An Overview of Data Activities at NIST

prepared for the
Board on Research Data and Information
National Academy of Sciences

National Institute of Standards and Technology
Gaithersburg, Maryland
April 7, 2009

Building and Fire Research Laboratory (BFRL)
Chemical Science and Technology Laboratory (CSTL)
Information Technology Laboratory (ITL)
Materials Science and Engineering Laboratory (MSEL)
Physics Laboratory (PL)
Technology Services (TS)
### NIST and Standards Setting Organizations

- NIST is a research agency that provides **critical data and measurement technologies** for use in science and industry
- NIST is *not a standard setting body*, but provides reference data for “realizing” standards which are formally adopted by standards setting organizations

#### The International Temperature Scale (for example)
- ITS-90 is realized, maintained and disseminated by NIST to provide a standard scale of temperature and was adopted by the International Committee of Weights and Measures (CIPM) as the official international temperature scale on January 1, 1990
- NIST reference tables of thermocouple electromotive force (emf) vs temperature have been adopted as standards by the American Society for Testing and Materials (ASTM)

### International System of Units (SI)
- American National Standards Institute (ANSI)
- American Society for Testing and Materials (ASTM)
- International Organization for Standardization (ISO)
- International Bureau of Weights and Measures (BIPM)
- General Conference on Weights and Measures (CGPM)
- Committee on Data for Science and Technology (CODATA)
- International Union for Pure and Applied Physics (IUPAP)
- International Union for Pure and Applied Chemistry (IUPAC)
- International Commission on Radiation Units & Measurements (ICRU)
- International Association for the Properties of Water and Steam (IAPWS)
NIST and Metadata Standards
Extensible Markup Language (XML)
(and other data exchange formats)

NIST staff are substantially involved (lead roles) in the development of standardized formats for data exchange

Atomic and Molecular Data Markup Language (AMDML)
Analytical Information Markup Language (AnIML)
Thermodynamics Markup Language (ThermoML)
Numerical Data Markup Language (UnitsML)
Materials Markup Language (MatML)

International Chemical Identifier (InChI)

Information Technology Standards
Cyber and Network Security
Biometric Data Interchange
Identity Management
Cryptographic Tools
NIST Data Activities

Fundamental and Reference DATA for Science and Industry

Identify
Collect
Evaluate
Recommend
Measure
Develop Measurement Technologies
Calculate
Model
Estimate
Calibrations
Reference Data
Critical Data
Standard Reference Data
Standard Reference Materials
Many Sectors
Many Applications

Industry
Education
Academic Research
National Laboratories

NIST
Reference Data
Enabling Measurements
Science
Applications
NIST Data Products and Activities

- Online Databases
- Electronic Databases (PC)
- Print Databases

- Standard Reference Materials
- Calibrations

- Journal Editors
- International Standards Committees
- XML (Extensible Markup Languages)

- Measurement Technologies

- Some FREE
- Some FEE ($)
  - nominal costs for distributing databases (~$100-200)
  - maintaining, expanding, and improving databases (~$1500-5000)
### NIST as a Source of Data and Information

- NIST is not just another source of data
- NIST is the primary source for most fundamental and reference data used in science & industry
- NIST provides critical data and measurement technologies enabling other data measurements

<table>
<thead>
<tr>
<th>Description</th>
<th>Source(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fundamental Physical Constants</td>
<td>[PL]</td>
</tr>
<tr>
<td>The Official U.S. Time (atomic clock)</td>
<td>[PL,TS]</td>
</tr>
<tr>
<td>Atomic Spectroscopic Data</td>
<td>[PL]</td>
</tr>
<tr>
<td>International Temperature Standard</td>
<td>[CSTL]</td>
</tr>
<tr>
<td>Equation of State for Water (steam table)</td>
<td>[CSTL]</td>
</tr>
<tr>
<td>Equation of States for Refrigerants (including cryogenic)</td>
<td>[CSTL]</td>
</tr>
<tr>
<td>Thermochemical Data</td>
<td>[CSTL]</td>
</tr>
<tr>
<td>Chemical Kinetic Data</td>
<td>[CSTL]</td>
</tr>
<tr>
<td>NIST/EPA/NIH Mass Spectral Library</td>
<td>[CSTL]</td>
</tr>
<tr>
<td>Microwave Transition Frequencies for Interstellar Molecules</td>
<td>[PL]</td>
</tr>
<tr>
<td>NIST/EPA/NIH Mass Spectral Library</td>
<td>[CSTL]</td>
</tr>
<tr>
<td>Dosimetry Standards for X-rays, Gamma Rays, and Electrons</td>
<td>[PL]</td>
</tr>
<tr>
<td>FASTData Fire Test Database</td>
<td>[BFRL]</td>
</tr>
<tr>
<td>Heat Transmission Properties of Insulating and Building Materials</td>
<td>[BFRL]</td>
</tr>
<tr>
<td>Phase Equilibria Diagrams Database</td>
<td>[MSEL]</td>
</tr>
<tr>
<td>Crystallographic Structure Databases</td>
<td>[MSEL]</td>
</tr>
</tbody>
</table>
NIST as a Source of Data and Information

