REFERENCE DATA CHALLENGE

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

Webinar for interested participants in the Reference Data Challenge

Heather Evans,
Challenge Manager

Wednesday, September 2, 2015

Welcome

- Introduction to NIST experts
- Background on NIST
- Overview of the Reference Data Challenge purpose and rules
- Review of Eligible NIST Data
- Q&A

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NIST experts on today's webinar:

Don Burgess
Research Chemist

Peter Linstrom
Chemical Engineer

Russ Johnson
Research Chemist

Adam Morey
Supervisory IT Specialist

Karen Olsen
Computer Scientist

Heather Evans
Challenge Manager
Moderator

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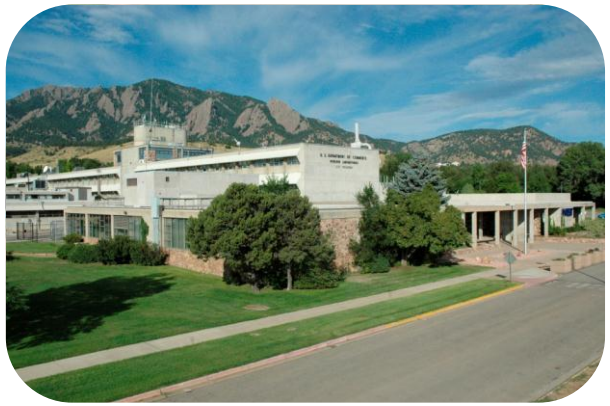
What is NIST?

The National Institute of Standards and Technology, NIST, is a non-regulatory agency of the United States Department of Commerce.

Founded in 1901, NIST's mission is to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life.

Two main sites in Gaithersburg, MD and Boulder, CO



NIST Standard Reference Data

- Formalized in the Standard Reference Data Act of 1968, NIST is responsible to make "critically evaluated reference data readily available to scientists, engineers, and the general public."
- Today, there are more than 100 reference data products available from NIST online.
- The NIST Data Gateway provides easy access to NIST scientific and technical data:

http://srdata.nist.gov/gateway/

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The purpose of the Reference Data Challenge is to spur the development of mobile applications that use freely available NIST datasets.

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- **Key Dates:**
  - Submission Period July 27 – Sept 28, 2015
  - Announcement of Winners Nov 16, 2015

- **Prizes:**
  - 1st Prize $30,000
  - 2nd Prize $10,000
  - 3rd Prize $5,000

- **Rules:**
  - http://nistdata.devpost.com/rules
  - https://federalregister.gov/a/2015-17865

Eligibility Rules for Participating

- **An individual, whether participating singly or with a group, must be over the age of 18 and a citizen or permanent resident of the United States.**
- Multiple entries are permitted. Each entry will be reviewed independently.
- Multiple individuals and/or legal entities may collaborate as a group to submit a single entry, in which case all members of the group must satisfy the eligibility requirements, and a single individual from the group must be designated as an official representative for each entry. That designated individual will be responsible for meeting all entry and evaluation requirements.
- Participation is subject to all U.S. federal, state and local laws and regulations. Void where prohibited or restricted by law. Participants are responsible for checking applicable laws and regulations in their jurisdiction(s) before participating in this Competition, to ensure that their participation is legal. Individuals entering on behalf of or representing a company, institution or other legal entity are responsible for confirming that their entry does not violate any policies of that company, institution or legal entity.
- NIST employees and Guest Researchers are not eligible to enter.
- Federal entities and non-NIST Federal employees acting in their official capacities are not eligible to enter.
- Non-NIST Federal employees acting in their personal capacities should consult with their respective agency ethics officials to determine whether their participation in this Competition is permissible.

- **What does a submission require?**

(1) your App software provided to the Competition Sponsor at no cost (for testing and evaluation)

(2) a brief (less than 250 words) text description of your App

(3) at least one screenshot image of your App in use on a mobile phone or tablet device

(4) a brief (less than five minutes) video demonstrating the functionality of your App

What is an App for the purposes of this contest?

App is defined in the rules as “a working software application that operates on a mobile device using one of three operating systems, i.e., iOS, Android, or Windows, together with relevant documentation and code to install and run the application.”

An app must use at least one of the Eligible NIST Datasets and may also include other freely available data.

• Minimum App Criteria for Consideration of a Prize:

- **General:** App submission should include detailed instructions on how to install and operate the App, and system requirements to run the App.
- **NIST Acknowledgment:** The following notice should be displayed prominently within the application: "This product uses data provided by the National Institute of Standards and Technology (NIST) but is not endorsed or certified by NIST." The NIST SRD number must also be displayed prominently in the application. Use of the NIST or Department of Commerce logos is prohibited.
- **Functionality/Accuracy:** A Submission may be disqualified if the software application fails to function as expressed in the description submitted by the Participant.
- **Privacy:** Participants should keep in mind that NIST considers protection of personal information an essential element of App security. Apps must seek user permission to access and use personal information.
- **Security Vulnerabilities:** Participants must agree that NIST may conduct testing on the App to determine whether malware or other security threats may be present. NIST may disqualify the App if, in NIST's sole judgment, the App may damage government or others' equipment or operating environment. For guidance about minimizing security vulnerabilities in mobile applications, Participants can consult NIST Special Publication 800-163, "Vetting the Security of Mobile Applications" (http://dx.doi.org/10.6028/NIST.SP.800-163).
- **Completeness:** other required components of the submission are complete.

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- **Judging**
- **Potential impact:** How strong is the potential of the submission to help students and other technical experts use NIST Standard Reference Data?
- **Creativity and Innovation:** To what degree is this submission innovative? Does it bring new thinking and creativity to improving access to NIST Standard Reference Data?
- **Implementation:** Does the App work well? Does it provide an engaging user experience and have interactive capabilities?
- **Uses scientific reference data:** Does the App use at least one of the eligible datasets? Preference will be given to applications that integrate more than one dataset.

