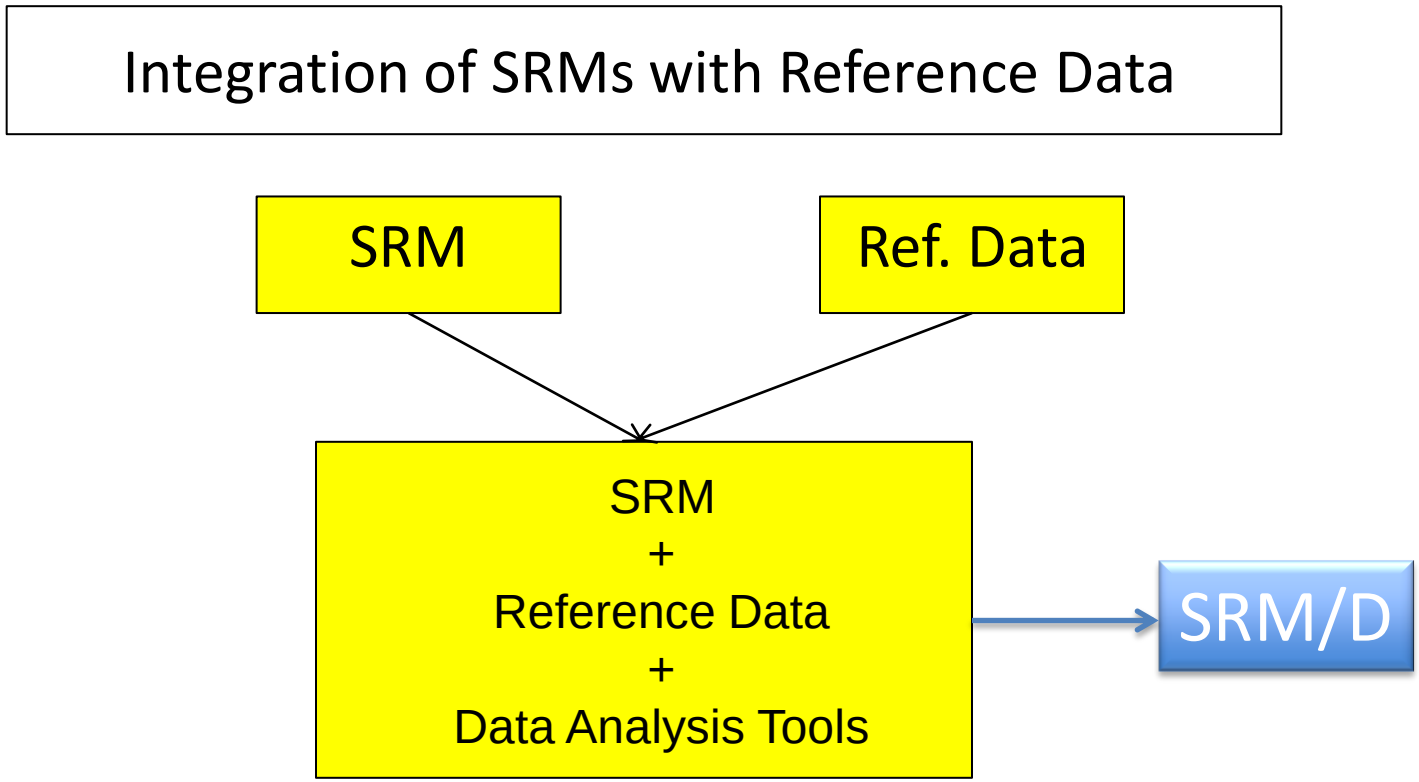


- Schematic of cataloging data within documents
- Standards such as InchI-ER enable details to be captured

