

# Computers in Chemistry – Lecture I

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## This class (handouts)

- Please check: <http://qc.chem.nagoya-u.ac.jp>
- Click on “Teaching”
- Username: qcguest, password: qcigf!  
(memorization help: quantum chemistry is great fun!)

*(today the Department website does not work due to hacker attack on Nagoya University's website)*

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## What you need for this class

- Nagoya University ID, e.g.:
- Your password
- In case of problems or questions, please contact: [sirle@chem.nagoya-u.ac.jp](mailto:sirle@chem.nagoya-u.ac.jp) (also on your hand-out)
- Prof. Irle's office hours: Mondays, 13:00-14:30, location: SA building, 4<sup>th</sup> floor, 424.
- Student TA in this class: Hong En Lim, E-Mail: [lim.hong.en@b.mbox.nagoya-u.ac.jp](mailto:lim.hong.en@b.mbox.nagoya-u.ac.jp)

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## The general contents of this class

- **Question:** *Why FORTRAN 90?*
- **Answer:** According to Robert Harrison, Director, Joint Institute for Computational Sciences (USA):
  - Not “old”
  - 70% of applications in FORTRAN



[www.iics.utk.edu](http://www.iics.utk.edu)



# What is chemistry? I

First in use: 1646

- **Answer I** (commonly quoted): Chemistry is the study of **matter** and **energy** and the interactions between them.
- **Answer II** (Webster's dictionary):
  - a) the science that deals with composition, structure, and properties and with the **transformations** that they undergo
  - b) a strong mutual attraction, attachment, or sympathy ("this couple has a great chemistry")



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The Explosion in the Alchemist's Laboratory Justus Gustav van Bentum (Leiden 1670–1727) Holland, 17th or 18th century Oil on canvas

- Alchemists: Ignis mutat rei (Latin: Fire changes matter)
- Goal: Change lead into gold (Pb → Au)

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Periodic table (standard form) [hide]

Group →	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
↓ Period	1	2																2
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
	* Lanthanides		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
	** Actinides		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

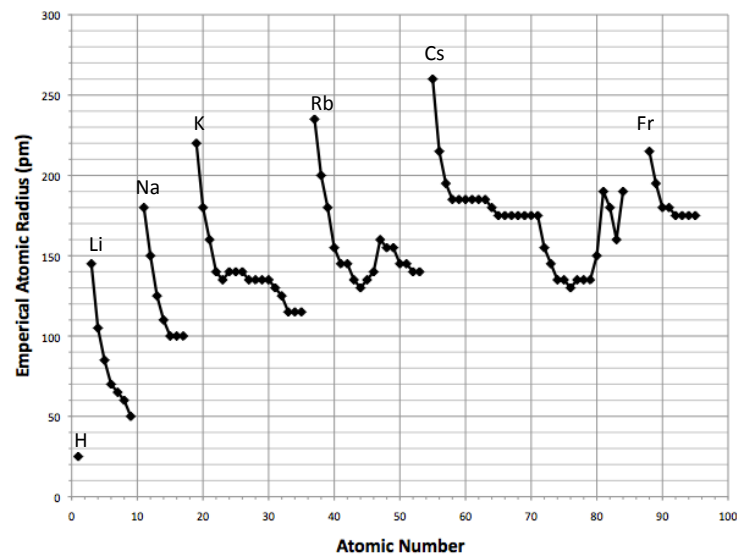
This is an 18-column periodic table layout, which has come to be referred to as the **common** or **standard form**, on account of its popularity. It is also sometimes referred to as the *long form*, in comparison to the *short form* or *Mendeleev-style* [table](#), which omits groups 3–12. The *wide periodic table* incorporates the lanthanides and the actinides, rather than separating them from the main body of the table. The *extended periodic table* adds the 8th and 9th periods, including the superactinides.