Bibiana Campos-Seijo, Editor, C&EN, and VP, C&EN Media Group

Vint Cerf, VP and Chief Internet Evangelist, Google

Stuart Chalk, Associate Professor of Chemistry, UNF

Robert Hanisch, Director, NIST Office of Data and Informatics

Ian Kalin, Chief Data Officer, Department of Commerce

Diana Ortiz-Montalvo, NIST Research Chemist & NRC Postdoc

Chris Sloop, CTO, Earth Networks

- **Intellectual Property Rights:**
- NIST does not make any claim to ownership of your Entry or any of your intellectual property or third party intellectual property that it may contain therein. By participating in the Competition, you are not granting any rights in any patents or pending patent applications related to your Entry; provided that by submitting an Entry, you are granting NIST certain limited rights as set forth herein.
- You grant to NIST the right to review your entry
- NIST may use your name, likeness, biographical information, image, any other personal data submitted with your Entry and the contents in your Entry (including any created works, such as YouTube® videos, but not including any App software submitted with or as part of your Entry), in connection with the Competition.

How to submit

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You know code. Scientists know data. Help NIST improve the way we share our scientific reference data by building an App today!

Scientists and engineers need data—from the atomic weight of carbon and the structure of benzene, to the most precise value for the speed of light. High quality physical and chemical reference data help researchers design experiments, build better products, solve health and environmental problems, and even study the stars. The National Institute of Standards and Technology, NIST, is a non-regulatory agency of the United States Department of Commerce. NIST provides some of the most accurate and comprehensive datasets in the world. Physicists, biochemical engineers, environmental researchers, and many other technically trained experts routinely use NIST Standard Reference Data in their workday. Students from high school through graduate school use the same datasets to master the ropes of scientific discovery. Help drive innovation and support research by developing your own mobile applications that use NIST Standard Reference Data!

View full rules

Enter a submission

Look for teammates

You're registered for this hackathon.
Unregister

34 days to submit
Jul 27 – Sep 28, 2015
view all dates

Invite others to compete

$45,000 in prizes

First Place
First Place Prize - $30,000 - will be selected

ELIGIBILITY

Participants (individuals or teams) should meet these eligibility guidelines:

- Competition is open to individuals over the age of 18 that are residents of the 50 United States, the District

Submit to Reference Data Challenge

34 MORE DAYS TO SUBMIT

Select one of your portfolio projects or add a new project:

+

Add a new project

test

tests

Submit this project

Post a new project

Please respect our community guidelines.

Import from GitHub Save time by importing your project name, tagline, and README from GitHub.

* **I'm developing a project called** Project name 54

Save and continue Cancel

Post a new project

Please respect our community guidelines.

* **Project name**

test2 49

Save

Cancel

* **Tagline**

Make it exciting: "Insanely easy keyboard shortcuts" or "Artisanal multi-touch library for JavaScript"

117

Thumbnail image

JPG, PNG or GIF format, 5 MB max file size. For best results, use a 3:2 ratio (e.g., 600px x 400px)

Change image

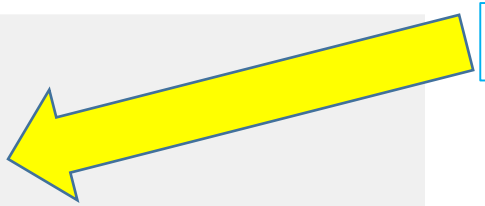
test2

Add team members

We'll email people added here and ask them to confirm they want to be added to your team.

someone@example.com Send invite

Heather Evans (that's you!)



Add team members here.

Save

Cancel

* **What's the story behind test2?**

Format your description with Markdown

Inspiration...

Description (less than 250 words) is Required.

Which tools and resources did you use?

Tag languages, APIs, hardware, hosts, libraries, UI Kits, and frameworks – even Pokémon if it fits!

e.g., Android, JavaScript, Twilio, Myo, Bootstrap, Heroku, Google Analytics...

Links

Link to your project's website, app store listing, repository, deck, etc.

http://

ADD ANOTHER LINK

Video

Great videos go viral. Learn how to make an awesome video

YouTube, Vimeo or Youku URL

Video (under five minutes) is Required.

Image gallery

The first image added will be used as your project thumbnail image.

Choose files

or drag and drop

JPG, PNG or GIF format
5 MB max file size
3:2 aspect ratio

At least one image is Required.

DEVPOST formerly ChallengePost Explore projects Find a hackathon Heather's Portfolio

Submit to Reference Data Challenge

34 DAYS TO SUBMIT

Your edits have been saved! ×

Step 1: select a project

test
tests

CREATED BY:
Heavans

Edit project details

Step 2: complete your challenge submission

Your submission must include:

- A working software application that uses at least one dataset from the list of eligible datasets under the tab "Eligible NIST Data".
- A description (should be less than 250 words) of the application.
- At least one image of your application running on a mobile device.
- A YouTube or Vimeo video (five minutes maximum) that demonstrates the functionality of the application via screencast or video. You must have permission to use all content in your video, including footage, music and images.
- A way for us to access your applicationfor testing/judging, such as a URL, installation file or shared test build. You must also provide

Platforms: Android, iOS, Windows Phone

Upload a File
Upload a zipped file containing an installation file for your app (35MB limit) (Note: you must either provide a link to access your app or upload your installation file.)

