Mass Spectrometry, Chromatography, Chemistry …..what is the purpose?

Egmont Rohwer

Head: Department of Chemistry

“Science without religion is lame, religion without science is blind “
(Albert Einstein)
Structure of lecture

• Introduction

• Historical perspective

• Personal research experience, with emphasis on recent years

• Vision for the Department
Understanding the exponential growth in scientific knowledge

Older view:

theory (models)  \leftrightarrow  experiment (reality check)
Understanding the exponential growth in scientific knowledge

- Technology (facilities)
- Theory (models)
- Experiment (reality check)

Motivation ??
Exponential growth in the discipline: Chemistry

Analytical technology (facilities) “Toolbox” MS, NMR, Xray Diff… Computers

Motivation:
Curiosity/Aesthetics
Quality of life
Power/control

Chemical theory (models)

Application to real problems. Experiment (reality check)
Chemistry – the central science

• The scientific discipline that bridges the mathematical, physical and biological sciences

The non-living (inorganic) and living world can in principle be described in exact chemical terms considering atomic and molecular building blocks. In many instances we are still, however, quite far from such a detailed understanding.
Chemistry plays a critical role in most modern research programmes, including those of medicine, veterinary science and engineering.

- The science that studies the composition, interaction, transformation of matter and the associated energy transformations,
  (internal combustion engines, digestion, photosynthesis, batteries, fuel cells, photoluminescence, oil-from-coal)

- The science that studies the properties and reactivity of matter by considering its atomic and molecular building blocks,
  (bioprospecting, design of new drugs, MR and PET scans, diagnosis and treatment of cancer, design of new composite materials, photovoltaics, understanding the immune system, neurological activity)
Application: Revolutionary breakthroughs in Chemistry are required to address the major challenges of modern society.

Addressing poverty, improving the quality of life: “Sustainable Development”

- Reliable energy supply (also off-grid, transportable forms of energy)
- Environmental issues (especially considering global warming and carbon dioxide emission; dangerous pollutants like endocrine disrupters)
- Sustainable, safe food supply (GM foods, fertilizers, pest control and pesticide residues…)
- Health (stem cell research, antibiotics, AIDS, TB, Malaria, depression, Alzheimers, diabetes …)
- Clean water (sterilization, recycling, desalination ….)
- Safety and security (forensic chemistry in e.g. murder cases, detecting narcotics, explosives or other contraband)
- Education (- is the most powerful weapon to change the world (Nelson Mandela))
Exponential growth in the discipline: Chemistry

Analytical technology (facilities) “Toolbox” MS, NMR, X-ray Diff… Computers

Motivation:
Curiosity/Aesthetics
Quality of life
Power/control

Chemical theory (models)

Applications. experiment (reality check)
Exponential growth in sub-discipline: Mass Spectrometry

Motivation:
(i) Sustainable development
(ii) Expanding the technology toolbox ("senses") of chemistry

MS Equipment development

Sample Analysis
Analytical information
SERVICE to others
Structure of lecture

• Introduction

• Historical perspective (MS, Chrom.)

• Personal research experience, with emphasis on recent years

• Vision for the Department
Aston’s first “mass spectrograph” from the book (1933):

Mass Spectra and Isotopes

by

FW Aston (Nobel laureate)

Resolution, R=130
Figure 2.48
Orientation of the magnetic force on a moving ion.

