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*)

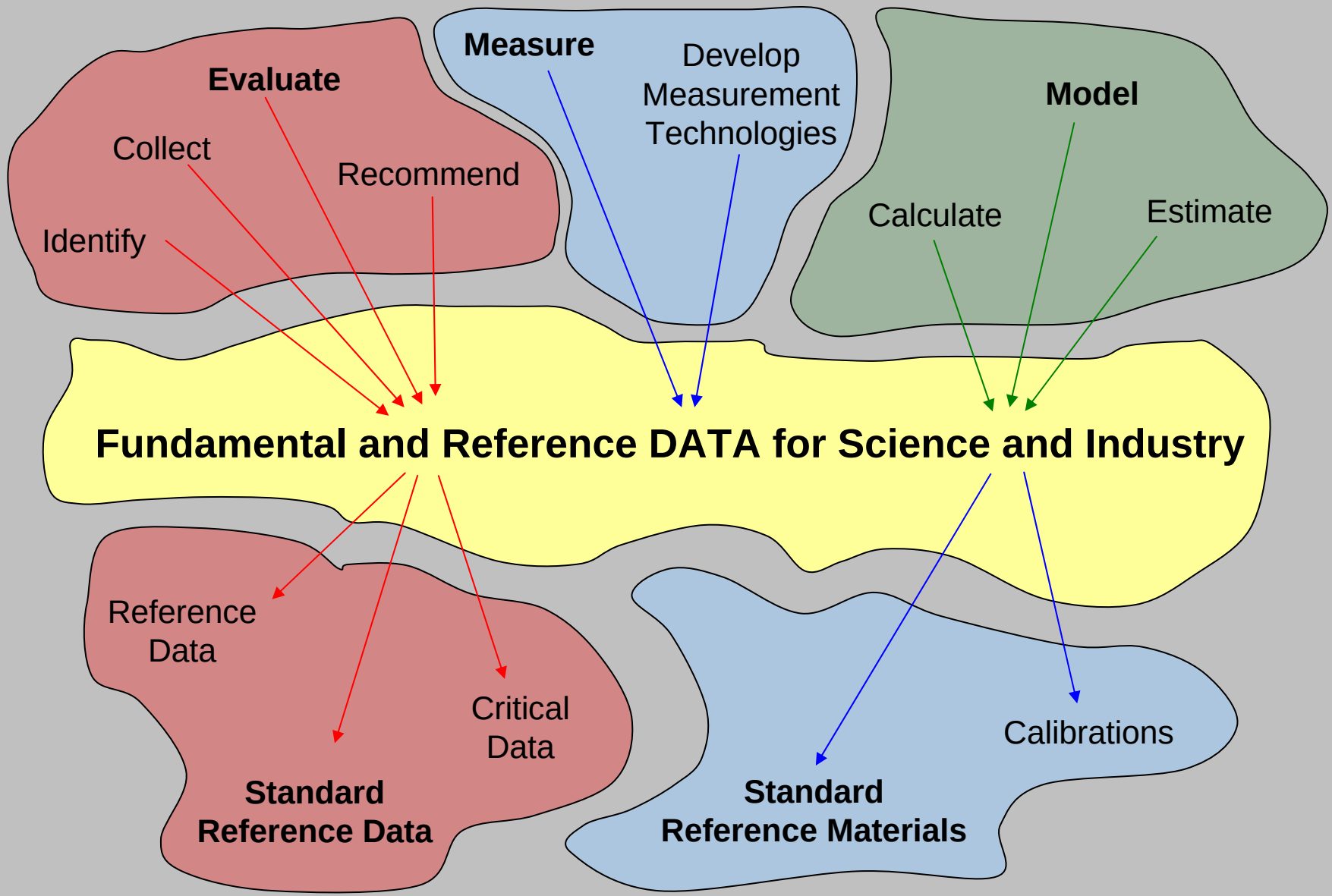
NIST staff are substantially involved (lead roles) in the development of standardized formats for data exchange

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*)

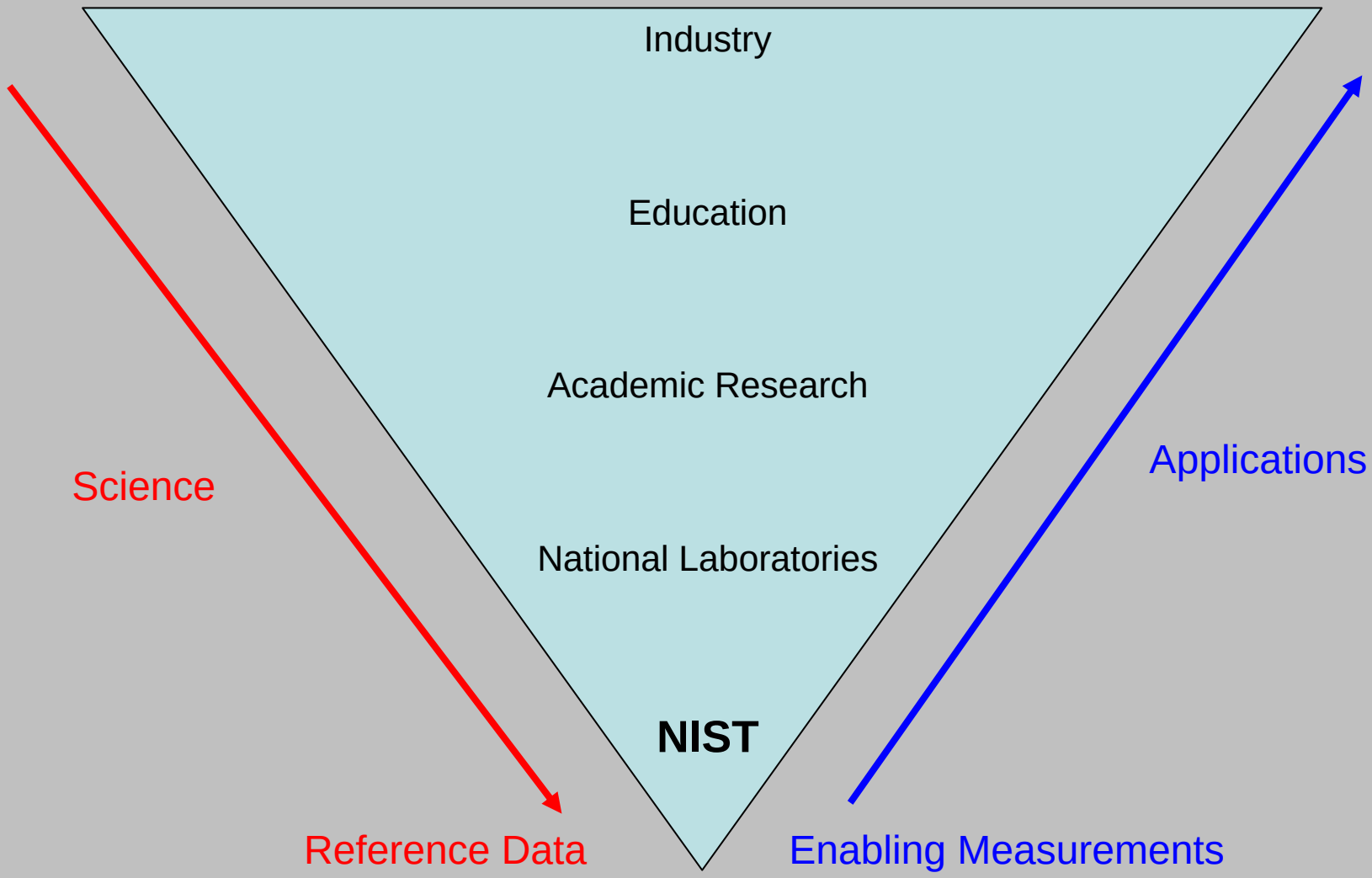
International Chemical Identifier (*InChI*)

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

NIST Data Activities



Many Sectors
Many 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

o Some FREE
o Some FEE ($)
    - nominal costs for distributing databases (~$100-200)
    - maintaining, expanding, and improving databases (~$1500-5000)

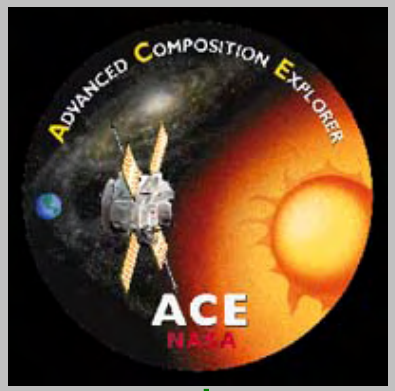
NIST as a Source of Data and Information

- 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

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

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**



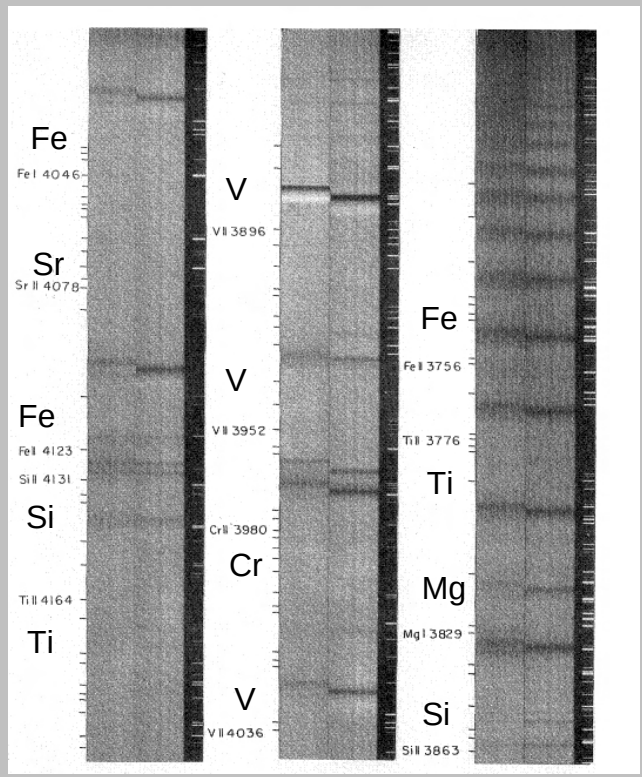
Data

NASA/Observatories

Information

NIST Atomic Spectra Database (ASD)

Knowledge



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.