- NIST provides critical data and measurement technologies enabling other data measurements.
- The amount of data collected or generated by NIST is minuscule in comparison to the Petabytes of data collected or generated by NASA, NOAA, and NIH …………….. However
## Elemental Data Index

Access database holdings organized by element. Use the databases below to access all information.

Examples of how to reference these online databases are provided in the "Version History" pages.

<table>
<thead>
<tr>
<th>Physical Constants</th>
<th>Periodic Table: Atomic Properties of the Elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Updated!</td>
<td>Contains NIST critically-evaluated data on atomic properties of the elements. Suitable for high-resolution color printing for desk or wall chart display.</td>
</tr>
<tr>
<td>Fundamental Physical Constants</td>
<td></td>
</tr>
<tr>
<td>Searchable Bibliography on the Constants</td>
<td></td>
</tr>
<tr>
<td>International System of Units (SI) or see Special Publication 811</td>
<td></td>
</tr>
<tr>
<td>Guidelines for Evaluating and Expressing Measurement Uncertainty</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Atomic Spectroscopy Data</th>
<th>Atomic Spectra Database</th>
</tr>
</thead>
<tbody>
<tr>
<td>Updated!</td>
<td>Handbook of Basic Atomic Spectroscopic Data</td>
</tr>
<tr>
<td>Status of Atomic Spectroscopy Data</td>
<td>Energy Levels of Hydrogen and Deuterium</td>
</tr>
<tr>
<td></td>
<td>Ground Levels and Ionization Energies for the Neutral Atoms</td>
</tr>
<tr>
<td></td>
<td>Spectral Data for the Chandra X-ray Observatory</td>
</tr>
<tr>
<td></td>
<td>NLTE Databases and Codes</td>
</tr>
<tr>
<td></td>
<td>FLYCHK Collisional-Radiative Code</td>
</tr>
<tr>
<td></td>
<td>SAHA Plasma Population Kinetics Database</td>
</tr>
<tr>
<td></td>
<td>NLTE4 Plasma Population Kinetics Database</td>
</tr>
<tr>
<td></td>
<td>Spectrum of Platinum Lamp for Ultraviolet Spectrograph Calibration</td>
</tr>
<tr>
<td></td>
<td>X-ray Transition Energies</td>
</tr>
<tr>
<td></td>
<td>Bibliographic Databases on Atomic Spectroscopy</td>
</tr>
<tr>
<td></td>
<td>Updated! Atomic Transition Probabilities</td>
</tr>
<tr>
<td></td>
<td>Updated! Atomic Spectral Line Broadening</td>
</tr>
<tr>
<td></td>
<td>NEW! Atomic Energy Levels and Wavelengths</td>
</tr>
</tbody>
</table>
| Molecular Spectroscopic Data          | Microwave Spectral Data: Diatomics, Triatomics, and Hydrocarbons  
Wavenumber Tables for Calibration of Infrared Spectrometers  
Frequencies for Interstellar Molecular Microwave Transitions  
Photoionization of CO_{2} (ARPES)  
Equations & Underpinning Theory  
Diatom Rotational Calculations  
Methane Symmetry Operators |
|-------------------------------------|------------------------------------------------------------------|
| Atomic and Molecular Data           | Electron-Impact Cross Sections for Ionization and Excitation  
Potential Energy Surface Database of Group II Dimer Molecules |
| X-Ray and Gamma-Ray Data            | Note on the X-Ray Attenuation Databases  
X-Ray Attenuation and Absorption for Materials of Dosimetric Interest  
XCOM: Photon Cross Sections Database  
Bibliography of Photon Attenuation Measurements  
X-Ray Form Factor, Attenuation and Scattering Tables  
X-ray Transition Energies |
| Radiation Dosimetry Data            | Stopping-Power and Range Tables for Electrons, Protons, and Helium Ions |
| Nuclear Physics Data                | Radionuclide Half-life Measurements Made at NIST  
Atomic Weights and Isotopic Compositions |
| Condensed Matter Physics Data       | Atomic Model Data for Electronic Structure Calculations |
| Other NIST Data                     | Data Gateway  
Online Reference Databases  
Standard Reference Data Catalog |
Latest (2006) values of the constants

