



OPCW

Organisation for the Prohibition of Chemical Weapons

Illuminating Chemical Reactivity an event guaranteed to brighten up your day...

Science for Diplomats at EC-91 The Hague, 9 July 2019

Starring Dr Marc-Michael Blum, Head OPCW Laboratory

With supporting cast

Mr Cheng Tang (SAB Chair), Mr Lucas Benderitter (OSP), Mr Peter Brud (OSP), Dr Jonathan E. Forman (Science Policy Adviser and SAB Secretary), Ms Giovanna Pontes (OSP), Ms Ayah Wafi (OSP) and special guest Ms Andrea Dymytrova

Let us Know You are Here!

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Let us Know You are Here!



Chemistry Lessons





Guidelines for Schedule 1

The following criteria shall be taken into account in considering whether a toxic chemical or precursor should be included in Schedule 1:

Schedule 1

- (a) It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article II;
- (b) It poses otherwise a high risk to the object and purpose of this Convention by virtue of its high potential for use in activities prohibited under this Convention because one or more of the following conditions are met:
 - It possesses a chemical structure closely related to that of other toxic (i) chemicals listed in Schedule 1, and has, or can be expected to have, comparableproperties;
 - (ii) It possesses such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon;
 - (iii) It may be used as a precursor in the final single technological stage of production of a toxic chemical listed in Schedule 1, regardless of whether this stage takes place in facilities, in munitions or elsewhere;

(c) It has little or no use for purposes not prohibited under this Convention.



Schedule 2

Guidelines for Schedule 2

The following criteria shall be taken into account in considering whether a toxic chemical not listed in Schedule 1 or a precursor to a Schedule 1 chemical or to a chemical listed in Schedule 2, part A, should be included in Schedule 2:

- (a) It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon;
- (b) It may be used as a precursor in one of the chemical reactions at the final stage of formation of a chemical listed in Schedule 1 or Schedule 2, part A;
- (c) It poses a significant risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 1 or Schedule 2, part A;
- (d) It is not produced in large commercial quantities for purposes not prohibited under this Convention.

Schedule 2 Part A, Toxic Chemicals

Thiodialycol

2B(13)



3B(14)

Relationship between Schedules, illustrated with sulfur mustard.

Sulfur mustard

1A(4)

Schedule 3

Guidelines for Schedule 3

The following criteria shall be taken into account in considering whether a toxic chemical or precursor, not listed in other Schedules, should be included in Schedule 3:

- (a) It has been produced, stockpiled or used as a chemical weapon;
- (b) It poses otherwise a risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that might enable it to be used as a chemical weapon;
- (c) It poses a risk to the object and purpose of this Convention by virtue of its importance in the production of one or more chemicals listed in Schedule 1 or Schedule 2, part B;
- (d) It may be produced in large commercial quantities for purposes not prohibited under this Convention.





Scheduled chemicals, including those in schedules 1 and 2, can have scientifically and economically important uses. This chart captures the number of yearly scientific publications that refer to them.























Degradation and Environmental Fate of Sulfur Mustard



Environmental fate in:

Cement & Soil Sea Water Synthesis Routes

Present in ton containers

Toxicology

Reported Impurities

Decontamination •Scheduled Chemical



Degradation and Environmental Fate of Sulfur Mustard

Darcy van Eerten

@opcw @opcw_st

f /opewonline 🔚 /opewonline in /company/opew 👰 /opew





HO

~

HS

(HMD Process)

=CH

Degradation and Environmental Fate of Sulfur Mustard

Darcy van Eerten



"delivery device"

Sea Water

Environmental fate in:

Cement & Soil

+ SO42.

Synthesis Routes

Present in ton containers

Toxicology

Reported Impurities

Levinstein mustards

@opcw st f /opcwonline book /opcwonline in /company/opcw 0 /opcw

What you see may not look exactly like the chemists Explanation! ("language" describes things, but objects do not always look like words!)

Today's Briefing:

What does chemistry really look like? (and how does it actually relate to the world you see and feel?)



What you see may not look exactly like the chemists Explanation! ("language" describes things, but objects do not always look like words!)



What you see may not look exactly like the chemists Explanation! ("language" describes things, but objects do not always look like words!)



Before we Begin...





Before we Begin...





Before we Begin...