Physical Constants
Updated! Fundamental Physical Constants
Updated! Searchable Bibliography on the Constants
International System of Units (SI) or see Special Publication 811
Guidelines for Evaluating and Expressing Measurement Uncertainty

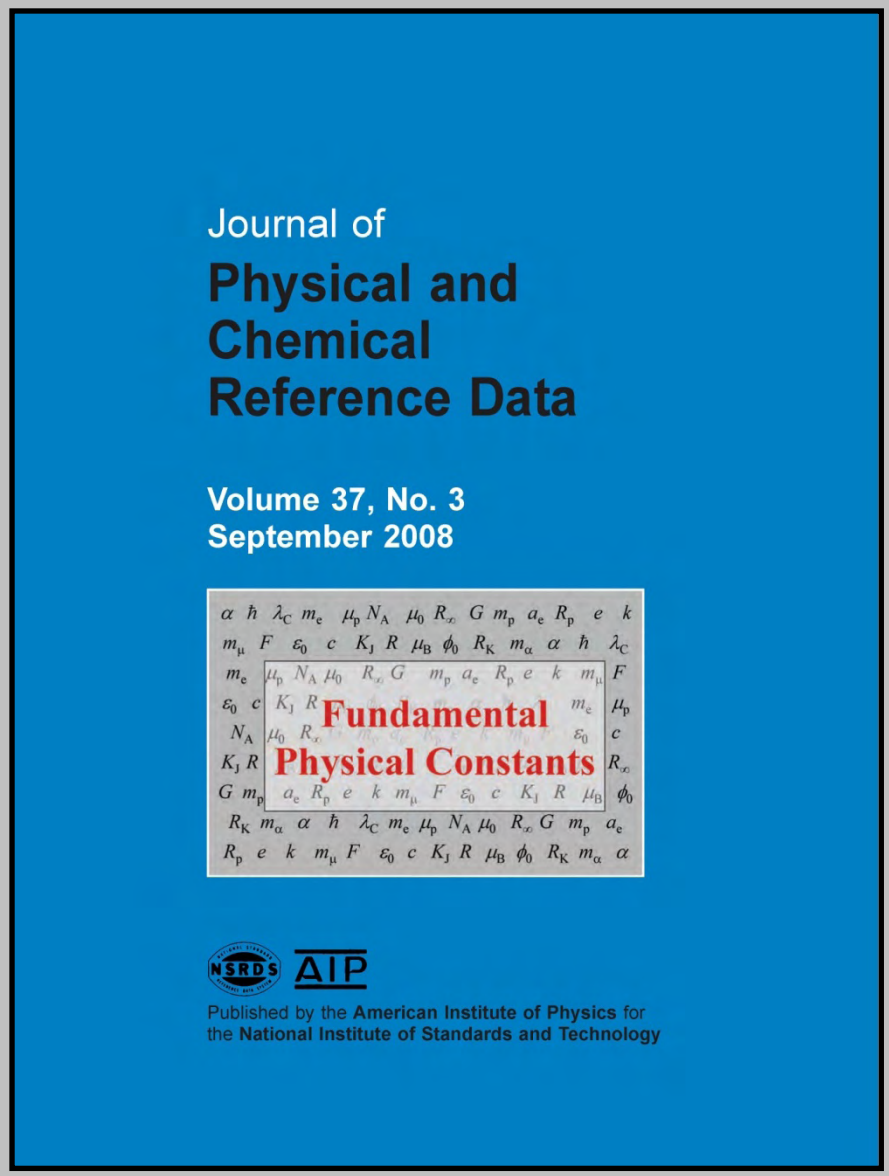
Periodic Table of the Elements
Periodic Table: Atomic Properties of the Elements
Contains NIST critically-evaluated data on atomic properties of the elements.
Suitable for high-resolution color printing for desk or wall-chart display.

Atomic Spectroscopy Data
Status of Atomic Spectroscopy Data
Updated! Atomic Spectra Database
Handbook of Basic Atomic Spectroscopic Data
Energy Levels of Hydrogen and Deuterium
Ground Levels and Ionization Energies for the Neutral Atoms
Spectral Data for the Chandra X-ray Observatory
NLTE Databases and Codes
FLYCHK Collisional-Radiative Code
SAHA Plasma Population Kinetics Database
NEW! NLTE4 Plasma Population Kinetics Database
Spectrum of Platinum Lamp for Ultraviolet Spectrograph Calibration
X-ray Transition Energies
Bibliographic Databases on Atomic Spectroscopy
Updated! Atomic Transition Probabilities
Updated! Atomic Spectral Line Broadening
NEW! Atomic Energy Levels and Wavelengths

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 CO2 (ARPES) Equations & Underpinning Theory Diatomic Rotational Calculations Methane Symmetry Operations
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

CODATA Fundamental Physical Constants

NIST Standard Reference Database 121



The NIST Reference on Constants, Units, and Uncertainty

Information at the foundation of modern science and technology from the Physics Laboratory of NIST

CODATA Internationally recommended values of the Fundamental Physical Constants

Constants Topics:

Values

Energy Equivalents

Searchable Bibliography

Background

Constants Bibliography

Constants, Units & Uncertainty home page

Latest (2006) values of the constants

Version history and disclaimer

(e.g., **electron mass**, most misspellings okay)

Search for value by name [ ] Search

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

by clicking a category below

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

Find the correlation coefficient between any pair of constants

Data from the least-squares adjustment of the values of the constants

Fundamental Physical Constants — Frequently used constants

Quantity	Symbol	Value	Unit	Relative std. uncert. u_r
speed of light in vacuum	c, c_0	299 792 458	$\mathrm{m\,s^{-1}}$	(exact)
magnetic constant	μ_0	$4\pi \times 10^{-7}$	$\mathrm{N\,A^{-2}}$	
		$= 12.566\,370\,614... \times 10^{-7}$	$\mathrm{N\,A^{-2}}$	(exact)
electric constant $1/\mu_0 c^2$	ϵ_0	$8.854\,187\,817... \times 10^{-12}$	$\mathrm{F\,m^{-1}}$	(exact)
Newtonian constant of gravitation	G	$6.674\,28(67) \times 10^{-11}$	$\mathrm{m^3\,kg^{-1}\,s^{-2}}$	1.0×10^{-4}
Planck constant	h	$6.626\,068\,96(33) \times 10^{-34}$	J s	5.0×10^{-8}
$h/2\pi$	$\hbar$	$1.054\,571\,628(53) \times 10^{-34}$	J s	5.0×10^{-8}
elementary charge	e	$1.602\,176\,487(40) \times 10^{-19}$	C	2.5×10^{-8}
magnetic flux quantum $h/2e$	Φ_0	$2.067\,833\,667(52) \times 10^{-15}$	Wb	2.5×10^{-8}
conductance quantum $2e^2/h$	G_0	$7.748\,091\,7004(53) \times 10^{-5}$	S	6.8×10^{-10}
electron mass	m_e	$9.109\,382\,15(45) \times 10^{-31}$	kg	5.0×10^{-8}
proton mass	m_p	$1.672\,621\,637(83) \times 10^{-27}$	kg	5.0×10^{-8}
proton-electron mass ratio	m_p/m_e	1836.152 672 47(80)		4.3×10^{-10}
fine-structure constant $e^2/4\pi\epsilon_0\hbar c$	α	$7.297\,352\,5376(50) \times 10^{-3}$		6.8×10^{-10}
inverse fine-structure constant	α^{-1}	137.035 999 679(94)		6.8×10^{-10}
Rydberg constant $\alpha^2 m_e c/2h$	R_∞	10 973 731.568 527(73)	$\mathrm{m^{-1}}$	6.6×10^{-12}
Avogadro constant	N_A, L	$6.022\,141\,79(30) \times 10^{23}$	$\mathrm{mol^{-1}}$	5.0×10^{-8}
Faraday constant $N_A e$	F	96 485.3399(24)	C $\mathrm{mol^{-1}}$	2.5×10^{-8}
molar gas constant	R	8.314 472(15)	J $\mathrm{mol^{-1}\,K^{-1}}$	1.7×10^{-6}
Boltzmann constant R/N_A	k	$1.380\,6504(24) \times 10^{-23}$	$\mathrm{J\,K^{-1}}$	1.7×10^{-6}
Stefan-Boltzmann constant $(\pi^2/60)k^4/\hbar^3 c^2$	σ	$5.670\,400(40) \times 10^{-8}$	$\mathrm{W\,m^{-2}\,K^{-4}}$	7.0×10^{-6}
Non-SI units accepted for use with the SI				
electron volt: (e/C) J	eV	$1.602\,176\,487(40) \times 10^{-19}$	J	2.5×10^{-8}
(unified) atomic mass unit 1 u $= m_u = \frac{1}{12}m(^{12}\mathrm{C})$ $= 10^{-3}$ kg $\mathrm{mol^{-1}}/N_A$	u	$1.660\,538\,782(83) \times 10^{-27}$	kg	5.0×10^{-8}

The NIST Reference on Constants, Units, and Uncertainty

Information at the foundation of modern science and technology from the Physics Laboratory of NIST

Fundamental Physical Constants

Constants Topics:

Values

Energy Equivalents

Searchable Bibliography

Background

Constants Bibliography

Constants, Units & Uncertainty home page

Searchable bibliography on the constants

Version history

Introduction Detailed search instructions Disclaimer

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

Word(s) in title or assigned keyword(s): e.g., `alpha`

Allow similar spelling ☐

Author (s): Allow similar spelling ☐

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

Boltzmann Constant (k_B) and Universal Gas Constant (R)

The ***Boltzmann Constant*** k_B and
the ***Universal Gas Constant*** $R = N_A \times k_B$
connect ***Energy*** with ***Temperature*** T

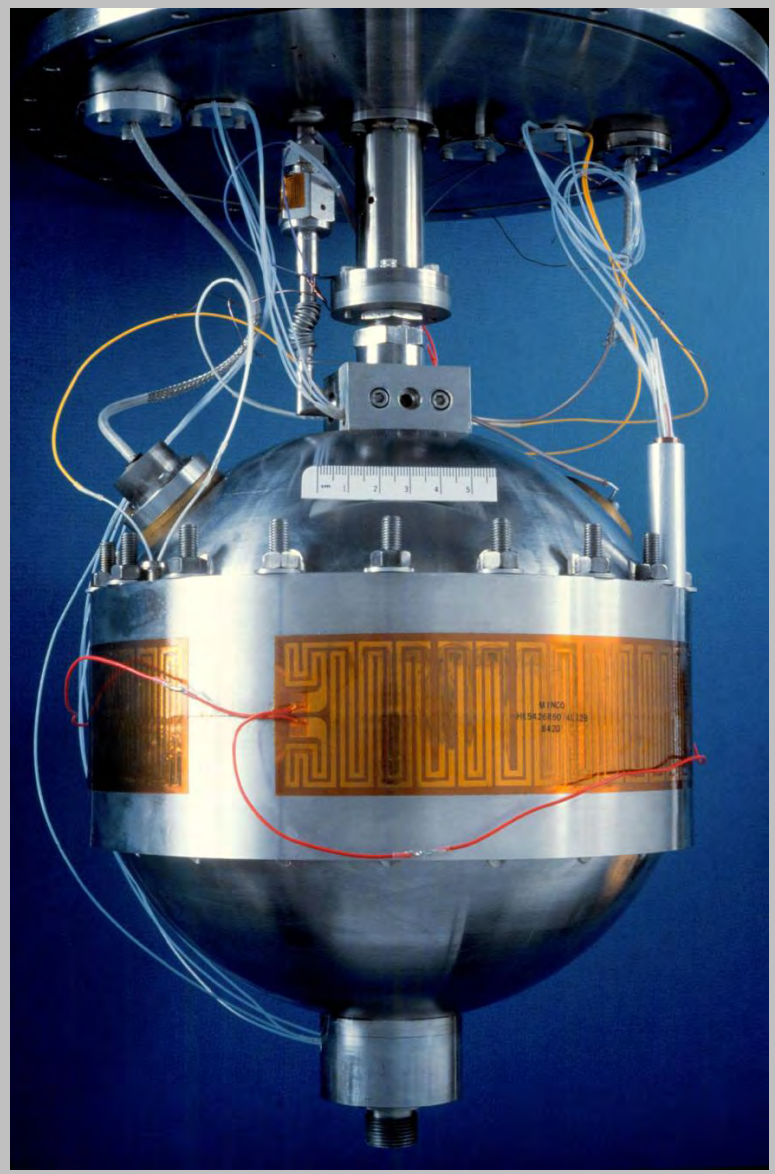
Examples

dilute gas: $pV = nRT(1 + \cdots$

black body radiation:

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

CSTL has determined R from the acoustic resonances of an argon-filled spherical cavity with a relative uncertainty of 1.8×10^{-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

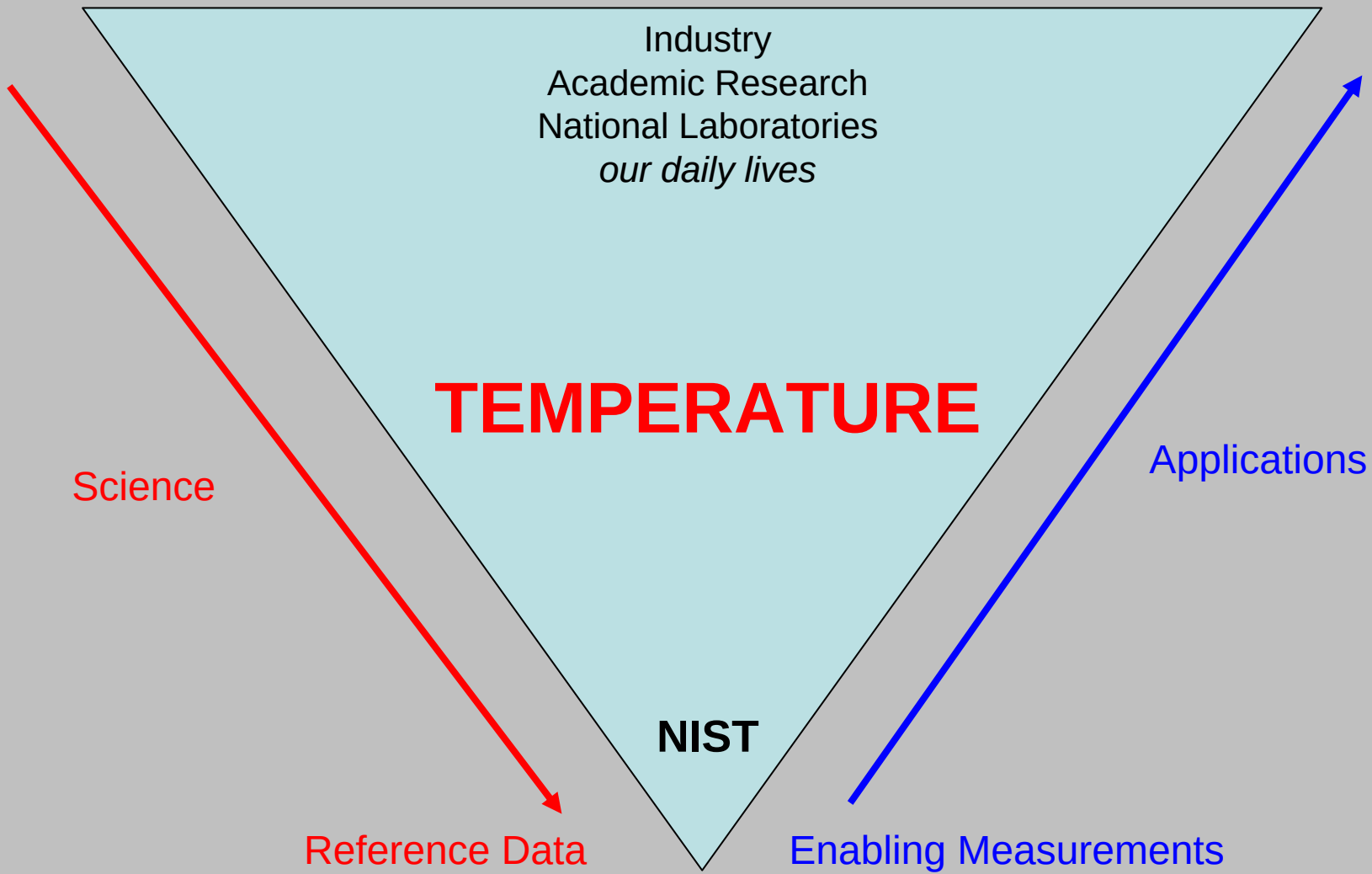
- IAPWS Formulation for the Thermodynamic Properties of Water
- Vapor-Liquid Distribution Constants for Gaseous Solutes in Water at High Temp.

- 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
- Enthalpies of Sublimation of Organic Compounds, 1910-2001
- 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



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

Thermocouple Grade
– 328 to 2282°F
– 200 to 1250°C

Extension Grade
32 to 392°F
0 to 200°C

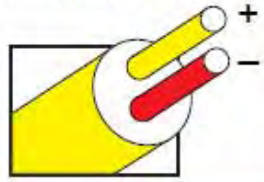
LIMITS OF ERROR
(whichever is greater)
Standard: 2.2°C or 0.75% Above 0°C
2.2°C or 2.0% Below 0°C
Special: 1.1°C or 0.4%

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

Thermocouple Grade

Nickel-Chromium vs. Nickel-Aluminum



Extension Grade

Revised Thermocouple Reference Tables

TYPE K

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

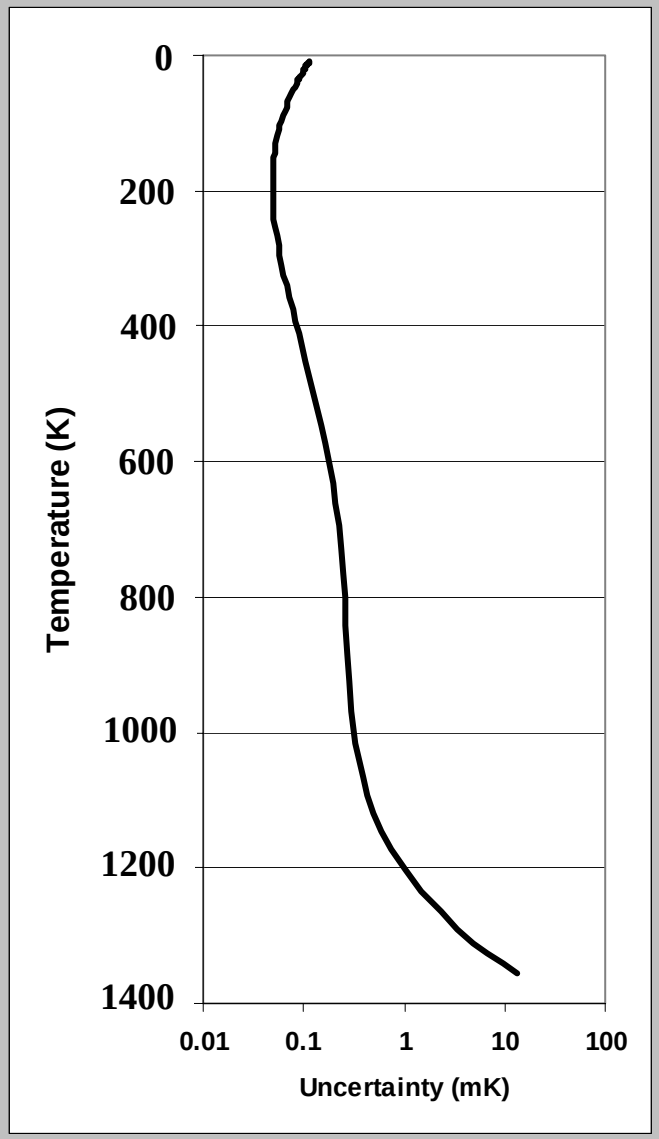
Thermoelectric Voltage in Millivolts

°C	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	°C
-260	-6.458	-6.457	-6.456	-6.455	-6.453	-6.452	-6.450	-6.448	-6.446	-6.444	-6.441	-260
-250	-6.441	-6.438	-6.435	-6.432	-6.429	-6.425	-6.421	-6.417	-6.413	-6.408	-6.404	-250
-240	-6.404	-6.399	-6.393	-6.388	-6.382	-6.377	-6.370	-6.364	-6.358	-6.351	-6.344	-240
-230	-6.344	-6.337	-6.329	-6.322	-6.314	-6.306	-6.297	-6.289	-6.280	-6.271	-6.262	-230
-220	-6.262	-6.252	-6.243	-6.233	-6.223	-6.213	-6.202	-6.192	-6.181	-6.170	-6.158	-220
-210	-6.158	-6.147	-6.135	-6.123	-6.111	-6.099	-6.087	-6.074	-6.061	-6.048	-6.035	-210
-200	-6.035	-6.021	-6.007	-5.994	-5.980	-5.965	-5.951	-5.936	-5.922	-5.907	-5.891	-200
-190	-5.891	-5.876	-5.861	-5.845	-5.829	-5.813	-5.797	-5.780	-5.763	-5.747	-5.730	-190
-180	-5.730	-5.713	-5.695	-5.678	-5.660	-5.642	-5.624	-5.606	-5.588	-5.569	-5.550	-180
-170	-5.550	-5.531	-5.512	-5.493	-5.474	-5.454	-5.435	-5.415	-5.395	-5.374	-5.354	-170
-160	-5.354	-5.333	-5.313	-5.292	-5.271	-5.250	-5.228	-5.207	-5.185	-5.163	-5.141	-160
-150	-5.141	-5.119	-5.097	-5.074	-5.052	-5.029	-5.006	-4.983	-4.960	-4.936	-4.913	-150

°C	0	1	2	3	4	5	6	7	8	9	10	°C
250	10.153	10.194	10.235	10.276	10.316	10.357	10.398	10.439	10.480	10.520	10.561	250
260	10.561	10.602	10.643	10.684	10.725	10.766	10.807	10.848	10.889	10.930	10.971	260
270	10.971	11.012	11.053	11.094	11.135	11.176	11.217	11.259	11.300	11.341	11.382	270
280	11.382	11.423	11.465	11.506	11.547	11.588	11.630	11.671	11.712	11.753	11.795	280
290	11.795	11.836	11.877	11.919	11.960	12.001	12.043	12.084	12.126	12.167	12.209	290
300	12.209	12.250	12.291	12.333	12.374	12.416	12.457	12.499	12.540	12.582	12.624	300
310	12.624	12.665	12.707	12.748	12.790	12.831	12.873	12.915	12.956	12.998	13.040	310
320	13.040	13.081	13.123	13.165	13.206	13.248	13.290	13.331	13.373	13.415	13.457	320
330	13.457	13.498	13.540	13.582	13.624	13.665	13.707	13.749	13.791	13.833	13.874	330
340	13.874	13.916	13.958	14.000	14.042	14.084	14.126	14.167	14.209	14.251	14.293	340
350	14.293	14.335	14.377	14.419	14.461	14.503	14.545	14.587	14.629	14.671	14.713	350
360	14.713	14.755	14.797	14.839	14.881	14.923	14.965	15.007	15.049	15.091	15.133	360
370	15.133	15.175	15.217	15.259	15.301	15.343	15.385	15.427	15.469	15.511	15.554	370
380	15.554	15.596	15.638	15.680	15.722	15.764	15.806	15.849	15.891	15.933	15.975	380
390	15.975	16.017	16.059	16.102	16.144	16.186	16.228	16.270	16.313	16.355	16.397	390