Search for value by name

Display ○ alphabetical list, ○ table (image), or ○ table (pdf)

by clicking a category below

Universal
Adopted values
Electromagnetic
Non-SI units
Conversion factors for energy equivalents
Extensive listings
Atomic and nuclear
Extensive listings
Physico-chemical
Extensive listings
X-ray values
Extensive listings
Frequently used constants
Extensive listings
All values (ascil)

Find the correlation coefficient between any pair of constants
Data from the least-squares adjustment of the values of the constants
<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
<th>Relative std. uncert. u_r</th>
</tr>
</thead>
<tbody>
<tr>
<td>speed of light in vacuum</td>
<td>c, c₀</td>
<td>299 792 458</td>
<td>m s⁻¹</td>
<td>(exact)</td>
</tr>
<tr>
<td>magnetic constant</td>
<td>µ₀</td>
<td>4π × 10⁻⁷</td>
<td>N A⁻²</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>= 12.566 370 614... × 10⁻⁷</td>
<td>N A⁻²</td>
<td>(exact)</td>
</tr>
<tr>
<td>electric constant 1/µ₀ c²</td>
<td>ε₀</td>
<td>8.854 187 817... × 10⁻¹²</td>
<td>F m⁻¹</td>
<td>(exact)</td>
</tr>
<tr>
<td>Newtonian constant of gravitation</td>
<td>G</td>
<td>6.674 28(67) × 10⁻¹¹</td>
<td>m³ kg⁻¹ s⁻²</td>
<td>1.0 × 10⁻⁴</td>
</tr>
<tr>
<td>Planck constant</td>
<td>h</td>
<td>6.626 068 96(33) × 10⁻³⁴</td>
<td>J s</td>
<td>5.0 × 10⁻⁸</td>
</tr>
<tr>
<td>h/2π</td>
<td></td>
<td>1.054 571 628(53) × 10⁻³⁴</td>
<td>J s</td>
<td>5.0 × 10⁻⁸</td>
</tr>
<tr>
<td>elementary charge</td>
<td>e</td>
<td>1.602 176 487(40) × 10⁻¹⁹</td>
<td>C</td>
<td>2.5 × 10⁻⁸</td>
</tr>
<tr>
<td>magnetic flux quantum h/2e</td>
<td>φ₀</td>
<td>2.067 833 667(52) × 10⁻₁⁵</td>
<td>Wb</td>
<td>2.5 × 10⁻⁸</td>
</tr>
<tr>
<td>conductance quantum 2ε²/h</td>
<td>G₀</td>
<td>7.748 091 7004(53) × 10⁻⁵</td>
<td>S</td>
<td>6.8 × 10⁻¹⁰</td>
</tr>
<tr>
<td>electron mass</td>
<td>mₑ</td>
<td>9.109 382 15(45) × 10⁻³¹</td>
<td>kg</td>
<td>5.0 × 10⁻⁸</td>
</tr>
<tr>
<td>proton mass</td>
<td>mₚ</td>
<td>1.672 621 637(83) × 10⁻²⁷</td>
<td>kg</td>
<td>5.0 × 10⁻⁸</td>
</tr>
<tr>
<td>proton-electron mass ratio</td>
<td>mₚ/mₑ</td>
<td>1836.152 672 47(80) × 10⁻¹⁰</td>
<td>kg</td>
<td>4.3 × 10⁻¹⁰</td>
</tr>
<tr>
<td>fine-structure constant ε²/4πε₀h c</td>
<td>α</td>
<td>7.297 352 5376(50) × 10⁻³</td>
<td>J m⁻¹</td>
<td>6.8 × 10⁻¹⁰</td>
</tr>
<tr>
<td>inverse fine-structure constant</td>
<td>α⁻¹</td>
<td>137.035 999 679(94) × 10⁻¹⁴</td>
<td>J m⁻¹</td>
<td>6.8 × 10⁻¹⁰</td>
</tr>
<tr>
<td>Rydberg constant α²mₑc²/2h</td>
<td>R₆₀</td>
<td>10.973 731 568 527(73)</td>
<td>m⁻¹</td>
<td>6.6 × 10⁻¹²</td>
</tr>
<tr>
<td>Avogadro constant</td>
<td>Nₐ, L</td>
<td>6.022 141 79(30) × 10⁻²³</td>
<td>mol⁻¹</td>
<td>5.0 × 10⁻⁸</td>
</tr>
<tr>
<td>Faraday constant Nₐ e</td>
<td>F</td>
<td>96 485.3399(24)</td>
<td>C mol⁻¹</td>
<td>2.5 × 10⁻⁸</td>
</tr>
<tr>
<td>molar gas constant</td>
<td>R</td>
<td>8.314 472(15)</td>
<td>J mol⁻¹ K⁻¹</td>
<td>1.7 × 10⁻⁶</td>
</tr>
<tr>
<td>Boltzmann constant R/Nₐ</td>
<td>k</td>
<td>1.380 6504(24) × 10⁻²³</td>
<td>J K⁻¹</td>
<td>1.7 × 10⁻⁶</td>
</tr>
<tr>
<td>Stefan-Boltzmann constant (π²/60)k₄/h³ c²</td>
<td>σ</td>
<td>5.670 400(40) × 10⁻⁸</td>
<td>W m⁻² K⁻⁴</td>
<td>7.0 × 10⁻⁵</td>
</tr>
<tr>
<td>electron volt: (ε₀/C) J</td>
<td>eV</td>
<td>1.602 176 487(40) × 10⁻¹⁹</td>
<td>J</td>
<td>2.5 × 10⁻⁸</td>
</tr>
<tr>
<td>(unified) atomic mass unit</td>
<td></td>
<td>1 u = mₚ = 1/12 m(¹²C)</td>
<td>kg</td>
<td>5.0 × 10⁻⁸</td>
</tr>
<tr>
<td></td>
<td></td>
<td>= 10⁻³ kg mol⁻¹/Nₐ</td>
<td>kg</td>
<td>5.0 × 10⁻⁸</td>
</tr>
</tbody>
</table>
Searchable bibliography on the constants