ions at the source outlet leads to

$$mv^2 = 2qV_s$$

Hence

$$\frac{m}{q} = \frac{r^2B^2}{2V_s}$$

Each mass has a different radius. Compare prism and light
Figure 6.7
Useful isotope combinations in mass spectrometry. Isotopes of other atoms that are possibly associated must always be taken into account, as is shown in the framed section.
Table 6.1 Isotopic abundances.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Relative abundance (%)</th>
<th>Mass (u)</th>
<th>Mean atomic mass&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Calculated</td>
<td>Measured</td>
</tr>
<tr>
<td>&lt;sup&gt;1&lt;/sup&gt;H</td>
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<td>1.007 825</td>
<td>1.007 976</td>
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<tr>
<td>&lt;sup&gt;2&lt;/sup&gt;H</td>
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<td>2.014 0</td>
<td></td>
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<tr>
<td>&lt;sup&gt;12&lt;/sup&gt;C</td>
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<td>12.000 000</td>
<td>12.011 036</td>
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<td>13.003 355</td>
<td>12.011 1</td>
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<tr>
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<td>14.003 074</td>
<td>14.006 762</td>
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<tr>
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<td>15.000 108</td>
<td>15.003 346</td>
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<td>&lt;sup&gt;16&lt;/sup&gt;O</td>
<td>99.76</td>
<td>15.994 915</td>
<td>15.999 324</td>
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<td>16.999 131</td>
<td>15.999 43</td>
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<td>17.999 160</td>
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<td>100</td>
<td>18.998 403</td>
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<tr>
<td>&lt;sup&gt;23&lt;/sup&gt;Na</td>
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<td>100</td>
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<td>22.989 76</td>
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<td>&lt;sup&gt;32&lt;/sup&gt;S</td>
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<td>30.973 762</td>
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<td>&lt;sup&gt;34&lt;/sup&gt;S</td>
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<td>33.967 866</td>
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<td>79.903 526</td>
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<tr>
<td>&lt;sup&gt;81&lt;/sup&gt;Br</td>
<td>49.31</td>
<td>80.916 289</td>
<td>79.904 1</td>
</tr>
</tbody>
</table>

<sup>a</sup> Mean value for the natural mixture of isotopes.
From the book (1933): Mass Spectra and Isotopes by FW Aston (Nobel laureate)
Origin of mass defect in mass spectrometry – nuclear binding

\[ \Delta E = (\Delta m)c^2 \]

Nuclear fusion

\[ 2n + 2p \rightarrow ^4\text{He} \]

\[ n + n + p + p \]

\[ ^4\text{He} \ (2n+2p) \]
RESOLVING POWER: \( R = \frac{m}{\delta m} \) (20% valley) if our criterion is say 20% valley between peaks before we term peaks resolved. (The RESOLUTION in this case is \( \delta m \))

\[ R = \frac{m}{\delta m} \text{ with } \delta m \text{ measured from two peaks resolved at say 20\% valley or from the width of one peak at 10\% peak height.} \]
An illustration of the information attainable with increasing resolving power $R$: $R(a) > 100$; $R(b) > 1000$; $R(c) > 10,000$ and $R(d) > 100,000$

Increase in MS resolution over a century

<table>
<thead>
<tr>
<th>Year</th>
<th>$R = m/\Delta m$</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>1913</td>
<td>13</td>
<td>Thomson</td>
</tr>
<tr>
<td>1918</td>
<td>100</td>
<td>Dempster</td>
</tr>
<tr>
<td>1919</td>
<td>130</td>
<td>Aston</td>
</tr>
<tr>
<td>1937</td>
<td>2000</td>
<td>Aston</td>
</tr>
<tr>
<td>1998</td>
<td>8 000 000</td>
<td>Marshall &amp; co</td>
</tr>
</tbody>
</table>
Figure 7
Atmospheric pressure photoionization negative ion 9.4-T Fourier transform–ion cyclotron resonance (FT-ICR) mass spectrum of a South American crude oil, showing the largest total number (and largest number spanning one Dalton) of assigned elemental compositions published to date. Figure adapted with permission from Reference 73.
Figure 6.3
Exact masses and corresponding formulae for various possible ions of $m/z$ 180 containing only carbon, hydrogen, nitrogen and oxygen atoms in limited number ($C_{6-15}$, $H_{0-24}$, $N_{0-4}$ and $O_{0-4}$).
MS-MS via Q-TOF analysers
High definition MS?
Ion mobility in the millisecond time domain
NASA’s Sample Analysis at Mars (SAM) for Curiosity Mars rover