International Temperature Scale (ITS-90)

NIST Standard Reference Database 60



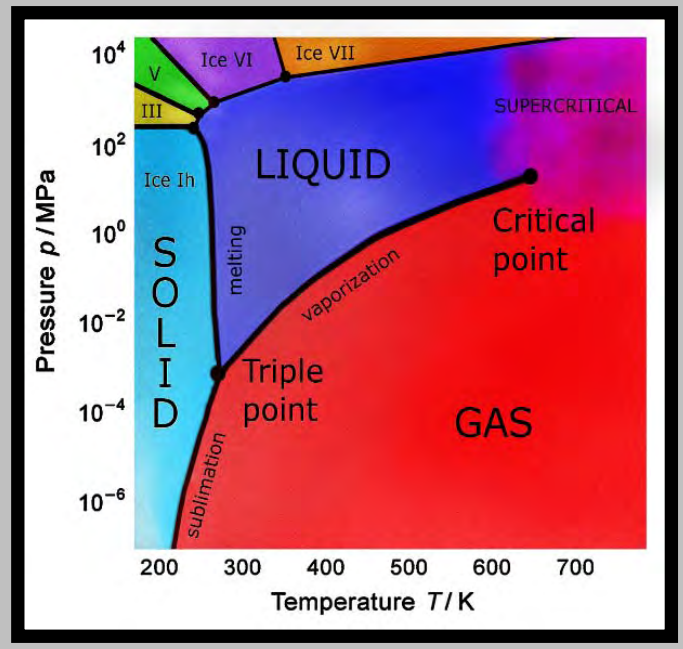
Fixed Pt	T / K	Substance	State
1	3 to 5	He	vapor press
2	13.8033	e-H_2	triple pt
3	~17	e-H_2/He	vapor press gas thermometry
4	~20.3	e-H_2/He	vapor press gas thermometry
5	24.5561	Ne	triple pt
6	54.3584	O_2	triple pt
7	83.8058	Ar	triple pt
8	234.3156	Hg	triple pt
9	273.16	H_2O	triple pt
10	302.9146	Ga	melting pt
11	429.7485	In	freezing pt
12	505.078	Sn	freezing pt
13	692.677	Zn	freezing pt
14	933.473	Al	freezing pt
15	1234.93	Ag	freezing pt
16	1337.33	Au	freezing pt
17	1357.77	Cu	freezing pt

Thermophysical Properties of Water and Steam

NIST Standard Reference Database 10

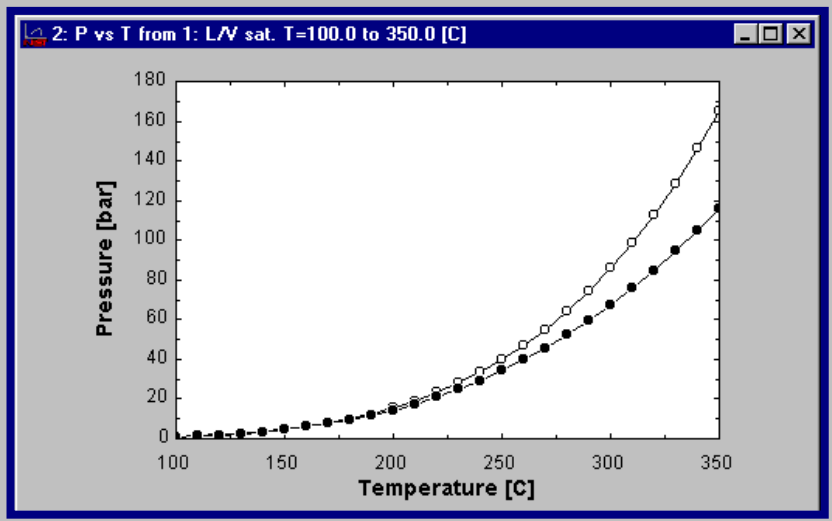
- Thermodynamic Properties
- Transport Properties
- Dielectric Constant, Refractive Index

Implements standards adopted by IAPWS
Inter. Assoc. for the Properties of Water & Steam



1: V/L sat. T=300.0 to 500.0 [K]

	Temperature [K]	Pressure [MPa]	Density (L) [kg/m³]	Density (V) [kg/m³]
1	300.0	0.003537	996.5	0.02559
2	320.0	0.01055	989.4	0.07166
3	340.0	0.02719	979.5	0.1744
4	360.0	0.06219	967.4	0.3786
5	380.0	0.1289	953.3	0.7483
6	400.0	0.2458	937.5	1.369
7	420.0	0.4373	919.9	2.352
8	440.0	0.7337	900.6	3.833
9	460.0	1.171	879.6	5.983
10	480.0	1.790	856.5	9.014
11	500.0	2.639	831.3	13.20



Reference Fluid Thermodynamic and Transport Properties Database (REFPROP)

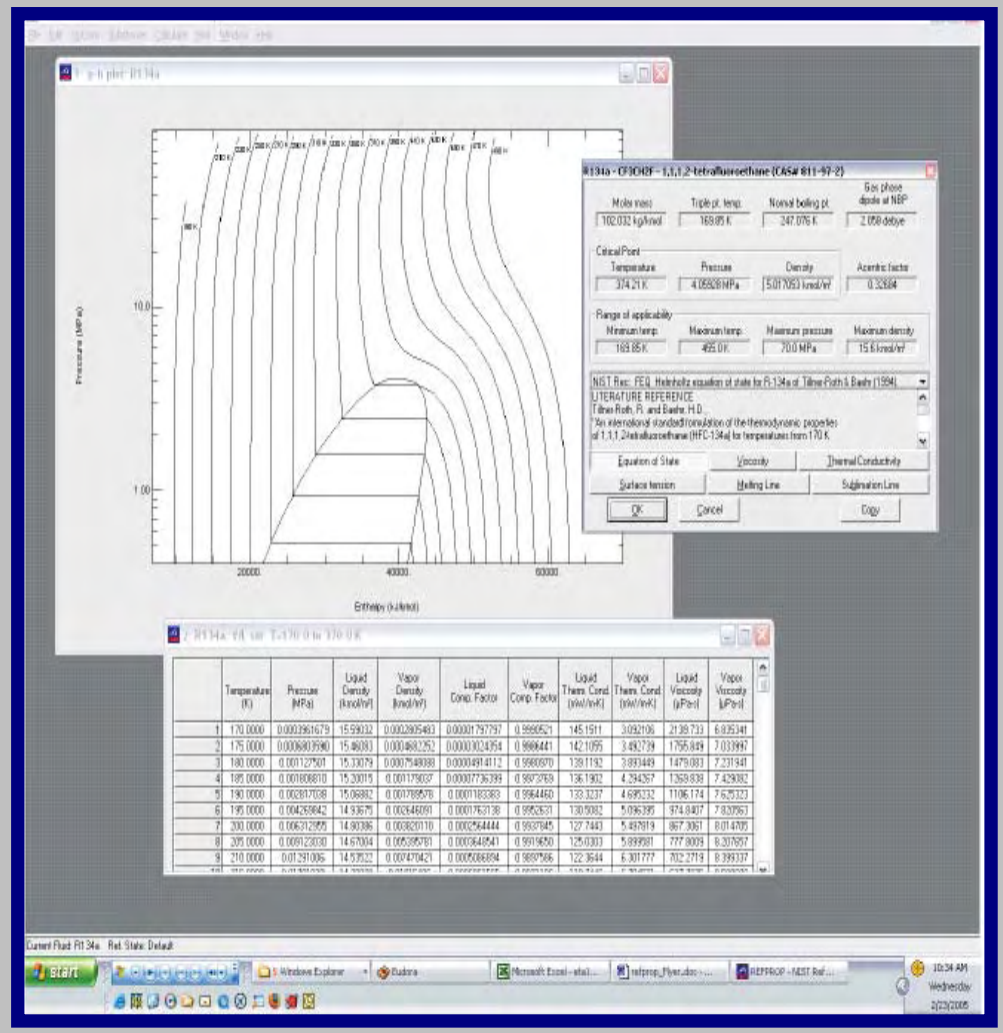
NIST Standard Reference Database 23

- Thermodynamic Properties
- Transport Properties

<u>Pure fluids and mixtures</u>

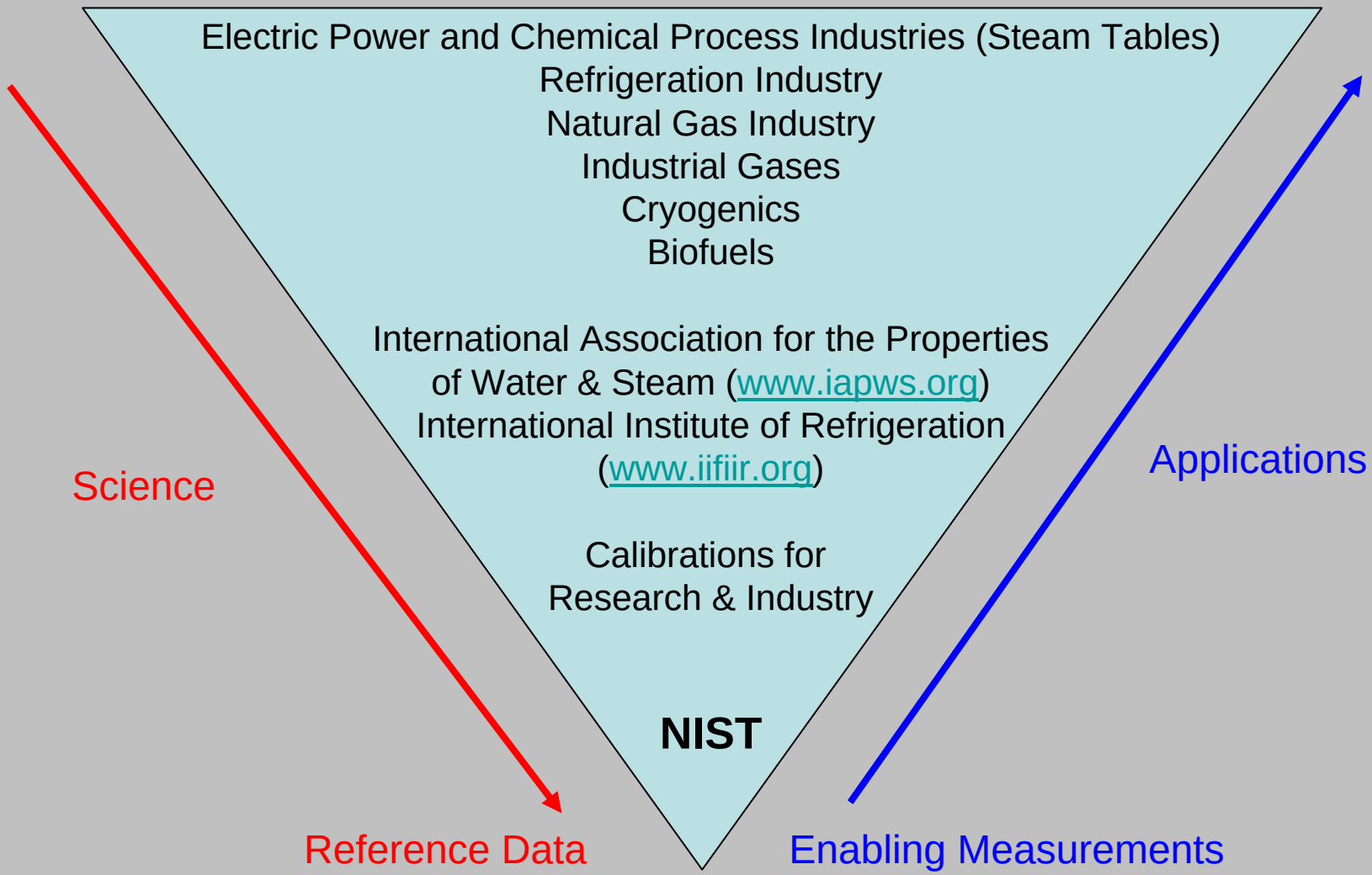
Implements standards and best available equations of state (EOS)