**Obtain** bibliographic citations by completing one or more items:

- **Word(s) in title or assigned keyword(s):** e.g., alpha
- **Author(s):**
- **Year(s):** from [ ] to [ ]

Include the following:
- Types of research: [ ] Experimental  [ ] Theoretical
- Types of papers: [ ] Original research  [ ] Review

[Search for Papers]  [Reset]

See also
- [Values of the constants](#)
- [Background information](#) related to the constants

NIST Standard Reference Database 123
The Boltzmann Constant $k_B$ and the Universal Gas Constant $R = N_A \times k_B$ connect Energy with Temperature $T$.

Examples

**Dilute gas:** $pV = nRT (1 + \cdots$

**Black body radiation:**

\[
\text{power per area} = \frac{\pi^2}{60h^3c^2}(k_B T)^4
\]

CSTL has determined $R$ from the acoustic resonances of an argon-filled spherical cavity with a relative uncertainty of $1.8 \times 10^{-6}$ (best in the world).
The Journal of Physical and Chemical Reference Data

“print” version of some NIST databases plus much reference data from international committees

- CODATA Recommended Values of the Fundamental Physical Constants
- Atomic Weights of the Elements
- IAPWS Formulation for the Thermodynamic Properties of Water
- Vapor-Liquid Distribution Constants for Gaseous Solutes in Water at High Temp.
- IUPAC-NIST Solubility Data Series (many volumes)
- Recommended Liquid-Liquid Equilibrium Data (many volumes)
- Physical Properties of Ionic Liquids: Database and Evaluation
- JANAF Thermochemical Tables
- IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals
- Heat Capacity of Liquids: Critical Review and Recommendations (many articles)
- IUPAC Evaluated Kinetic Data for Combustion Modeling (many articles)
- IUPAC Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry
- Handbook of Basic Atomic Spectroscopic Data
- Atomic Spectra Data Tables (many volumes)
- Microwave Transition Frequencies for Interstellar Molecules (many articles)
- Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules
Virtually Every Area
Virtually Every Application

Industry
Academic Research
National Laboratories
our daily lives

TEMPERATURE

Science
Reference Data
Enabling Measurements
Applications

NIST
EMF versus Temperature

I get everything I need from Omega Engineering Inc.
or, What's NIST got to do with it? (an Engineer's question)

### Maximum Temperature Range

<table>
<thead>
<tr>
<th>Thermocouple Grade</th>
<th>32°F to 2282°F</th>
<th>200°F to 1250°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extension Grade</td>
<td>32 to 392°F</td>