SAM is a suite of three instruments totaling 40 kg, located in the Curiosity rover’s interior: a 6-column Gas Chromatograph (GC), a Quadrupole Mass Spectrometer (QMS), and a Tunable Laser Spectrometer (TLS). These instruments are coupled through solid and gas processing systems to provide complementary information on the same samples. Each sample may be analyzed by one, two, or all three of the SAM instruments.
The search for organic molecules is particularly important in the search for life on Mars because life as we know it cannot exist without them (though they can exist without life). SAM will be able to detect lower concentrations of a wider variety of organic molecules than any other instrument yet sent to Mars.
Structure of lecture

• Introduction

• Historical perspective

• Personal research experience, with emphasis on recent years

• Vision for the Department
Phases in my career

• Interest in the fundamentals

• Need to feel useful

• A growing feeling of responsibility
Organic analysis of complex mixtures are a challenge

Literally hundreds and thousands of compounds are present in:

- Natural products
- Petrochemicals
- Aroma of food and beverages
- All trace analysis

These analyses all require combined chromatography – mass spectrometry instrumentation
Typical trace analysis consists of:

Concentration  Separation  Selective detection

Our research programme addresses all three aspects, trying to improve the sensitivity, selectivity, time and costs.
Concentration

Multichannel silicone rubber traps

Separation

Multidimensional chromatography

Selective detection

High resolution MS
Special ionization techniques MS
Human nose
Insect antennae
Two-dimensional separation

hexane

hexane
GCXGC/TOFMS

Comprehensive two-dimensional gas chromatography Time-of-flight mass spectrometry
Results: Two-dimensional Chromatogram
Chemisorption

A chemical understanding of Lubricity
Physisorption

A chemical understanding of Lubricity
Figure 7
Atmospheric pressure photoionization negative ion 9.4-T Fourier transform–ion cyclotron resonance (FT-ICR) mass spectrum of a South American crude oil, showing the largest total number (and largest number spanning one Dalton) of assigned elemental compositions published to date. Figure adapted with permission from Reference 73.
Figure 6.3
Exact masses and corresponding formulae for various possible ions of m/z 180 containing only carbon, hydrogen, nitrogen and oxygen atoms in limited number (C_{6-15}, H_{0-24}, N_{0-4} and O_{0-4}).
Increasing unsaturation

Increasing chain length

\[ C_nH_{2n+2}X_x \]
Figure 4: SFCxGC analysis of an petrochemical standard containing alkanes, ethers and alcohols. CO$_2$ at a pressure of 150 atm and a temperature of 28°C was used as mobile phase in the SFC analysis. The flow through the PLOT column was collected for intervals of 5 seconds. The GC was repeatedly temperature programmed from -50 to 250°C at 450 °C/min while hydrogen was supplied as carrier gas to obtain a linear flow rate of 1m/sec.
Figure 3. Gas chromatogram obtained at the optimum ramp rate where the maximum attainable separation of the analytes was attained in the shortest time. The sample contained n-alkanes from decane to tetracosane. The temperature was ramped from 50 to 300 °C. A ramp rate of 450 °C/min at a flow rate of 100 cm/s was used. Peak capacity of 60 peaks in 30 seconds
Electroantennography

- Insect antenna
- GC effluent
- Electrode
Electroantennography
Male vs. Female (40-300°C)

Female - EAD
Male - EAD
Gland Extract - FID

Retention time (min)
Pheromones

1. Search

2. Identify

3. Behaviour

4. Field trial - female control
What are Persistent organic pollutants (POPs)?

• POPs are chemical substances that persist in the environment, bio-accumulate through the food web, and pose a risk of causing adverse effects to human health and the environment at locations near and far from their source.

