InChI and Data Management

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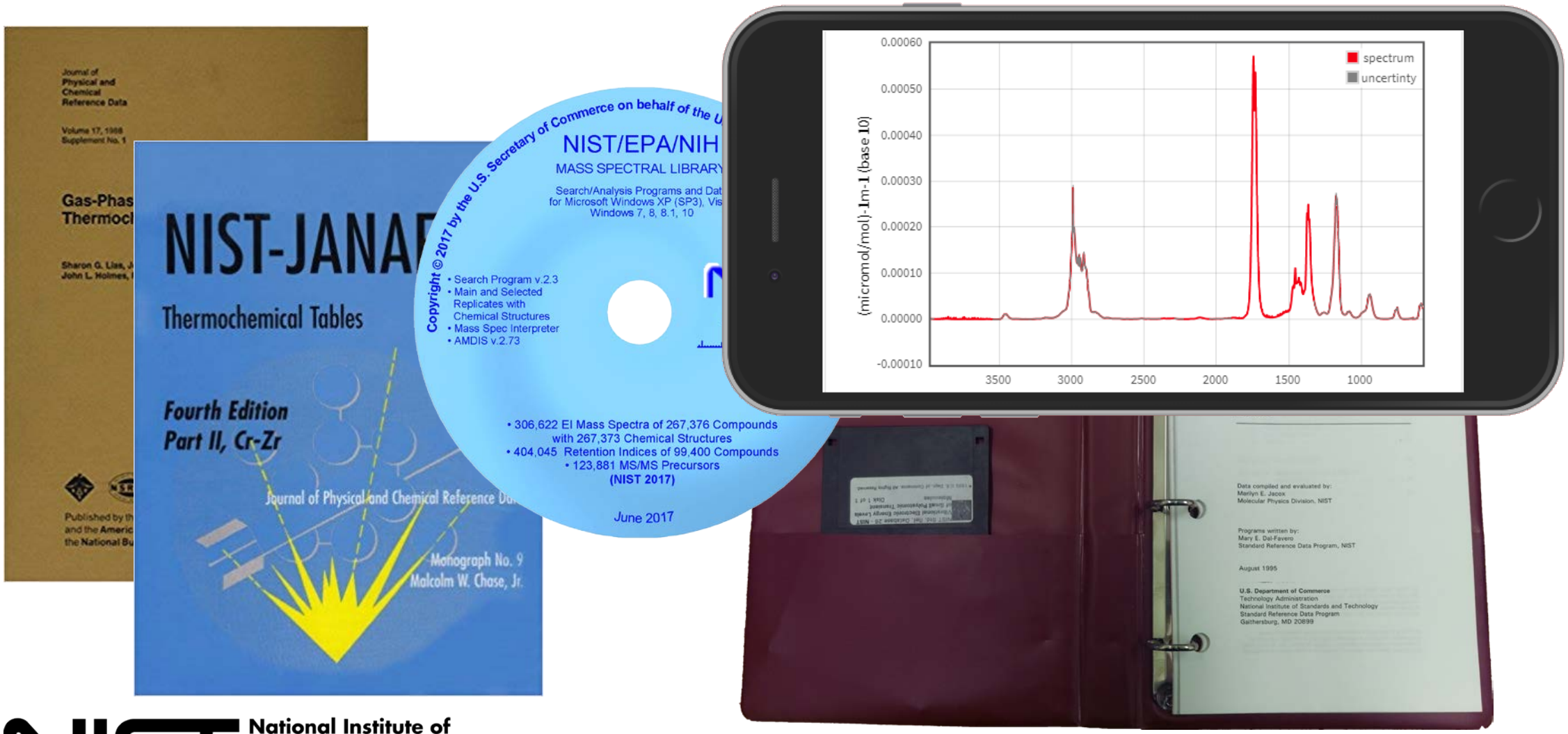
NIST, Office of Data and Informatics

NIST – History of ~~publishing~~ managing data



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

InChI and data management

- Data applies to *something*.
  - Is there any value in data which corresponds to an undefined object?
  - Types of errors
    - Numerical
    - Units of measure
    - **Wrong object! ← Bad, really bad!**
- When *something* is an atom or molecule.
  - Good news: people have been working on describing these systems for some time.
  - Bad news: there is a reason people have been working on this problem for some time

InChI is a tool!