Scie Dr Blum





Presentation by Dr Blum







OPCW

Organisation for the Prohibition of Chemical Weapons

Chemical reactivity

or why Chemistry is basically the same as Politics

Marc-Michael Blum, Ph.D. Head, OPCW Laboratory



Politics is more difficult than physics

Albert Einstein



Chemistry is basically the same as politics

Marc-Michael Blum Head, OPCW Laboratory

(somehow implying that Chemistry is more difficult than Physics)





Chemistry:

Chemistry is the study of matter, its properties, *how and why substances combine or separate to form other substances*, and how substances interact with energy.



The Chemical Weapons Convention is quite focused on chemicals themselves:

- Declarations based on production, consumption and/or transfers of chemicals
- Annex on Chemicals of the CWC listing those chemicals for which special verification measures are in place
- Sampling & Analysis is conducted to confirm the presence or absence of a CWC relevant chemical



But we also deal with REACTIONS of chemicals:

- We discuss the meaning of "production by synthesis"
- We discuss the the productions of DOCs via biomediated processes
- Sampling & Analysis is looking for precursors and degradation products of chemical agents in IAUs
- Reaction products of agents with biomolecules ("adducts") are valuable biomarkers and important in biomedical verification



So why do chemicals react with each other?





What are the laws that determine in what direction a chemical reaction is proceeding?




The <u>first law</u> of thermodynamics is a version of the law of conservation of energy, adapted for thermodynamic systems. The law of conservation of energy states that the total energy of an isolated system is constant; energy can be transformed from one form to another, but can be neither created nor destroyed.



The <u>second law of thermodynamics states that the</u> total entropy of an isolated system can never decrease over time. The total entropy of a system and its surroundings can remain constant in ideal cases where the system is in thermodynamic equilibrium. In all processes that occur, including spontaneous processes, the total entropy of the system and its surroundings increases and the process is irreversible in the thermodynamic sense. The increase in entropy accounts for the irreversibility of natural processes, and the asymmetry between future and past.



Chemical equilibrium

$$A+B \longrightarrow C+D$$

Thermodynamics determine if A and B or C and D are the favoured products and where the equilibrium is located. It does NOT determine reaction rates.





Activation Energy and reaction rates



Reaction coordinate



A practical example





Fritz Haber (1868-1934)

"Father" of chemical warfare in World War I

But also Nobel Laureate in Chemistry 1918









Carl Bosch (1874-1940)

Chemist and Industrialist

Nobel Laureate in Chemistry 1931





The Haber-Bosch process

Making ammonia with nitrogen from the air

$$N_2 + 3 H_2 \rightleftharpoons 2 NH_3$$

- Nitrogen is a very stable and unreactive molecule.
- Process has high activation barrier.
- Raising the temperature makes reaction faster but shifts equilibrium from ammonia towards starting products



Reaction rate and temperature





The Haber-Bosch process

The solution:

- Lowering activation energy a using metal catalyst
- Temperature for reasonable reaction rates now lower but still favouring the starting products
- Shifting the equilibrium towards ammonia by applying high pressure.



The Haber-Bosch process

Major technological breakthrough (high pressure reactions in industry). Uses about 1-2% of world energy consumption.







- Enabled Imperial Germany to continue to fight World War I despite being blocked from accessing natural nitrate deposits Enabled the mass production of nitrogen fertilizers
- Enabling massive growth of agricultural production
- Without the Haber process the current world population would not be possible
- About half of all nitrogen atoms in the human body are derived from air nitrogen via the Haber process.



Chemical warfare and reactivity

 Nerve agents should have high reactivity with the biological target (Acetylcholinesterase) but low reactivity towards water (hydrolytic stability). Fluoridates better than chloridates.







But back to Chemistry and Politics....

$A+B \xleftarrow{C+D}$

How can this be similar to politics? Clearly defined start and end states? Predictable reaction rates and equilibrium? No room for negotiations?

Chemistry can be a little bit more complicated.....



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## Looks like the org chart of the UN? Reminds you of political decision making?





## Sometimes even a chemical reaction does not know in what direction it wants to run...





## Sometimes even a chemical reaction does not know in what direction it wants to run...







Ok you say. Colour changes are nice but I need a green light from capital. How can chemistry help me with that?