Some element categories in the periodic table										
Metals						Nonmetals				Unknown chemical properties
Alkali metals	Alkaline earth metals	Inner transition metals	Transition metals	Post-transition metals	Metalloids	Other nonmetals	Halogens	Noble gases		
		Lanthanides	Actinides							

Color of the atomic number shows state of matter  
Border shows natural occurrence:

[http://en.wikipedia.org/wiki/Periodic\\_table](http://en.wikipedia.org/wiki/Periodic_table)

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Atomic DATA  
[http://en.wikipedia.org/wiki/Periodic\\_table](http://en.wikipedia.org/wiki/Periodic_table)

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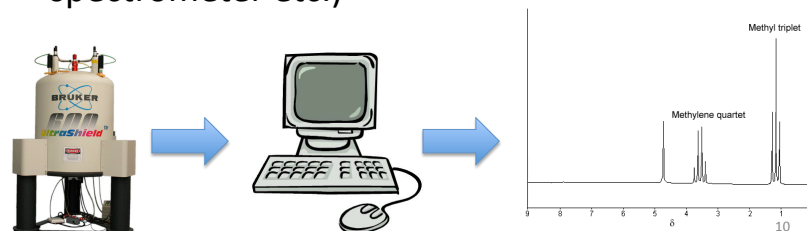
## Chemistry is the “Study of Change”

- Chemistry of the **Universe** (interstellar clouds)
- Chemistry of the **Earth** (geological chemistry)
- **Darwinian Evolution** (biochemistry)
- **Chemistry of Nature** (Organic/inorganic chemistry, physical chemistry, analytical chemistry [**collect knowledge**])
- **Chemistry of Man** (Medical chemistry, chemical technology [**apply knowledge**])

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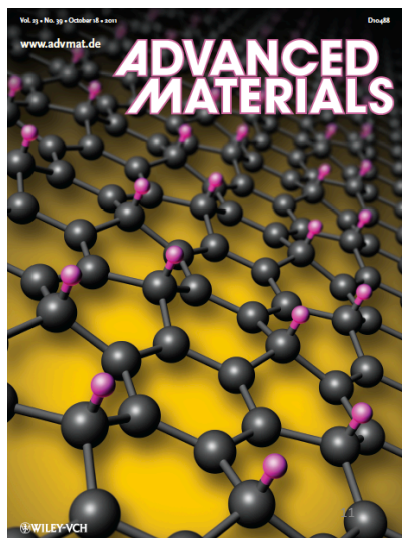
## Computers in Chemistry?

- Finding DATA in literature or databases
- Produce DATA (theoretical/computational chemistry)
- Analyze DATA (computer attached to spectrometer etc.)



## Chemical Knowledge

- Papers written in books and scientific journals
- Peer-reviewed
- Open-access?
- Many many journals
- Many, many studies
- **Science nowadays is run like a business!**



## Chemical Knowledge

- Impact factor of a journal

Mark	Rank	Abbreviated Journal Title (linked to journal information)	ISSN	JCR Data <sup>(j)</sup>					Eigenfactor™ Metrics <sup>(j)</sup>		
				Total Cites	Impact Factor	5-Year Impact Factor	Immediacy Index	Articles	Cited Half-life	Eigenfactor™ Score	Article Influence™ Score
<input type="checkbox"/>	1	<a href="#">ACCOUNTS CHEM RES</a>	0001-4842	33869	21.852	20.330	3.235	149	7.4	0.09692	7.076
<input type="checkbox"/>	2	<a href="#">ACS NANO</a>	1936-0851	9914	9.865	9.962	1.478	986	1.8	0.05575	3.393
<input type="checkbox"/>	3	<a href="#">ACTA CHIM SINICA</a>	0567-7351	2287	0.611	0.586	0.043	415	4.9	0.00319	0.072
<input type="checkbox"/>	4	<a href="#">ACTA CHIM SLOV</a>	1318-0207	959	1.011	1.233	0.076	132	4.1	0.00340	0.311
<input type="checkbox"/>	5	<a href="#">ACTA PHARMACOL SIN</a>	1671-4083	4364	1.909	2.033	0.338	207	5.8	0.01005	0.484
<input type="checkbox"/>	6	<a href="#">ACTUAL CHIMIQUE</a>	0151-9093	116	0.145	0.125	0.012	82	5.3	0.00036	0.039
<input type="checkbox"/>	7	<a href="#">ADV FUNCT MATER</a>	1616-301X	22516	8.508	9.442	1.202	481	3.8	0.11097	3.075
<input type="checkbox"/>	8	<a href="#">ADV MATER</a>	0935-9648	68115	10.880	11.306	2.097	777	5.2	0.24245	3.765
<input type="checkbox"/>	9	<a href="#">AFINIDAD</a>	0001-...	183	0.233	0.244	0.000	21	7.0	0.00028	0.044

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# Chemical Science as a Business

Schematic flow-chart for the research of a chemistry professor

- Perform research
- 10 • Write papers
- **Give talks, get cited by others**
- Write proposal to government agency (JSPS, NSF, DFG, ...)
- Get more money
- Hire more people
- Perform more research
- Go to 10