• They are typically characterized as having low water solubility and high fat solubility, they are prone to long range transport and most of them are anthropogenic in origin.
The POP group includes, amongst others, twelve substances (“the dirty dozen”):

– aldrin, chlordane, 2,2-bis(4-chlorophenyl)-1,1,1-trichloroethane (DDT), dieldrin, endrin, heptachlor, hexachloro benzene (HCB), mirex and toxaphene;

– Three are *industrial substances* - polychlorinated biphenyls (PCBs), polychlorinated dibenzo-\(p\)-dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs)
“Dioxin” PCDDs

PCBs

“Furan” PCDFs
Atmospheric pressure photoionization negative ion 9.4-T Fourier transform–ion cyclotron resonance (FT-ICR) mass spectrum of a South American crude oil, showing the largest total number (and largest number spanning one Dalton) of assigned elemental compositions published to date. Figure adapted with permission from Reference 73.
Selectivity: Column Combinations

Tetra

Penta

Hexa

Hepta

Octa

Initial 80.00 1.00
20.00 220.00 0.00
2.00 240.00 0.00
1.00 250.00 0.00
5.00 260.00 0.00
1.00 270.00 0.00
Surface plot - SA sample

2,3,7,8-TeCDF

2,3,7,8-TeCDD
Multichannel Silicone (PDMS) Rubber Trap (MCT) Sorption volume 300 µl

Unique and the heart of a number of our techniques:
1 concentration
2 multi-dimensional chromatography
3 detection

Example 1: Monitoring atmospheric combustion products

Novelty in our methodology:

- Screening for impacted areas to reduce numbers of expensive GC-MS analyses
- Laser fluorescence measurements in tube
- Denuder properties of open tubes
NO2 Pollution
Polycyclic aromatic hydrocarbons (PAHs)
Molecular fluorescence spectrometry

![Diagram of molecular fluorescence spectrometry](image)
LIF of PAHs

- PAHs have large absorption cross sections and quantum yields (ratio of no. photons emitted to no. photons absorbed thus indicates efficiency of fluorescence process)
- Usually the $\pi \rightarrow \pi^*$ transitions are most probable
- Fluorescence thus used in HPLC detectors for PAHs in solution for many years

<table>
<thead>
<tr>
<th>PAH</th>
<th>Excitation (nm)</th>
<th>Emission (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Naphthalene</td>
<td>292</td>
<td>323</td>
</tr>
<tr>
<td>Phenanthrene</td>
<td>298</td>
<td>364</td>
</tr>
<tr>
<td>Fluoranthene</td>
<td>365</td>
<td>462</td>
</tr>
<tr>
<td>Pyrene</td>
<td>341</td>
<td>395</td>
</tr>
</tbody>
</table>
Multi-channel silicone rubber sample traps

Quartz tube: 3.5 mm i.d.; 160 mm long.
22 PDMS channels, each 0.64 mm o.d. & 0.3 mm i.d.
& 55 mm long
Applications
Sugar cane burn
Human health effects of PAHs

Naphthalene causes haemolytic anaemia and is a possible human carcinogen.
Benzo(a)pyrene is a suspected human carcinogen.
Monitoring particulate and non-particulate air pollutants
Figure 2. Serially coupled low pressure-drop denuder MCT – quartz micro-fibre filter – MCT system. The MCTs and filter fit a commercial glass desorption tube. The MCTs are connected in series with Tefon (PTFE) tubing.
Denuder/filter/denuder after smoke sampling
Example 2: Monitoring atmospheric and soil contamination by DDT

Novelty in our methodology:

• Denuder properties of open tubes allow measurement of exposure to free molecular as well as aerosol bound DDT

• Capture of GC peaks allows re-injection for chiral analysis of o,p DDT and o,p DDD (forensic environmental application)
Persistent organic pollutant: DDT

- In rural parts of South Africa the pesticide 1,1,1-trichloro-2,2-bis(4-chlorophenyl)ethane (DDT) is still used for malaria vector control.
- 1 120 cases of malaria reported between July 2009 - January 2010 in Limpopo, South Africa.
- According to the strict international Stockholm (POPs) convention, traditional dwellings are sprayed on the inside with small quantities of technical DDT.
Controlled spraying of huts with DDT
Controlled spraying of huts with DDT
Denuder MCT

Separate but simultaneous sampling of free molecular and particle bound DDT

Portable sampling pump

MCT 1 collects vapour phase DDT/D/E

MCT 2 back-up particle bound

Quartz micro-fibre filter collects particle bound DDT/D/E

Dust particles on quartz micro-fibre filter

Portable, battery operated, field sampling system.
Indoor Air of Huts in the Limpopo Province

Denuder MCT + GC - MS: Vapour phase

Time delay between spraying and sampling (hours)

Denuder MCT + GC - MS: Particle bound (Airborne)

Time delay between spraying and sampling (hours)
• Technical DDT consists of approximately 65-75% $p,p'$-DDT and 15-25% $o,p'$-DDT.