Choose File No file chosen

*** Testing Instructions**
Please provide step-by-step instructions for testing your application (including minimum operating system or browser version required) any private links for downloading it, log in information (if applicable), and anything else we may need to access your app free of charge for testing and evaluation.

iOS Build Link (non-public iOS Apps Only)
If your app is not yet publicly available, send it to us via one of the beta distribution methods listed on the FAQ page. Enter our email address to share a build with us for testing. Our testing email is appchallenge@nist.gov.

App submission via one of 3 mechanisms:

1. Provide a weblink in your project page and in the Testing Instructions field
2. Upload a file
3. Send an iOS build link (for non-public iOS Apps)

Testing Instructions are Required.

Eligible NIST Datasets

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- Your App must use at least one of these Eligible NIST Datasets:
  - CODATA Fundamental Physical Constants (SRD 121)
  - Ground Levels and Ionization Energies for the Neutral Atoms (SRD 111)
  - Atomic Weights and Isotopic Compositions (SRD 144)
  - Computational Chemistry Comparison and Benchmark Database (SRD 101)
  - NIST-JANAF Thermochemical Tables (SRD 13)
  - ITS-90 Thermocouple Database (SRD 60)

Links to each Dataset: http://nistdata.devpost.com/details/data

Your App may also use other freely available scientific data (from NIST or other third party providers) but you must have the right and authority to submit the App entry (see Warranties section of Rules).

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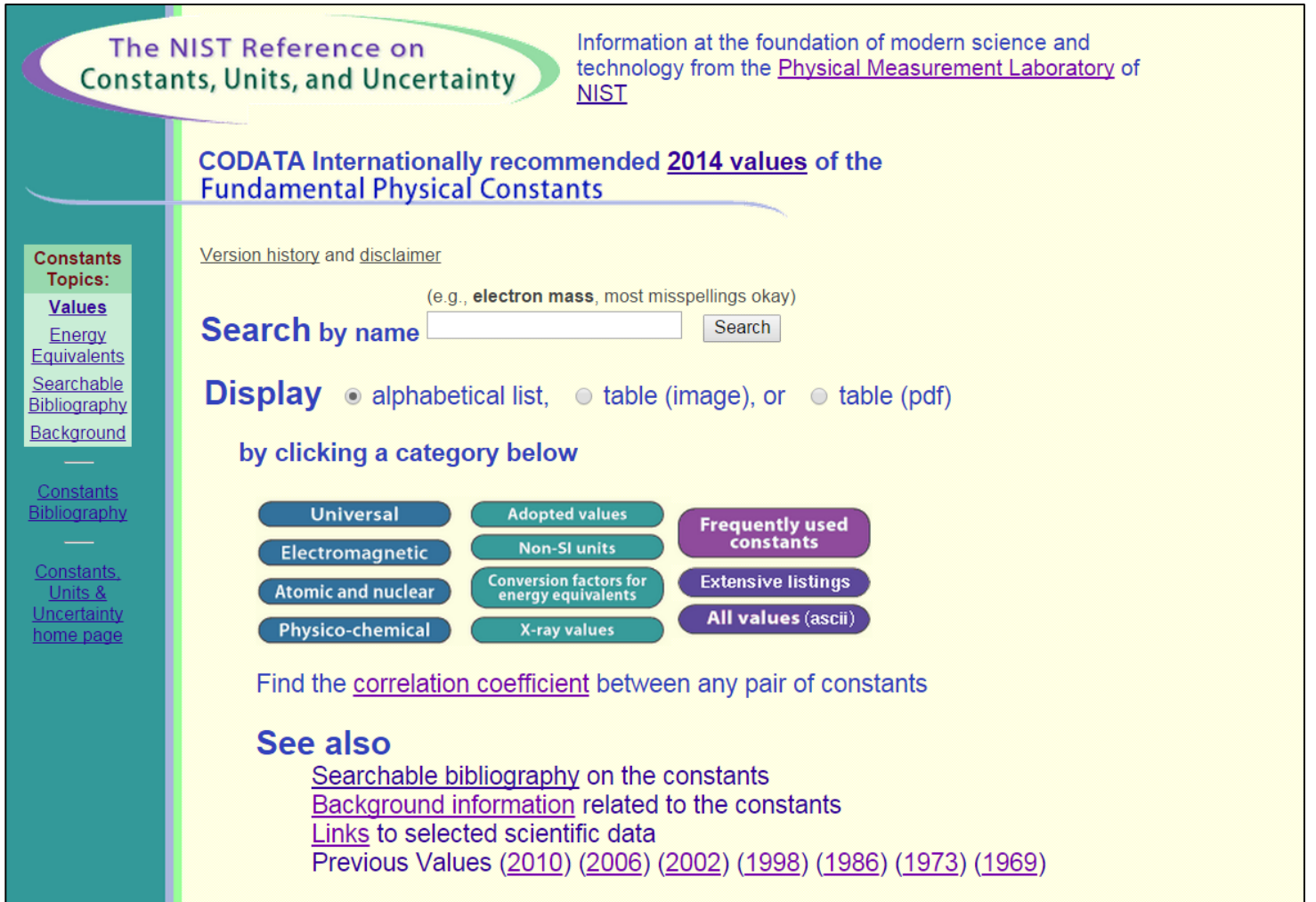
- **CODATA Fundamental Physical Constants (NIST SRD 121):** The fundamental physical constants have specific and universally-used symbols, including the velocity of light in vacuum (c), charge of the electron (e), and Planck's constant (h). These constants are essential to basic theories of physics and our quantitative understanding of the physical universe. This resource provides the most accurate internationally recommended values of these constants available. NIST currently makes this dataset available on its website. This data is available in machine readable format.