<td>0 to 200°C</td>
</tr>
</tbody>
</table>

### Limits of Error

(whichever is greater)

- **Standard**: 2.2°C or 0.75% Above 0°C
- 2.2°C or 2.0% Below 0°C
- **Special**: 1.1°C or 0.4%

### Comments, Bare Wire Environment:

- Clean Oxidizing and Inert; Limited Use in Vacuum or Reducing; Wide Temperature Range; Most Popular Calibration

### Temperature in Degrees °C Reference Junction at 0°C

<table>
<thead>
<tr>
<th>°C</th>
<th>-10</th>
<th>-9</th>
<th>-8</th>
<th>-7</th>
<th>-6</th>
<th>-5</th>
<th>-4</th>
<th>-3</th>
<th>-2</th>
<th>-1</th>
<th>0</th>
<th>°C</th>
</tr>
</thead>
</table>

### Revised Thermocouple Reference Tables

**TYPE K**

- Reference Tables
- N.I.S.T. Monograph 175
- Revised to ITS-90

### Thermoelectric Voltage in Millivolts

<table>
<thead>
<tr>
<th>°C</th>
<th>-10</th>
<th>-9</th>
<th>-8</th>
<th>-7</th>
<th>-6</th>
<th>-5</th>
<th>-4</th>
<th>-3</th>
<th>-2</th>
<th>-1</th>
<th>0</th>
<th>°C</th>
</tr>
</thead>
</table>
International Temperature Scale (ITS-90)

NIST Standard Reference Database 60

<table>
<thead>
<tr>
<th>Fixed Pt</th>
<th>T/K</th>
<th>Substance</th>
<th>State</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3 to 5</td>
<td>He</td>
<td>vapor press</td>
</tr>
<tr>
<td>2</td>
<td>13.8033</td>
<td>e-H₂</td>
<td>triple pt</td>
</tr>
<tr>
<td>3</td>
<td>~17</td>
<td>e-H₂/He</td>
<td>vapor press</td>
</tr>
<tr>
<td>4</td>
<td>~20.3</td>
<td>e-H₂/He</td>
<td>vapor press</td>
</tr>
<tr>
<td>5</td>
<td>24.5561</td>
<td>Ne</td>
<td>triple pt</td>
</tr>
<tr>
<td>6</td>
<td>54.3584</td>
<td>O₂</td>
<td>triple pt</td>
</tr>
<tr>
<td>7</td>
<td>83.8058</td>
<td>Ar</td>
<td>triple pt</td>
</tr>
<tr>
<td>8</td>
<td>234.3156</td>
<td>Hg</td>
<td>triple pt</td>
</tr>
<tr>
<td>9</td>
<td>273.16</td>
<td>H₂O</td>
<td>triple pt</td>
</tr>
<tr>
<td>10</td>
<td>302.9146</td>
<td>Ga</td>
<td>melting pt</td>
</tr>
<tr>
<td>11</td>
<td>429.7485</td>
<td>In</td>
<td>freezing pt</td>
</tr>
<tr>
<td>12</td>
<td>505.078</td>
<td>Sn</td>
<td>freezing pt</td>
</tr>
<tr>
<td>13</td>
<td>692.677</td>
<td>Zn</td>
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<tr>
<td>14</td>
<td>933.473</td>
<td>Al</td>
<td>freezing pt</td>
</tr>
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<td>15</td>
<td>1234.93</td>
<td>Ag</td>
<td>freezing pt</td>
</tr>
<tr>
<td>16</td>
<td>1337.33</td>
<td>Au</td>
<td>freezing pt</td>
</tr>
<tr>
<td>17</td>
<td>1357.77</td>
<td>Cu</td>
<td>freezing pt</td>
</tr>
</tbody>
</table>
Thermophysical Properties of Water and Steam