• $o,p'$-DDT shows enantioselective estrogenicity and biodegradability.

• Thus, it is important to analyse enantiomers of $o,p'$-DDT and its chiral degradation product, $o,p'$-DDD, for both health and environmental-forensic considerations.
Table 1  Structure, nomenclature, molecular formula and weight of the chiral isomers \(o,p'\)-DDT and \(o,p'\)-DDD

<table>
<thead>
<tr>
<th></th>
<th>(o,p')- DDT</th>
<th>(o,p')- DDD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Structure</td>
<td><img src="image" alt="Structure DDT" /></td>
<td><img src="image" alt="Structure DDD" /></td>
</tr>
<tr>
<td>Nomenclature</td>
<td>1,1,1-trichloro-2-((o\text{-chlorophenyl}))-2-((p\text{-chlorophenyl}))ethane</td>
<td>1,1-dichloro-2-((o\text{-chlorophenyl}))-2-((p\text{-chlorophenyl}))ethane</td>
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<tr>
<td>Molecular Formula</td>
<td>(\text{C}<em>{14}\text{H}</em>{9}\text{Cl}_{5})</td>
<td>(\text{C}<em>{14}\text{H}</em>{10}\text{Cl}_{4})</td>
</tr>
<tr>
<td>Weight</td>
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<td>320.04</td>
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</table>
Fig. 2. Removed detector top assembly and collector. MCT placed on GC-FID flame tip to recapture single peaks or various fractions [17].
Heart-cuts separated on a chiral column (β-cyclodextrin). Non-chiral separation of the corresponding o,p′-DDT/D peaks. Enantiomeric order of elution [1].
Example 3: Analysis of environmental trace hydrocarbons of geological origin

Novelty in our methodology:

• Solvent and Artifact-free trace hydrocarbon analysis

• Soil analysis with silicone loops in contact with a few gram of sample (in field or lab)
Sorptive extraction with Multichannel Silicone Rubber (PDMS) Traps (MCTs) and Loops

Figure 2. A Cross section of a MCT. B, D MCT/Loop fits a commercial glass desorption tube.

- Geobotanical manifestation of natural gas microseeps
- Portable, rugged (desert!)
- Sand: PDMS loop for passive extraction

"Traditional Himba belief holds that beneath the edge of the Namib Desert, the oldest desert in the world, lies a crack in the earth’s crust. A dragon lives there. Whenever he exhales, bubbles of fire rise to the surface, burning the vegetation, causing it to completely vaporise, forming circles.”
Example 4: Aroma investigations

Novelty in our methodology:

• Screening by nose of full trap contents
• GC- fraction or single peak capture for olfactometric assessment (synergism !)
• Re-injection of positive fractions for GC-MS or GCxGCMS identification of components
Fig. 2. Removed detector top assembly and collector. MCT placed on GC-FID flame tip to recapture single peaks or various fractions [17].
Off-line Olfactometry: Slow Release of Aroma or off-odours from MCTs

MCT loaded with full sample or recaptured GC peak or peaks

N\textsubscript{2} gas flow control 20ml.min\textsuperscript{-1}

Temperature Control

Blank MCT
Synergistic perception of aroma compounds

2-Nonanone + 2-Heptanone = Blue Cheese

Fruity + Soapy + Sweet + Floral

This blue cheese aroma was absent when 2-Heptanone and 2-Nonanone were sniffed individually!