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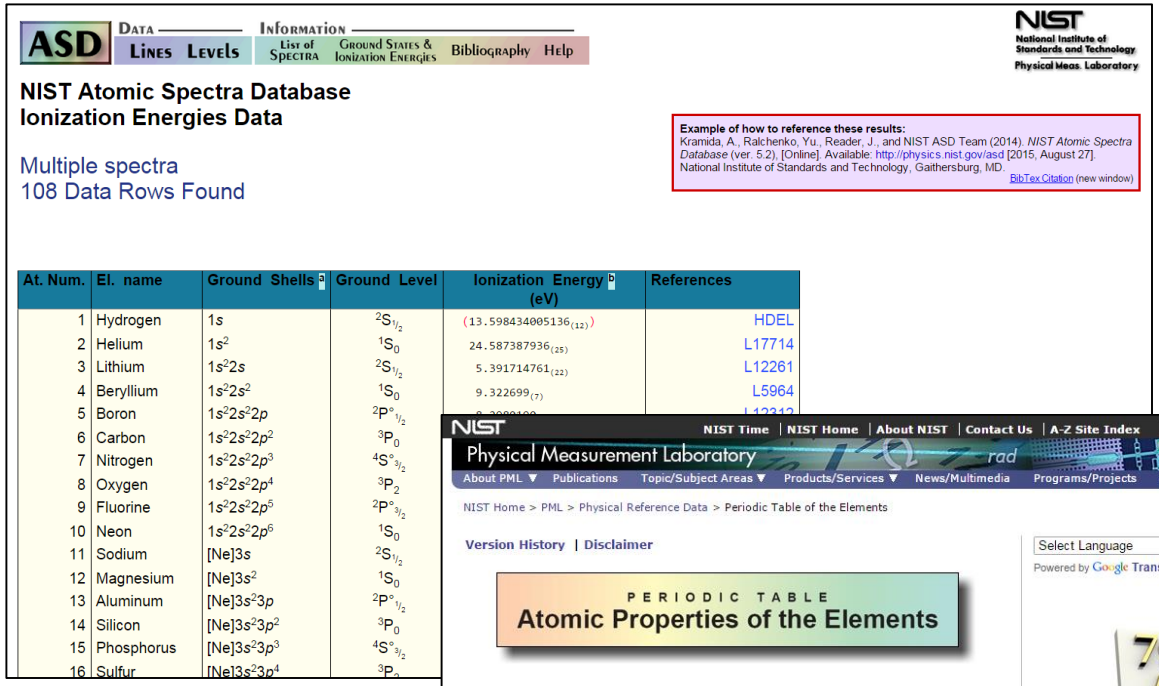
- **Ground Levels and Ionization Energies for the Neutral Atoms (NIST SRD 111):** This resource provides scientific values of ground levels and ionization energies for neutral atoms. The data is primarily used by chemists and astronomers to calculate thermodynamic properties of atoms in chemical reactions and other kinetic processes. Atomic physicists use the values to benchmark experimental data for advanced atomic theories. NIST currently makes this dataset available on its website. The data is available in machine readable format.



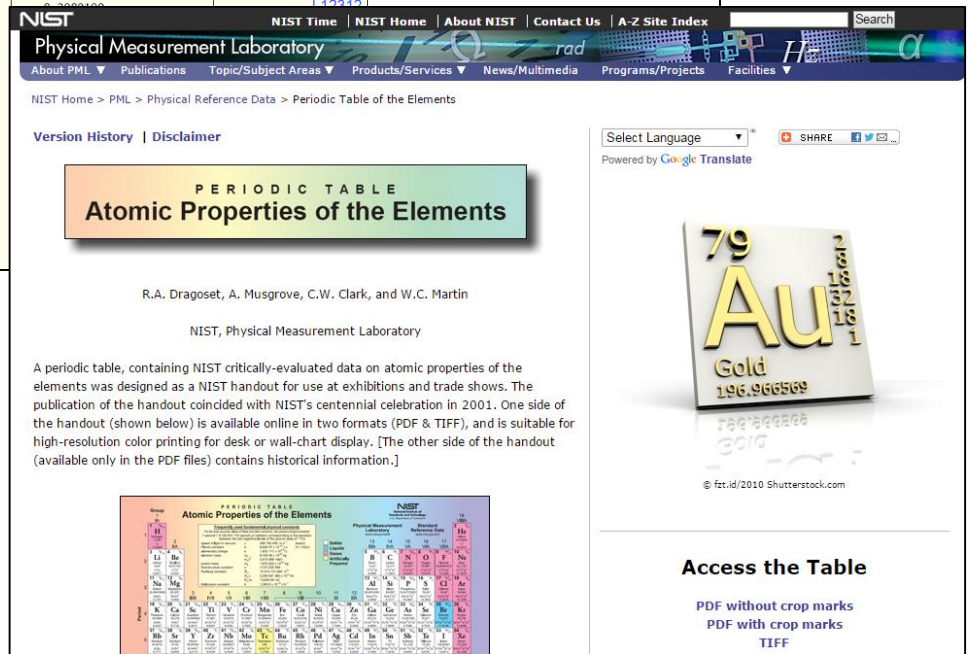
ASD Data — Lines Levels — Information — List of Spectra — Ground States & Ionization Energies — Bibliography — Help

NIST Atomic Spectra Database
Ionization Energies Data

Multiple spectra
108 Data Rows Found

Example of how to reference these results:
Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team (2014). *NIST Atomic Spectra Database* (ver. 5.2). [Online]. Available: http://physics.nist.gov/asd [2015, August 27]. National Institute of Standards and Technology, Gaithersburg, MD.
BibTex Citation (new window)