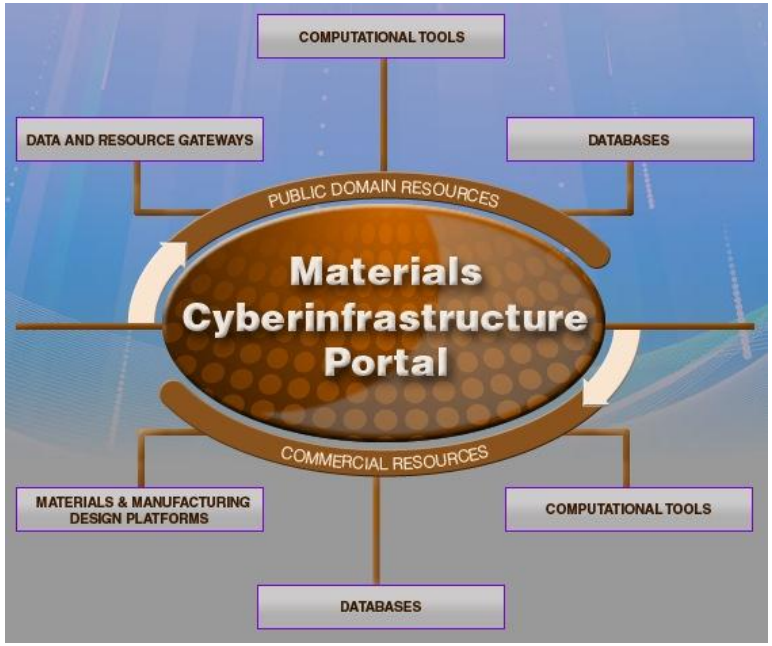
$CH_3CH_3 \rightarrow CH_3CH_2^* + H$	**bond fission**
C2H6/c1-2/h1-2H3	/r1-3
$CH_3CH_3 \rightarrow CH_2{=}CH_2 + H_2$	**1,2-elimination**
C2H6/c1-2/h1-2H3	/r1,2-3,4
$CH_3CH_3 + CH_3 \rightarrow CH_3CH_2^* + CH_4$	**abstraction**
C2H6.CH3/c1-2;/h1-2H3;1H3	/r1-3+1'
$CH_3CH_2CH_2^* \rightarrow CH_3C^*HCH_3$	**H-atom transfer**
C3H7/c1-3-2/h1,3H2,2H3	/r2-4+1

SRM/D Vision

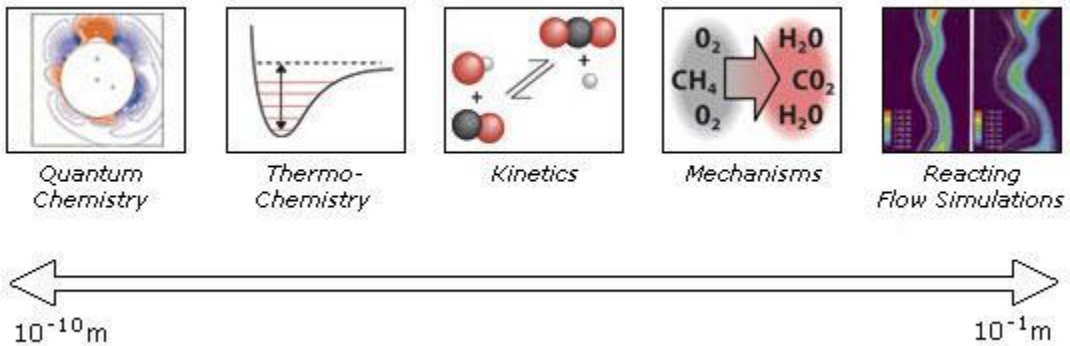
- Foster the creation of scientific communities/environments behind SRMs and Reference Data that will enable advances in science and technology



Benefits to the Combustion Cyberinfrastructure



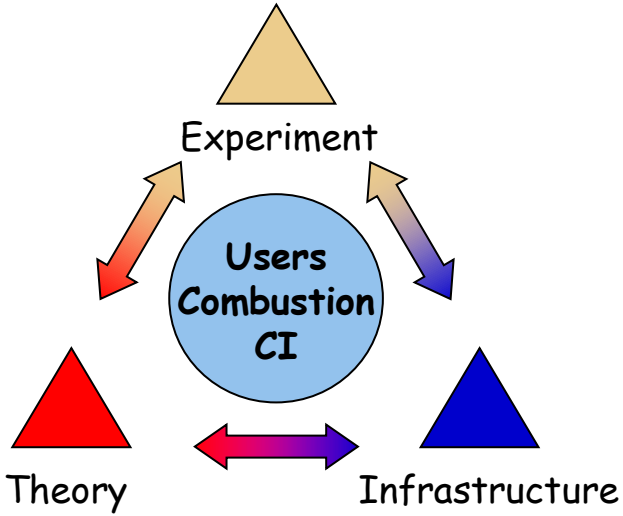
Combustion is Multi-Scale, Multidisciplinary



- Data at small scales needed to support models at larger scales.
- Few experts across scales/disciplines
- Many Data Needs
  - Information Exchange Standards
  - Data Pedigree
  - Data Evaluation
  - Identify and Fill Data Gaps
- A Cyberinfrastructure would accelerate progress

Combustion Cyberinfrastructure – Ways forward

- Integration of combustion related databases with WebBook development & enhancements
- SRM/D on a high community priority material (e.g. surrogate) to enhance comparability of community-wide measurements & data
- Develop new software tools & standards to foster community data exchange



Thank You!