# Ok you say. Colour changes are nice but I need a green light from capital. How can chemistry help me with that?





### **Captured on Video!**



https://www.youtube.com/watch?v=shZtgWBWFAA&feature=youtu.be





## The Science For Diplomats Flow Chemistry System

### You are in possession of a DIY flow chemistry kit!

#### Your kit contains:

- 1 Lego laboratory bench
- 1 flow chemistry assembly (consisting of three fluidic blocks with 5 connecters, tubing and a stopcock)
- 2 syringe to tubing connectors
- 1 syringe (3 ml) containing precursor A (blue)
- 1 syringe (3 ml) containing precursor B (yellow)

(B)

(A)

1 product collection container

Syringes containing precursors

Flow chemistry assembly

Lego laboratory bench

Product collection

container

Syringe to tubing connectors

Your kit includes all the parts you will need to safely mix component chemicals (precursors) together to produce and collect a new chemical product.



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- 1 product collection con

Syringes containing precursors

Flow chemistry

assembly



Lego laboratory

bench

Your kit includes all the parts you will need to safely mix component chemicals (precursors) together to produce and collect a new chemical product.

#### A fully assembled flow chemistry system should look like this:





#### Your task:

- 1. Figure out how to assemble the system
- 2. Mix precursors A and B
- 3. Collect the product (without spilling, leaking or otherwise contaminating your work space!)

Prizes will awarded for the perfect combination of system assembly, chemical containment, product purity and product yield. Good luck diplochemists!

### Assembly instructions?

We keep hearing how easy it is to produce chemicals using DIY approaches, now you can show us how!

... in case you really want instructions... just ask! A cheat sheet is available upon request.

### A fully assembled flow chemistry system should look like this:



rity and

Your task 1. Figure of 2. Mix press 3. Collect the OPCW LAB

Prizes will c product yiel

Assembly We keep he

... in case you really want instructions... just ask! A cheat sheet is available upon request.
















### **Chemistry Lessons**





### **Chemistry Lessons**



ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

### THE "SCIENCE FOR DIPLOMATS" ANNEX ON CHEMICALS

A user friendly and scientifically annotated version of the Chemical Weapons Convention Annex on Chemicals







OPCW gene before... What is missing

areconats at ec-go

CI to CIO and beyond



### How can we make the "Unnofficial" Annex on Chemicals more informative?

## ses explanations of cemic more real chemical exerci hal compositions links

What is miss

rule



From the audience:

23



# **Scientific Advisory Board Update**







# **Scientific Advisory Board Update**



Working Together For a World Free of Chemical Weapons

### **Temporary Working Group on Investigative Science and Technology**

Reporting to the Scientific Advisory Board (SAB), the Temporary Working Group (TWG) will in particular consider the following questions:

### Question 1:

Which methods and capabilities used in the forensic sciences could usefully be developed and/or adopted for Chemical Weapons Convention-based investigations?



/opcwonline

### **Question 2:**

What are the best practices and analysis tools used in the forensic sciences for effectively cross-referencing, validating, and linking together information related to investigation sites, materials collected/analysed, and individuals interviewed?



Which technologies and methodologies (whether established or new) can be used in the provenancing of chemical and/or material samples collected in an investigation?

### **Question 4:**

What are the best practices for the collection, handling, curation and storage, and annotation of evidence?

### **Question 10:**

Do collections of physical objects, samples, and other information for chemical weapons-related analysis exist and can they be made available to investigators for retrospective review? How might these collections be used to support investigations?

@opcw

@opcw_st

**Ouestion 8:** 

Which technologies and methodologies (whether established or new) can be used in ensuring chain of custody and verifying authenticity (sepecially in regard to digital images and video recordings)?

### Question 11:

could usefully engage with to leverage their capa on investigative matters?

**Ouestion 9:** 

**Question 6:** 

Which technologies and methodologies (whether established or new) can be used to ensure the integrity of an investigation site?

In addition, the TWG will provide advice on Technical Secretariat proposals for methodologies, procedures, technologies, and equipment for investigative purposes. TWG will meet twice more, then produce a final report.

opcw



### **Some Acknowledgements: Interns!**





### Thank you for Joining Us!





### Periodic Table of States Parties to the Chemical Weapons Convention



### Good Luck Dr Blum, we will miss you!







# OPCW

منظمة حظر الأسلحة الكيميائية

禁止化学武器组织

Organisation for the Prohibition of Chemical Weapons Organisation pour l'Interdiction des Armes Chimiques Организация по запрещению химического оружия Organización para la Prohibición de las Armas Químicas