At. Num.	El. name	Ground Shells	Ground Level	Ionization Energy (eV)	References
1	Hydrogen	$1s$	$^2S_{1/2}$	$(13.598434005136_{(12)})$	HDEL
2	Helium	$1s^2$	$^1S_0$	$24.587387936_{(25)}$	L17714
3	Lithium	$1s^2 2s$	$^2S_{1/2}$	$5.391714761_{(22)}$	L12261
4	Beryllium	$1s^2 2s^2$	$^1S_0$	$9.322699_{(7)}$	L5964
5	Boron	$1s^2 2s^2 2p$	$^2P^o_{1/2}$		
6	Carbon	$1s^2 2s^2 2p^2$	$^3P_0$		
7	Nitrogen	$1s^2 2s^2 2p^3$	$^4S^o_{3/2}$		
8	Oxygen	$1s^2 2s^2 2p^4$	$^3P_2$		
9	Fluorine	$1s^2 2s^2 2p^5$	$^2P^o_{3/2}$		
10	Neon	$1s^2 2s^2 2p^6$	$^1S_0$		
11	Sodium	$[Ne]3s$	$^2S_{1/2}$		
12	Magnesium	$[Ne]3s^2$	$^1S_0$		
13	Aluminum	$[Ne]3s^2 3p$	$^2P^o_{1/2}$		
14	Silicon	$[Ne]3s^2 3p^2$	$^3P_0$		
15	Phosphorus	$[Ne]3s^2 3p^3$	$^4S^o_{3/2}$		
16	Sulfur	$[Ne]3s^2 3p^4$	$^3P_2$		



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Physical Measurement Laboratory

About PML | Publications | Topic/Subject Areas | Products/Services | News/Multimedia | Programs/Projects | Facilities

NIST Home > PML > Physical Reference Data > Periodic Table of the Elements

Version History | Disclaimer

PERIODIC TABLE
Atomic Properties of the Elements

R.A. Dragoset, A. Musgrove, C.W. Clark, and W.C. Martin

NIST, Physical Measurement Laboratory

A periodic table, containing NIST critically-evaluated data on atomic properties of the elements was designed as a NIST handout for use at exhibitions and trade shows. The publication of the handout coincided with NIST's centennial celebration in 2001. One side of the handout (shown below) is available online in two formats (PDF & TIFF), and is suitable for high-resolution color printing for desk or wall-chart display. [The other side of the handout (available only in the PDF files) contains historical information.]

Select Language | Powered by Google Translate | SHARE

79 Au Gold 196.966569

© fzt.id/2010 Shutterstock.com

Access the Table

PDF without crop marks
PDF with crop marks
TIFF

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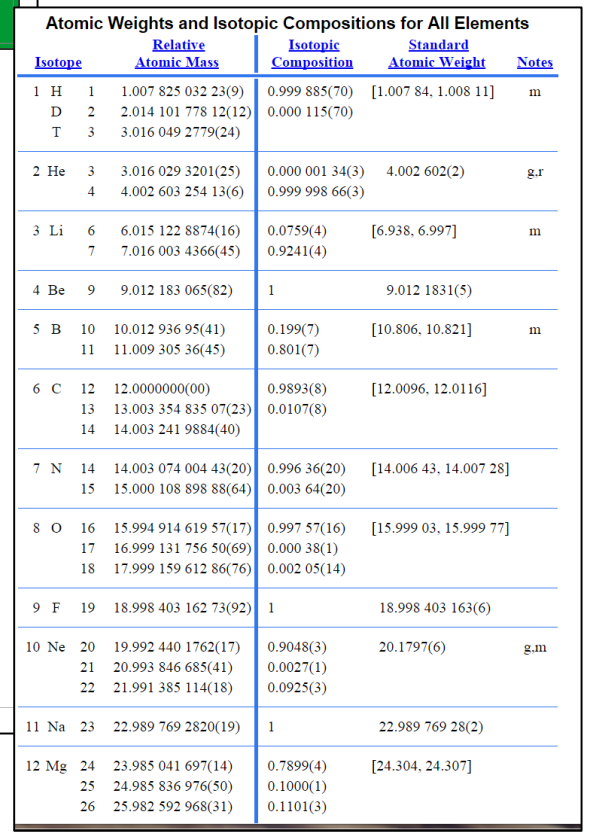
- **Atomic Weights and Isotopic Compositions (NIST SRD 144):** This compilation of data provides atomic weights for elements 1 through 118, noting isotopic compositions or abundances when appropriate. Physicists and other scientists working with high-resolution optical spectra use this data for many applications, including detection of radioactive isotopes, dating of paintings and sculptures, and determining the origins of meteor samples. NIST currently makes this dataset available on its website. The data is available in machine readable format.



Atomic Weights and Isotopic Compositions for All Elements

Isotope		Relative Atomic Mass	Isotopic Composition	Standard Atomic Weight	Notes
1 H	1	1.007 825 032 23(9)	0.999 885(70)	[1.007 84, 1.008 11]	m
D	2	2.014 101 778 12(12)	0.000 115(70)		
T	3	3.016 049 2779(24)			
2 He	3	3.016 029 3201(25)	0.000 001 34(3)	4.002 602(2)	g,r
	4	4.002 603 254 13(6)	0.999 998 66(3)		
3 Li	6	6.015 122 8874(16)	0.0759(4)	[6.938, 6.997]	m
	7	7.016 003 4366(45)	0.9241(4)		
4 Be	9	9.012 183 065(82)	1	9.012 1831(5)	
5 B	10	10.012 936 95(41)	0.199(7)	[10.806, 10.821]	m
	11	11.009 305 36(45)	0.801(7)		
6 C	12	12.0000000(00)	0.9893(8)	[12.0096, 12.0116]	
	13	13.003 354 835 07(23)	0.0107(8)		
	14	14.003 241 9884(40)			
7 N	14	14.003 074 004 43(20)	0.996 36(20)	[14.006 43, 14.007 28]	
	15	15.000 108 898 88(64)	0.003 64(20)		
8 O	16	15.994 914 619 57(17)	0.997 57(16)	[15.999 03, 15.999 77]	
	17	16.999 131 756 50(69)	0.000 38(1)		
	18	17.999 159 612 86(76)	0.002 05(14)		
9 F	19	18.998 403 162 73(92)	1	18.998 403 163(6)	
10 Ne	20	19.992 440 1762(17)	0.9048(3)	20.1797(6)	g,m
	21	20.993 846 685(41)	0.0027(1)		
	22	21.991 385 114(18)	0.0925(3)		
11 Na	23	22.989 769 2820(19)	1	22.989 769 28(2)	
12 Mg	24	23.985 041 697(14)	0.7899(4)	[24.304, 24.307]	
	25	24.985 836 976(50)	0.1000(1)		
	26	25.982 592 968(31)	0.1101(3)		