NIST Standard Reference Database 10

• Thermodynamic Properties
• Transport Properties
• Dielectric Constant, Refractive Index

Implements standards adopted by IAPWS
Inter. Assoc. for the Properties of Water & Steam
Reference Fluid Thermodynamic and Transport Properties Database (REFPROP)

- Thermodynamic Properties
- Transport Properties

Pure fluids and mixtures implements standards and best available equations of state (EOS)
  - GERG-2004 and AGA-8 standards for natural gas
  - REFPROP is a de facto standard in the refrigeration industry
  - Also includes water and other industrially important fluids
  - Upcoming version will include biofuel constituents
Industrial Process Design
Standardized Properties of Industrially Important Fluids

Electric Power and Chemical Process Industries (Steam Tables)
Refrigeration Industry
Natural Gas Industry
Industrial Gases
Cryogenics
Biofuels

International Association for the Properties of Water & Steam (www.iapws.org)
International Institute of Refrigeration (www.iifiir.org)

Calibrations for Research & Industry

NIST

Science
Reference Data
Applications
Enabling Measurements
Global Environment
Various NIST Data Contributions

- Refrigerant Properties
- Steam Tables
- Power
- Ozone-depleting & GHGs
- Greenhouse Gases (GHGs)
- Temp Measurement & Control
- Sensing of ODPGs & GHGs & Pollutants
- Photochemistry of ODPGs & GHGs
- Refrigerant Properties
Climate Change and Carbon Cap & Trading
Spectroscopic reference data for remote sensing of greenhouse gases

High-resolution spectral line parameters
- \( \text{O}_2, \text{H}_2\text{O}; \) Greenhouse gases (GHGs)
- uncertainties < 0.5%

HITRAN Database (2008) updated with NIST \( \text{O}_2 \) data

Satellite Measurements of \( \text{CO}_2 \)
AIRS, 2002
ASCENDS, 2013-16
Quality-Assured Infrared Absorption Coefficient Data

- Absorption coefficients: intrinsic molecular property
- Directly traceable to: national primary gas standards

Northwest-Infrared
vapor phase infrared spectral library
http://nwir.pnl.gov

NIST Standard Reference Database 79

http://webbook.nist.gov/chemistry/
Global Environment, Health Sciences, and Homeland Security
Chemical and Biological Agents; Environmental Regulations
Air Pollutants, Greenhouse Gases, Ozone-Depleting Chemicals

Edgewood Chemical Biological Center (Army)
Environmental Protection Agency (EPA)
Pacific Northwest Laboratories (DOE)

Orbiting Carbon Observatory (OCO)
ASCENDS (Active Sensing CO2 Satellite)
Atmospheric Infrared Sounder (AIRS Satellite)
Harvard-Smithsonian Center for Astrophysics
Caltech/JPL (Jet Propulsion Labs)
HITRAN database

NASA

NIST

Science

Reference Data

Applications

Enabling Measurements
## Gas Phase Chemical Kinetics

### NIST Standard Reference Database 133

<table>
<thead>
<tr>
<th>Reference</th>
<th>Temp [K]</th>
<th>A</th>
<th>n</th>
<th>Ea [kJ]</th>
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Global Environment
Air Pollutants, Greenhouse Gases, Ozone-Depleting Chemicals

Atmospheric Modeling

IUPAC Subcommittee for Kinetic, Photochemical, and Heterogeneous Data Evaluation for Atmospheric Chemistry

NASA/JPL Evaluation Panel for Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies

Chemical Kinetics Database

NIST

Science

Applications

Reference Data

Enabling Measurements
Accurate Photochemical Data for Atmospheric Lifetimes of Halogenated Compounds
Global Warming Potential (GWP) and Ozone Depletion Potential (ODP)

Halogenated hydrocarbons are the most important industrial greenhouse gases (GHGs) whose IR absorption spectra need to be measured.