- Well known useful properties
  - Canonical representation of molecule
  - Modular structure enables discovery of related species
  - Search engine friendly hash
- Limitations
  - Labor: drawing or finding structures
  - Can’t deal with poorly defined systems
  - Chemists are human

- A craftsman chooses and uses tools carefully!

NIST Chemistry WebBook

- A collection of data compilations
  - Many developed by small groups of scientists
  - Historical data – not designed to integrate with other databases
- Challenges
  - Combining data from databases with vastly different designs
  - Helping users find data (SEO)

NIST National Institute of Standards and Technology U.S. Department of Commerce — NIST Chemistry WebBook, SRD 69

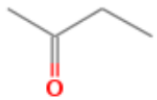
Search ▾ | NIST Data ▾ | About ▾

2-Butanone

- **Formula:** C_4H_8O
- **Molecular weight:** 72.1057
- **IUPAC Standard InChI:**
  - InChI=1S/C4H8O/c1-3-4(2)5/h3H2,1-2H3
  - Download the identifier in a file.

InChI TRUST CERTIFIED 2011

- **IUPAC Standard InChIKey:** ZWEHNKRNPOVVGH-UHFFFAOYSA-N
- **CAS Registry Number:** 78-93-3
- **Chemical structure:**



This structure is also available as a 2d Mol file or as a computed 3d SD file
The 3d structure may be viewed using Java or Javascript.

- **Other names:** Butan-2-one; Butanone; Ethyl methyl ketone; Ketone, methyl ethyl; Methyl ethyl ketone; MEK; C2H5COCH3; Acetone, methyl-; Aethylmethylketon; 3-Butanone; Butanone 2; Ethyl methyl cetone; Ethylmethylketon; Ketone, ethyl methyl; Meetco; Methyl acetone; Metiletilchetone; Metyloetyloketon; Rcra waste number U159; UN 1193; 2-Oxobutane; 2-Butanal; 2-butanone (MEK; methyl ethyl ketone); 2-butanone (MEK)
- **Permanent link** for this species. Use this link for bookmarking this species for future reference.

InChI and the NIST Chemistry WebBook

- Database development
  - Draw structures, find matches
- Identify species across data collections
  - Are these species the same?
- Create invariant URLs
  - Inbound links
- Identify isotopologues
- Help users find data
  - Internet search engines

Database development

Skilled chemist

- Abstracts data (including identifiers: name, CAS #, etc.)
- Draws or obtains structures

Chemical informatics person

- Identifies duplicate structures ← InChI!
- Identifies "bad" structures ← InChI makes this easier (disconnections, undefined stereo)
- May identify values inconsistent with the structure

Skilled chemist

- Acts on analyses: updates data or finds error in analysis

Identify species across data collections

Merging data collections based on molecular identifiers can be difficult.

If we are lucky the collections have structures

- Most likely with different drawing conventions
- InChI can still find matching molecules!
- Unless the conventions are really different
  - Acid drawn for conjugate base
  - Coordination compounds
  - Chrages on nitro groups, ring tautomers, etc.

InChI is not immune to Murphy's Law

Nothing is…

- Bad structures can come from numerous causes
- Unexpected hydrogens may present in the structure but not shown on the screen
- Where possible, confirm match with other identifiers
- **Knowledge of chemistry and likely failure modes is still essential**

Invariant URLs – Use InChI to create link

Pros

- Stable
- Can provide some response for valid InChIs that don't resolve

Cons

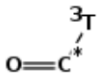
- URLs look ugly
  - Characters in InChI need to be URL-encoded
  - URLs are long (~2000 character limit in Internet Explorer)
- Why not use InChIKey?