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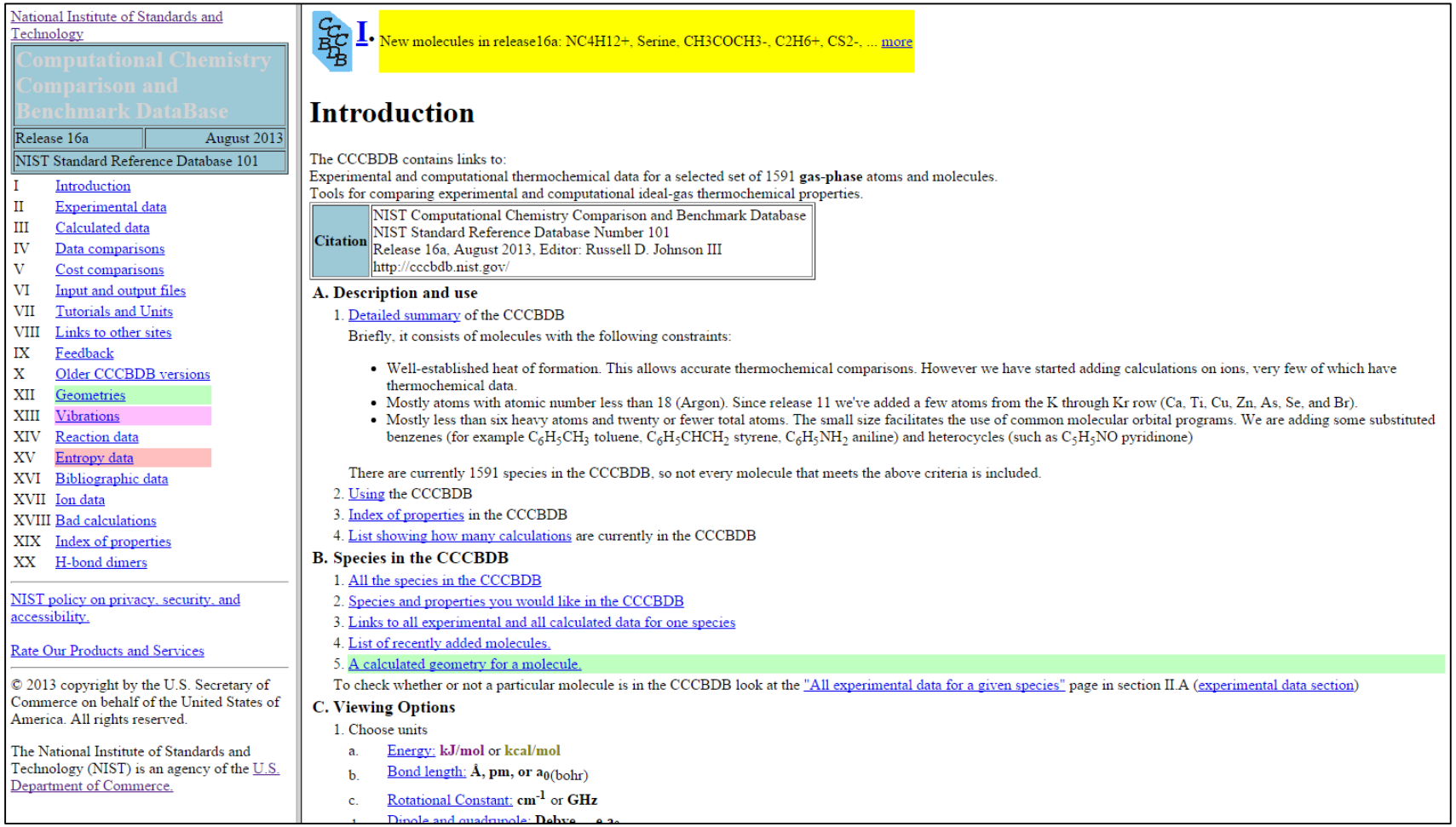
- **NIST Computational Chemistry Comparison and Benchmark Database (CCCBDB, NIST SRD 101):** The CCCBDB provides thermochemical data for a selected set of over 1,000 gas-phase atoms and molecules. It is used by chemists to compare experimental results with computational ideal-gas properties. NIST currently makes this dataset available on its website. The data is available in machine readable format.



National Institute of Standards and Technology

Computational Chemistry Comparison and Benchmark DataBase

Release 16a | August 2013

NIST Standard Reference Database 101

I Introduction
II Experimental data
III Calculated data
IV Data comparisons
V Cost comparisons
VI Input and output files
VII Tutorials and Units
VIII Links to other sites
IX Feedback
X Older CCCBDB versions
XII Geometries
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XV Entropy data
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XVII Ion data
XVIII Bad calculations
XIX Index of properties
XX H-bond dimers

NIST policy on privacy, security, and accessibility.

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The National Institute of Standards and Technology (NIST) is an agency of the U.S. Department of Commerce.