- 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



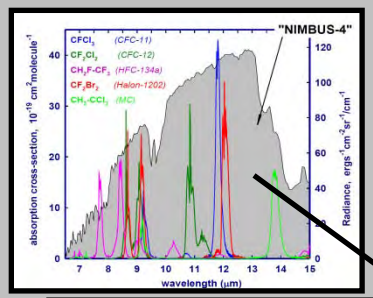
Industrial Process Design

Standardized Properties of Industrially Important Fluids

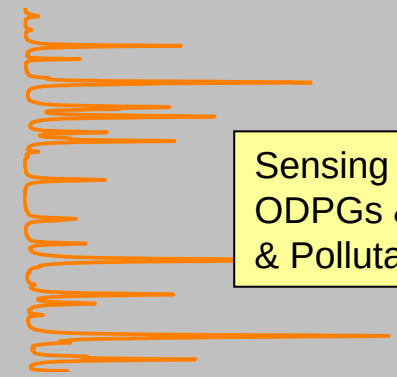


Global Environment

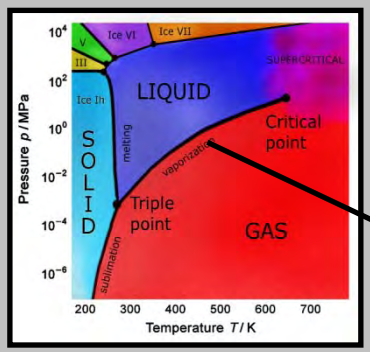
Various NIST Data Contributions



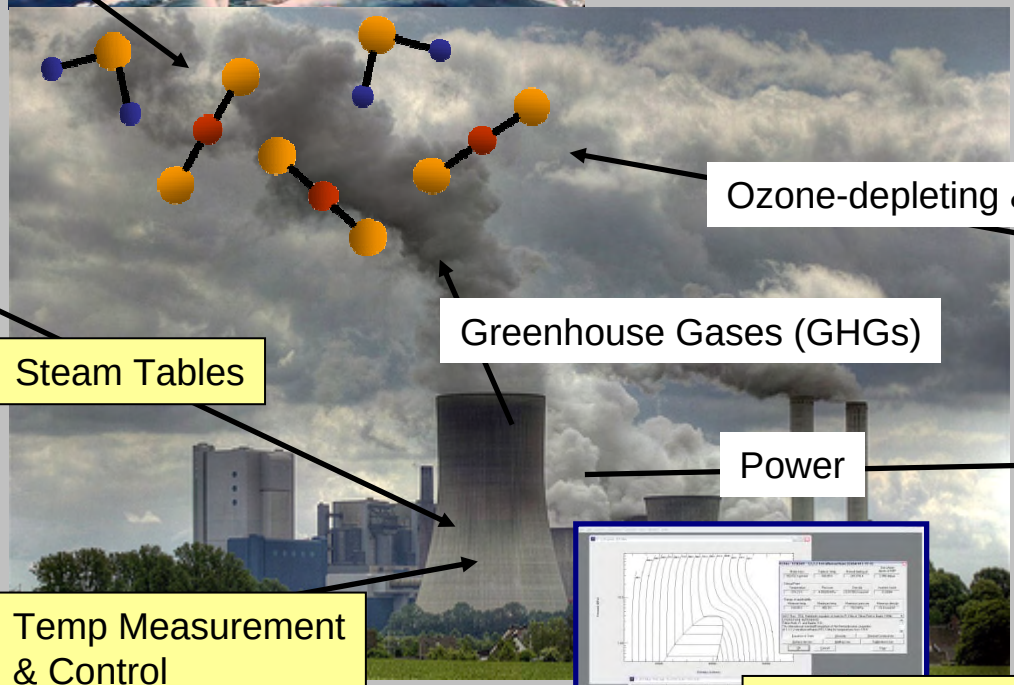
Photochemistry of ODPGs & GHGs



Sensing of ODPGs & GHGs & Pollutants



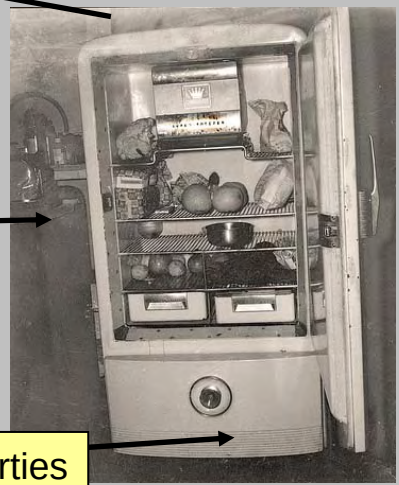
Steam Tables

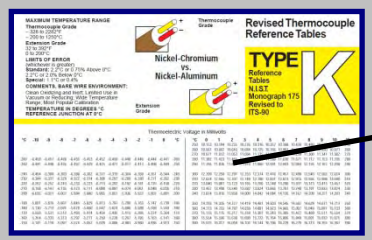


Ozone-depleting & GHGs

Greenhouse Gases (GHGs)