Invariant URLs – InChI does not resolve

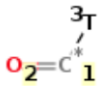
Information from the InChI

There are no matching entries in the database for this IUPAC International Chemical Identifier. The following information was obtained from the identifier.

- **Formula:** CTO
- **Molecular weight:** 31.0261
- **IUPAC Standard InChI:**
  - `InChI=1S/CHO/c1-2/h1H/i1T`
- **IUPAC Standard InChIKey:** `CFHIDWOYWUOIHU-CNRUNOGKSA-N`
- Connectivity:

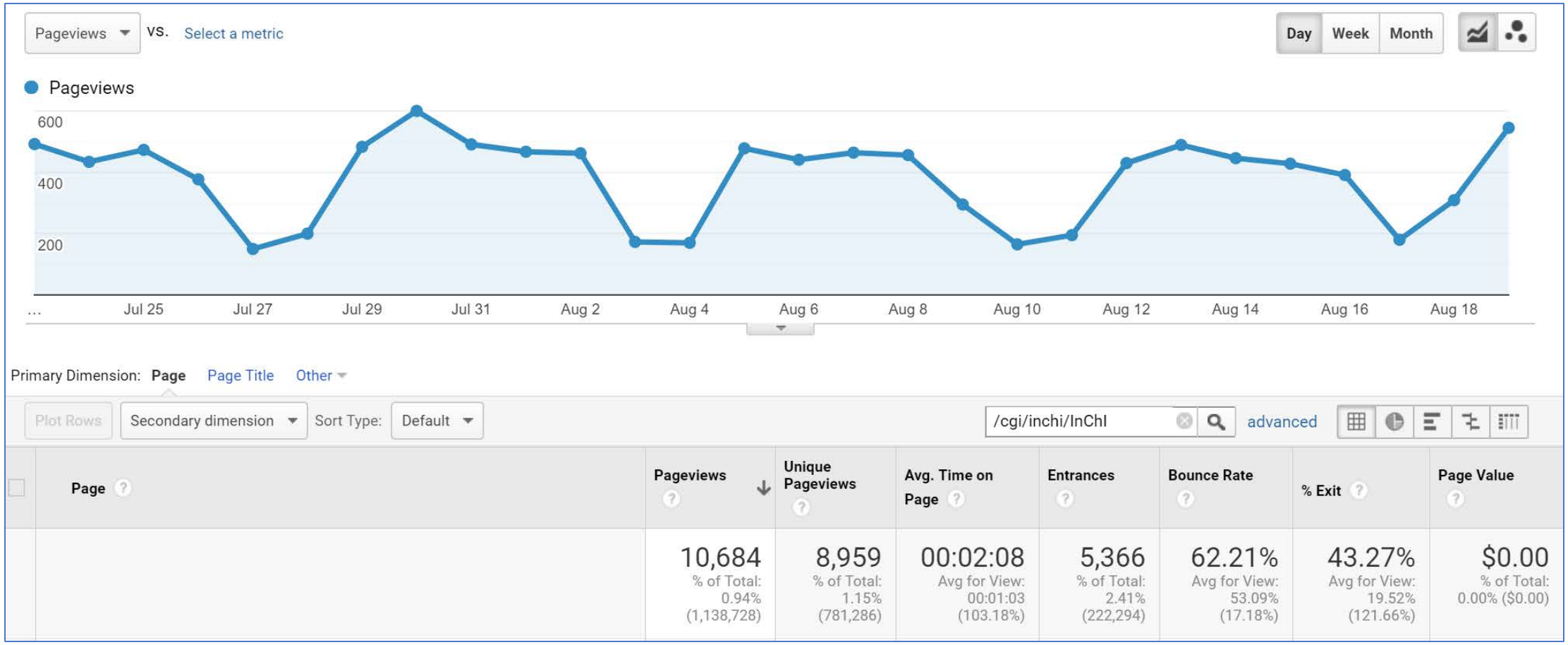


- 2-d Mol File from the identifier
- Canonical atom numbers:



  Note: stereochemistry is currently not indicated in the items above.
- **Permanent link** for this search. Use this link for bookmarking this species for future reference.
- **Isotopologues:**
  - Methyl-d1 radical, oxo-
  - Formyl radical

Invariant URLs – Less than 1% of page views



Page	Pageviews	Unique Pageviews	Avg. Time on Page	Entrances	Bounce Rate	% Exit	Page Value
	10,684 % of Total: 0.94% (1,138,728)	8,959 % of Total: 1.15% (781,286)	00:02:08 Avg for View: 00:01:03 (103.18%)	5,366 % of Total: 2.41% (222,294)	62.21% Avg for View: 53.09% (17.18%)	43.27% Avg for View: 19.52% (121.66%)	$0.00 % of Total: 0.00% ($0.00)

Screenshot from Google Analytics

Isotopologues – Parsing InChIs

Formyl radical

- **Formula:** CHO
- **Molecular weight:** 29.0180
- **IUPAC Standard InChI:**
  - `InChI=1S/CHO/c1-2/h1H`
  - Download the identifier in a file.

InChITRUST CERTIFIED 2011

- **IUPAC Standard InChIKey:** `CFHIDWOYWUOIHU-UHFFFAOYSA-N`
- **CAS Registry Number:** 2597-44-6
- **Chemical structure:**

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

The 3d structure may be viewed using Java or Javascript.

- **Isotopologues:**
  - Methyl-d1 radical, oxo-

Search engines

- Marketing hyperbole:

  InChIKey is an important part of a search engine optimization strategy for web pages dealing with molecules or atoms!

- But:
  - Using “InChIKey + relevant search text” can be a useful search strategy
  - “relevant search text” is part of a SEO strategy!
- Search engines don’t know some synonyms

Search engine example

CFHIDWOYWUOIHU-UHFFFAOYSA-N microwave spectra

Web Images Videos News Maps Settings

All Regions Safe Search: Moderate Any Time

PDF Microwave (Rotational) Spectroscopy

sci.tanta.edu.eg/files/Microwave spectroscopy BSc-Lect-2.pdf

From **microwave** spectroscopy, bond lengths can be determined with a correspondingly high precision, as illustrated in this example. From the rotational **microwave** spectrum 35of 1H Cl, we find that B = 10.59342 cm-1. Given that 35the masses of 1H and Cl are 1.0078250 and 34.9688527 amu, respectively, determine the bond

Formyl radical - webbook.nist.gov

https://webbook.nist.gov/cgi/cbook.cgi?ID=C2597446

IUPAC Standard InChIKey: **CFHIDWOYWUOIHU-UHFFFAOYSA-N**; CAS Registry Number: 2597-44-6; Chemical structure: This structure is also available as a 2d Mol file or as a computed 3d SD file The 3d structure may be viewed using Java or Javascript. Isotopologues: Methyl-d1 radical, oxo-Permanent link for this species. Use this link for bookmarking this species for future reference.

Screenshot from Duck Duck Go

Integrating InChI into work flows

- Chemists should never have to see InChI strings.

- Drawing programs:
  - Control them programmatically
  - Support chemistry beyond mol file v2000
  - Make it easy to show hydrogens?

- In the future this may all be done in web browsers?

A real problem – Ag^{+47}, InChI=1S/Ag/q+47

Molecular Formula "Ag" > substances (183) > **181588-83-0** > get references (3)

SUBSTANCE DETAIL | **Get References**

Return | Previous

97. CAS Registry Number 181588-83-0

~6

Ag

Silver, ion (Ag^{47+})

Other Names

Silver(47+)

Ag^{47+}

Screenshot from CAS SciFinder

Our most valuable resource

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Links

- NIST Chemistry WebBook: https://webbook.nist.gov/chemistry/
- NIST Standard Reference Data (SRD): https://www.nist.gov/srd

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