I. New molecules in release16a: NC4H12+, Serine, CH3COCH3-, C2H6+, CS2-, ... more

Introduction

The CCCBDB contains links to:
Experimental and computational thermochemical data for a selected set of 1591 **gas-phase** atoms and molecules.
Tools for comparing experimental and computational ideal-gas thermochemical properties.

Citation	NIST Computational Chemistry Comparison and Benchmark Database NIST Standard Reference Database Number 101 Release 16a, August 2013, Editor: Russell D. Johnson III http://cccbdb.nist.gov/

A. Description and use

1. Detailed summary of the CCCBDB
   Briefly, it consists of molecules with the following constraints:
   - Well-established heat of formation. This allows accurate thermochemical comparisons. However we have started adding calculations on ions, very few of which have thermochemical data.
   - Mostly atoms with atomic number less than 18 (Argon). Since release 11 we've added a few atoms from the K through Kr row (Ca, Ti, Cu, Zn, As, Se, and Br).
   - Mostly less than six heavy atoms and twenty or fewer total atoms. The small size facilitates the use of common molecular orbital programs. We are adding some substituted benzenes (for example $C_6H_5CH_3$ toluene, $C_6H_5CHCH_2$ styrene, $C_6H_5NH_2$ aniline) and heterocycles (such as C_5H_5NO pyridinone)

   There are currently 1591 species in the CCCBDB, so not every molecule that meets the above criteria is included.
2. Using the CCCBDB
3. Index of properties in the CCCBDB
4. List showing how many calculations are currently in the CCCBDB

B. Species in the CCCBDB

1. All the species in the CCCBDB
2. Species and properties you would like in the CCCBDB
3. Links to all experimental and all calculated data for one species
4. List of recently added molecules.
5. A calculated geometry for a molecule.

To check whether or not a particular molecule is in the CCCBDB look at the "All experimental data for a given species" page in section II.A (experimental data section)

C. Viewing Options

1. Choose units
   a. Energy: **kJ/mol** or **kcal/mol**
   b. Bond length: **Å, pm, or a_0**(bohr)
   c. Rotational Constant: **cm^{-1}** or **GHz**
   d. Dipole and quadrupole: **Debye**, **e a_0**

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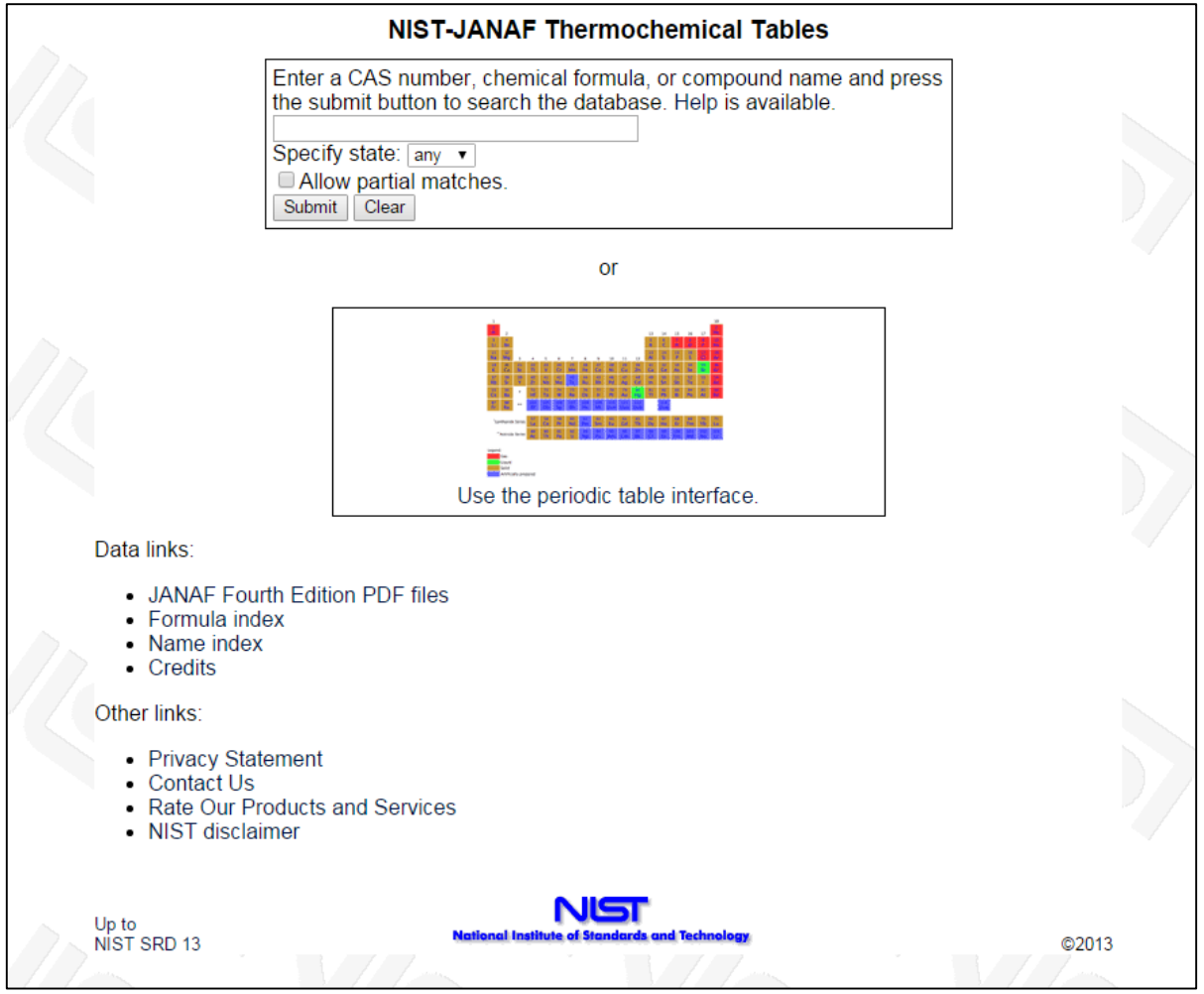
- **NIST-JANAF Thermochemical Tables (NIST SRD 13):** This dataset contains critically evaluated thermochemical data for a range of chemical substances. Originally used by the aerospace industry to understand rocket propellant combustion, today the data are used world-wide as thermodynamic reference data in a range of chemistry, environmental, and materials applications. Industry scientists use these tables to predict thermodynamic information about chemical substances including equilibrium mixtures and heat release. NIST currently makes this dataset available on its website. The data is available in machine readable format.