Exponential growth in sub-discipline: Mass Spectrometry

Motivation:
(i) Sustainable development
(ii) Expanding the technology toolbox ("senses") of chemistry

Mass Spectrometry

Electronics
Vacuum technology
Physics
Computers
Lasers
New devices

MS Equipment development

Sample Analysis
Analytical information
SERVICE to others
The bigger picture

• Make yourself useful, also do applied work, and you and your very expensive infrastructure will survive! (Nobody finances your personal hobby)
• Academia has a longer term vision and has a responsibility to lead where industry and government cannot (yet). Alliances come later.
• There is synergy between the curiosity driven “blue sky” research and applied science. Both drive your discipline and satisfy your curiosity.
• I discovered the ultimate satisfaction of combining my playful and innovative character with my desire to make a difference.
Thanks to the post graduate students involved in recent work

- Yvette Naudé
- Patricia Forbes
- Jayne de Vos
- Elize Smit
- Marc Bouwer
- Niel Malan
- All former post grad students
Thanks to collaborators involved from other Departments

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- Prof Gretel van Rooyen Botany
- Prof Mike Wingfield FABI
- Prof Bernard Slippers FABI
- Prof Lise Korsten Plant Pathology
- Prof Elna Buys Food Science
- Prof Riette de Kock Food Science
- Prof Riana Bornman Urology
- Prof Tian de Jager Urology
- Dr Duncan Cromarty Pharmacology
- Prof Ralf Zimmermann Univ Rostock
Thanks to the Sponsors

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• SABMiller
• NRF ; Thrip (DTI)
• National Laser Centre (NLC)
Thanks

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- Dr Fanie van der Walt
- Dr Jack Cochran
- Mr David Masemula
- Nico van Vuuren
- Leon Engelbrecht
- Naomi Steenkamp
Structure of lecture

- Introduction
- Historical perspective
- Personal research experience, with emphasis on recent years
- Vision for the Department
Vision 2025 of the University

“to be a leading research-intensive university in Africa, recognised for its quality, relevance and impact, and also for developing people, creating knowledge and making a difference locally and globally.”
President Barack Obama (Nobel laureate)

• at the US National Academy of Science (NAS) annual meeting (27 April 2009), referring to present economic problems:

“At such a difficult moment, there are those who say we cannot afford to invest in science, that support for research is somehow a luxury at moments defined by necessities. I fundamentally disagree. Science is more essential for our prosperity, our security, our health, our environment, and our quality of life than it has ever been before.”

• C&EN; Jan 2010

“The nation that out-educates us today is going to out-compete us tomorrow. To continue to cede our leadership in education is to cede our position in the world.”
The True Size of Africa

A small contribution in the fight against rampant immaturity, by Kai Krause

Graphic layout for visualization only (some countries are cut and rotated). But the conclusions are very accurate: refer to table below for exact data.

### COUNTRY

<table>
<thead>
<tr>
<th>Country</th>
<th>AREA x 1000 km²</th>
</tr>
</thead>
<tbody>
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<td>9.597</td>
</tr>
<tr>
<td>USA</td>
<td>9.629</td>
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<td>India</td>
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<td>Norway</td>
<td>324</td>
</tr>
<tr>
<td>Italy</td>
<td>301</td>
</tr>
<tr>
<td>New Zealand</td>
<td>270</td>
</tr>
<tr>
<td>United Kingdom</td>
<td>243</td>
</tr>
<tr>
<td>Nepal</td>
<td>147</td>
</tr>
<tr>
<td>Bangladesh</td>
<td>144</td>
</tr>
<tr>
<td>Greece</td>
<td>132</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>30.102</strong></td>
</tr>
<tr>
<td><strong>AFRICA</strong></td>
<td><strong>30.221</strong></td>
</tr>
</tbody>
</table>

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In addition to the well-known social issues of illiteracy and immaturity, there also should be such a concept as "immaturity", meaning insufficient geographical knowledge.

A survey with random American schoolkids let them guess the population and land area of their country. Not entirely unexpected, but still rather unsettling, the majority chose "1-2 billion" and "largest in the world", respectively.

Even with Asian and European college students, geographical estimates were often off by factors of 2-3. This is partly due to the highly distorted nature of the predominantly used mapping projections (such as Mercator).