Power



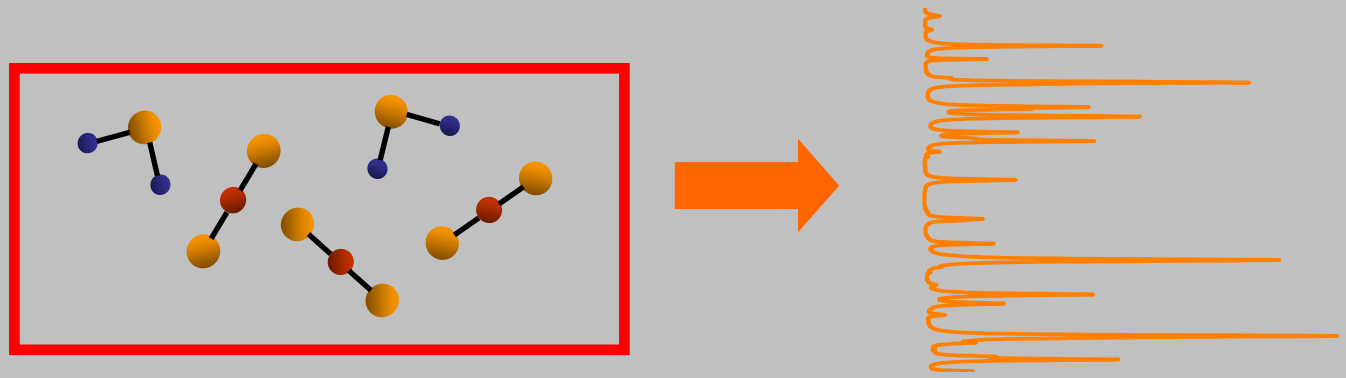


Temp Measurement & Control

Refrigerant Properties

Climate Change and Carbon Cap & Trading

Spectroscopic reference data for remote sensing of greenhouse gases



High-resolution spectral line parameters

- O_2, H_2O; Greenhouse gases (GHGs)
- uncertainties < 0.5%

HITRAN Database (2008) updated with NIST O_2 data

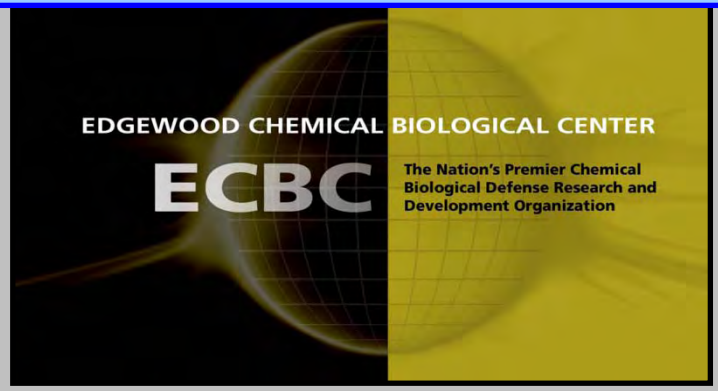
AIRS, 2002

Satellite Measurements of CO_2

ASCENDS, 2013-16

Quality-Assured Infrared Absorption Coefficient Data

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

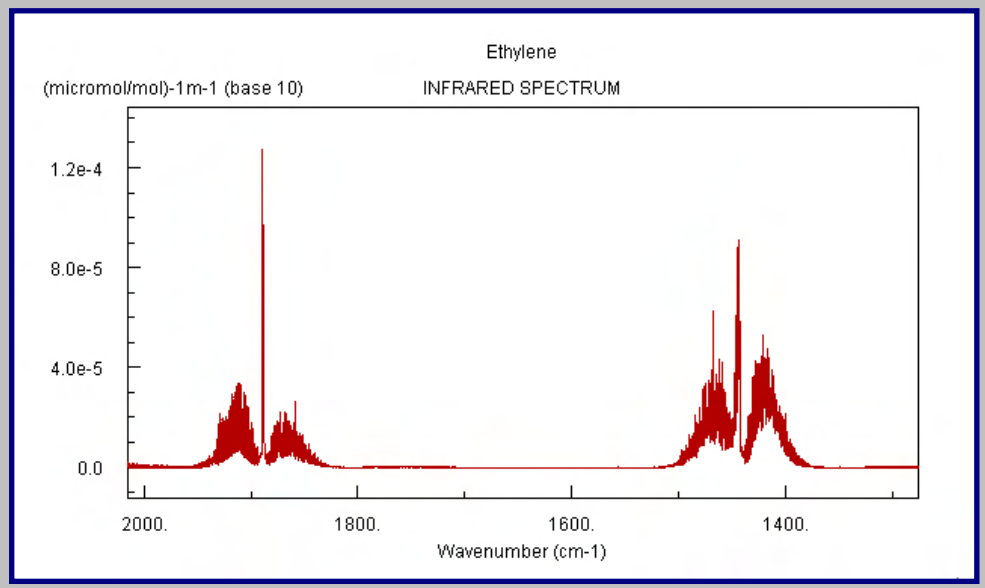


Northwest-Infrared

vapor phase infrared spectral library

http://nwir.pnl.gov

NIST Standard Reference Database 79

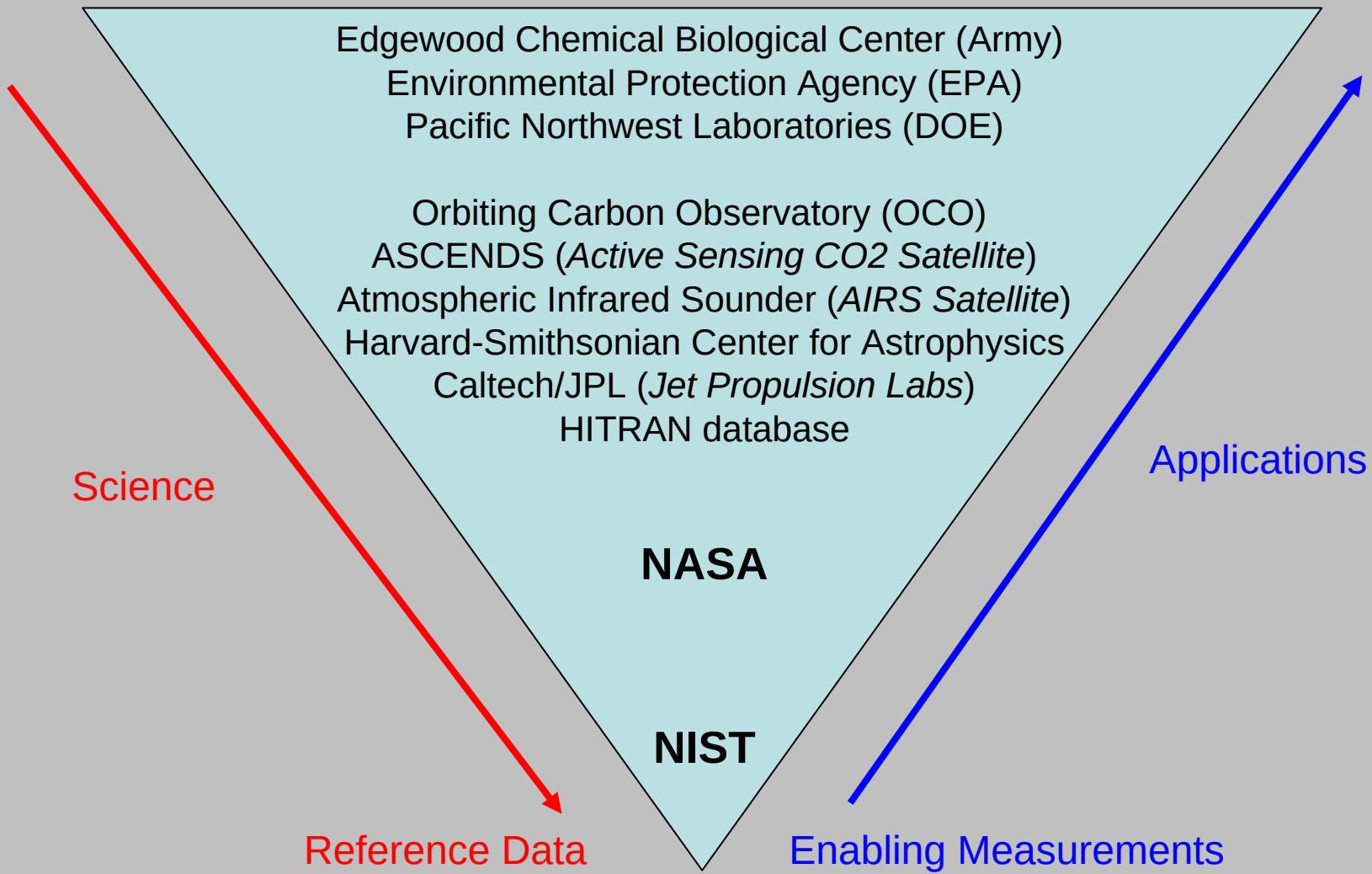


http://webbook.nist.gov/chemistry/

Global Environment, Health Sciences, and Homeland Security

Chemical and Biological Agents; Environmental Regulations

Air Pollutants, Greenhouse Gases, Ozone-Depleting Chemicals



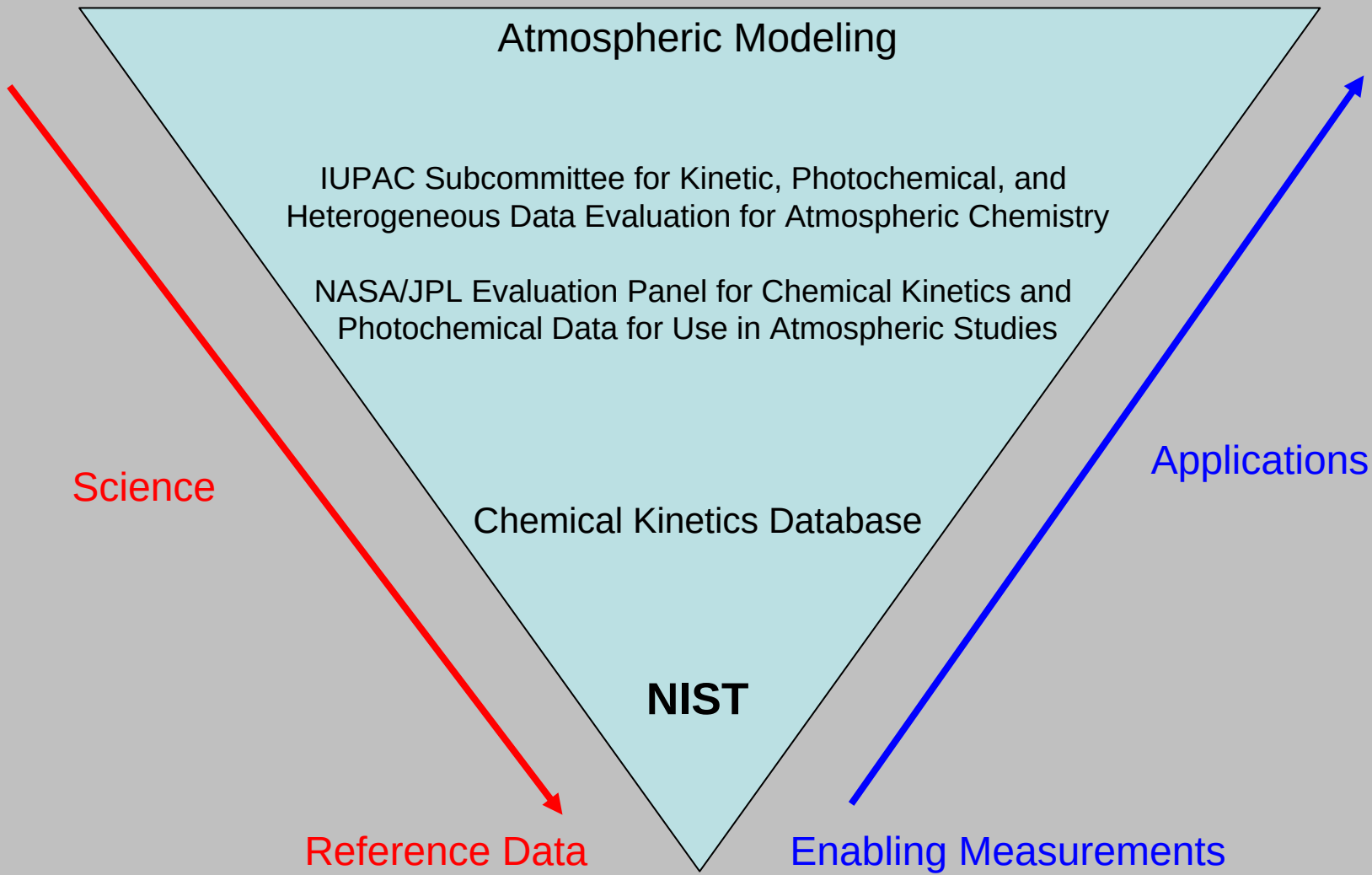
Gas Phase Chemical Kinetics

NIST Standard Reference Database 133

Reference	Temp [K]	A	n	Ea [kJ]	k(298 K)
2001ATK/BAU1-56	200 - 300	6.90E-12		8.31	2.41E-13
1997DEM/SAN1-266	200 - 300	8.70E-12		8.9	2.40E-13
1997ATK/BAU521-1011	240 - 300	7.89E-12		8.56	2.49E-13
1996DON/CLA5821-5838	300	2.54E-13			
1994DEM/SAN	200 - 300	8.70E-12		8.9	2.40E-13
1992BAU/COB411-429	250 - 2000	1.06E-12	2	3.62	2.47E-13
1992ATK/BAU1125-1568	240 - 300	7.80E-12		8.48	2.55E-13
1989ATK/BAU881-1097	230 - 300	7.41E-12		8.23	2.67E-13
1986TSA/HAM1087	300 - 2500	5.50E-12	1.04	7.59	
1986BAU/BOW465	250 - 1200	2.32E-11		11.14	2.59E-13
1986ATK69	238 - 850	1.22E-12	2	3.69	2.75E-13
1984WAR197C	300 - 2000	9.27E-13	2	2.7	
1983COH/WES531	300 - 2000	1.84E-12	1.9	4.74	
1972WIL535-573	300 - 2000	1.08E-10		14.97	
2004KRA/MIC5643-5648	822 - 1367	1.10E-10		21.09	
1998HEA/ANA711-717	298	2.81E-13			2.81E-13
1998DON/AND3121-3126	300 - 390	9.43E-12		8.9	
1998CLA/KRO9847-9857	298	2.52E-13			2.52E-13
1998CAV/GLA3767-3773	295	4.2			
1996KOF/COH79-87	970	8.39E-12			
1996CRO/CAM3601-3606	247 - 303	1.33E-11		9.89	2.46E-13
1996ANC/VAN1009-1016	1530 - 1790	2.92E-10		32.01	
1994TAL/MEL973-990	231 - 377	1.03E-11		9.23	2.49E-13
1993SHA/SMI631-638	138 - 298	4.92E-14	6.93	-4.54	