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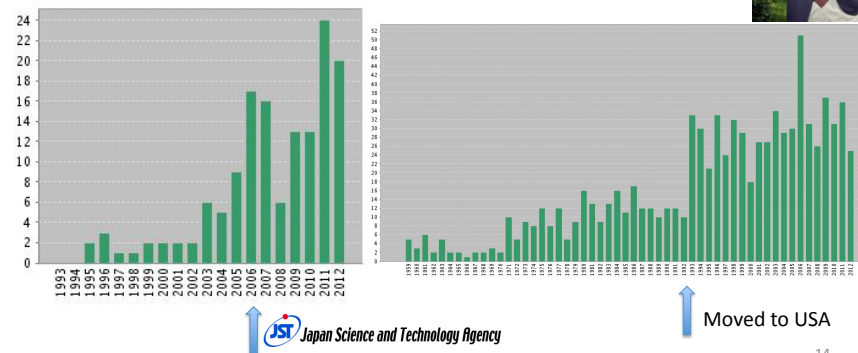
# Chemical Science as a Business

Number of papers of a researcher as function of time



Irle, S\* (45)

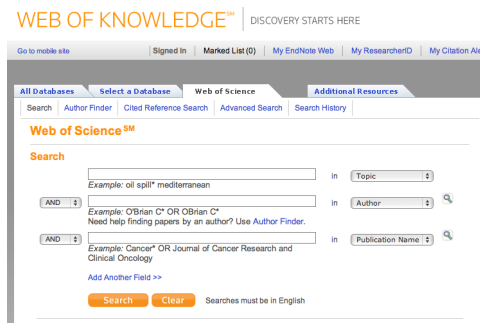
Morokuma, K\* (78)



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## Chemistry Knowledge

- How to find chemistry papers?
  - - ISI Web of Knowledge
- <http://www.webofknowledge.com/WOS>



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## Chemistry Knowledge

- Databases
  - Example: QCLDB II
- <http://qcldb2.ims.ac.jp>



USER-ID:

PASSWORD:

[Forgot your password?](#)

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# Chemistry Knowledge

- How to access journals
  - Nagoya University electronic journals  
<http://sfx.nul.nagoya-u.ac.jp/nagoya/az/>

The screenshot shows the Nagoya University electronic Journal DataBase interface. At the top, it says '名古屋大学 電子ジャーナル・アクセスサービス' and 'Nagoya University electronic Journal DataBase'. Below that, there's a search bar with 'English' selected. A navigation menu includes 'Title', 'Category', 'Locate', and 'CitationLinker'. A large green box contains a search grid with letters A-Z and 'Others', and a search bar with 'GO' button. Below the search area, there's a section for '障害情報・メンテナンス情報' (Disability Information / Maintenance Information) in English, listing dates and times for system downtime.

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# Chemistry Knowledge

- Social Networks
  - For instance, Facebook  
<http://www.facebook.com>

The screenshot shows the Facebook page for 'Chemistry Nagoya University 名古屋大学理学部化学科'. The page features a large group photo of the department members. The profile picture is a logo with the text 'CHEMISTRY Nagoya University'. The page has 82 likes and 1 person talking about it. There are navigation tabs for 'About', 'Photos', and 'Likes'. A 'ChemComm' link is visible in the top right.

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# Chemistry Knowledge

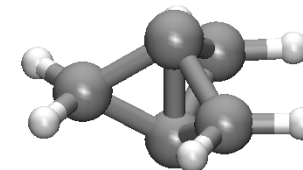
- Social Networks
  - 2<sup>nd</sup> Example: academia.edu (pushes publications up in Google searches), others: ResearchGate.com

The screenshot shows the Academia.edu profile for 'Stephan Irle', a faculty member at Nagoya University. The profile includes a photo, a bio, and research interests in 'Ionic Liquids, Fullerenes, Graphene, and 31 more'. It also shows statistics: 1,370 profile views and 689 document views. A list of books and papers is visible, including 'Spectroscopy, Dynamics, and Molecular Theory of Carbon Plasmas and Vapor' and 'DFT calculations on fullerenes and carbon nanotubes'.

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# Interactive Task:

- Find a research paper on the [1.1.1]propellane ( $C_5H_6$ ) molecule.



- Write on the back of the Assignment I sheet:
- a) the name of the paper, and
- b) how you found this paper.

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