NIMBUS-4
Spectrum of radiation from Earth
Accurate Photochemical Data for Atmospheric Lifetimes of Halogenated Compounds
Global Warming Potential (GWP) and Ozone Depletion Potential (ODP)

Hydroxy Radical Reaction Rates – Nature’s Vacuum

UV Absorption Spectra

Photoinduced Chemistry
NIST Mass Spectrometer Database

NIST Standard Reference Database 1

NIST/EPA/NIH Mass Spectral Database
• World’s most widely used mass spectral reference library
• Used by environmental, toxicology, forensic, and biomedical labs
• Distributed ($$$) as an option by mass spectrometer manufacturers.

Molecules $\rightarrow$ e$^-(E)$ $\rightarrow$ Neutral and Ion Fragments
# Ion and Neutral Thermochemistry
Ionization Potentials, Appearance Potentials and Heats of Formation

## Table 1. Ionization Potentials, Appearance Potentials, and Heats of Formation of Gaseous Positive Ions—Continued

<table>
<thead>
<tr>
<th>Ion</th>
<th>Reactant</th>
<th>Other products</th>
<th>AP or IP (eV)</th>
<th>Method</th>
<th>Heat of formation (kcal mol⁻¹)</th>
<th>Ref</th>
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<tr>
<td>C₆H₆O₅⁻</td>
<td>C₆H₄OHCOOC₆H₄ (Methyl hydroxybenzoate)</td>
<td>H</td>
<td>10.39 ± 0.05</td>
<td>RPD</td>
<td>66</td>
<td>1139</td>
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<tr>
<td>C₆H₅O₇⁻</td>
<td>C₆H₄OHCOOC₆H₄ (Methyl hydroxybenzoate)</td>
<td>CH₄</td>
<td>10.39 ± 0.10</td>
<td>RPD</td>
<td>78</td>
<td>1139</td>
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<td>C₆H₅O₇⁻</td>
<td>C₆H₄OHCOOC₆H₄ (Methyl hydroxybenzoate)</td>
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<td>RPD</td>
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<td>1139</td>
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<td>C₈H₅O₅⁻</td>
<td>C₆H₄OHCOOC₆H₄ (Methyl hydroxybenzoate)</td>
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<td>TC</td>
<td>94</td>
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<td>C₈H₆O₅⁻</td>
<td>C₆H₄OHCOOC₆H₄ (Methyl hydroxybenzoate)</td>
<td>CH₄</td>
<td>8.48 ± 0.04</td>
<td>CS</td>
<td>90*</td>
<td>2126</td>
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<tr>
<td>C₈H₇O₇⁻</td>
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<td>TC</td>
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<td>2194</td>
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<tr>
<td>C₉H₁₀O₅⁻</td>
<td>C₆H₄OHCOOC₆H₄ (Methyl hydroxybenzoate)</td>
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<tr>
<td>C₉H₁₁O₅⁻</td>
<td>C₆H₄OHCOOC₆H₄ (Methyl hydroxybenzoate)</td>
<td>CH₆O</td>
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<td>2035</td>
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<tr>
<td>C₉H₁₂O₅⁻</td>
<td>C₆H₄OHCOOC₆H₄ (Methyl hydroxybenzoate)</td>
<td>CH₆O</td>
<td>13.5 ± 0.16</td>
<td>EVD</td>
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<td>2035</td>
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<td>HNO₃</td>
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<td>11.03 ± 0.01</td>
<td>PI</td>
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<tr>
<td>C₃H₂BO⁺</td>
<td>(CH₃O)₂B</td>
<td>CH₃O + OH</td>
<td>16.6 ± 0.3</td>
<td>EVD</td>
<td>187</td>
<td>115</td>
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<tr>
<td>C₃H₃BO⁺</td>
<td>(CH₃O)₂B</td>
<td>CH₃O + H₂</td>
<td>13.2 ± 0.2</td>
<td>EVD</td>
<td>117</td>
<td>115</td>
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<tr>
<td>C₃H₃BO⁺</td>
<td>(CH₃O)₂B</td>
<td>H₂</td>
<td>9.0 ± 0.2</td>
<td>SL</td>
<td>16</td>
<td>364</td>
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<tr>
<td>C₃H₃BO⁺</td>
<td>(CH₃O)₂B</td>
<td>CH₃O</td>
<td>13.0 ± 0.2</td>
<td>EVD</td>
<td>85</td>
<td>115</td>
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<tr>
<td>C₃H₃BO⁺</td>
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<td>CH₃O</td>
<td>9.6 ± 0.2</td>
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Biosciences and Health
Improving success rate of discovery experiments in proteomics