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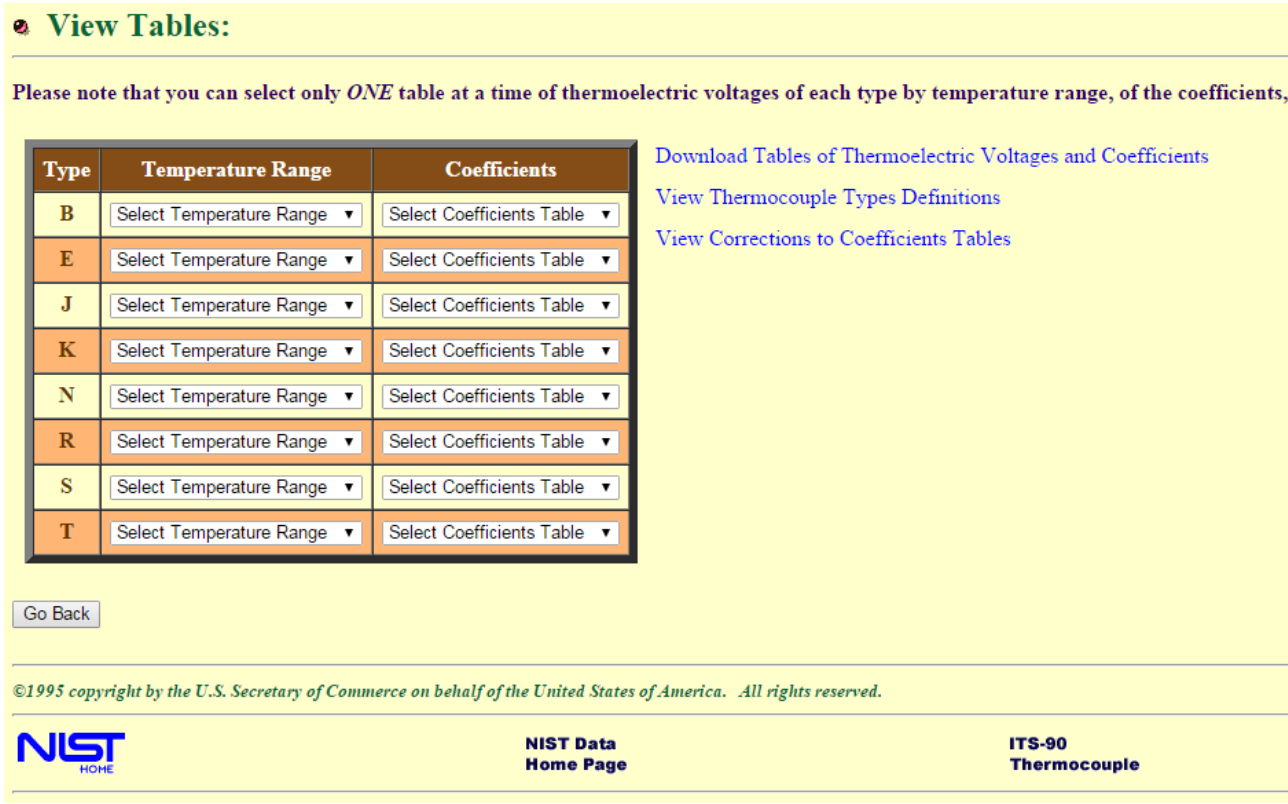
- **NIST ITS-90 Thermocouple Database (NIST SRD 60):** This thermometry database reproduces a subset of the tables and reference functions of NIST Monograph 175, "Temperature Electromotive Force Reference Functions and Tables for the Letter-Designated Thermocouple Types Based on the ITS-90." It provides temperature calibration data that is used by scientists and engineers to convert a measured voltage to temperature, and is the basis for calibration of thermometers, instrument controllers, and other devices that rely on temperature for process control. These types of devices are found in virtually every technology including kitchen ovens, hot water heaters, residential and commercial furnaces, power plants, and more. NIST currently makes this database available on its website. The data is available in machine readable format.



View Tables:

Please note that you can select only *ONE* table at a time of thermoelectric voltages of each type by temperature range, of the coefficients,

Type	Temperature Range	Coefficients
B	Select Temperature Range	Select Coefficients Table
E	Select Temperature Range	Select Coefficients Table
J	Select Temperature Range	Select Coefficients Table
K	Select Temperature Range	Select Coefficients Table
N	Select Temperature Range	Select Coefficients Table
R	Select Temperature Range	Select Coefficients Table
S	Select Temperature Range	Select Coefficients Table
T	Select Temperature Range	Select Coefficients Table

Download Tables of Thermoelectric Voltages and Coefficients
View Thermocouple Types Definitions
View Corrections to Coefficients Tables

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Questions?

Thank You

Links to the slides and this presentation will be posted in the FAQ section on the challenge website:

http://nistdata.devpost.com/details/faq

Use the Discussion Board on the website or email appchallenge@nist.gov with any questions!