A particularly extreme example is the worldwide misjudgement of the true size of Africa. This single image tries to embody the massive scale, which is larger than the USA, China, India, Japan and all of Europe......combined!

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Department of Chemistry research focus areas:

• **Separation Science** (Prof E Rohwer, Dr T Laurens, Dr P Forbes, Dr S Bauermeister, Ms A Botha.)

• **Synthesis and Applications in Organometallic Chemistry** (Prof S Lotz, Dr M Landman, Dr D Bezuidenhout)

• **Synthesis of Biologically-active Compounds** (Prof R Vleggaar Dr L Pilcher, Dr N October, Dr M Nkwelo)

• **Materials and computational chemistry** (Prof P van Rooyen Dr. M Rademeyer, Dr E van der Merwe, Dr J Pretorius, Extr. Prof Casper Schutte)

• **Electrochemistry** (Prof. I. Cukrowski, Extr. Prof K Ozoemena (CSIR) )

• **Chemical Education** (Prof. M. Potgieter)

• **Forensic Toxicology** (Dr T Laurens)
New overarching themes of local relevance, to synergistically strengthen the traditional disciplines in Chemistry

- Molecular diagnostic and therapeutic techniques (NECSA, Health sciences, Petlabs …)

- Computer modeling and synthesis of catalysts used for renewable fuels production (IBM, Johnson Matthey, …)
Cost of facilities/ sub-disciplines

- Capital cost/replacement cost
- Running cost, maintenance
- Repair costs
- Skilled, dedicated scientists and operators

All in an environment ("intellectual home") where the sub-discipline is mastered and taught
Exponential growth in the discipline: Chemistry

Analytical technology (facilities) “Toolbox” MS, NMR, Xray Diff…Computers

Motivation:
Curiosity/Aesthetics
Quality of life
Power/control

Chemical theory (models)

Application to real problems. Experiment (reality check)
Evolutionary survival of expensive experimental disciplines in a developing world can only be achieved symbiotically, with a vigilant adaptation to needs

- We, our discipline and our facilities cannot achieve critical mass without reaching out to other fields of science
- We want to make alliances with other UP departments, industry and government to chase our dreams and serve theirs
- We are thankful to have been identified as a base discipline department in need of special help
- We have big dreams and need lots of help to upgrade the facilities we host for all researchers at UP
Anton Rupert, ex-staff member of the Chemistry Department

“He who does not believe in miracles is not a realist”

aan studente by Tukkies (1987):
“Streef nie daarna om bloot suksesvol te wees nie, maar probeer mense van waarde wees. Die suksesvolle man haal dikwels meer uit die lewe as wat hy terugplaas. Die man van waarde, daarenteen, gee meer as wat hy ontvang.”
Thanks

• Ms Ria Swart
• All other Colleagues from Chemistry

• Prof Willem Engelbrecht (US)
• Dr Daan Kemp (UCOR/ NECSA)
• Prof Piet van Berge (RAU/ UJ)
• Prof Victor Pretorius
Thanks for planned Departmental collaboration

• Prof Debra Meyer (Biochemistry)
• Prof Philip de Vaal (Chemical Engineering)
• Prof Oppel Greef (Pharmacology)
• Prof Mike Wingfield (FABI)
• Prof Chris Theron (Physics)
• Prof Elna Buys (Food Science)
• Prof Walter Focke (Materials Institute)
• Prof Philip Crouse (SARCHI)
• Prof Ncholu Manyala (SARCHI)
• Prof Innocent Pikirayi (Anthropology & Archeology)
• Prof Fanus Venter (Microbiology and Plant Pathology)
• Prof Hannes Rautenbach (Department of Geography, Geoinformatics and Meteorology)

• And all other Departments yet to join in....
“As we celebrate the achievements of the past, we must think about our stewardship going forward: If we conduct ourselves with integrity, diligence, competence and a deep commitment to serve South Africa, we will build an institution that will last: an institution that will make a unique contribution to the socioeconomic advancement of our country. However, if we allow ourselves to be engulfed by mediocrity and populism, the edifice that has been bequeathed to us will collapse in our own hands to the detriment of the whole country “