Proteome Software Inc
ProteomeCommons (http://www.proteomecommons.org)
Global Proteome Machine (http://www.thegpm.org)
PeptideAtlas (http://www.peptideatlas.org)

Johns Hopkins Medical Institutions
Vanderbilt School of Medicine
Harvard Medical School

National Cancer Institute
(http://proteomics.cancer.gov)

National Center for Biotechnology Information

NIST

Science
Reference Data
Applications
Enabling Measurements
NIST Chemistry WebBook
Convenient, Centralized Source of Physical and Chemical Property Data

NIST Standard Reference Database 69

NIST Chemistry WebBook
• Most widely used NIST data product
• Used by scientists, engineers, educators, and students

Applications in areas of
• Chemical Engineering
• Physical Chemistry
• Analytical Chemistry
• Chemical Informatics
NIST Chemistry WebBook
Convenient, Centralized Source of Physical and Chemical Property Data

NIST Standard Reference Database 69

NIST Chemistry WebBook “Chapters”
1. Organic thermochemistry archives
2. Heat capacities & entropies of condensed phase organic compounds
3. Positive and negative ion energetics database
4. Organometallic thermochemistry database
5. JANAF thermochemical tables
6. Chemical structures and properties thermochemical prediction database
7. Constants of diatomic molecules
8. Computed 3-D structures of organic compounds
9. Vibrational & electronic energy levels of small polyatomic transient molecules
10. Gas-phase infrared database
11. UV/Visible spectra database
12. Quantitative infrared database
13. Gas chromatographic retention indices database
14. Thermophysical properties of fluids
Naphthalene

**Formula:** $C_{10}H_8$

**Molecular weight:** 128.1705

**InChI:** 1S/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H

**CAS Registry Number:** 91-20-3

**Chemical structure:**

Isotopomers: [Naphthalene-d8](#)

**Other names:** Albocarbon; Dezodorator; Moth flakes; Naphthalin; Naphthaline; Naphthene; Tar camphor; White tar; Camphor tar; Moth balls; Naftalen; NCI-C52904; Mighty 150; Mighty rd1; Naphthalene, molten; Rcra waste number U165; UN 1334; UN 2304

**Other data available:**

… … …

… …

…
Naphthalene

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)
- UV/Visible spectrum
- Gas Chromatography

Data at other public NIST sites:
- Computational Chemistry Comparison and Benchmark Database
- Gas Phase Kinetics Database
- X-ray Photoelectron Spectroscopy Database, version 3.5
NIST Thermodynamics Research Center
• TRC Ideal Gas Database
• TRC Web Thermo Tables
• Thermophysical Properties of Hydrocarbon Mixtures Database
• ThermoData Engine (TDE) for Pure Mixtures
• ThermoData Engine (TDE) for Binary Compounds
• Thermodynamics Markup Language (ThermoML)
• TRC Guided Data Capture (GDC)
• Used by scientists, engineers, educators, and students

Applications in areas of
• Chemical Engineering
• Physical Chemistry
### NIST/TRC Web Thermo Tables (WTT)

**Professional Edition**  
**NIST Standard Reference Subscription Database 3**

WTT - Professional Edition, a Web version of the TRC Thermodynamic Tables, represents a complete collection of **critically evaluated** thermodynamic property data primarily for pure organic compounds. References to experimental data sources and information and methodology related to the evaluations can be found in complementary hard-copy publications:


#### Compound Options:
- **CAS registry number:**  
- **Formula (case-sensitive):** C2H6O  
- **Name (exaxt or part):**  
- **Molecular weight (approximate value or range, e.g. 20-30):**

#### Property Options:

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Reference Data

Applications
Enabling Measurements