Global Environment

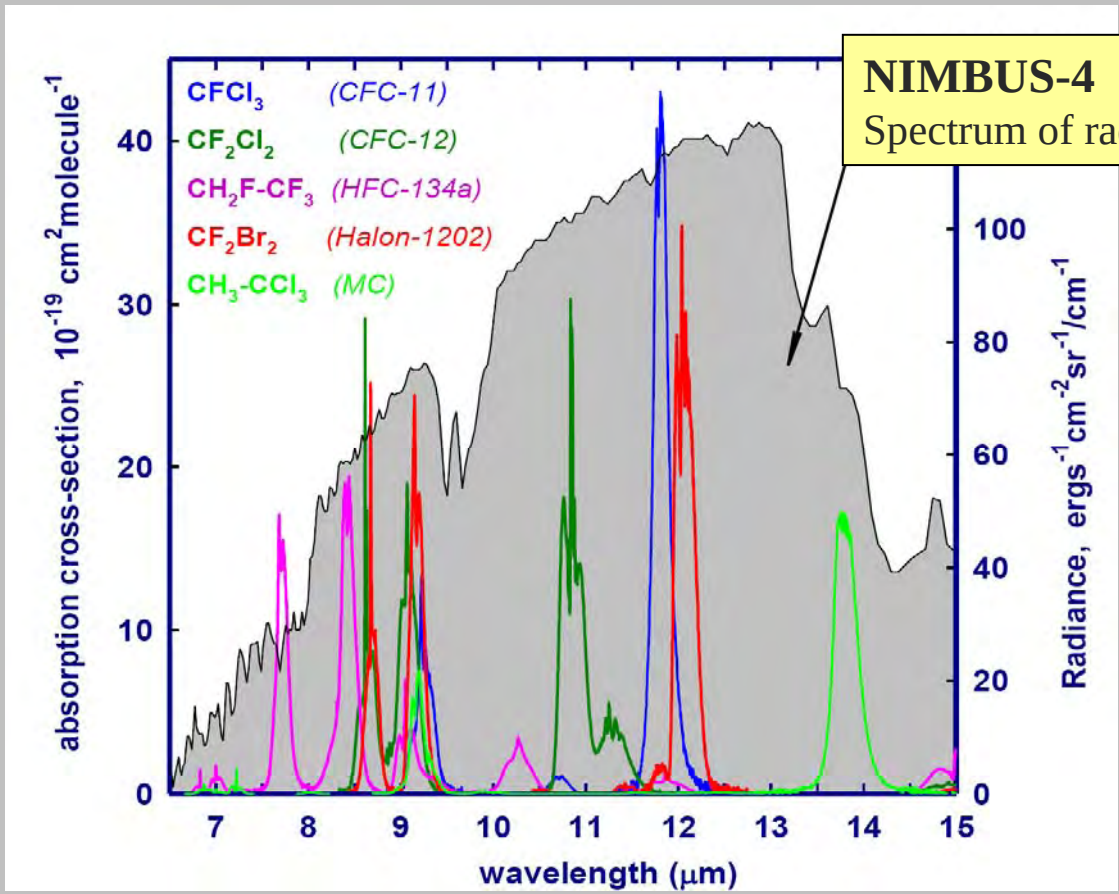
Air Pollutants, Greenhouse Gases, Ozone-Depleting Chemicals



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.

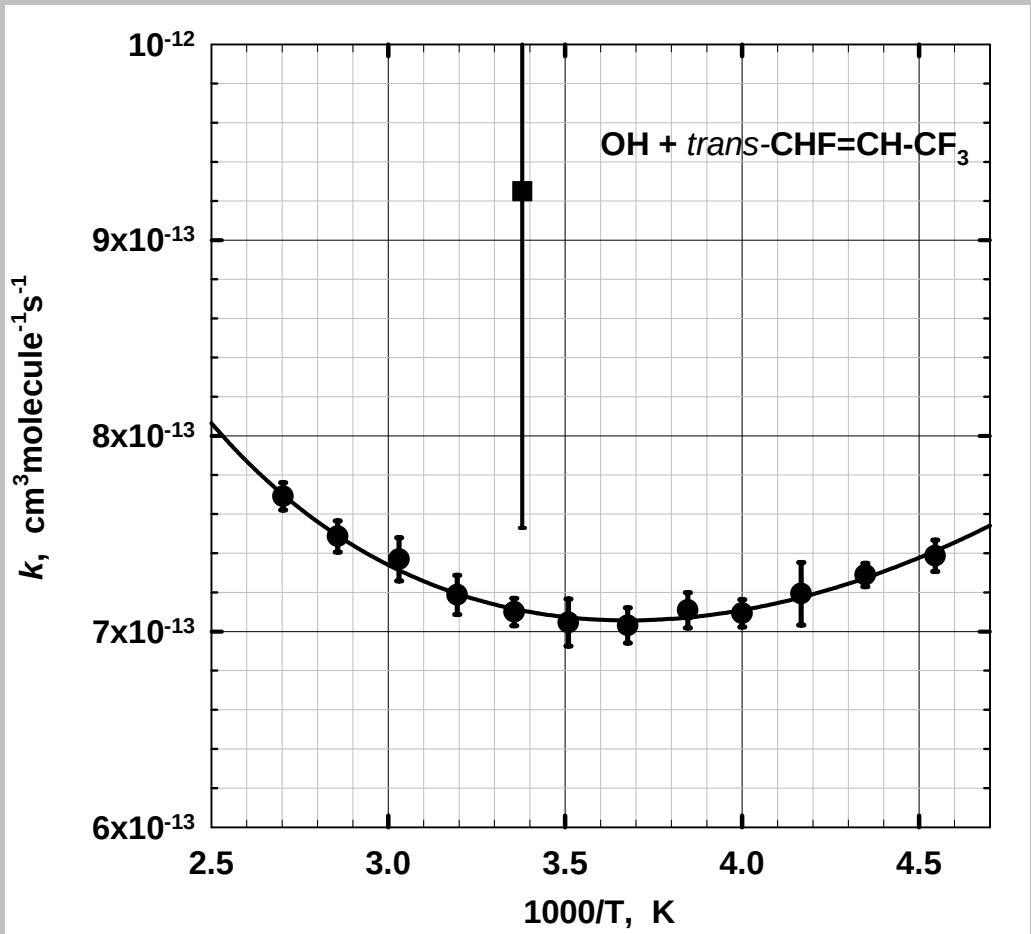


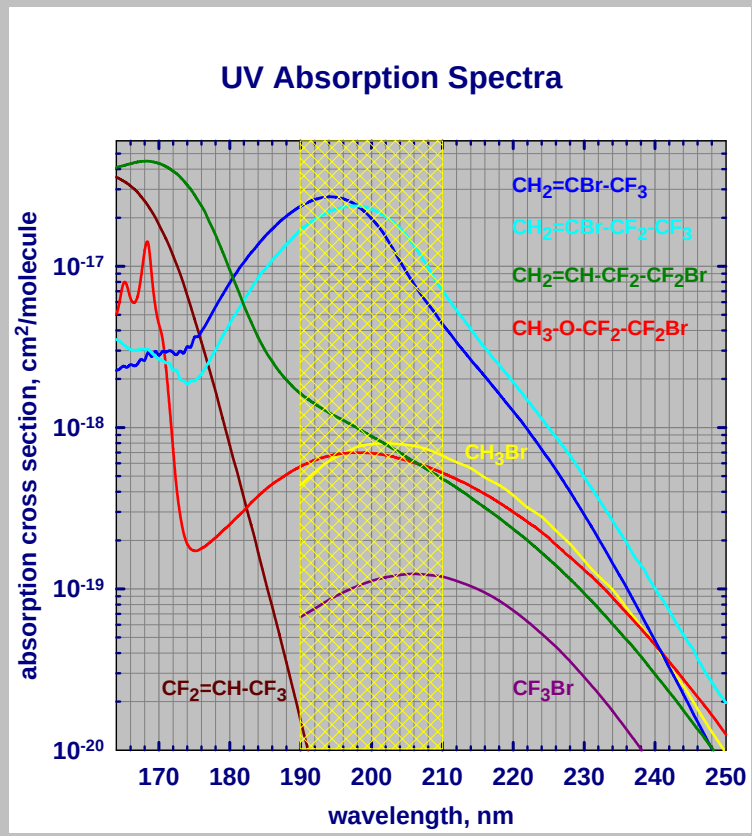
NIMBUS-4
Spectrum of radiation from Earth

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





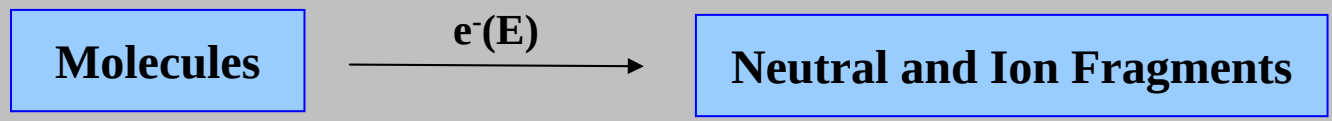
Photoinduced Chemistry

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.



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*

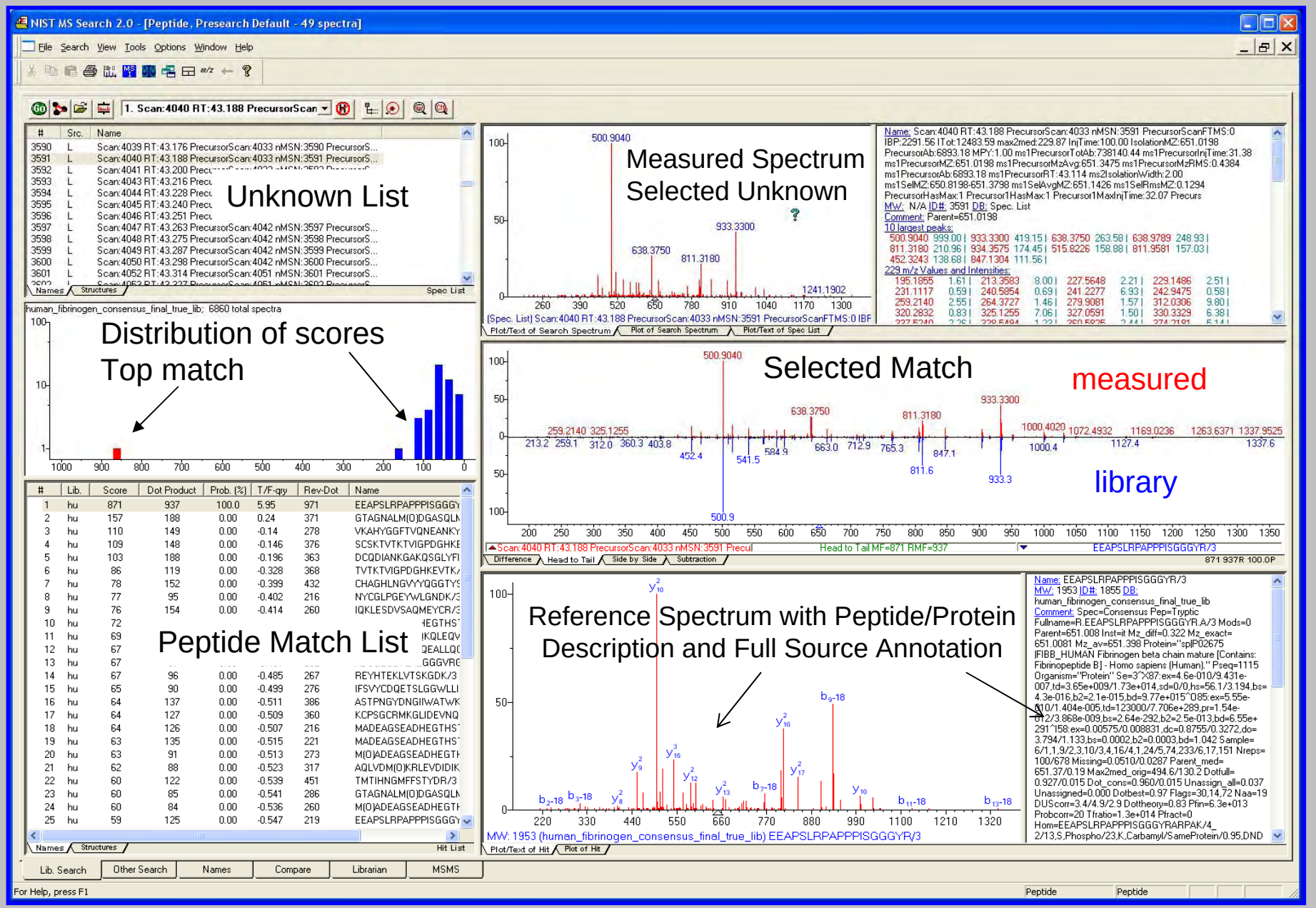
Ion	Reactant	Other products	AP or IP (eV)	Method	Heat of formation (kcal mol^{-1})	Ref.
		$C_4H_9O_3^+$				
$C_4H_9O_3^+$	$(CH_3O)_3CH$	H	10.39 ± 0.05	RPD	66	1139
$C_4H_9O_3^+$	$(CH_3O)_3CCH_3$	CH_3	10.39 ± 0.10	RPD	78	1139
$C_4H_9O_3^+$	$(CH_3O)_4C$	CH_3O	10.32 ± 0.10	RPD	80	1139
		$C_8H_8O_3^+$				
$C_8H_8O_3^+$ (Methyl hydroxybenzoate)	$C_6H_4OHCOOCH_3$		9.03	TC	94	2194
		$C_9H_{10}O_3^+$				
$C_9H_{10}O_3^+$ (Methyl *p*-methoxybenzoate)	$C_6H_4OCH_3COOCH_3$		8.43 ± 0.04	CS	90*	2026
$C_9H_{10}O_3^+$ (Methyl methoxybenzoate)	$C_6H_4OCH_3COOCH_3$		8.73	TC	97	2194
		$C_{13}H_{10}O_3^+$				
$C_{13}H_{10}O_3^+$ (Diphenyl carbonate)	$(C_6H_5)_2CO_3$		9.01 ± 0.05	SL	122*	1237
		$C_6H_{11}O_5^+$				
$C_6H_{11}O_5^+$ (α-Methyl-(D)-glucoside)	$C_7H_{14}O_6$	CH_3O	12.9 ± 0.16	EVD	28	2036
$C_6H_{11}O_5^+$ (β-Methyl-(D)-glucoside)	$C_7H_{14}O_6$	CH_3O	13.5 ± 0.16	EVD	42	2036
		HNO_3^+				
HNO_3^+	HNO_3		11.03 ± 0.01	PI	222	1253
		$C_2H_6BO^+$				
$C_2H_6BO^+$	$(CH_3O)_3B$	$CH_2O + OH$	16.6 ± 0.3	EVD	187	115
		$C_2H_5BO_2^+$				
$C_2H_5BO_2^+$	$(CH_3O)_3B$	$CH_2O + H_2$	13.2 ± 0.2	EVD	117	115
		$C_2H_6BO_2^+$				
$C_2H_6BO_2^+$	$(CH_3O)_2BH$	H	9.0 ± 0.2	SL	16	364
$C_2H_6BO_2^+$	$(CH_3O)_3B$	CH_3O	13.0 ± 0.2	EVD	85	115
$C_2H_6BO_2^+$	$(CH_3O)_3B$	CH_3O	9.6 ± 0.2	SL	7	364

Molecules

$e^-(E)$

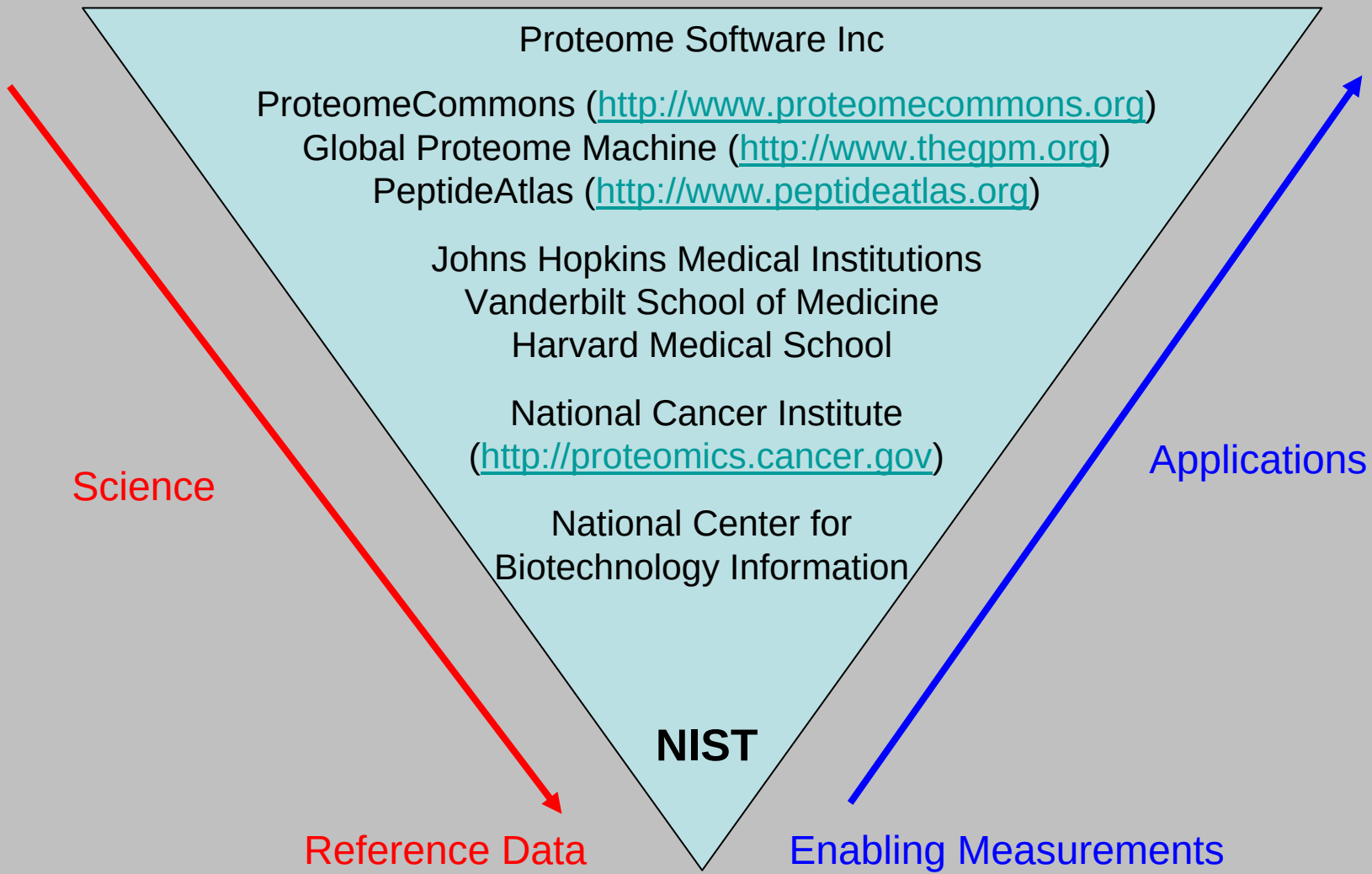
Neutral and Ion Fragments

NIST MS Search 2.0 – Peptide Version (free)



Biosciences and Health

Improving success rate of discovery experiments in proteomics



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

NIST Chemistry WebBook

Naphthalene

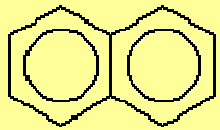
Formula: $C_{10}H_8$

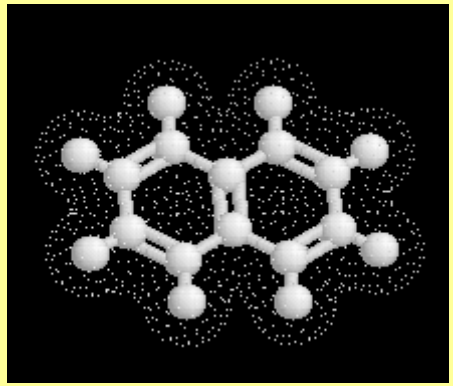
Molecular weight: 128.1705

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; Napthalene, molten; Rcra waste number U165; UN 1334; UN 2304

Other data available:

… … …

… …

…

NIST Chemistry WebBook

Naphthalene

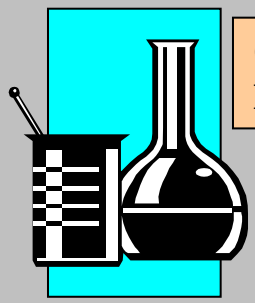
Other data available:

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

Thermodynamics Research Center (TRC)

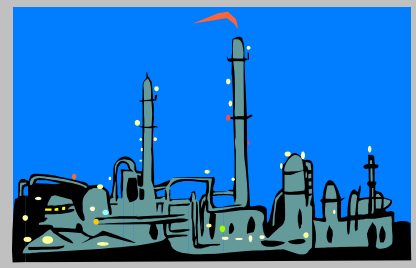


Experimentalists

Committee on Printed & Electronic Publication (CPEP)

International Association of Chemical Thermodynamics (IACT)

IUPAC



Industrial Engineers

NIST Guided Data Capture (GDC)

Measurements

Applications

Products

Users

- J. Chem. Eng. Data *(ACS)*
- J. Chem. Thermodyn. *(Elsevier)*
- Fluid Phase Equilib. *(Elsevier)*
- Int. J. Thermophys. *(Springer)*
- Thermochimica Acta *(Elsevier)*

ThermoML

"Reader" Software

NIST ThermoML Archive

WEB

- AspenTech *(USA)*
- Virtual Materials Group *(Canada)*
- Nat'l Engineering Lab *(UK)*
- Fiz Chemie *(Germany)*

Industry: **DIPPR**

Thermodynamics Research Center (TRC)

NIST Standard Reference Databases 4, 88, 103, S3

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

Thermodynamics Research Center (TRC)

Physical and Chemical Properties Division
TRC Group
NIST National Institute of Standards and Technology
Supplying physical and chemical properties data, models, standards, and research for industry, public health & safety, and the environment

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:

- *TRC Thermodynamic Tables - Hydrocarbons, Ed. M. Frenkel, National Institute of Standards and Technology, Boulder, CO, Standard Reference Data Program, Publication Series NSRDS-NIST- 75 (1942-2007), Gaithersburg, MD.*
- *TRC Thermodynamic Tables - Non-Hydrocarbons, Ed. M. Frenkel, National Institute of Standards and Technology, Boulder, CO, Standard Reference Data Program, Publication Series NSRDS-NIST- 74 (1955-2007), Gaithersburg, MD.*

Search | Clear/Reset

Compound Options:

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

Web Thermo Tables Information Center
About WTT
How to use WTT/Help
WTT statistical information

Property Options:

Critical Properties	Any available	**Vapor Pressure and Boiling Temperatures**	Any available
Phase Transition Properties	Any available	**Volumetric Properties**	Any available
Heat Capacities and Derived Properties	Any available	**Transport Properties**	Any available
Refraction, Surface Tension, and Speed of Sound	Any available	**Reaction State-Change Properties**	Any available

Many Sectors
Many Applications